

## Statistical mechanics of a coevolving spin system

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(Received 3 May 2018; published 24 September 2018)

We propose a statistical mechanics approach to a coevolving spin system with an adaptive network of interactions. The dynamics of node states and network connections is driven by both spin configuration and network topology. We consider a Hamiltonian that merges the classical Ising model and the statistical theory of correlated random networks. As a result, we obtain rich phase diagrams with different phase transitions both in the state of nodes and in the graph topology. We argue that the coupling between the spin dynamics and the structure of the network is crucial in understanding the complex behavior of real-world systems and omitting one of the approaches renders the description incomplete.

DOI: [10.1103/PhysRevE.98.030301](https://doi.org/10.1103/PhysRevE.98.030301)

During the past few decades, there has been rapid development in the interdisciplinary area of network science. This may be because of the availability of vast amounts of data, much of it from such complex systems as financial markets, social and biological structures, and transportation networks. Studies of the network structure of such real-world systems as the World Wide Web [1] indicate that their topology has numerous nontrivial properties that the classical random graph model cannot explain [2]. This has produced new network models able to recreate some of these observed phenomena [3,4]. Initially, most of these models focused on the graph evolution, often the growth in the number of nodes and edges [5]. On the other hand, a different approach has been developed that considers a statistical ensemble of graphs [6] called “exponential random graphs” [7]. This formalism, borrowed from statistical physics, has proven successful and has led to a phenomenological theory of the topological phase transitions in evolving networks [8–10].

This newly discovered concept of networks with a complex structure moved rapidly through the spin models community. Important critical properties were observed for both scalefree and small-world network versions of the canonical Ising model of ferromagnetism [11–13]. The use of complex networks became popular because they more closely resemble real-world structures than regular lattices or Poissonian graphs. This has been particularly important when modeling social and financial phenomena for which spin models are the simplest and the most common [14,15]. Although the topology of many systems can be described using complex networks, the evolution of the model is limited to changes in the spin configuration. This implies that connection dynamics evolve more slowly than node state dynamics. Unfortunately, this assumption is not valid in most complex adaptive systems,

which are describable using network tools. An Ising model with slowly evolving interactions was used as a model of a neural network [16] and as a possible tool for simulating magnetostriction in nanoscale magnetic structures [17]. A particularly interesting case involved models in which the connections and state dynamics coevolve with each other, one evolution depending on the other and resulting in nontrivial feedback. Most of these models focus on socioeconomic systems and describe their dynamics [18,19] rather than their statistical mechanics [20,21]. Some of them produce intriguing topological properties, mainly when the dynamics is driven by the structural characteristics of the network [22].

We here use the Hamiltonian formalism to describe Ising-like models with coevolution of spins and connections, and we want the connection dynamics to depend on both the spin configuration and network topology. Following the approach taken in Ref. [9], we use the degree as a topological variable and focus on nearest neighbor interactions. We consider undirected graphs with a fixed number  $N$  of vertices and a fixed number  $M$  of edges. The partition function  $Z$  for our ensemble we define to be

$$Z = \sum_{\{c_{ij}\}, \{s_i\}} e^{-\beta H(\{c_{ij}\}, \{s_i\})}, \quad (1)$$

where  $\{\cdot\}$  is all possible configurations with respect to a fixed number of links and nodes. Parameter  $\beta$  is the strength of fluctuations and is the inverse temperature. A general form of the Hamiltonian that lies within the scope of this paper is

$$H(\{c_{ij}\}, \{s_i\}) = \sum_{i < j} c_{ij} f(k_i, k_j, s_i, s_j) + \sum_i g(k_i, s_i), \quad (2)$$

where  $c_{ij}$  is the adjacency matrix,  $k_i = \sum_j c_{ij}$  and  $s_i$  are respectively the degree and the spin of node  $i$ , and  $f(\cdot)$  and  $g(\cdot)$  are functions to be determined. More specifically, we

