PAPER

Bipartite quantum states and random complex networks

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Bipartite quantum states and random complex networks

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Abstract. We introduce a mapping between graphs and pure quantum bipartite states and show that the associated entanglement entropy conveys non-trivial information about the structure of the graph. Our primary goal is to investigate the family of random graphs known as complex networks. In the case of classical random graphs, we derive an analytic expression for the averaged entanglement entropy $\bar{S}$ while for general complex networks we rely on numerics. For a large number of nodes n we find a scaling $\bar{S} \sim c \log n + g_e$ where both the prefactor c and the sub-leading $O(1)$ term g_e are characteristic of the different classes of complex networks. In particular, g_e encodes topological features of the graphs and is named network topological entropy. Our results suggest that quantum entanglement may provide a powerful tool for the analysis of large complex networks with non-trivial topological properties.

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1. Introduction

Complex networks are models of graphs that appear capable of capturing the phenomenology of a plethora of systems, from biology to the World Wide Web [1]. The departure from regular lattices, the most common background geometry in solid state physics, allows for the rich static and dynamic behavior of complex networks. This is due to the simultaneous presence of a global compact structure and a sophisticated architecture of interactions. By *compact structures* we refer to the typical small distance (with respect to a regular lattice) between nodes in the network. The complexity of the network architecture is manifest in the entangled pattern of links and paths that such objects display; see figure 1. This architecture encodes a type of strong disorder that requires for its analysis some of the techniques developed in statistical mechanics [2]. There exist a plethora of phenomenological quantities that provide information on the architecture of a network: degree distribution, the clustering coefficient, community structure measures and many others [1]. In particular, a few classical entropic measures have been introduced to describe the structure of complex networks [3].

In this paper, we address the problem of the entropic analysis and discrimination of networks using quantum information tools, notably entanglement entropy. Entanglement, a purely quantum measure of correlation, is one of the fundamental concepts in quantum information [4]. We provide a recipe, in a way the simplest possible one, to construct a pure bipartite quantum state for a given graph. This allows us to study entanglement properties of quantum states that are related to the topological features of the original graphs and that are able to distinguish between different complex network topologies. Although at first sight it may seem a bit artificial to look for a graph-entropy measure in a quantum context, the synergy between quantum information and complex network tools is not new. For example, in [5, 6], the authors have discussed different interesting ways of associating graphs with quantum states and investigated in what sense complex networks may play a role in the quantum domain. All these constructions are then similar in spirit but substantially different from the present approach.

This paper is organized as follows. We first describe the construction of the quantum bipartite network states. Then we introduce the families of complex networks that we consider in this work. Subsequently, we define the notion of topological network entropy and apply it to study the structure of different complex network topologies. Finally, we briefly discuss the relation to former works and present our conclusions.

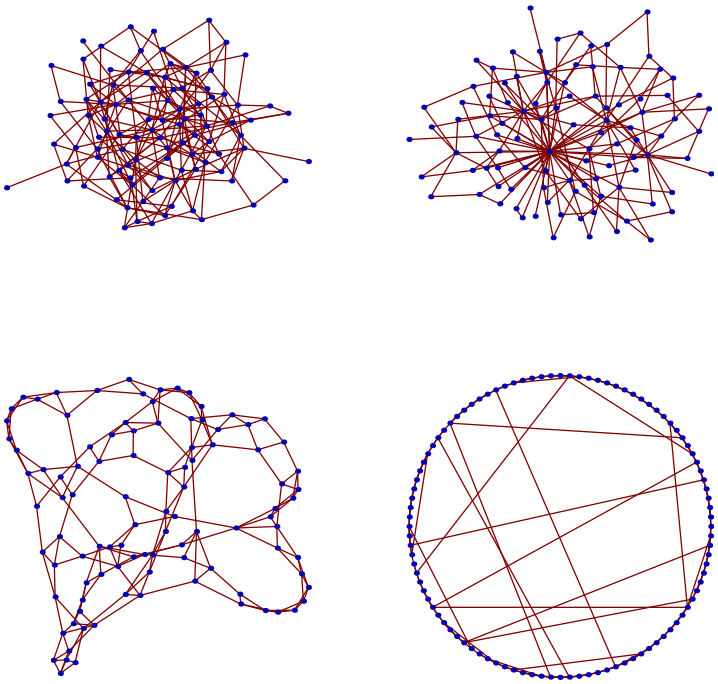

Figure 1. Random graphs belonging to different ensembles: the Erdős–Rényi (top left corner), preferential attachment (top right corner), small-world (bottom left corner) and the same graph but with a different embedding (bottom right corner).

