Antiferromagnatic Ising model in scale-free networks

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(Dated: August 25, 2009)

The antiferromagnatic Ising model in uncorrelated scale-free networks has been studied by means of Monte Carlo simulations. These networks are characterized by a connectivity (or degree) distribution \( P(k) \sim k^{-\gamma} \). The disorder present in these complex networks frustrates the antiferromagnatic spin ordering, giving rise to a spin-glass (SG) phase at low temperature. The paramagnetic-SG transition temperature \( T_c \) has been studied as a function of the parameter \( \gamma \) and the minimum degree present in the networks. \( T_c \) is found to increase when the exponent \( \gamma \) is reduced, in line with a larger frustration caused by the presence of nodes with higher degree.

PACS numbers: 64.60.De, 05.50.+q, 75.10.Nr, 89.75.Hc

I. INTRODUCTION

Several types of natural and artificial systems have a network structure, where nodes represent typical system units and edges play the role of interactions between connected pairs of units. This kind of description of complex systems as networks or graphs has attracted much interest in recent years. Thus, complex networks have been used to model various types of real-life systems (biological, social, economic, technological), and to study several processes taking place on them [1, 2, 3, 4, 5]. Some models of networks have been designed to explain empirical data in various fields. This is the case of the so-called small-world [6] and scale-free networks [7], which incorporate different aspects of real systems.

In scale-free (SF) networks the degree distribution \( P(k) \), where \( k \) is the number of links connected to a node, has a power-law decay \( P(k) \sim k^{-\gamma} \) [8, 9]. This kind of networks have been found in the internet [10], in the world-wide web [11], for protein interactions [12], and in social systems [13]. The origin of such power-law degree distributions was addressed by Barabási and Albert [7], who found that two ingredients are sufficient to explain the scale-free character of networks: growth and preferential attachment. They concluded that the combination of these criteria yields non-equilibrium SF networks with an exponent \( \gamma = 3 \). One can also consider equilibrium SF networks, defined as statistical ensembles of random networks with a given degree distribution \( P(k) \) [8, 13], for which it is possible to analyze various properties as a function of the exponent \( \gamma \).

Cooperative phenomena in complex networks display unusual characteristics due to their peculiar topology [13, 14, 15, 16, 17, 18, 19, 20]. In particular, the ferromagnetic (FM) Ising model has been thoroughly studied in scale-free networks [21, 22, 23, 24], and its critical behavior was found to be dependent on the exponent \( \gamma \). For finite \( \langle k^2 \rangle \), a ferromagnetic to paramagnetic transition occurs at a finite temperature \( T_c \). However, when \( \langle k^2 \rangle \) diverges (as happens for \( \gamma \leq 3 \)), the spin system remains in an ordered FM phase at any temperature, so that no phase transition appears in the thermodynamic limit.

Here we study the antiferromagnetic (AFM) Ising model in equilibrium (uncorrelated) scale-free networks with several values of the exponent \( \gamma \). This model contains the two basic ingredients necessary to produce a spin-glass (SG) phase at low temperature: disorder and frustration. In some spin-glass models, such as the Sherrington-Kirkpatrick model, all spins are assumed to be mutually connected [25, 26], whereas in others random graphs with finite (low) connectivity are considered [27, 28, 29, 30]. For the AFM Ising model on scale-free networks, we expect to find features intermediate between these two cases.

Spin glasses on complex networks have been studied in recent years by using several techniques, such as transfer matrix analysis [31], replica symmetry breaking [32], defect-wall calculations [33], and an effective field theory [34]. In this paper, we employ Monte Carlo (MC) simulations to study the paramagnetic to spin-glass phase transition appearing in scale-free networks. In this line, MC simulations have been carried out earlier to analyze spin-glass phases appearing for the AFM Ising model in Barabási-Albert scale-free networks [35], as well as in small-world networks [36].

The paper is organized as follows. In Sec. II we describe the networks and the computational method used here. In Sec. III we present results for the heat capacity, energy, and spin correlation, as derived from MC simulations. In Sec. IV we characterize the spin-glass phase through the overlap parameter and transition temperature. The paper closes with the conclusions in Sec. V.