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assume that the functions are such that

$$H(\{c_{ij}\}, \{s_i\}) = \sum_{i<j} c_{ij} \left( \frac{k_i k_j}{\langle k \rangle} \right)^\phi s_i s_j - \sum_i k_i^\gamma - h \sum_i s_i, \quad (3)$$

where  $\phi$  and  $\gamma$  are model parameters,  $\langle k \rangle = 2M/N$ , and  $h$  is the external field acting on spins set to zero. This simple concrete form shows (i) that parameters  $\phi$  and  $\gamma$  allow us to continuously switch from complicated topological interactions to the classical Ising model and (ii) that the multiplication of degrees is the simplest interaction expression. In an Ising framework, we treat it as a weight  $J_{ij}$  assigned to an edge  $(i, j)$ . In addition,  $J_{ij} = \left( \frac{k_i k_j}{\langle k \rangle} \right)^\phi$  is in accordance with real-world weighted network characteristics [23]. The second sum term is an external field that interacts with each local node degree and drives the preference for high- or low-degree nodes. In addition to the classical ferromagnetic interpretation, if we use a socioeconomic model to examine the proposed Hamiltonian, we find an accurate interpretation of its terms. Using an opinion model, we determine the influence of a given agent by examining its connectivity. The external field term forces each agent to reach as many people as possible. In contrast, the interaction term allows the energy of the system to be strongly affected by the connections among influential high-degree nodes. This works in two ways. High-degree agents with opposite spins are energetically unstable and agents with the same spins lower the energy level.

We perform Monte Carlo simulations of the model using the METROPOLIS algorithm [24–26]. We start every simulation with a random configuration. Every time step of the simulation consists of two basic mechanisms. The first one is spin switching and the second one is edge rewiring. For the spin switching, we randomly select one node, and we compute the energy difference between the system in a current state and with the chosen spin in the opposite state. The decision of whether to flip the spin or not is made according to the standard METROPOLIS rule. Subsequently, in the same time step, the edge rewiring is performed as follows. One link is randomly selected from the network, with equal probability for every link. Then two nodes are chosen randomly for possible ends of a new edge. Note that the new edge cannot overlap with any of the existing ones. Next, the energy difference between the new configuration and the old configuration is calculated. Again, the decision of whether to rewire the edge or not is made according to the METROPOLIS algorithm. More details can be found in the Supplemental Material [27].

The topological portion of the Hamiltonian changes the behavior of the Ising model. We find a variety of different effects. Some are structural, others are associated with spin configurations, and still others are a result of both. Figure 1 shows the simulation results for the phase diagram of  $\gamma$  and  $T$  with a fixed  $\phi = 0$ . Here, no structural portion of the Hamiltonian describes interactions; i.e., the network structure is only locally important. Note that there are two separate topological phases and also a continuous phase transition in magnetization, with a small impact by parameter  $\gamma$ .

Figure 2 shows the case  $\phi = 0$  and  $\gamma = 1.6$ . Note that the topological transition of the highest degree is discontinuous, but also that the magnetization behaves in a way similar to a standard Ising model on a coevolving network [20]. These

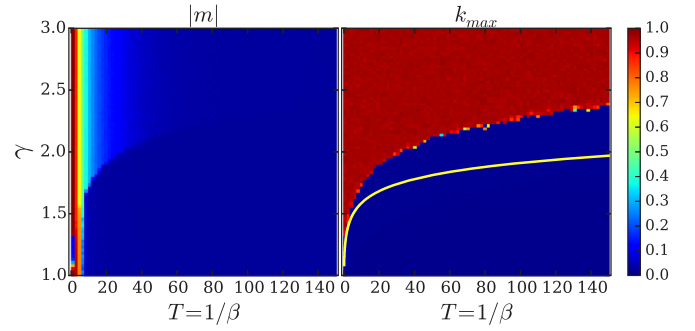


FIG. 1. Absolute magnetization  $|m|$  (left) and the largest degree  $k_{\max}$  (right), as a function of the temperature  $T = 1/\beta$  and  $\gamma$ , for  $\phi = 0$ . Solid line represents analytical approximation of the transition according to the equation (5). Results averaged over  $5 \times 10^5$  time steps for a network with  $N = 1000$  nodes and  $M = 3000$  edges.

effects belong to different transition classes and occur at different temperatures, and we see a striking behavior in energy  $E$ , i.e., the value of the Hamiltonian. It exhibits multiple jumps, one of which occurs at the same temperature as the highest-degree topological phase transition. In addition, all jumps are approximately equal. This energy behavior suggests a multistar configuration in which the maximum number of stars is restricted by a fraction  $\frac{M}{N}$ . Figure 5(a) shows that when  $M = 3N$  three vertices are connected to approximately every network node. The number of stars decreases with the temperature. Eventually, the system becomes more homogeneous, and we see a sharp transition in the largest degree.

