# Non glassy ground-state in a long-range antiferromagnetic frustrated model in the hypercubic cell

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We analyze the statistical mechanics of a long-range antiferromagnetic model defined on a $D$-dimensional hypercube, both at zero and finite temperatures. The associated Hamiltonian is derived from a recently proposed complexity measure of Boolean functions, in the context of neural networks learning processes. We show that, depending of the value of $D$, the system either presents a low temperature antiferromagnetic stable phase or the global antiferromagnetic order disappears at any temperature. In the last case the ground state is an infinitely degenerated non-glassy one, composed by two equal size anti-aligned antiferromagnetic domains. We also present some results for the ferromagnetic version of the model.

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## INTRODUCTION

The success in understanding the collective behavior of conventional magnets lead in the past decade to an increased interest in systems that exhibit a novel type of ordering as a consequence of "frustration". In particular, geometrically frustrated systems (having as a basic building block triangles of antiferromagnetic bonds) have been the object of extensive theoretical studies (see [1] and references therein). It was found that frustration gives rise to spectacular and often unexpected behaviors at low temperatures due to the high degeneracy of the ground state. Recently, more and more experimental realizations of such geometrically frustrated systems have been achieved. 2D and 3D materials have been assembled from triangles and tetrahedra such that neighbouring geometrical units share either a common edge or a common corner [2]. Such new materials have stirred a new debate, whether frustration alone is strong enough to destroy magnetic long range order. Spin glass behavior is usually associated to the presence of both disorder and frustration. It has been argued that frustration alone can lead to large ground-states degeneracies, accompanied by extensive ground-state entropies, but cannot produce a sufficiently "rough" free energy landscape necessary for the development of a thermodynamical "glassy" state[4, 5].

In contrast with the previously mentioned systems, non-geometrical frustration may arise as an effect of antiferromagnetic long-ranged interactions (e.g., dipolar, Coulomb, etc.). It is well known that the competition between short-range ferromagnetic exchange interactions and long-range antiferromagnetic ones in hypercubic Bravais lattices give rise to low temperature long range order associated with lamellar structures[3, 6]. Although those systems presents a very rich behaviour concerning both its equilibrium[3]-[6] and non-equilibrium[7, 9] properties, in all these cases the ground state presents a finite degeneracy. Even in the case of a 3D system with Coulomb interactions, where some evidence of glassy behaviour has been obtained[9], it is of purely dynamical origin, the ground state still having a finite degeneracy.

In this work we analyze the zero and low temperature equilibrium properties of a long range antiferromagnetic spin model defined on a $D$-dimensional hypercubic cell. The associated Hamiltonian is related to a recently proposed complexity measure of Boolean functions in the context of neural networks learning processes and it is described in section . Although the original motivation for studying the statistical mechanics of this model is related to the the field of Boolean functions complexity and neural networks [10], we found that it presents some very peculiar properties that provide new insights about the relationship between frustration and order-disorder low temperature properties. Spin models defined on hypercubic cells have been repeatedly used in the past to study both equilibrium and dynamical properties of spin glasses[11]-[13]. In that context, the main interest in hypercubic cell models is to analyze how their properties change as the dimension (and therefore the connectivity of the lattice) increases, thus resembling fully

connected models like the Sherrington-Kirkpatrick one[14], whose general properties are rather well understood[15, 16]. One of the main questions

today concerning spin glasses is whether the physical scenario that emerges in long-range fully connected models holds in systems with short range interactions or not. One step further towards the answer of that question is to consider systems with long range interactions that decay with the distance between spins. In this work we analyze the effects of frustrating long range antiferromagnetic interactions in an hypercuibc cell without disorder. The interactions in our model decay with the Hamming distance between spins, a natural metric in hypercubic cells, instead of the Euclidean distance. Notice that the Hamming distance in the hypercubic cell is equivalent to the chemical distance (i.e., the number of steps required to go from one node to another along the shortest path). Hence, the present study may also provide some insigths about the possible effects of frustrating interactions we expect in models defined on lattices with complex network topologies, such as small world networks (see Ref.[17] and references therein).

