Statistical mechanics of scale-free networks at a critical point: Complexity without irreversibility?

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Based on a rigorous extension of classical statistical mechanics to networks, we study a specific microscopic network Hamiltonian. The form of this Hamiltonian is derived from the assumption that individual nodes increase or decrease their utility by linking to nodes with a higher or lower degree than their own. We interpret utility as an equivalent to energy in physical systems and discuss the temperature dependence of the emerging networks. We observe the existence of a critical temperature T_c where total energy (utility) and network architecture undergo radical changes. Along this topological transition we obtain ensemble averages of scale-free networks with complex hierarchical topology. The scale-free nature emerges strictly within equilibrium, with a clearly defined microcanonical ensemble and the principle of detailed balance fulfilled. This provides evidence that "complex" networks may arise without irreversibility. The utility approach establishes a link between classical statistical physics and a wide variety of applications in socioeconomic statistical systems.

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I. INTRODUCTION

Triggered by the vast number of nontrivial networks observed in nature, a respectable number of models has been introduced recently to understand their statistical properties. Many of these networks differ considerably from pure random graphs [1], leading to the notion of complex networks which is a well established concept nowadays [2,3]. Perhaps the most apparent property distinguishing "complex" real-world networks from pure random graphs is their scale-free degree distribution $P(k) \sim k^{-\gamma}$, which seems to be ubiquitous in nature [3,4]. Further, many real-world networks exhibit a high amount of clustering, and sometimes even a nontrivial dependence of the clustering coefficient, C_i of node i, when seen as a function of its degree k_i. A power form of $\langle C(k) \rangle \sim k^{-\delta}$ can be associated with the "complex" topological property of hierarchical clustering [5]. Almost all of the microscopic models proposed to describe such "complex"—growing or static—networks involve nonequilibrium and evolutionary elements, manifesting themselves in different procedures of preferential attachment [6–9] or other structured rewirement schemes [10–12]. Further, these procedures often involve the need for nonlocal information.

Aiming at a statistical description of complex networks, generalized concepts of preferential attachment have been applied in the definition of network ensembles with fixed degree distribution [13,3]. Another way of generating scale-free networks which is based on appropriately tuning "macroscopic" weights of "network-Feynman graphs" [14] can be related to this approach. Other views of ensembles of networks include generalizations of random graphs to networks with arbitrary degree distributions via methods of superstatistics [15]. So far, comparatively little has been done to understand complex networks from a purely classical statistical mechanics point of view where phase space is not constrained. Clearly, its possible foundations on, e.g., the maximum entropy principle would allow for a very broad range of applications. A few serious equilibrium approaches have been proposed [16–18], where topological properties of networks associated with specific Hamiltonians have been studied. In [16] an equilibrium partition function of the form (2), see below, was established, giving an arbitrary degree distribution. In [18] it was shown that along topological transitions scale-free networks can be recovered at a certain point in time during a relaxation process to equilibrium, implying that scale-free graphs are temporary configurations not typical for equilibrium.

The aim of this paper is to present a form of a network Hamiltonian leading to *ensemble averages* of networks which correspond to distinct "phases" of networks, depending on the temperature of the system. By increasing temperature we observe a transition from starlike to scale free to eventually Poissonian networks. In addition to previous work, we present numerical evidence that scale-free networks may indeed be obtained within a pure equilibrium approach as suggested in [16]. Moreover, we demonstrate that the introduced Hamiltonian leads to nontrivial hierarchic features. The form of the Hamiltonian is derived from simple and general assumptions about individual utilities of nodes, in a way that is standard in economics. Nodes act as utility maximizers, in analogy to physical systems minimizing energy.

II. MODEL

We consider symmetric networks with a fixed number of distinguishable nodes $i=1,\ldots,N$, connected by a fixed number of $\ell=1,\ldots,L$ indistinguishable links. The network is represented by its adjacency matrix $\mathbf{c}$, where $c_{ij}=1$, if a link connects nodes i and j and $c_{ij}=0$, otherwise; there are no self-connections or multiple edges. Thus we define the microcanonical partition function as

$$\Omega(E,N,L) = \sum_{P(\mathbf{c})} \frac{1}{L!} \delta(E - \mathcal{H}(\mathbf{c})) \delta\left(L - \mathrm{Tr}\left(\frac{\mathbf{c}^2}{2}\right)\right), \qquad (1)$$

