Sequences of phase transitions in Ising models on correlated networks

Jörg Menche,* Angelo Valleriani, and Reinhard Lipowsky
Theory & Bio-Systems, Max Planck Institute of Colloids and Interfaces, D-14424 Potsdam, Germany
(Received 7 October 2010; revised manuscript received 31 March 2011; published 20 June 2011)

Using the generic example of Ising spins on scale-free networks, we demonstrate that degree-degree correlations can induce a large number of thermodynamically stable states in networks that otherwise exhibit only the two completely ordered states. The additional stable states are related to the layered network structure. As one increases the temperature, a cascade of first-order phase transitions is found, at which some layers of the network become disordered, while others remain ordered. Negative degree-degree correlations are found to stabilize ordered layers against thermal fluctuations. Positively correlated networks can exhibit an infinite number of ground states and phase transitions, while in negatively correlated networks both numbers are finite.

DOI: 10.1103/PhysRevE.83.061129 PACS number(s): 64.60.Cn, 05.50.+q, 89.75.Hc

I. INTRODUCTION

A vast variety of systems can be described as networks of interacting units that evolve with time. In the last decade, many universal characteristics in the topology of such networks have been revealed; important examples include degree distributions, degree-degree correlations, and community structures [1]. A key question of current research in the field of complex networks is how the *structure* of networks is related to the properties of *dynamical* processes that take place on them.

An important class of dynamical processes with numerous applications are pairwise-interacting two-state systems. The paradigmatic model of such systems is the Ising model. It can be viewed as a simple dynamical system, which describes, e.g., the process of opinion formation [2–4]. In many applications, thermodynamic properties, such as the number of stable patterns and their robustness against thermal fluctuations, are of great interest, since they can often be identified with relevant states of the underlying system. Furthermore, Ising models are equivalent to maximum entropy models for the average values and correlations of binary variables as used, e.g., for the activity patterns in neural networks [5].

Ising models have been studied for many years on different topologies, from regular lattices in the classical model to recent studies on complex networks; see [6] for a comprehensive overview. The randomness of the connectivity in networks generally favors globally ordered dynamical states [2,7]. Networks with a broad degree distribution and without correlations in the degrees of adjacent vertices remain in the ordered phase for all finite temperatures [8].

In this paper, we study the general question of how *local* ordering can be induced in networks that usually only show *global* ordering. In particular, we demonstrate that degree-degree correlations can lead to a large number of thermodynamically stable states with local ordering. We characterize these states in terms of the underlying network structure and determine their total number. Further, we show that correlated networks exhibit a sequence of phase transitions, at which some parts of the network become disordered, while others remain in the ordered phase; see Fig. 1.

II. NETWORK STRUCTURE

We consider scale-free networks with their vertex degrees k characterized by the degree distribution

$$P(k) = \frac{1}{\mathcal{A}} k^{-\gamma} \quad \text{for} \quad k_0 \leqslant k \leqslant k_{\max}\,, \tag{1}$$

with the normalization constant $\mathcal{A} \equiv \sum_k k^{-\gamma}$. The structural parameters of these networks are the size N, the exponent γ of the degree distribution, and the lower cutoff k_0. We use the so-called natural cutoff $k_{\max} = \min(N-1, k_0 N^{\frac{1}{\gamma-1}})$ [9]. In general, the degree distribution does not completely describe the structure of a network, since it may have correlations in the degrees of adjacent vertices [10]. Networks are called *assortative* or *positively* correlated if vertices with similar degree are preferably connected to each other. Networks are called *dissortative* or *negatively* correlated if vertices with high degree are linked to vertices with low degree.

Several measures have been proposed to describe the correlations of a given network [10–13]. In this work, we use a rewiring scheme from [14]. Starting from uncorrelated networks as obtained from the configuration model [15], the algorithm allows for the gradual increase of positive or negative correlations: In each step of the iterative algorithm, two edges with four vertices at their ends are chosen at random. Rewiring the two edges such that the two vertices with the highest degree are connected leads to a more assortative network. Connecting the vertex with the highest degree to the vertex with the lowest degree leads to a more dissortative network. In this work we consider only simple networks, so we check at every step whether the new connections are allowed, and return to the previous configuration otherwise. Repeated iteration of this procedure eventually leads to asymptotic network configurations with *maximal* correlations. As shown in [13], these networks exhibit a number of distinctive and well-defined features. The key

*Present address: Center for Complex Network Research, Northeastern University, Boston, Massachusetts 02115, USA; Center for Cancer Systems Biology, Dana-Farber Cancer Institute, Boston, Massachusetts 02115, USA.

