## Fluctuation-dissipation relations in complex networks

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In this paper, we study fluctuations over several ensembles of maximum-entropy random networks. We derive several fluctuation-dissipation relations characterizing the susceptibilities of different networks to changes in external fields. In the case of networks with a given degree sequence, we argue that the scale-free topologies of real-world networks may arise as a result of the self-organization of real systems into sparse structures with low susceptibility to random external disruptions. We also show that the ensembles of networks with a given degree sequence and networks characterized by two-point correlations are equivalent to random networks with hidden variables.

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## I. INTRODUCTION

Recently, the statistical properties of real networks (including biological, social, and technological systems) have attracted a large amount of attention among physicists (see, e.g., [1-3]). It has been realized that, despite functional diversity, most real weblike systems share important structural features, e.g., small average path length, high clustering, and scale-free degree distribution. A number of network models have been proposed to embody the fundamental characteristics. The models can be roughly divided into two classes: static (homogeneous, equilibrium) and evolving (causal, nonequilibrium). The second class of causal networks encompasses, in particular, the famous Barabási-Albert (BA) model [4], whereas the configuration model [5-7] and the large group of networks with hidden variables [8–10] belong to the first class of static networks. Although very intuitive, the mentioned representatives of static random networks are not properly defined from the point of view of equilibrium statistical mechanics. Below we briefly outline what the mentioned lack of appropriateness means with reference to random networks.

To start with, let us concentrate on the phrase *random network*. What does it mean if a network is random? One possible answer is that there is a large amount of randomness in the process of network construction. It applies to all the examples of homogeneous and causal networks quoted in the previous paragraph. The answer, however, has a few disadvantages, the most striking of which is the issue of the quantification of the randomness. Another answer could be that a random network is a member of a statistical *ensemble* of networks and the probability of the occurrence of a given network in random sampling is proportional to its statistical weight. Without a doubt, the last treatment directly follows the principles of equilibrium statistical mechanics.

A simple example could be the configuration model. In this model, the total number of nodes is fixed to N and degrees of all nodes i=1,2,...,N create a specific degree sequence  $\{k_i\}$ . Until now, nothing has been said about the connections between nodes. As a rule, random graphs with a given degree sequence are constructed in the following way: first, attach to each node *i* a number  $k_i$  of *stubs* (ends of edges); next, choose pairs of these stubs uniformly at random and join them together to make complete edges. Of course, such a procedure represents a large randomness, justifying the phrase *random networks*. On the other hand, however, the second definition treats the resulting networks as members of the ensemble of graphs with the desired degree sequence, which seems to be more familiar to physicists.

The concepts of statistical mechanics (including statistical ensembles, partition functions, averages over ensemble, and so forth) have already been applied to analyses of complex networks. Although the majority of recently submitted articles still define network models through construction procedures, there have also been several interesting papers published on the *genuine* statistical mechanics of random networks (cf. [11–20]). The general idea is similar to all the above-mentioned papers. The statistical ensemble of networks is defined by specifying a set of networks  $\mathcal{G}$  that one wants to study (e.g., simple graphs, digraphs, weighted graphs) and a rule that associates probability distribution P(G) with these networks  $G \in \mathcal{G}$ . The differences between the approaches consist of different weight assignment strategies.

In this study, we develop the information-theoretic approach to random networks that has been very recently proposed by Park and Newman [18] (see also [13]). Information theory [21,22] provides a criterion for setting up probability distributions over a given ensemble on the basis of partial knowledge and leads to a type of statistical inference. It is the least biased estimate possible on the given information, i.e., it is maximally noncommittal with regard to missing information. Since the procedure consists in entropy maximization under constraints imposed by the physical conditions of the ensemble, it is also known as a maximumentropy estimate [23].

In this paper, following Park and Newman [18], we use Shannon entropy in order to establish probability distribution over analyzed networks [24]. Park and Newman have presented a few exact solutions (in the sense of weighted averages over ensembles) of specific network models, including undirected networks with a given degree sequence and networks incorporating arbitrary but independent edge probabilities. Here, we analyze these models from the point of view of fluctuations over ensembles. We discuss several fluctuation-dissipation relations for the mentioned ensembles. We also show that the quoted maximum-entropy models are equivalent to random networks with hidden variables [9].

### **II. GENERAL DEFINITIONS**

In this section, we review the fundamentals of maximumentropy random networks presented by Park and Newman [18].

In order to correctly define a statistical 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 [26] with a fixed number of nodes N. A simple graph has, at most, one link between any pair of vertices and it does not contain self-loops connecting vertices to themselves. Also note that a one-to-one correspondence (isomorphism) exists between simple graphs and symmetric matrices of size N with elements  $\sigma_{ij}$  equal to either 0 or 1.