with $\mathcal{H}(\mathbf{c})$ being the network Hamiltonian. $P(\mathbf{c})$ denotes all permutations of links in a $N \times N$ adjacency matrix. The number of links is fixed by the term $\delta(L - \mathrm{Tr}(\mathbf{c}^2/2))$, so that the sum finally extends over all permutations of L links which

are possible in a $N \times N$ adjacency-matrix. The canonical partition function may be obtained by the Laplace transform of Eq. (1), or via the maximum entropy principle, as shown in [17],

$$Z(T,N,L) = \sum_{P(\mathbf{c})} \frac{1}{L!} \delta\left(L - \frac{\mathrm{Tr}(\mathbf{c}^2)}{2}\right) e^{-\beta \mathcal{H}(\mathbf{c})}, \tag{2}$$

using the usual definition of temperature $T \equiv 1/\beta$. In simulations the canonical ensemble can be generated, e.g., by the Metropolis algorithm: Starting from an adjacency matrix $\mathbf{c}$ at time t, a graph $\hat{\mathbf{c}}$ is generated by replacing a randomly chosen edge between nodes i and j with a new edge between randomly chosen, previously unconnected, nonidentical nodes m and n. In the next time step $\mathbf{c}$ is replaced by $\hat{\mathbf{c}}$ with probability $p_{\mathrm{replace}} = \min\{1, \exp[-\beta(\mathcal{H}(\hat{\mathbf{c}}) - \mathcal{H}(\mathbf{c}))]\}$. Differing from structured rewirement schemes as used in [10], this procedure guarantees that *every possible* configuration of the adjacency matrix is realized with the same *a priori* probability.

Given Eq. (2) any reasonable Hamiltonian depending on any properties of the network can be studied. Here, we adopt the view of modeling *microscopic* interactions, where the total utility of a network can be expressed as the sum over all utility contributions of individual nodes, U_i.

In the spirit of utility theory, U_i is a function which describes the preferences of nodes between different alternatives [19,20]. In our case these alternatives are the different possibilities for establishing links. Therefore, node utility will depend on properties or states Π_i of node i itself, and on properties of the node j, Π_j, whereto a link is going. For simplicity we assume linearity and define the utility of a link l (which connects nodes i and j) as

$$u_\ell(\Pi_i, \Pi_j) = U_i(\Pi_i, \Pi_j) + U_j(\Pi_i, \Pi_j). \tag{3}$$

In the following we specify the model such that the utility of a node increases if it connects to a node that is "more important" than itself. Similarly, its utility decreases if it establishes a (potentially costly) link to a "less important" node. As the argument of the individual utility functions U_i we therefore take the relative importance between two nodes, defined via $\Delta k \equiv |k_i - k_j|$, which is the most obvious measure satisfying the specification above.

For the functional form of the utility function we chose a standard, monotonically increasing, concave utility function, which incorporates the concept of decreasing marginal utility, $U = (x^\alpha - 1)/\alpha$. One of the most used variants of this utility in economics and social sciences is the limit, $\alpha \to 0$, the log utility [19]. We thus model node utility by

$$U_i(k_i, k_j) = \begin{cases} c_1 + a_1 \ln(b_1 + \Delta k) & \text{for } k_j > k_i, \\ c_2 - a_2 \ln(b_2 + \Delta k) & \text{for } k_j < k_i, \end{cases} \tag{4}$$

with shape parameters a and b, and offsets c. To avoid discontinuity in the utility function we set $c_2 = c_1 + a_1 \ln(b_1) + a_2 \ln(b_2)$. This function is shown in Fig. 1. For the sake of further simplicity, we assume $b_1 = b_2 = b$, to obtain a particularly simple form for the link utility,

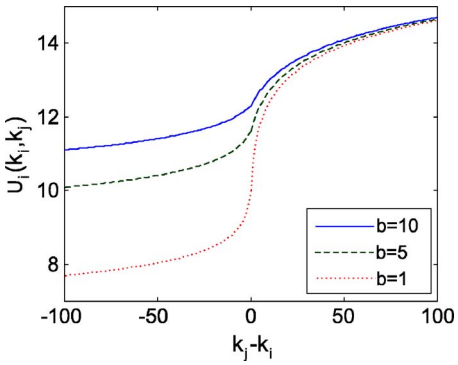

FIG. 1. (Color online) Node utility as a function of $k_j - k_i$ for different values of b. The parameters in Eq. (4) are $a_1 = 1$, $c_1 = 10$, $a_2 = 0.5$, and $c_2 = 1.5$.

