

First- and second-order phase transitions in scale-free networks

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We study first- and second-order phase transitions of ferromagnetic lattice models on scale-free networks, with a degree exponent γ . Using the example of the q -state Potts model we derive a general self-consistency relation within the frame of the Weiss molecular-field approximation, which presumably leads to exact critical singularities. Depending on the value of γ , we have found three different regimes of the phase diagram. As a general trend first-order transitions soften with decreasing γ and the critical singularities at the second-order transitions are γ dependent.

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Complex networks, which have more complicated connectivity structure than periodic lattices (PLs) have attracted considerable interest recently [1,2]. This research is motivated by empirical data collected and analyzed in different fields. Small-world (SW) networks [3], which can be generated from PLs by replacing a fraction p of bonds by new random links of arbitrary lengths, are suitable to model neural networks [4] and transportation systems [5]. On the other hand, scale-free (SF) networks [6] are realized among others in social systems [7], in protein interaction networks [8], in the Internet [9] and in the World-Wide Web [10]. In a SF network the degree distribution $P_D(k)$, where k is the number of links connected to a vertex, has an asymptotic power-law decay $P_D(k) \sim k^{-\gamma}$, thus there is no characteristic scale involved. In natural and artificial networks the value of the degree exponent is usually in the range $2 < \gamma < 3$ [11].

Cooperative processes such as spread of epidemic disease [12], percolation [13], Ising model [14,15], etc., have also been studied in the SW and the SF networks. For SW networks numerical studies show [16] that any finite fraction of new, long-range bonds, $p > 0$, brings the transition into the classical, mean-field (MF) universality class. It is understandable since for systems with long-range interactions the MF approximation is exact. In the SF networks, where links between remote sites exists, too, at first thought one could expect also a traditional MF critical behavior. In specific problems, however, it turned out that it is only true for loosely connected networks, when the degree exponent γ is large enough. Otherwise the critical singularities of the transition are model independent, but nonuniversal; the critical exponents continuously depend on the value of the degree exponent. In particular, for $2 < \gamma \leq 3$, when $\langle k^2 \rangle$ is divergent the systems are in their ordered phase for any value of the control parameter (temperature, percolation probability, transition rate, etc.), and the critical properties can be investigated in the limit of infinitely strong fluctuations.

Till now investigations on cooperative processes in the SF networks are almost exclusively limited to continuous phase transitions. However, in many problems the phase transitions on PLs are first order and it seems natural to ask what happens with these transitions on the SF networks? There is a general tendency that the discontinuities (e.g., the latent heat)

in the pure system are reduced due to inhomogeneities, which often change the transition into a continuous one. This has been observed in the vicinity of free surfaces [17], when there are missing bonds, or in the bulk when random [18] or aperiodic [19] perturbations are present.

In the present paper, we investigate this issue on the SF networks. In particular we are interested in the combined effect of strong connectivity and irregularities, present in the SF networks, on the properties of discontinuous phase transitions. In the actual calculations we start with the ferromagnetic q -state Potts model and solve it in the frame of the Weiss molecular-field approximation, which represents a lattice version of the MF method. Then we generalize this procedure for any lattice model and show how the MF equation on the SF networks can be deduced from the corresponding one for PLs. The MF equation is analyzed by standard methods [21] and the properties of the phase transitions, in particular those related to a first- to second-order crossover are calculated. Since the MF method is expectedly exact for the SF networks our results are presumably exact.

In the following, we consider the q -state ferromagnetic Potts model [22] defined by the Hamiltonian:

$$-\frac{H}{k_B T} = \sum_{\langle ij \rangle} K_{ij} \delta(s_i, s_j) + \sum_i h_i \delta(s_i) \quad (1)$$

in terms of Potts spin variables, $s_i = 0, 1, \dots, q-1$, at site i . The interaction K_{ij} is equal to $K > 0$ if the bond $\langle ij \rangle$ is occupied and zero, otherwise. As is well known, the Potts model contains as special cases as the Ising model for $q = 2$ and the bond percolation problem in the limit $q \rightarrow 1$. On regular, d -dimensional lattices in the absence of external fields the phase transition of the homogeneous model is first order, as in the MF theory, for $q > q_c(d)$ and continuous for $q \leq q_c(d)$ where $q_c(2) = 4$, $q_c(3) \leq 3$ and $q_c(d \geq 4) = 2$.