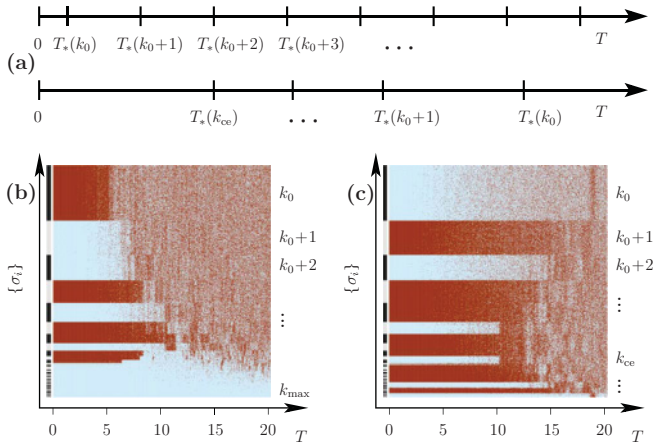

FIG. 1. (Color) (a) Sequence of transition temperatures T_* for maximally correlated networks. The assortative case (top sequence) exhibits an infinite number of equidistant transition temperatures, while this number is finite in the dissortative case (bottom sequence). (b),(c) Snapshots of Monte Carlo simulations on a network with $N = 2^{10}$ vertices and a scale-free degree distribution as in (1) with $\gamma = 2.5$, $k_0 = 6$, and (b) assortative or (c) dissortative correlations. Each column parallel to the y axis shows the spin values $\{\sigma_i\}$ of all the vertices in the network. The vertices are ordered according to their degree, from the k_0 vertices at the top to the k_{max} vertex at the bottom. Spin-up and spin-down states are shown in red and blue, respectively. As the temperature increases, one after another the ordered layers become disordered.

features that are important for the present study are the following:

Assortative networks are characterized by pronounced layers of vertices in which vertices are mostly connected to vertices of the same degree. These layers correspond to square regions in the adjacency matrix; see Fig. 2. Since scale-free networks are characterized by the presence of a relatively small number of vertices with high degree, there is a certain degree k_s such that vertices with degree $k \leqslant k_s$ are essentially saturated with vertices of the same degree whereas vertices with degree $k > k_s$ are not able to saturate all of their edges by connecting them only to other vertices of the same degree, simply because the number of such vertices in the network is too small. The high-degree vertices with $k > k_s$ therefore form a large cluster that is connected by the hubs. The degree k_s is directly visible in the average nearest neighbor degree $K_{NN}(k)$ of the k vertices, which exhibits an essentially linear k dependence with $K_{nn}(k) \approx k$ for $k \leqslant k_s$, see Fig. 5 in Ref. [13].

By comparing the total number of edges emanating from all vertices with a certain degree k with the available vertices of degree k, one can derive an analytical expression for the degree k_s. In the asymptotic limit of totally assortative networks, for which the layers of vertices with degree $k \leqslant k_s$ are completely separated from the rest of the network, k_s is given by [13]

$$k_s = k_0^{(\gamma-1)/(\gamma+1)}(\gamma-1)^{1/(\gamma+1)}\left(\frac{3\gamma}{2\gamma-1}\right)^{1/(2-\gamma)} N^{1/(\gamma+1)}. \tag{2}$$

The low-degree vertices with degree $k \leqslant k_s$ form monolayers that consist of vertices with a single degree. The total number N_{mono} of these monolayers is given by the number of all degrees smaller than or equal to k_s:

$$N_{mono} \equiv k_s - k_0 + 1. \tag{3}$$

Comparing with Eq. (2) we see that the number of such layers increases with network size N.

Dissortative networks also exhibit a pronounced layered structure. As correlations become more and more negative, a number of well-separated *bilayers* emerges that are nested around each other and around a central cluster of degree k_{ce};[1] see Fig. 2. Each bilayer consists of all low-degree vertices with a single degree $k < k_{ce}$ on one side and all vertices within a range of high degrees on the other side.