$$u_\ell(k_i, k_j) = c + (a_1 - a_2)\ln(b + \Delta k). \tag{5}$$

Parameter $c \equiv c_1 + c_2$ can be chosen to ensure positive total utility for each link. Parameter b is the curvature of the utility function. Equation (5) can be interpreted as the inverse energy contribution of each link. Simulations of the associated maximum entropy ensemble, Eq. (2), can now be performed. The collective amount of "irrationality" of individual nodes is captured by the "temperature" T (bounded rationality). For $a_1 = a_2$, utility is independent of Δk and random networks are obtained, as expected. For $a_1 \neq a_2$, the constants a and c can be absorbed in the temperature scale of the system; hence they are omitted in the following without loss of generality. Assuming $a_1 > a_2$, i.e., putting more emphasis on wins than on losses, we finally base our simulations on the Hamiltonian,

$$\mathcal{H}(\mathbf{c}) = -\sum_\ell \ln(b + \Delta k). \tag{6}$$

III. RESULTS

We simulate networks of the canonical ensemble, Eq. (2), ranging from $N = 500$ to 10^4 nodes. For computational reasons, temperature-dependent results are presented for $N = 10^3$. All ensemble averages have been calculated from at least 2×10^3 configurations, separated by at least $20 \times N$ update steps. We analyze the obtained networks as a function of the model parameters—temperature (irrationality) T, link density $\rho = 2L/N$, and the "sensitivity" parameter b.

Figure 2(a) shows the ensemble average of the total energy of the system, $\mathcal{U} \equiv -\Sigma_{i=1}^N U_i$, as a function of T for different values of ρ. Also shown is the specific heat $\mathcal{C}$, obtained as the derivative of the energy. One clearly finds a radical change in the energy and a characteristic maximum of the specific heat at about $T_c \approx 0.84$ for $N = 1000$, indicating the presence of a critical point. The transition softens for higher link densities ρ, as well as for lower values of b (not shown). The question arises whether the observed transition is a phase transition or a crossover. To clarify this point we perform a finite-size scaling analysis. The finite-size dependence of the maximum of the specific heat, $C_{\max} \equiv \max(C)$, and of

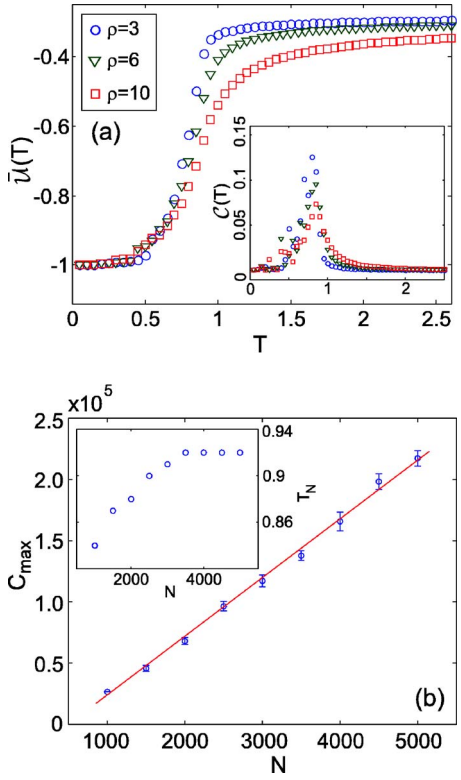

FIG. 2. (Color online) (a) Ensemble average of normalized internal energy $\bar{\mathcal{U}}(T)=\mathcal{U}(T)/\min(\mathcal{U}(T))$ and specific heat $\mathcal{C}(T)$ (inset) as a function of T, for $N=10^3$, $b=5$, and various densities ρ. (b) Finite-size dependence of the maximum of the specific heat $C_{\max}$. Points represent average values of $C_{\max}$ over 50 identical, independent computations of $C(T)$. Each point of a single $C(T)$ curve was obtained from averages based on 10^5 values. The line is a linear least-squares fit $C_{\max}\sim N^{1.0}$. The inset shows the associated finite-size dependence of temperature, i.e., the location of the maximum of $C_{\max}$.