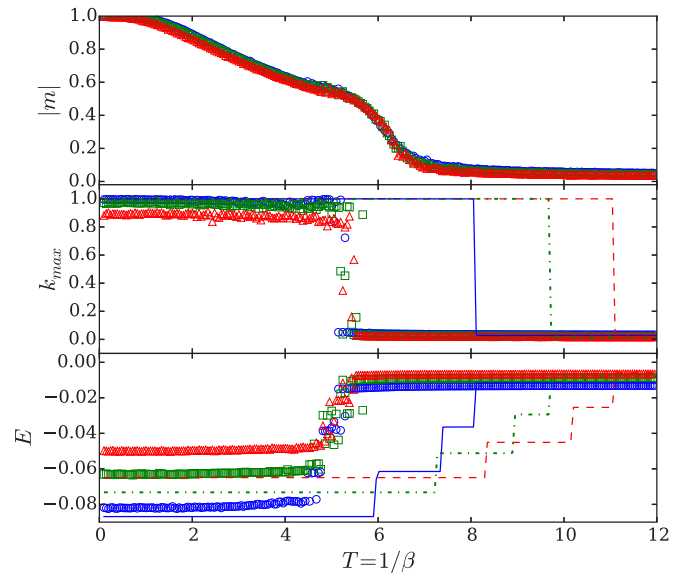


FIG. 2. Absolute magnetization  $|m|$ , the largest degree  $k_{\max}$ , and energy  $E$  as a function of the temperature  $T = 1/\beta$ , for  $\gamma = 1.6$  and  $\phi = 0$ . Lines represent analytical approximations according to Eq. (5) and symbols correspond to numerical simulations averaged over  $10^6$  time steps for a network with  $N = 500$  (blue circles and solid line),  $N = 750$  (green squares and dotted line),  $N = 1000$  (red triangles and dashed line), with  $c = M/N = 3$ . All quantities are normalized to the range  $[0, 1]$ , except the energy, which is given in arbitrary units.

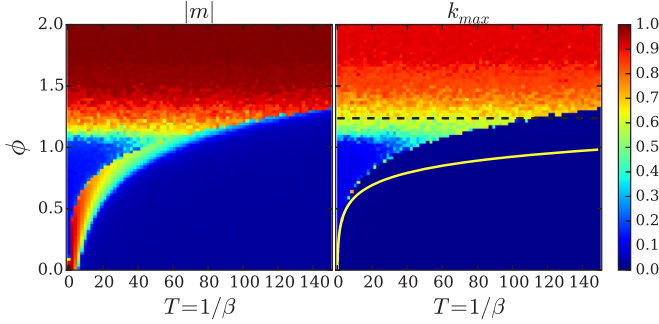


FIG. 3. Absolute magnetization  $|m|$  (left) and the largest degree  $k_{\max}$  (right), as a function of the temperature  $T = 1/\beta$  and  $\phi$ , for  $\gamma = 1$ . Solid and dashed lines represent analytical approximations of the transitions according to Eqs. (7) and (8) respectively. Results are averaged over  $5 \times 10^5$  time steps for a network with  $N = 1000$  nodes and  $M = 3000$  edges.

Here  $k_{\max} \ll N$ , and the degree distribution is approximately Poissonian.

When we remove the external field associated with the degree of each node and turn on the combination of structural terms in the interaction portion of the Hamiltonian, we find a different behavior. Figure 3 shows this in the phase diagram with respect to  $\phi$  and  $T$  when there is a neutral value of  $\gamma = 1$ . Figure 4 shows the same when we fix  $\phi = 0.6$ . When we examine the largest degree and the magnetization, we see four phases. Figure 4 shows that in the one-dimensional phase diagram the topological transition is characterized by a sharp