2. Network quantum states

Any graph $\mathcal{G}_A$ with n nodes is completely specified by its adjacency matrix A: a two-dimensional (2D) array of size n, where each entry $a_{i,j}$ characterizes the connection between nodes i and j. The domain of $a_{i,j}$ determines the kind of graph one is considering: directed, undirected, weighted or unweighted. In this work, we focus on undirected unweighted graphs, the so-called simple graphs, for which $a_{i,j} \in \{0, 1\}$ (the same analysis can be naturally extended to directed and weighted graphs). In particular, if $a_{i,j} = 0$ it means that there is no edge connecting the two nodes i and j; otherwise $a_{i,j} = 1$. Sometimes it will be useful to refer also to non-simple graphs with loops. Given the graph $\mathcal{G}_A$ ($A \neq 0$) we define the following bipartite quantum state:

$$|A\rangle \equiv \frac{1}{\|A\|_F} \sum_{i,j=1}^{n} a_{i,j}|i\rangle|j\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2, \tag{1}$$

where $\|A\|_{\mathrm{F}} := \sqrt{\mathrm{Tr}A^{\dagger}A}$ denotes the Frobenius norm of the matrix A and $\mathcal{H}_1 \cong \mathcal{H}_2 \cong \mathbb{C}^n$. In the fixed local basis $\{|i\rangle : i = 1, \ldots, n\}$ we refer to $|A\rangle$ as a *pure network state*. It corresponds to the state of two n-level systems, or analogously to the state of two n-qubit systems where each subsystem of n qubits is constrained to the one-excitation manifold. The isomorphism class of a graph corresponds to the orbit of the permutation group on the adjacency matrix: PAP^t, where $P \in S_n$ are permutation matrices. This implies that the adjacency matrix of isomorphic graphs is unique up to permutations of rows and columns, and the same holds true for the bipartite states in equation (1). The reduced density matrix of the subsystem whose Hilbert space is $\mathcal{H}_1$ is given

(in the given basis) by

$$\rho_A \equiv \mathrm{Tr}_2|A\rangle\langle A| = \frac{AA^\dagger}{\|A\|_{\mathrm{F}}^2} \in \mathcal{H}_1. \tag{2}$$

We refer to this reduced density matrix as the *mixed network state*. Note that both definitions (1) and (2) do not rely on A being symmetric and therefore extend immediately to oriented (and weighted) graphs. We are interested in the correlation properties between $\mathcal{H}_1$ and $\mathcal{H}_2$, quantified by the entanglement entropy [7]. Since this quantity depends only on the spectrum of the adjacency matrix, it is a property of the isomorphism class of the graph, i.e. isomorphic graphs will have the same entanglement entropy. Indeed, if P is an (orthogonal) permutation matrix: $|PAP^t\rangle = \hat{P}^{\otimes 2}|A\rangle$, where $\hat{P} = \sum_{i,j=1}^{n} P_{i,j}|i\rangle\langle j|$. Namely, isomorphic graphs give rise to locally equivalent network states.

Before considering complex topologies, it is instructive to play with the simplest possible examples and try to characterize maximally and minimally entangled network states. Note that the unnormalized bipartite state can be written as $A \otimes I|I\rangle$, where $|I\rangle = \sum_i^n |i, i\rangle$ is an unnormalized maximally entangled state. The network corresponding to the state $|I\rangle$ consists of n nodes with loops, and by construction its adjacency matrix is the identity. Entanglement does not change under local unitary transformations [7], so in order to construct other maximally entangled network states we need to characterize all the adjacency matrices that correspond to unitary operators. It is easy to prove that the set of unitary adjacency matrices coincides with the set of permutation involutions, i.e. the permutation matrices that square to the identity. This is also consistent with the fact that the square of the adjacency matrix is the unnormalized totally mixed network state. Unitary adjacency matrices correspond to networks made of only loops or disconnected linked pairs of nodes. On the other hand, factorized states (i.e. unentangled) correspond to complete graphs with loops.

In the following, we study the properties of ensembles of random network states. The probability measure in the space of network states is the one induced by the measure on the space of random networks, according to the construction in equations (1) and (2).