the critical temperature T_c, for networks with size N with $\rho=3$, are shown in Fig. 2(b). The simulation data suggests that the finite-size dependence of the maximum of the specific heat is consistent with linear scaling $C_{\max}\sim N^{1.0}$, within the limits of observation. The finite-size dependence of the critical temperature shown in the inset of Fig. 2(b) suggests convergence to a limit of $T_c^{\infty}\approx 0.92$. Even though the approximately linear increase of $C_{\max}$ is undoubtedly evidence for a phase transition, one has to be careful. For a first-order phase transition a scaling $C_{\max}\sim N^d$ is expected, whereas for a second order transition one would expect $C_{\max}\sim N^{\alpha/\nu}$, where α is the critical exponent of the specific heat and ν the critical exponent of the correlation length. Thus conclusive statements are difficult for two reasons: First, the definition of the correlation length ξ on fluctuating networks, which are not embedded in some metric space, is not clear. Any definition of a correlation length and its finite-size scaling behavior will depend on the chosen metrics. Second, the system is overextensive with respect to ρ, which makes it hard to use standard arguments from finite-size scaling. As long as neither the effective dimension, d, nor the exponent for the correlation length, ν, can be reasonably estimated, we cannot decide between the two cases. The only piece of evidence for a phase transition is the direct measurement of $C_{\max}$ as displayed in Fig. 2(b).

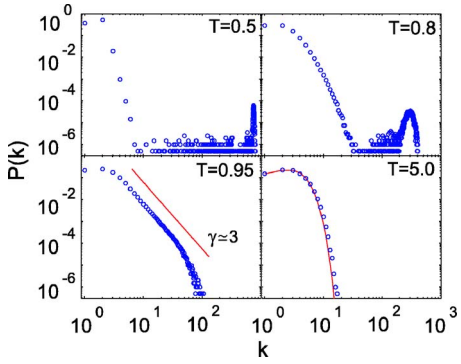

FIG. 3. (Color online) Ensemble averages of degree distributions at different temperatures for $N=10^3$, $\rho=3$, and $b=5$. The line for $T=5$ is the Poissonian $p(k)=e^{-\rho}\rho^k/k!$, expected for random graphs.

The change in energy is associated with considerable restructuring of the underlying networks. To discuss this in more detail we calculated ensemble averages of degree distributions along the transition; see Fig. 3. At low temperatures networks are dominated by stars (i.e., nodes which are linked to nearly all of the other nodes of the networks) of different degrees. In this low-temperature regime the system is dominated by the energy of the network and the entropy plays a rather meager role. The energy resulting from the Hamiltonian Eq. (6) is maximized when there are only a few nodes with very large degree of the order of N; then, due to the constraint $\Sigma_i k_i=2L$ the other degrees are small and hence most of the individual energy contributions are of the order $\ln(b+N)$, so that the overall energy is approximately $N\ln(b+N)$. From $T\sim 0.5$ upward, the starlike structure shifts to lower degrees. At $T\sim 0.8$ self-similar patterns emerge (Fig. 3): The highest connected starlike structures are accompanied by more interconnected stars of smaller, less favorable degree to the left. This organization is mirrored in the structure of nodes of lower degree whose tail becomes power-law–like. At T_c the situation inverts and energy changes drastically: Thermal excitation surmounts the "repelling" Δk term when merging different zones of starlike structures; the starlike phase ceases to exist. Still the network is organized in a self-similar way—at $T\sim 0.95$ the degree distribution follows a power law $P(k)\sim k^{-\gamma}$ with exponent $\gamma\sim 3$. [For a larger system where the power law extends for an order of magnitude more, see Fig. 4(a).] As many statistical physical systems lose their characteristic length scale at the phase transition it is not surprising that the structure of a network, measured by its degree distribution, becomes scale free.

Further temperature increase shifts the exponential cutoff to the left, ultimately leading to random networks with Poissonian distributions. In this high-temperature regime, where $\beta=1/T$ is small, the system basically does not depend on the particular form of the Hamiltonian and network structure is almost solely dominated by the entropy, as heat excitations result in total randomness of the system; see Fig. 3.

Finite-size effects of the degree distributions and the role of parameter b for the scale-free region are captured in Fig.