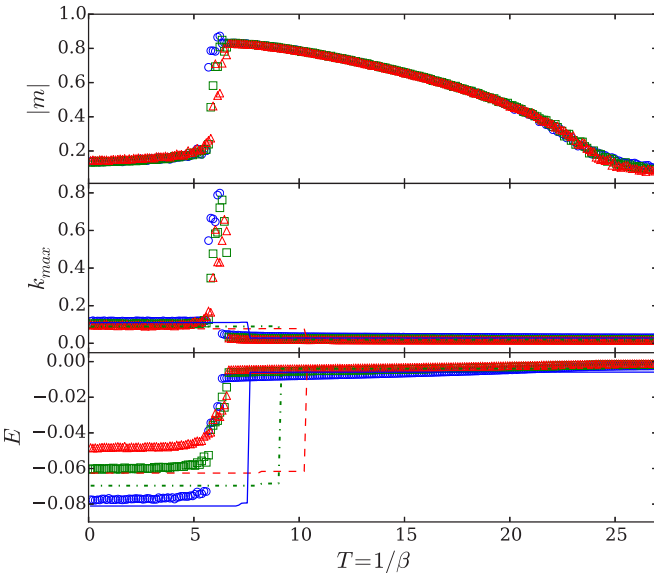


FIG. 4. Absolute magnetization  $|m|$ , the largest degree  $k_{\max}$ , and energy  $E$  as a function of the temperature  $T = 1/\beta$ , for  $\phi = 0.6$  and  $\gamma = 1$ . Lines represent analytical approximations according to Eq. (7) and symbols correspond to numerical simulations averaged over  $10^6$  time steps for a network with  $N = 500$  (blue circles and solid line),  $N = 750$  (green squares and dotted line), and  $N = 1000$  (red triangles and dashed line), with  $c = M/N = 3$ . All quantities are normalized to the range  $[0, 1]$ , except the energy, which is given in arbitrary units.

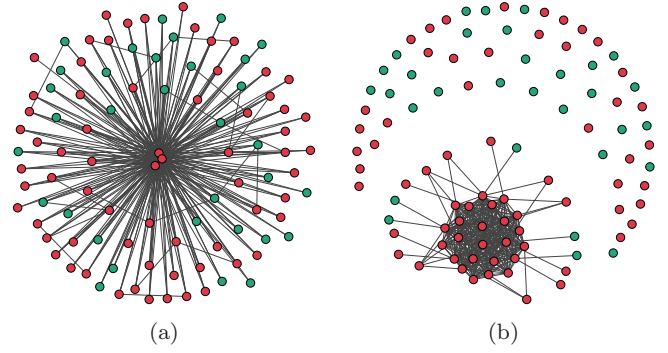


FIG. 5. Exemplary networks obtained in the simulation. Green nodes indicate  $+1$  spin, and red nodes indicate  $-1$  spin. (a) Model  $\phi = 0$ ,  $\gamma = 2$ ; (b) model  $\phi = 1$ ,  $\gamma = 1$ .

jump in the maximum degree. Thus there is an abrupt change in the magnetization. Unlike the case with a varying  $\gamma$ , there is also a transition that is triggered by a change in parameter  $\phi$  and that is unaffected by temperature. The critical value of  $\phi$  in this transition is notated  $\phi_c$ .

Examining the structural properties of the different phases mentioned above, we find that when  $\gamma = 1$  and  $\phi < \phi_c$  in a low-temperature regime there are many disconnected nodes and one big component with high-degree clustering [see Fig. 5(b)]. At the critical temperature, the network recombines into one component, and the highest-degree  $k_{\max}$  reaches its maximum value at the transition point. Increasing the temperature decreases the highest degree and the degree distribution to become Poissonian. When we increase  $\phi$  above  $\phi_c$ , the system transitions into a multistar configuration, a phase similar to the one previously observed for high  $\gamma$  values.

We next analytically describe the system to produce an approximation of our numerical results. Because the structural heterogeneity disallows a simple mean-field approach, we use a semi-mean-field method and focus on the nonhomogeneous elements of the system that most strongly impact the Hamiltonian.

Figures 1 and 2 show the results when  $\phi = 0$  and the  $\gamma$  value varies. We here assume that the most important part of the Hamiltonian is the contribution from the largest hubs, i.e., the stars connected to all other nodes. We assume nonhubs to have a degree equal to the average degree. Thus we approximate the Hamiltonian

$$H \approx -n_h k_m^\gamma - (N - n_h) k_a^\gamma, \quad (4)$$

where  $n_h \in \{0, 1, 2, \dots, \lfloor \frac{M}{N} \rfloor \equiv [c]\}$  is the number of stars,  $k_m = N - 1$  is the degree of each star,  $k_a$  is the average degree of the remaining nodes, and  $k_a \equiv k_a(n_h) = n_h + \frac{2(M - L(n_h))}{N - n_h}$ , where  $L(n_h) = k_m + k_m - 1 + \dots + k_m - (n_h - 1) = n_h \frac{2N - 1 - n_h}{2}$  is the number of links required to create  $n_h$  stars. Taking into account all possible configurations, the partition function becomes