[1]The degree k_{ce} of the central cluster was denoted by k_{me} in Ref. [13].

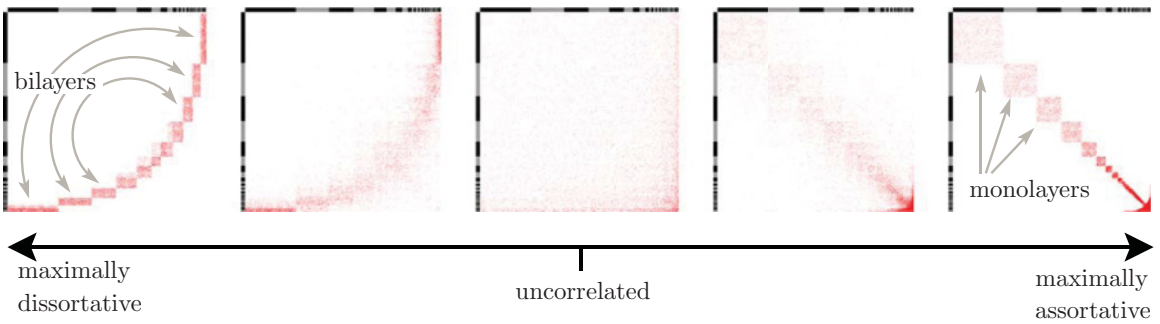

FIG. 2. (Color) Different correlation profiles of a scale-free network with $N = 2^{10}$, $\gamma = 2.5$, and $k_0 = 6$ as provided by its ordered adjacency matrices $\mathbf{A}$. The matrices have $N \times N$ entries A_{ij}, with $A_{ij} = 1$ (red) if the vertices i and j are connected and $A_{ij} = 0$ (white) otherwise. The vertices are arranged according to their degree k with $k_0 < k_1 < \cdots < k_{max}$. The black and white bars at the left and upper boundary have a length proportional to the number of vertices with a certain degree. The square regions in maximally assortative networks correspond to monolayers of vertices with a certain degree $k \leqslant k_s$ that are connected only to other vertices of the same degree. The vertices with degree $k > k_s$ form a big component that is connected via the hubs. Maximally dissortative networks consist of bilayers, where all k vertices of the low-degree side are connected to a range of high-degree vertices. The degree k_{ce} belongs to the central cluster around which the bilayers are nested and therefore determines their total number.

The value of k_{ce} can be computed using the condition that the total number of edges emanating from all vertices with $k < k_{ce}$ must equal the total number of edges attached to vertices with $k > k_{ce}$:

$$\sum_{k=k_0}^{k_{ce}} N P(k) k = \sum_{k=k_{ce}}^{k_{max}} N P(k) k. \tag{4}$$

Solving Eq. (4) in the limit of large and maximally dissortative networks, we find that the degree k_{ce} becomes independent of N and attains the asymptotic value [16]

$$k_{ce} \approx k_{ce}^{\infty} \equiv 2^{1/(\gamma-2)} k_0. \tag{5}$$

The total number of bilayers N_{bi} in the network is simply given by the number of degrees smaller than k_{ce}. Contrary to the assortative case, this number is bounded from above and satisfies

$$N_{bi} \leqslant \max(N_{bi}) = k_{ce}^{\infty} - k_0. \tag{6}$$

III. DYNAMICS

Each vertex i of the network is occupied by an Ising spin $\sigma_i = \pm 1$. We study the standard Ising model as defined by the configurational energy

$$\mathcal{H} = -J \sum_{NN} \sigma_i \sigma_j, \tag{7}$$

with uniform ferromagnetic interactions $J > 0$ between connected vertices and without external magnetic field. The sum in (7) runs over all pairs of nearest neighbors. The pattern $\{\sigma_i\}$ of all spins σ_i evolves according to the Glauber update [17]: At each Monte Carlo step, a spin i is chosen at random and its value σ_i changed to $-\sigma_i$ with the probability $P(\sigma_i \to -\sigma_i) \equiv 1/[1 + \exp(2\Delta\mathcal{H}/k_B T)]$, where $\Delta\mathcal{H} = \mathcal{H}_+ - \mathcal{H}_-$ denotes the energy difference of the two states with the spin being in either state σ_i or $-\sigma_i$. One Monte Carlo sweep consists of the sequential update of N randomly chosen vertices and defines the macroscopic time step Δt. At zero temperature, the Glauber update rule is equivalent to the so-called majority rule with random update [2–4].

