Ising model in scale-free networks: A Monte Carlo simulation

Carlos P. Herrero
Instituto de Ciencia de Materiales, Consejo Superior de Investigaciones Científicas (CSIC), Campus de Cantoblanco, 28049 Madrid, Spain
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The Ising model in uncorrelated scale-free networks has been studied by means of Monte Carlo simulations. These networks are characterized by a degree (or connectivity) distribution $P(k) \sim k^{-\gamma}$. The ferromagnetic-paramagnetic transition temperature has been studied as a function of the parameter γ. For $\gamma > 3$ our results agree with earlier analytical calculations, which found a phase transition at a temperature $T_c(\gamma)$ in the thermodynamic limit. For $\gamma \leq 3$, a ferromagnetic-paramagnetic crossover occurs at a size-dependent temperature T_{co}, and the system is in the ordered ferromagnetic state at any temperature for a system size $N \to \infty$. For $\gamma = 3$ and large enough N, the crossover temperature is found to be $T_{co} \approx A \ln N$, with a prefactor A proportional to the mean degree. For $2 < \gamma < 3$, we obtain $T_{co} \sim \langle k \rangle N^z$, with an exponent z that decreases as γ increases. This exponent is found to be lower than predicted by earlier calculations.

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Complex networks describe several kinds of natural and artificial systems (social, biological, technological, economic), and are currently employed as models to study various processes taking place in real-life systems [1–3]. In last years, new models of complex networks have been introduced, motivated by empirical data in different fields. Thus, the so-called small-world [4] and scale-free (SF) networks [5] incorporate various aspects of real systems. These complex networks provide us with the underlying topological structure to study processes such as spread of infections [6], signal propagation [1,7], and cooperative phenomena [8–11].

In a SF network the degree distribution, $P(k)$, where k is the number of links connected to a node, has a power-law decay $P(k) \sim k^{-\gamma}$. This kind of networks have been found in particular in social systems [12], in protein interaction networks [13], in the internet [14], and in the world-wide web [15]. In both natural and artificial networks, the exponent γ controlling the degree distribution is usually in the range $2 < \gamma < 3$ [3,16].

Cooperative phenomena in complex networks are expected to display unusual characteristics, associated to the peculiar topology of these systems. In this context, the Ising model on SF networks has been studied with several theoretical techniques [9,17,18], and its critical behavior was found to be dependent on the exponent γ. In particular, when $\langle k^2 \rangle$ is finite, there appears a ferromagnetic (FM) to paramagnetic (PM) transition at a finite temperature T_c. On the contrary, when $\langle k^2 \rangle$ diverges (as happens for $\gamma \leq 3$), the system remains in its ordered FM phase at any temperature, and no phase transition occurs in the thermodynamic limit.

Here we investigate the FM-PM transition for the Ising model in scale-free networks with various values of the exponent γ. We employ Monte Carlo (MC) simulations to obtain the transition temperature, and compare it with that predicted in earlier calculations. Our results confirm those of analytical calculations for $\gamma > 3$, and are used to check the precision of those obtained earlier with approximate methods for $\gamma \leq 3$.

Our networks are defined, apart from γ, by the maximum and minimum degrees, denoted $k_{\rm cut}$ and k_0, respectively. Thus, the number of sites with degree k is given by $N_k = (k_{\rm cut}/k)^\gamma$ for $k_0 \leq k \leq k_{\rm cut}$, and $N_k = 0$ otherwise. This gives $N_{k_{\rm cut}} = 1$, and a system size $N = \sum_{k_0}^{k_{\rm cut}} N_k$, which for large $k_{\rm cut}$ scales as $N \sim k_{\rm cut}^\gamma$. Once $\{N_k\}$ is defined [or the corresponding probability density $P(k) = N_k/N$], one has a total number of ends of links (total degree) $K = \sum_{k_0}^{k_{\rm cut}} k N_k$. Then we ascribe a degree to each node according to $\{N_k\}$, and finally connect at random ends of links (giving a total of $L = K/2$ 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, in the sense that the joint probability $P(k,k')$ for degrees of nearest neighbors fulfills the relation $P(k,k') = k\,k' P(k) P(k') / \langle k \rangle^2$ [3].