To find the thermodynamical properties of the model we use the MF method, when the problem is transformed to a set of independent spins in the presence of effective local fields, which are created by the nearest neighbors. The partition function is then given as a product of single site contributions, $Z = \prod_i z_i$, and the free energy F takes the form,

$$-\frac{F}{k_B T} = \sum_i \sum_j \frac{K_{ij}}{2q} [1 - 2m_j - (q-1)m_i m_j] + \sum_i \ln \left[\exp \left(\sum_j K_{ij} m_j + h_i \right) + q - 1 \right]. \quad (2)$$

Here we introduced the local magnetization $0 \leq m_i \leq 1$ as

$$m_i = \frac{q \langle \delta(s_i) \rangle - 1}{q - 1}, \quad (3)$$

the value of which follows from the extremal condition of the free energy $\partial F / \partial m_i = 0$, leading to a set of self-consistency (SC) equations:

$$\sum_i K_{ij} m_i = \sum_i K_{ij} \frac{\exp \left(\sum_j K_{ij} m_j + h_i \right) - 1}{\exp \left(\sum_j K_{ij} m_j + h_i \right) + q - 1}. \quad (4)$$

On a PL with coordination number, z , $m_i = m_0$, and $h_i = h$ one obtains the relation,

$$m = G(zK m_0 + h), \quad G(x) = G_P(x) = \frac{e^x - 1}{e^x + q - 1}, \quad (5)$$

which is compatible with a first-order (second-order) transition for $q > 2$ ($q \leq 2$).

For a SF network we consider no correlations (anticorrelations) between the degrees of connected sites and assume that the probability of having a link between sites i and j , p_{ij} is proportional to the number of links connected to each sites, i.e., $p_{ij} \sim k_i k_j$. Furthermore, in the spirit of the MF method we replace the interaction, K_{ij} , in Eq. (4) by its average value [20], $K_{ij} = K(k_i k_j / \sum_i k_i)$. Now in terms of the average order parameter, $m = \sum_i k_i m_i / \sum_i k_i$ and for homogeneous field $h_i = h$ one obtains from Eq. (4) the SC equation for the SF networks:

$$m = \int dk P_D(k) k G(kK m + h) / \langle k \rangle = G_{SF}(K m, h), \quad (6)$$

where summation with respect to i is replaced by integration over the degree k as $(1/N) \sum_i \rightarrow \int dk P_D(k)$, where N is the number of vertices. Note that the SC equations for PLs in Eq. (5) and for the SF networks in Eq. (6) are in similar form, and the SC function for networks, $G_{SF}(K m, h)$ is directly related to that in a PL, $G(x)$. This latter transformation, as given in Eq. (6) remains the same for any type of lattice model. Therefore, Eq. (6) sets a direct connection between the MF solutions in PLs and in the SF networks and thus it is a fundamental relation.

Next, we turn to analyze the critical behavior of the SF networks compatible with the general SC equation in Eq. (6). First, we recall that the SC function, $G(x)$ is monotonically increasing from 0 to 1 as x varies from 0 to ∞ and the first few terms of its Taylor expansion, $G(x) = \sum_{n=1}^{\infty} a_n x^n$ are essential for the properties of the phase transition [21]. For the

Potts model the first three coefficients are given by $a_1 = 1/q$, $a_2 = (q-2)/(2q^2)$, and $a_3 = (q^2 - 6q + 6)/(6q^3)$. For the SF networks, the analogous SC function, $G_{SF}(K m, h)$, is generally not analytical due to singularities caused by integration over the degree distribution. For small m (and for small h) it has generally a regular part which is a polynome of finite degree \tilde{n} where \tilde{n} is the largest natural number smaller than $\gamma - 2$:

$$G_{SF}^r(K m, h) = \sum_{n=1}^{\tilde{n}} a_n \frac{\langle k^{n+1} \rangle}{\langle k \rangle} (K m)^n + a_1 h, \quad (7)$$

and a singular contribution, which in the small m limit is given by

$$G_{SF}^s(K m) = \begin{cases} a_s (K m)^{\gamma-2}, & \tilde{n} + 2 < \gamma < \tilde{n} + 3 \\ B |\ln K m| (K m)^{\tilde{n}+1}, & \gamma = \tilde{n} + 3. \end{cases} \quad (8)$$

Here

$$a_s = C \int_0^{\infty} dx x^{1-\gamma} \left[G(x) - \sum_{n=1}^{\tilde{n}} a_n x^n \right] \quad (9)$$

and the constants B and C are positive.

