Alma Mater Studiorum · University of Bologna

School of Science
Department of Physics and Astronomy
Master Degree in Physics

Network theory and Out of Equilibrium Statistical Mechanics: A Quantum Density Matrix Approach

Supervisor:
Prof. Armando Bazzani

Co-supervisor:
Dr. Giulio Colombini

Submitted by:
Matteo Shqemza

Academic Year 2023/2024

Abstract

The complex network framework has been successfully applied across various fields, from biochemistry to artificial intelligence. This dissertation studies an information-theoretic approach to complex networks based on quantum information.

We define a network entropy using the von Neumann entropy, where the density matrix is proportional to the exponential of the Laplacian matrix, scaled by a parameter β. This formulation provides a novel perspective on network dynamics, enabling the characterization of structural complexity.

Furthermore, we establish a connection between this density matrix approach and the evolution of quantum walks in the presence of thermal noise. Specifically, we show that the stationary distribution of a quantum walk on a network in contact with a thermal bath at temperature $T = 1/\beta$ leads to the same formulation. The interactions with the bath are models as Markovian and the system is analyzed through the Lindblad master equation. The temperature T regulates the spatial correlation between the nodes: at lower temperatures, long-range correlations become more significant, influencing the system's relaxation dynamics. However, the quantum walk requires that the Laplacian is hermitian. Thus, the analogy holds only for network that satisfies the detailed balance condition.

Finally, we introduce Kullback-Leibler and Jensen-Shannon divergences based on network entropy, which define a distance between networks according to their relaxation behavior. However, these measures rely solely on the network spectrum and thus cannot distinguish between different networks with the same spectral properties.

These findings provide a deeper understanding of network complexity and open new avenues for applying quantum information tools to the study of complex systems.

Contents

Introduction **1**

1 Introduction to Network Theory **3**
- 1.1 Introduction to Graph Theory . . . 3
- 1.2 Random Networks . . . 4
  - 1.2.1 Erdős-Rényi Random Graph . . . 5
  - 1.2.2 Barabábi-Albert Scale-Free Network . . . 5
  - 1.2.3 Watts-Strogatz Small World Network . . . 6
- 1.3 Random Walk on Networks . . . 7
- 1.4 Quantum Walk . . . 10
  - 1.4.1 1-D Quantum Random Walk . . . 13
  - 1.4.2 Double tree network . . . 14

2 Density Matrix and Entropy for Networks **17**
- 2.1 Communicability matrix . . . 17
  - 2.1.1 Analogy with Hamiltonian systems . . . 19
  - 2.1.2 Network of classic harmonic oscillators . . . 20
  - 2.1.3 Network of quantum harmonic oscillators . . . 22
- 2.2 Density matrix and Entropy for networks . . . 24
  - 2.2.1 Kullback-Leibler and Jensen-Shannon Divergences . . . 28

3 Lindblad Master Equation **31**
- 3.1 Derivation of the formula . . . 31
- 3.2 Time evolution . . . 35
- 3.3 Properties of the Lindblad equation . . . 36
- 3.4 Entropy production . . . 36

4 Quantum Network Master Equation **41**
- 4.1 Quantum Stochastic Random Walk . . . 41
  - 4.1.1 Stationary distribution . . . 43
- 4.2 Quantum Network Master Equation . . . 43
  - 4.2.1 Return to node's basis . . . 45
  - 4.2.2 Interpretation . . . 47
- 4.3 Generalization to other dynamic . . . 47
- 4.4 Symmetry breaking . . . 48

Conclusion **51**

A Mastubara Green Function **53**

B Sub-additivity of the network's entropy **55**

C Mathematical method to solve differential equation from matrix **57**

Bibliography **59**

Introduction

Traffic congestion in the morning, airport scheduling, and even the functioning of the brain are all systems that can be naturally analyzed through complex networks. In such networks, vertices represent elements, and links define their interactions: airports and neurons serve as vertices, while flights and synapses act as links.

The foundations of graph theory trace back to 1736, when Euler introduced his famous problem about the Seven Bridges of Königsberg [1]. The challenge was about finding a route, if it exist, that cross all the seven bridges connecting the two island on the Pregel river with the rest of the city once and only one. Euler solved the problem eliminating all the irrelevant information and focusing just on the sequence of the bridges. In other words, he reformulates the problem considering the island and the rivers banks as nodes and the bridges as links. Graph theory was begun. One of the success of this theory was the proof of the five color problem. It declared that given a plane divided into regions, such as a political map, those regions could be always colored using no more that five different colors, such that two neighboring regions did not have the same color [2, 3].

With the spread of the graph theory through different fields and the complexity of the networks, the necessity to find a way to reproduce reliable artificial networks with basic algorithm was crucial. The first answer was given by Erdős and Rényi [4, 5] with their random graphs. This model is widely studied and understood; it was used a base to for ages. However, due to the increasing of the data and computational power, the Erdős-Rényi model started failing to capture the behavior of the real network like Internet. In fact, real networks present strong hubs and short distances, features that this model did not have. To answer the new question, in the last 40 years many model has been proposed and studied, each one with their unique properties [6, 7]. The network theory was born.

Real-world network problems are intrinsic dynamic, necessitating the integration of dynamical models. The simplest dynamics we can consider is the random walk, a single particle wandering across the network. Despite its simplicity, the random walk on network has proven to be a powerful tool, forming the basis of various algorithms [8, 9, 10].

With the progress in quantum computing, many point of contact between quantum information and network theory arose. One of the most important model is the quantum walk. It is the quantum equivalent of the classic random walk on network but, because of the quantum effects, its behavior is different [11]. There are two different way to deal with time. We can consider time discrete and the motion is ruled by a quantum coin tossed at each timestep [12]. Otherwise, we consider the time continuous and the evolution is ruled by the Schrödinger equation with the Laplacian of the network as Hamiltonian [13]. In this dissertation we focus on the latter.

However, there is a lack of a unified theoretical framework in the network theory, particularly concerning information theory and entropy. In the literature, there have been various attempts to formulate entropy for networks. A notable contribution was made by Bianconi [14, 15], who considered an ensemble of all possible graphs with specific properties, but this approach neglected the dynamical aspects of the system. Another attempt was made by De Domenico [16]. Starting from the Estrada communicability matrix [17], he defined the network entropy at time t as $\mathrm{Tr}[\rho \ln \rho]$ with $\rho = e^{-tL}$ as density matrix and L as the Laplacian matrix. This type of entropy not only captured the topological features of the network but also its dynamical behavior. In fact, the entropy held the property of the relaxation of a random walk on the network. Starting from there, we expanded the information related quantities introducing The Kullback Leibler divergence and the Jensen Shannon divergence. This two quantities could be employed to distinguish between networks [18].

The density matrix introduced by De Domenico is reminiscent of the density matrix of a quantum canonical ensemble with the Laplacian as Hamiltonian. This observation suggests a deep connection between network entropy and continuous time quantum walks. The aim of this dissertation is to explore this connection using techniques borrowed from open quantum system, specifically the Lindblad master equation. These results can be use in several fields: from the study of the interaction between the amino acids in the proteins, to the management of the urban traffic, passing through the social interaction on the Internet. The theoretical calculations come with numerical simulations made in python.

The dissertation is structured as follows. The Chapter 1 is an introduction to the Network theory. There we explain the foundation of network, the classic random walk and the quantum version.

The Chapter 2 focuses on the network entropy. Starting from the Estrada communicability matrix, it defines the density matrix for network and the network entropy and their applications.

Before entering the last argument, in the Chapter 3 there is an introduction to the Markovian open quantum system and the Gorini-Kossakowski-Sudarshan-Lindblad master equation.

The last Chapter explains the connection between the quantum walk with thermal noise and the network entropy.

Chapter 1

Introduction to Network Theory

From social interactions and transportation systems to the intricate connections within biological organisms and the internet, networks provide a powerful framework to understand complex systems. Graph theory, the mathematical foundation of network theory, offers the tools needed to analyze these interconnected structures.

In this chapter, we introduce the fundamental concepts of network and graph theory, along with various types of random graphs. Then, we focus on random walks and diffusion processes on networks, considering both classical and quantum cases, which play a crucial role in modeling real-world phenomena such as information spread, epidemic modeling, and quantum transport.

1.1 Introduction to Graph Theory

A graph is defined by an ordinate couple (V, E) where $V = \{1, 2, 3, ..., n\}$ is the set of nodes or vertices and $E = \{(i, j) : i, j \in V; i \text{ is linked to } j\}$ is the set of links or edges. Usually, a general graph is denoted as $G = (N, M)$ where N and M are the cardinality of V and E respectively.

A graph can be described with a $N \times N$ matrix called Adjacency matrix which is defined as

$$A_{ij} = \begin{cases} +1 & \text{if } j \text{ is linked to } i \\ 0 & \text{otherwise} \end{cases} . \tag{1.1}$$

The degree d_i of a node i is the number of nodes to which it is connected. We can introduce the degree matrix D as $D_{ij} = d_i \delta_{ij}$ It can be computed from the adjacency matrix as

$$d_i = \sum_j A_{ij}. \tag{1.2}$$

Graphs can be grouped mainly into two type: *undirected* and *directed* graph. In the first one if the node i is linked to j then j is linked to i, namely $(i, j) = (i, j)$; its adjacency matrix is symmetric. In contrast, in the second one, if the node i is linked to j not necessary j is linked to i, namely $(i, j) \neq (i, j)$; its adjacency matrix is not symmetric.

An important concept in graph theory is the study of connections between nodes that are not directly linked by an edge. As a matter of fact, two nodes can be connected by passing through multiple other nodes. A *walk* of length k from node i to node j is a sequence of nodes $(x_0, x_1, ..., x_k)$ such that $x_0 = i$, $x_k = j$ and $(x_l, x_{l+1}) \in E$ for all $l \in \{0, ..., k-1\}$. A node can be crossed multiple times. If a walk visits each node only once, it is called a *path*. A particularly important concept is the *shortest path* or *geodesic* that is the path that crosses the minimum number of nodes. The number of walks $N_{ij}(k)$ of length k from node i to node j can be computed using the adjacency matrix as

$$N_{ij}(k) = (A^k)_{ij}. \tag{1.3}$$

A undirected graph is said to be *connected* if, for each pair of distinct nodes i and j, there exists a walk that connects them.

We can defined $G' = (V', E')$ a subgraph of $G = (V, E)$ if $V' \subseteq V$ and $E' \subseteq E$. A *component* of a graph $G = (V, E)$ is a connected subgraph $G' = (V', E')$ meaning that not connected to any external node of the graph, that is $(i, j) \notin E$ for each $i \in V'$ and $j \in V \setminus V'$. A important concept is the *giant component*: a connected subgraph that has approximately the same number of nodes of the total graph.

A directed graph is said to be *weakly connected* if replacing all its links with undirected ones it produces a connected graph. It is said to be *unilaterally connected* if there exists a walk from node i to j or a walk from node j to i for each pair of vertex i and j. It is said to be *strongly connected* if there exists a walk from node i to j and a walk from node j to i each pair of nodes i and j. A strongly connected graph is *irreducible*, its adjacency matrix is not similar by permutation to a block upper triangular matrix. In other word, that exchanging two or more raws the adjacency matrix such that the it can be written in the form

$$A = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1N} \\ 0 & A_{22} & \cdots & A_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdot & A_{NN} \end{pmatrix}. \tag{1.4}$$

Some systems present interactions with different strength between the elements. Thus, the binary representation, the link exist or not, is no more sufficient. To model this kind of system we introduce the *weight graphs* $G(V, E, W)$, where W is the set of real weights attached to the links. It can be described with the $N \times N$ weight matrix which entries are the weight w_{ij} of each link. If there is no link between two nodes $w_{ij} = 0$. The weight matrix is not necessary symmetric.

Figure 1.1 shows three examples for undirected, directed and weight networks.

1.2 Random Networks

In network theory, random networks play a crucial role in understanding the structure and behavior of complex systems. These networks are often used to model real-world networks, such as the Internet and social networks. There are several methods to generate random networks, each with its own specific focus, such as the degree distribution, the average path length, or the presence of particular structural properties. In this section, we will explore some of the most important models used to generate random networks, highlighting their characteristics and differences.

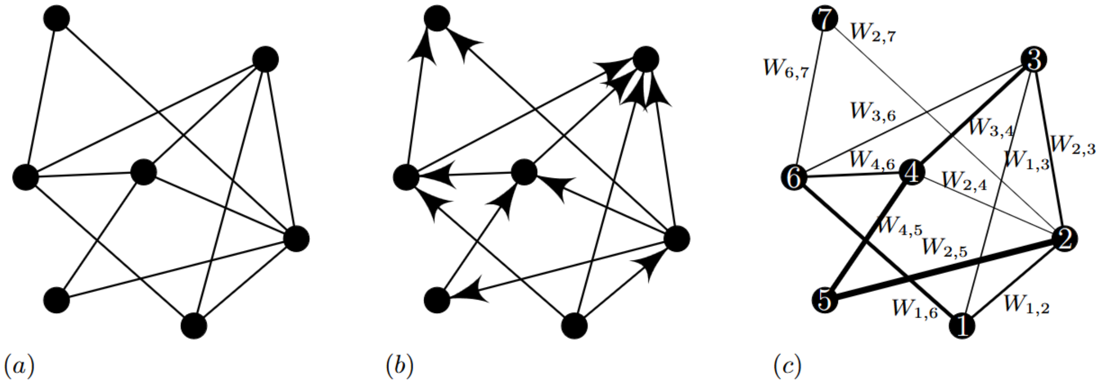

Figure 1.1: Examples of undirected (a), directed (b), weight (c) networks with $N = 7$ and $M = 12$. The arrows indicates the direction of each link. In the weight graph the thickness of the links represents its weight.

1.2.1 Erdős-Rényi Random Graph

The Erdős-Rényi (E-R) random graph $G(N, M)$, where N and M are the number of nodes and links respectively, is one of the first attempts to generate a random network [4, 5]. The network is built by randomly choosing M links from all the possible ones. Usually, is used the variation proposed by Gilbert $G(N, p)$ [19] , where p is the probability that two distinct node are connected. The two formulations converge in the thermodynamic limit $N \to \infty$ and they are interchangeable. This type of random graph has peculiar properties, such as the degree distribution of the nodes $P(k)$ is binomial

$$P(k) = \binom{n-1}{k} p^k (1-p)^{n-1-k} \tag{1.5}$$

Additionally, if $p > \frac{1}{N}$ then is almost sure that the network presents a giant component. In this work we use the second formation $G(N, p)$. Figure 1.2 shows two examples of E-R random graph, one below and one above the giant component threshold.

However, the E-R algorithm does not reproduce networks similar to those found in nature, which tend to be more clustered and to have hubs (nodes with very high degree). To simulate these properties, new algorithms have been proposed like the Barabábi-Albert scale-free network and the Watts-Strogatz small-world network.

1.2.2 Barabábi-Albert Scale-Free Network

Barabábi and Albert (B-A) proposed a scale-free network $G(N, m)$, where N is the number of nodes and m is a parameter, that mimics the behavior of real graph like the Internet [6]. This type of graph exhibits some preferential nodes with a degree order of magnitude higher than the average and it presents a power law as degree distribution.