$$Z = 2^N \sum_{n_h=0}^{[c]} \binom{N}{n_h} R(n_h) e^{\beta[n_h k_m^\gamma + (N - n_h) k_a^\gamma]}, \quad (5)$$

where  $2^N$  is all spin configurations,  $\binom{N}{n_h}$  is the number of star combinations, and  $R(n_h)$  is the number of possible link configurations with  $n_h$  stars in the network. We approximate this as  $R(n_h) \approx \binom{(N-n_h)(N-n_h-1)/2}{M-L(n_h)}$ . Although this is a slight overcounting when  $n_h < c$ , the number of incorrect configurations is negligible when compared to the number of all other configurations.

Figures 1 and 2 show that the partition function allows us to analytically determine the energy and the highest degree. Although the estimated critical temperature diverges from the observed temperature, using this simple approach allows us to recreate the steplike behavior of the energy.

When  $\gamma = 1$  and the  $\phi < \phi_c$  value varies, there is a shattering transition with a decreasing temperature. Some nodes disconnect from other nodes and become inactive. In contrast, when the temperature is high, and  $c = 3$ , the graph becomes random and highly connected. Thus we describe the state of the system in terms of the number of active nodes, and we assume that their degree can be approximated using the mean field approach. We denote the number of these nodes  $n_s$  and write the Hamiltonian

$$H \approx -M \frac{\langle k \rangle_s^{2\phi}}{\langle k \rangle^\phi}, \quad (6)$$

where  $\langle k \rangle_s = 2M/n_s$  and  $\lceil n_{\min} \rceil \leq n_s \leq N$  with  $n_{\min} = (1 + \sqrt{1 + 8M})/2$ . We approximate the number of configurations for a particular  $n_s$  with  $\binom{N}{n_s} \binom{n_s(n_s-1)}{M}$  and derive the partition function

$$Z = \sum_{n_s=\lceil n_{\min} \rceil}^N 2^{N-n_s+1} \binom{N}{n_s} \binom{n_s(n_s-1)}{M} e^{\beta 2^\phi N^\phi M^{\phi+1} n_s^{-2\phi}}. \quad (7)$$

We assume that the spin direction of all active nodes is the same and that there are  $2^{N-n_s+1}$  possible spin configurations. Figures 3 and 4 show the results when we analytically obtain the energy and the highest degree level. As in the previous case, we can use our estimation to approximate the system behavior but not the critical temperature.

We approximate  $\phi_c$  to fully describe the phase diagrams. The critical value of  $\phi$  separates the homogeneous active node

phase from the multistar configuration phase. We assume that the energy of both phases is the same when  $\phi = \phi_c$  and define the critical value

$$\begin{aligned} \phi_c \ln \frac{(n_{\min} - 1)^2}{N - 1} + \ln \frac{M}{c} \\ = \ln \left[ \frac{c - 1}{2} (N - 1)^{\phi_c} + c^{\phi_c} (N - c) \right], \quad (8) \end{aligned}$$

where both  $c$  and  $n_{\min}$  retain the previous definitions. An analysis of the order parameter behavior and variance shows that our simple approximation is always overestimating the transition point. Nevertheless, it provides a clear indication of the border between the two phases. For the complete calculation of all cases, see the Supplemental Material [27].

To statistically describe a coevolving spin system, we have used a Hamiltonian that merges exponential random graphs and Ising-like models. A Hamiltonian that simultaneously depends on topological properties and node states has not been previously analyzed, and we have found complex behavior and have generated rich phase diagrams. The most striking aspect of our results is the existence, at specific temperatures, of topological phase transitions in which there are no node state transitions. There are also transitions that influence order parameters, but this suggests that we must take into account both the topology and the state of the nodes to fully describe the system, and if we do not we miss essential aspects of systemic behavior.

Although the results presented here concern networks in which  $c \equiv \frac{M}{N} = 3$ , we did extend our simulations to other cases and found the same qualitative results. These extended results and a detailed analysis of the asymptotic and topological properties of the transitions will be supplied in a future publication [28].

M.W. would like to acknowledge the support from the National Science Centre under Grant No. 2015/19/N/ST2/02701. T.R. and M. W. would like to acknowledge the support from the Young Researchers of the Complex Systems Society under Bridge Grant 2018.

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