Thermodynamic forces, flows, and Onsager coefficients in complex networks

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(Received 12 June 2007; published 5 December 2007)

In this paper the linear theory of nonequilibrium thermodynamics, developed by Onsager and others, is applied to random networks with arbitrary degree distribution. Using the well-known methods of nonequilibrium thermodynamics we identify thermodynamic forces and their conjugated flows induced in networks as a result of single node degree perturbation. The forces and the flows can be understood as a response of the system to events, such as random removal of nodes or intentional attacks on them. Finally, we show that cross effects (such as thermodiffusion, or thermoelectric phenomena), in which one force may not only give rise to its own conjugated flow, but to many other flows, can be observed also in complex networks.

Onsager relations [1] constitute one of the most prominent results of the traditional nonequilibrium statistical physics [2,3]. In short, they explain why and how small perturbations of some system parameters can induce fluctuations of other parameters.

The relations are derived from the assumption that the response of the system, which is close to equilibrium, to small external perturbation is the same as its response to a spontaneous fluctuation. Since the considered systems are close to equilibrium the change in entropy dS is mainly due to entropy production d_iS, the rate of which can be written as

$$\sigma = \frac{d_iS}{dt} = \sum_j F_j J_j, \qquad (1)$$

where F_j are thermodynamic forces, such as the gradient of $1/T$, and J_j are flows, such as the heat flow. In the vicinity of thermodynamic equilibrium, the following linear relation between the flows and the forces holds:

$$J_j = \sum_i L_{ji} F_i, \qquad (2)$$

where L_{ji} represent the so-called phenomenological coefficients, which have been proved to fulfill the Onsager reciprocal relations

$$L_{ji} = L_{ij}. \qquad (3)$$

The relation (2) implies that not only can a force such as the gradient of $1/T$ cause the heat flow but it can also drive other flows, such as a flow of matter or an electrical current. In other words, an entropic force F_i may not only give rise to its corresponding flux J_i, but to many other fluxes J_j in a dazzling variety. Moreover, due to Eq. (3), one flow J_j causes the other J_i in exactly the same way and to exactly the same extent. The thermoelectric effect is one such cross effect. Thermodiffusion is another example. The proliferation of fluxes described above is the main reason why it is so difficult to perceive causality in complex systems, in which relationships between constituents may give rise to very complicated behaviors. Notwithstanding these difficulties, in the paper we examine effects of the Onsager causality in complex networks, which during the last decade have broadened the purview of physics.

In a nutshell, real-world networks and their theoretical models are called complex by virtue of a set of nontrivial topological features among which the most prominent are heavy tails in the degree distribution, tendency of nodes to form clusters, small world effect, assortativity or disassortativity among vertices, community structure at many scales, and evidence of a hierarchical structure (for an extensive review, see Refs. [4,5]). Since Onsager relations operate when the considered systems are close to equilibrium, in the following we will concentrate on equilibrium networks, precisely on exponential random graphs, also known as p^* models, neglecting a huge class of evolving nonequilibrium networks.

Exponential random graphs are ensemble models. They are already well known for mathematicians [6,7], and recently have also aroused interest among physicists [8–10]. As a matter of fact, the methodology behind the models directly follows the methodology behind the maximum entropy school of thermodynamics [11]. In order to correctly define an ensemble of networks, one has to specify a set of graphs $\mathcal{G}$ that one wants to study. In the following we restrict ourselves to labeled simple graphs with a fixed number of nodes N. Next, since the set $\mathcal{G}$ of possible networks has been established, one has to decide what kind of constraints should be imposed on the ensemble. The choice may be, for example, encouraged by properties of real networks such as high clustering, significant modularity, or scale-free degree distribution $P(k) \sim k^{-\gamma}$. Then, one specifies probability distribution $P(G)$ $(G \in \mathcal{G})$ over the ensemble, which consists in maximization of the Shannon entropy $S = -\sum_G P(G)\ln(G)$ subject to the given constraints. The procedure leads to the Boltzmann-like probability distribution