The model works by preferential attachment: we begin from a small network and connect other nodes such that is more likely that a new nodes are connected to nodes with a high degree.

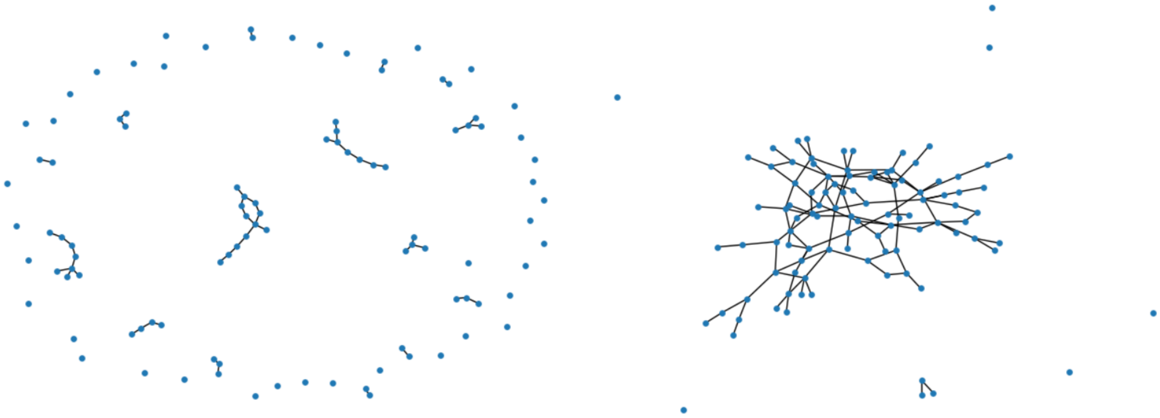

Figure 1.2: Two examples of Erdős-Rényi random graphs with 100 nodes: on the left, it has $p = 0.01$; on the right, it has $p = 0.02$. Overcoming the threshold $p > 0.01$ can be seen the formation of the giant component.

The algorithm is defined as follow:

1. It is initialized a complete graph of $m_0 > m$ node, usually $m_0 = m + 1$;
2. The other nodes are connected to this graph: for each new node, it is connected to m nodes with probability $p_i = \frac{k_i}{\sum_i k_i}$, where k_i is the degree of the i node.

Figure 1.3 shows two examples of B-A networks.

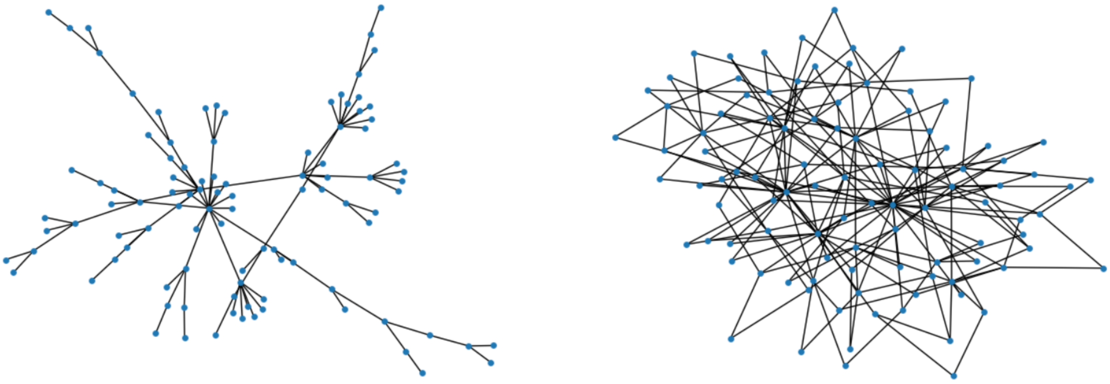

Figure 1.3: Two example of Barabábi-Albert scale-free networks: on the left, it has 100 nodes and $m = 1$; on the right, it has 100 nodes and $m = 2$.

1.2.3 Watts-Strogatz Small World Network

The Watts-Strogatz small-world network $G(N, K, p)$, where N is the number of nodes, K is the average degree (it must be even) and p is the rewiring probability, is a model that exhibits high clustering and short average path lengths [7]. The degree distribution follows a power law and the network is homogeneous, meaning that all nodes have similar degree.

The algorithm is defined as follows:

1. A ring network with N nodes is created, where each node is connected to the $K/2$ nearest neighbors on each side;
2. For each edge, with probability p the link is removed and a new one is created to random node. There is no preferential attachments. The new link must be a not existing one.

Figure 1.4 it shows two example of W-S networks.

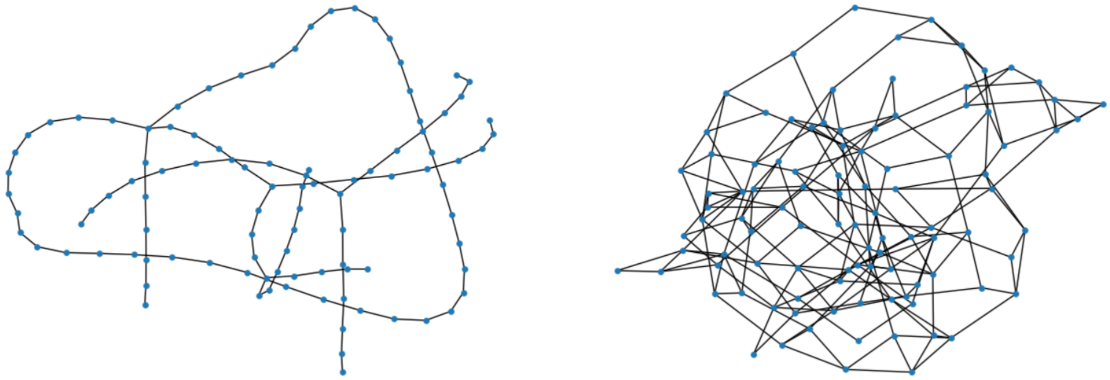

Figure 1.4: Two example of Watts-Strogatz small world networks: on the left, it has 100 nodes, $K = 2$ and $p = 0.1$; on the right, it has 100 nodes, $K = 4$ and $p = 0.3$.

The B-A and W-S algorithms produce more realistic networks compared to the E-R one, but both focus on their specific feature: the B-A networks fail to reproduce the high clustering of real networks and the W-S ones fail to reproduce the hubs characteristic of networks like Internet.

1.3 Random Walk on Networks

The study of random walks on networks is fundamental in understanding various dynamical processes, such as diffusion, search algorithms, and transport phenomena. In this section, we formalize the mathematical framework of random walks on networks and explore their key properties, including stationary distributions, transition probabilities, and their connection to the Laplacian matrix.

Consider a network $G(N, M)$ where a particle moves randomly between the nodes at each time step, with transition probability $P_{ij}^{\Delta t}$ to go to the node j starting from the node i after a time interval Δt. If the link between them does not exist then $P_{ij}^{\Delta t} = 0$. The dynamics of this system is a Markov chain: it has no memory of the past states and the future state depends only on the current position. Let $\rho_i(t)$ be the probability of finding the particle at the node i at time t. The discrete time evolution of the system is given by the law

$$\rho_i(n + \Delta t) = \sum_j P_{ij}^{\Delta t} \rho_j(n). \tag{1.6}$$

In order to conserve the total probability the transition probability must be a stochastic matrix, namely it must hold

$$\sum_i P_{ij}^{\Delta t} = 1. \tag{1.7}$$

We define a regular random walk when

$$P_{ij}^{\Delta t} = \pi_{ij} \Delta t + o(\Delta t) \qquad i \neq j \tag{1.8}$$

$$P_{jj}^{\Delta t} = 1 - \sum_{k \neq j} P_{kj}^{\Delta t} \tag{1.9}$$

where π_{ij} are the transition rates, namely the transition probability per units of time, we set $\pi_{ii} = 0$. In un unweighted network, the transition rates can be identified with the adjacency matrix as

$$\pi_{ij} = \frac{A_{ij}}{\sum_j A_{ij}}. \tag{1.10}$$

In a weight network, the transition rate can be computed starting from the weights of the links

$$\pi_{ij} = \frac{w_{ij}}{\sum_j w_{ij}}. \tag{1.11}$$

Taking the continuum limit of the evolution (1.6) we obtain the master equation [8]

$$\dot{\rho}_i(t) = \sum_j \pi_{ij} \rho_j(t) - \pi_{ji} \rho_i(t) = -\sum_j L_{ij} \rho_j(t), \tag{1.12}$$

where

$$L_{ij} = \sum_k \pi_{kj} \delta_{ij} - \pi_{ij} \tag{1.13}$$

is the Laplacian matrix. The first term represents incoming transitions to node i, while the second term accounts for outgoing transitions.

The Laplacian matrix has the property that $L_{ij} < 0$ for $i \neq j$ and also it satisfies the relation

$$\sum_i L_{ij} = 0. \tag{1.14}$$

The eigenvalues of the Laplacian matrix have always a not negative real part and its spectrum contains at least one zero eigenvalue, therefore it is not invertible [20]. The multiplicity of the zero eigenvalue is equal to the number of connected component of the network: in fact that if the network is not connected the Laplacian should be a block matrix, one block for each connected component, each component can be seen as an independent network with its zero eigenvalue.

The solution of master equation (1.12) is

$$\rho(t) = e^{-tL}\rho(0). \tag{1.15}$$

We can prove that

$$\sum_i \dot{\rho}_i(t) = -\sum_i \sum_j L_{ij}\rho_j(t) = -\sum_j \left(\sum_i L_{ij} \right) \rho_j(t) = 0. \tag{1.16}$$

This implies a first integral of motion

$$\sum_i \rho_i(t) = \sum_i \rho_i(0). \tag{1.17}$$

If the network is irreducible the master equation (1.12) has a unique stationary solution ρ^* that satisfies

$$\sum_j (\pi_{ij}\rho_j^* - \pi_{ji}\rho_i^*) = -\sum_j J_{ij}^* = 0 \tag{1.18}$$

where we introduce the stationary density currents $J_{ij}^* = \pi_{ji}\rho_i^* - \pi_{ij}\rho_j^*$.

Consider a system that hold the detailed balance condition

$$\pi_{ij}\rho_j^* = \pi_{ji}\rho_i^*, \tag{1.19}$$

in other word, where each stationary density current J_{ij}^* vanishes. In this case, the Laplacian matrix can be reduced to a symmetric matrix

$$S_{ij} = \frac{1}{\sqrt{\rho_i^*}} L_{ij} \sqrt{\rho_j^*}, \tag{1.20}$$

so that the eigenvalues are real and the eigenvectors are orthogonal. In particular the master equation becomes

$$\tilde{p}_i = -\sum_j S_{ij}\tilde{p}_j \tag{1.21}$$

where $\tilde{p}_i = p_i\sqrt{\rho_i^*}$. For these systems we can introduce a vector field on the network as

$$v_{ij} = \ln \pi_{ij} - \ln \pi_{ji}, \tag{1.22}$$

it admits a potential V_i such that

$$v_{ij} = V_j - V_i \qquad \forall\ (i,j). \tag{1.23}$$

The stationary distribution can be written in the form

$$\rho_i^* \propto \exp(-V_i). \tag{1.24}$$

such that

$$\sum_j L_{ij}\rho_j^* = 0. \tag{1.25}$$

Thus, the stationary distribution (1.24) is the eigenvector with eigenvalue 0 of the Laplacian matrix. We have recovered the Boltzmann distribution.

Let us now assume the network satisfies the detailed balance condition (1.19), then there exists a hyperplane Σ_0 that is orthogonal to the stationary distribution and this subspace is invariant under the dynamics. Let be $w \in \Sigma_0$, this subspace is identify by the relation

$$\sum_i w_i = 0. \tag{1.26}$$

Therefore, any probability vector can be decomposed as a direct sum of the stationary state and a vector $w(t) \in \Sigma_0$

$$\rho(t) = \rho^* + w(t). \tag{1.27}$$

Thus, all the eigenvectors with not zero eigenvalues belong to this subspace.

The uncertainty in the particle's location can be captured by the Shannon entropy

$$S(t) = -\sum_i \rho_i(t) \ln \rho_i(t). \tag{1.28}$$

It is a bounded function $0 \geq S \geq \ln N$.

The random walk process is irreversible, the entropy (1.28) increases by time. In fact, the entropy's derivative for the random walk is

$$\dot{S}(t) = -\sum_i \dot{\rho}_i(t) \ln \rho_i(t) = -\sum_{ij} L_{ij} \rho_j(t) \ln \rho_i(t). \tag{1.29}$$

We can diagonalize the Laplacian such that ρ_λ the probability to find the system in the eigenstate of λ eigenvalue. The eigenvalues of the Laplacian are not negative. Thus, the entropy's derivative becomes

$$\dot{S} = -\sum_\lambda \lambda \rho_\lambda(t) \ln \rho_\lambda(t) \geq 0. \tag{1.30}$$

It can been shown that the stationary distribution maximizes the Shannon entropy $S = \ln N$.

Figure 1.5 shows the Shannon entropy (1.28) as a function of time for a random walk on different networks:[1] a ring graph, a Erdős-Rényi (E-R) random graph, a Barabábi-Albert (B-A) scale-free network, and a Watts-Strogatz (W-S) small world network. The Shannon entropy is a monotonic increasing function and the stationary distribution has maximal entropy.

1.4 Quantum Walk

We can extend the random walk model to quantum particles. They must follow the Schrödinger equation with the Laplacian as Hamiltonian. However, the Schrödinger

---

[1] The python scripts can be found in the GitHub page of the author at the link: `https://github.com/ShqemzaMatteo/Master_thesis`

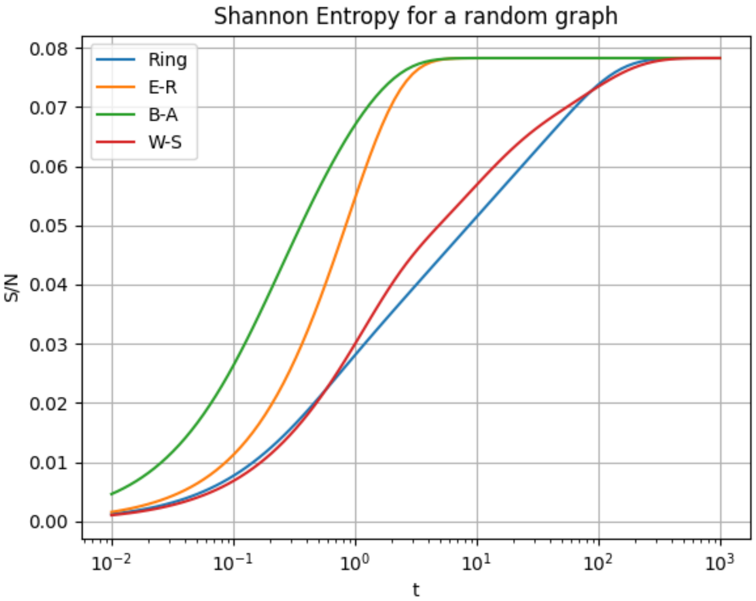

Figure 1.5: Plot of the Shannon entropy per node as a function of time t for a random walk over different types of networks with 50 nodes: a ring graph (blue), a Erdős-Rényi (E-R) random graph with connectivity probability 0.7 (orange), a Barabábi-Albert (B-A) scale-free network with parameter m = 3 (green), and a Watts-Strogatz (W-S) small world network with parameter K = 6 and rewire probability 0.2 (red). The x-axis has a logarithmic scale. In every network the entropy is monotonically increasing. For large t the entropy per node is equal to $S/N = \ln(50)/50 \approx 0.0782$.

equation requires that the Laplacian is hermitian; therefore, the network must hold the detailed balance condition (1.19). This model is known as "continuos time quantum walk" [13, 21]. This model is used to build quantum algorithms [22, 23].