On these scale-free networks, we consider the Hamiltonian

$$H = -\sum_{i<j} J_{ij} S_i S_j \,, \tag{1}$$

where $J_{ij} = J(>0)$ if nodes i and j are connected, and $J_{ij} = 0$ otherwise. $S_i = \pm 1$ ($i = 1, ..., N$) are Ising spin variables. Sampling of the configuration space has been carried out by the Metropolis local update algorithm [19]. This allows us to study the temperature dependence of the magnetization, and in particular the transition from a FM to a PM regime as T is increased. Depending on the value of the exponent γ, this transition: (i) can occur at a well-defined temperature in the thermodynamic limit ($N \to \infty$), or (ii) may display a FM-PM crossover temperature shifting with system size and diverging to

infinity as $N \to \infty$. For the sake of clarity we will employ a different notation for the temperature of phase change in both cases. In the first case, we will call it T_c as for thermodynamic phase transitions ($T_c < \infty$). In the second case, it will be called crossover temperature, T_{co}, to emphasize its size dependence.

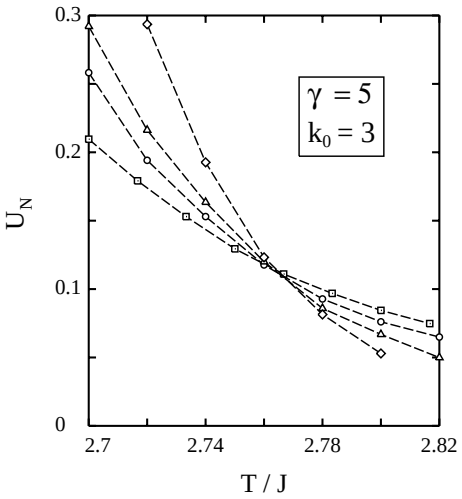

FIG. 1. Fourth-order Binder's cumulant U_N as a function of temperature for scale-free networks with $\gamma = 5$ and $k_0 = 3$. Symbols represent different system sizes: squares, $k_{\rm cut} = 15$; circles, $k_{\rm cut} = 17$; triangles, $k_{\rm cut} = 19$, and diamonds, $k_{\rm cut} = 22$. These values of $k_{\rm cut}$ correspond to system sizes N ranging from 4300 to 29300.

When a FM-PM transition occurs in the thermodynamic limit, the transition temperature T_c has been determined by using Binder's fourth-order cumulant [19]

$$U_N(T) \equiv 1 - \frac{\langle M^4 \rangle_N}{3\langle M^2 \rangle_N^2}\,, \qquad (2)$$

where the magnetization M of a given spin configuration $\{S_i\}$ is $M = \sum_{i=1}^{N} S_i/N$. The average values in Eq. (2) are taken over different network realizations and different spin configurations for a given network at temperature T. In this case, the transition temperature is obtained from the unique crossing point for several sizes N.

In the second case, the size-dependent crossover temperature $T_{co}(N)$ has been determined from the maximum of the magnetization fluctuations, $(\Delta M)^2_N = \langle M^2 \rangle_N - \langle M \rangle^2_N$, as a function of temperature. We have checked that the crossover temperatures obtained by using this criterion agree within error bars with those derived from the maximum derivative of the heat capacity. In particular, both procedures give the same size-dependence of T_{co} in the cases presented below.

The largest networks considered here included about 5×10^5 sites. Such network sizes are required in particular to determine the power law characterizing the size dependence of the crossover temperature T_{co} for scale-free networks with $2 < \gamma < 3$. On the contrary, for the cases in which a phase transition exists in the thermodynamic limit ($\gamma > 3$), smaller sizes are necessary (see below). The results presented below were obtained by averaging in each case over 1000 networks, except for the largest system sizes, for which 400 network realizations were considered.