IV. THE GROUND STATES AT ZERO TEMPERATURE

As shown in [2], uncorrelated networks exhibit only two stable fixed points which correspond to the two completely ordered states. The absolute value of the magnetization per spin as defined by $|m| = |\frac{1}{N}\sum_{i=1}^{N} \sigma_i|$ then has the value $|m| = 1$. In contrast, the strongly correlated networks in Fig. 3 show additional fixed points with $|m| \neq 1$. As demonstrated in [16] for the special case of parallel update of all spins and dissortative networks, this behavior is closely related to the layered structure of the underlying networks which becomes more and more pronounced as correlations increase. Each individual layer is ordered locally, with all its vertices being in the same state. Figure 3 shows that different layers can exhibit different local ordering. In the limit of maximally correlated and infinitely large networks the layers are expected to separate completely and the network then falls apart into disconnected components. In this limit the observed fixed points with local ordering become true global ground states. Their total number $\mathcal{N}_g$ is then simply given by all possible combinations of the local states of N_l layers,

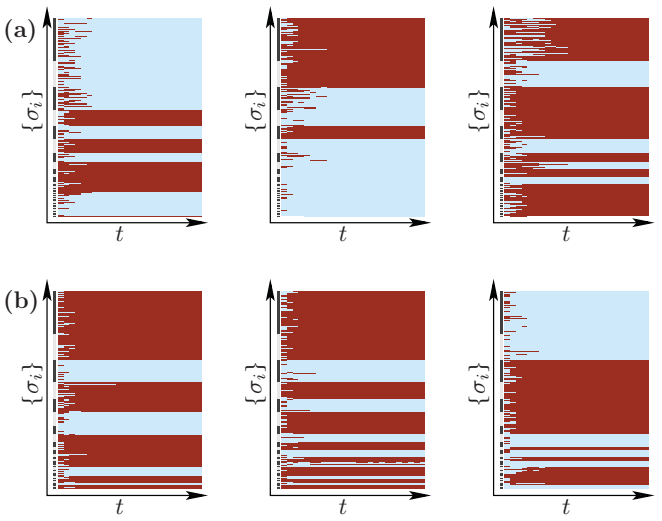

FIG. 3. (Color) Time evolution of three spin patterns $\{\sigma_i\}$ at zero temperature on (a) maximally assortative and (b) maximally dissortative networks with $N = 2^{10}$, $\gamma = 2.5$, and $k_0 = 6$. Time t is measured in Monte Carlo sweeps. As in Fig. 1, each column parallel to the y axis shows the spin values $\{\sigma_i\}$ of all vertices, ordered by their degree. The initial configurations at $t = 0$ are random. Both networks in (a) and (b) exhibit many ground states with locally ordered layers.

$$\ln \mathcal{N}_g = N_l \ln 2\,. \tag{8}$$

For finite networks, Eq. (8) provides an upper bound for the total number of fixed points. Note that these fixed points correspond to real ground states in the thermodynamic limit; they are therefore qualitatively different from metastable states observed for Ising models on square and cubic lattices [18,19]. Note also that, for random sequential (or asynchronous) update as used here, the long time dynamics is always governed by fixed points and cannot lead to limit cycles, in contrast to parallel (or synchronous) update as used in Ref. [16], where a large number of blinkers or two-cycles was found in addition to fixed points.

Assortative networks consist of N_{mono} low-degree monolayers and the cluster of all remaining vertices; the total number of layers is therefore given by $N_l = N_{mono} + 1$. Dissortative networks consist of N_{bi} bilayers plus the central cluster with degree k_{ce}, so the total number of layers is $N_l = N_{bi} + 1$. Note that the number of ground states behaves very differently for assortative and dissortative networks. According to Eqs. (5) and (6) the number of layers and subsequently $\mathcal{N}_g$ attain a constant value for large dissortative networks. In assortative networks, on the other hand, the number of layers in (3) and therefore $\mathcal{N}_g$ grow continuously with network size.