Let $G(N, M)$ ba a network. We introduce an Hilbert space $\mathcal{H}$ with an orthonormal basis $\{|i\rangle\}_{i<N}$, where each element $|i\rangle$ indicates their corresponding node i, satisfying $\langle i \,|\, j\rangle = \delta_{ij}$. A general general state of the network can be encoded in the ket state $|\psi\rangle$ is define as

$$|\psi\rangle = \sum_i \sqrt{\rho_i(t)}|i\rangle, \tag{1.31}$$

in this way $\rho_i = |\langle i \,|\, \psi\rangle|^2$ is the projection of the state in the node i, in other words the probability that the system can be measured in the node i. The norm of $|\psi\rangle$ is normalize to 1, therefore, the projections ρ_i satisfy the condition $\sum_i \rho_i = 1$. The Schrödinger equation can be written as

$$\frac{d}{dt}|\psi\rangle = -i\frac{1}{2}\hat{L}|\psi\rangle. \tag{1.32}$$

where

$$\hat{L} = \sum_{ij} L_{ij}|i\rangle\langle j| \tag{1.33}$$

is the Laplacian operator. If we apply a Wick rotation into the equation (1.32) we recover the master equation of the classic random walk (1.12).

The solution of the equation (1.32) takes the form

$$|\psi(t)\rangle = \hat{U}(t,0)|\psi(0)\rangle = e^{-\frac{i}{2}\hat{L}t}|\psi(0)\rangle, \tag{1.34}$$

where $\hat{U}(t,t') = e^{-\frac{i}{2}\hat{L}(t-t')}$ is the evolution operator and it is unitary. It holds the following property

$$\hat{U}(t,t')\hat{U}(t',t'') = U(t,t''). \tag{1.35}$$

The quantum walk does not converge to a stationary distribution. However, it is possible to define a limiting transition probability for a quantum walk as follow: suppose the system starts at node $|i\rangle$, we measure it after a time t, random variable uniformly distributed over the interval $t \in [0,T]$ [21]. The transition probability from node i to j is given by

$$\begin{aligned}
\rho_{i\to j}(T) &= \frac{1}{T}\int_0^T |\langle i|e^{-i\frac{t}{2}\hat{L}}|j\rangle|^2 dt \\
&= \frac{1}{T}\int_0^T \sum_{\lambda,\lambda'}\langle i|e^{i\frac{t}{2}\hat{L}}|\lambda\rangle\langle\lambda\,|\,j\rangle\langle j|e^{-i\frac{t}{2}\hat{L}}|\lambda'\rangle\langle\lambda'\,|\,i\rangle dt \\
&= \sum_{\lambda,\lambda'}\langle i\,|\,\lambda\rangle\langle\lambda\,|\,j\rangle\langle j\,|\,\lambda'\rangle\langle\lambda'\,|\,i\rangle\frac{1}{T}\int_0^T e^{-i(\lambda-\lambda')\frac{t}{2}}dt \\
&= \sum_{\lambda}|\langle i\,|\,\lambda\rangle\langle\lambda\,|\,j\rangle|^2 + 2\sum_{\lambda\neq\lambda'}\langle i\,|\,\lambda\rangle\langle\lambda\,|\,j\rangle\langle j\,|\,\lambda'\rangle\langle\lambda'\,|\,j\rangle\frac{1-e^{-i(\lambda-\lambda')\frac{T}{2}}}{i(\lambda-\lambda')T},
\end{aligned} \tag{1.36}$$

where $|\lambda\rangle$ are the eigenstates of $\hat{L}$ with eigenvalues λ. In the limit $T\to\infty$ it tend to

$$\rho_{i\to j}(T) \xrightarrow[T\to\infty]{} \sum_{\lambda}|\langle i\,|\,\lambda\rangle\langle\lambda\,|\,j\rangle|^2. \tag{1.37}$$

Let the system be in the state $|\psi\rangle$, also called pure state, we can define the density matrix as

$$\hat{\rho} = |\psi\rangle\langle\psi| = \sum_{ij}\sqrt{\rho_i}\sqrt{\rho_j}|i\rangle\langle j|, \tag{1.38}$$

It is a self-adjoint operator and $\mathrm{Tr}[\hat{\rho}] = 1$.

For a generic operator $\hat{O}(t) = O_{ij}|i\rangle\langle j|$, the expectation value of the respective observable can be found as [24]

$$\left\langle\hat{O}\right\rangle = \mathrm{Tr}\left[\hat{O}\hat{\rho}\right]. \tag{1.39}$$

The probability ρ_k to be in the node k can be express using the operator $\hat{P}_k = |k\rangle\langle k|$ such that

$$\mathrm{Tr}\left[\hat{P}_k\hat{\rho}(t)\right] = \rho_k. \tag{1.40}$$

In the Heisenberg picture, the density operator's evolution can be found solving the different equation called von Neumann equation

$$\frac{d}{dt}\hat{\rho}(t) = -\frac{i}{2}\left[\hat{L}, \rho\right] \tag{1.41}$$

where $[\cdot,\cdot]$ is the commutator. The solution of the differential equation is

$$\hat{\rho}(t) = \hat{U}(t,0)\hat{\rho}(0)\hat{U}^{\dagger}(t,0) = e^{-\frac{i}{2}t\hat{L}}\hat{\rho}\, e^{\frac{i}{2}t\hat{L}}. \tag{1.42}$$

Using the cyclic property of the trace and the unity of the evolution operator, it can be proved that the $\mathrm{Tr}[\hat{\rho}]$ is time invariant.

If the initial distribution over the network is uncertain, we can introduce the density matrix for mixed state. Let be $\{|\psi_k\rangle\}_{k<K\in\mathbb{R}}$ a set of different probability state that can describe the system with probability p_k, such that $\sum_k^K p_k = 1$, then the mixed density matrix is define as

$$\hat{\rho} = \sum_{k=1}^{K} p_k \hat{\rho}_k \qquad \hat{\rho}_k = |\psi_k\rangle\langle\psi_k|. \tag{1.43}$$

The temporal evolution of the operator is defined as in eq. (1.41); the probability to be at node a at time t is the same as in eq. (1.40). All the properties for the pure state still holds; this can be easily proven using the linearity of the trace.

Using the mixed density matrix we can consider a system that does not start from a defined distribution, but from an ensemble of possible distribution with their probability.

To study the mixed state we introduce the von Neumann entropy

$$S[\hat{\rho}] = -\,\mathrm{Tr}[\hat{\rho}\ln\hat{\rho}]. \tag{1.44}$$

It is the quantum counterpart of the Shannon entropy for classical information theory. The von Neumann entropy (1.44) is bounded $0 \geq S[\hat{\rho}] \geq \ln N$. It vanishes for pure states. The von Neumann entropy is a time invariance, thus, the evolution operator takes pure state into pure state [24].

1.4.1 1-D Quantum Random Walk

Consider a toy model: the quantum random walk over a discrete line [13]. The probability of moving left or right is $\frac{1}{2}$. To analyze this model, it is useful to introduce the momentum state $|p\rangle$ such that $\langle j\,|\,p\rangle = e^{ijp}$, where $-\pi < p < \pi$.

In line the Laplacian is defined as

$$\hat{L}|j\rangle = 2|j\rangle - |j-1\rangle - |j+1\rangle. \tag{1.45}$$

Therefore, applying this to the momentum state

$$\begin{aligned}\langle j|\hat{L}|p\rangle &= \langle j\,|\,p\rangle - \frac{1}{2}\langle j-1\,|\,p\rangle - \frac{1}{2}\langle j+1\,|\,p\rangle \\ &= e^{ijp} - \frac{1}{2}e^{i(j-1)p} - \frac{1}{2}e^{i(j+1)p} \\ &= e^{ijp}(\cos(p)-1) = (\cos(p)-1)\langle j\,|\,p\rangle\end{aligned} \tag{1.46}$$

Thus, the amplitude of the walk can be computed as the integral over all the momenta, leading to

$$\begin{aligned}\langle j|e^{-i\frac{t}{2}\hat{L}}|k\rangle &= \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-i\frac{t}{2}(\cos(p)-1)}\langle j\,|\,p\rangle\langle p\,|\,k\rangle dp \\ &= \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-ip(j-k)-i\frac{t}{2}(\cos(p)-1)} \\ &= e^{i\frac{t}{2}}(-i)^{k-j}J_{k-j}\left(\frac{t}{2}\right),\end{aligned} \tag{1.47}$$

where $J_n(x)$ is the Bessel function of the first kind of order n.

Applying the Wick rotation we obtain

$$\left|\langle j|e^{-i\frac{t}{2}\hat{L}}|k\rangle\right|^2 = e^{-t}\left(I_{k-j}\left(\frac{t}{2}\right)\right)^2, \tag{1.48}$$

where $I_n(x) = i^n J_n(ix)$ is the modified Bessel function of the first kind. In the limit $t \gg 1$ it tends to a gaussian centered in the origin and variance $\sqrt{t}$, in accordance with the classical model [25].

1.4.2 Double tree network

Another important toy model is the quantum walk on a network consisting of two binary trees of depth n with the ending connected as shown in figure 1.6. We start from one root and analyze the probability to reach the other one [21]. Classically, the probability of crossing the network scales exponentially as 2^{-n}, and it is not computable for big n. However, using the quantum version it remains computable.

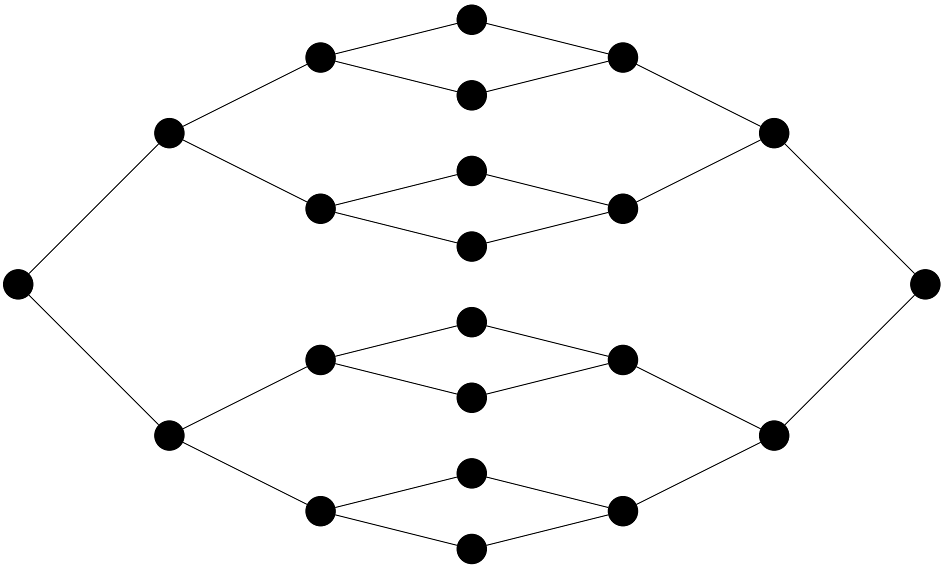

Figure 1.6: The picture of a glued double tree network.

To simplify the analysis, we can introduce a new basis $|\text{col } j\rangle_{j<2n}$ that indicates a column and not the single node, except at the two root nodes where they coincide. This basis is defined as

$$|\text{col } j\rangle = \frac{1}{\sqrt{N_j}} \sum_{a \in \text{column}} |a\rangle, \tag{1.49}$$

where the renormalization factor N_j is

$$N_j = \begin{cases} 2^j & 0 \leq j \leq n \\ 2^{2n-j} & n \leq j \leq 2n \end{cases}. \tag{1.50}$$

In this basis, the Laplacian act as

$$\begin{aligned} \langle \text{col } j|\hat{L}|\text{col } j\rangle &= 1 \\ \langle \text{col } j \pm 1|\hat{L}|\text{col } j\rangle &= \begin{cases} \dfrac{\sqrt{2}}{2} & j = 0, n, 2, \\ \dfrac{\sqrt{2}}{3} & \text{otherwise} \end{cases} \end{aligned} \tag{1.51}$$

Thus, the dynamics along the network reduces to a 1-D quantum walk which has a known computable solution (1.48)

$$\langle 0|e^{i\frac{t}{2}\hat{L}}|2n\rangle = e^{-t} I_{2n}\left(\frac{t}{2}\right), \tag{1.52}$$

where $I_n(x) = i^n J_n(ix)$ is the modified Bessel function of the first kind.

Chapter 2

Density Matrix and Entropy for Networks

In many complex systems, one element can be influenced by others with which does not directly interact. For instance, considering the city mobility, the road forms a network, closing one road may create traffic in other roads that do not intersect the closed one. To study the correlations between the nodes of a network the communicability matrix was introduced [17]. This matrix captures the way the information spreads across the network. Thus, it should depend on the dynamical aspects of the network. We call it communicability because correlation as a different meaning in social science, where it typically describes interactions.

Interestingly, this matrix behave as quantum density matrix, making it is a possible candidate to the role of network's density matrix. As a consequence, we can introduce an entropy function analogous to the von Neumann entropy found in quantum many body and quantum computing, opening a connection between the network theory and quantum realm.

2.1 Communicability matrix

Most studies on complex networks focus on the spread of information following the shorter path, namely the shortest sequence of links that connects two different nodes. However, this is not the only way the information can flow, there are plenty of other more long route that are also available, and the shorter path description ignores completely the complexity of the network. To overcome that we introduce the communicability matrix, defined to accounts for all possible paths, not just the shortest ones [26]. this matrix considers the influence of all the path that cross the chosen node, weighted by their length.

Let $G = (V, E)$ be an undirected graph composed of N nodes and E links and let A be the adjacency matrix of the graph. We can define the communicability matrix as

$$G(A) = \sum_{k=0}^{\infty} c_k A^k. \tag{2.1}$$

The communicability from node i to node j is given by G_{ij}. The power of the adjacency matrix $(A^k)_{ij}$ give us the number of path of length k starting from node i ending in node j. The coefficients c_k indicates the weight of the paths, with longer paths being penalized. This is made to give more relevance to the short ones respect to the long ones. These coefficients must be chosen such that the series is convergent. For weight network the adjacency matrix A can be substitute by the weight matrix W.