3. Complex networks

In order to make the paper self-contained, let us briefly introduce three network structures that we will use in the following. The seminal paper of Erdős and Rényi (ER) in 1959 defined what is now the standard example of a random network [8]. The ER random graph model, denoted by $\mathcal{G}_{n,m}^{\mathrm{ER}}$, is an ensemble of graphs where each element has n nodes and m edges. ER graphs are also related to the so-called Gilbert models [9], denoted by $\mathcal{G}_{n,p}^{\mathrm{ER}}$, where an edge between each pair of n nodes is present with a probability p. The Gilbert model is better suited for analytical investigations, while $\mathcal{G}_{n,m}^{\mathrm{ER}}$ graphs are numerically easier to study. In the thermodynamic limit, fixing the average degree $\overline{q}$ of a node, one can constrain the two models to be related by $\overline{q} = 2m/n = pn$. If, for $n \to \infty$, $\overline{q}/n \to 0$, the network is said to be sparse. The other example of a complex network that we consider is known as the Barabási–Albert model [10], denoted by $\mathcal{G}^{\mathrm{BA}}$, based on a growth process and a preferential attachment mechanism. The rationale is that nodes with higher degree acquire new nodes at higher rates than other lower-degree nodes. Nodes are added successively, and for each node a number d of edges is generated, with bias towards connections with higher-degree nodes. The distribution for the number of links emanating from a node is not Poissonian, like for ER graphs, but rather follows a power law.

Another way of modelling stochasticity in the connectivity pattern of a graph is by randomly destroying the periodicity of a regular lattice. This is the idea behind small-world networks, denoted by $\mathcal{G}^{\mathrm{SW}}_{p,k}$, as proposed by Watts and Strogatz [11]. They can be created by randomly adding bonds to a regular 1D ring, this way building a superposition between regular lattices and classical random graphs. The probability p according to which new bonds are added at random is a parameter characterizing the ensemble, and it allows us to interpolate from regular graphs ($p = 0$) to ER random graphs ($p = 1$). The other parameter for this kind of network is denoted by k, and it quantifies the number of next-nearest-neighbor links present in the original regular graph. For each of the above complex network ensembles, we shall construct the associated ensemble of random network states denoted by ψ^{ER}, ψ^{BA} and ψ^{SW}, and we will consider scaling properties of the average entanglement entropies.

4. Topological network entanglement

We start by evaluating analytically the averaged Rényi entropy of network states in ψ^{ER}, the states associated with the ensemble of ER random graphs. The α-Rényi entropy of a state is defined by $R_\alpha(\rho) \equiv (1-\alpha)^{-1} \log_2 \mathrm{Tr}\, \rho^\alpha$. Using the definition of ρ_A given in equation (2) we have

$$R_\alpha(\rho_A) = \frac{\log_2 \mathrm{Tr} A^{2\alpha} - \alpha \log_2 \mathrm{Tr} A^2}{1-\alpha}. \tag{3}$$

We are interested in the scaling in n of the average Rényi entropy $\overline{R_\alpha}$. In order to provide an explicit expression for $\overline{R_\alpha}$ we use the fact that for each α there exists a constant $c_{2\alpha}$ such that $\lim_{n\to\infty} n^{-1}\overline{\mathrm{Tr} A^{2\alpha}} = c_{2\alpha}$, i.e. for sparse ER graphs the thermodynamic limits of the moments of the graph spectrum exist and are finite [12]. Furthermore, one can check numerically that the difference between the quenched average $(1-\alpha)^{-1}\overline{\log_2 \rho^\alpha}$ and the annealed average $(1-\alpha)^{-1} \log_2 \overline{\rho^\alpha}$ scales as n^{-1}. Putting this together we can write

$$\overline{R_\alpha(\rho_A)}[n] = \log_2 n + g(\alpha) + O\left(\frac{1}{n}\right), \tag{4}$$

