

Statistical mechanics of multiplex networks: Entropy and overlap

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There is growing interest in multiplex networks where individual nodes take part in several layers of networks simultaneously. This is the case, for example, in social networks where each individual node has different kinds of social ties or transportation systems where each location is connected to another location by different types of transport. Many of these multiplexes are characterized by a significant overlap of the links in different layers. In this paper we introduce a statistical mechanics framework to describe multiplex ensembles. A multiplex is a system formed by N nodes and M layers of interactions where each node belongs to the M layers at the same time. Each layer α is formed by a network G^α . Here we introduce the concept of correlated multiplex ensembles in which the existence of a link in one layer is correlated with the existence of a link in another layer. This implies that a typical multiplex of the ensemble can have a significant overlap of the links in the different layers. Moreover, we characterize microcanonical and canonical multiplex ensembles satisfying respectively hard and soft constraints and we discuss how to construct multiplexes in these ensembles. Finally, we provide the expression for the entropy of these ensembles that can be useful to address different inference problems involving multiplexes.

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I. INTRODUCTION

Much attention has been paid to single networks [1–4] with breakthroughs revealing the deep relation between topological properties of the networks and their dynamics [5,6]. Nevertheless, many systems are not formed by isolated networks; instead they are formed by a network of networks [7–9]. Examples include multimodal transportation networks [10, 11], climatic systems [12], economic markets [13], energy-supply networks [14], and the human brain [15]. Moreover, many networks are multiplex, indicating the fact that two nodes can belong to different networks at the same time. For example, this is the case of social networks in which agents can be linked at the same time, by familiar relationships, friendship, professional collaboration, colocation, email communication, and so on. The offshoot of the network theory’s fundamental insights is that for us working in statistical mechanics it is now possible (in a sense it is mandatory) to move into the field to shed light on the complexity on interdependent networks and multiplexes. In this context, alternative measures for multiplexes [8,16,17] and models of growing multiplexes [18,19] have been proposed. Moreover, several works have studied dynamical processes taking place on multiplexes and interacting networks and different surprising phenomena have been observed in this context involving percolation [14,20–22], cascades [23], diffusion [24], epidemic spreading [25] cooperation [26], opinion dynamics [27], and community detection [7,28,29].

Yet we are only at the beginning of the research on interacting networks and multiplexes and we need to develop further theoretical frameworks to extract information from multiplex data. For this purpose we need alternative statistical mechanics methods to analyze data on multiplexes and interacting networks.

An important tool to study real networks is to compare them with null models represented by randomized network ensembles. For single networks an equilibrium statistical mechanics framework has been formulated [30–42] in order

to characterize network ensembles. A network ensemble is defined as a set of networks that satisfy a given number of structural constraints, i.e., degree sequence, community structure, etc. Every set of constraints can give rise to a microcanonical network ensemble, satisfying the hard constraints, or to a canonical network ensemble in which the constraints are satisfied on average. This construction is symmetric to the classical ensemble in statistical mechanics where one considers system configurations compatible with either a fixed value of the energy (microcanonical ensembles) or a fixed average of the energy determined by the thermal bath (canonical ensembles). For example, the $G(N, L)$ random graphs formed by networks of N nodes and L links are an example of a microcanonical network ensemble, while the $G(N, p)$ ensembles, where each pair of links is connected with probability p , are an example of a canonical network ensemble since the number of links can fluctuate but has a fixed average given by $\langle L \rangle = pN(N-1)/2$. A theoretical question that arises in the study of network ensembles is whether the microcanonical ensemble and the corresponding canonical ensemble are equivalent in the thermodynamic limit. It turns out [34,35] that when the number of constraints in two conjugated network ensembles is extensive, the ensembles are no longer equivalent in the thermodynamic limit and it is important to characterize their differences. For example, microcanonical and canonical network ensembles with a given degree sequence are nonequivalent in the thermodynamic limit.

The entropy of network ensembles is given by the logarithm of the number of typical networks in the ensemble. The entropy of a network ensemble quantifies the complexity of the ensemble. In particular we have that the smaller the entropy of the ensemble, the smaller the number of networks satisfying the corresponding constraints and implying that these networks are more optimized. Both the network ensembles and their entropy can be used in several inference problems to extract information from a given network [43,44]. Given the relevance

of the statistical mechanics of randomized network ensembles for describing real networks, it is important to extend this successful approach to describe multiplex ensembles. In this paper we have chosen to consider only simple multiplexes, but the results can be easily extended to directed and weighted networks.

In this paper we will show how to treat multiplex ensembles as null models for multiplexes. We will introduce a distinction between uncorrelated multiplex ensembles and correlated multiplex ensembles in which the existence of a link in one layer is correlated to the existence of a link in another layer. We will characterize the overlap between links in two different layers in the case of uncorrelated and correlated multiplex ensembles. We will evaluate the entropy of microcanonical and canonical multiplex ensembles for a large variety of constraints. Finally, this work creates a scenario for building null models of multiplex ensembles that has the promise to be used in a large variety of inference problems. The paper is organized as follows. In Sec. II we introduce multiplexes and the global and local overlap of the links in the two layers. In Sec. III we introduce multiplex ensembles, their entropy, and correlations. In Sec. IV we describe canonical multiplex ensembles and distinguish these ensembles as correlated or uncorrelated. We give relevant examples of these ensembles, calculate their entropy and their overlap, and give algorithms to construct multiplexes in these ensembles. In Sec. V we describe microcanonical multiplex ensembles. We give relevant examples of both correlated and uncorrelated microcanonical multiplex ensembles and calculate their entropy. Finally, in Sec. VI we present a summary.

II. MULTIPLEXES AND OVERLAP BETWEEN TWO LAYERS

Consider a multiplex formed by N labeled nodes $i = 1, 2, \dots, N$ and M layers. We can represent the multiplex as described, for example, in [7]. To this end we indicate by $\vec{G} = (G^1, G^2, \dots, G^M)$ the set of all the networks G^α at layer $\alpha = 1, 2, \dots, M$ forming the multiplex. Each of these networks has an adjacency matrix with matrix elements $a_{ij}^\alpha = 1$ if there is a link between node i and node j in layer $\alpha = 1, 2, \dots, M$ and zero otherwise. Moreover, for a multiplex we can define multilinks and multidegrees in the following way. Let us consider the vector $\vec{m} = (m_1, m_2, \dots, m_\alpha, \dots, m_M)$ in which every element m_α can take only two values $m_\alpha = 0, 1$. We define a multilink \vec{m} , the set of links connecting a given pair of nodes in the different layers of the multiplex and connecting them in the generic layer α only if $m_\alpha = 1$. We can therefore introduce a multiadjacency matrix $A^{\vec{m}}$ with elements $A_{ij}^{\vec{m}}$ equal to 1 if there is a multilink \vec{m} between node i and node j and zero otherwise, i.e., the multiadjacency matrices have elements $A_{ij}^{\vec{m}} = 0, 1$ given by

$$A_{ij}^{\vec{m}} = \prod_{\alpha=1}^M [a_{ij}^\alpha m_\alpha + (1 - a_{ij}^\alpha)(1 - m_\alpha)]. \quad (1)$$

Therefore, we can define the total number of multilinks \vec{m} in a network as the total number of pairs of nodes connected by a multilink \vec{m} . Moreover, we can define the multidegree \vec{m} of a node i , $k_i^{\vec{m}}$, as the total number of multilinks \vec{m} incident to

node i , i.e.,

$$k_i^{\vec{m}} = \sum_{j=1}^N A_{ij}^{\vec{m}}. \quad (2)$$

We note here that the multilink $\vec{m} = \vec{0}$ between two nodes represents the situation in which in all the layers of the multiplex the two nodes are not directly linked. To have a uniform notation we refer also in this case to a multilink. Moreover, we observe that the multiadjacency matrices are not all independent. In fact, they satisfy the normalization condition

$$\sum_{\vec{m}} A_{ij}^{\vec{m}} = 1 \quad (3)$$

for every fixed pair of nodes (i, j) .

For two layers α and α' of the multiplex we can define the global overlap $O^{\alpha, \alpha'}$ as the total number of pair of nodes connected at the same time by a link in layer α and a link in layer α' , i.e.,

$$O^{\alpha, \alpha'} = \sum_{i < j} a_{ij}^\alpha a_{ij}^{\alpha'}. \quad (4)$$

For a node i of the multiplex, we can define the local overlap $o_i^{\alpha, \alpha'}$ of the links in two layers α and α' as the total number of nodes j linked to the node i at the same time by a link in layer α and a link in layer α' , i.e.,

$$o_i^{\alpha, \alpha'} = \sum_{j=1}^N a_{ij}^\alpha a_{ij}^{\alpha'}. \quad (5)$$

We expect the global or the local overlap between two layers to characterize important correlations between the two layers in real-world situations. For example, in a transportation multiplex, where the different layers can represent different kinds of transport such as bus and train connections or private commuting, we expect that the links in the different layers of this multiplex have an overlap that is statistically significant with respect to a null hypothesis of uncorrelation between the different layers. Also, if we consider in social sciences the multiplex formed by different means of communication between people (emails, mobile, sms, etc.), two people that are linked in one layer are also likely to be linked in another layer, forming a multiplex of correlated networks. We note also that for a two-layer multiplex, i.e., $M = 2$, the multilink $k_i^{1,1}$ is equal to the local overlap o_i . Reversibly, the multidegree $k_i^{\vec{m}}$ of a node i in a multiplex with a generic number of layers M can be seen as a higher-order local overlap.

III. MULTIPLEX ENSEMBLES, ENTROPY, AND CORRELATIONS

A multiplex ensemble is specified when the probability $P(\vec{G})$ for each possible multiplex is given. In a multiplex ensemble, if the probability of a multiplex is given by $P(\vec{G})$, the entropy of the multiplex S is defined as

$$S = - \sum_{\vec{G}} P(\vec{G}) \ln P(\vec{G}) \quad (6)$$

and measures the logarithm of the typical number of multiplexes in the ensemble. As it occurs for single networks, we can construct microcanonical or canonical multiplex ensembles according to the equilibrium statistical mechanics approach applied to complex networks. Moreover, two layers in a multiplex network ensemble might be either correlated or uncorrelated. We will say that a multiplex ensemble is uncorrelated if the probability $P(\vec{G})$ of the multiplex is factorizable into the probability of each single network G^α in the layer α . Therefore, in an uncorrelated multiplex ensemble we have

$$P(\vec{G}) = \prod_{\alpha=1}^M P_\alpha(G^\alpha), \quad (7)$$

where $P_\alpha(G^\alpha)$ is the probability of network G^α on layer α . If Eq. (7) does not hold, i.e.,

$$P(\vec{G}) \neq \prod_{\alpha=1}^M P_\alpha(G^\alpha), \quad (8)$$

we will say that the multiplex ensemble is correlated.