We show that, for some particular values of the dimension $D$ the frustrating long range interaction gives rise to a ground state that is neither disordered (i.e., non-glassy) nor completely ordered but, it is composed of two equal size anti-aligned antiferromagnetic domains. The ground state is thus partially ordered. Moreover, it has an infinite degeneracy in the thermodynamic limit (although this degeneracy grows logarithmically with the number of spins, and hence its entropy per spin goes to zero).

In section  we analyze the frustrated ground state of the system for the particular set of values of $D$ such that it exhibit global frustration. In section  we analyze the finite temperature behaviour of the model using Monte Carlo simulations. In section  we present Monte Carlo results for the ferromagnetic version of the model, which are of interest in the general context of long range interacting systems. Finally, we present some general conclusions in section .

## THE MODEL

In Ref.[10] a measure for the complexity of Boolean functions of $D$ Boolean variables was introduced in the context of feed-forward neural networks learning processes. The $2^D$ possible inputs of a Boolean function of this type are located at the corners of a $D$-dimensional hypercubic cell. If we associate a spin variable $S_i = \pm 1$ to each corner $i$ of the cell every possible Boolean function corresponds to a particular spin configuration of this system. The complexity measure is based on the concept that complex Boolean functions assign different outputs to similar inputs, where the similarity is measured by the Hamming distance between them. Thus, in the magnetic analogy, configurations where neighbour spins tend to be anti-aligned correspond to functions of increasing complexity. The complexity measure can be then mapped into minus the long range antiferromagnetic Hamiltonian[10]

$$H = \sum_{i,j} J(r_{ij}) S_i S_j \tag{1}$$

where $r_{ij}$ is the Hamming distance between spins $i$ and $j$ in the hypercubic cell and

$$J(r) = \begin{cases} \frac{1}{M(r)} & \text{if } r \leq D/2 \\ 0 & \text{otherwise} \end{cases} \tag{2}$$

$M(r)$ being the number of nearest neighbors at distance $r$ of a given spin and equals the binomial coefficient

$$M(r) = C(D,r) = \frac{D!}{(D-r)!\, r!}. \tag{3}$$

The distribution of Boolean functions with high complexity is then associated with the low energy spectrum of Hamiltonian (1) which can be characterized by the low temperature statistical mechanics behaviour of the associated spin model. The Hamiltonian (1) can be rewritten as a sum of terms, each of them taking into account the interactions between pair of spins at a different Hamming distance:

$$H = \sum_{r=1}^{r=D/2} J(r) \sum_{[i,j/Hamming(i,j)=r]} S_i S_j, \tag{4}$$

Notice that the number of interaction terms in Hamiltonian (4) depends on $D$; as $D$ increases a new term is included every time $D$ takes an even value. For instance, in the cases $D = 2$ and 3 only nearest neighbor spins interact; in the

cases $D = 4$ and 5 an interaction between next nearest neighbor spins is added, etc.. Hence, the antiferromagnetic nature of the interactions introduce local frustration for $D \geq 4$, in the sense that not all the couplings inside groups of spins closely located can be simultaneously minimized. However, this does not necessarily generate global frustration, in the sense of a non-ordered ground state with high degeneracy, due to the particular form Eq.(2) of the interaction coupling $J(r)$. Global frustration appears only when the number of interaction terms included in the Hamiltonian (4) is even, that is, when the dimension $D$ is a multiple of four $D = 4l$, $l = 1, 2, 3, \ldots$. In all the other cases the ground state is the antiferromagnetic one (i.e., the Nèel state with every pair of nearest neighbor spins anti-aligned), with degeneracy 2 (corresponding to the inversion of all the spins). To see this let us calculate the energy of the Nèel state. Every term in Eq.(4) corresponding to a fixed Hamming distance $r$ equals in this case $(-1)^r N\, M(r)$, $N = 2^D$ being the total number of spins (notice that the interaction between every pair of spin in Hamiltonian (1) is counted twice for simplicity; this corresponds to a renormalization of the energy units by a factor two, and does not affect the results). Hence, the energy of the Nèel state is given by

$$E_N = N \sum_{r=1}^{r=D/2} (-1)^r \tag{5}$$

which equals zero when $D/2$ is even and $E_N/N = -1$ when $D/2$ is odd. Moreover, in the last case is easy to see that a single spin flip increases the energy in a quantity $\Delta E = 2$. Therefore, the Nèel state is stable against small perturbations. Monte Carlo simulations presented in section  provide further evidence that the ground state is the Néel one. Moreover, the finite temperature simulations show that there is a finite critical temperature below which the system presents long range antiferromagnetic order when $D/2$ is odd.