An convenient choice for the coefficients is $c_k = \frac{1}{k!}$, which transforms the communicability into an exponential function [17]

$$G^E(A) = \sum_{k=0}^{\infty} \frac{A^k}{k!} = e^A. \tag{2.2}$$

We can generalize it adding a constant term β to further penalize the longer paths

$$G^E(A) = \sum_{k=0}^{\infty} \frac{\beta^k A^k}{k!} = e^{\beta A}, \tag{2.3}$$

which resembles to the Boltzmann distribution with Hamiltonian A and temperature $T = \frac{1}{\beta}$.

Alternatively, we can choose $c_k = \alpha^k$ with $\alpha < \frac{1}{\lambda_N}$, where λ_N is the largest eigenvalue of the adjacency matrix [27]. In this case, it becomes a geometrical series yielding

$$G^R(A) = \sum_{k=0}^{\infty} \alpha^k A^k = (I - \alpha A)^{-1}. \tag{2.4}$$

In the limit $\alpha \to \frac{1}{\lambda_N}$ and $\lambda_N - \lambda_{N-1}$ large, the two formulations for the communicability matrix $G^E(A)$ and $G^R(A)$ converge leading to the same communicability for the network [28].

From this, we can introduce a global index for the network that considers the communication between the different nodes as

$$EE(A) = \mathrm{Tr}\left[e^{\beta A}\right]. \tag{2.5}$$

In the literature, it is called Estrada index [17] and can be interpreted as the sum of all the self-communication, which the sum of the paths that start and end in the same node. This index resembles the partition function from statistical mechanics.

However, the communicability matrices (2.2) and (2.4) focus only on the network's topology and they ignore the presence of a dynamics over the network that may change how information spreads. Consider the simplest dynamics, the random walk, the information's flow is governed by the Laplacian matrix L. Therefore, we define the dynamical communicability matrices for random walk as follow [26]

$$\begin{aligned} G^E(L) &= \sum_{k=0}^{\infty} \frac{\beta^k L^k}{k!} = e^{\beta L}, \\ G^R(L) &= \sum_{k=0}^{\infty} \alpha^k L^k = (I - \alpha L)^{-1}, \end{aligned} \tag{2.6}$$

with $\alpha < \frac{1}{\lambda_N}$, where λ_N is the largest eigenvalue of the Laplacian matrix.

Lastly, the Laplacian Estrada index is define as

$$EE(L) = \mathrm{Tr}\left[e^{\beta L}\right]. \tag{2.7}$$

The exponential communicability matrix resembles the Boltzmann density matrix with the Laplacian Estrada index as partition function. In fact, in the following section we demonstrate how this matrix is a suitable candidate for representing the network's density matrix. With this framework, we can define an entropy function and introduce an information theory for networks.

2.1.1 Analogy with Hamiltonian systems

The formulae (2.6) can be motivated by studying a classical and quantum harmonic oscillator on a network under specific conditions. Consider a set of N harmonic oscillators with a coupling matrix K proportional to the symmetric adjacency matrix A of the network. In this framework, the nodes are treated as particle of mass $m = 1$ connected by springs with elastic constant A_{ij}/d_i. The network should not have self interacting nodes, thus $A_{ii} = 0$. The system is submerged in a thermal bath at the temperature T. We assume there is no damping or external forces acting on the system aside the thermal fluctuation. Let us introduce a set of coordinates q_i that indicates the displacement of the i particle from the equilibrium position. The elastic elastic potential can be defined as

$$V(q) = \frac{1}{4}\sum_{i\neq j} K_{ij}(q_i - q_j)^2 = \frac{1}{2}\sum_{j} K_{jj} q_j^2 - \frac{1}{2}\sum_{i\neq j} K_{ij} q_i q_j, \tag{2.8}$$

where

$$K_{jj} = \sum_{j\neq i} K_{ij}. \tag{2.9}$$

We define the matrix $H_{ij} = K_{jj}\delta_{ij} - K_{ij}$, allowing us to express the potential as

$$V(q) = \frac{1}{2}\sum_{i,j} H_{ij} q_i q_j. \tag{2.10}$$

The matrix H is a laplacian matrix and it is equal to the Laplacian of the network (1.13). It holds the property $\sum_j H_{ij} = 0$, which implies that it has not negative eigenvalues and one must be equal to zero. The presence of zero eigenvalue ensures us that the motion of the center of mass is conserved.

We can write the Lagrangian of the system as

$$\mathcal{L} = \frac{1}{2}\sum_{ij} \dot{q}_i \dot{q}_j - \frac{1}{2}\sum_{ij} q_i H_{ij} q_j. \tag{2.11}$$

The equations of motion are

$$\ddot{q}_i = -H_{ij} q_j. \tag{2.12}$$

The eigenmodes of the system are defined by the solution of the equation

$$\omega^2\phi_i = H_{ij}\phi_j. \tag{2.13}$$

Rewriting it in matrices form yields

$$|\Omega^2 - H| = 0. \tag{2.14}$$

Therefore, the spectral signature of the matrix $H = L$ is the same as that of the harmonic oscillator. This establishes a connection between the harmonic oscillator and the master equation of a network and vice versa. Since M is diagonal, H and L have the same support, eigenvectors and eigenvalues, leading to $E = \omega^2 = \lambda$, which creates a natural ranking among the eigenvectors.

However, in order to achieve the analogy with the communicability matrix (2.6), we should impose a constrain on the system: each particle is connected by a spring with elastic constant K' to the ground. The elastic constant must be larger than the largest eigenvalue of the Laplacian. Thus, the Hamiltonian of the system is given by

$$H_L = \sum_i \frac{p_i^2}{2} + \sum_{ij} \frac{1}{2} H'_{ij} q_i q_j, \tag{2.15}$$

where

$$H'_{ij} = K'\delta_{ij} - L_{ij}. \tag{2.16}$$

With the constrain, the potential is no more singular. We will study this system in both classic and quantum cases.

2.1.2 Network of classic harmonic oscillators

Let consider a hamiltonian system with Hamiltonian (2.15) in contact with a thermal bath using the Langevin equation

$$\begin{aligned} \dot{q}_i &= p_i; \\ \dot{p}_i &= -H'_{ij} q_j - \gamma p_i + \sqrt{2T\gamma}\,\xi_i(t), \end{aligned} \tag{2.17}$$

where γ is the friction coefficient, T is the temperature (with Boltzmann constant $K_B = 1$). The term $\xi_i(t)$ represents white noise defined as

$$\langle \xi_i(t) \rangle = 0 \qquad \langle \xi_i^2(t) \rangle = 1 \tag{2.18}$$

The white noises must hold the condition $\sum_i \xi_i = 0$, that leaves invariant the motion of system's center of mass but $\xi_i(t)$ are no more independent. As a matter of fact, the total momentum $P = \sum_i p_i$ is an integral of motion

$$\frac{d}{dt}\sum_i \dot{p}_i = -\gamma \sum_i p_i + \cancel{\sqrt{2T\gamma}\sum_i \xi_i(t)} = 0. \tag{2.19}$$

The condition over the white noises $\sum_i \xi_i = 0$ breaks the independence between them and it adds correlation. We can rewriting the noise using i.i.d. white noise $w_i(t)$ as

$$\xi_i(t) = w_i(t) + \frac{1}{N}\sum_k w_k(t). \tag{2.20}$$

The covariance matrix of $\xi_i(t)$ yields

$$\langle \xi_i(t)\xi_j(s)\rangle = [\delta_{ij} - 1_{ij}]\,\delta(t-s) \tag{2.21}$$

The distribution $\rho(q,p,t)$ is a Gaussian and satisfies the Fokker-Planck equation [29]

$$\frac{\partial \rho}{\partial t} = -\sum_i p_i \frac{\partial \rho}{\partial q_i} + \sum_{ij} H'_{ij} q_j \frac{\partial \rho}{\partial p_i} + \gamma \sum_i \left[\frac{\partial}{\partial p_i} p_i \rho + T \frac{\partial^2 \rho}{\partial p_i^2}\right]. \tag{2.22}$$

The dynamics converges to a stationary distribution, with the time scale depending on the eigenvalues of the Laplacian matrix. The solution at equilibrium is give by

$$\rho(q,p) = Z(\beta)^{-1} \exp\left[-\beta\left(\sum_j p_j^2 + \sum_{ij} \frac{1}{2} q_i H'_{ij} q_j\right)\right], \tag{2.23}$$

where $\beta = \frac{1}{T}$ and $Z(\beta)$ is the partition function defined as

$$Z(\beta) = \int \prod_i dp_i dq_i \; \exp\left[-\beta\left(\sum_j p_j^2 + \sum_{ij} q_i H'_{ij} q_j\right)\right]. \tag{2.24}$$

The marginal distribution over the coordinates is a Boltzmann distribution

$$\rho(q) = Z(\beta)^{-1} e^{-\beta\left(\sum_{ij} q_i H_{ij} q_j\right)}. \tag{2.25}$$

If H' is symmetric, namely the detailed balance condition (1.19) holds, we can diagonalize the marginal distribution obtaining the motion of independent oscillators in the same thermal bath. Therefore, changing the basis from q_i to Q_λ eigenvectors with λ eigenvalue of the Hamiltonian H', the marginal distribution becomes

$$\rho(q) = Z(\beta)^{-1} e^{-\beta\left(\sum_{\lambda \neq 0} Q_\lambda \lambda Q_\lambda\right)}, \tag{2.26}$$

with the partition function

$$Z(\beta) = \int \prod_{\lambda \neq 0} dQ_\lambda e^{-\beta\left(\sum_{\lambda \neq 0} \lambda Q_\lambda^2\right)}. \tag{2.27}$$

The thermal distribution does not involve the center of mass motion since the thermal bath does not interact with it. Thus, we can project the system into an invariant subspace orthogonal to the stationary distribution. The oscillator modes Q_λ remain the same of the unperturbed case. This is a consequence of the condition $\sum_i \xi_i = 0$. The distribution has mean $\langle Q_\lambda \rangle = 0$ and the covariance matrix is diagonal with entries $\langle Q_\lambda^2 \rangle = \frac{1}{\beta\lambda}$.

The variance can be expressed as

$$\mathrm{Cov}(Q) = \frac{1}{\beta} H^{-1}, \tag{2.28}$$

where $H^{-1} = \sum_{i=2}^{N} \frac{1}{\lambda_i} v_i^T v_i$ is the Moore-Penrose generalized inverse of the Hamiltonian. Here, λ are the eigenvalues ordered from the smallest to the biggest such that $\lambda_1 < \lambda_2 < ... < \lambda_N$, and v_i are the respective eigenvectors of the Hamiltonian matrix [30].

Substituting the equation (2.16) into the correlation (2.28) we obtain

$$\mathrm{Cov}(Q) = \frac{1}{\beta} \left(K'\mathbb{I} - L_{ij}\right)^{-1} = \frac{1}{\beta K'} \left(\mathbb{I} - K'^{-1} L_{ij}\right)^{-1} \tag{2.29}$$

where $\mathbb{I}$ is the identity matrix. This is proportional to the Communicability matrix $G^R(L)$ (2.6) when $K' = 1/\alpha$. The parameter K' suppresses the motion along the eigenvectors with high eigenvalues. In the limit $K' \to \infty$, all the eigenvectors are suppressed except for the zero eigenvector.

2.1.3 Network of quantum harmonic oscillators

If we consider a system as quantum in place of a classic one the covariance matrix changes and becomes similar to te exponential communicability matrix. In the quantum case, the quantities H'_L, q_i and p_j are promoted to operators $\hat{H}'_L$, $\hat{q}_i$ and $\hat{p}_j$ and they satisfy the commutator relation $[\hat{q}_i, \hat{p}_j] = i\delta_{ij}$ ($\hbar = 1$). Thus, the Hamiltonian becomes

$$\hat{H}'_L = \sum_i \left(\frac{\hat{p}_i^2}{2} + \frac{K'}{2}\hat{q}_i^2\right) + \sum_{ij} \frac{1}{2} L_{ij} \hat{q}_i \hat{q}_j. \tag{2.30}$$

We introduce the creation and annihilation operators as

$$\hat{a}_i = \frac{1}{\sqrt{2}} \left(\sqrt{\Omega}\hat{q}_i + \frac{i}{\sqrt{\Omega}}\hat{p}_i\right) \qquad \hat{a}_i^\dagger = \frac{1}{\sqrt{2}} \left(\sqrt{\Omega}\hat{q}_i - \frac{i}{\sqrt{\Omega}}\hat{p}_i\right), \tag{2.31}$$

and the inverse as

$$\hat{q}_i = \sqrt{\frac{1}{2\Omega}} \left(\hat{a}_i + \hat{a}_i^\dagger\right) \qquad \hat{p}_i = i\sqrt{\frac{\Omega}{2}} \left(\hat{a}_i - \hat{a}_i^\dagger\right), \tag{2.32}$$

where $\Omega = \sqrt{K'}$. They satisfy the commutation relation $\left[\hat{a}_i, \hat{a}_j^\dagger\right] = \delta_{ij}$.

The Hamiltonian can be written as

$$\hat{H}_L = \sum_i \Omega \left(\hat{a}_i \hat{a}_i^\dagger + \frac{1}{2}\right) + \frac{1}{4\Omega} \sum_{ij} \left(\hat{a}_i + \hat{a}_i^\dagger\right) L_{ij} \left(\hat{a}_i + \hat{a}_i^\dagger\right). \tag{2.33}$$

Assuming the network satisfies the detailed balance condition (1.19), L is symmetric and, therefore, we can diagonalize it. The diagonalized laplacian is written in the form

$\Lambda = OLO^T$, where O is a orthogonal matrix. This generates a new pair of creation and annihilation operators respect the eigenvalue μ of the Laplacian

$$b_\mu = \sum_j a_j O_{\mu j} \qquad \hat{b}^\dagger_\mu = \sum_j a^\dagger_j O^T_{\mu j}. \tag{2.34}$$

Thus, the new Hamiltonian becomes a sum of independent Hamiltonians

$$\hat{H}_L = \sum_\mu \hat{H}_\mu, \tag{2.35}$$

with

$$\hat{H}_\mu = \Omega\left(\hat{b}_\mu \hat{b}^\dagger_\mu + \frac{1}{2}\right) + \frac{1}{4\Omega}\mu\left(\hat{b}_\mu + \hat{b}^\dagger_\mu\right)^2. \tag{2.36}$$

With some algebra, it reduces to

$$\hat{H}_\mu = \Omega\left[1 + \frac{1}{2\Omega}\mu\right]\left(\hat{b}_\mu \hat{b}^\dagger_\mu + \frac{1}{2}\right) + \frac{1}{4\Omega}\mu\left[\left(\hat{b}_\mu\right)^2 + \left(\hat{b}^\dagger_\mu\right)^2\right]. \tag{2.37}$$

We now consider the system as fermionic so the modes do not excite beyond the first excitation state. As a consequence, we can restrict the Hilbert state of a mode to the span of the ground state $|g\rangle$ and the first excited state $|e_\mu\rangle = b^\dagger_\mu |g\rangle$. Therefore, the second term in the Hamiltonian cancel out.