Using Eq. (7) we can show that the entropy of any uncorrelated multiplex ensemble is given by

$$S = \sum_{\alpha=1}^M S^\alpha = - \sum_{\alpha=1}^M P_\alpha(G^\alpha) \ln P_\alpha(G^\alpha), \quad (9)$$

where S^α is the entropy of the network ensemble in layer α with probability $P_\alpha(G^\alpha)$. In an uncorrelated multiplex the links in any two layers α and α' are uncorrelated; therefore we have

$$\langle a_{ij}^\alpha a_{ij}^{\alpha'} \rangle = \langle a_{ij}^\alpha \rangle \langle a_{ij}^{\alpha'} \rangle \quad (10)$$

for every choice of pair of nodes i, j . On the contrary, if the multiplex is correlated there will be at least two layers α and α' in a multiplex ensemble and a pair of nodes i and j for which

$$\langle a_{ij}^\alpha a_{ij}^{\alpha'} \rangle \neq \langle a_{ij}^\alpha \rangle \langle a_{ij}^{\alpha'} \rangle. \quad (11)$$

IV. CANONICAL MULTIPLEX ENSEMBLES OR EXPONENTIAL RANDOM MULTIPLEXES

The canonical multiplex ensembles are the set of multiplexes that satisfy a series of constraints on average. The construction of the canonical multiplex ensembles or exponential random multiplex follows closely the derivation of the exponential random graphs.

We can build a canonical multiplex ensemble by maximizing the entropy of the ensemble given by Eq. (6) under the condition that the soft constraints we want to impose are satisfied. We assume to have K of such constraints determined by the conditions

$$\sum_{\vec{G}} P(\vec{G}) F_\mu(\vec{G}) = C_\mu \quad (12)$$

for $\mu = 1, 2, \dots, K$, where $F_\mu(\vec{G})$ determines one of the structural constraints that we want to impose to the network. For example, $F_\mu(\vec{G})$ might characterize the total number of links in a layer of the multiplex \vec{G} or the degree of a node in a layer of the multiplex \vec{G} , etc. In the following we will specify

in detail different major examples for the constraints $F_\mu(\vec{G})$. In order to build the maximal entropy ensemble satisfying the soft constraints defined Eq. (12), we maximize the entropy S given by Eq. (6) under the condition that the ensemble satisfies the K soft constraints given by Eq. (12). Introducing the Lagrangian multipliers λ_μ enforcing the conditions given by Eq. (12) and the Lagrangian multiplier Λ enforcing the normalization of the probabilities $\sum_{\vec{G}} P(\vec{G}) = 1$, we find the expression for the probability $P(\vec{G})$ of a multiplex by solving the system of equations

$$\frac{\partial}{\partial P(\vec{G})} \left[S - \sum_{\mu=1}^K \lambda_\mu \sum_{\vec{G}} F_\mu(\vec{G}) P(\vec{G}) - \Lambda \sum_{\vec{G}} P(\vec{G}) \right] = 0. \quad (13)$$

Therefore, we get that the probability of a multiplex $P_C(\vec{G})$ in a canonical multiplex ensemble is given by

$$P_C(\vec{G}) = \frac{1}{Z_C} \exp \left[- \sum_{\mu} \lambda_\mu F_\mu(\vec{G}) \right], \quad (14)$$

where the normalization constant Z_C is called the partition function of the canonical multiplex ensemble. The values of the Lagrangian multipliers λ_μ are determined by imposing the constraints given by Eq. (12) assuming for the probability $P_C(\vec{G})$ the structural form given by Eq. (14).

In this ensemble, we can relate the entropy S [given by Eq. (6)] to the canonical partition function Z_C getting

$$\begin{aligned} S &= - \sum_{\vec{G}} P_C(\vec{G}) \ln P_C(\vec{G}) \\ &= - \sum_{\vec{G}} P_C(\vec{G}) \left[- \sum_{\mu} \lambda_\mu F_\mu(\vec{G}) - \ln(Z_C) \right] \\ &= \sum_{\mu} \lambda_\mu C_\mu + \ln Z_C. \end{aligned} \quad (15)$$

We call the entropy S of the canonical multiplex ensemble the Shannon entropy of the ensemble.

A. Uncorrelated or correlated canonical multiplex ensembles

For a canonical uncorrelated multiplex ensemble in which each multiplex \vec{G} has probability $P_C(\vec{G})$, we have that Eq. (7) is satisfied, i.e.,

$$P_C(\vec{G}) = \prod_{\alpha=1}^M P_C^\alpha(G^\alpha), \quad (16)$$

where $P_C^\alpha(G^\alpha)$ is the probability of network G^α on layer α . Given the structure of the probability $P_C(\vec{G})$ in the canonical multiplex ensemble given by Eq. (14), in order to have an uncorrelated multiplex the functions $F_\mu(\vec{G})$ should be equal to a linear combination of constraints $f_{\mu,\alpha}(G^\alpha)$ on the networks G^α on a single layer α , i.e.,

$$F_\mu(\vec{G}) = \sum_{\alpha=1}^M f_{\mu,\alpha}(G^\alpha). \quad (17)$$

A special case of this type of constraint is when each constraint depends on a single network G^α in a layer α . In this case typical sets of constraints can be the average total number of links in each layer, the expected degree sequence in each layer, the expected degree sequence and the expected community structure in each layer, etc. Instead, in the case in which the multiplex is correlated, also quantities such as the expected overlap can be fixed. For a multiplex formed by two layers, we can therefore construct multiplex ensembles with an expected total number of links in each layer and expected global overlap between the two layers or with an expected degree sequence and expected local overlap between the two layers, etc.

We can therefore construct a large class of canonical uncorrelated and correlated multiplex ensembles enforcing a different number of constraints. Starting with a minimal number of constraints, when we introduce further constraints in our ensemble we expect that the typical number of multiplexes that satisfy the constraints will decrease and therefore we expect that the entropy of the multiplex ensemble will decrease. Multiplexes in network ensembles with a typical number of realizations are more complex and more optimized. Therefore, the entropy of the multiplex can be used in solving inference problems and is a first-principles measure to quantify the complexity of the ensemble. In the following we give some examples of uncorrelated and correlated canonical multiplex ensembles.

B. Examples of uncorrelated canonical multiplex ensembles

1. Multiplex ensemble with given expected total number of links in each layer

We can fix the average number of links in each layer α to be equal to L^α . In this case we have $K = M$ constraints in the system indicated with a label $\alpha = 1, 2, \dots, M$. These constraints are given by

$$\sum_{\vec{G}} F_\alpha(\vec{G}) P(\vec{G}) = \sum_{\vec{G}} \sum_{i < j} a_{ij}^\alpha P(\vec{G}) = L^\alpha, \quad (18)$$

with $\alpha = 1, 2, \dots, M$. Therefore, the explicit expression for $F_\alpha(\vec{G})$ is given by

$$F_\alpha(\vec{G}) = \sum_{i < j} a_{ij}^\alpha. \quad (19)$$

The probability of the multiplex is given by Eq. (14). Using this expression, we observe that the probability $P_C(\vec{G})$ can be written as

$$P_C(\vec{G}) = \frac{1}{Z_C} \exp \left[- \sum_{\alpha=1}^M \lambda_\alpha \sum_{i < j} a_{ij}^\alpha \right], \quad (20)$$

where Z_C is the canonical partition function and λ_α is the Lagrangian multiplier enforcing the constraint given by Eq. (18). The probability of a link between node i and node j in layer α is given by

$$p_{ij}^\alpha = p^\alpha = \langle a_{ij}^\alpha \rangle = \frac{e^{-\lambda_\alpha}}{1 + e^{-\lambda_\alpha}}. \quad (21)$$

The Lagrangian multipliers are fixed by the condition

$$\sum_{i < j} p_{ij}^\alpha = \frac{N(N-1)}{2} p^\alpha = L^\alpha, \quad (22)$$

i.e., $p^\alpha = 2L^\alpha/[N(N-1)]$ and $e^{-\lambda_\alpha} = \frac{2L^\alpha}{N(N-1)-2L^\alpha}$. Using the definition of the entropy of the multiplex and the expression for $P_C(\vec{G})$ given by Eq. (20) it is easy to show that the entropy of the canonical multiplex ensemble S , which we call Shannon entropy, is given by

$$S = - \frac{N(N-1)}{2} \sum_{\alpha=1}^M [p^\alpha \ln p^\alpha + (1-p^\alpha) \ln(1-p^\alpha)], \quad (23)$$

where $p^\alpha = 2L^\alpha/[N(N-1)]$. If the number of layers M is finite, it can be shown that this expression in the large- N limit is equal to

$$S = \sum_{\alpha=1}^M \ln \left(\frac{N(N-1)}{2L^\alpha} \right).$$

2. Multiplex ensemble with given expected degree sequence in each layer

We can fix the expected degree k_i^α of every node i in each layer α . In this case we have $K = M \times N$ constraints in the system indicated with the labels $\alpha = 1, 2, \dots, M$ and $i = 1, 2, \dots, N$. These constraints are given by

$$\sum_{\vec{G}} F_{i,\alpha}(\vec{G}) P(\vec{G}) = \sum_{\vec{G}} \sum_{j=1, j \neq i}^N a_{ij}^\alpha P(\vec{G}) = k_i^\alpha. \quad (24)$$

Therefore, the explicit expression for $F_{i,\alpha}(\vec{G})$ is given by

$$F_{i,\alpha}(\vec{G}) = \sum_{j=1, j \neq i}^N a_{ij}^\alpha. \quad (25)$$

The probability of the multiplex is given by Eq. (14). Using this expression we observe that the probability $P_C(\vec{G})$ can be written as

$$P_C(\vec{G}) = \frac{1}{Z_C} \exp \left[- \sum_{\alpha=1}^M \sum_{i=1}^N \lambda_{i,\alpha} \sum_{j=1, j \neq i}^N a_{ij}^\alpha \right], \quad (26)$$

where Z_C is the canonical partition function and $\lambda_{i,\alpha}$ is the Lagrangian multiplier enforcing the constraint given by Eq. (24). The probability of a link between node i and node j in layer α is given by

$$p_{ij}^\alpha = \langle a_{ij}^\alpha \rangle = \frac{e^{-\lambda_{i,\alpha} - \lambda_{j,\alpha}}}{1 + e^{-\lambda_{i,\alpha} - \lambda_{j,\alpha}}}, \quad (27)$$

where the Lagrangian multipliers $\lambda_{i,\alpha}$ are fixed by the conditions

$$\sum_{j=1, j \neq i}^N p_{ij}^\alpha = k_i^\alpha. \quad (28)$$

Using the definition of the entropy of the multiplex (6) and the expression for $P_C(\vec{G})$ given by Eq. (26), it is easy to show

that the entropy of the canonical multiplex ensemble S , which we call Shannon entropy, is given by

$$S = - \sum_{\alpha=1}^M \sum_{i < j} [p_{ij}^{\alpha} \ln p_{ij}^{\alpha} + (1 - p_{ij}^{\alpha}) \ln (1 - p_{ij}^{\alpha})]. \quad (29)$$

If $k_i^{\alpha} < \sqrt{\langle k^{\alpha} \rangle N} \forall i = 1, 2, \dots, N$ then each network G^{α} is uncorrelated and therefore $e^{-\lambda_{i,\alpha}} \simeq \frac{k_i^{\alpha}}{\sqrt{\langle k^{\alpha} \rangle N}}$ and $p_{ij}^{\alpha} \simeq \frac{k_i^{\alpha} k_j^{\alpha}}{\langle k^{\alpha} \rangle N}$. In this limit the Shannon entropy S is given by

$$S \simeq \sum_{\alpha=1}^P \left[- \sum_i k_i^{\alpha} \ln \left(\frac{k_i^{\alpha}}{\langle k^{\alpha} \rangle} \right) + \frac{1}{2} \langle k^{\alpha} \rangle N \ln \left(\frac{\langle k^{\alpha} \rangle N}{\langle k^{\alpha} \rangle} \right) + \frac{1}{2} \langle k^{\alpha} \rangle N - \frac{1}{4} \left(\frac{\langle (k^{\alpha})^2 \rangle}{\langle k^{\alpha} \rangle} \right)^2 \right]. \quad (30)$$