In the next section we analyze the frustrated ground state for the case $D = 4l$, $l = 1, 2, 3, \ldots$.

## THE FRUSTRATED GROUND STATE

From exhaustive enumeration of the energy values for the case $D = 4$, where the Hamiltonian contains two terms, it was found that the ground state of the system consist of two equal size antiferromagnetic domains with an energy value equal to $-0.5$. Monte Carlo simulations in higher dimensions ($D = 4, 8, 12, 16$) have also shown that the energy value of the ground state of the system is equal to $-0.5$ and has the same structure found for the case for $D = 4$. (Long relaxation times and very low cooling were used in different simulations, all of them confirming the structure and energy value of the ground state). Energy calculations for states composed by 4 and 8 anti-aligned antiferromagnetic domains($D = 8, 16$) also yield values higher than $-0.5$. Moreover, as we will demonstrate next, the energy per spin of the state composed by two antiferromagnetic domains equals $-0.5$ for arbitrary values of $D$. Since the antiferromagnetic state has always zero energy, all these result suggests that the two antiferromagnetic domains structure has the minimal energy for arbitrary dimension $D = 4l$, $l = 1, 2, 3, \ldots$. The total magnetization and staggered magnetization is zero for the ground state. In figure 1 a representation of the ground state for $D = 4$ is depicted, where the state of the spins is indicated by filled or empty circles. The antiferromagnetic domains correspond to two hypercubes of dimension $D - 1$ each (see Fig. 1). Each spin in this state has $D - 1$ nearest neighbor spins anti-aligned, which belong to the same domain, and one nearest neighbor spin aligned, which belong to the other domain. Once we fixed two nearest neighbor spins to be aligned, the rest of the structure is completely determined. Since every spin has $D$ nearest neighbors, the degeneracy of the state is $2\,D = 2\,\log_2 N$, where the factor 2 results from the inversion operation of all the spins.

We now demonstrate that the energy per spin $E_d$ of the state composed of two antiferromagnetic domains equals $-0.5$ for any dimension $D = 4l$, $l = 1, 2, 3, \ldots$. $E_d$ can be written as

$$E_d = \sum_{n=1}^{n=D/2} E_d(n) \tag{6}$$

$E_d(n)$ being the interaction energy between an arbitrary chosen reference spin and all its neighbors located at a Hamming distance $n$.

We denote the two antiferromagnetic domains as regions A and B. Consider now an arbitrary spin $S_1$ that belongs to the domain A. Spin $S_1$ has $D - 1$ anti-aligned nearest neighbors (NN) spins in the domain A and only one first

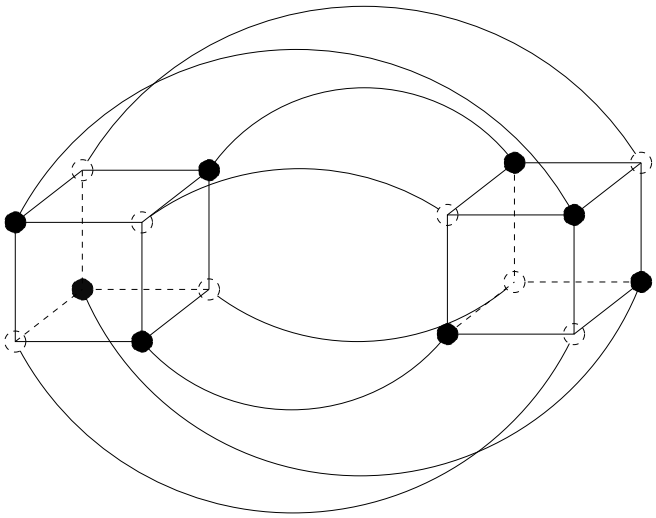

FIG. 1: Ground state of the antiferromagnetic Hamiltonian for $D = 4$ . Spin states are represented by empty or filled circles and the bond between spins indicate that they are first nearest neighbors.

