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Numerical Study of the Antiferromagnetic Ising Model in Hyperdimensions

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Abstract

We built a model where all spins are in interaction with each other via an antiferromagnetic Ising Hamiltonian. The geometry of such a model is a tetrahedron placed on a hypersphere in spaces of dimensions enclosed between 1 and 9. Due to confinement and to the fact that all spins interact which each other, our spin system exhibit frustration. The temperatures of the observed antiferro-paramagnetic transformations are equal for all space dimensions to one of two given values depending on the parity of the space dimension. Moreover, the order parameter $< m >$, i.e. the magnetization of the system, has been also studied.

Keywords: Ising model, finite syze system, high dimension, antiferromagnetism

1 Introduction

The Ising model [1] has been widely studied to understand physical phenomena that occur in ferroelectric compounds, lattice gas, binary alloys etc. The Ising model is one of the most studied method in statistical physics [2, 3]. The Ising model has played a crucial role in the development of concepts about critical phenomena, from scaling [4, 5] and universality [6, 7], to the renormalization group [8]. In addition, critical phenomena in Ising models have been under study by Monte Carlo simulations since about thirty years. Recently, these studies have reached an accuracy that is competitive with the most accurate renormalization group estimates. Despite this impressive progress, there are still many problems left that are less well understood.

But, there are very few articles on confinement effects [9, 10, 11, 12] on the Ising model. Up to now, the Ising model has been widely used for simulating large size systems by using periodic boundary conditions in order to recover the properties of these large scale systems. Here we will use a small scale system with no periodic boundary conditions.

Understanding the statistical mechanics of classical systems in confined geometries and in systems of small sizes is important for the future studies of nanocompounds.

This article deals of $N+2$ Ising spins on a $d = N$ dimensional hypersphere. The geometry of the spins corresponds to the following: each spin is located on the apex of the tetrahedron corresponding to the space dimension. Due to the geometry of the tetrahedron and specifically to the number of bonds per spin, what can occur to the order parameter? We will use here finite size scaling which is here adequate as we use a finite size system.

2 Numerical model

We used an Ising model on a tetrahedron in hyperspace. For the sake of confinement, we assume that the space is closed: it corresponds to a d dimensional hypersphere on which the tetrahedron is located. This tetrahedron is located on the hypersphere so as each spin is at equal distance from each other. Hence the curvature of the hypersphere is very large and is directly related to the distance between spins. The number of apex of the tetrahedron is also directly related to the dimension of space: if d is the dimension of hyperspace, the number of apex is equal to $d+2$. So, like in a 1-dimensional circle or a 2-dimensional sphere, each spin located at an apex of the tetrahedron is at equal distance from all other spins.

Hence the Hamiltonian of such an Ising model writes:

$$H = -\sum_i \sum_{j \neq i} -J s_i s_j \tag{1}$$

were s_i is Ising spin number i and $J <$ is the antiferromagnetic coupling. We took here the magnetisation $m =< |s_i| >$ of the assembly of spins as the order parameter in a finite size analysis. The algorithm used here was the Wolff one.

The finite size analysis [13] is a very efficient way to study phase transitions by Monte-Carlo simulations. Indeed, the notion of phase transition has a sense only for the thermodynamical limit, while simulations can only be done on finite size systems. For the case of second order phase transitions, for infinite size systems with periodic boundary conditions, the correlation length diverges at the critical temperature T_c. Here, we have a closed and finite space. We will use the finite size analysis which applies here as we have a finite size system. But due to the small size of this system we will not use the finite size scaling. As we are in a finite space, the notion of phase transition has no sense, therefore we will use the word transformation instead of transition.

We shall define here the physical parameters necessary to the finite size analysis. The specific heat per spin c writes:

$$c(t) = \frac{< E^2 > - < E >^2}{N k_B T^2} \tag{2}$$

where E is the total energy of the assembly of spins, T is the the absolute temperature, k_B is Boltzmann constant and $t = T/T_c - 1$ where T_c is the critical temperature. For the order parameter per spin m we have:

$$m(t) = \frac{< |M| >}{N} \tag{3}$$

where M is the magnetization of the whole assembly of spins.