Having the small m behavior of the SC function for the SF network at hand, we can analyze the corresponding critical behavior. Due to the presence of the singular contribution in Eq. (8) the critical behavior of the SF network can be different from that in PLs. Generally we can define three regions of the degree exponent γ with different types of critical behavior. In the following, we are going to describe these regimes.

$\gamma > \gamma^u$: Conventional mean-field regime. If the degree exponent is larger than an upper critical value γ^u the critical behavior on the SF network is the same as on a PL. This happens when the singular term in Eq. (8) does not modify the usual Landau-type analysis [21]. Here, depending on the order of the transition in the PL, there are two different possibilities:

(i) If the transition in the PL is second order, then the first two nonvanishing terms of the small m expansion of $G_{SF}(K m, h)$ should be regular, i.e., $\tilde{n} \geq 2$ and $\sum_{n=2}^{\tilde{n}} |a_n| > 0$. In this case $\gamma^u = n_2 + 2$, where $n_2 > 1$ is the smallest integer for which $a_{n_2} < 0$. As an example for the ($q < 2$)-state Potts model (including percolation for which $q = 1$) the upper critical degree exponent is $\gamma^u = 4$, since here $a_2 < 0$. On the other hand for the Ising model, where $a_2 = 0$ and $a_3 < 0$ the upper critical value is $\gamma^u = 5$.

(ii) In the second case, when the transition in the PL is first order, we are looking for the condition that the transition stays first order in the SF network, too. This will happen, provided (a) the linear regular term of $G_{SF}(K m, h)$ exists and (b) the next-order contribution (either regular or singular) is positive. It is then easy to see that the upper critical value of γ^u is given by the conditions $\tilde{n} = 1$ and $a_s(\gamma^u) = 0$. Indeed, for strongly connected networks, when $a_s < 0$ the transition is softened into a second-order one, the uncon-

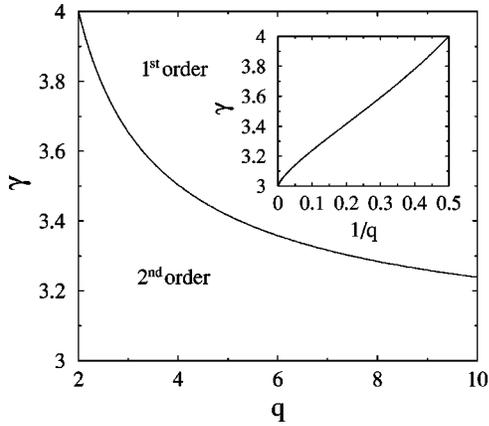


FIG. 1. Regions of first- and second-order phase transitions for the q -state Potts model on scale-free networks with a degree exponent γ . In the second-order regime, i.e., below the upper critical value γ^u the singularities are γ dependent.

ventional properties of which will be described later. As an example the first-order transition of the ($q > 2$)-state Potts model in PLs, where $a_2 > 0$ and $a_3 < 0$, will turn into a continuous one on the SF networks for $\gamma < \gamma^u$, where the upper critical exponent obtained numerically is shown in Fig. 1 for different values of q .

As a general trend γ^u is monotonously decreasing with q and approaching the limiting value of 3 as $1/q$ for large q (see the inset to Fig. 1). This is consistent with our expectations; a stronger first-order transition on a PL, which has a larger latent heat, can be destroyed only in a more connected network, i.e., with a smaller value of γ .

Thus we can conclude at this point that for $\gamma \leq \gamma^u$ the effect of the connectivity of the SF network is *relevant*, so that the singularities of the thermodynamical quantities of the system are different from the conventional mean-field behavior, which can be observed in PLs. The relevant perturbation region is still divided into two parts, depending on the position of the singularity, whether it is at finite or at zero coupling. In the following, we describe these regions.

$3 < \gamma \leq \gamma^u$: Unconventional critical regime. The critical behavior in this regime is due to an interplay between a regular linear term (which does exist, since $\gamma > 3$) and a negative singular next-to-leading term in the expansion of $G_{SF}(Km, h)$. As a result the transition is second order and takes place at a finite coupling, which in the MF method is given by $K_c = \langle k \rangle / (\langle k^2 \rangle a_1)$. Due to the γ dependence of the singular term the singularity of the order parameter is unconventional:

$$m(K) \sim (\Delta K)^{1/(\gamma-3)}, \quad 3 < \gamma < \gamma^u, \quad (10)$$

where $\Delta K = K - K_c$. At the upper critical value of the degree exponent $\gamma = \gamma^u$ according to the result in Eq. (8), there are logarithmic corrections of the form

$$m(K) \sim \left(\frac{\Delta K}{|\ln \Delta K|} \right)^{1/(\gamma_u-3)}, \quad \gamma = \gamma^u, \quad (11)$$

at least if the transition in the PL is second order.