Case $\gamma > 3$.— For scale-free networks with $\gamma > 3$, the average value $\langle k^2 \rangle$ converges to a finite value as $k_{\rm cut} \to \infty$. In this case, analytical calculations [9,17] predict a well-defined FM-PM transition temperature T_c given by

$$\frac{J}{T_c} = \frac{1}{2} \ln \left(\frac{\langle k^2 \rangle}{\langle k^2 \rangle - 2\langle k \rangle} \right)\,. \qquad (3)$$

We have calculated Binder's cumulant U_N for several values of γ and different network sizes. As an example, in Fig. 1 we present U_N as a function of temperature for $\gamma = 5$, $k_0 = 3$, and various values of $k_{\rm cut}$. The transition temperature is obtained from the crossing point for different system sizes (or cutoffs $k_{\rm cut}$).

The same procedure has been repeated for other values of k_0. The resulting values of T_c are presented in Fig. 2 (open symbols), along with the transition temperature predicted by Eq. (3) (solid line). In fact, this line was obtained by joining values of T_c derived from Eq. (3) for integer values of k_0 in the limit $k_{\rm cut} \to \infty$. The MC results agree within error bars with the transition temperature given by Eq. (3). For comparison, we also present the critical temperature obtained in a simple mean-field approach [9]: $T_c^{MF} = \langle k^2 \rangle / \langle k \rangle$, which is displayed as a dashed line.

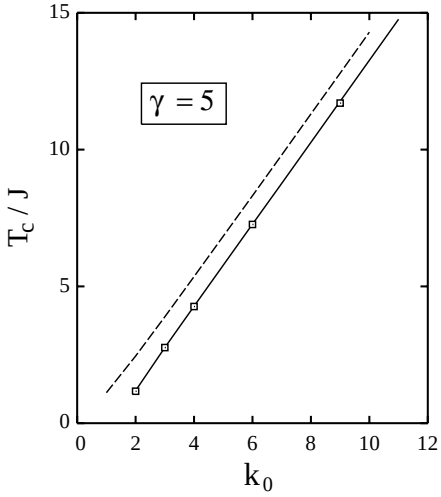

FIG. 2. Transition temperature T_c for scale-free networks with $\gamma = 5$ as a function of the minimum degree k_0. Symbols represent results of MC simulations, as obtained from Binder's cumulant. Error bars are less than the symbol size. The solid line was plotted by connecting points obtained from Eq. (3) for integer values of k_0 and $k_{\rm cut} \to \infty$. The dashed line shows the mean-field result for T_c.

The critical temperature T_c obtained from Eq. (3) for $\gamma = 5$ and $k_0 > 3$ can be fitted linearly with good precision as $T_c = ak_0 + b$, with the parameters $a = 1.50$ and $b = -1.72$. The value of a can in fact be estimated by approximating by integrals the sums giving the average values $\langle k \rangle$ and $\langle k^2 \rangle$ in Eq. (3). This approach gives for large k_0, $T_c \approx \frac{3}{2} k_0$. We note that for $k_0 = 2$ and 3, the actual values of T_c deviate slightly from such a linear fit. For $k_0 = 1$, Eq. (3) is not defined, since $\langle k^2 \rangle - 2\langle k \rangle < 0$. In this case, the simulated networks consist of many different (not connected) components, and Binder's cumulant does not give a crossing for different system sizes.

Case $\gamma = 3$.— The transition temperature given by Eq. (3) increases for increasing γ and eventually diverges for $\gamma \to 3$, as a consequence of the divergence of $\langle k^2 \rangle$. For $\gamma = 3$, analytical calculations [17,18] predict a FM-PM crossover at a size-dependent temperature T_{co}, which scales as $\log N$. Such a logarithmic increase of T_{co} with N has been also obtained by Aleksiejuk *et al.* [20,21] from Monte Carlo simulations of the Ising model in Barabási-Albert growing networks. We note that these networks have $\gamma = 3$, but display correlations between degrees of adjacent nodes [5].