We took $J = 1$ and $k_B = 1$. The results are the following.

3 Results and discussion

In fig.1, one can see the evolution of the specific heat c as a function of β. For low space dimensions $d < 10$ it appears a smooth maximum in this graph which can be interpreted as a transformation at a critical temperature β_c. It is easy to see that if the curved space has a dimension which is odd the inverse of the critical temperature is equal to $\beta_c = 0.6$; if the hypersphere has an even space dimension the critical temperature is equal to $\beta_c = 1.25$. This is valid for all space dimensions enclosed between $d = 1$ and $d = 9$. But for high dimensions, the evolution of the peak of c seems to flatten as a function of β. Though, we have checked that transformations always occur for $N \to \infty$ and that the two values of β_c remain.

Let us look now at fig.2 which is the evolution of the order parameter $< m >$ as a function of the inverse temperature $\beta = 1/k_B T$. For $d = 2$ and $d = 4$, $< m >$ tends to zero when β tends to infinity. For the space dimension $d = 1, 3, 5, 6, 7, 8, 9$ even for $\beta \to \infty$ the magnetization $< m >$ does not tend to zero.

To resume fig.2 we plotted in fig. 3 the values of $< m >$ at $\beta = 0$ (squares) and at $\beta = 5$ (circles). For $d = 100$ we add the value of $< m >= 0.156$ at $\beta = 0$ and $< m >= 0$ at $\beta = 5$.

Geometrical frustration [15] is the explanation of the behavior of both $< m >$ and c as a function of β. $< m >$ at $1/k_B T = 5$ is equal to zero for $d = 2$ and for $d = 4$ because the number of antiferromagnetic spins is even in such spaces and geometrical frustration is not too strong. Hence it is possible that the number of spins up and the number of spins down is equal even if geometrical frustration remains because of the tetrahedral geometry. For even space dimensions larger than 4, geometrical frustration is too strong, and the number of spins up and down is different leading to a non zero value of the magnetization as the temperature goes to zero (i.e. $\beta \to \infty$). If the space dimension is even, the number of spins is also even, hence the transformation from an antiferromagnetic state to a paramagnetic one will occur at a lower temperature, i.e. at a larger β value because the spins can create pairs. Hence the antiferromagnetic state is temporarily and locally possible even with frustration. For odd space dimensions, the odd number of spins renders it impossible to create pairs, transformations occur at a larger temperature (i.e. lower β) because the antiferromagnetic state is unstable. The values of the critical temperature are the same for all odd (resp. even) space dimensions: the tetrahedral geometry is the same in all dimensions, no critical dimension has been observed because of the curvature of space.

The temperature of the transformation from an antiferromagnetic state to a paramagnetic state is the same for the systems with an odd (resp. even) number of spins because for an odd (resp. even) space dimension the energy necessary to create antiferromagnetic pairs of spins does not depend on the number of spins but on the number of spins divided by the number of interaction per spin. As this number is equal for all odd (resp. even) space dimensions this yields the equality between the temperature of transformation for odd (resp. even) dimensional spaces.

The fact that the space is finite yields no periodic boundary conditions. This is a consequence of the curvature of space. Our model may be compared to finite size systems with long range interactions where all spins interact with each others.

To conclude this discussion, we can say that it is necessary to use a numerical method to compute the order parameter and the behavior of the antiferromagnetic spins. Indeed, it is not as is usually found in the literature a conventional lattice with periodic boundary conditions. Moreover, the spins interact with all other spins for each space dimension so the number of interactions increases as $(d+1)!$. And the number of interaction per spin is equal to $d+1$. The calculation of Z the partition function is therefore not simple and not found in the literature at the moment for this kind of geometry.