V. PROPERTIES AT FINITE TEMPERATURE

Correlated networks exhibit a heterogeneous layered structure, where the individual layers vary greatly in the number

of vertices they contain and in their internal connectivity. We therefore expect that the individual layers of the network also behave differently when temperature is introduced. Figure 1 shows snapshots of the spin patterns $\{\sigma_i\}$ of maximally correlated networks for increasing temperatures. At $T = 0$, all individual layers are locally ordered. When temperature is increased, we see that one after another the ordered layers become disordered. In the assortative network depicted in Fig. 1(a) the low-degree layers are the first to undergo such a transition as temperature increases. In the dissortative network in Fig. 1(b) we see the opposite. Here, the outer bilayers are more stable against thermal fluctuations.

For a more detailed analysis of the temperature-driven transition from order to disorder, we consider the Binder cumulant [20]

$$C_b(T,k,N) \equiv 1 - \frac{\langle M^4 \rangle}{3\langle M^2 \rangle^2}. \tag{9}$$

The nth moment of the magnetization M is computed by $\langle M^n \rangle = \frac{1}{s}\sum_{i=1}^{s} M_i^n$, where the average is taken over s independent simulations. The Binder cumulant can be used to determine the transition temperature T_* by plotting $C_B(T,k,N)$ for different system sizes N as a function of temperature. The transition temperature T_* is given by the temperature of the intersection point of the different curves, and the shape of these curves provides additional insight into the order of the transition [21].

According to the previous finding that the different layers of the system become disordered at different temperatures, we analyzed the subsets of all vertices of a single degree k separately. In assortative networks, these subsets correspond to a low-degree monolayer, in dissortative networks to the low-degree part of a bilayer. Figure 4 shows examples for the Binder cumulant as a function of temperature, plots for other k layers are qualitatively similar.

Figure 5 shows the transition temperatures $T_*(k)$ for the different k layers, as determined from the corresponding Binder cumulant. Curves for different network sizes intersect at a common temperature, indicating clearly a temperature-driven phase transition. These results can be understood using the mean-field theory in Ref. [8], according to which the transition temperature scales as $T_* \sim \langle k^2 \rangle / \langle k \rangle$. For homogeneous k layers in assortative networks, this expression leads to $\langle k^2 \rangle / \langle k \rangle = k$, which implies a linear dependence of T_* on k: As temperature increases, a sequence of transition temperatures $T_*(k)$ appears, at which the monolayers undergo subsequent transitions into the disordered phase, beginning with the k_0 layer.

The vertices of the bilayers in dissortative networks, on the other hand, are highly inhomogeneous in their degrees and $\langle k^2 \rangle / \langle k \rangle$ decreases with k. This is consistent with the decrease of T_* as k increases for the dissortative case in Fig. 5. In effect, the inner parts of the nested bilayer structure around k_{ce} are the first to undergo a transition into the disordered phase as the temperature increases. Note that the heterogeneity of the vertex degrees within the outer bilayers strongly enhances the stability of dissortative networks against thermal fluctuations: The transition temperatures are much larger than those of assortative networks.