Now, we can compute the thermal Green function or Matsubara Green function for fermions. This quantity describes the probability amplitude for the particle to travel from one state to the other in a given time τ (more details in the Appendix A). In the Heisenberg picture, the annihilation and creation operator depend on time [31] as

$$\hat{b}_\mu(\tau) = e^{-\mu t}\hat{b}_\mu \qquad \hat{b}^\dagger_\mu(\tau) = e^{\mu t} \tag{2.38}$$

For $\tau > 0$ it is

$$G^L_{ij}(\beta, \tau > 0) = \frac{\mathrm{Tr}\left[e^{-\beta \hat{H}_L}\hat{a}_i(\tau)\hat{a}^\dagger_j\right]}{\mathrm{Tr}\left[e^{-\beta \hat{H}_L}\right]} = \sum_{\mu\nu} O_{\mu i}\frac{\mathrm{Tr}\left[e^{-\beta \hat{H}_L}\hat{b}_\mu(\tau)\hat{b}^\dagger_\nu\right]}{\mathrm{Tr}\left[e^{-\beta \hat{H}_L}\right]} O_{j\nu} \tag{2.39}$$

The equation (2.39) reduces, the calculation are in the Appendix A, to

$$G^L_{ij}(\beta, \tau > 0) = \sum_\mu O_{i\mu}\left\{-e^{-\mu\tau}\left[\left(1 - f\left(\Omega + \frac{1}{2\Omega^2}\mu\right)\right)\right]\right\} O_{j\mu}, \tag{2.40}$$

where $f(\epsilon)$ is the Fermi-Dirac distribution

$$f(\epsilon) = \frac{1}{e^{\beta\epsilon} + 1}. \tag{2.41}$$

With some algebra we obtain

$$G^L_{ij}(\beta, \tau > 0) = \sum_\mu O_{i\mu} \left\{ \frac{e^{-\mu\tau}}{e^{-\beta\left[\Omega + \frac{1}{2\Omega^2}\mu\right]} + 1} \right\} O_{j\mu} \tag{2.42}$$

In the limit $\tau \to 0^+$ and β large enough it tend to

$$G^L(\beta) = \sum_\mu O_{i\mu} e^{\beta\left[\Omega + \frac{1}{2\Omega^2}\mu\right]} O_{\mu i}, \tag{2.43}$$

that can be written also as

$$G^L_{ij}(\beta) = e^{\beta\Omega} e^{\frac{\beta}{2\Omega}L}. \tag{2.44}$$

Redefining the temperature $\beta \to \frac{\beta}{2\Omega}$ the equations (2.44) is related to equation (2.6)

$$G^E(L) = e^{-\beta\Omega} G^L(\beta). \tag{2.45}$$

When the temperature $T \to 0$ the communicability between the nodes drops to zero and the perturbation does not spread across the network. Instead, when $T \to \infty$ the communicability tend to infinity and the perturbation spread instantaneously.

In the high temperature limit, $\beta \to 0$, the correlation of the quantum system (2.43) converges to the correlation of the classic one (2.28). This is well known, since in the high temperature limit the quantum effects should be negligible.

2.2 Density matrix and Entropy for networks

The communicability matrix defined above possesses peculiar properties that make it suitable for use as a density matrix. Moreover, the presence of the Laplacian matrix ensures that it consider not only the topological features of the network but also its dynamics. Taking the exponential communicability matrix as a reference, we can define a density matrix as

$$\hat{\rho}(\beta) = \frac{1}{Z} e^{-\beta\hat{L}} \qquad \text{with} \qquad Z(\beta) = \mathrm{Tr}[e^{-\beta\hat{L}}], \tag{2.46}$$

where Z is the partition function, which is equal to the Laplacian Estrada index of the network (2.7). The density matrix $\hat{\rho}(\beta)$ is a Hermitian and positive definite matrix with trace equal to unity. the density matrix $e^{-\beta L}$ is similar to the propagator of the master equation (1.15) considering time $t = \beta$.

From this, we can define the network's entropy as the von Neumann entropy

$$S(\hat{\rho}) = -\,\mathrm{Tr}[\hat{\rho} \ln \hat{\rho}]. \tag{2.47}$$

The entropy is not negative and equal to zero if and only if the $\hat{\rho}$ is a pure state. It has a upper bound give by $S \leq \ln(N)$, [24]. The entropy satisfies the sub-additivity property [16]: Let $\hat{\rho}$, $\hat{\tau}$ and $\hat{\sigma}$ be density matrices corresponding to the networks G, H, I respectively. If the networks H and I are subgraphs of the network G such that

$G = H + I$. If the sub-additivity is satisfied we have that $S(\hat{\rho}) \leq S(\hat{\tau}) + S(\hat{\sigma})$, the equivalence is obtain if the two subgraphs do not have nodes from the same component of G. A mathematical proof can be found in appendix B.

Figure 2.1 shows the entropy (2.47) for different types of networks[1]: a ring graph, an Erdős-Rényi (E-R) random graph, a Barabási-Albert (B-A) scale-free graph, and a Watts-Strogatz (W-S) small-sworld graph.

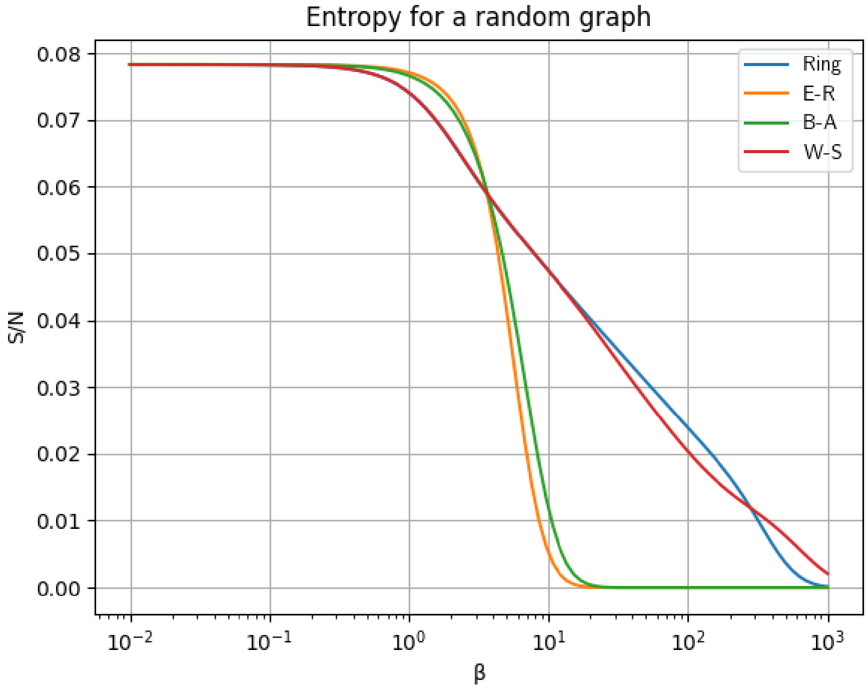

Figure 2.1: Plot of the network's entropy per node as a function of β for different network types with 50 nodes: a ring graph (blue), a Erdős-Rényi (E-R) random graph with connectivity probability 0.7 (orange), a Barabási-Albert (B-A) scale-free graph with parameter $m = 3$ (green), and a Watts-Strogatz (W-S) small world graph with parameter $K = 3$ and rewire probability 0.2 (red). The x-axis is on logarithmic scale. For large β, the entropy tends to zero for all the networks.

The parameter β in the network's entropy suppresses the spread of information along eigenvector with high eigenvalue. In fact, increasing β, more eigenvalues are suppressed until only the zero eigenvector remains. Figure 2.2 shows the eigenvalues of the same networks we have studied in figure 2.1. In the ER and BA networks the eigenvalues are clustered around 1, consequently, their entropy drops rapidly because, when β is high enough, their eigenvector are suppressed simultaneously. In contrast, in the ring and WS network the eigenvalues are closer to zero, thus the suppressed of their eigenvectors is slower.

A possible interpretation of this density matrix is given by De Domenico [32]. Consider a network $G(N, M)$, represented by the adjacency matrix A. In this network, a classic

---

[1] The Python scripts can be found on the author's GitHub page at the following link: `https://github.com/ShqemzaMatteo/Master_thesis`

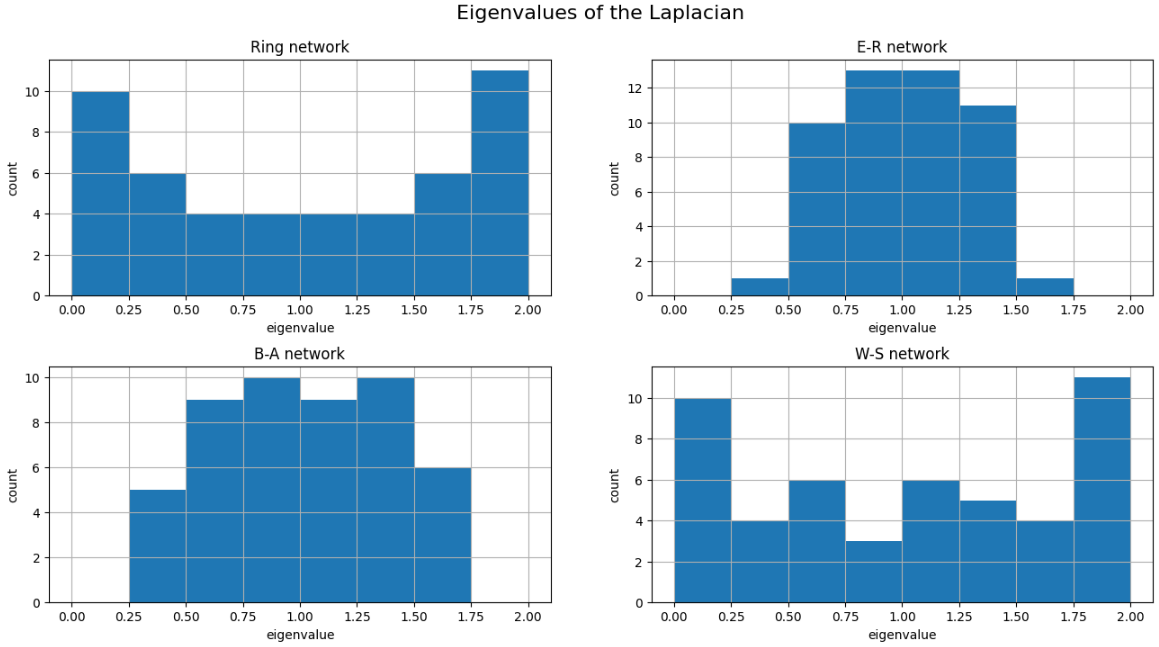

Figure 2.2: The figure shows the eigenvalue of the Laplacian matrix for different networks with 50 nodes: the top left graph is for a ring network, the top right one is for a Erdős-Rényi (E-R) random graph with connectivity probability 0.7, the bottom left one is for a Barabási-Albert (B-A) scale-free graph with parameter $m = 3$, the bottom right one shows a Watts-Strogatz (W-S) small world graph with parameter $K = 3$ and rewire probability 0.2. In the ring and WS networks the eigenvalues are clustered close to zero and near the value 2. In contrast, in the ER and BA networks the eigenvalues are clustered around the value 1.

particle performs a random walk. The network can be described using the Dirac notation. Let be $|\psi\rangle = \sum_i \rho_i |i\rangle$ the state of the system, where $|i\rangle$ is the canonical vector identifying node i and ρ_i is the probability of finding the particle on top of node i. Thus, the scalar product $\langle i \,|\, \psi\rangle = \rho_i$ is already an observable. The set $\{|i\rangle\}_{i=0}^{N}$ forms an orthogonal basis, satisfying $\langle i \,|\, j\rangle = \delta_{ij}$, where δ_{ij} is the Kronecker delta. The evolution of the dynamics is governed by the Laplacian operator $\hat{L} = L_{ij}|i\rangle\langle j|$ following the equation

$$\partial_t|\psi(t)\rangle = -\hat{L}|\psi(t)\rangle, \tag{2.48}$$

with the solution

$$|\psi(t)\rangle = \hat{G}(t,0)|\psi(0)\rangle \tag{2.49}$$

where $\hat{G}(t,0) = e^{-t\hat{L}}$ is the propagator and $|\psi(0)\rangle$ is the initial state.

If the detailed balance condition (1.19) holds, $\hat{L}$ is Hermitian. Therefore, the propagator can be diagonalized in the orthogonal basis $\{|v_\lambda\rangle\}_\lambda$ of eigenvectors of the control operator as

$$\hat{G}(t,0) = \sum_\lambda e^{-t\lambda}|v_\lambda\rangle\langle v_\lambda| = \sum_\lambda e^{-t\lambda}\hat{\sigma}_\lambda, \tag{2.50}$$

where $\hat{\sigma}_\lambda = |v_\lambda\rangle\langle v_\lambda|$ is the projector into the left and right eigenvectors with the λ eigenvalue. The operators do not depend on time; they are constant throughout the process, only the coefficients change. The system relaxes to a stationary state $|\psi_0\rangle$ corresponding to the zero eigenvector.

We consider the system in the initial state $|\psi\rangle = |\psi_0\rangle + |\Delta\psi\rangle$, where $|\Delta\psi\rangle$ is a small perturbation relative to the stationary state. The initial perturbation can be decomposed between the different nodes as $|\Delta\psi_0\rangle = \sum_i \Delta_i|i\rangle$. The time evolution of the initial state becomes

$$|\psi(t)\rangle = G(t,0)|\psi(0)\rangle = |\psi_0\rangle + G(t,0)|\Delta\psi\rangle = |\psi_0\rangle + |\Delta\psi(t)\rangle \tag{2.51}$$

with $|\Delta\psi(t)\rangle = e^{-t\hat{L}}|\Delta\psi\rangle$.

Since the stationary component is constant in time, we focus on the evolution of the perturbation $|\Delta\psi_0\rangle$. The value of the perturbation on top of node j at time t is

$$\langle j\,|\,\Delta\psi(t)\rangle = \langle j|e^{-t\hat{L}}|\Delta\psi\rangle = \sum_\lambda \langle j|e^{-t\lambda}\hat{\sigma}_\lambda|\Delta\psi\rangle = \sum_i\sum_\lambda \Delta_i e^{-t\lambda}\langle j|\hat{\sigma}_\lambda|i\rangle. \tag{2.52}$$

We have used equation (2.50) and the definition of the perturbation. This equation shows that the perturbation can travel through N different streams, one for each projector σ_λ, with stream's size $\Delta_i e^{-t\lambda}$. If $\Delta_i e^{-t\lambda} > 0$ the stream is active; if $\Delta_i e^{-t\lambda} = 0$ it is inactive. Negative stream coefficients imply an inverted flux from j to i. Now, we assume that there is maximal uncertainty in the perturbation, therefore $\Delta_i = \Delta$. The dynamics can trap part of the perturbation in a specific node. The size of the trapped perturbation can be compute as

$$T = \sum_i\sum_\lambda \Delta e^{-t\lambda}\langle i|\hat{\sigma}_\lambda|i\rangle = \Delta\,\mathrm{Tr}[\hat{G}(t,0)] \tag{2.53}$$

We can introduce a density matrix defined as

$$\hat{\rho}(t) = \frac{1}{Z}\sum_\lambda e^{-t\lambda}\hat{\sigma}_\lambda = \frac{1}{Z}e^{-t\hat{L}}, \tag{2.54}$$

where $Z = \mathrm{Tr}[e^{-t\hat{L}}]$ is the partition function. Thus, the evolution of the perturbation yields

$$\langle j\,|\,\Delta\psi(t)\rangle = \sum_i \Delta Z\langle j|\hat{\rho}(t)|i\rangle = \sum_i T\langle j|\hat{\rho}(t)|i\rangle. \tag{2.55}$$

The size of the streams is proportional to the trapped field. The density matrix can be interpreted as the probability that the perturbation will flow through a specific stream $\hat{\sigma}_l$ at time t in the ensemble of all the possible streams [32]. We have recovered the density matrix (2.46) considering the time t as the parameter β.