where $g(\alpha) := \log_2 c_2 + (1-\alpha)^{-1}(\log_2 c_{2\alpha} - \log_2 c_2)$ is a sub-leading $O(1)$ term. This equation tells us that the Rényi entropy is almost maximal for any α. Note that, even though the logarithmic scaling for these network states is consistent with the one of general (Haar distributed) random states [14], one could not predict *a priori* this behavior for the particular family of random states we introduced. Remarkably, the sub-leading term contains information about the topology of the graphs. In fact, the term $c_{2\alpha}$ is directly related to the average number of closed paths of length 2α in the graph. In figure 2(a), we provide a numerical check of equation (4), which supports in particular the approximation of the quenched with the annealed average. The figure shows perfect agreement between equation (4) and the results of the simulation. It is tempting to extrapolate our analysis from the Rényi entropy to the von Neumann entanglement entropy, which is defined by $\overline{S} \equiv \lim_{\alpha\to 1} \overline{R_\alpha}$. By construction it follows immediately the logarithmic scaling of the von Neumann entropy, while for the sub-leading term we have $g_{\mathrm{e}} := \lim_{\alpha\to 1} g(\alpha) = \log_2 c_2 - \frac{\mathrm{d}\log c_{2x}}{\mathrm{d}x}|_{x=1}$ and then, using the definition of $c_{2\alpha}$, one finds that

$$g_{\mathrm{e}} = \log_2 c_2 - \frac{\overline{\mathrm{Tr} A^2 \log_2 A^2}}{\overline{\mathrm{Tr} A^2}}. \tag{5}$$

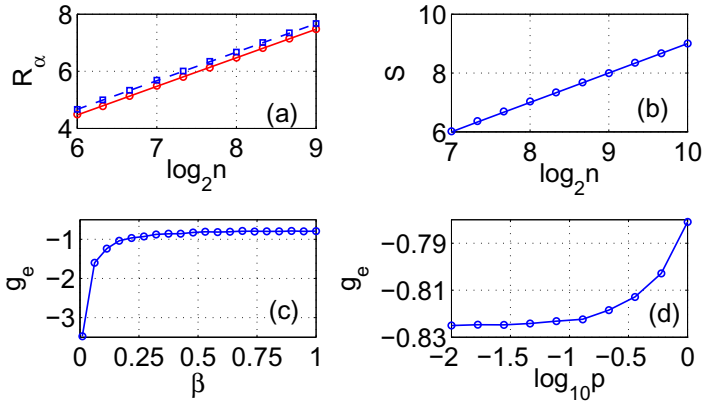

Figure 2. (a) The average Renyi entropy R_α obtained numerically and the analytical prediction (dashed and continuous lines) for ER quantum random states. The open square symbols correspond to the $\alpha = 2$ data points, while the open circles are for $\alpha = 3$. (b) The average von Neumann entropy obtained numerically and the analytical prediction for the states corresponding to $\mathcal{G}^{\mathrm{ER}}_{n,n}$. (c) g_{e} as a function of β in $\mathcal{G}^{\mathrm{ER}}_{n,\beta n \log_2 n}$. (d) g_{e} as a function of the rewiring probability p, for small-world networks in $\mathcal{G}^{\mathrm{SW}}_{p,2}$.

It is interesting to observe that the second term in equation (5) can be regarded as a sort of topological susceptibility of the given family of networks. In fact this term is equal to $-\frac{\log c_{2x}}{\mathrm{d}x}|_{x=1}$, and it tells us how the logarithm of the rescaled averaged number of loops of length 2α changes as the length is changed continuously around $\alpha = 1$. For this reason, and in view of its conceptual similarity to the topological entanglement entropy introduced in [13], we call the $O(1)$ quantity in equation (5) the *topological network entanglement*.

In figure 2(b), we show a comparison between the analytical expression for the von Neumann entropy, obtained using equation (5), and the empirical average of the entanglement entropy over different realizations. As can be seen from the figure there is perfect overlap between the two. The ensemble $\mathcal{G}^{\mathrm{ER}}_{n,m}$ is parameterized by the number of edges m. One can wonder about the behavior of g_{e} as m varies in some particular interval, but in such a way that the graph is always sparse. Figure 2(c) shows the value of g_{e} as a function of a parameter $\beta \in (0, 1]$, which is related to the number of edges by $m = \beta n \log_2 n$. The figure shows that for ER graphs, the greater the number of links the greater the entanglement. We now evaluate g_{e} numerically for small worlds and preferential attachment networks. Considering first networks in $\mathcal{G}^{\mathrm{SW}}_{p,k}$ we checked numerically that the scaling is logarithmic and that the prefactor is always 1. In figure 2(d), we see the dependence of g_{e} on p, the probability of rewiring edges. The figure shows that g_{e} increases monotonically from regular to more random graphs. This is consistent with the intuition that adding randomness to a graph increases its entropy, as measured by g_{e}. From these results it is clear that the properties of the entanglement entropy provide information on the complex network structure, supporting its interpretation as a graph entropic quantity. Considering the ability to discriminate between different network topologies, in figure 3 we compare the scaling of the average von Neumann entropy of $\psi^{\mathrm{ER}}_{n,n}$, $\psi^{\mathrm{SW}}_{0.1,2}$ and ψ^{BA} random network states. The simulations show that, unlike for ER and small-world networks, the logarithmic prefactor for ψ^{BA} states is slightly smaller than 1. From the figure, it is clear that