If the transition in the PL is first order, then $\gamma = \gamma^u$ corresponds to a tricritical point in the SF network and the tricritical exponents depend on other details of the degree distribution, such as the next-to-leading decay exponent.

The behavior of the susceptibility at the transition point is calculated from the small h expansion of the SC function in Eq. (7). Since the leading contributions are regular, the singularity of the susceptibility follows the conventional Curie-Weiss law, $\chi(K) \sim 1/|\Delta K|$, and is not modified by the connectivity effect of the SF network.

The singularity in the specific heat is directly related to that of the order parameter and can be deduced from the known relation for the energy density $e \sim m^2$ valid in the MF theory.

$\gamma \leq 3$: Ordered regime. If the degree exponent of the SF network is $\gamma \leq 3$ (but $\gamma > 2$, in order to ensure a finite average degree, $\langle k \rangle < \infty$), then the singular properties of the system are exclusively determined by the leading singular term of the SC function in Eq. (8). As a consequence the system in the SF network is in its ordered phase at any finite value of the coupling and singularities take place only at zero coupling (or at infinite temperature). The order parameter vanishes at $K = 0$ as

$$m(K) \sim K^{(\gamma-2)/(3-\gamma)}, \quad 2 < \gamma < 3, \quad (12)$$

whereas at the borderline value, $\gamma = 3$, there is an essential singularity:

$$m(K) \sim K^{-1} \exp(-1/BK), \quad \gamma = 3. \quad (13)$$

The susceptibility at $K = 0$ is generally finite, $\chi = a_1/(3 - \gamma)$, except for $\gamma = 3$, when it is divergent as $\chi \sim 1/K$.

In a finite network with N vertices the order in the system disappears already at a nonzero coupling, $K_c(N)$, which can be estimated as follows. The typical value of the largest degree in the finite network, k_{max} , is obtained from the usual condition for extreme events: $\int_{k_{max}}^{\infty} P_D(k) dk \sim 1/N$, thus $k_{max} \sim N^{1/(\gamma-1)}$. In a finite system the different moments of k are also finite, and we obtain for the finite-size scaling behavior of the second moment $\langle k^2 \rangle \sim k_{max}^{3-\gamma} \sim N^{(3-\gamma)/(\gamma-1)}$. From this result the size dependent value of the coupling at the transition point can be calculated as

$$K_c(N) \sim \langle k^2 \rangle^{-1} \sim N^{-(3-\gamma)/(\gamma-1)}, \quad 2 < \gamma < 3, \quad (14)$$

from which the finite-size scaling behavior of the order parameter at the transition point

$$m(N) \sim K_c(N)^{(\gamma-2)/(3-\gamma)} \sim N^{-(\gamma-2)/(\gamma-1)} \quad (15)$$

follows. For $\gamma = 3$ the size dependence of the transition point is logarithmic:

$$K_c(N) \sim (\ln N)^{-1}, \quad \gamma = 3, \quad (16)$$

which has been observed in Monte Carlo simulations for the Ising model [14].

To summarize we have studied the properties of first- and second-order phase transitions of ferromagnetic lattice models on scale-free networks. Using the Weiss molecular-field

approximation we have derived a general SC equation that has been analyzed by standard methods. Three regions of the phase diagram are identified as a function of the degree exponent γ . First-order transitions can only take place in the first regime, where $\gamma > \gamma''$, and where the effect of connectivity of the network is irrelevant. In the second regime, for $3 < \gamma \leq \gamma''$ the phase transition is always continuous and takes place at a finite temperature. The magnetization critical exponent, however, is nonconventional, γ dependent. In the third regime, for $\gamma \leq 3$, the system is in its ordered phase at any temperature and a singularity can develop only for diverging temperature (or vanishing coupling).

As far as the properties of the critical singularities are concerned the MF method presumably gives exact results. The location of the transition point is not necessarily exact.

Indeed, our results coincide with others, obtained by different methods on specific problems [13,15].

After this work has been completed we became aware of a preprint by Goltsev, Dorogovtsev, and Mendes [23], in which some results about the q -state Potts model on the SF networks have been announced.

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