Once 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. In fact, due to the mentioned isomorphism between graphs and matrices, there can be exactly solved only such ensembles which constraints are simply expressed in terms of an adjacency matrix.

Now, suppose that one would like to establish probability distribution over G in such a way that the expected values (i.e., averages over the ensemble) of several observables  $\{x_i(G)\}, i=1,2,\ldots,r$  were, respectively, equal to  $\{\langle x_i \rangle\}$ . Due to information theory, the best choice for probability distribution P(G) is the one that maximizes the Shannon entropy

$$S = -\sum_{G} P(G) \ln P(G), \qquad (1)$$

subject to the constraints

$$\langle x_i \rangle = \sum_G x_i(G) P(G)$$
 (2)

for  $i=1,2,\ldots,r$ , plus the normalization condition

$$\sum_{G} P(G) = 1.$$
(3)

The Lagrangian for the above problem is given by the expression

$$\mathcal{L} = -\sum_{G} P(G) \ln P(G) + \alpha \left(1 - \sum_{G} P(G)\right)$$
(4)

$$+\sum_{i=1}^{r} \theta_i \bigg( \langle x_i \rangle - \sum_G x_i(G) P(G) \bigg), \tag{5}$$

where the multipliers  $\alpha$  and  $\theta_i$  are to be determined by Eqs. (2) and (3).

Differentiating  $\mathcal{L}$  with respect to P(G) and then equating the result to zero, one obtains the desired probability distribution over the ensemble of graphs with given properties (2),

$$P(G) = \frac{e^{-H(G)}}{Z},\tag{6}$$

where H(G) is the network Hamiltonian

$$H(G) = \sum_{i=1}^{r} \theta_{i} x_{i}(G),$$
(7)

and Z represents the partition function (normalization constant)

$$Z = \sum_{G} e^{-H(G)} = e^{\alpha + 1}.$$
 (8)

Finally, in order to complete the section devoted to general considerations, it is useful to define the free energy of the ensemble

$$F = -\ln Z. \tag{9}$$

The last quantity is of wide use in the rest of the paper.

Now, let us examine the introduced formalism with a few examples. In the next section, we will analyze fluctuations over the ensembles presented below.

### A. Microcanonical ensemble of random networks

First, let us study the equivalent of the microcanonical ensemble for maximum-entropy random networks. Maximizing Shannon entropy (1) subject to only normalization condition (3), i.e., omitting other constraints (2), one obtains the uniform distribution over all simple graphs of size N,

$$P(G) = \frac{1}{\Omega},\tag{10}$$

where  $\Omega = 2^{\binom{N}{2}}$  represents the total number of the considered networks, i.e., the total number of 0–1 symmetric matrices of size *N*. The uniform distribution (10) means that each graph in the ensemble has the same weight regardless of its properties.

Since all graphs in the ensemble are equiprobable, one can simply argue that the probability of a graph having m links is given by

$$P(m) = \frac{\binom{\binom{N}{2}}{m}}{2\binom{\binom{N}{2}}{2\binom{\binom{N}{2}}{2}}}$$
(11)

and, respectively,

$$\langle m \rangle = \sum_{m=0}^{\binom{N}{2}} mP(m) = \frac{\binom{N}{2}}{2}.$$
 (12)

Similarly, the probability of an arbitrary node to have *k* nearest neighbors equals  $P(k) = \binom{N-1}{k}/2^{N-1}$ , and the average connectivity is  $\langle k \rangle = (N-1)/2$ .

In fact, the considered microcanonical ensemble of random networks is equivalent to the ensemble of classical random graphs with the connection probability  $p=\frac{1}{2}$ . Ensembles of classical random graphs with an arbitrary linkage probability will be considered in the next subsection.

#### **B.** Classical random graphs

Now, let us consider an ensemble of networks with an expected number of links  $\langle m \rangle$  (the ensemble is equivalent to random graphs introduced by Erdös-Rényi). The Hamiltonian (7) for this ensemble is given by

$$H(G) = \theta m(G), \tag{13}$$

where  $\theta$  represents a field or an inverse temperature. The value of  $\theta$  is fixed and depends only on  $\langle m \rangle$ . Park and Newman [18] have shown that the partition function (8) for the ensemble is equal to

$$Z = (1 + e^{-\theta}) {\binom{N}{2}}$$
(14)

and, respectively, the free energy (9) can be written as

$$F = -\ln Z = -\binom{N}{2}\ln(1 + e^{-\theta}).$$
 (15)