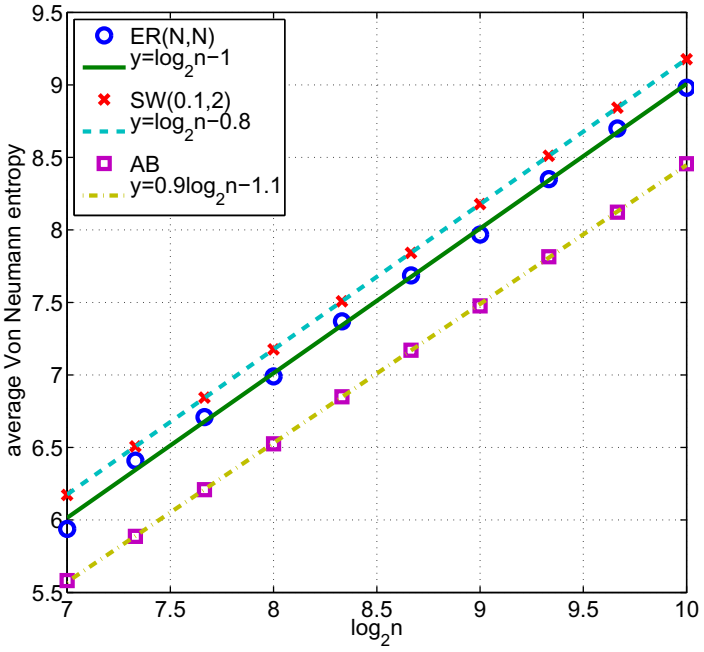

Figure 3. The average von Neumann entropy obtained numerically for different quantum random states and the linear fit of the data points.

the von Neumann entropy distinguishes different complex network ensembles. For sufficiently big networks the fluctuations due to disorder are strongly suppressed. On the one hand, this is an indication of the robustness of this graph-entropic measure; on the other hand, it can also be useful from a computational point of view. In fact, one has a very good estimate of the entanglement entropy already from a few realizations. Hence, if the network is big enough, the scaling analysis could in principle be performed on a single realization, for example evaluating the entanglement entropy on sub-graphs of increasing size. Furthermore, whenever computational efficiency is an issue, we point out that instead of the von Neumann entropy one could evaluate the so-called single-copy entanglement ($\lim_{\alpha\to\infty} R_\alpha$) [15], for which efficient numerical techniques can be used [16].

5. Discussion and conclusions

In this paper, we have exploited a natural mapping from graphs to quantum bipartite states and we have defined the entropy of a graph as the entanglement entropy of the associated quantum state. We have then used this quantum measure of correlations to study the structure of complex networks. The scaling of the entanglement entropy is logarithmic in the system dimension, and both the prefactor and the sub-leading $O(1)$ term (topological network entropy) can be used to characterize the network family and to distinguish between different network topologies. In particular, we showed that the Barabási–Albert model has scaling behavior that differs significantly from that of small-world and ER graphs. While the last two have a similar scaling, they still are distinguishable comparing graphs with the same number of edges. This is consistent with the fact that small-world networks are a mixture of regular lattices and ER graphs. Furthermore, we provided an analytic expression, exact in the thermodynamic limit, for the averaged Rényi and von Neumann entropy associated with ER random graphs. It is desirable

to achieve a clear and general understanding of the relations between the quantum entropic measures we introduced and the standard graph-theoretic observables analyzed in the complex-network community. One would like to also gain a deeper insight into the measure concentration (large-size convergence) properties of the various probabilistic objects we discussed for the different families of complex networks. While the primary goal of this paper has been to show how to use quantum tools to investigate complex networks, it should be clear that also the converse task, i.e. using properties of a complex network to study the novel class of random quantum states we introduced, is of interest in its own right. Moreover, on the quantum side, it is a challenge to find a consistent inverse mapping that allows one to associate a specific network with a general bipartite quantum state. Finally, one would like to devise efficient and physically feasible preparation schemes for the network quantum states we proposed.

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