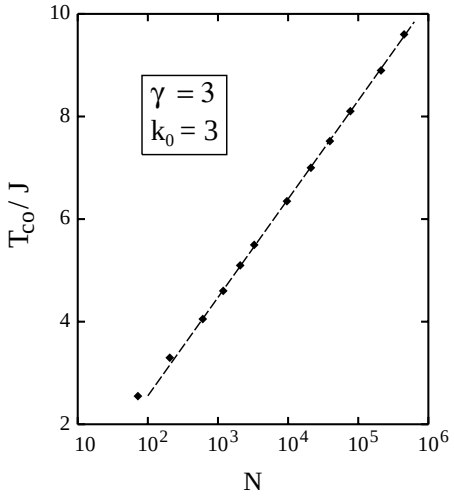

FIG. 3. Crossover temperature T_{co} for scale-free networks with $\gamma = 3$ and $k_0 = 3$, as a function of the system size N, presented in a logarithmic plot. Symbols indicate results derived from MC simulations, with error bars less than the symbol size. The dashed line is a least-square fit to the data points for $N > 500$.

Our results for T_{co} in the case $\gamma = 3$ and $k_0 = 3$ are shown in Fig. 3 as a function of the system size N in a logarithmic plot. We indeed find a logarithmic dependence of T_{co} on N, as in earlier works. In Fig. 3, symbols represent simulation results and the dashed line is a least-square fit to the data points with $N > 500$ (smaller sizes give T_{co} values that deviate from the asymptotic trend). Thus, our results indicate a dependence: $T_c/J = A \ln N + B$, with constants $A = 0.83$ and $B = -1.28$. We have repeated the MC simulations for $k_0 = 5$ and 9, and obtained the same logarithmic dependence as for $k_0 = 3$. The prefactor A increases linearly with k_0, and in fact we found: $A/k_0 = 0.28 \pm 0.01$. For Barabási-Albert networks with $k_0 = 5$, Aleksiejuk *et al.* [20] found from a fit similar to ours $A = 2.6$, which means $A/k_0 = 0.52$.

For uncorrelated scale-free networks with $\gamma = 3$, Dorogovtsev *et al.* [17] found $T_{co}/J \approx \frac{1}{4}\langle k \rangle \ln N$. For $k_0 = 3$ and $k_{\rm cut} \to \infty$, one has $\langle k \rangle = 5.125$, and thus their calculations predict $T_{co}/J \approx 1.28 \ln N$, with a prefactor A on the order of unity, as that obtained here. Mean-field calculations for $\gamma = 3$ give $T_c = \frac{1}{2} J k_0 \ln N$ [9,21], which translates into a ratio $A/k_0 = 0.5$, somewhat larger than that found from our MC simulations.

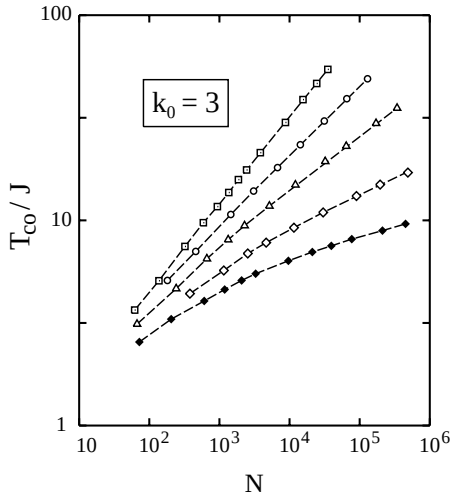

FIG. 4. Crossover temperature T_{co} for scale-free networks with $2 \leq \gamma \leq 3$, as a function of the system size N, in a log-log plot. From top to bottom: $\gamma = 2$, 2.2, 2.4, 2.7, and 3. Error bars are less than the symbol size. Dashed lines are guides to the eye.

Case $2 < \gamma < 3$.— For scale-free networks with $\gamma < 3$, analytical calculations [17,18] predict a size-dependent crossover temperature T_{co} scaling as $\sim J\langle k \rangle N^z$, with an exponent z dependent of the parameter γ. In Fig. 4 we show the temperature T_{co} as a function of the system size N for several values of γ in a log-log plot, as derived from our MC simulations (for $k_0 = 3$). The exponent γ decreases from top to bottom: $\gamma = 2$, 2.2, 2.4, 2.7, and 3. For a given system size, T_{co} decreases as γ increases, as a consequence of the reduction in $\langle k^2 \rangle$. For a given $\gamma < 3$ and large-enough networks, $\log T_{co}$ displays a linear dependence on $\log N$, as expected for a crossover temperature T_{co} diverging as a power of the system size N. This linear dependence is obtained for system sizes $N \gtrsim N_0$, N_0 increasing with γ and eventually diverging for $\gamma \to 3$. This means that the present MC procedure cannot be applied to obtain accurately the exponent z close to $\gamma = 3$, unless one employes much larger system sizes. However, for $\gamma < 2.8$, z can be found with enough precision for the system sizes considered here.