nearest neighbor spin $S_2$ in the domain B. Spin $S_2$ has the same orientation as the spin $S_1$. As the total number of NN spins in dimension $D$ is exactly $D$, the first term of Eq.(6) equals

$$E_d(1) = -\frac{(D-1)}{D} + \frac{1}{D} \tag{7}$$

which can be expressed as

$$E_d(1) = 2\frac{C(D,0)}{C(D,1)} - 1 \tag{8}$$

Let us now consider the next nearest neighbors (NNN) term $n = 2$ in Eq.(6). Note that the NNN spins of $S_1$ in the domain B (anti-aligned to $S_1$) are the $D-1$ spins NN of $S_2$ in B; the remaining spins NNN to $S_1$ in A have the same orientation of it. Since the total number of NNN spins is $C(D,2)$ we have that

$$\begin{aligned} E_d(2) &= -\frac{(D-1)}{C(D,2)} + \frac{C(D,2)-(D-1)}{C(D,2)} \\ &= -2\frac{C(D,1)-C(D,0)}{C(D,2)} + 1 \end{aligned} \tag{9}$$

Following the same analysis the $3rd$ term of Eq.(6) equals

$$E_d(3) = 2\frac{C(D,2)-C(D,1)+C(D,0)}{C(D,3)} - 1 \tag{10}$$

and the $n-th$ order term can be written as

$$E_d(n) = 2\frac{\sum_{k=0}^{n-1}(-1)^k C(D,k)}{C(D,n)} + (-1)^n. \tag{11}$$

Equation (11) can be rewritten as

$$E_d(n) = (-1)^{n+1}\,(2\,a(n) - 1) \tag{12}$$

where

$$a(n) \equiv (-1)^{n+1}\frac{\sum_{k=0}^{n-1}(-1)^k C(D,k)}{C(D,n)}. \tag{13}$$

It is s easy to verify that $a(n)$ satisfy the recurrence equation

$$a(n+1) = \frac{C(D,n)(1-a(n))}{C(D,n+1)} = \frac{n+1}{D-n}\,(2\,a(n) - 1) \tag{14}$$

from which it can be proved by induction that $a(n) = n/D$. Replacing into Eqs.(6) and (12) we finally obtain

$$\begin{aligned} E_d &= \sum_{n=1}^{n=D/2} (-1)^{n+1}\left(\frac{2n}{D} - 1\right) \\ &= -\frac{2}{D}\sum_{n=1}^{n=D/2}(-1)^n\, n = -\frac{1}{2} \end{aligned} \tag{15}$$

where in the last step we have used that

$$\sum_{n=1}^{n=D/2}(-1)^n n = \frac{D}{4} \tag{16}$$

## FINITE TEMPERATURE EQUILIBRIUM PROPERTIES

We now present some numerical simulation results at finite temperature. Monte Carlo simulations were performed using heat bath dynamics. We first analyze the frustrated case $D = 4l$, $l = 1, 2, \ldots$. In Fig. 2 we show the results for the internal energy per spin for system sizes $D = 4, 8, 12$. The different curves were obtained by starting at high temperature with random or ferromagnetic initial conditions (there were no difference between both cases in the final results) and slowly cooling, that is, the initial configuration at every subsequent temperature was taken as the last configuration of the previous temperature. At every temperature we left the system thermalize during a varying transient period, which was higher at low temperatures.

For low values of $D$ we see that the energy converges to the value $-0.5$. Direct inspection of the final configurations obtained at $T = 0$ shows always the conjectured state composed by two antiferromagnetic domains. Notice from Fig.2 that there seems to be a change of behaviour around $T \sim 0.2$. An analysis of the energy distribution at low temperatures showed that this effect is related to a gap between the ground state and the first excited states that decreases as $D$ increases and hence, it is a finite size effect. Both the magnetization and the staggered magnetization are always $\mathcal{O}(N^{-1/2})$ at any temperature and also the specific heat does not show any type of anomaly. So the system does not (globally) order at any temperature.