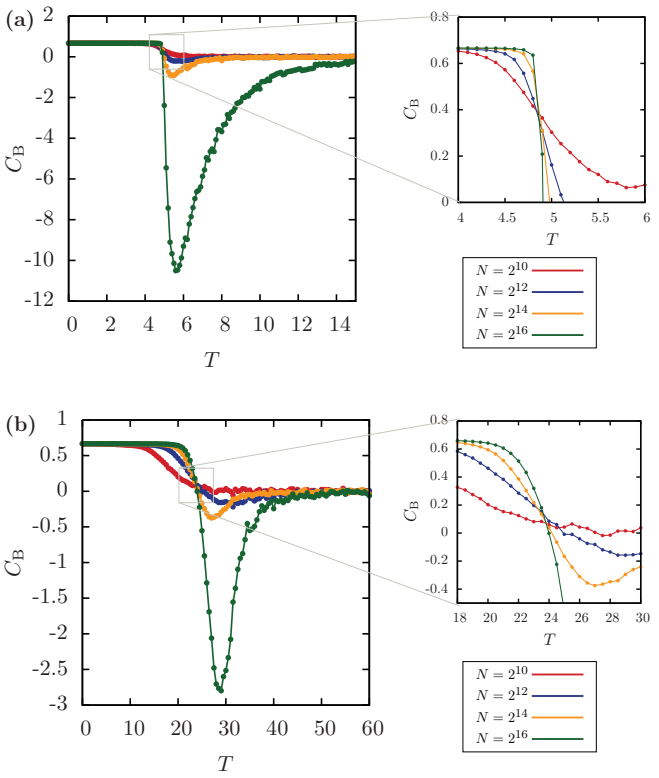

FIG. 4. (Color) Binder cumulant C_B as a function of temperature T for maximally correlated networks of different sizes N, $\gamma = 2.5$, and $k_0 = 6$. (a) The $k = 6$ layer of an assortative network and (b) the $k = 11$ layer of a dissortative network. Each data point is an average over 100 networks and 1000 random initial configurations for each network. The temperature at which the curves for different network sizes N intersect provides an estimate of the transition temperature T_*.

Finally, we address the nature of the individual phase transitions. The plots of the Binder cumulant in Fig 4 exhibit minima for temperatures slightly above T_* that become more pronounced and whose position approaches T_* with growing network size. These features are typical for first-order phase transitions [21]. Because of finite size effects, it is difficult to observe the discontinuity at T_* directly. To provide

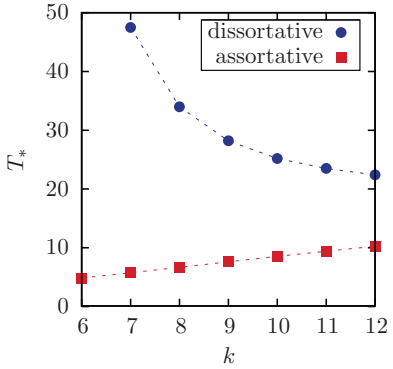

FIG. 5. (Color online) Transition temperatures in units of J/k_B of the individual k layers for maximally correlated networks with $\gamma = 2.5$ and $k_0 = 6$ as obtained from the intersections of the corresponding Binder cumulants.