3. Multiplex ensemble with given expected number of links present in each layer between nodes in different communities

We can fix the expected number of links present in each layer between nodes belonging to different communities. We assign to each node i a discrete variable $q_i = 1, 2, \dots, Q$ indicating the community of the node. We can consider canonical uncorrelated multiplex ensembles in which we fix the expected number of links $e_{q,q'}^{\alpha}$ between nodes in community q and nodes in community q' in layer α . In this case we have $K = M \times Q(Q+1)/2$ constraints in the system indicated with the labels $\alpha = 1, 2, \dots, M$ and $q, q' = 1, 2, \dots, Q$. These constraints are given by

$$\sum_{\vec{G}} F_{q,q',\alpha}(\vec{G}) P(\vec{G}) = e_{q,q'}^{\alpha}, \quad (31)$$

where the explicit expression for $F_{q,q',\alpha}(\vec{G})$ is given by

$$F_{q,q',\alpha}(G^{\alpha}) = \sum_{i,j} a_{ij}^{\alpha} \delta_{q,q_i} \delta_{q',q_j} \quad \text{for } q \neq q', \quad (32)$$

$$F_{q,q,\alpha}(G^{\alpha}) = \sum_{i < j} a_{ij}^{\alpha} \delta_{q,q_i} \delta_{q,q_j}.$$

The probability of the multiplex is given by Eq. (14). Using this expression, we observe that the probability $P_C(\vec{G})$ can be written as

$$P_C(\vec{G}) = \frac{1}{Z_C} \exp \left[- \sum_{\alpha=1}^M \sum_{q \leq q'} \lambda_{q,q',\alpha} F_{q,q',\alpha}(\vec{G}) \right], \quad (33)$$

where Z_C is the canonical partition function and $\lambda_{q,q',\alpha}$ is the Lagrangian multiplier enforcing the constraint given by Eq. (31). The probability of a link between node i and node j in layer α is given by

$$p_{ij}^{\alpha} = \langle a_{ij}^{\alpha} \rangle = \frac{e^{-\lambda_{q_i,q_j,\alpha}}}{1 + e^{-\lambda_{q_i,q_j,\alpha}}}, \quad (34)$$

where the Lagrangian multipliers are fixed by the conditions

$$\sum_{i,j} p_{ij}^{\alpha} \delta_{q,q_i} \delta_{q',q_j} = e_{q,q'}^{\alpha} \quad \text{for } q \neq q', \quad (35)$$

$$\sum_{i < j} p_{ij}^{\alpha} \delta_{q,q_i} \delta_{q,q_j} = e_{q,q}^{\alpha}.$$

As can be seen by Eq. (34), the probabilities p_{ij}^{α} depend only on q_i, q_j , and α ; therefore, we have $p_{ij}^{\alpha} = p^{\alpha}(q_i, q_j)$ with

$$p^{\alpha}(q, q') = \frac{e_{q,q'}^{\alpha}}{n_q n_{q'}} \quad \text{for } q \neq q', \quad (36)$$

$$p^{\alpha}(q, q) = \frac{e_{q,q}^{\alpha}}{n_q(n_q - 1)/2},$$

where n_q indicates the total number of nodes in community q . Using the definition of the entropy of the multiplex (6) and the expression for $P_C(\vec{G})$ given by Eq. (33), it is easy to show again that the entropy of the canonical multiplex ensemble S , which we call Shannon entropy is given by

$$S = - \sum_{\alpha=1}^M \sum_{i < j} [p_{ij}^{\alpha} \ln p_{ij}^{\alpha} + (1 - p_{ij}^{\alpha}) \ln (1 - p_{ij}^{\alpha})]. \quad (37)$$

If the number of constraints is nonextensive $M \times Q(Q+1)/2 \ll N$, this expression in the large- N limit is given by

$$S = - \sum_{\alpha=1}^M \sum_{q \neq q'} \ln \left(\frac{n_q n_{q'}}{e_{q,q'}^{\alpha}} \right) - \sum_{\alpha=1}^M \sum_q \ln \left(\frac{n_q(n_q-1)}{e_{q,q}^{\alpha}} \right).$$

4. Multiplex ensemble with given expected degree sequence in each layer and given expected number of links present in each layer between nodes in different communities

We assign to each node i the label $q_i = 1, 2, \dots, Q$ indicating the community to which node i belongs. We can consider canonical uncorrelated multiplex ensembles in which we fix the expected degree k_i^{α} of every node i in each layer α together with the expected number of links $e_{q,q'}^{\alpha}$ between nodes in community q and nodes in community q' in layer α . In this case we have $M \times N$ constraints in the system indicated with the labels $\alpha = 1, 2, \dots, M$ and $i = 1, 2, \dots, N$ and other $M \frac{Q(Q+1)}{2}$ constraints indicated with the labels $\alpha = 1, 2, \dots, M$ and $q, q' = 1, 2, \dots, Q$. These constraints are given by

$$\sum_{\vec{G}} F_{i,\alpha}(\vec{G}) P(\vec{G}) = k_i^{\alpha}, \quad (38)$$

$$\sum_{\vec{G}} F_{q,q',\alpha}(\vec{G}) P(\vec{G}) = e_{q,q'}^{\alpha}, \quad (39)$$

where the explicit expressions for $F_{i,\alpha}(\vec{G})$ and $F_{q,q',\alpha}(\vec{G})$ are given by

$$F_{i,\alpha}(\vec{G}) = \sum_{j=1, j \neq i}^N a_{ij}^{\alpha},$$

$$F_{q,q',\alpha}(G^{\alpha}) = \sum_{i,j} a_{ij}^{\alpha} \delta_{q,q_i} \delta_{q',q_j} \quad \text{for } q \neq q', \quad (40)$$

$$F_{q,q,\alpha}(\vec{G}) = \sum_{i < j} a_{ij}^{\alpha} \delta_{q,q_i} \delta_{q,q_j}.$$

The probability of the multiplex is given by Eq. (14). Using this expression we observe that the probability $P_C(\vec{G})$ can be

written as

$$P_C(\vec{G}) = \frac{1}{Z_C} \exp \left[- \sum_{\alpha=1}^M \sum_{i=1}^N \lambda_{i,\alpha} F_{i,\alpha}(\vec{G}) \right] \times \exp \left[- \sum_{\alpha=1}^M \sum_{q \leq q'} \lambda_{q,q',\alpha} F_{q,q',\alpha}(\vec{G}) \right], \quad (41)$$

where Z_C^α is the normalization factor, $\lambda_{i,\alpha}$ is the Lagrangian multiplier enforcing the constraint given by Eq. (38), and $\lambda_{q,q',\alpha}$ is the Lagrangian multiplier enforcing the constraint given by Eq. (39). The probability of a link between node i and node j in layer α is given by

$$p_{ij}^\alpha = \langle a_{ij}^\alpha \rangle = \frac{e^{-\lambda_{i,\alpha} - \lambda_{j,\alpha} - \lambda_{q,q',\alpha}}}{1 + e^{-\lambda_{i,\alpha} - \lambda_{j,\alpha} - \lambda_{q,q',\alpha}}}, \quad (42)$$

where the Lagrangian multipliers are fixed by the conditions

$$\begin{aligned} \sum_{j=1, j \neq i}^N p_{ij}^\alpha &= k_i^\alpha, \\ \sum_{i,j} p_{ij}^\alpha \delta_{q,q_i} \delta_{q',q_j} &= e_{q,q'}^\alpha \quad \text{for } q \neq q', \\ \sum_{i < j} p_{ij}^\alpha \delta_{q,q_i} \delta_{q',q_j} &= e_{q,q'}^\alpha. \end{aligned} \quad (43)$$

Using the definition of the entropy of the multiplex (6) and the expression for $P_C(\vec{G})$ given by Eq. (41), it is easy to show that the Shannon entropy is given by

$$S = - \sum_{\alpha} \sum_{i < j} [p_{ij}^\alpha \ln p_{ij}^\alpha + (1 - p_{ij}^\alpha) \ln (1 - p_{ij}^\alpha)]. \quad (44)$$

C. Properties of the uncorrelated canonical multiplex ensembles under consideration

In all the ensembles taken into consideration in the preceding section the existence of any link is independent of the presence of other links in the multiplex and the probability of a given multiplex \vec{G} is given by

$$P_C(\vec{G}) = \prod_{\alpha=1}^M \prod_{i < j} [p_{ij}^\alpha a_{ij}^\alpha + (1 - p_{ij}^\alpha)(1 - a_{ij}^\alpha)]. \quad (45)$$

Using the definition of the entropy of the multiplex (6) and the expression for $P_C(\vec{G})$ given by Eq. (45), we can show once again that the Shannon entropy is given by for all the cases under consideration in Sec. IV B.

In the considered ensembles we can calculate the average global overlap $\langle O^{\alpha,\alpha'} \rangle$ between two layers α and α' and the average local overlap $\langle o_i^{\alpha,\alpha'} \rangle$ between two layers α and α' where the global overlap $O^{\alpha,\alpha'}$ is defined in Eq. (4) and the local overlap $o_i^{\alpha,\alpha'}$ is defined in Eq. (5). These quantities are given by

$$\langle O^{\alpha,\alpha'} \rangle = \sum_{i < j} p_{ij}^\alpha p_{ij}^{\alpha'}, \quad \langle o_i^{\alpha,\alpha'} \rangle = \sum_{j=1, j \neq i}^N p_{ij}^\alpha p_{ij}^{\alpha'}. \quad (46)$$

For a multiplex ensemble with fixed expected total number of links L^α in each layer α we have $p_{ij}^\alpha = p^\alpha = 2L^\alpha /$

$[N(N-1)]$ and therefore

$$\langle O^{\alpha,\alpha'} \rangle = \frac{2L^\alpha L^{\alpha'}}{N(N-1)}, \quad \langle o_i^{\alpha,\alpha'} \rangle = \frac{4L^\alpha L^{\alpha'}}{N^2(N-1)}. \quad (47)$$

Therefore, if $L^\alpha = \mathcal{O}(N) \forall \alpha = 1, 2, \dots, M$, then the average global overlap is a finite number in the large network limit and the local overlap is vanishing in the large network limit. Therefore, in this case the overlap of links is a totally negligible phenomenon in the multiplex. In fact, the average global overlap $\langle O^{\alpha,\alpha'} \rangle$ is much smaller than the total number of links in layer α , i.e., L^α , or the total number of links in layer α' , i.e., $L^{\alpha'}$. Moreover, the average local overlap $\langle o_i^{\alpha,\alpha'} \rangle$ is much smaller than the expected degree of node i in layer α or in layer α' . For multiplex ensembles with a given expected degree of the nodes in each layer and with $k_i^\alpha < \sqrt{\langle k^\alpha \rangle N}$ we have $p_{ij}^\alpha = \frac{k_i^\alpha k_j^\alpha}{\langle k^\alpha \rangle N}$ and therefore

$$\langle O^{\alpha,\alpha'} \rangle = \frac{1}{2} \left(\frac{\langle k^\alpha k^{\alpha'} \rangle^2}{\langle k^\alpha \rangle \langle k^{\alpha'} \rangle} \right), \quad \langle o_i^{\alpha,\alpha'} \rangle = k_i^\alpha k_i^{\alpha'} \frac{\langle k^\alpha k^{\alpha'} \rangle}{\langle k^\alpha \rangle \langle k^{\alpha'} \rangle N}, \quad (48)$$

where $\langle k^\alpha k^{\alpha'} \rangle = \sum_{i=1}^N k_i^\alpha k_i^{\alpha'} / N$.