Having probability distribution (6) over an ensemble, one can, for example, find the relation between the average number of links  $\langle m \rangle$  and  $\theta$ ,

$$\langle m \rangle = \frac{\partial F}{\partial \theta} = \frac{\binom{N}{2}}{e^{\theta} + 1}.$$
 (16)

Now, since  $\theta$  is fixed, one can express the last formula in terms of the linkage probability p, which is known from the theory of classical random graphs

$$\langle m \rangle = \binom{N}{2} p,$$
 (17)

where

$$p = \frac{1}{e^{\theta} + 1}.\tag{18}$$

Finally, let us point out that in the limit of very small fields  $\theta \rightarrow 0$  (high temperatures), the ensemble of random networks with an expected number of links is equivalent to the microcanonical ensemble of random networks (10) introduced in the previous subsection.

#### C. Networks with a given degree sequence

At the moment, suppose that one would like to deal with random networks with an expected degree sequence

$$\{\langle k_i \rangle\}$$
 for  $i = 1, 2, ..., N.$  (19)

In this case, the network Hamiltonian is given by

$$H(G) = \sum_{i=1}^{N} \theta_{i} k_{i}(G),$$
 (20)

where the multipliers  $\theta_i$  represent a kind of potential assigned to each node and they only depend on the expected degrees  $\langle k_i \rangle$  [see Eqs. (24) and (27)]. The partition function for the considered ensemble can be written as [18]

$$Z = \prod_{i < j} \left( 1 + e^{-(\theta_i + \theta_j)} \right) \tag{21}$$

and the free energy is

$$F = -\sum_{i < j} \ln(1 + e^{-(\theta_i + \theta_j)}).$$
(22)

By performing weighted averages over the ensemble, one can easily prove the following identities: the first one describes the connection probability between two nodes i and j,

$$p_{ij} = \frac{1}{e^{(\theta_i + \theta_j)} + 1},$$
 (23)

and the second describes the identity for the average connectivity of a node characterized by the local field  $\theta_i$ ,

$$\langle k_i \rangle(\theta_i) = \frac{\partial F}{\partial \theta_i} = \sum_{j=1}^N \frac{1}{e^{(\theta_i + \theta_j)} + 1} = \sum_{j=1}^N p_{ij}.$$
 (24)

Both expressions show the reverse relation between the two parameters (i.e.,  $\langle k_i \rangle$  and  $\theta_i$ ) that characterize each node. The relation consists of the following statement: small degrees correspond to large multipliers and, vice versa, nodes with a large number of connections possess small multipliers.

Park and Newman [18] have pointed out that instead of studying networks with an expected degree sequence (19), one can deal with networks characterized by an expected degree distribution  $P(\langle k_i \rangle)$  [27]. They have argued that one can produce any degree distribution by a judicious choice of the distribution of multipliers  $\rho(\theta_i)$ . In fact, due to Eq. (24),  $\rho(\theta_i)$  resulting in the desired  $P(\langle k_i \rangle)$  can be determined from the expression

$$\rho(\theta_i) = P(\langle k_i \rangle) \left| \frac{d\langle k_i \rangle}{d\theta_i} \right|, \qquad (25)$$

where  $\langle k_i \rangle(\theta_i)$  is given by Eq. (24). There are, however, a few subtleties related to the transition between the sequence  $\{\langle k_1 \rangle, \langle k_2 \rangle, \dots, \langle k_N \rangle\}$  and  $P(\langle k_i \rangle)$ . First, Eq. (25) defines  $\rho(\theta_i)$ as an implicit function that, except for a very few cases, cannot be explicitly calculated. Second, when performing such a transition, one has to keep in mind that the phase space consists of labeled graphs in which every node *i* =1,2,...,*N* has been assigned its own multiplier  $\theta_i$  (i.e., is distinguishable). Using  $\rho(\theta_i)$  implies that the nodes lose their identities. In such a case, there is a threat of widening the original phase space.

To proceed further, let us consider *sparse* networks. In this case, connection probabilities (23) factorize

$$p_{ij} \simeq e^{-(\theta_i + \theta_j)} = \frac{\langle k_i \rangle \langle k_j \rangle}{\langle k \rangle N}, \qquad (26)$$

where

$$\langle k_i \rangle(\theta_i) \simeq e^{-\theta_i} \sqrt{\langle k \rangle N}.$$
 (27)

As shown in [9,10], such ensembles are equivalent to uncorrelated networks. The relation (27) between expected degrees and their multipliers makes the ensembles very simple for both Monte Carlo simulations and analytical treatment. In particular, the distribution of multipliers (25) corresponding to  $P(\langle k_i \rangle)$  is simply

$$\rho(\theta_i) = \langle k_i \rangle P(\langle k_i \rangle), \qquad (28)$$

where  $\langle k_i \rangle$  is given by Eq. (27).