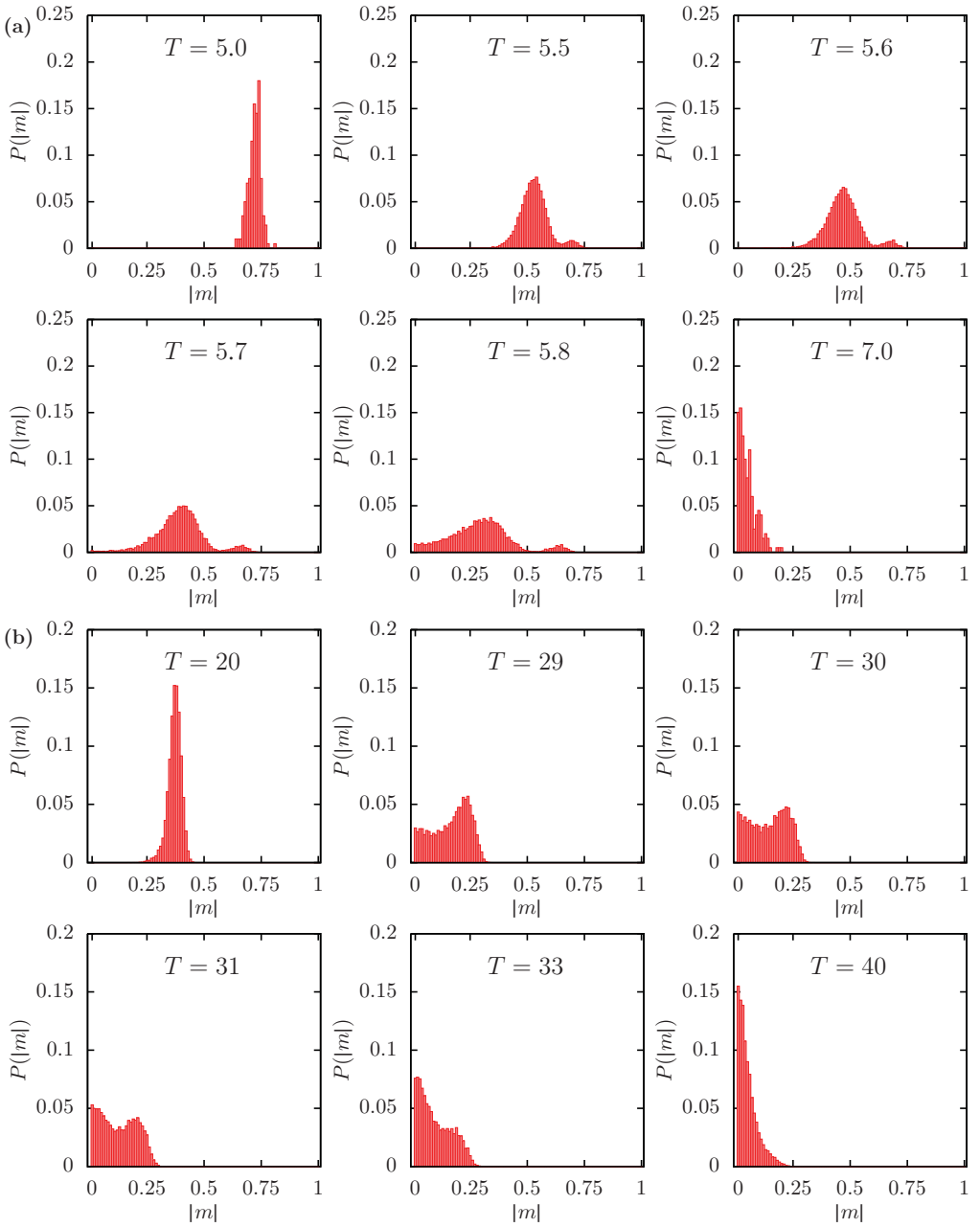

FIG. 6. (Color online) The distribution $P(|m|)$ of the absolute values $|m|$ of the magnetization for (a) the $k = 7$ layer of an assortative network and (b) the $k = 8$ layer of a dissortative network for different temperatures close to the critical temperature $T_* \simeq 5.75$ and $T_* \simeq 34$, respectively. The remaining network parameters are $N = 2^{16}$, $\gamma = 2.5$, and $k_0 = 6$. All data points are averages over 1000 random initial configurations. Both temperature trajectories clearly show the emergence of a second peak, indicating a metastable state, and thus a first-order phase transition.

further evidence for first-order transitions, we analyzed the distribution $P(|m|)$ of the absolute values of the magnetization for different temperatures; see Fig. 6. For both assortative and dissortative layers, the distributions around T_* develop a second peak, indicating the existence of metastable states. We also observed hysteresis in $|m|$, when T_* is crossed from above and from below; see Fig. 7. We performed additional simulations on random networks for which all vertices had the same degree k, for different values of k and different network sizes. The latter networks showed no negative values in $C_B(T)$, no double-peaked distributions $P(|m|)$, and no hysteresis. We conclude that the coupling between adjacent layers is crucial for the details of the phase transition and that adjacent layers are not completely separated but remain connected by a small number of edges. Because of this overlap the vertices of one layer receive input not only from within the layer, but also from adjacent layers. Generally, this input can be different from the spin value of the locally ordered layer and thus be regarded as an effective small external field, acting on a fraction of spins. This situation is similar to the bimodal random-field Ising model, for which a first-order phase transition has been discussed previously [22].

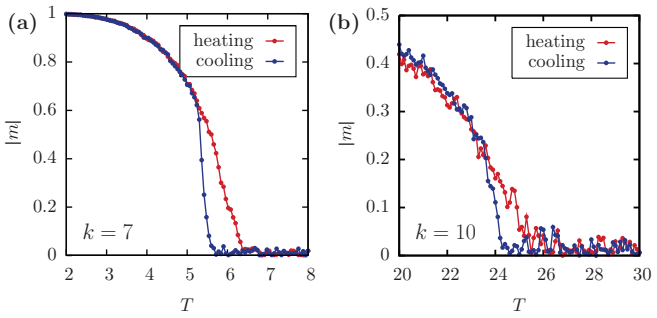

FIG. 7. (Color online) Absolute value of the magnetization $|m|$ as a function of temperature for (a) the $k = 7$ layer of an assortative network and (b) the $k = 10$ layer of a dissortative network. The remaining network parameters are $N = 2^{18}$, $\gamma = 2.5$, and $k_0 = 6$. At each temperature, ten Monte Carlo sweeps were performed before measuring $|m|$ and proceeding to the next adjacent temperature. The values of the critical temperatures are given by $T_* \simeq 5.75$ in (a) and $T_* \simeq 25.2$ in (b).