If the degrees in the different layers are uncorrelated (i.e., $\langle k^\alpha k^{\alpha'} \rangle = \langle k^\alpha \rangle \langle k^{\alpha'} \rangle$) then the global and local overlaps are given by

$$\begin{aligned} \langle O^{\alpha,\alpha'} \rangle &= \frac{1}{2} (\langle k^\alpha \rangle \langle k^{\alpha'} \rangle) \ll N, \\ \langle o_i^{\alpha,\alpha'} \rangle &= \frac{k_i^\alpha k_i^{\alpha'}}{N} \ll \min(k_i^\alpha, k_i^{\alpha'}). \end{aligned} \quad (49)$$

Therefore, also in this case the overlap is negligible. Degree correlation in between different layers can enhance the overlap, but as long as $\langle k^\alpha k^{\alpha'} \rangle \ll N$ the average global $\langle O^{\alpha,\alpha'} \rangle$ and the local $\langle o_i^{\alpha,\alpha'} \rangle$ overlaps continue to remain negligible with respect to the total number of nodes in the two layers and the degrees of node i in the two layers. Similarly using Eq. (46) it is possible to calculate the expected global overlap and local overlap also in the multiplex ensemble in which we fix the number of links that in the layer connect nodes belonging to different communities and in the multiplex ensemble in which we fix at the same time the average degree of each node in each layer and the average number of links in between nodes of different communities at any given layer. In all the considered multiplex ensembles, if we want to have a given significant overlap we need to consider correlated multiplex ensembles.

D. Construction of a uncorrelated multiplex in an uncorrelated canonical multiplex ensemble under consideration

In all the cases taken into consideration in the previous sections, the probability of a network G^α on layer α is uncorrelated with the other networks in the other layers. In particular, the probability of a multiplex \vec{G} can be written as in Eq. (45).

Therefore, in order to construct a multiplex in the canonical network ensembles it is sufficient to follow the following scheme.

(i) Calculate the probability p_{ij}^α to have a link between nodes i and j in layer α .

(ii) For every pair of nodes i and j put a link in layer α with probability p_{ij}^α . Do this for every layer $\alpha = 1, 2, \dots, M$ independently.

E. Examples of correlated canonical multiplex ensembles

If the probability of a multiplex $P_C(\vec{G})$ does not factorize into the probabilities $P_C^\alpha(G^\alpha)$ of the networks in the different layers α of the multiplex, i.e., if

$$P_C(\vec{G}) \neq \prod_{\alpha=1}^M P_C^\alpha(G^\alpha), \quad (50)$$

the multiplex is correlated. In these ensembles the existence of a link in one layer can be correlated with the existence of a link in another layer. For single networks, when we want to treat ensembles in which the links are correlated we need to make use of a parametrization that takes into account not only single independent links but also a correlated set of links called subgraphs, such as triangles and triples [37,38]. Similarly, if we want to treat correlated multiplexes, it is convenient to consider multilinks. In this way our multiplex is no longer described by M adjacency matrices describing the networks at each multiplex layer, but the network is described by a much larger set of variables corresponding to correlated links, i.e., multilinks, and is fully characterized by 2^M multiadjacency matrices. The simplest case of a correlated multiplex ensemble is an ensemble in which we fix the expected total number of multilinks \vec{m} in the network defined in Sec. II. Starting from this example of a correlated canonical multiplex ensemble, we can generate more refined models in which we fix the expected multidegree sequence $k_i^{\vec{m}}$ defined in Sec. II or the expected number of multilink \vec{m} linking nodes of different communities, etc. In the following we will describe in detail some of the more relevant examples of correlated canonical multiplex ensembles.

1. Multiplex ensemble with given expected total number of multilinks \vec{m}

We can fix the average number $L^{\vec{m}}$ of multilinks \vec{m} with the condition $\sum_{\vec{m}} L^{\vec{m}} = N(N-1)/2$. In this case we have $K = 2^M$ constraints indicated by the label $\vec{m} = (m_1, m_2, \dots, m_\alpha, \dots, m_M)$ with $m_\alpha = 0, 1$. These constraints are given by

$$\sum_{\vec{G}} F_{\vec{m}}(\vec{G}) P_C(\vec{G}) = \sum_{\vec{G}} \sum_{i<j} A_{ij}^{\vec{m}} P_C(\vec{G}) = L^{\vec{m}}, \quad (51)$$

where the multiadjacency matrices of elements $A_{ij}^{\vec{m}}$ are defined in Eq. (1). In this case the functions $F_{\vec{m}}(\vec{G})$ are given by

$$F_{\vec{m}}(\vec{G}) = \sum_{i<j} A_{ij}^{\vec{m}}. \quad (52)$$

The probability $P_C(\vec{G})$ of a multiplex in the ensemble is given by Eq. (14), which reads in this specific case

$$P_C(\vec{G}) = \frac{1}{Z_C} \exp \left[- \sum_{\vec{m}} \lambda_{\vec{m}} \sum_{i<j} A_{ij}^{\vec{m}} \right], \quad (53)$$

where Z_C is the canonical partition function and $\lambda_{\vec{m}}$ is the Lagrangian multiplier enforcing the constraint given by

Eq. (51). The probability $p_{ij}^{\vec{m}}$ of a multilink \vec{m} between node i and node j is given by

$$p_{ij}^{\vec{m}} = p^{\vec{m}} = \langle A_{ij}^{\vec{m}} \rangle = \frac{e^{-\lambda_{\vec{m}}}}{\sum_{\vec{m}} e^{-\lambda_{\vec{m}}}}, \quad (54)$$

with $\sum_{i<j} p_{ij}^{\vec{m}} = L^{\vec{m}}$ and $\sum_{\vec{m}} p_{ij}^{\vec{m}} = 1$, implying

$$p^{\vec{m}} = \frac{L^{\vec{m}}}{N(N-1)/2}. \quad (55)$$

The entropy of the canonical multiplex ensemble S given by Eq. (6) can be calculated using the expression for $P_C(\vec{G})$ [Eq. (53)], obtaining

$$S = - \frac{N(N-1)}{2} \sum_{\vec{m}} (p^{\vec{m}} \ln p^{\vec{m}}), \quad (56)$$

with $p^{\vec{m}}$ is given by Eq. (55). If the number of layers M is finite this entropy S is given by

$$S = \ln \left[\frac{\left(\frac{N(N-1)}{2} \right)!}{\prod_{\vec{m}} (L^{\vec{m}}!)} \right]. \quad (57)$$

2. Multiplex ensemble with given expected multidegree sequence

We can fix the average multidegree $k_i^{\vec{m}}$ of node i with the condition $\sum_{\vec{m}} k_i^{\vec{m}} = N-1$. In this case we have $K = 2^M \times N$ constraints indicated by the label $\vec{m} = (m_1, m_2, \dots, m_\alpha, \dots, m_M)$ with $m_\alpha = 0, 1$ and the label $i = 1, 2, \dots, N$. In particular we have

$$\sum_{\vec{G}} F_{i,\vec{m}}(\vec{G}) P_C(\vec{G}) = \sum_{\vec{G}} \sum_j A_{ij}^{\vec{m}} P_C(\vec{G}) = k_i^{\vec{m}} \quad (58)$$

for all \vec{m} with $m_\alpha = 0, 1$ and all $i = 1, 2, \dots, N$, where the multiadjacency matrices of elements $A_{ij}^{\vec{m}} = 0, 1$ are given by Eq. (1). Therefore, the functions $F_{i,\vec{m}}(\vec{G})$ are given in this case by

$$F_{i,\vec{m}}(\vec{G}) = \sum_{j=1, j \neq i}^N A_{ij}^{\vec{m}}. \quad (59)$$

The probability of the multiplex is given by Eq. (14), which in this case reads

$$P(\vec{G}) = \frac{1}{Z_C} \exp \left[- \sum_{\vec{m}} \sum_{i=1}^N \lambda_{i,\vec{m}} \sum_{j=1}^N A_{ij}^{\vec{m}} \right], \quad (60)$$

where Z_C is the canonical partition function and $\lambda_{i,\vec{m}}$ is the Lagrangian multiplier enforcing the constraint given by Eq. (58). The probability of a multilink \vec{m} between node i and node j is given by

$$p_{ij}^{\vec{m}} = \langle A_{ij}^{\vec{m}} \rangle = \frac{e^{-\lambda_{i,\vec{m}} - \lambda_{j,\vec{m}}}}{\sum_{\vec{m}} e^{-\lambda_{i,\vec{m}} - \lambda_{j,\vec{m}}}}, \quad (61)$$

with the Lagrangian multipliers $\lambda_{i,\vec{m}}$ fixed by the constraints

$$\sum_{\vec{m}} p_{ij}^{\vec{m}} = 1, \quad \sum_{j=1}^N p_{ij}^{\vec{m}} = k_i^{\vec{m}}. \quad (62)$$

The entropy of the canonical multiplex ensemble S , the Shannon entropy, is given by Eq. (6) and can be calculated

using the expression for $P_C(\vec{G})$ [Eq. (60)], obtaining

$$S = - \sum_{\vec{m}} \sum_{i < j} (p_{ij}^{\vec{m}} \ln p_{ij}^{\vec{m}}). \quad (63)$$

If the multiplex is sparse, i.e., $k_i^{\vec{m}} < \sqrt{\langle k^{\vec{m}} \rangle N}$ provided that in the multilink \vec{m} there is at least a link, i.e., $\sum_{\alpha=1}^M m_\alpha > 0$, we have

$$p_{ij}^{\vec{m}} = \frac{k_i^{\vec{m}} k_j^{\vec{m}}}{\langle k^{\vec{m}} \rangle N} \quad (64)$$

for all \vec{m} such that $\sum_{\alpha=1}^M m_\alpha > 0$. In this limit the entropy S is given by

$$S \simeq \sum_{\vec{m} | \sum_{\alpha=1}^M m_\alpha > 0} \left[- \sum_i k_i^{\vec{m}} \ln(k_i^{\vec{m}}) + \frac{1}{2} \langle k^{\vec{m}} \rangle N + \frac{1}{2} \langle k^{\vec{m}} \rangle N \ln(\langle k^{\vec{m}} \rangle N) - \frac{1}{4} \left(\frac{\langle (k^{\vec{m}})^2 \rangle}{\langle k^{\vec{m}} \rangle} \right)^2 \right]. \quad (65)$$

3. Multiplex ensemble with given expected number of multilinks \vec{m} between nodes in different communities

We can fix the expected number of multilinks \vec{m} between nodes in different communities of the multiplex. We assign to each node i a discrete variable $q_i = 1, 2, \dots, Q$ indicating the community of the node.