$$P(G) = \frac{e^{-H(G)}}{Z}, \qquad (4)$$

where Z stands for the partition function, whereas $H(G) = \sum_j \theta_j m_j(G)$ is called the graph Hamiltonian. The set $\{m_j\}$ represents ensemble free parameters (like energy E in the

canonical ensemble) upon which the relevant constraints act, and $\{\theta_j\}$ is a set of fields conjugated to these parameters [like $\beta = (kT)^{-1}$ representing field conjugated to the energy E]. Further in the paper, we will consider network ensembles characterized by a desired degree sequence $\{h_1, h_2, \ldots, h_N\}$, i.e., by the Hamiltonian of the form [8]

$$H(G) = \sum_{i=1}^{N} \theta_i k_i(G). \tag{5}$$

The ensembles are formally equivalent to uncorrelated networks with a given node degree distribution $P(k)$ [9], which have been repeatedly used in recent years as the simplest (but not yet trivial!) models of real networks [12–14]. The Onsager formalism applied to this ensemble will allow us to study dynamical response of the considered networks to external perturbations.

In the following, we will study the simplest kind of perturbation consisting in a sudden change of single node's connectivity, e.g., $k_i(t_0) = 0$. The perturbation is particularly well suited for the Hamiltonian (5) because node degrees are ensemble free parameters in the case. Let us also stress that the perturbation directly corresponds to frequently discussed problems of random or intentional removal of sites and links in complex networks, which have been considered in relation with such important issues as resilience of real networks to random breakdowns, their susceptibility to intentional attacks, and finally the issue of cascading failures in these networks. Although, however, a number of analyses in the field have been performed, most of them may be classified into one of two categories: the first one focusing on static, percolation properties of new networks arising as a result of a given perturbation [14,15], and the second one encompassing a variety of processes which excel at imitating specific phenomena (like clogging in the Internet) and give some insight into dynamical behavior of the considered networks after such a perturbation [16–18]. The approach presented in this paper does not fall into either category. Although in the paper we concentrate on a similar kind of perturbation the true challenge of our approach is to present how the most fundamental results of nonequilibrium thermodynamics can help in the understanding of complex networks. The approach is all the more important, since it can be applied to any ensemble of networks with an arbitrary graph Hamiltonian (4).

Thus let us apply the Onsager formalism to the ensemble of networks described by the Hamiltonian (5). Our first aim is to determine thermodynamic flows and forces (1) which appear in the networks after the perturbation consisting in a sudden change of a single node's degree. In order to do it one has to expand the ensemble entropy $S(k_1, k_2, \ldots, k_N)$ about equilibrium as a power series in its independent variables,

$$d_i S = S - S_{eq} = \frac{1}{2} \sum_{i,j} \frac{\partial^2 S}{\partial k_i \, \partial k_j} (k_i - h_i)(k_j - h_j), \tag{6}$$

where $\partial S / \partial k_i = 0$. Next, computing the time derivative of the above expression one obtains a new microscopic expression for the rate of the entropy production,

$$\sigma = \frac{d_i S}{dt} = -\sum_{i,j} g_{ij} (k_i - h_i) \frac{d(k_j - h_j)}{dt}, \tag{7}$$

where $g_{ij} = -\partial^2 S / (\partial k_i \partial k_j)$. Identifying the derivative

$$J_j = \frac{d(k_j - h_j)}{dt} \tag{8}$$

as a thermodynamic flow, and then comparing Eq. (7) with Eq. (1) allows one to show that the term

$$F_j = -\sum_i g_{ij} (k_i - h_i) \tag{9}$$

corresponds to the thermodynamic force.