4 Conclusion

We analyzed the behavior of antiferromagnetic spins interacting all with each other in a tetrahedron configuration in high dimensions. The resulting specific heat shows that the transformation from a paramagnetic state to an anti ferromagnetic configuration , depends on the parity of the number of spins i.e. on the parity of the space dimension and not on the number of spins. The analysis of the magnetization shows that depending on this number of spins, the perfect antiferromagnetic state depends also on the number of spins. If the space dimension equals to 2 or 4, the resulting number of spins leads to a perfect antiferromagnetic state shown by a magnetization equal to zero. Geometrical frustration is the explanation of these behaviors. Our model may be applied to confined antiferromagnetic spins, like nanometric dots of an antiferromagnetic compound.

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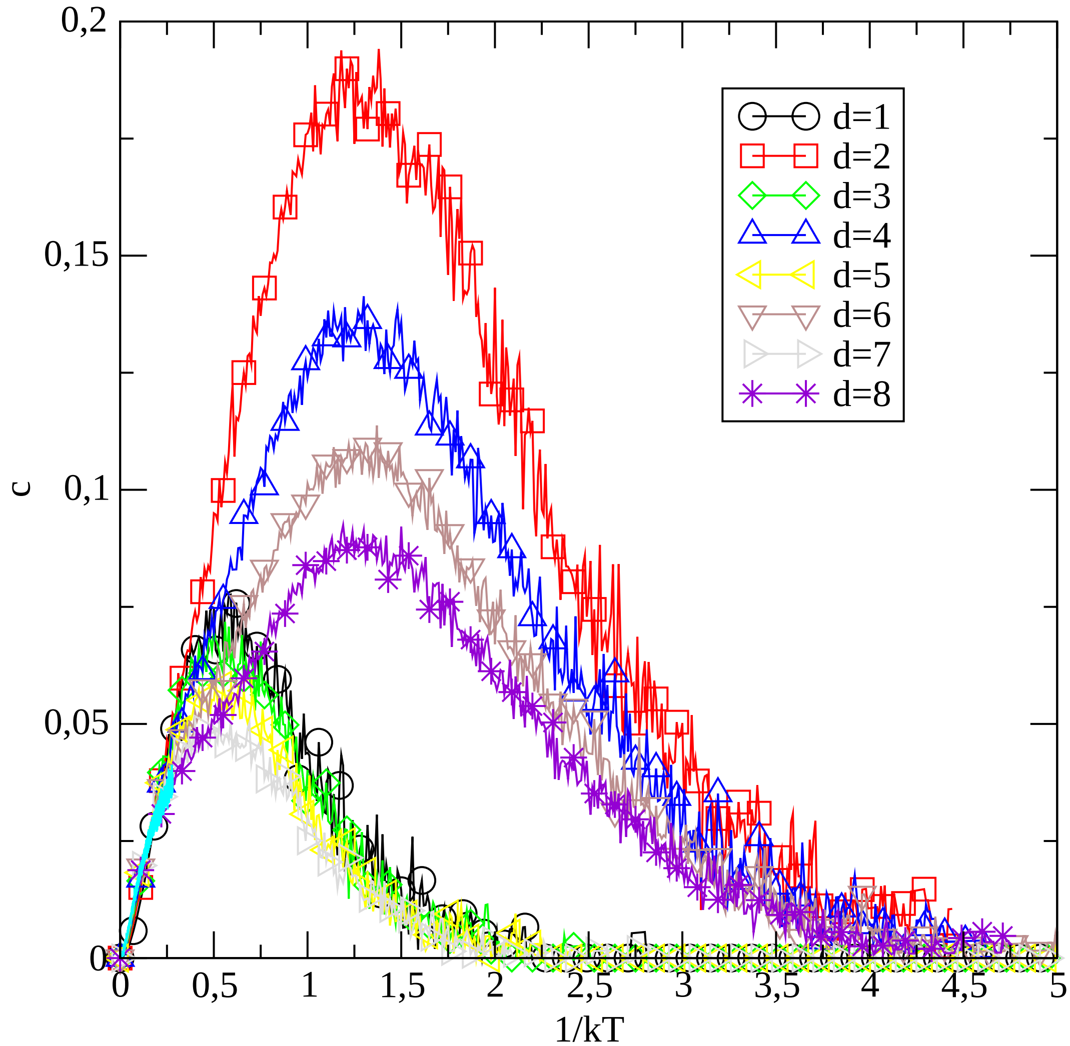