We can consider canonical uncorrelated multiplex ensembles in which we fix the expected number of multilinks \vec{m} , $e_{q,q'}^{\vec{m}}$, between nodes in community q and nodes in community q' . Moreover, we choose $e_{q,q'}^{\vec{m}}$ such that they satisfy the condition that the sum over the different multilinks \vec{m} of $e_{q,q'}^{\vec{m}}$ is equal to the total number of links in between nodes in community q and nodes in community q' . In this case we have $K = 2^M \times Q(Q+1)/2$ constraints in the system indicated with the label $\vec{m} = (m_1, m_2, \dots, m_M)$ with $m_\alpha = 0, 1$ and the labels $q, q' = 1, 2, \dots, Q$. These constraints are given by

$$\sum_{\vec{G}} F_{q,q',\vec{m}}(\vec{G}) P_C(\vec{G}) = e_{q,q'}^{\vec{m}}, \quad (66)$$

where the explicit expression for $F_{q,q',\vec{m}}(\vec{G})$ is given by

$$F_{q,q',\vec{m}}(\vec{G}) = \sum_{i,j} A_{ij}^{\vec{m}} \delta_{q,q_i} \delta_{q',q_j} \quad \text{for } q \neq q', \quad (67)$$

$$F_{q,q,\vec{m}}(\vec{G}) = \sum_{i < j} A_{ij}^{\vec{m}} \delta_{q,q_i} \delta_{q,q_j},$$

and the multiadjacency matrices of elements $A_{ij}^{\vec{m}}$ are defined in Eq. (1). The probability of the multiplex is given by Eq. (14) and in this specific case is given by

$$P_C(\vec{G}) = \frac{1}{Z_C} \exp \left[- \sum_{\vec{m}} \sum_{q \leq q'} \lambda_{q,q',\vec{m}} F_{q,q',\vec{m}}(\vec{G}) \right], \quad (68)$$

where Z_C is the canonical partition function and $\lambda_{q,q',\vec{m}}$ is the Lagrangian multiplier enforcing the constraint given by Eq. (66). The probability of a multilink \vec{m} between node i and

node j is given by

$$p_{ij}^{\vec{m}} = \langle A_{ij}^{\vec{m}} \rangle = \frac{e^{-\lambda_{q_i,q_j,\vec{m}}}}{\sum_{\vec{m}} e^{-\lambda_{q_i,q_j,\vec{m}}}}, \quad (69)$$

where the Lagrangian multipliers are fixed by the conditions

$$\sum_{\vec{m}} p_{ij}^{\vec{m}} = 1, \quad (70)$$

$$\sum_{i,j} p_{ij}^{\vec{m}} \delta_{q,q_i} \delta_{q',q_j} = e_{q,q'}^{\vec{m}} \quad \text{for } q \neq q',$$

$$\sum_{i < j} p_{ij}^{\vec{m}} \delta_{q,q_i} \delta_{q,q_j} = e_{q,q}^{\vec{m}}.$$

As can be seen by Eq. (69), the probabilities $p_{ij}^{\vec{m}}$ depend only on q_i, q_j , and \vec{m} ; therefore we have $p_{ij}^{\vec{m}} = p^{\vec{m}}(q_i, q_j)$ with

$$p^{\vec{m}}(q, q') = \frac{e_{q,q'}^{\vec{m}}}{n_q n_{q'}} \quad \text{for } q \neq q', \quad (71)$$

$$p^{\vec{m}}(q, q) = \frac{e_{q,q}^{\vec{m}}}{n_q (n_q - 1)/2},$$

where n_q indicates the total number of nodes in community q . The entropy of the canonical multiplex ensemble S is given by Eq. (6). Evaluating this expression using the probability of the multiplex $P_C(\vec{G})$ given by (68) we obtain

$$S = - \sum_{\vec{m}} \sum_{i < j} (p_{ij}^{\vec{m}} \ln p_{ij}^{\vec{m}}). \quad (72)$$

If the number of constraints is nonextensive $2^M Q(Q+1)/2 \ll N$, this expression in the large- N limit is given by

$$S = \sum_{q \neq q'} \ln \left[\frac{(n_q n_{q'})!}{\prod_{\vec{m}} (e_{q,q'}^{\vec{m}})!} \right] + \sum_q \ln \left[\frac{(n_q(n_q-1))!}{\prod_{\vec{m}} (e_{q,q}^{\vec{m}})!} \right]. \quad (73)$$

4. Multiplex ensemble with fixed expected multidegree sequence and expected number of multilinks \vec{m} between nodes in different communities

We assign to each node i the label $q_i = 1, 2, \dots, Q$ indicating the community to which node i belongs. We can consider canonical uncorrelated multiplex ensembles in which we fix the expected multidegree $k_i^{\vec{m}}$ of every node i (with the condition $\sum_{\vec{m}} k_i^{\vec{m}} = N - 1$) together with the expected number of multilinks $e_{q,q'}^{\vec{m}}$ between nodes in community q and nodes in community q' (with the condition that the sum over the different multilinks \vec{m} of $e_{q,q'}^{\vec{m}}$ is equal to the total number of links in between nodes in community q and nodes in community q'). In this case we have $2^M \times N$ constraints indicated with the labels $\vec{m} = (m_1, m_2, \dots, m_M)$ with $m_\alpha = 0, 1$ and $i = 1, 2, \dots, N$ and other $2^M \times \frac{Q(Q+1)}{2}$ constraints indicated with labels \vec{m} and $q, q' = 1, 2, \dots, Q$.

These constraints are given by

$$\sum_{\vec{G}} F_{i,\vec{m}}(\vec{G})P(\vec{G}) = k_i^{\vec{m}}, \quad (74)$$

$$\sum_{\vec{G}} F_{q,q',\vec{m}}P_C(\vec{G}) = e_{q,q'}^{\vec{m}} \quad \text{for } q \neq q', \quad (75)$$

$$\sum_{\vec{G}} F_{q,q,\vec{m}}(\vec{G})P_C(\vec{G}) = e_{q,q}^{\vec{m}}, \quad (76)$$

where the explicit expressions for $F_{i,\vec{m}}(\vec{G})$ and $F_{q,q',\vec{m}}(\vec{G})$ are given by

$$\begin{aligned} F_{i,\vec{m}}(\vec{G}) &= \sum_j A_{ij}^{\vec{m}}, \\ F_{q,q',\vec{m}}(\vec{G}) &= \sum_{i,j} A_{ij}^{\vec{m}} \delta_{q,q_i} \delta_{q',q_j} \quad \text{for } q \neq q', \\ F_{q,q,\vec{m}}(\vec{G}) &= \sum_{i<j} A_{ij}^{\vec{m}} \delta_{q,q_i} \delta_{q,q_j}, \end{aligned} \quad (77)$$

where the element $A_{ij}^{\vec{m}}$ of the multiadjacency matrices is defined in Eq. (1). The probability of the multiplex is given by Eq. (14), which reads in this case

$$\begin{aligned} P_C(\vec{G}) &= \frac{1}{Z_C} \exp \left[- \sum_{\vec{m}} \sum_i \lambda_{i,\vec{m}} F_{i,\vec{m}}(\vec{G}) \right] \\ &\times \exp \left[- \sum_{\vec{m}} \sum_{q \leq q'} \lambda_{q,q',\vec{m}} F_{q,q',\vec{m}}(\vec{G}) \right], \end{aligned} \quad (78)$$

where Z_C is the canonical partition function, $\lambda_{i,\vec{m}}$ is the Lagrangian multiplier enforcing the constraint given by Eq. (74), and $\lambda_{q,q',\vec{m}}$ is the Lagrangian multiplier enforcing the constraint given by Eq. (75) or (76). The probability of a multilink \vec{m} between node i and node j is given by

$$p_{ij}^{\vec{m}} = \langle A_{ij}^{\vec{m}} \rangle = \frac{e^{-\lambda_{i,\vec{m}} - \lambda_{j,\vec{m}} - \lambda_{q,q',\vec{m}}}}{\sum_{\vec{m}} e^{-\lambda_{i,\vec{m}} - \lambda_{j,\vec{m}} - \lambda_{q,q',\vec{m}}}}, \quad (79)$$

where the Lagrangian multipliers are fixed by the conditions

$$\begin{aligned} \sum_{\vec{m}} p_{ij}^{\vec{m}} &= 1, \\ \sum_j p_{ij}^{\vec{m}} &= k_i^{\vec{m}}, \\ \sum_{i,j} p_{ij}^{\vec{m}} \delta_{q,q_i} \delta_{q',q_j} &= e_{q,q'}^{\vec{m}} \quad \text{for } q \neq q', \\ \sum_{i<j} p_{ij}^{\vec{m}} \delta_{q,q_i} \delta_{q,q_j} &= e_{q,q}^{\vec{m}}. \end{aligned} \quad (80)$$

The entropy of the canonical multiplex ensemble that we call Shannon entropy is given by

$$S = - \sum_{\vec{m}} \sum_{i<j} (p_{ij}^{\vec{m}} \ln p_{ij}^{\vec{m}}), \quad (81)$$

where the probabilities $p_{ij}^{\vec{m}}$ are given by Eq. (79) and satisfy Eqs. (80).

F. Overlap in correlated canonical ensembles under consideration

In all the cases taken into consideration in the preceding section, the probability of a network G^α on layer α is correlated with the other networks in the other layers. Therefore, the probability $P_C(\vec{G})$ cannot be factorized in the probability for single layers. Nevertheless, $P_C(\vec{G})$ takes a simple form in the cases that we have investigated so far, i.e.,

$$P_C(\vec{G}) = \prod_{i<j} \left[\prod_{\vec{m}} p_{ij}^{\vec{m}} A_{ij}^{\vec{m}} \right], \quad (82)$$

where $\vec{m} = (m_1, m_2, \dots, m_M)$ is a vector of elements $m_\alpha = 0, 1$ and $A_{ij}^{\vec{m}}$ are the multiadjacency matrices defined in Eq. (1). In these ensembles the Shannon entropy S given by Eq. (6) takes the simple form

$$S = - \sum_{i<j} \sum_{\vec{m}} p_{ij}^{\vec{m}} \ln p_{ij}^{\vec{m}}. \quad (83)$$

In the considered ensembles we can calculate the average total overlap $\langle O^{\alpha,\alpha'} \rangle$ between two layers α and α' and the average local overlap $\langle o_i^{\alpha,\alpha'} \rangle$ between two layers α and α' , where the global overlap $O^{\alpha,\alpha'}$ is defined in Eq. (4) and the local overlap $o_i^{\alpha,\alpha'}$ is defined in Eq. (5). These quantities are given by

$$\begin{aligned} \langle O^{\alpha,\alpha'} \rangle &= \sum_{\vec{m}|m_\alpha=1, m_{\alpha'}=1} \sum_{i<j} p_{ij}^{\vec{m}}, \\ \langle o_i^{\alpha,\alpha'} \rangle &= \sum_{\vec{m}|m_\alpha=1, m_{\alpha'}=1} \sum_{j=1}^N p_{ij}^{\vec{m}}. \end{aligned} \quad (84)$$

These quantities now can be significant also for sparse networks, as we will see in the next section in the simple case of a multiplex with just two layers, i.e., $M = 2$.