There exist, however, some difficulties with the approximation. First, the connection probability  $p_{ij} \leq 1$ , Eq. (26) and thus the assumption of sparse networks is only valid for networks with non-negative Lagrange multipliers (i.e.,  $\theta_i, \theta_j \geq 0$ ). This restriction causes a failure of the approach in the case of scale-free networks  $P(k) \sim k^{-\gamma}$  with  $2 < \gamma < 3$ . The existence of hubs  $k_{\max} \sim N^{1/(\gamma-1)}$  [28], i.e., nodes with negative multipliers [see the comment after Eq. (24)], spontaneously develops degree correlations [29,30]. It was argued [14,31,32] that one can omit the correlations by applying the so-called structural cutoff, i.e., forcing the largest degree to scale as  $k_{\max} \sim \sqrt{N}$ . At the moment, let us stress that the structural cutoff in uncorrelated networks naturally results in Eq. (24) when  $\theta_i \rightarrow 0$ .

## D. Networks with two-point correlations

In order to study random networks with two-point correlations, one may consider a class of Hamiltonians (7) constructed on the basis of an expected linkage probability,

$$H(G) = \sum_{i < j} \Theta_{ij} \sigma_{ij}(G).$$
<sup>(29)</sup>

In the preceding expression,  $\sigma_{ij}(G)$  is an element of the adjacency matrix representing the graph *G*, and  $\Theta_{ij}$  characterizes field coupled to the hypothetical link  $\{i, j\}$ . The partition function and the free energy for the ensemble are given by

$$Z = \prod_{i < j} (1 + e^{-\Theta_{ij}}), \quad F = -\sum_{i < j} \ln(1 + e^{-\Theta_{ij}}).$$
(30)

Comparing Eqs. (21) and (30), one can see that the previous ensemble of networks with an expected degree sequence is a special case (for  $\Theta_{ij} = \theta_i + \theta_j$ ) of networks with arbitrary twopoint correlations. Similar to Eq. (23), one can also find that

$$p_{ij} = \langle \sigma_{ij} \rangle = \frac{\partial F}{\partial \Theta_{ij}} = \frac{1}{e^{\Theta_{ij}} + 1}.$$
 (31)

## **III. FLUCTUATIONS AND RESPONSES**

In classical thermodynamics, fields interacting with a system have conjugate variables that represent the response of the system to changes in the corresponding field. For example, the response of a gas to a change in pressure is a change in volume. The pressure p is the conjugate variable to the volume V. Similarly, the magnetization M of a magnet changes in response to the applied field B. These relations are produced by terms in the Hamiltonian of the form  $\Theta X$ , where  $\Theta$  is a field and X is the conjugate variable to which it couples. Note that the above also holds for maximum-entropy random networks [see Eq. (7)],

$$H(G) = \sum_{i=1}^{\prime} \theta_i x_i(G).$$
 (32)

Taking advantage of Eqs. (6)–(9), expectation values  $\langle x_i \rangle$  of observables  $x_i$  can be calculated as first derivatives of the free energy with the appropriate field  $\theta_i$  [cf. Eqs. (16), (24), and (31)],

$$\langle x_i \rangle = \sum_G x_i(G) P(G) = \frac{\partial F}{\partial \theta_i}.$$
 (33)

Similarly, second derivatives of the free energy F give the mean-square fluctuations of the variables

$$\langle x_i^2 \rangle - \langle x_i \rangle^2 = -\frac{\partial^2 F}{\partial \theta_i^2}.$$
 (34)

Now, inserting Eq. (33) into Eq. (34), one obtains a very important result

$$\langle x_i^2 \rangle - \langle x_i \rangle^2 = -\frac{\partial \langle x_i \rangle}{\partial \theta_i} = \chi_i^{(\theta)}, \qquad (35)$$

which is known as the *fluctuation-dissipation theorem* (FDT). The theorem states that fluctuations in an observable  $x_i$  are proportional to the susceptibility  $\chi_i^{(\theta)}$  of the observable to its conjugate field  $\theta_i$ . Remember that the susceptibility  $\chi_i^{(\theta)}$  measures the strength of the response of  $x_i$  to changes in  $\theta_i$ . In reality, due to practical purposes, it is often simpler to analyze the susceptibility  $\chi_i^{(\phi)}$  to another field  $\phi_i$  that directly depends on  $\theta_i$  (35),

$$-\frac{\partial \langle x_i \rangle}{\partial \theta_i} = -\frac{\partial \langle x_i \rangle}{\partial \phi_i} \frac{\partial \phi_i}{\partial \theta_i} = \frac{\partial \phi_i}{\partial \theta_i} \chi_i^{(\phi)}, \qquad (36)$$

where  $\partial \phi_i / \partial \theta_i$  is the transitional derivative.