We next performed Monte Carlo simulations for the antiferromagnetic system when $D/2$ is odd.

In figure 3 we show the absolute value of the staggered magnetization, the energy per spin and the staggered susceptibility vs temperature for $D = 6, 10, 14$. These results not only confirms that the ground state is antiferromagnetic, but also show that the system undergoes a second order phase transition at a finite critical temperature $T_c \approx 1$. The comparison of the magnetization curves with the solution of the Curie-Weiss equation $m = tanh(\beta m)$ suggests that mean field behaviour is exact in this case at any temperature.

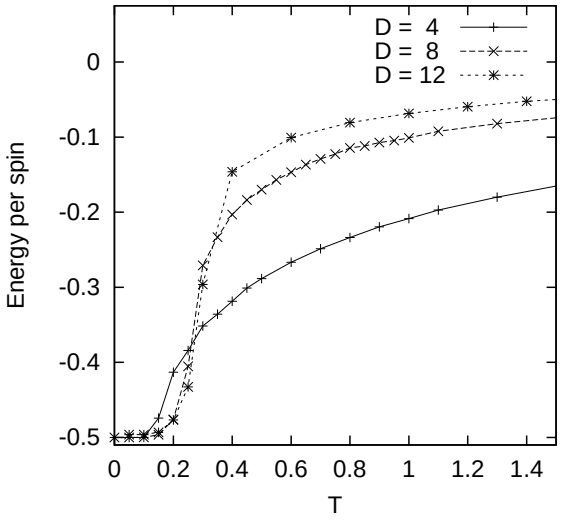


FIG. 2: Monte Carlo calculation of the mean energy per spin vs temperature for an antiferromagnetic Hamiltonian with $D = 4, 8, 12$.

## THE FERROMAGNETIC MODEL

Finally we consider the ferromagnetic version of the model, that is, the model defined by the Hamiltonian (1) with $J(r) = -\frac{1}{M(r)}$. This system is non-extensive, in the sense that the quantity

$$\phi = -\sum_{j \neq i} J(r_{ij}) = D/2 = \frac{\log_2(N)}{2} \tag{17}$$

diverges for $N \to \infty$, and therefore the thermodynamic limit is not defined[18, 19]. In this situation the magnetization per spin $m(T)$ and the internal energy per spin $u(T)$ are expected to scale as[20, 21]

$$\begin{aligned} m(T) &\sim m'(T/\phi) \\ u(T) &\sim \phi u'(T/\phi) \end{aligned} \tag{18}$$

when $N \gg 1$, $m'(x)$ and $u'(x)$ being scaling functions independent of $N$. In the case of $d$-dimensional hypercubic *lattices* with interactions that decay with the distance $r$ between spins as $1/r^\alpha$ the quantity $\phi$ is proportional to[21]

$$N^* = \frac{1}{1-\alpha/d}\left(N^{1-\alpha/d} - 1\right) \tag{19}$$

This scaling factor generalizes the traditional scaling $J \to J/N$ of the couplings in the Curie-Weiss model, i.e., a fully connected Ising spin system with distance-independent interactions, which corresponds to the $\alpha = 0$ case. For $\alpha > d$ the scaling factor (19) becomes independent of $N$ in the thermodynamic limit and the system is extensive, while for $\alpha \to d$ (this corresponds, for instance, to the case of three dimensional systems wtih dipolar interactions that decay as $1/r^3$ for $r \gg 1$) we have that $N^* \to \ln N$. Thus, the behavior of the present hypercell model is expected to be analog to that of the borderline case between short and long range interactions $\alpha = d$ in hypercubic Bravais lattices.