G. Case of a two-layer multiplex, i.e., $M = 2$

Let us consider the simple case of a correlated multiplex ensemble formed by $M = 2$ layers: network 1 and network 2. The probability $P_C(\vec{G})$ of a multiplex in all the cases taken into consideration in Sec. IV E is given by Eq. (82), which reads in this case

$$\begin{aligned} P(\vec{G}) &= \prod_{i<j} [p_{ij}^{00} (1 - a_{ij}^1)(1 - a_{ij}^2) + p_{ij}^{10} a_{ij}^1 (1 - a_{ij}^2) \\ &+ p_{ij}^{01} (1 - a_{ij}^1) a_{ij}^2 + p_{ij}^{11} a_{ij}^1 a_{ij}^2], \end{aligned} \quad (85)$$

where $p_{ij}^{n_1 n_2}$ is the probability to have $n_1 = 0, 1$ links between node i and node j in network 1 and $n_2 = 0, 1$ links between the same nodes in network 2. The probabilities $p_{ij}^{n_1 n_2}$ satisfy the constrain $p_{ij}^{00} + p_{ij}^{01} + p_{ij}^{10} + p_{ij}^{11} = 1$. The entropy of such a multiplex is then given by Eq. (83), which reads in this case

$$S = - \sum_{n_1, n_2} \sum_{i<j} p_{ij}^{n_1 n_2} \ln p_{ij}^{n_1 n_2}. \quad (86)$$

In the considered ensembles we can calculate the average total overlap $\langle O^{1,2} \rangle = \langle O \rangle$ between two layers 1 and 2 and the average local overlap $\langle o_i^{1,2} \rangle = \langle o_i \rangle$ defined in Eqs. (84). For

the ensembles in which we fix the expected total number of multilinks \bar{m} , $L^{\bar{m}}$, considered in Sec. IV E1 we have

$$\langle O \rangle = L^{11}, \quad \langle o_i \rangle = \frac{2L^{11}}{N-1}. \quad (87)$$

Assuming $L^{11}, L^{10}, L^{01} \propto N$, Eq. (87) implies that the fraction of links that overlap is not negligible (globally and locally) also if both network 1 and network 2 are sparse. For the ensemble in which we fix the expected multidegree (considered in Sec. IV E2), considering the additional condition $k_i^{\bar{m}} < \sqrt{\langle k^{\bar{m}} \rangle N}$ for all multilinks \bar{m} formed at least by a link, i.e., $\sum_{\alpha=1}^M m_\alpha > 0$, we have $p_{ij}^{\bar{m}} = \frac{k_i^{\bar{m}} k_j^{\bar{m}}}{\langle k^{\bar{m}} \rangle N}$ and therefore

$$\langle O \rangle = \frac{1}{2} \langle k^{11} \rangle N, \quad \langle o_i \rangle = k_i^{11}. \quad (88)$$

Provided $\langle k^{11} \rangle$ is finite, we find that also in this case the global and local overlaps can be significant also if both network 1 and network 2 are sparse. A similar conclusion can be drawn for the other two cases of correlated multiplex ensembles taken into consideration in the previous paragraphs.

H. Construction of correlated multiplex in the canonical multiplex ensemble

Since in the considered cases of correlated multiplex ensembles the probability of a multiplex can be expressed as in Eq. (82), in order to construct a correlated multiplex in the canonical network ensembles it is sufficient to follow the following scheme.

(i) Calculate the probability $p_{ij}^{\bar{m}}$ to have a multilink \bar{m} between node i and j .

(ii) For every pair of node i and j , draw a multilink \bar{m} with probability $p_{ij}^{\bar{m}}$ and consequently put a link in every layer α where $m_\alpha = 1$ and put no link in every layer α where $m_\alpha = 0$.

V. MICROCANONICAL MULTIPLEX ENSEMBLES

The microcanonical multiplex ensembles are formed by the multiplexes that satisfy some hard constraints. Every multiplex in a microcanonical multiplex ensemble has equal probability. We note here that we consider only graphical constraints [45], i.e., constraints that can be satisfied at least by one realization of the multiplex. This is a condition that, for example, is automatically satisfied if we consider network ensembles that are a randomization of a real multiplex with some given structural features. Therefore, the probability $P_M(\vec{G})$ of a microcanonical multiplex ensemble is given by

$$P_M(\vec{G}) = \frac{1}{Z_M} \prod_{\mu=1}^K \delta(F_\mu(\vec{G}), C_\mu), \quad (89)$$

where $\delta(\cdot)$ is the Kronecker delta function and Z_M is the microcanonical partition function of the multiplex given by

$$Z_M = \sum_{\vec{G}} \prod_{\mu=1}^K \delta(F_\mu(\vec{G}), C_\mu). \quad (90)$$

Therefore, the microcanonical partition function Z_M of the multiplex ensemble counts the number of multiplexes satisfying the hard constraints $F_\mu(\vec{G}) = C_\mu$ for $\mu = 1, 2, \dots, K$. We

call the entropy of these multiplex ensembles $N\Sigma$ and using the definition of the entropy of an ensemble given by Eq. (9) together with the expression for the probability of a multiplex in the microcanonical ensemble given by Eq. (89) we have

$$N\Sigma = - \sum_{\vec{G}} P_M(\vec{G}) \ln P_M(\vec{G}) = \ln Z_M, \quad (91)$$

where we call Σ the Gibbs entropy of the multiplex ensemble. The Gibbs entropy Σ of microcanonical multiplex ensembles is related to the Shannon entropy S of the associated canonical multiplex ensemble S , which enforces the same constraint of the microcanonical network ensemble on average (the conjugated canonical ensemble), by a simple relation. In fact, we have

$$N\Sigma = S - N\Omega, \quad (92)$$

where $N\Omega$ is equal to the logarithm of the probability that in the conjugated canonical multiplex ensemble the hard constraints $F_\mu(\vec{G})$ are satisfied, i.e.,

$$N\Omega = - \ln \left\{ \sum_{\vec{G}} P_C(\vec{G}) \prod_{\mu=1}^K \delta(F_\mu(\vec{G}), C_\mu) \right\}. \quad (93)$$

In order to verify the relation (92) we observe that the canonical multiplex probability $P_C(\vec{G})$ is given by Eq. (14), which we rewrite here for convenience as

$$P_C(\vec{G}) = \frac{1}{Z_C} \exp \left(- \sum_{\mu=1}^K \lambda_\mu F_\mu(\vec{G}) \right), \quad (94)$$

and therefore, using Eq. (93), we get

$$\begin{aligned} & \exp(-N\Omega) \\ &= \sum_{\vec{G}} \frac{1}{Z_C} \exp \left(- \sum_{\mu=1}^K \lambda_\mu F_\mu(\vec{G}) \right) \prod_{\mu=1}^K \delta(F_\mu(\vec{G}), C_\mu) \\ &= \frac{1}{Z_C} \exp \left(- \sum_{\mu=1}^K \lambda_\mu C_\mu \right) \sum_{\vec{G}} \prod_{\mu=1}^K \delta(F_\mu(\vec{G}), C_\mu) \\ &= \frac{Z_M}{e^S} = \exp(N\Sigma - S), \end{aligned} \quad (95)$$

where in the last relation we have used Eqs. (15), (90), and (91). Given Eq. (92), if Ω is larger than zero in the limit $N \gg 1$, the microcanonical and the conjugated canonical multiplex ensembles are not equivalent.

A. Uncorrelated microcanonical multiplex ensembles

In an uncorrelated multiplex ensemble we have that the probability of a multiplex \vec{G} is factorizable into the product of probabilities $P_\alpha(G^\alpha)$ of the networks G^α in layer α , i.e.,

$$P_M(\vec{G}) = \prod_{\alpha=1}^M P_M^\alpha(G^\alpha). \quad (96)$$

Given the general expression for $P_M(\vec{G})$ provided by Eq. (89), we can conclude that a microcanonical multiplex ensemble is uncorrelated only if the hard constraints $F_\mu(\vec{G}) = C_\mu$ with $\mu = 1, 2, \dots, K$ involve for every constraint μ only one

network G^α in one layer α of the multiplex. Therefore, we will indicate the function $F_{\mu}(\vec{G})$ with a label indicating the layer α and one label ν counting the number of constraints in each layer, i.e., $F_{\nu,\alpha}(G^\alpha)$.

Given the condition Eq. (96), the Gibbs entropy Σ of the multiplex can be expressed as

$$N\Sigma = - \sum_{\vec{G}} P_M(\vec{G}) \ln P_M(\vec{G}) = \sum_{\alpha} N\Sigma^\alpha, \quad (97)$$

where Σ^α is the Gibbs entropy of the network ensemble induced in layer α ,

$$N\Sigma^\alpha = - \sum_{G^\alpha} P_M^\alpha(G^\alpha) \ln P_M^\alpha(G^\alpha) \quad (98)$$

with $P_M^\alpha(G^\alpha) = \prod_{\nu} \delta(F_{\nu,\alpha}(G^\alpha), C_{\nu,\alpha}) / Z_M^\alpha$, and

$$Z_M^\alpha = \sum_{G^\alpha} \prod_{\nu} \delta(F_{\nu,\alpha}(G^\alpha), C_{\nu,\alpha}). \quad (99)$$

Using the same arguments used to derive Eq. (92), it is straightforward to show that the Gibbs entropy Σ^α of each network ensemble at layer α is given by

$$N\Sigma^\alpha = S^\alpha - N\Omega^\alpha, \quad (100)$$

where S^α is the Shannon entropy of the canonical network ensemble, which enforces the same constraint of the microcanonical network ensemble on average, i.e.,

$$S^\alpha = - \sum_{G^\alpha} P_C^\alpha(G^\alpha) \ln P_C^\alpha(G^\alpha), \quad (101)$$

where $P_C^\alpha(G^\alpha)$ is the probability for a network G^α in layer α . Moreover, Ω^α in Eq. (100) satisfies

$$N\Omega^\alpha = - \ln \left\{ \sum_{G^\alpha} P_C^\alpha(G^\alpha) \prod_{\nu} \delta(F_{\nu,\alpha}(G^\alpha), C_{\nu,\alpha}) \right\}. \quad (102)$$

Examples of uncorrelated microcanonical multiplex ensembles are given by ensembles in which we fix the total number of links at each layer, the degree sequence at each layer, the number of links between nodes in different communities in each layer, etc. In the following section we present in detail several examples of uncorrelated microcanonical multiplex ensembles.