Probably the best known example of the theorem (35) is the one arising from fluctuations of energy in the canonical ensemble,

$$\langle E^2 \rangle - \langle E \rangle^2 = -\frac{\partial E}{\partial \beta} = kT^2 C_V,$$
 (37)

where  $C_V = \partial \langle E \rangle / \partial T$  is the heat capacity (or thermal susceptibility), whereas  $kT^2 = \partial \beta / \partial T$  is the respective transitional derivative. Another example relates fluctuations in the magnetization to the magnetic susceptibility

$$\langle M^2 \rangle - \langle M \rangle^2 = \frac{1}{\beta} \frac{\partial M}{\partial B} = \frac{1}{\beta} \chi^{(B)}.$$
 (38)

The fluctuation-dissipation theorems (35)–(38) are interesting for a number of reasons. First, they join both the microscopic description (left-hand side) and macroscopic properties (right-hand side) of the considered systems. Second, they relate the actual state (fluctuations) of the systems to their future behavior (response). Third, due to the FDT, phase transitions certified by singularities in susceptibilities can also be reported by large-scale fluctuations.

Extending the idea of susceptibility, one can consider what happens with a variable  $x_i$  when one changes the value of a field  $\theta_j$ . To study the problem, one can define a generalized susceptibility  $\chi_{ij}^{(\theta)}$ , which is a measure of the response of  $\langle x_i \rangle$  to the variation of the field  $\theta_j$ ,

$$\chi_{ij}^{(\theta)} = -\frac{\partial \langle x_i \rangle}{\partial \theta_j}.$$
(39)

Again, the susceptibility  $\chi_{ij}^{(\theta)}$  is a second derivative of the free energy,

$$\chi_{ij}^{(\theta)} = -\frac{\partial^2 F}{\partial \theta_i \partial \theta_j} = \langle x_i x_j \rangle - \langle x_i \rangle \langle x_j \rangle.$$
(40)

The issue of generalized susceptibilities is of special interest in lattice systems (32), where the variables  $x_i$  may represent the same observable x but are measured in different spatial points i=1,2,...,r. Then, susceptibility  $\chi_{ij}^{(\theta)}$  is just the twopoint correlation function between sites *i* and *j*.

In the following, we will concentrate on fluctuations over a few selected ensembles of random networks.

### A. Classical random graphs

At the beginning, let us consider the ensemble of classical random graphs. By definition, the average number of links  $\langle m \rangle$  is fixed in the ensemble. As stressed at the beginning of the section, fluctuations exist around the average. In fact, the probability of a graph *G* with *m* links is given by

$$P(G) = \frac{e^{-\theta m(G)}}{Z} = p^m (1-p)^{\binom{N}{2}-m}.$$
 (41)

The variance of the above distribution calculated from Eq. (35) is very similar to Eq. (37),

$$\langle m^2 \rangle - \langle m \rangle^2 = -\frac{\partial \langle m \rangle}{\partial \theta} = -\frac{\partial \langle m \rangle}{\partial p} \frac{\partial p}{\partial \theta} = p(1-p)C_m, \quad (42)$$

where  $C_m = \partial \langle m \rangle / \partial p = {N \choose 2}$  is the link capacity in classical random graphs. Note that for a given network size *N*, the link capacity does not depend on the linkage probability  $C_m(p)$ =const [classical ideal gas reveals the analogous behavior  $C_V(T)$ =const].

#### B. Networks with a given degree sequence

Now, let us continue with random networks characterized by an expected degree sequence (19).