Figure 1: Evolution of the specific heat c as a function of $\beta = 1/k_B T$ for space dimensions : $d = 1, 2, 3, 4, 5, 6, 7, 8, 9$

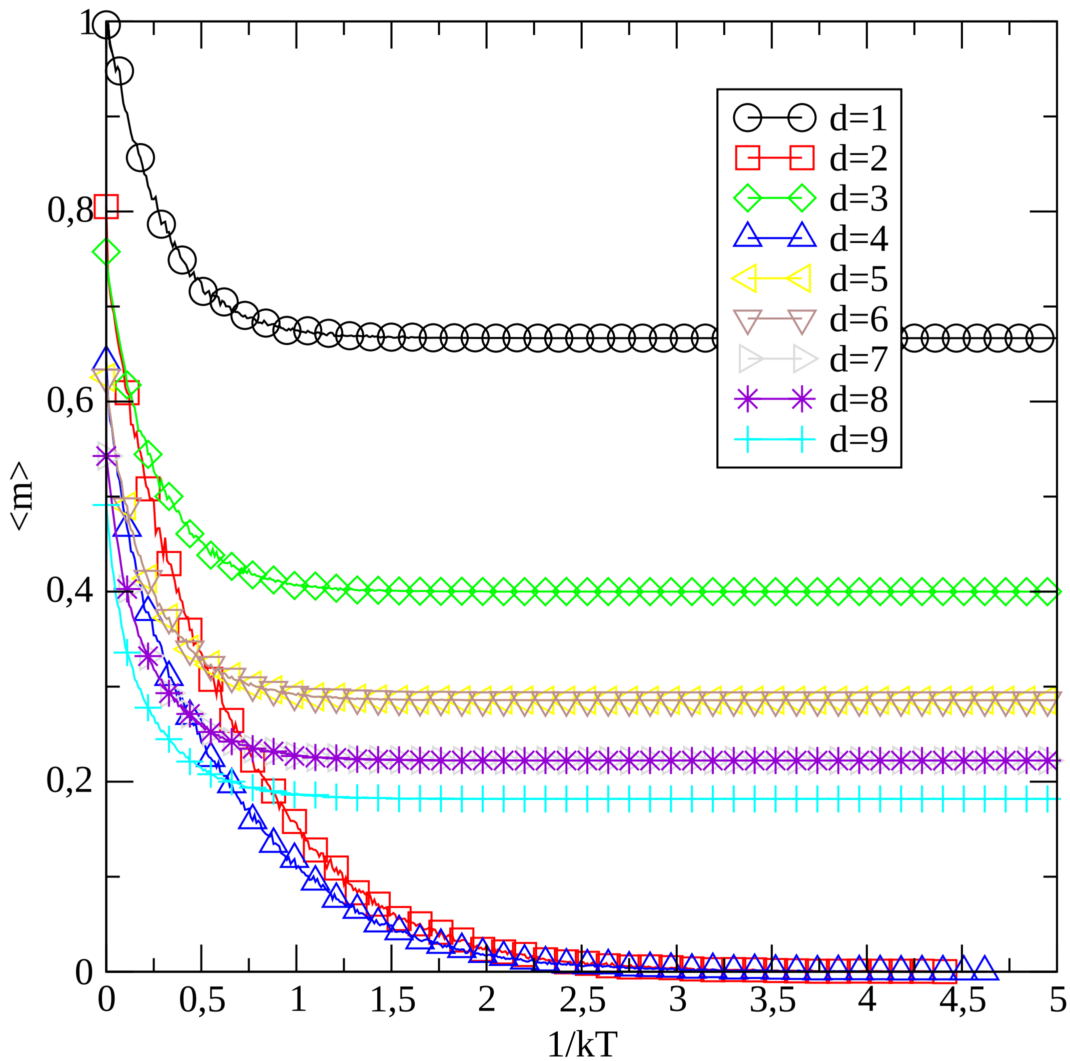

Figure 2: Evolution of the order parameter $< m >$ as a function of $\beta = 1/k_B T$ for space dimensions : $d = 1, 2, 3, 4, 5, 6, 7, 8, 9$