B. Examples of uncorrelated microcanonical multiplex ensembles

1. Multiplex ensemble with given total number of links in each layer

We can fix the total number of links L^α in each layer α of the multiplex. In this case we have $K = M$ constraints in the system indicated with the label $\alpha = 1, 2, \dots, M$. These constraints are given by

$$F_\alpha(\vec{G}) = L^\alpha \quad (103)$$

with $\alpha = 1, 2, \dots, M$ and $F_\alpha(\vec{G})$ given by

$$F_\alpha(\vec{G}) = \sum_{i < j} a_{ij}^\alpha. \quad (104)$$

The microcanonical partition function Z_M is equal to the number of multiplexes in these ensemble, which is given by

the product over the layers $\alpha = 1, 2, \dots, M$ of the number of networks G^α satisfying the constraints $F_\alpha(\vec{G}) = L^\alpha$. The number of networks G^α with L^α links is given by the number of ways of choosing L^α links out of $N(N-1)/2$ possible links; we have therefore

$$Z_M = \prod_{\alpha=1}^M \binom{N}{L^\alpha}. \quad (105)$$

Using Eq. (91) we find that the Gibbs entropy for this ensemble is given by

$$N\Sigma = \ln \left(\binom{N}{L^\alpha} \right). \quad (106)$$

As long as the number of constraints M is sublinear with respect to N we have that the microcanonical and canonical ensembles studied in Sec. IV B1 are equivalent in the thermodynamic limit and $\Sigma \simeq S/N$.

2. Multiplex ensemble with given degree sequence in each layer

We can fix the degree k_i^α of every node i in each layer α . In this case we have $K = M \times N$ constraints in the system indicated with the labels $\alpha = 1, 2, \dots, M$ and $i = 1, 2, \dots, N$. These constraints are given by

$$F_{i,\alpha}(\vec{G}) = k_i^\alpha, \quad (107)$$

with $F_{i,\alpha}(\vec{G})$ given by

$$F_{i,\alpha}(\vec{G}) = \sum_{j=1, j \neq i}^N a_{ij}^\alpha. \quad (108)$$

For this ensemble we can use the results of [33,35], getting

$$N\Sigma = S - N\Omega, \quad (109)$$

with S given by Eq. (29) and $N\Omega$ for sparse networks given by

$$N\Omega = - \sum_{\alpha=1}^M \sum_{i=1}^N \ln \pi_{k_i^\alpha}(k_i^\alpha), \quad (110)$$

where $\pi_y(x)$ is the Poisson distribution with the average y , $\pi_y(x) = 1/x! y^x \exp(-y)$. In this case, if the number of layers M is finite, then in the large network limit $N \gg 1$, Ω is finite and we have $\Sigma = S/N - \Omega$. Therefore, the Gibbs entropy Σ is lower than S/N and the microcanonical ensemble is not equivalent in the thermodynamic limit $N \gg 1$ to the conjugated canonical ensemble. In the case in which $k_i^\alpha < \sqrt{\langle k^\alpha \rangle N}$ we can use for S the expression in Eq. (30). Therefore, the Gibbs entropy Σ can be approximated by

$$N\Sigma = \sum_{\alpha=1}^M \ln \left\{ \frac{(\langle k^\alpha \rangle N)!!}{\prod_{i=1}^N k_i^\alpha!} \exp \left[-\frac{1}{4} \left(\frac{\langle (k^\alpha)^2 \rangle}{\langle k^\alpha \rangle} \right)^2 \right] \right\}. \quad (111)$$

This last expression is a generalization of the Bender formula [34,46] for the entropy of networks with a given degree sequence.

3. Multiplex ensemble with given number of links in each layer between nodes of different communities

We can fix the total number of links between nodes of different communities in each layer α . We assign to each node i a discrete variable $q_i = 1, 2, \dots, Q$ indicating the community of the node. We consider a microcanonical uncorrelated multiplex ensemble in which we fix the total number of links $e_{q,q'}^\alpha$ between nodes in community q and nodes in community q' in layer α . In this case we have $K = M \times Q(Q+1)/2$ constraints in the system indicated with the labels $\alpha = 1, 2, \dots, M$ and $q, q' = 1, 2, \dots, Q$. These constraints are given by

$$F_{q,q',\alpha}(\vec{G}) = e_{q,q'}^\alpha, \quad (112)$$

where the explicit expression for $F_{q,q',\alpha}(\vec{G})$ is given by

$$F_{q,q',\alpha}(\vec{G}) = \sum_{i,j} a_{ij}^\alpha \delta_{q,q_i} \delta_{q',q_j} \quad \text{for } q \neq q',$$

$$F_{q,q,\alpha}(\vec{G}) = \sum_{i<j} a_{ij}^\alpha \delta_{q,q_i} \delta_{q,q_j}. \quad (113)$$

The microcanonical partition function Z_M is equal to the number of multiplexes in this ensemble, which is given by the product over the layers $\alpha = 1, 2, \dots, M$ of the number of networks G^α satisfying the constraints $F_{q,q',\alpha}(\vec{G}) = e_{q,q'}^\alpha$. The number of networks G^α with $e_{q,q'}^\alpha$ links is given by the number of ways of choosing $e_{q,q'}^\alpha$ links out of the total number of possible links between nodes in community q and community q' ; we have therefore

$$Z_M = \prod_{\alpha=1}^M \left[\prod_{q<q'} \binom{n_q n_{q'}}{e_{q,q'}^\alpha} \prod_q \binom{n_q(n_q-1)/2}{e_{q,q}^\alpha} \right], \quad (114)$$

where n_q indicates the number of nodes in community q . Finally, the Gibbs entropy Σ for this ensemble is given by Eq. (90) and therefore we obtain

$$N\Sigma = \sum_{\alpha=1}^M \ln \left[\prod_{q<q'} \binom{n_q n_{q'}}{e_{q,q'}^\alpha} \prod_q \binom{n_q(n_q-1)/2}{e_{q,q}^\alpha} \right]. \quad (115)$$

In this case the Gibbs entropy $\Sigma = S/N$ in the limit $N \gg 1$ only if the number of constraints K is sublinear with respect to N .

4. Multiplex ensemble with given degree sequence in each layer and given number of links in between nodes in different communities in each layer

We assign to each node i the label $q_i = 1, 2, \dots, Q$ indicating the community to which node i belongs. We can consider microcanonical uncorrelated multiplex ensembles in which we fix the degree k_i^α of every node i in every layer α together with the total number of links $e_{q,q'}^\alpha$ between nodes in community q and nodes in community q' in layer α . In this case we have $M \times N$ constraints in the system indicated with the labels $\alpha = 1, 2, \dots, M$ and $i = 1, 2, \dots, N$ and other $M \frac{Q(Q+1)}{2}$ constraints indicated with the labels $\alpha = 1, 2, \dots, M$ and $q, q' = 1, 2, \dots, Q$. These constraints are given by

$$F_{i,\alpha}(\vec{G}) = k_i^\alpha, \quad F_{q,q',\alpha}(\vec{G}) = e_{q,q'}^\alpha, \quad (116)$$

where the explicit expressions for $F_{i,\alpha}(\vec{G})$ and $F_{q,q',\alpha}(\vec{G})$ are given by

$$F_{i,\alpha}(\vec{G}) = \sum_{j=1, j \neq i}^N a_{ij}^\alpha,$$

$$F_{q,q',\alpha}(G^\alpha) = \sum_{i,j} a_{ij}^\alpha \delta_{q,q_i} \delta_{q',q_j} \quad \text{for } q \neq q', \quad (117)$$

$$F_{q,q,\alpha}(\vec{G}) = \sum_{i<j} a_{ij}^\alpha \delta_{q,q_i} \delta_{q,q_j}.$$

The Gibbs entropy for this ensemble satisfies

$$N\Sigma = S - \sum_{\alpha} N\Omega^\alpha, \quad (118)$$

where S is given by Eq. (44), and using the results of [35] the entropy of large variations Ω^α for sparse networks is given by

$$N\Omega^\alpha = - \sum_{i=1}^N \ln [\pi_{k_i^\alpha}(k_i^\alpha)] - \sum_{q \leq q'} \ln [\pi_{e_{q,q'}^\alpha}(e_{q,q'}^\alpha)], \quad (119)$$

where $\pi_y(x)$ is the Poisson distribution with average y given by $\pi_y(x) = \frac{1}{x!} y^x \exp(-y)$. In this case, if the number of layers M is finite, then in the large network limit $N \gg 1$, Ω is finite and we have $\Sigma = S/N - \Omega$. Therefore, the Gibbs entropy Σ is lower than S/N and the microcanonical ensemble is not equivalent in the thermodynamic limit to the conjugated canonical ensemble.

5. Multiplex with given degree-degree correlations in each layer α

We can construct a microcanonical uncorrelated multiplex ensemble with given degree-degree correlations in each layer α by fixing the degree k_i^α of each node i in layer α and the total number of links $e_{k,k'}^\alpha$ between nodes of degree k and degree k' in layer α . This case is a small modification of the previous case in which for every different layer we identify a community of nodes at a given layer α as the set of nodes with given degree, i.e., $q_i = k_i^\alpha$. The Gibbs entropy Σ satisfies

$$N\Sigma = \sum_{\alpha=1}^M S^\alpha - \sum_{\alpha=1}^M N\Omega^\alpha. \quad (120)$$

Using the results of [35] the entropy of large variations Ω^α for sparse networks is given by

$$N\Omega^\alpha = - \sum_{i=1}^N \ln [\pi_{k_i^\alpha}(k_i^\alpha)] - \sum_{k \leq k'} \ln [\pi_{e_{k,k'}^\alpha}(e_{k,k'}^\alpha)]. \quad (121)$$

Moreover, the Shannon entropy S^α for each layer α is given by

$$S^\alpha = - \sum_{i<j} p_{ij}^\alpha \ln p_{ij}^\alpha - \sum_{i<j} (1 - p_{ij}^\alpha) \ln (1 - p_{ij}^\alpha), \quad (122)$$

with

$$p_{ij}^\alpha = \frac{e^{-\lambda_{i,\alpha} - \lambda_{j,\alpha} - \lambda_{k,k',\alpha}}}{1 + e^{-\lambda_{i,\alpha} - \lambda_{j,\alpha} - \lambda_{k,k',\alpha}}} \quad (123)$$

and the Lagrangian multipliers $\lambda_{i,\alpha}$ and $\lambda_{k,k',\alpha}$ fixed by the conditions

$$\begin{aligned} \sum_{j=1, j \neq i}^N p_{ij}^\alpha &= k_i^\alpha, \\ \sum_{i,j} p_{ij}^\alpha \delta_{k_i^\alpha, k} \delta_{k_j^\alpha, k'} &= e_{k,k'}^\alpha \quad \text{for } k \neq k', \\ \sum_{i < j} p_{ij}^\alpha \delta_{k_i^\alpha, k} \delta_{k_j^\alpha, k} &= e_{k,k}^\alpha. \end{aligned} \quad (124)$$

C. Correlated microcanonical multiplex ensembles

In a correlated multiplex ensemble we have that the probability of a multiplex \vec{G} is not factorizable into the product of probabilities $P_\alpha(G^\alpha)$ of the networks G^α in layer α , i.e.,

$$P_M(\vec{G}) \neq \prod_{\alpha=1}^M P_M^\alpha(G^\alpha). \quad (125)$$

The simplest example of a correlated multiplex ensemble is the ensemble in which we fix the total number of multilinks \vec{m} in the multiplex. Starting from this model, different more refined multiplex ensemble can be determined, fixing, for example, the multidegree sequence or the total number of multilinks \vec{m} in between nodes of different communities, etc. In Sec. VD we discuss in detail some relevant examples of correlated multiplex ensembles.