Taking advantage of Eqs. (23) and (24), fluctuationdissipation relations (35) for the ensemble may be written in the following form:



FIG. 1. Schematic representation of networks possessing N=19 nodes with one nearest neighbor  $\langle k \rangle = 1$  and the supernode (the gray one) with the tunable connectivity  $\langle k^* \rangle = 1, 2, ..., N$ .

$$\chi_i^{(\theta)} = -\frac{\partial \langle k_i \rangle}{\partial \theta_i} = \langle k_i^2 \rangle - \langle k_i \rangle^2 = \sum_j p_{ij} (1 - p_{ij}) = \langle k_i \rangle - \sum_j p_{ij}^2.$$
(43)

At the moment, before delving into the discussion of the last expression, let us note that the susceptibility  $\chi_i^{(\theta)}$  is also given by the following formula:

$$\chi_i^{(\theta)} = -\sum_j \frac{\partial \langle k_i \rangle}{\partial p_{ij}} \frac{\partial p_{ij}}{\partial \theta_i} = -\sum_j \frac{\partial p_{ij}}{\partial \theta_i} C_{ij}, \qquad (44)$$

where  $C_{ij} = \partial \langle k_i \rangle / \partial p_{ij}$  represents the link capacity. Here, since  $C_{ij} = 1$ , the fluctuations in node degrees result only from the transitional derivative  $\partial p_{ij} / \partial \theta_i$ .

The importance of the two above identities lies in the fact that, from the fluctuations over degrees of nodes characterized by the same local field  $\theta_i$ , one can deduce the future behavior of the nodes in the face of possible changes in  $\theta_i$ . Large (small) fluctuations correspond to high (low) local susceptibility  $\chi_i^{(\theta)}$ .

Now, let us note that in the case of small degrees [see also the assumption of sparse networks (27)], the fluctuationdissipation relation (43) gets a simplified form

$$\langle k_i^2 \rangle - \langle k_i \rangle^2 = \langle k_i \rangle, \tag{45}$$

indicating the Poissonian fluctuations. However, in the case of sparse homogeneous networks, one can omit the last term in Eq. (43). In sparse scale-free networks with the characteristic exponent  $2 < \gamma < 3$ , the mentioned term is dominated by hubs and the nodes' susceptibilities  $\chi_i^{(\theta)}$  are much smaller than their expected degrees  $\langle k_i \rangle$ . The total network susceptibility decreases, making the system resistant against random changes in the landscape of multipliers and simultaneously susceptible to the behavior of supernodes (i.e., hubs) [33,34].

In order to establish a better understanding of the statement included in the last paragraph, let us consider a trivial network consisting of N nodes with expected degrees  $\langle k \rangle = 1$  and one supernode with the tunable desired degree  $\langle k^* \rangle = 1, 2, ..., N$  (in the sequel, the parameters denoted by the star apply to the supernode). Adjusting the degree of the supernode makes it possible to smoothly pass between regular graphs (for  $\langle k^* \rangle = 1$ ) and star networks (for  $\langle k^* \rangle = N$ ) (see Fig. 1). The transition enables an understanding of what the reduced network susceptibility consists in.



FIG. 2. (Color online) (a) Lagrange multipliers  $\theta$  and  $\theta^*$  as a function of  $\langle k^* \rangle$ ; (b) relative susceptibilities  $\chi$  and  $\chi^*$  as a function of  $\langle k^* \rangle$ . Here, we have assumed N=100.

First, let us find the Lagrange multipliers  $\theta$  and  $\theta^*$  corresponding to the nodes of the considered ensemble. Using Eq. (24), one can see that the parameters fulfill the set of equations

$$1 = \frac{N-1}{e^{2\theta}+1} + \frac{1}{e^{\theta+\theta^*}+1},$$
$$\langle k^* \rangle = \frac{N}{e^{\theta+\theta^*}+1}.$$

Solving the above equations for  $\theta$  and  $\theta^*$  [see Fig. 2(a)], one gets

$$\theta = \frac{1}{2} \ln \left[ \frac{N^2 - 2N + \langle k^* \rangle}{N - \langle k^* \rangle} \right],$$
$$\theta^* = \ln \left[ \frac{N - \langle k^* \rangle}{\langle k^* \rangle} \right] - \theta.$$

Next, inserting the multipliers into Eq. (23) and then using Eq. (43), one obtains the susceptibilities of expected degrees due to changes in the nodes' intensive parameters. The relative susceptibilities are given, respectively, by

$$\chi = -\frac{1}{\langle k \rangle} \frac{\partial \langle k \rangle}{\partial \theta} = 1 - \frac{(N - \langle k^* \rangle)^2}{N^2 (N - 1)} - \frac{\langle k^* \rangle^2}{N^2}$$
(46)

for the bulk of nodes and

$$\chi^* = -\frac{1}{\langle k^* \rangle} \frac{\partial \langle k^* \rangle}{\partial \theta^*} = 1 - \frac{\langle k^* \rangle}{N}$$
(47)

for the supernode.