The data collapse of the rescaled quantities for different values of $D$ shown in Fig.(4) verify the scaling (18). Moreover, the comparison of the magnetization curves with the solution of the Curie-Weiss equation $m = tanh(m/T^*)$ (where $T^* \equiv T/\phi$) shows that mean field behavior is asymptotically exact for a system of this type when the thermodynamic variables are properly rescaled, as was previously conjectured for general systems with long-range ferromagnetic interactions[22]. Also the specific heat calculation shown in Fig.(5) displays a convergence to a discontinuous curve at the rescaled critical temperature when $N \to \infty$, consistently with the mean field behaviour.

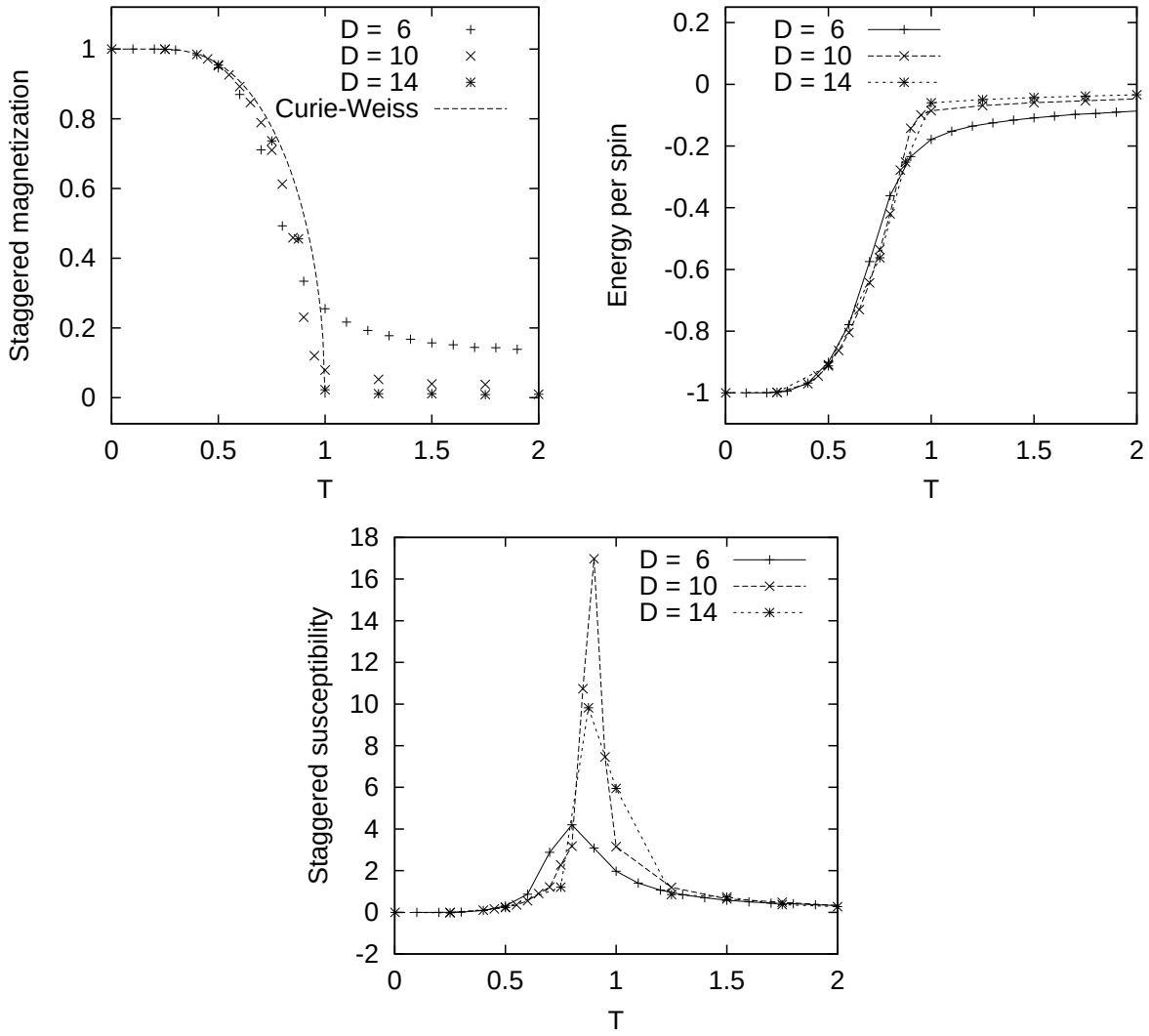


FIG. 3: Monte Carlo calculation of the mean staggered magnetization per spin, energy per spin and staggered susceptibility vs temperature for an antiferromagnetic Hamiltonian with $D = 6, 10, 14$.