Thus, we have derived the exponent z from our simulation results for $\gamma < 2.8$ by obtaining the slope of $\log[T_{co}/(J\langle k\rangle)]$ vs $\log N$ for large N. Our results are shown in Fig. 5 (open symbols) as a function of γ. The solid line represents the analytical prediction [17,18]:

$$z = \frac{3-\gamma}{\gamma-1} \, . \tag{4}$$

Our results agree with the analytical calculations in that the ratio $T_{co}/(J\langle k\rangle)$ diverges with N as a power law, with exponent z increasing for decreasing γ. However, our MC simulations give values of z lower than Eq. (4). In particular, for $\gamma \to 2$ Eq. (4) gives $z = 1$, and our numerical procedure yields $z = 0.43 \pm 0.02$.

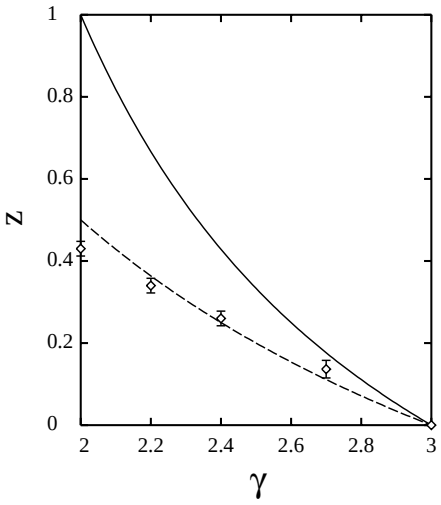

FIG. 5. The exponent z giving the power-law dependence of the crossover temperature T_{co} is plotted vs the parameter γ for scale-free networks. Open symbols are results derived from Monte Carlo simulations. The solid line corresponds to the analytical prediction given by Eq. (4). The dashed line represents the dependence $z = (3-\gamma)/\gamma$.

The exponent z in Eq. (4) is related to the divergence of $\langle k^2\rangle$ in networks with $\int_{k_{\rm cut}}^{\infty} P(k)dk \sim 1/N$, which means that $k_{\rm cut} \sim N^{1/(\gamma-1)}$ [17,18]. However, for the networks considered here, for practical computational reasons we have defined a sharp cutoff $k_{\rm cut}$, which gives a dependence $\langle k^2\rangle \sim N^{(3-\gamma)/\gamma}$, or $k_{\rm cut} \sim N^{1/\gamma}$. Therefore, assuming that T_{co} diverges with the same exponent as $\langle k^2\rangle$, we have $z = (3-\gamma)/\gamma$. This dependence of z on γ is plotted in Fig. 5 as a dashed line. Our MC results follow this line, but separate from it at $\gamma = 2$. It is not clear the reason for this discrepancy. One can argue, however, that in the limit $\gamma \to 2$ the average value $\langle k\rangle$ diverges logarithmically, and thus the convergence of the exponent for the ratio $\langle k^2\rangle/\langle k\rangle$ should be very slow, in spite of the apparent convergence shown in Fig. 4. This point may require further theoretical consideration.

In summary, we have studied the FM-PM transition for the Ising model in uncorrelated scale-free networks, by means of Monte Carlo simulations. For $\gamma > 3$ our results for the temperature transition fully agree with earlier analytical calculations, confirming the appearance of a well-defined transition in the thermodynamic limit. For $\gamma \leq 3$ we find a crossover temperature which increases with system size. In particular, for $\gamma = 3$ such an increase is found to be $T_{co} \approx 0.28 k_0 \ln N$, whereas for $\gamma < 3$ we obtained $T_{co} \sim J\langle k\rangle N^z$, with an exponent z lower than predicted by earlier analytical calculations. We finally note that some care should be taken when comparing analytical results for scale-free netwoks with those derived from simulations, since the cutoff definition for the actually simulated networks may appreciably change the results in some cases.

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