D. Examples of correlated microcanonical ensembles

1. Multiplex ensemble with given total number of multilinks \vec{m}

In a correlated multiplex ensemble we can fix the total number $L^{\vec{m}}$ of multilinks \vec{m} in the multiplex, i.e.,

$$F_{\vec{m}}(\vec{G}) = L^{\vec{m}} \quad (126)$$

for all $\vec{m} = (m_1, m_2, \dots, m_\alpha, \dots, m_M)$ with $m_\alpha = 0, 1$ as long as $\sum_{\vec{m}} L^{\vec{m}} = N(N-1)/2$. In this case the functions $F_{\vec{m}}(\vec{G})$ are given by

$$F_{\vec{m}}(\vec{G}) = \sum_{i < j} A_{ij}^{\vec{m}}, \quad (127)$$

where the multiadjacency matrices of elements $A_{ij}^{\vec{m}}$ are defined as in Eq. (1). Since any pair of nodes is linked by one multilink \vec{m} , we have that the total number of multiplexes Z_M in this ensemble is given by the multinomial

$$Z_M = \frac{\binom{N}{2}!}{\prod_{\vec{m}} L^{\vec{m}}!}. \quad (128)$$

Using this result, we can easily derive the Gibbs entropy $N\Sigma = \ln(Z_M)$, i.e.,

$$N\Sigma = \ln \left[\frac{\binom{N}{2}!}{\prod_{\vec{m}} L^{\vec{m}}!} \right]. \quad (129)$$

As long as the number of constraints $K = 2^M$ is sublinear with respect to N we have that the microcanonical and the conjugated canonical ensemble are equivalent in the thermodynamic limit $N \gg 1$ and $\Sigma \simeq S/N$.

2. Multiplex ensemble with given multidegree sequence

In a correlated multiplex ensemble we can fix the multidegree $k_i^{\vec{m}}$ of node i ,

$$F_{i,\vec{m}}(\vec{G}) = k_i^{\vec{m}} \quad (130)$$

for all \vec{m} with $m_\alpha = 0, 1$ and all $i = 1, 2, \dots, N$ as long as $\sum_{\vec{m}} k_i^{\vec{m}} = N-1$ and the constraints are graphical. In this case we have that $F_{i,\vec{m}}(\vec{G})$ is given by

$$F_{i,\vec{m}}(\vec{G}) = \sum_{j=1, j \neq i}^N A_{ij}^{\vec{m}}, \quad (131)$$

where the multiadjacency matrices of elements $A_{ij}^{\vec{m}} = 0, 1$ are given by Eq. (1). The Gibbs entropy Σ of this ensemble satisfies Eq. (100), which we rewrite here for convenience as

$$N\Sigma = S - N\Omega, \quad (132)$$

with S given by Eq. (63). Using a similar derivation as the one reported in [33,35], it is possible to prove that for sparse networks Ω is given by

$$N\Omega = - \sum_{\vec{m} | \sum_{\alpha=1}^M m_\alpha > 0} \sum_{i=1}^N \ln \pi_{k_i^{\vec{m}}}(k_i^{\vec{m}}), \quad (133)$$

where $\pi_y(x)$ is the Poisson distribution with average y , $\pi_y(x) = \frac{1}{x!} y^x \exp(-y)$, calculated at x . In this case, if the number of layers M is finite, then in the large network limit $N \gg 1$, Ω is finite and we have $\Sigma = S/N - \Omega$. Therefore, the Gibbs entropy Σ is lower than S/N and the microcanonical ensemble is not equivalent in the thermodynamic limit to the conjugated canonical ensemble. For networks with $k_i^{\vec{m}} < \sqrt{\langle k^{\vec{m}} \rangle N}$ where \vec{m} satisfies the inequality $\sum_{\alpha=1}^M m_\alpha > 0$, using Eq. (65) we can find a simple expression for the Gibbs entropy extending Bender result [34,46] to a correlated multiplex, i.e.,

$$N\Sigma = \ln \left\{ \prod_{\vec{m}} \frac{(2L^{\vec{m}})!}{\prod_{i=1}^N k_i^{\vec{m}}!} \exp \left[-\frac{1}{4} \left(\frac{\langle (k^{\vec{m}})^2 \rangle}{\langle k^{\vec{m}} \rangle} \right)^2 \right] \right\}. \quad (134)$$

3. Multiplex ensemble with given number of multilinks \vec{m} in between nodes of different communities

We assign to each node i the label $q_i = 1, 2, \dots, Q$ indicating the community to which node i belongs. We consider a microcanonical correlated multiplex ensemble in which we fix the total number of multilinks \vec{m} , $e_{q,q'}^{\vec{m}}$, between nodes in community q and nodes in community q' with the condition that the constraint is graphical. In this case we have $2^M \times \frac{Q(Q+1)}{2}$ constraints indicated with labels $\vec{m} = (m_1, m_2, \dots, m_\alpha, \dots, m_M)$ with $m_\alpha = 0, 1$ and $q, q' = 1, 2, \dots, Q$. The constraints are given by

$$\begin{aligned} F_{q,q',\vec{m}}(\vec{G}) &= \sum_{i,j} A_{ij}^{\vec{m}} \delta_{q,q_i} \delta_{q',q_j} = e_{q,q'}^{\vec{m}} \quad \text{for } q \neq q', \\ F_{q,q,\vec{m}}(\vec{G}) &= \sum_{i < j} A_{ij}^{\vec{m}} \delta_{q,q_i} \delta_{q,q_j} = e_{q,q}^{\vec{m}}. \end{aligned} \quad (135)$$

For every pair of nodes, one in community q and one in community q' , we will have one multilink \vec{m} ; therefore, the

total number of multiplexes in this ensemble is given by Z_M , which has the explicit expression

$$Z_M = \left[\prod_{q < q'} \frac{(n_q n_{q'})!}{\prod_{\vec{m}} e_{q,q'}^{\vec{m}}!} \prod_q \frac{[n_q(n_q - 1)/2]!}{\prod_{\vec{m}} e_{q,q}^{\vec{m}}!} \right], \quad (136)$$

where n_q is the number of nodes in community q . Finally, the Gibbs entropy Σ of this ensemble, with $N\Sigma = \ln Z_M$, satisfies

$$N\Sigma = \ln \left[\prod_{q < q'} \frac{(n_q n_{q'})!}{\prod_{\vec{m}} e_{q,q'}^{\vec{m}}!} \prod_q \frac{[n_q(n_q - 1)/2]!}{\prod_{\vec{m}} e_{q,q}^{\vec{m}}!} \right]. \quad (137)$$

As long as the number of constraints P is sublinear with respect to N we have that the microcanonical and canonical ensembles are equivalent in the thermodynamic limit and $\Sigma \simeq S/N$.

4. Multiplex ensemble with given multidegree sequence and given number of multilinks in between nodes of different communities

We assign to each node i the label $q_i = 1, 2, \dots, Q$ indicating the community to which node i belongs. We can consider a microcanonical correlated multiplex ensemble in which we fix the multidegree $k_i^{\vec{m}}$ of every node i together with the total number of multilinks $e_{q,q'}^{\vec{m}}$ between nodes in community q and nodes in community q' with the condition that the constraints are graphical. In this case we have $2^M \times N$ constraints indicated with the labels $\vec{m} = (m_1, m_2, \dots, m_M)$ with $m_\alpha = 0, 1$ and $i = 1, 2, \dots, N$ and other $2^M \times \frac{Q(Q+1)}{2}$ constraints indicated with labels \vec{m} and $q, q' = 1, 2, \dots, Q$. The constraints are given by

$$\begin{aligned} F_{i,\vec{m}}(\vec{G}) &= \sum_{j=1, j \neq i}^N A_{ij}^{\vec{m}} = k_i^{\vec{m}}, \\ F_{q,q',\vec{m}}(\vec{G}) &= \sum_{i,j} A_{ij}^{\vec{m}} \delta_{q,q_i} \delta_{q',q_j} = e_{q,q'}^{\vec{m}} \quad \text{for } q \neq q', \\ F_{q,q,\vec{m}}(\vec{G}) &= \sum_{i < j} A_{ij}^{\vec{m}} \delta_{q,q_i} \delta_{q,q_j} = e_{q,q}^{\vec{m}}. \end{aligned} \quad (138)$$

The Gibbs entropy Σ of this ensemble satisfies

$$N\Sigma = S - N\Omega, \quad (139)$$

where S is given by Eq. (81) and by following arguments similar to the ones in [35] it can be proved that for sparse networks Ω satisfies the relation

$$\begin{aligned} N\Omega &= - \sum_{i=1}^M \sum_{\vec{m} | \sum_{\alpha=1}^M m_\alpha = 0} \ln [\pi_{k_i^{\vec{m}}} (k_i^{\vec{m}})] \\ &\quad - \sum_{q \leq q'} \sum_{\vec{m} | \sum_{\alpha=1}^M m_\alpha = 0} \ln [\pi_{e_{q,q'}^{\vec{m}}} (e_{q,q'}^{\vec{m}})], \end{aligned} \quad (140)$$

where $\pi_y(x)$ is the Poisson distribution with average y $\pi_y(x) = \frac{1}{x!} y^x \exp(-y)$ calculated at x . In this case, if the number of constraints $P \propto N$, then in the large network limit $N \gg 1$, Ω is finite and we have $\Sigma = S/N - \Omega$. Therefore, the Gibbs entropy Σ is lower than S/N and the microcanonical ensemble is not equivalent in the thermodynamic limit to the conjugated canonical ensemble.

VI. CONCLUSION

We have presented a statistical mechanics approach for microcanonical and canonical multiplex ensembles. We have defined both uncorrelated and correlated multiplex ensembles. Uncorrelated multiplex ensembles are characterized by a probability of the multiplex that factorizes into the probability of the networks G^α for every layer α of the multiplex. Therefore, for uncorrelated multiplex ensembles the probability of a link in one network is independent of the presence of other links in the other layers. We have considered uncorrelated networks in which we fix the expected number of links in each layer, the expected degree sequence in each layer, the expected number of links in between different communities in each layer, or the expected degree sequence and the expected total number of links between communities in each layer. These ensembles, when describing multiplexes formed by sparse networks, have negligible global and local overlap; therefore, they cannot model situations in which the overlap of links in different layers is significant. In order to describe the situation in which the overlap is significant we introduced canonical correlated multiplex ensembles in which we fix the expected number of multilinks \vec{m} given by $L^{\vec{m}}$, the expected multidegree $k_i^{\vec{m}}$ sequence, the expected number of multilinks \vec{m} between nodes in different communities, or even the expected multidegree sequence and expected number of multilinks between nodes of different communities. Finally, we characterize both microcanonical uncorrelated and correlated networks showing that the microcanonical ensembles and canonical ensembles are not equivalent as long as the number of constraints is extensive. This paper presents a scenario for studying multiplex ensembles and characterizes null models of multiplexes including a significant global or local overlap of the links in the different layers. The extension of this statistical mechanics of multiplex ensembles to more complex situations, such as to directed and weighted networks, and the application of the entropy of multiplexes for extracting information from multiplex data sets are beyond the scope of the present paper. Moreover, different entropy measures for quantifying the complexity of complex networks have been proposed using tools of quantum information theory [47,48]. The generalization of also these measures to multiplexes and the use of these measures to uncover hidden statistical features of multiplex data sets are left for future work.

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