VI. DISCUSSION

We have shown that degree-degree correlations give rise to a large number of stable dynamical patterns with local ordering in networks that only exhibit global ordering when no correlations are present.

A detailed analysis of the resulting network structure provides analytical bounds for the total number of ground states, as well as estimates for the transition temperatures where the local ordering is destroyed. Interestingly, we find very different behavior for assortative and dissortative networks. Dissortative networks exhibit a lower complexity in terms of the number of possible stable patterns, but at the same time their patterns are more stable against thermal fluctuations. These structural and dynamical properties are generic and robust. We have found rather similar properties for Ising models with more complex interactions, for systems with more than two degrees of freedom as described, e.g., by Potts models, and for networks with other types of degree distribution that are sufficiently broad to allow the formation a several layers of vertices.

[1] *The Structure and Dynamics of Networks*, edited by M. E. J. Newman, A.-L. Barabási, and D. J. Watts (Princeton University Press, Princeton, NJ, 2006); A.-L. Barabási, Science **325**, 412 (2009).
[2] H. Zhou and R. Lipowsky, Proc. Natl. Acad. Sci. USA **102**, 10052 (2005); **102**, 10052 (2005); J. Stat. Mech. **2007**, P01009.
[3] P. L. Krapivsky and S. Redner, Phys. Rev. Lett. **90**, 238701 (2003).
[4] R. Lambiotte, J. Phys. A **41**, 224021 (2008).
[5] E. Schneidman, M. J. Berry II, R. Segev, and W. Bialek, Nature (London) **440**, 1007 (2006).
[6] S. N. Dorogovtsev, A. V. Goltsev, and J. F. F. Mendes, Rev. Mod. Phys. **80**, 1275 (2008).
[7] J. Shao, S. Havlin, and H. E. Stanley, Phys. Rev. Lett. **103**, 18701 (2009).
[8] M. Leone, A. Vázquez, A. Vespignani, and R. Zecchina, Eur. Phys. J. B **28**, 191 (2002).
[9] R. Cohen, K. Erez, D. ben-Avraham, and S. Havlin, Phys. Rev. Lett. **85**, 4626 (2000).
[10] M. E. J. Newman, Phys. Rev. Lett. **89**, 208701 (2002).
[11] S. Maslov and K. Sneppen, Science **296**, 910 (2002).
[12] R. Pastor-Satorras, A. Vázquez, and A. Vespignani, Phys. Rev. Lett. **87**, 258701 (2001).
[13] J. Menche, A. Valleriani, and R. Lipowsky, Phys. Rev. E **81**, 046103 (2010).
[14] R. Xulvi-Brunet and I. M. Sokolov, Phys. Rev. E **70**, 066102 (2004).
[15] M. Molloy and B. Reed, Random Struct. Algorithms **6**, 161 (1995).
[16] J. Menche, A. Valleriani, and R. Lipowsky, Europhys. Lett. **89**, 18002 (2010).
[17] R. J. Glauber, J. Math. Phys. **4**, 294 (1963).
[18] V. Spirin, P. L. Krapivsky, and S. Redner, Phys. Rev. E **63**, 36118 (2001).
[19] V. Spirin, P. L. Krapivsky, and S. Redner, Phys. Rev. E **65**, 16119 (2001).
[20] K. Binder, Z. Phys. B **43**, 119 (1981).
[21] K. Vollmayr, J. Reger, M. Scheucher, and K. Binder, Z. Phys. B **91**, 113 (1993).
[22] N. G. Fytas, A. Malakis, and K. Eftaxias, J. Stat. Mech. (2008), P03015.