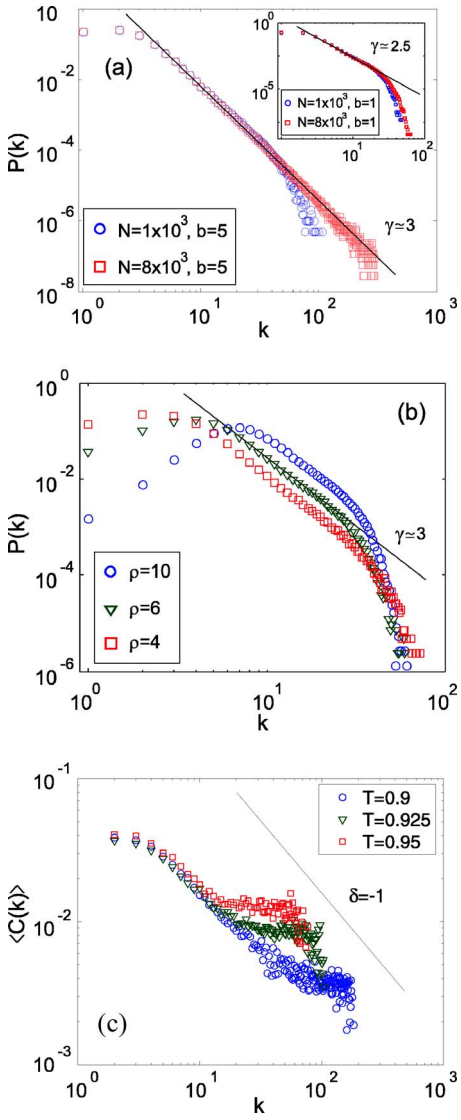

FIG. 4. (Color online) (a) Finite size dependence of the ensemble-averaged degree distribution for various N and b (inset) at $\rho=3$. For $b=5$, we have $T=0.95$, being somewhat higher for $b=1$. (b) Averaged degree distributions for different link densities ρ, $N=10^3$, and $b=5$. Temperatures are adjusted to be in the scale-free region. (c) Degree dependence of the average cluster coefficient $\langle C(k)\rangle$ at different temperatures. $N=10^3$, $\rho=3$, and $b=5$. Plots are normalized to the first point.

4(a). Sizes $N=10^3$ and $N=8\times10^3$ are compared for $b=1$ and $b=5$; both indicate scaling within the limits of observation. Power-law fits yield a degree exponent of $\gamma\approx3$ and 2.5 for $b=5$ and $b=1$, respectively, regardless of system size. Variation of b therefore allows us to model different exponents occurring in real-world networks [3]. The fact that the cutoff of the degree distribution lies at lower $k_{\max}$ for $b=1$ than for $b=5$ can be understood qualitatively when taking the b dependence of $U_i(k_i,k_j)$ into account: As can be seen from Fig. 1, lower b results in a comparatively higher sensitivity at small Δk. Consequently, sensitivity at higher degree differences becomes more negligible (for the same system size N) compared to the circumstances at, e.g., $b=5$.

In Fig. 4(c) we show the degree dependence of ensemble averages of the cluster coefficient $\langle C_i\rangle=\langle 2n_i/k_i(k_i-1)\rangle$, where n_i is the number of links between the neighbors of node i. For $T=0.85$, we obtain scaling $\langle C(k)\rangle=k^{\delta}$ with $\delta\sim-1$. This is in very good agreement with many empirical data on socioeconomic systems [5] and demonstrates that our model reproduces the "complex" topological property of hierarchical clustering found in many socioeconomical networks. In Fig. 4(c) one observes that for increasing temperatures a plateau of constant $C(k)$ is emerging for large k; however, the exponent in the scaling region appears to remain rather robust at $\delta\sim-1$. We have checked this point more closely in a $N=8000$ run at $T=0.95$ (not shown). The existence of self-similar, "complex" hierarchical structures can be associated with the Δk term in the utility function. Actually, this specific form leads to a significant correlation of degrees which can be understood when looking at the dynamics imposed by the Metropolis algorithm more closely: If the Hamiltonian $\mathcal{H}$ depends on the degrees of both nodes, $\mathcal{H}_\ell=\mathcal{H}(k_i,k_j)$, the correct expression of the energy exchange $\Delta E=\mathcal{H}(\hat{\mathbf{c}})-\mathcal{H}(\mathbf{c})$ associated with a random rewirement $\ell(i,j)\to\ell(m,n)$ is given by

$$\Delta E=\mathcal{H}(k_m+1,k_n+1)-\mathcal{H}(k_i,k_j)+\sum_{\tau\in\{i,j,m,n\}}\sum_{\xi\in N(\tau)}[\mathcal{H}(\hat{k}_\tau,k_\xi)-\mathcal{H}(k_\tau,k_\xi)],\qquad(7)$$