Now, assuming that the probability of a fluctuation in our ensemble is given by the Einstein formula $P(d_i S) \sim \exp[d_i S]$ one can show that elements of the matrix $\mathbf{g}^{-1}$ (which is the inverse of $\mathbf{g}$) describe correlations between fluctuations [2,3],

$$g_{ij}^{-1} = \langle (k_i - h_i)(k_j - h_j) \rangle = \langle k_i k_j \rangle - h_i h_j. \tag{10}$$

At this point it is also worthwhile to stress that from a physical point of view the parameters g_{ij}^{-1} correspond to generalized susceptibilities $\chi_{ij}^{(\theta)} = -\partial h_i / \partial \theta_j$ [see Eq. (39) in Ref. [9]], which measure the response of h_i to the variation of the field θ_j. Having the ensemble averages [19]

$$\langle k_i k_j \rangle = h_i \left(1 - \frac{h_i \langle h^2 \rangle}{\langle h \rangle^2 N} \right) \delta_{ij} + h_i h_j, \tag{11}$$

one immediately finds that in sparse and uncorrelated networks described by the Hamiltonian (5), for which $\langle h^2 \rangle / \langle h \rangle \leq \ln N$ [9,21], the matrix $\mathbf{g}$ is always diagonal,

$$g_{ij} \simeq \frac{\delta_{ij}}{h_i}. \tag{12}$$

The last result is interesting for two reasons. First, it allows us to simplify the expression for the thermodynamic force F_j acting on the node j when the studied networks are thrown out of equilibrium. Namely, inserting Eq. (12) into Eq. (9) one finds that the force is equivalent to the normalized fluctuation on the considered node,

$$F_j = \frac{h_j - k_j}{h_j}. \tag{13}$$

Second, it shows that correlations between fluctuations on various nodes are negligibly small. Although at first glance the remark seems to contradict the expected cross effects, further in the paper we show that the effects consisting in cascading development of different flows between the nodes do really exist in the considered networks.

In the following, in order to examine the mentioned cross effects we will write the rate equation for $k_j - h_j$, which will make possible the detailed analysis of the thermodynamic flows J_j (8) in the considered ensemble. Before, however, we proceed with this equation let us discuss structural and dynamical properties of the studied networks. First, since the networks are uncorrelated the probability of a link between any pair of nodes i and j with degrees respectively equal to k_i

and k_j is given by $p_{ij} = k_i k_j / (\langle k \rangle N)$. Next, due to the fact that the networks are close to equilibrium one can assume that their dynamics after a small perturbation is the same as their dynamics in equilibrium. One can expect that the analyzed networks make only small steps in the configuration space $\mathcal{G}$ forming a sort of reasonable physical trajectory, along which successive networks G appear with probabilities proportional to their weights, that is, proportional to $e^{-H(G)}$ (4). The simplest and physically the most reasonable method providing such a sampling is known as the Metropolis algorithm [22]. In the algorithm the ratio

$$w = \frac{P(G_1)}{P(G_2)} = \frac{e^{-H(G_1)}}{e^{-H(G_2)}} = e^{-\Delta H} \quad (14)$$

is interpreted as the probability of making a transition from one network configuration G_1 to the other configuration G_2 (if $\Delta H < 0$ then $w > 1$ and such a transition is always accepted). The considered difference between the two configurations G_1 and G_2 should not be too large, since then the acceptance probability w would be small.

Now, having in mind the expounded properties of the considered ensemble, and assuming that during a single time step only one link may be added or removed from the network, one can easily write the rate equation for $k_j - h_j$

$$\frac{\partial (k_j - h_j)}{\partial t} = \frac{1}{\binom{N}{2}} \sum_{i \neq j} \left[(-1) \frac{k_i k_j}{\langle k \rangle N} \min[e^{\theta_i + \theta_j}, 1] \right.$$
$$\left. + (+1) \left(1 - \frac{k_i k_j}{\langle k \rangle N} \right) \min[e^{-(\theta_i + \theta_j)}, 1] \right]. \quad (15)$$