## DISCUSSION

We analyzed the statistical mechanics of a long-range model defined on a $D$-dimensional hypercube, which is related to the complexity of Boolean functions. Besides its interest in Boolean functions complexity and neural networks fields, the model exhibits several features that contribute to the understanding of general long-range systems. Thus, the statistical mechanics of the model is of interest on its own.

In the antiferromagnetic (AF) version of the model, the particular form of the coupling terms in Eq.(2) actually define two different models, according to the value of $D$. When $D/2$ is an odd number the model presents a low temperature AF phase and undergoes a mean-field like second order phase transition at a finite critical temperature $T_c = 1$. The most interesting situation appears when $D/2$ is and even number. In this case long range AF order is suppressed at any finite temperature, while the ground state is composed by two equal size anti-aligned AF domains; this state becomes infinitely degenerated in the thermodynamic limit, but its entropy per spin goes to zero. This result shows that the frustration produced by the interplay between long range interactions and lattice topology can produce large ground state degeneracies without the generation of a "rough" free energy landscape. This result is of importance in spin glasses studies, where models defined on an hypercube are used to analyze the influence of large dimensionalities[11, 13]. We have shown that this type of lattice can introduce effects of large ground state

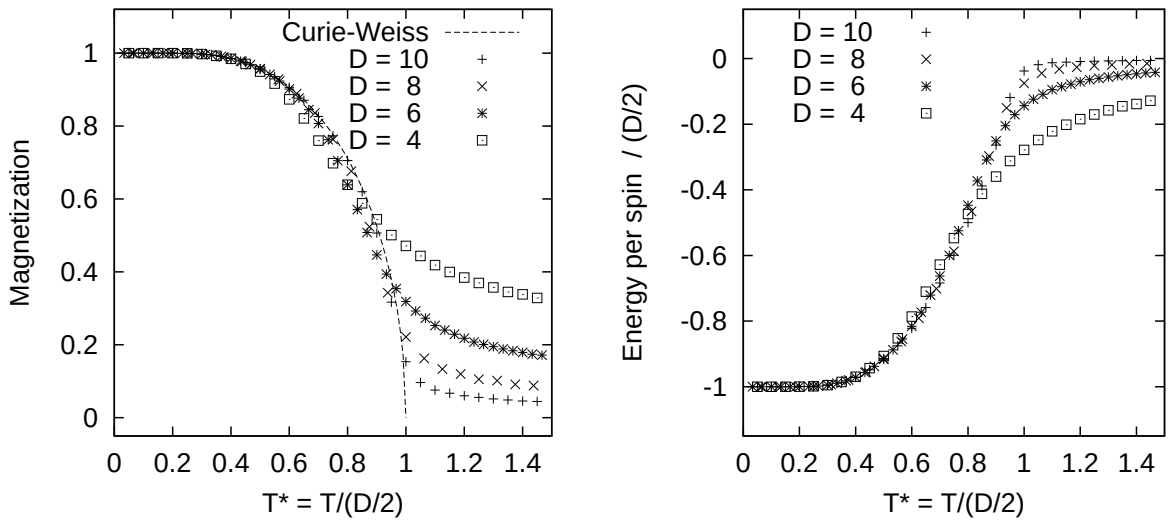


FIG. 4: Monte Carlo calculation of the mean magnetization per spin and energy per spin vs rescaled temperature $T^*$ for a ferromagnetic Hamiltonian with $D = 4, 6, 8, 12$.

degeneracies which are independent of the presence of disorder, at least in the case of long range interactions. Although the contribution of such effects to the entropy per spin goes to zero in the thermodynamic limit, its importance could not be negligible for finite systems, as in the case of numerical simulation studies. It is worth to stress that the antiferromagnetic model do not have a well defined thermodynamic limit for general dimension of the hypercell $D$. The system exhibit a well defined thermodynamic limit only when the dimension $D$ is restricted to a particular set of values, that is, to be a multiple of four or not. This peculiar behavior illustrates the type of subtleties that may arise when working with long range frustrating interactions in hypercubic cells.