The complexity of information streams can be quantified by the von Neumann entropy. When the information dynamics is described by a single information stream, entropy vanishes: the density matrix is a pure state. In contrast, as the information dynamics becomes more complex and diverse, the number of information streams increases, resulting in higher entropy: the density matrix becomes a mixed state.

Considering the analogy with the quantum mechanics, in the following chapters we propose an alternative way to obtain the density matrix (2.46) starting from the quantum walk instead of the classical one. The new description, based on open quantum systems, adds new meaning to the network's entropy (2.47).

2.2.1 Kullback-Leibler and Jensen-Shannon Divergences

Starting from the concept of entropy, we can introduce the Kullback-Leibler (KL) divergence or relative entropy [33] as

$$D_{KL}(\hat{\rho}||\hat{\sigma}) = \mathrm{Tr}\left[\hat{\rho}\ln\left(\frac{\hat{\sigma}}{\hat{\rho}}\right)\right]. \tag{2.56}$$

It measures how closely the distribution $\hat{\sigma}$ reproduces an event to real distribution $\hat{\rho}$. The KL divergence is always non negative and it equals zero when $\hat{\rho} = \hat{\sigma}$. It is not symmetric and unbounded [34].

The KL divergence can be used to make comparisons between networks. Moreover, this concept can be applied to the reconstruction of networks starting from real data using the maximum likelihood estimation: it consists of finding the best model that reproduces the experimental data by minimizing the Kullback-Leibler divergence between a chosen network model and the dataset [16]. This opens the door to the application of machine learning techniques in network theory.

However the Kullback-Leibler divergence is not symmetric, therefore it cannot be use as a metric. But, we can symmetrize introducing the Jensen-Shannon (JS) divergence [34] defined as

$$\mathcal{D}_{JS}(\hat{\rho}||\hat{\sigma}) = \frac{1}{2}D_{KL}(\hat{\rho}||\hat{\mu}) + \frac{1}{2}D_{KL}(\hat{\sigma}||\hat{\mu}) = S(\hat{\mu}) - \frac{1}{2}\left[S(\hat{\rho}) + S(\hat{\sigma})\right], \tag{2.57}$$

where $\hat{\mu} = \frac{1}{2}(\hat{\rho} + \hat{\sigma})$.

The JS divergence is a bounded function [34]

$$0 \geq \mathcal{D}_{JS}(\hat{\rho}||\hat{\sigma}) \geq 1. \tag{2.58}$$

The quantity $(\mathcal{D}_{JS})^{\frac{1}{2}}$ defines a metric: it is symmetric, positive definite, and it satisfies the triangle inequality [35].

Figure 2.3 shows the Jensen-Shannon divergence between an Erdős-Rényi (E-R) random graph, a Barabási-Albert (B-A) scale-free graph and a Watts-Strogatz (W-S) small-sword graph [2].

The JS divergence has been use successfully used to measure the distance between the layers of a multiplex network. In some systems, the elements can interacts through different type of interaction. To models them, we create a set of networks with the same number of nodes but different links, one for each interaction's type. Each network forms a layer in a multiplex. For example, the mobility within a city can be mapped into a multiplex, one layer for each means of transport. Multiplex with many layers are difficult to handle; in order to simplify the model we can use the JS divergence to aggregate the redundant layers [18].

However, both the KL and JS divergences study only the spectral properties of the system. Thus, they do not distinguish between different networks with same spectrum but different eigenvectors.

---

[2] TThe Python scripts can be found on the author's GitHub page at the following link: `https://github.com/ShqemzaMatteo/Master_thesis`

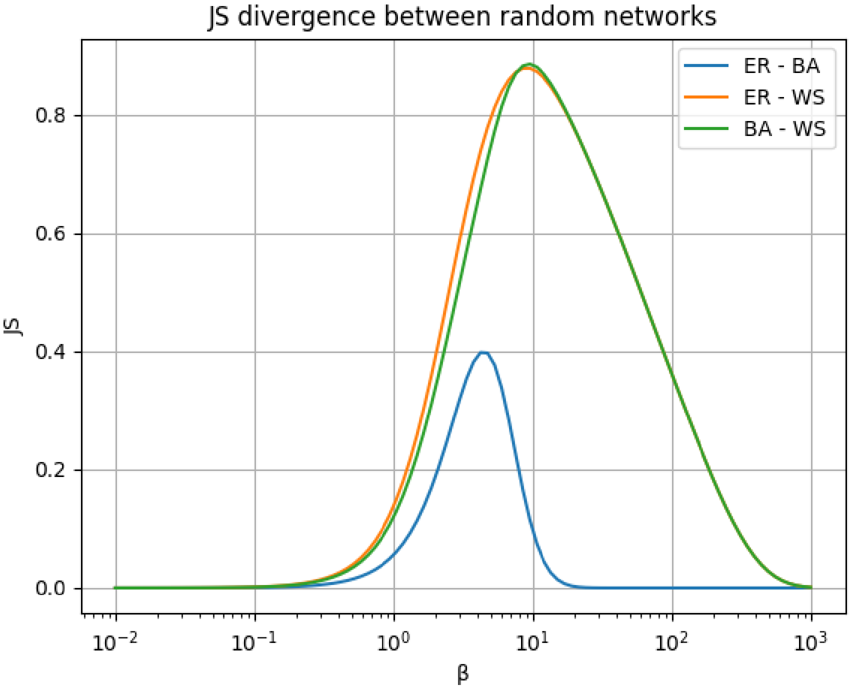

Figure 2.3: Plot of the KL divergence as a function of β between different network types with 50 nodes: a Erdős-Rényi (E-R) random graph with connectivity probability 0.7 and a Barabási-Albert (B-A) scale-free graph with parameter $m = 3$ (blue); a Erdős-Rényi (E-R) random graph with connectivity probability 0.7 and Watts-Strogatz (W-S) small world graph with parameter $K = 3$ and rewire probability 0.2 (orange); a Barabási-Albert (B-A) scale-free graph with parameter $m = 3$ and a Watts-Strogatz (W-S) small world graph with parameter $K = 3$ and rewire probability 0.2 (green). The x-axis is on logarithmic scale. The ER and BA networks are closer in terms of KL divergence compared to the WS network. Notably, the divergence reaches its maximum around $\beta = 10$.

Chapter 3

Lindblad Master Equation

Before exploring the following chapter, it is useful to introduce the Lindblad master equation, also called Gorini-Kossakowski-Sudarshan-Lindblad equation [36, 37]. This equation was introduced to describe the behavior of an open quantum system, namely a quantum system in contact with the environment. This is important because the Schrödinger equation applies only to closed systems, which are idealized and not realistic: all the quantum experiments we can build are influenced to the external environment.

The model investigates the evolution of a quantum system coupled to a Markovian environment, the interaction has no memory of the past. The Schrödinger equation requires a unitary time operator that does not permit energy dissipation. In contrast, the time operator of Lindblad master equation allows the system to exchange energy with its surroundings. Despite this, the Lindblad dynamics remains trace preserving and completely positive.

3.1 Derivation of the formula

We show the derivation of the Lindblad equation following [38, 39]. First, let $\mathcal{H}_T$ be the Hilbert space of the system and the environment combined, which can be divided into the Hilbert space $\mathcal{H}$ of the proper system and $\mathcal{H}_E$ of the environment. The combined system is a closed quantum system and evolves following the von Neumann equation

$$\partial_t \hat{\rho}_T(t) = -i[\hat{H}_T, \hat{\rho}_T(t)], \tag{3.1}$$

where $\hat{H}_T$ is the Hamiltonian of the total universe. Since we are only interesting in the system's dynamics without the environment, we can trace out the degrees of freedom associated with it, obtaining $\hat{\rho}(t) = \mathrm{Tr}_E[\hat{\rho}_T]$. The total Hamiltonian can be separated as

$$H_T = H \otimes \mathbb{I}_E + \mathbb{I}_S \otimes H_E + \alpha H_I, \tag{3.2}$$

where H is the Hamiltonian of the system, H_E the Hamiltonian of the environment and H_I is the interaction Hamiltonian, α measure the strength of the interaction. Tha Hamiltonians H and H_E commutes. It is useful to work in the interaction picture, where the operators becomes

$$\tilde{O}(T) = e^{i(\hat{H}+\hat{H}_E)t}\hat{O}e^{-i(\hat{H}+\hat{H}_E)t}, \tag{3.3}$$

and the von Neumann equation reduces to

$$\frac{d\tilde{\rho}_T(t)}{dt} = -i\alpha\left[\tilde{H}_I(t), \tilde{\rho}_T(t)\right]. \tag{3.4}$$

The solution to (3.4) is

$$\tilde{\rho}_T(t) = \tilde{\rho}_T(0) - i\alpha\int_0^t ds\left[\tilde{H}_I(s), \tilde{\rho}_T(s)\right]. \tag{3.5}$$

Even though the equation (3.5) has an exact solution, it is complicated to compute. To simplify the calculation, a perturbative approach is useful. We apply the equation (3.5) into the equation (3.4) yielding

$$\frac{d\tilde{\rho}_T(t)}{dt} = -i\alpha\left[\tilde{H}_I(t), \tilde{\rho}_T(0)\right] - \alpha^2\int_0^t ds\left[\tilde{H}_I(t), \left[\tilde{H}_I(s), \tilde{\rho}_T(s)\right]\right] \tag{3.6}$$

Applying this method again, we obtain

$$\frac{d\tilde{\rho}_T(t)}{dt} = -i\alpha\left[\tilde{H}_I(T), \tilde{\rho}_T(0)\right] - \alpha^2\int_0^t ds\left[\tilde{H}_I(t), \left[\tilde{H}_I(s), \tilde{\rho}_T(t)\right]\right] + O(\alpha^3) \tag{3.7}$$

Now, we make an approximation: we consider the strength of the interaction α to be weak, allowing us to neglect the last term. Then, we can trace out the environment, obtaining

$$\frac{d\tilde{\rho}}{dt} = -i\alpha\,\mathrm{Tr}_E\left[\tilde{H}_I(T), \tilde{\rho}_T(0)\right] - \alpha^2\int_0^t ds\,\mathrm{Tr}_E\left[\tilde{H}_I(t), \left[\tilde{H}_I(s), \tilde{\rho}_T(t)\right]\right]. \tag{3.8}$$

However, the equation (3.8) still depends on the total density matrix. To proceed, we make two more assumptions. First, we consider the initial state of the universe to be a separable state $\hat{\rho}_T(0) = \hat{\rho}(0) \otimes \hat{\rho}_E(0)$. This holds if the system has just been put in contact with the environment or if the correlation between the system and the environment is short-lived. This is called Born approximation. Second, we consider the environment as a thermal reservoir, which is in a thermal state

$$\hat{\rho}_E(0) = \frac{e^{-\hat{H}_E/T}}{\mathrm{Tr}\left[e^{-\hat{H}_E/T}\right]}, \tag{3.9}$$

where T is the temperature (the Boltzmann constant $k_B = 1$). Moreover, without loss of generality, we can write the interaction Hamiltonian in the form

$$\hat{H}_I(t) = \sum_i \hat{S}_i \otimes \hat{E}_i, \tag{3.10}$$

where $\hat{S}_i$ is an operator acting on $\mathcal{H}$ (it is not a spin operator) and $\hat{E}_i$ is an operator acting on $\mathcal{H}_E$. After making this assumption, the equation (3.8) becomes

$$\begin{aligned}\frac{d\tilde{\rho}}{dt} = &- i\alpha\sum_i\left(\tilde{S}_i(t)\tilde{\rho}(0)\,\mathrm{Tr}_E\left[\tilde{E}_i(t)\tilde{\rho}_E(0)\right] - \tilde{\rho}(0)\tilde{S}_i(t)\,\mathrm{Tr}_E\left[\tilde{\rho}_E(0)\tilde{E}_i(t)\right]\right)\\ &- \alpha^2\int_0^t ds\,\mathrm{Tr}_E\left[\tilde{H}_I(t), \left[\tilde{H}_I(s), \tilde{\rho}(t)\otimes\tilde{\rho}_E(t)\right]\right].\end{aligned} \tag{3.11}$$

The first term on the r.h.s. vanishes because $\mathrm{Tr}_E\left[\tilde{E}_i(t)\tilde{\rho}_E(0)\right] = \langle E_i(t)\rangle$ can be considered to be zero. It may seem strange, however, if it does not vanish, we can always redefine the environmental Hamiltonian as $\hat{E}_i' = \hat{E}_i - \langle E_i(t)\rangle$. The extra term is a constant and does not modify the von Neumann equation. The second term requires a stronger assumption: since α is small, the system and the environment should remain uncorrelated throughout the evolution, meaning that the timescale of the correlation should be much shorter than the timescale of the system. Thus, we can consider that the total density matrix is always separable, with the environment in the thermal state. Nevertheless, the equation is still not markovian, since it still depends on a specific initial time $t = 0$. To add this property, we can extend the lower limit of the integration to infinity with no real change in the outcome; this is valid when the integrand disappears sufficiently fast [39]. Then, changing the integration variable to $t - s$, we arrive at

$$\frac{d\tilde{\rho}(t)}{dt} = -\alpha^2 \int_0^\infty ds\, \mathrm{Tr}_E\left[\tilde{H}_I(t), \left[\tilde{H}_I(t-s), \tilde{\rho}(t) \otimes \tilde{\rho}_E(t)\right]\right]. \tag{3.12}$$

This is called Redfield equation [40]. This is the Markov approximation, which is justified if the timescale over which the state of the system varies appreciably is large compared to the timescale over which the reservoir correlation functions decay. The approximations made before are called Born-Markov approximation [39].