The behavior of susceptibilities (46) and (47) is depicted in Fig. 2(b). One can see that the susceptibilities decrease to 0 when the expected degree of hub  $\langle k^* \rangle$  approaches N. In the region of the vanishing susceptibilities, the small changes in the fields  $\theta$  and  $\theta^*$  poorly affect the topological features (i.e.,  $\langle k^* \rangle$ ) of the considered networks [cf. Fig. 2(a)]. The last statement supports our previous claim of the resilience of such networks against random external interference. The large  $\langle k^* \rangle$  makes it so that the supernode accumulates most of the links present in the system and causes a relatively small number of network realizations that both (i) fulfill physical constraints of the ensemble and (ii) possess significant statistical weight. For example, only one such a realization exists in the limiting case of the star network with  $k^* = N$ .

# IV. EQUIVALENCE OF MAXIMUM ENTROPY NETWORKS AND NETWORKS WITH HIDDEN VARIABLES

In this section, we continue the thread of Poissonian fluctuations (45).

Random networks with hidden variables are simply defined through the construction procedure that consists of only two steps.

(i) First, prepare N nodes and assign them hidden variables that are independently drawn from the probability distribution R(h).

(ii) Next, link each pair of nodes  $\{i, j\}$  with a probability  $r_{ij}$ .

One can show that the uncorrelated networks with hidden variables arise from the factorized connection probability

$$r_{ij} = \frac{h_i h_j}{\langle h \rangle N},\tag{48}$$

whereas networks with two-point correlations require more sophisticated expressions for  $r_{ii}$ .

Comparing the above short review to our previous results on sparse networks with an expected degree sequence [Eq. (26)] allows one to deduce the equivalence of the two approaches. In the course of the section, we will argue that the claimed equivalence also holds for networks with two-point correlations. We will prove it by recovering the so-called Poissonian propagators characterizing both correlated and uncorrelated sparse networks with hidden variables [9].

## A. Networks with a given degree sequence

At the moment, it is clear that the expected degree of node i is  $\langle k_i \rangle$ , but due to ensemble fluctuations, its actual degree  $k_i$  changes from network to network. Our aim is to find the so-called propagator  $P(k_i | \theta_i)$ , i.e., the degree distribution of the node given that it is characterized by the multiplier  $\theta_i$ .

First, let us reformulate the probability of a graph G in the ensemble

$$P(G) = \frac{e^{-H(G)}}{Z},$$
 (49)

where H(G) and Z are, respectively, the graph Hamiltonian (20) and the partition function (21). Taking advantage of the connection probability  $p_{ij}$  (23), P(G) can be written in a similar form, as in the case of classical random graphs (41),

$$P(G) = \prod_{i < j} \Phi(i, j), \tag{50}$$

where

$$\Phi(i,j) = p_{ij}^{\sigma_{ij}} (1 - p_{ij})^{(1 - \sigma_{ij})},$$
(51)

whereas  $\sigma_{ij}$  are elements of the adjacency matrix describing *G* and they are equal to either 1 or 0 depending on whether *i* and *j* are connected or not.

In the following, without the loss of generality, we will concentrate on node *i*=1. Having *P*(*G*), one can calculate the probability *P*({ $\sigma_{1j}$ }) of the node to have a given linkage profile { $\sigma_{1i}$ } (e.g., {0,0,0,1,0,1,...,0}),

$$P(\{\sigma_{1j}\}) = \sum_{G^*} P(G)$$
$$= \prod_{j} \Phi(1,j) \prod_{2 \le i < j} \sum_{\sigma_{ij}=0}^{1} \Phi(i,j)$$
$$= \prod_{j} \Phi(1,j),$$
(52)

where the first sum runs over all networks  $G^*$  with the fixed sequence  $\{\sigma_{1j}\}$  (i.e., the fixed neighborhood of the node i=1). Now, in order to obtain  $P(k_1|\theta_1)$ , one has to sum the probabilities (52) over different sequences  $\{\sigma_{1j}\}^*$  representing the same degree  $k_1 = \sum_j \sigma_{1j}$ ,

$$P(k_1|\theta_1) = \sum_{\{\sigma_{1j}\}^*} P(\{\sigma_{1j}\}).$$
(53)

Let us also stress that formula (43) describes the variance of the above distribution. In fact, both expressions (43) and (53) certify that fluctuations are intrinsic to the construction scheme based on Lagrange multipliers and it is impossible to avoid them. It means that the considered approach allows one to recover the desired degree distribution only up to fluctuations. In particular, the relation (43) shows that the standard deviation of the propagator  $P(k_1 | \theta_1) = P(k_1 | \langle k_1 \rangle)$ (53) grows slower than  $\sqrt{\langle k_1 \rangle}$ , therefore the fluctuations are significant in sparse networks (with values of connectivity of order 1) and, respectively, they are unimportant in dense networks.