Finally, in the ferromagnetic version of the model we verified a previous conjecture[22] for non-extensive (ferromagnetic) systems, that is, all the thermodynamic behaviour of the model can be exactly described at any temperature by mean field theory if the thermodynamic variables are properly rescaled with the system size.

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[1] T. Ogawa and Y. Nakajima, Prog. Theor. Phys. Supp. **87**, 90 (1986).
[2] M.A. Girtu, C.M. Wynn, W. Fujita, K. Awaga, and A.J. Epstein, Phys. Rev. B **57**, R11058 (1998).
[3] K. De'Bell, A. B. MacIsaac and J. P. Whitehead, Rev. Mod. Phys. **72**, 225 (2000).
[4] P. Chandra, P. Coleman and I. Ritchey, J. de Phys. I **3**, 591 (1993).
[5] R. Rammal, Rev. Mod. Phys. **58**, 765 (1986).
[6] M. Grousson, G. Tarjus and P. Viot, Phys. Rev. E **64**, 036109 (2001)
[7] J. H. Toloza, F. A. Tamarit and S. A. Cannas, Phys. Rev. B 58, R8885 (1998)
[8] D. A. Stariolo and S. A. Cannas Phys. Rev. B **60**, 3013 (1999).
[9] M. Grousson, G. Tarjus and P. Viot, Phys. Rev. E **65**, 065103 (R) (2002).
[10] L. Franco, cond-mat/0111169 (2002).
[11] G. Parisi, F. Ritort and J.M. Rubí, J. Phys. A: Math. and Gen., **24**, 5307 (1991).
[12] P.M. Gleiser and F.A. Tamarit, Phys. Rev. E **57**, 1410 (1998)
[13] D. A. Stariolo, Physica A **253**, 1 (1998).
[14] D. Sherrington and S. Kirkpatrick, Phys. Rev. Lett. **35**, 1972 (1975).
[15] G. Parisi, J. Phys. A **13**, L371 (1980).
[16] L. Cuglinadolo and J. Kurchan, J. Phys. A. **27**, 5749 (1994).

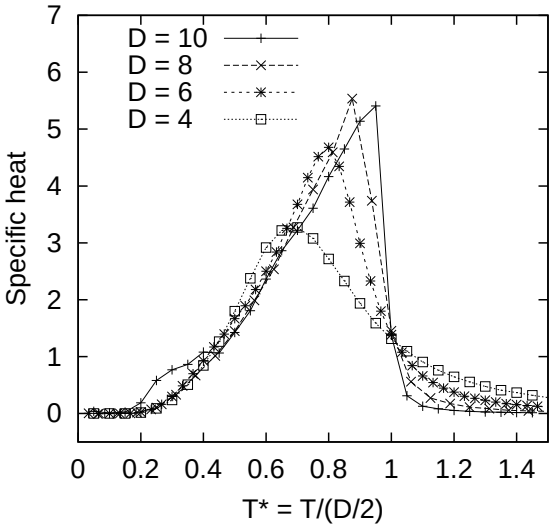


FIG. 5: Monte Carlo calculation of the specific heat vs rescaled temperature $T^*$ for $D = 4, 6, 8, 10$.

[17] S. H. Strogatz, Nature **40**, 268 (2001).
[18] C. J. Thompson, *Classical Equilibrium Statistical Mechanics* (Clarendon Press, Oxford, 1988).
[19] M. Ainzenman, J. T. Chayes, L. Chayes and C. M. Newman, J. Stat. Phys. **50**, 1 (1988).
[20] C. Tsallis, Fractals **3**, 541 (1995).
[21] S.A. Cannas and F.A. Tamarit, Phys. Rev. B, **54**, R12661 (1996).
[22] S.A. Cannas, A.C.N. de Magalhaes and F.A. Tamarit, Phys. Rev. B **61**, 11521 (2000).