as long as nodes m and n and/or nodes i and j are not neighbors of each other; if they are neighbors the expression is somewhat more lengthy. τ runs over the involved nodes, $N(\tau)$ denotes the neighbors of node τ, and $\hat{k}_\tau$ is the "new" degree of node τ (i.e. the degree *after* rewirement). The contribution $\mathcal{H}(k_m+1,k_n+1)-\mathcal{H}(k_i,k_j)$ is given by $\ln((b+\Delta k_{ij})/(b+\Delta k_{mn}))$, thus making clear how the parameter b governs the strength of the influence of degree difference. It is also clear that this contribution drives the system to reduce link differences, i.e., the system shows an assortative tendency. The secondary sums in Eq. (7) can be written as

$$\sum_{\xi\in N(\tau)}-\ln\left(1\pm\frac{1}{b+\Delta k_{\tau\xi}}\right).\qquad(8)$$

Here the sign is positive (negative) for nodes τ where a link is added in the case of $k_\tau>k_\xi$ ($k_\tau<k_\xi$) and positive (negative) for nodes where a link is removed for the case $k_\tau<k_\xi$ ($k_\tau>k_\xi$). The sum over $N(\tau)$ in Eq. (8) has k_τ elements and is thus dominated by some kind of "preferential attachment." Additionally, it can be easily checked that the secondary term favors disassortative tendencies. The correlation resulting from Eq. (8) couples the cluster coefficient C_i to the degree k_i and results in a hierarchic organization of the network resembling the well known $\delta=-1$ slope for many real-world data. As expected, the secondary terms dominate the overall behavior of the clustering coefficient as a function of degree, see Fig. 4(c).

The results presented so far hold qualitatively for relatively small ρ. For ρ larger than 5, a characteristic scale gradually emerges, due to the fact that the mean $\langle k\rangle$, corresponding to high-temperature random networks, shifts to

larger values. Despite this characteristic scale, for an appropriate temperature window, the power law with the characteristic exponent of $\gamma=3$ remains, Fig. 4(b). For $\rho<1/2$ the networks contain only very few links. The transition gets very sharp and we were not able to find a regime of scale-free networks. Still, the transition between random networks and a starlike phase is visible.

Finally, we mention that the computation of the energy associated with relinking is computationally expensive since it involves a number of secondary terms, some of them given in Eq. (7): A number of k_ξ contributions have to be reevaluated for each node participating in the rewirement, which makes simulations demanding at $T\to T_c$. This fact imposes a limit on our analysis to networks of $N<8000$ nodes.

IV. CONCLUSION

We proposed a very general model of socioeconomical statistical systems, where individuals are utility maximizers with bounded rationality. We found that—for low link densities—scale-free networks with hierarchical clustering naturally emerge as maximum entropy expectation values in the vicinity of a critical point. We argue that the hierarchical clustering results from degree correlations, which are understandable from the form of the chosen Hamiltonian. Further, different from work conducted earlier, no modifications of the sampling of phase space have been used and the degree distribution was not predefined by macroscopic weights, or similar approaches. Our results emphasize that scale-free networks also exist within a pure equilibrium concept, in addition to [18] where they have been reported as a transient relaxation phenomenon. It is also important to point out the generality of our results from a socioeconomic point of view. The Hamiltonian has been derived from the most frequently used utility functions in economics. Similar utility functions like $U=[(b+\Delta k)^\alpha-1]/\alpha$ (see [19]) do not change our results qualitatively for small α.

We further showed the existence of different phases of network structure. We find numerical evidence for a first-order transition, however, for conclusive statements a renormalization analysis of the matter would be needed, which is beyond the scope of this work.

We think that it would be interesting to investigate systems of opinion formation on networks within the proposed approach of identifying the network Hamiltonian with individual utilities, i.e., to couple internal degrees of freedom to the network ensemble, Eq. (2), by methods of statistical mechanics. This would allow us to juxtapose nonequilibrium models of opinion formation or equilibrium models on "hard-wired" networks with results from a maximum entropy ensemble of scale-free networks. Of course, such a juxtaposition would not be possible in an unbiased way when taking nonequilibrium network formation processes into account.

Finally, as the notion of complexity is usually tightly connected to dissipative structures far from equilibrium, our results could stimulate a discussion about the actual complexity of "complex" networks.

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