Up to this point, the derivation of  $P(k_1 | \theta_1)$  has been exact. Now, before proceeding with approximations, let us test the formula (53) against the simplest ensemble, i.e., networks with an expected homogeneous degree sequence  $P(k) = \delta(k, \langle k \rangle)$ . In the ensemble, all nodes have the same desired degree  $\langle k \rangle$  and also  $\forall_{i=1}^N \theta_i = \theta$ . It is easy to check that the degree distribution of an arbitrary node (53) is given by

$$P(k|\theta) = \binom{N-1}{k} p^k (1-p)^{N-1-k},$$
(54)

where the binomial factor in the front of the expression arises from the fact that  $\binom{N-1}{k}$  different connection profiles corresponding to degree k and  $p = (e^{2\theta} + 1)^{-1}$  (23) exist [please do not confuse it with Eq. (18), where  $\theta$  has a different meaning]. One should not be surprised with the last result. If it is not obvious, let us stress that the ensemble of networks with an expected homogeneous degree sequence is in fact equivalent to the ensemble of classical random graphs. To become familiar with the statement, compare the formulas (14) and (21).

Now, in order to recover the claim of equivalence between the considered maximum-entropy models and random networks with hidden variables, one has to apply the meanfield approximation to the expression (53),

$$P(k_1|\theta_1) \simeq \binom{N-1}{k_1} \langle p_{1j} \rangle^{k_1} (1 - \langle p_{1j} \rangle)^{(N-1-k_1)}, \quad (55)$$

where  $\langle p_{1j} \rangle = \sum_j p_{1j} / (N-1) = \langle k_1 \rangle / (N-1)$  (24). The assumption of sparse networks enables further simplification of the distribution

$$P(k_1|\theta_1) \simeq \frac{e^{-\langle k_1 \rangle} \langle k_1 \rangle^{k_1}}{k_1!}.$$
(56)

The Poissonian propagator (56) indicates the mentioned equivalence of the considered maximum-entropy networks and the well-known class of uncorrelated random networks with hidden variables [8] (Lagrange multipliers correspond to hidden attributes).

The key point to notice with reference to the last expression is that due to the Poissonian fluctuations in the region of small degrees, *real* connectivity distributions  $\tilde{P}(k)$  observed in single realizations of the considered network may strongly differ from the *desired* degree distribution P(k). In general, the observed degree distributions are given by the expression below [35],

$$\widetilde{P}(k) = \sum_{\langle k \rangle} P(k|\langle k \rangle) P(\langle k \rangle) = \sum_{\langle k \rangle} \frac{e^{-\langle k \rangle} \langle k \rangle^k}{k!} P(\langle k \rangle), \quad (57)$$

where  $P(k|\langle k \rangle) = P(k|\theta)$  (56). Averaging the connectivity distribution  $\tilde{P}(k)$  over many networks also does not reduce the effect of Poisson transformation (57). Only the average over many instances of given nodes will show the desired degree distribution.

#### B. Networks with two-point correlations

One can show that the probability of a graph G in the ensemble (29) can be transformed into the same form (50) as the one for random networks with an expected degree sequence, where the linkage probability is given by Eq. (31). Performing the same calculations as in the case of ensembles analyzed in the previous subsection, one can prove that, in the limit of sparse networks, the degree distribution of a specific node is Poissonian (56),

$$P(k_1|\{\Theta_{1,i}\}) \simeq \frac{e^{-\langle k_1 \rangle} \langle k_1 \rangle^{k_1}}{k_1!},\tag{58}$$

where  $\langle k_1 \rangle = \sum_i p_{1i}$  and  $p_{1i}$  represents the connection probability given by Eq. (31). Again, the last formula supports the claimed equivalence between the analyzed maximumentropy networks with two-point correlations and the class of correlated networks with hidden variables [9].

#### **V. CONCLUSIONS**

In this paper, we have developed the information-theoretic approach to random networks that has been very recently proposed by Park and Newman [18]. We have concentrated on fluctuations over ensembles of undirected networks with a given degree sequence and networks characterized by twopoint correlations. We have studied a few fluctuationdissipation relations characterizing the susceptibilities of different networks to changes in the external fields. In the case of networks with a given degree sequence, we have argued that the scale-free topologies of real networks may arise as a result of the self-organization of real systems into sparse structures with low susceptibility to random external disruptions. Finally, we have revealed that maximum-entropy networks are equivalent to random networks with hidden variables. We have also shown that Poissonian fluctuations can destroy the validity of the construction scheme in sparse networks, based on Lagrange multipliers.

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