The first term on the right-hand side of Eq. (15) corresponds to the node's degree decrement by a link removal, and respectively the second term represents the node's degree increment by a link addition. At the moment, our aim is to reformulate the last equation into the form similar to relation (2). In order to do it let us recall two properties of the analyzed ensemble (5), which have been proved in Ref. [9]. The first property $\langle k \rangle = \langle h \rangle$ is trivial and does not require any comment. The second property, that is of our interest, relates the expected node's degree h_j with its conjugated field θ_j, i.e., $h_j \simeq e^{-\theta_j} \sqrt{\langle h \rangle N}$. The last expression is only true in sparse and uncorrelated networks for which fields $\{\theta_i\}$ conjugated to nodes' degrees are positive. Putting the mentioned expressions into Eq. (15), after some algebra one gets a new rate equation,

$$\frac{\partial (k_j - h_j)}{\partial t} = -\frac{2}{N^2} \left[k_j \left(1 + \frac{h_j \langle h^2 \rangle}{N \langle h \rangle^2} \right) - h_j \right]$$
$$- \frac{2 k_j h_j}{\langle h \rangle^2 N^4} \sum_{i \neq j} h_i (k_i - h_i), \quad (16)$$

which after putting $k_j = h_j$ in the second term (since we operate in the vicinity of equilibrium the assumption is reasonable) simplifies to the desired form (2),

$$\frac{\partial (k_j - h_j)}{\partial t} = \frac{2 h_j}{N^2} \left(\frac{h_j - k_j}{h_j} \right) + \sum_{i \neq j} \frac{2 h_i^2 h_j^2}{\langle h \rangle^2 N^4} \left(\frac{h_i - k_i}{h_i} \right), \quad (17)$$

having the exact solution

$$\vec{k}(t) - \vec{h} = e^{-\mathbf{L} \mathbf{g} t} (\vec{k}(t_0) - \vec{h}), \quad (18)$$

and providing us with the matrix of phenomenological coefficients $\mathbf{L}$ describing non-equilibrium phenomena occurring in the considered networks,

$$L_{ij} = \begin{cases} \dfrac{2 h_i}{N^2} & \text{for } i = j \\[2mm] \dfrac{2 h_i^2 h_j^2}{\langle h \rangle^2 N^4} & \text{for } i \neq j \end{cases}.$$

Now, let us discuss the results of the last paragraph. At the beginning let us note that Eq. (17) clearly shows that cross effects do really exist in complex networks. Furthermore, the obtained matrix $\mathbf{L}$ is symmetrical. It means that the Onsager relations (3) hold in the studied networks, i.e., the effect of a normalized fluctuation occurring in one node F_i (13) on the flow which is induced in another node J_j (8) is the same as the effect of F_j on J_i, regardless of the nodes' degrees h_i and h_j. Note also that Eq. (17) can be written as follows:

$$J_j = J_j^{(j)} + \sum_{i \neq j} J_j^{(i)}, \quad (19)$$

revealing the multicomponent nature of the analyzed flows. The partial flows introduced in the last expression can be easily identified from the initial equation (17). They respectively stand for flows $J_j^{(i)} = L_{ji} F_i$ generated on the node j by other nodes $i \neq j$, and for the flow $J_j^{(j)} = L_{jj} F_j$ induced on the node by itself. A simple comparison of the flows shows that in the studied case of sparse and uncorrelated networks (5) the following relation holds:

$$\forall_{i \neq j} J_j^{(j)} \gg J_j^{(i)}, \quad (20)$$

which stems from the analogous relation between Onsager coefficients, i.e., $\forall_{i \neq j} L_{jj} \gg L_{ij}$. The above relation causes that the partial flows $J_j^{(i)}$, giving rise to cross effects, are much smaller than the local flow $J_j^{(j)}$. In fact, the only networks for which the total effect of the cross flows is considerable are scale-free networks, in which highly connected nodes appear.