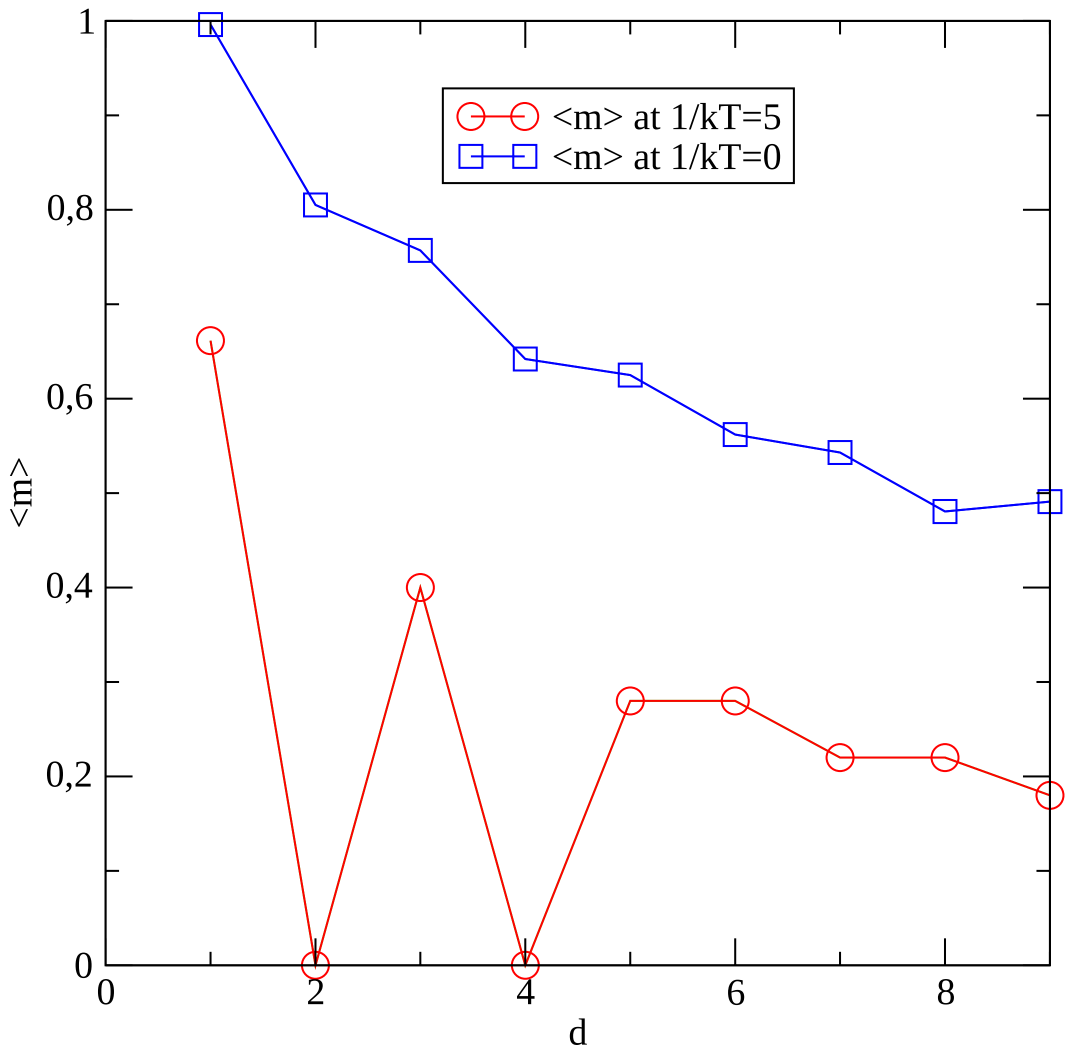

Figure 3: Evolution of the $< m >$ at $1/k_BT = 5$ (circles) and at $1/k_BY = 0$ (squares) as a function of space dimension d