Now, we perform the last approximation known as rapid wave approximation, which involves averaging over the rapid oscillating term. To do it, we consider the interaction Hamiltonian (3.10) and decompose it into eigenoperators if the the system Hamiltonian H. These eigenoperators generate a complete basis of the space $\{\hat{S}_i(\omega)\}$ of the bounded operators acting on the Hilbert $\mathcal{H}$, they satisfy the conditions

$$\left[H, \hat{S}_i(\omega)\right] = -\omega \hat{S}_i(\omega) \qquad \left[H, \hat{S}_i^\dagger(\omega)\right] = \omega \hat{S}_i^\dagger(\omega). \tag{3.13}$$

Here, ω indicates the energy difference after the operator $\hat{A}_i(\omega)$ has acted. The eigenoperators $\hat{S}_i(\omega)$ satisfy the relations

$$\begin{aligned} e^{i\hat{H}_S t}\hat{A}(\omega)e^{-i\hat{H}_S t} &= e^{-i\omega t} \\ e^{i\hat{H}_S t}\hat{A}^\dagger(\omega)e^{-i\hat{H}_S t} &= e^{i\omega t} \end{aligned} \tag{3.14}$$

We can decompose the operators S_i as $\hat{S}_i = \sum_\omega \hat{S}_i(\omega)$. To apply this decomposition in (3.12), we need to go back to the Schrödinger picture for the Hamiltonian acting on the proper system. Using $\tilde{S}_i(\omega) = e^{i\hat{H}t}\hat{S}_i(\omega)e^{-i\hat{H}t}$, we obtain the Hamiltonian

$$\tilde{H}_i(t) = \sum_{i,\omega} e^{-i\hat{H}t}\hat{S}_i(\omega) \otimes \tilde{E}_i(t) = \sum_{i,\omega} e^{i\hat{H}t}\hat{S}_i^\dagger(\omega) \otimes \tilde{E}_i(t) \tag{3.15}$$

We insert the equation (3.15) into (3.12). After expanding the commutators, we substitute the decomposition for $\hat{S}_i(\omega)$. Using the cyclic property of the trace and the fact that $\mathrm{Tr}[\hat{H}_e, \hat{\rho}_E(0)] = 0$, we arrive at the result

$$\frac{d\tilde{\rho}(t)}{dt} = \sum_{\omega,\omega',i,j} e^{i(\omega-\omega')t}\Gamma_{ij}\left[\hat{S}_j(\omega)\tilde{\rho}(t), \hat{S}_i^\dagger(\omega')\right] + e^{-i(\omega-\omega')t}\Gamma_{ji}^\dagger\left[\hat{S}_j(\omega), \tilde{\rho}(t)\hat{S}_i^\dagger(\omega')\right], \tag{3.16}$$

where $\Gamma_{kl}(\omega)$ contains the effect of the environment and it is defined as

$$\Gamma_{ij}(\omega) = \int_0^{\infty} ds e^{i\omega s} \operatorname{Tr}\left[\tilde{E}_i^{\dagger}(t)\tilde{E}_j(t-s)\hat{\rho}_E(0)\right]. \tag{3.17}$$

Here, the operator $\tilde{E}_j(t) = e^{i\hat{H}_E t}\hat{E}_j e^{-i\hat{H}_E t}$ is in the interaction picture. It does not depend on time since the environment is in a stationary state and the correlation function of the environment decay extremely fast.

Now, we make the final assumption: we consider the system in the rotating wave approximation. The terms proportional to $|\omega - \omega'| \gg \alpha^2$ will oscillate much faster than the timescale of the system; thus, they do not contribute to its evolution. In the low-coupling regime, $\alpha \to 0$, we can consider that only the resonant terms, $\omega = \omega'$, contribute to the dynamics and remove all the others. Therefore, the equation (3.16) reduces to

$$\frac{d\tilde{\rho}(t)}{dt} = \sum_{\omega,i,j} \Gamma_{ij}\left[\hat{S}_j(\omega)\tilde{\rho}(t), \hat{S}_i^{\dagger}(\omega)\right] + \Gamma_{ji}^{\dagger}\left[\hat{S}_j(\omega), \tilde{\rho}(t)\hat{S}_i^{\dagger}(\omega)\right]. \tag{3.18}$$

The operators $\Gamma_{ij}(\omega)$ are not necessarily Hermitian. Thus, we divide them into the Hermitian and not Hermitian parts, such that $\Gamma_{ij}(\omega) = \frac{1}{2}\gamma_{ij}(\omega) + i\pi_{ij}(\omega)$. They yields respectively

$$\begin{aligned}\gamma_{ij}(\omega) &= \Gamma_{ij}(\omega) + \Gamma_{ij}^{\dagger}(\omega) = \int_{-\infty}^{\infty} ds e^{i\omega s} \operatorname{Tr}\left[\left\{\tilde{E}_i^{\dagger}(t), \tilde{E}_j(t-s)\right\}\hat{\rho}_E(0)\right] \\ \pi_{ij}(\omega) &= \frac{-i}{2}\left(\Gamma_{ij}(\omega) - \Gamma_{ij}^{\dagger}(\omega)\right) = \int_{-\infty}^{\infty} ds e^{i\omega s} \operatorname{Tr}\left[\left[\tilde{E}_i^{\dagger}(t), \tilde{E}_j(t-s)\right]\hat{\rho}_E(0)\right]\end{aligned} \tag{3.19}$$

Inserting them into the equation (3.18) and returning to the Schrödinger picture, we obtain

$$\frac{d}{dt}\hat{\rho} = -i\left[\hat{H} + \hat{H}_{LS}, \hat{\rho}\right] + \sum_{i,j,\omega} \gamma_{ij}(\omega)\left(\hat{S}_i(\omega)\hat{\rho}\hat{S}_j^{\dagger}(\omega) - \frac{1}{2}\left\{\hat{S}_i^{\dagger}(\omega)\hat{S}_j(\omega), \hat{\rho}\right\}\right), \tag{3.20}$$

where $\hat{H}_{LS} = \sum_{\omega,i,j} \pi_{ij}(\omega)\hat{S}_i^{\dagger}(\omega)\hat{S}_j(\omega)$ is called Lamb shift Hamiltonian. It adjusts the energy levels due to the interaction with the environment. The equation (3.20) is the general version of the Markovian master equation. The matrix $\gamma(\omega)$ must be positive definite, although the trace preservation of the dynamics is not guaranteed.

If the matrix $\gamma(\omega)$ can be diagonalized, namely exist a diagonal matrix $D = \hat{O}\gamma(\omega)\hat{O}^{\dagger}$ with $\hat{O}$ being a unitary operator, we can write the Lindblad-Gorini-Kossakowski-Sudarshan master equation as

$$\frac{d}{dt}\hat{\rho} = \mathcal{L}\left[\hat{\rho}\right] = -i\left[\hat{H} + \hat{H}_{LS}, \hat{\rho}\right] + \sum_k \gamma_k(\omega)\left(\hat{J}_k(\omega)\hat{\rho}\hat{J}_k^{\dagger}(\omega) - \frac{1}{2}\left\{\hat{J}_k^{\dagger}(\omega)\hat{J}_k(\omega), \hat{\rho}\right\}\right). \tag{3.21}$$

The operators $\hat{J}_k(\omega) = \sum_i O_{ki}\hat{S}_i(\omega)$ are called jump operators, the superoperator $\mathcal{L}$ is called Lindblad superoperator and $\gamma_i(\omega)$ are the damping rates. In the limit $\gamma_k(\omega) = 0$ the von Neumann equation is recovered with the Hamiltonian $\hat{H} + \hat{H}_{LS}$.

3.2 Time evolution

In this section, we present a solution for the Lindblad master equation [41]. First, we vectorize the density matrix: let introduce an Hilbert space with dimension N^2 such that a vector is $|\rho\rangle\rangle = (\rho_{00}, \rho_{01}, ..., \rho_{NN-1}, \rho_{NN})^T$ and the scalar product is $\langle\langle\phi\,|\,\rho\rangle\rangle = \mathrm{Tr}[\hat{\phi}^\dagger\hat{\rho}]$. This is known as the Fock-Liouville space [38].

The follow operation can be vectorize as

$$\hat{A}\hat{\rho}\hat{B} \to (\hat{A}\otimes\hat{B})|\rho\rangle\rangle \qquad \hat{A}\hat{\rho} + \hat{\rho}\hat{B} \to \left(\hat{A}\otimes\mathbb{I} + \mathbb{I}\otimes\hat{B}\right)|\rho\rangle\rangle, \tag{3.22}$$

where $\mathbb{I}$ is the identity matrix, $\hat{A}$ and $\hat{B}$ are two generic operator. The symbol $\otimes$ denotes the tensorial product which generates a $N^2 \times N^2$ matrix defined as

$$\hat{A}\otimes\hat{B} = \begin{pmatrix} A_{11}\hat{B} & \cdots & A_{1N}\hat{B} \\ \vdots & \ddots & \vdots \\ A_{n1}\hat{B} & \cdots & A_{NN}\hat{B} \end{pmatrix}. \tag{3.23}$$

Further details can be found in the Appendix C.

In this space the Lindblad equation (3.21) becomes

$$\frac{d}{dt}|\rho(t)\rangle\rangle = \tilde{\mathcal{L}}|\rho(t)\rangle\rangle, \tag{3.24}$$

where $\tilde{\mathcal{L}}$ is the operator

$$\tilde{\mathcal{L}} = -i\left[\hat{H}\otimes\mathbb{I} - \mathbb{I}\otimes\hat{H}\right] + \sum_k \gamma_k \left[\hat{J}_k\otimes\hat{J}_k^\dagger + \hat{J}_k^\dagger\hat{J}_k\otimes\mathbb{I} + \mathbb{I}\otimes\hat{J}_k^\dagger\hat{J}_k\right]. \tag{3.25}$$

The solution to the equation (3.24) can be written as

$$|\rho(t)\rangle\rangle = \hat{U}(t,0)|\rho(0)\rangle\rangle, \tag{3.26}$$

where $U(t,0)$ is the evolution operator

$$\begin{aligned} \hat{U}(t,0) = \exp\Bigg\{&-it\left(\hat{H}\otimes\mathbb{I} - \mathbb{I}\otimes\hat{H}\right) \\ &+ t\sum_k \gamma_k \left[\hat{J}_k\otimes\hat{J}_k^\dagger - \frac{1}{2}\hat{J}_k\hat{J}_k^\dagger\otimes\mathbb{I} - \frac{1}{2}\mathbb{I}\otimes\hat{J}_k\hat{J}_k^\dagger\right]\Bigg\} \end{aligned} \tag{3.27}$$

The evolution operator is not unitary.

Depending on the choice of the jump operators and of the damping rates, the density matrix can converge to a stationary distribution. Some cases are discussed in [39] where the stationary distribution corresponds to the Boltzmann distribution. In other scenarios, some stationary currents between the states may persist leading to a not equilibrium stationary solution, or the system may not converge altogether.

3.3 Properties of the Lindblad equation

The Lindblad master equation satisfies some important properties.

It defines a set of dynamical maps $\phi_t\left(\hat{\rho}\right) = e^{\mathcal{L}t}\hat{\rho}(0)$ on the space of density matrices, such that

$$\hat{\rho}(t) = \phi_t\left(\hat{\rho}(0)\right). \tag{3.28}$$

These maps have the semigroup property, that is

$$\phi_s\left(\phi_t\left(\hat{\rho}(0)\right)\right) = \phi_{t+s}\left(\hat{\rho}(0)\right) \tag{3.29}$$

The Lindblad master equation is the most general form for the generator of a quantum dynamical semigroup. As a matter of fact, the Lindblad equation can also be derived from this assumption [39].

The Lindblad master equation is invariant under the following transformations [39]:

- Unitary transformation of the Lindblad operator:

$$\sqrt{\gamma_i}\hat{J}_i \rightarrow \sqrt{\gamma_i'}\hat{J}_i' = \sum_j u_{ij}\sqrt{\gamma_j}\hat{J}_j \tag{3.30}$$

  where u_{ij} is an unitary matrix.

- Inhomogeneous transformation:

$$\begin{aligned} \hat{J}_i &\rightarrow \hat{J}_i' = \hat{J}_i + a_i\mathbb{I} \\ \hat{H}_I &\rightarrow \hat{H}' = \hat{H} + \frac{1}{2i}\sum_j \gamma_j\left(a_j^*\hat{J}_j - a_j\hat{J}_j^\dagger\right) + b\mathbb{I} \end{aligned} \tag{3.31}$$

  where $a_i \in \mathbf{C}$ and $b \in \mathbf{R}$, $\mathbb{I}$ is the identity matrix.

The latter transformation allows us to always choose a traceless jump operator.

Lastly, we can prove that the dynamics (3.32) conserve the trace of the density matrix. As a matter of fact, its time derivative is given by

$$\frac{d}{dt}\operatorname{Tr}[\hat{\rho}] = \operatorname{Tr}\left[-i\left(\hat{H}\hat{\rho} - \hat{\rho}\hat{H}\right) + \hat{J}_k\hat{\rho}\hat{J}_k^\dagger - \frac{1}{2}\left(\hat{H}\hat{\rho} + \hat{\rho}\hat{H}\right)\right] = 0, \tag{3.32}$$

we have use the cyclic property of the trace. However, it is important to note that the Lindblad master equation does not conserve the purity $\operatorname{Tr}\left[\hat{\rho}^2\right]$ that decreases [38].

3.4 Entropy production

In thermodynamics, the irreversibility of a process is encoded in the entropy function: a process is reversible if and only if it does not produce entropy, otherwise it is irreversible. Thus, the entropy of the universe should be conserved, namely the entropy produce by the process is $\Delta S_T = 0$. This is the second law of the thermodynamics, which assures that the of the universe can not decrease, i.e. $\Delta S_T \geq 0$. The Lindblad equation should satisfy this requirement.