Therefore to numerically verify the obtained results we have analyzed the behavior of scale-free networks [i.e., networks characterized by a power law distribution of the desired nodes' degrees $P(h) \sim h^{-\gamma}$, which $2.4 \leq \gamma \leq 4$] after a sudden rewiring of all links attached to the node with the highest degree k_{max} to other nodes. A schematic illustration of the network response to this externally applied disturbance is shown in Fig. 1. The cross effects manifest themselves in a number of additional links which appear in the network during its return to equilibrium. In order to quantify the effects and check the correctness of our calculations we have measured the amplitude of the response function (see Fig. 1) obtained from Monte Carlo simulations and compare it with both numerical solutions of the set of initial rate Eqs.
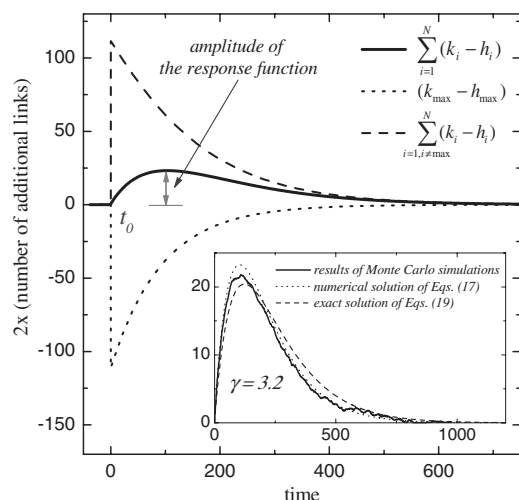
FIG. 1. Main stage: Schematic picture illustrating the behavior of a network after the perturbation consisting in a sudden rewiring of all links attached to the most connected node to other nodes. Subset: Response function of a scale-free network of sizes $N=512$ with $\gamma=3.2$. (All Monte Carlo simulations presented in the paper have been averaged 10^6 times.)

FIG. 2. Amplitude of the response function vs γ in scale-free networks of size $N=512$.

(15) and the exact solution (18) of the set of simplified Eqs. (17) (see the subset in Fig. 1). The results are presented in Fig. 2. One can see that for $\gamma \geq 3$ our analytical calculations fit numerical results very well. The visible discrepancy between the numerical results and their theoretical predictions for $\gamma < 3$ is due to the fact that the applied formalism does not take into account degree correlations which spontaneously develop in scale-free networks with $\gamma < 3$ [see the comment after Eq. (28) in Ref. [9]].

In summary, in this paper we present the Onsager formalism applied to random networks with arbitrary degree distribution. Using the well-known methods of nonequilibrium thermodynamics we identify thermodynamic forces and their conjugated flows induced in networks as a result of single node degree perturbation. The forces and the flows can be understood as a response of the system to events, such as random removal of nodes or intentional attacks on them. We show that cross effects (such as thermodiffusion, or thermo-
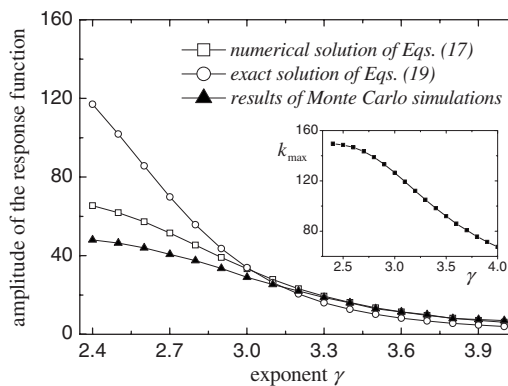
electric phenomena), in which one force may not only give rise to its own corresponding flow, but to many other flows, can be observed also in complex networks.

Finally, since the science of complex networks is a genuinely multidisciplinary domain, the approach if applied to social, economic, or even biological networks may open new horizons for the sciences, as it would provide them with a completely new understanding of how rumors, information, marketing, or crises can spread through these systems causing small, medium, or large responses. Moreover, if one can identify social (economic) equivalents of thermodynamic forces and flows, a social (economic) analog of thermodynamic cross effects, underlying complexity of the socioeconomic systems, will be within the grasp. We hope that the approach introduced in the paper will serve as a practical starting point for exploring a variety of nonequilibrium network-driven phenomena.

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