II. MODEL AND METHOD

We consider SF networks with degree distribution \( P(k) \sim k^{-\gamma} \). They are characterized, apart from the exponent \( \gamma \) and the system size \( N \), by the minimum degree \( k_0 \). We assume that \( P(k) = 0 \) for \( k < k_0 \). Our networks are uncorrelated, in the sense that degrees of nearest neighbors are statistically independent. This means that the distribution \( P(k, k') \) of degrees of nearest-neighbor
nodes fulfills the relation \[ P(k, k') = \frac{k k'}{\langle k \rangle^2} P(k) P(k') . \] (1)

Alternatively, one can use a correlation coefficient \( r \) defined as
\[ r = \frac{\langle k k' \rangle - \langle k \rangle \langle k' \rangle}{\sigma_k^2} , \] (2)

where the averages are taken over all links and \( \sigma_k^2 \) is the variance of the degree distribution. This coefficient \( r \) is zero for uncorrelated networks.

For the numerical simulations we have generated networks with several values of \( \gamma \), \( k_0 \), and \( N \). To generate a network, we first define the number of nodes \( N_k \) with degree \( k \), according to the distribution \( P(k) \), which can be conveniently done by using the so-called transformation method [3]. Then, we ascribe a degree to each node according to the set \{ \( N_k \) \}, and finally connect at random ends of links (giving a total of \( L = \sum_k k N_k / 2 \) connections), with the conditions: (i) no two nodes can have more than one bond connecting them, and (ii) no node can be connected by a link to itself. We have checked that networks generated in this way are uncorrelated, i.e. they fulfill Eq. (1), and \( r = 0 \). The networks considered here contain a single component, i.e. any node in a network can be reached from any other node by traveling through a finite number of links.

Given a network with a particular set of links, we consider an Ising model with the Hamiltonian:
\[ H = \sum_{i < j} J_{ij} S_i S_j , \] (3)

where \( S_i = \pm 1 \) (\( i = 1, \ldots, N \)), and the coupling matrix \( J_{ij} \) is given by
\[ J_{ij} \equiv \begin{cases} J(> 0), & \text{if } i \text{ and } j \text{ are connected}, \\ 0, & \text{otherwise}. \end{cases} \] (4)

This means that each edge in the network represents an AFM interaction between spins on the two linked nodes. Note that, contrary to the usually studied models for spin glasses in which both FM and AFM couplings are present, in our model all couplings are antiferromagnetic (similarly to Refs. [33, 38]).

For a given network, we carried out Monte Carlo simulations at several temperatures, sampling the spin configuration space by the Metropolis update algorithm [39], and using a simulated annealing procedure. Several variables characterizing the spin system have been calculated and averaged for different values of the considered parameters. For each set of parameters \( (\gamma, k_0, N) \), 1000 network realizations were generated, and the largest networks included 16000 nodes. In the sequel, we will use the notation \( \langle \ldots \rangle \) to indicate a thermal average for a network, and \( [\ldots] \) for an average over networks with a given parameter set.

\[ \text{Heat capacity per node (} c_v \text{), vs temperature for scale-free networks with } N = 8000 \text{ nodes and minimum degree } k_0 = 5. \text{ The plotted curves correspond to different values of the exponent } \gamma: 10 \text{ (solid line), 5 (dashed line), 4 (dotted line), and 3 (dashed-dotted line).} \]

**III. THERMODYNAMIC VARIABLES**

We present first results for the heat capacity per site, \( c_v \), as a function of temperature for several values of the exponent \( \gamma \). \( c_v \) has been derived from the energy fluctuations \( \Delta E \) at a given temperature, by using the expression
\[ c_v = \frac{[\langle \Delta E \rangle^2]}{NT^2} , \] (5)

where \( \langle \Delta E \rangle^2 = \langle E^2 \rangle - \langle E \rangle^2 \). We have checked that the results obtained in this way coincide within statistical noise with those derived by calculating the heat capacity as the energy derivative \( [\langle dE/dT \rangle]/N \). Note that we take the Boltzmann constant \( k_B = 1 \).

The temperature dependence of \( c_v \) is displayed in Fig. 1 for scale-free networks with various values of \( \gamma \) between 3 and 10. The data shown correspond to networks including 8000 nodes. For increasing \( \gamma \), we observe that the maximum of \( c_v \) shifts to lower \( T \), and the peak becomes narrower. This narrowing is in line with that observed earlier for the heat capacity in the AFM Ising model on small-world networks, when the disorder is reduced [36]. In our case of scale-free networks, larger values of the exponent \( \gamma \) correspond to networks with a higher homogeneity in the node connectivities (less dispersion in the degree distribution), causing a narrower peak in the heat capacity, as shown in Fig. 1. The peak shift to lower temperatures suggests a transition from a paramagnetic to a SG phase at a temperature \( T_c \) that decreases as the exponent \( \gamma \) rises. For increasing \( \gamma \), one reduces the presence of nodes with a large degree, which in turn reduces the degree of frustration in the spin distribution (see below).
AFM ordering on the considered random networks with power-law distribution of degrees is frustrated by the disorder in the link configuration, and in particular by the presence of loops with an odd number of nodes. The degree of frustration can be quantified by looking at the low-temperature energy of the system, which will be higher for larger frustration. Given the parameters $\gamma$ and $k_0$ defining the scale-free networks, we obtain a value for the minimum energy by extrapolating to infinite size the minimum energy reached in our simulations of finite-$N$ networks. This extrapolation has been performed by assuming a dependence of the energy on network size of the form:

$$e_m(N) = e_m + \frac{A}{N^{2/3}},$$

where $e_m(N)$ is the energy per link for size $N$, $e_m$ is its limit for $N \to \infty$, and $A$ is a fit parameter. This kind of dependence of the low-temperature energy in spin-glass systems was proposed by Boettcher [30], and has been found to be followed by the results of our calculations using the simulated-annealing method. We have checked that our method to obtain a minimum energy for the AFM Ising model on complex networks gives similar results to those found by using extremal optimization [30]. In particular, for spin glasses on random graphs with a Poisson distribution of connectivities, we found results very close to those obtained by using this technique [30].

In any case, the energy $e_m$ found here for each parameter set $(k_0, \gamma)$ will be an upper limit for the lowest energy of the system.

In Fig. 2, we show results for the minimum energy per link $e_m$ found for three values of $k_0$ and several values of the exponent $\gamma$. For a given $k_0$, one observes an increase in $e_m$ as the exponent $\gamma$ is reduced. This indicates that the presence of nodes with large degree (hubs), which is favored for small $\gamma$, plays in our context the role of increasing the frustration in the spin arrangement. For a given $\gamma$, one observes also in Fig. 2 an increase in the energy $e_m$ for rising $k_0$. This shows that an increase in the minimum connectivity (or in the average degree $\langle k \rangle$), causes also a higher frustration in the AFM ordering.

A quantification of the short-range order present in the spin system on scale-free networks can be obtained by calculating the spin correlation

$$\xi(r) = \langle S_i S_j \rangle_r,$$

where the subscript $r$ indicates that the average is taken for the ensemble of pairs of sites at distance $r$. Note that the dimensionless distance $r$ refers to the minimum number of links between two nodes, also called in the literature chemical or topological distance. The correlation $\xi(r)$ is shown in Fig. 3 for several values of the exponent $\gamma$ at a temperature $T = J$. This temperature is below the critical temperature $T_c$ of the paramagnetic-SG transition for all values of $\gamma$ (see below). As expected, $\xi(r)$ decreases faster for smaller $\gamma$, due to the presence of nodes with large degree, and consequently a larger frustration of the AFM ordering, as discussed above in connection with the minimum energy per link.

To obtain more direct insight into the reduction of $\xi(r)$ with the distance, we display in Fig. 4 $|\xi(r)|$ on a
FIG. 4: Absolute value of the spin correlation function $\xi$ vs distance in a semilogarithmic plot. Shown is $\ln|\xi(r)|$ for scale-free networks with minimum degree $k_0 = 3$ and several values of the exponent $\gamma$ at $T = J$. Symbols correspond to different values of $\gamma$. From top to bottom: $\gamma = \infty$ (regular networks, open squares), 10 (circles), 6 (triangles), 5 (open diamonds), 4 (filled diamonds), and 3 (filled squares). Error bars are on the order of the symbol size. These results were derived from Monte Carlo simulations for networks including $N = 8000$ nodes.

A semilogarithmic plot for various $\gamma$ values. In general, after a short transient for small $r$, one obtains an exponential decrease in the spin correlation with distance, as $|\xi(r)| \sim e^{-ar}$, $a$ being a parameter that depends on temperature as well as on the parameters defining the networks ($k_0$ and $\gamma$). For the results shown in Fig. 4, we find a parameter $a$ that decreases from 1.01(3) to 0.386(5) when increasing $\gamma$ from 3 to 10, and reaches the limit $a = 0.321(4)$ for regular random networks with constant degree $k = k_0 = 3$. We note that here the limit $\gamma \to \infty$ correspond to networks (called regular [40]), in which all nodes have the same degree $k_0$, and consequently do not include any hub with high degree.

IV. SPIN-GGLASS BEHAVIOR

A. Overlap parameter

In the study of spin glasses, it is usual to consider two copies of the same network, with a given realization of the disorder. Then, one considers a spin system on each network, both with different initial values of the spins, and follows their evolution with different random numbers for generating the spin flips [41,42]. A particularly relevant parameter is the overlap $q$ between the two copies, defined as

$$q = \frac{1}{N} \sum_i S_i^{(1)} S_i^{(2)},$$

where the superscripts (1) and (2) indicate the copies. This parameter $q$ is defined in the interval $[-1, 1]$, and the extreme values 1 and $-1$ correspond to pairs of networks with the same spin configuration (apart from a trivial overall flip in the $-1$ case).

We have calculated the overlap parameter $q$ for scale-free networks with various exponents $\gamma$, and derived the probability distribution $Q(q)$ from Monte Carlo simula-
tions. Results for \( Q(q) \) are presented in Fig. 5. In particular, in Fig. 5(a) we display the distribution of the overlap parameter for networks with \( \gamma = 3 \) at several temperatures. At high temperatures (\( T \gg J \)), the distribution \( Q(q) \) shows a single peak centered at \( q = 0 \), which is characteristic of a paramagnetic state. This peak has, however, a finite width, which results to be a finite-size effect. It should collapse to a Dirac delta function at \( q = 0 \) in the limit \( N \to \infty \). When the temperature is lowered, \( Q(q) \) broadens around \( q = 0 \), due to the appearance of an increasing number of frustrated links. At still lower temperatures, frustration is more apparent, and “freezing” of the spins causes the appearance of two peaks in \( Q(q) \), symmetric respect to \( q = 0 \), and characteristic of spin-glasses \cite{35,36,42,43}. Such a distribution \( Q(q) \) is associated to the break of ergodicity occurring in the spin system at low temperatures.

In Fig. 5(b) we show the distribution \( Q(q) \) for three values of the exponent \( \gamma \) at a fixed temperature \( T = 2J \). The effect of decreasing \( \gamma \) for a given \( T \) is similar to that shown in Fig. 5(a) for lowering the temperature for a given \( \gamma \), in the sense that in both cases one passes from a high-temperature paramagnetic phase to a spin-glass with broken ergodicity. From the results displayed in Fig. 5(b), along with those presented in Sect. III (especially Fig. 1 for the heat capacity and Fig. 2 for the minimum energy per link), we expect that the freezing of the spins in the SG phase occurs at lower \( T \) for larger \( \gamma \). In other words, one expects that the transition temperature from paramagnetic to SG will decrease for rising \( \gamma \).

### B. Transition temperature

The overlap parameter \( q \) can be further employed to obtain precise values of the paramagnetic-SG transition temperature. To this end, one can use the fourth-order Binder cumulant \cite{33,42}

\[
    g_N(T) = \frac{1}{2} \left( 3 - \frac{\langle q^4 \rangle_N}{\langle q^2 \rangle_N^2} \right) ,
\]

which is restricted to the interval \([0,1]\). On one side, this parameter \( g_N \) vanishes at high temperatures, as expected for a Gaussian distribution \( Q(q) \) in a paramagnetic state. On the other side, one has \( g_N = 1 \) whenever the distribution \( Q(q) \) vanishes everywhere except for \( |q| = 1 \), which corresponds to the case of a single ground state, and could be reached at low temperatures. This case (\( g_N = 1 \)) is clearly not expected here due to the onset of frustration, which gives rise to the spin-glass phase.

In general, \( g_N \) increases as temperature is lowered, and the transition temperature \( T_c \) can be obtained from the single crossing point for different network sizes \( N \) \cite{37,39}. By employing this method, we have calculated \( T_c \) for scale-free networks with several values of the parameters \( k_0 \) and \( \gamma \), and the results obtained are displayed in Fig. 6. In this figure, we have plotted \( T_c \) as a function of \( \gamma^{-1} \), and the limit \( \gamma \to \infty \) corresponds to regular random networks with \( k = k_0 \). This limit gives a reasonable extrapolation of the \( T_c \) values obtained for \( \gamma \) values up to \( \gamma = 10 \). For a given minimum degree \( k_0 \), the transition temperature increases as \( \gamma \) is lowered. Also, for a given value of \( \gamma \), \( T_c \) grows for increasing \( k_0 \), similarly to the case of the minimum energy \( e_m \) displayed in Fig. 2. We note that the transition temperature \( T_c \) derived from the Binder cumulant is in the order of the maximum (negative) temperature derivative of the heat capacity \( c_0 \) for finite networks, as can be seen by comparing results for \( k_0 = 5 \) in Figs. 1 and 6.

The average degree \( \langle k \rangle \) of scale-free networks can be estimated rather accurately by replacing the sum \( \sum_k k P(k) \) by an integral. Thus, one finds for networks with \( P(k) \sim k^{-\gamma} \) and \( \gamma > 2 \), that the average degree scales as

\[
    \langle k \rangle \approx \frac{\gamma - 1}{\gamma - 2} k_0 ,
\]

From this expression, it is clear that \( \partial\langle k\rangle/\partial k_0 > 0 \) and \( \partial\langle k\rangle/\partial \gamma < 0 \). Since rising \( k_0 \) or lowering \( \gamma \) cause an increase in the transition temperature, we observe that in fact a rise in \( \langle k \rangle \) is accompanied by a rise in \( T_c \).

In this context, it is interesting to compare our results for \( T_c \) in scale-free networks with those found for the paramagnetic-SG transition in other complex networks. In Ref. 36 it was studied the AFM Ising model on small-world networks generated by rewiring links in a regular lattice \cite{6}. It was found that the transition temperature decreases as the disorder (number of random connections) increases, in networks where the average degree was kept constant (\( \langle k \rangle = 4 \)). In the limit of
large disorder, those networks approach random networks with a Poisson distribution of degrees, and the transition temperature for the AFM Ising model was found to be $T_c = 1.71 J$. Going back to our random networks with power-law degree distribution, we have an average degree $\langle k \rangle \approx 4$ for $k_0 = 3$ and $\gamma = 5$ [see Eq. (10)]. For these networks, we find $T_c = 1.65 J$, as shown in Fig. 6, a value close to that obtained for small-world-type networks in the large-disorder limit and $\langle k \rangle = 4$.

All this could suggest that the transition temperature $T_c$ is proportional to the average degree $\langle k \rangle$, irrespective of the details of the networks under consideration. This is, however, not the case, as can be inferred directly from the results displayed in Fig. 6. Looking for example at the data for $k_0 = 3$, we observe that going from $\gamma = 3$ to the limit $\gamma \to \infty$, $\langle k \rangle$ decreases by a factor of 2 (from 6 to 3). On the other side, $T_c$ is reduced by a factor $\approx 4$. Since lowering $\gamma$ increases the inhomogeneity in the degree distribution, favoring the presence of nodes with degree much larger than $\langle k \rangle$, we find that this inhomogeneity helps to rise the transition temperature.

Bartolozzi et al. [35] studied the AFM Ising model on Barabási-Albert scale-free networks, and found a paramagnetic-SG transition temperature $T_c = 4.0(1) J$. These nonequilibrium networks are characterized by an exponent $\gamma = 3$, and those authors used the particular value of the minimum degree $k_0 = 5$. For these parameters, we find for equilibrium networks a transition temperature $T_c = 4.8(2) J$, a value somewhat higher than that obtained in Ref. [35].

We note that the error bar in the transition temperature grows when $\gamma$ is reduced. In fact, the actual value of the cumulant $g_N$ at the crossing point for different $N$ values (network sizes) decreases as $\gamma$ is lowered, and is near zero for $\gamma \sim 3$. This coincides with results shown for this cumulant in Ref. [35] for Barabási-Albert SF networks, where the value of $g_N$ at the crossing point was less than 0.01. This means that the signal-to-noise ratio in $g_N$ becomes poor, and one has an increasing uncertainty in $T_c$. For networks with $\gamma < 3$, we could not find a single crossing point for the cumulant corresponding to different network sizes, and a transition temperature cannot be given. We note that these $\gamma$ values correspond to SF networks with diverging $\langle k^2 \rangle$. In this respect, it is known that the ferromagnetic Ising model in such networks does not show a phase transition, and remains in an ordered FM phase at any temperature in the thermodynamic limit [21, 22, 23, 21]. Something similar could happen for the AFM Ising model in these networks. This point remains as a challenge for future research.

V. CONCLUSIONS

The AFM Ising model in random networks with a power-law distribution of degrees gives rise to a spin-glass phase at low temperature. This is a consequence of the combination of disorder in the networks and frustration caused by the presence of loops with odd number of links. The overlap parameter $q$ gives us evidence of this frustration at low temperatures.

The transition temperature $T_c$ from the high-temperature paramagnetic phase to the spin-glass has been studied as a function of the minimum degree $k_0$ and the exponent $\gamma$ in the degree distribution. $T_c$ is found to rise for increasing $k_0$ and for lowering $\gamma$.

For a given $k_0$, both the transition temperature and the minimum energy per link $e_m$ found from our simulations increase as the exponent $\gamma$ is lowered. This indicates that the degree of frustration in the spin configurations rises with the presence of nodes with large degree (hubs). The same conclusion can be reached by analyzing the spin correlation as a function of distance, which decays faster for smaller values of $\gamma$.

Acknowledgments

This work was supported by Ministerio de Ciencia e Innovación (Spain) under Contract No. FIS2006-12117-C04-03.

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