In fact, considering the derivative of the von Neumann entropy

$$\dot{S}\left(\hat{\rho}(t)\right) = -\operatorname{Tr}\left[\frac{d\hat{\rho}}{dt}\ln\hat{\rho}\right] + \operatorname{Tr}\left[\frac{d\hat{\rho}}{dt}\right]. \tag{3.33}$$

Knowing that the dynamics is trace preserving, $\operatorname{Tr}\left[\frac{d\hat{\rho}}{dt}\right] = 0$. the equation (3.33) reduces to

$$\dot{S}\left(\hat{\rho}(t)\right) = -\operatorname{Tr}\left[\frac{d\hat{\rho}}{dt}\ln\hat{\rho}\right]. \tag{3.34}$$

To prove that the Lindblad dynamics (3.21) satisfies the second law, we can substitute it into (3.34). The von Neumann dynamical part does not produce entropy, thus, we can only consider the dissipative one. We reach the equation

$$\dot{S}(\hat{\rho}) = -\operatorname{Tr}\left[\sum_k \gamma_k\left[\hat{J}_k\hat{\rho}\hat{J}_k^\dagger - \frac{1}{2}\left\{\hat{J}_k^\dagger\hat{J}_k, \hat{\rho}\right\}\right]\ln\hat{\rho}\right]. \tag{3.35}$$

We expand the commutator obtaining

$$\dot{S}(\hat{\rho}) = -\sum_k \gamma_k \operatorname{Tr}\left[\hat{J}_k\hat{\rho}\hat{J}_k^\dagger\ln\hat{\rho} - \frac{1}{2}\hat{J}_k^\dagger\hat{J}_k\hat{\rho}\ln\hat{\rho} - \frac{1}{2}\hat{\rho}\hat{J}_k^\dagger\hat{J}_k\ln\hat{\rho}\right]. \tag{3.36}$$

Since $\ln\hat{\rho}$ and $\hat{\rho}$ commute, the second and third terms can be summed.

$$\dot{S}(\hat{\rho}) = -\sum_k \gamma_k\left(\operatorname{Tr}\left[\hat{J}_k\hat{\rho}\hat{J}_k^\dagger\ln\hat{\rho}\right] - \operatorname{Tr}\left[\hat{J}_k^\dagger\hat{J}_k\hat{\rho}\ln\hat{\rho}\right]\right). \tag{3.37}$$

We can reduce the two traces. First, we diagonalize the density matrix. Let $|\lambda\rangle$ be the eigenstate with eigenvalue λ, the density matrix can be written as

$$\hat{\rho} = \sum_\lambda \rho_\lambda|\lambda\rangle\langle\lambda|. \tag{3.38}$$

We also transform the jump operator in this basis $\hat{\mathcal{J}}_k = \hat{O}\hat{J}_k\hat{O}^\dagger$. The first one with some algebra can be reduces to

$$\begin{aligned}\operatorname{Tr}\left[\hat{J}_k\hat{\rho}\hat{J}_k^\dagger\ln\hat{\rho}\right] &= \sum_{\lambda\mu}\operatorname{Tr}\left[\hat{\mathcal{J}}_k\rho_\lambda|\lambda\rangle\langle\lambda|\hat{\mathcal{J}}_k^\dagger\ln\rho_\mu|\mu\rangle\langle\mu|\right] \\ &= \sum_{\lambda\mu}\rho_\lambda\ln\rho_\mu\operatorname{Tr}\left[|\langle\mu|\hat{\mathcal{J}}_k|\lambda\rangle|^2\right] \\ &= N\sum_{\lambda\mu}\rho_\lambda\ln\rho_\mu x_{\lambda\mu}^{(k)}.\end{aligned} \tag{3.39}$$

where $x_{\lambda\mu}^{(k)} = |\langle\mu|\hat{\mathcal{J}}_k|\lambda\rangle|^2$ is a non negative scalar. It is symmetric respect the change $\lambda \leftrightarrow \mu$.

The other term becomes

$$\begin{aligned}\mathrm{Tr}\left[\hat{J}_k^\dagger \hat{J}_k \hat{\rho} \ln \hat{\rho}\right] &= \sum_{\lambda\mu} \mathrm{Tr}\left[\hat{\mathcal{J}}_k^\dagger \hat{\mathcal{J}}_k \rho_\lambda |\lambda\rangle\langle\lambda| \ln \rho_\mu |\mu\rangle\langle\mu|\right] \\ &= \sum_{\lambda\mu} \rho_\lambda \ln \rho_\lambda \, \mathrm{Tr}\left[\langle\mu|\hat{\mathcal{J}}_k^\dagger \hat{\mathcal{J}}_k|\lambda\rangle\langle\lambda\,|\,\mu\rangle\right] \\ &= \sum_{\lambda} \rho_\lambda \ln \rho_\lambda \, \mathrm{Tr}\left[\langle\lambda|\hat{\mathcal{J}}_k^\dagger \hat{\mathcal{J}}_k|\lambda\rangle\right].\end{aligned} \tag{3.40}$$

The second braket in the trace is simply a Kronecker delta. Using the completeness relation $I = \sum_\mu |\mu\rangle\langle\mu|$ we obtain

$$\begin{aligned}\mathrm{Tr}\left[\hat{J}_k^\dagger \hat{J}_k \hat{\rho} \ln \hat{\rho}\right] &= \sum_{\lambda\mu} \rho_\lambda \ln \rho_\lambda \, \mathrm{Tr}\left[\langle\lambda|\hat{\mathcal{J}}_k^\dagger|\mu\rangle\langle\mu|\hat{\mathcal{J}}_k|\lambda\rangle\right] \\ &= N \sum_{\lambda\mu} \rho_\lambda \ln \rho_\lambda x_{\lambda\mu}^{(ij)}.\end{aligned} \tag{3.41}$$

The the deivative of the system's entropy (3.37) yields

$$\dot{S}(\hat{\rho}) = -N \sum_{\lambda\mu} \gamma_{\lambda\mu}\rho_\lambda \ln \rho_\mu x_{\lambda\mu}^{(k)} + N \sum_{\lambda\mu} \gamma_{\lambda\mu}\rho_\lambda \ln \rho_\lambda x_{\lambda\mu}^{(k)}. \tag{3.42}$$

We can add and subtract the term $\ln \gamma_{\lambda\mu}$ such that the equation (3.42) becomes

$$\dot{S}(\hat{\rho}) = -\sum_{\lambda\mu} \gamma_{\lambda\mu}\rho_\lambda x_{\lambda\mu}^{(k)} \left(\ln\left(\rho_\mu \gamma_{\lambda\mu}\right) - \ln \gamma_{\lambda\mu}\right) + \sum_{\lambda\mu} \gamma_{\lambda\mu}\rho_\lambda x_{\lambda\mu}^{(k)} \left(\ln\left(\rho_\lambda \gamma_{\mu\lambda}\right) - \ln \gamma_{\mu\lambda}\right). \tag{3.43}$$

Rearrange the terms, we reach

$$\dot{S}(\hat{\rho}) = -\sum_{\lambda\mu} \gamma_{\lambda\mu}\rho_\lambda x_{\lambda\mu}^{(k)} \left(\ln\left(\rho_\mu \gamma_{\lambda\mu}\right) - \ln\left(\rho_\lambda \gamma_{\mu\lambda}\right)\right) + \sum_{\lambda\mu} \gamma_{\lambda\mu}\rho_\lambda x_{\lambda\mu}^{(k)} \left(\ln \gamma_{\lambda\mu} - \ln \gamma_{\mu\lambda}\right). \tag{3.44}$$

Here, the first term represent the entropy of the universe, in contrast, the second one represents the work done by the environment to the system. Thus, in order to satisfy the second law of thermodynamics the entropy of the universe must not decrease, meaning

$$\sum_{\lambda\mu} \gamma_{\lambda\mu}\rho_\lambda x_{\lambda\mu}^{(k)} \ln\left(\rho_\mu \gamma_{\lambda\mu}\right) \le \sum_{\lambda\mu} \gamma_{\lambda\mu}\rho_\lambda x_{\lambda\mu}^{(k)} \ln\left(\rho_\lambda \gamma_{\mu\lambda}\right). \tag{3.45}$$

We can rearrange the term in the two sum as

$$\begin{aligned}&\sum_{\lambda}\sum_{\mu<\lambda} \left(\gamma_{\lambda\mu}\rho_\lambda \ln\left(\gamma_{\lambda\mu}\rho_\mu\right) + \gamma_{\mu\lambda}\rho_\mu \ln\left(\gamma_{\mu\lambda}\rho_\lambda\right)\right) x_{\lambda\mu}^{(k)} + \sum_{\lambda} \gamma_{\lambda\lambda}\rho_\lambda \ln\left(\gamma_{\lambda\lambda}\rho_\lambda\right) x_{\lambda\lambda}^{(k)} \le \\ &\quad \sum_{\lambda}\sum_{\mu<\lambda} \left(\gamma_{\lambda\mu}\rho_\lambda \ln\left(\gamma_{\mu\lambda}\rho_\lambda\right) + \gamma_{\mu\lambda}\rho_\mu \ln\left(\gamma_{\lambda\mu}\rho_\mu\right)\right) x_{\lambda\mu}^{(k)} + \sum_{\lambda} \gamma_{\lambda\lambda}\rho_\lambda \ln\left(\gamma_{\lambda\lambda}\rho_\lambda\right) x_{\lambda\lambda}^{(k)}.\end{aligned} \tag{3.46}$$

Therefore, it is sufficient that the following equation is satisfied

$$\gamma_{\lambda\mu}\rho_\lambda \ln\left(\gamma_{\lambda\mu}\rho_\mu\right) + \gamma_{\mu\lambda}\rho_\mu \ln\left(\gamma_{\mu\lambda}\rho_\lambda\right) \le \gamma_{\lambda\mu}\rho_\lambda \ln\left(\gamma_{\mu\lambda}\rho_\lambda\right) + \gamma_{\mu\lambda}\rho_\mu \ln\left(\gamma_{\lambda\mu}\rho_\mu\right) \tag{3.47}$$

Moving all the term in the right hand side and collecting the terms, we reach

$$(\gamma_{\lambda\mu}\rho_\lambda - \gamma_{\mu\lambda}\rho_\mu)\ln\left(\frac{\gamma_{\lambda\mu}\rho_\mu}{\gamma_{\mu\lambda}\rho_\lambda}\right) \leq 0, \tag{3.48}$$

which is always satisfied. The equality is satisfied for the reversible processes. The last result tell us that the dynamics increases the entropy of the universe, thus, the Lindblad master equation (3.21) is in accordance with the second law of thermodynamics.

Chapter 4

Quantum Network Master Equation

In Chapter 2 we have introduced the concept of the density matrix for a network, derived by the communicability matrix. This quantity captures the correlations between the nodes in a random walk dynamics.

In this chapter, we aim to unify the two concept taken from the quantum realm we have introduced: the quantum walk and the network's density matrix. Specifically, by examining a quantum walk process subjected to thermal noise, we derive a stationary distribution which coincides with the network's density matrix. The interaction between the quantum system and the thermal noise are treated as Markovian, that is they do not depends on the past, and thus, we study them using the Lindblad master equation.

4.1 Quantum Stochastic Random Walk

One of the early approaches to a Open Quantum Walk on network was proposed by Whitfield, Rodríguez-Rosario and Aspuru-Guzik. [42]. They defined a quantum walk on network in contact with a thermal bath with the dynamics described by a Lindblad master equation. In this framework, the jump operators are proportional to the adjacency matrix A_{ij} of the network. The thermal bath introduces noise into the dynamics, causing it which to deviate from the von Neumann equation (1.41). The system dissipation is reminiscent of the classic random walk.

Let us consider a quantum walk on a network $G(N, M)$, the system in contact with a thermal bath that randomly interact with modifying the dynamic of the quantum particle. Let us introduce a Hilbert space $\mathcal{H}$ with an orthonormal basis $\{|i\rangle\}_{i<N}$, where each element $|i\rangle$ corresponds to the node i, satisfying $\langle i \mid j\rangle = \delta_{ij}$. The system is described by a density matrix $\hat{\rho}$ whose evolution follows the Lindblad master equation (3.32). The Laplacian operator $\hat{L}$, defined as in equation (1.33), serves as the Hamiltonian $\hat{H}$, while the jump operators $\{\hat{J}_k\}_{k<M}$ represent the thermal jumps between two node linked together. For convenience, we will denote the jump operator with two indeces referring to the starting node j and the ending node i of the jump: therefore, the jumps operator are $\hat{J}_{ij} = |i\rangle\langle j|$. The damping rates are $\gamma_{ij} = A_{ij}/d_i$, like the transition rates in the classical

random walk (1.10). The master equation can be expressed as follows:

$$\frac{d}{dt}\hat{\rho} = -\frac{i}{2}\left[\hat{L},\hat{\rho}\right] + \sum_{ij}\gamma_{ij}\left[\hat{J}_{ij}\hat{\rho}\hat{J}_{ij}^{\dagger} - \frac{1}{2}\left\{\hat{J}_{ij}^{\dagger}\hat{J}_{ij},\hat{\rho}\right\}\right], \tag{4.1}$$

where $[\cdot,\cdot]$ and $\{\cdot,\cdot\}$ denote respectively the commutator and the anticommutator. The equation (4.1) is composed by two distinct terms. The first term, also called coherent dynamics, is given by $\mathcal{L}^{qm}\left[\hat{\rho}(t)\right] = -i\left[H,\hat{\rho}\right]$ is equal to the quantum walk dynamics. In contrast, the second term, denoted as $\mathcal{L}^{cl}\left[\hat{\rho}(t)\right] = \sum_i \gamma_i\left(\hat{J}_i\hat{\rho}\hat{J}_i^{\dagger} - \frac{1}{2}\left\{\hat{J}_i^{\dagger}\hat{J}_i,\hat{\rho}\right\}\right)$, called decoherent dynamics, encodes the dissipation. When $\gamma_{ij} = 0$ we recover the von Neumann equation for the quantum walk (1.41). $\mathcal{L}\left[\hat{\rho}(t)\right]$ act as a superoperator in the space of the density matrix.

In the Fock-Liouville space, the quantum system evolves according the equation

$$|\rho(t)\rangle\rangle = U(t,0)|\rho(0)\rangle\rangle \tag{4.2}$$

where the evolution operator is defined as [43]

$$\begin{aligned}\hat{U}(t,0) = \exp\Bigg\{&-it\left(\hat{H}\otimes\mathbb{I} - \mathbb{I}\otimes\hat{H}\right)\\ &+ t\sum_{ij}\gamma_{ij}\left[\hat{J}_{ij}\otimes\hat{J}_{ij}^{\dagger} - \frac{1}{2}\hat{J}_{ij}\hat{J}_{ij}^{\dagger}\otimes\mathbb{I} - \frac{1}{2}\mathbb{I}\otimes\hat{J}_{ij}\hat{J}_{ij}^{\dagger}\right]\Bigg\}.\end{aligned} \tag{4.3}$$

The master equation (4.1) contains both the quantum and classical aspects of a random walk over a network. As a matter of fact, the classical random walk behavior emerges when we consider the evolution of the diagonal elements of the density matrix under the dissipative part alone. Let $\rho = |k\rangle\langle k|$ represent the density matrix of a system localized at node k. Its evolution is given by

$$\begin{aligned}\mathcal{L}^{cl}|k\rangle\langle k| &= \sum_{ij}\gamma_{ij}\left[\hat{J}_{ij}|k\rangle\langle k|\hat{J}_{ij}^{\dagger} - \frac{1}{2}\left\{\hat{J}_{ij}^{\dagger}\hat{J}_{ij},|k\rangle\langle k|\right\}\right]\\ &= \sum_{i}\left[\gamma_{ik}|i\rangle\langle i| - \gamma_{ik}|k\rangle\langle k|\right]\\ &= \sum_{i}\left(\gamma_{ki} - \gamma_{ki}\delta_{ki}\right)|i\rangle\langle i| = -\sum_{i}L_{ki}|i\rangle\langle i|.\end{aligned} \tag{4.4}$$

where d_i is the degree of the node i. This expression recovers the dynamics of the classical random walk over the network. Next, considering the off-diagonal terms, their evolution is described by

$$\begin{aligned}\mathcal{L}^{cl}|k\rangle\langle l| &= \sum_{ij}\gamma_{ij}\left[\hat{J}_{ij}|k\rangle\langle l|\hat{J}_{ij}^{\dagger} - \frac{1}{2}\left\{\hat{J}_{ij}^{\dagger}\hat{J}_{ij},|k\rangle\langle l|\right\}\right]\\ &= \sum_{j}\left[-\frac{1}{2}\gamma_{jk}|k\rangle\langle l| - \frac{1}{2}\gamma_{jl}|k\rangle\langle l|\right]\\ &= -|k\rangle\langle l|.\end{aligned} \tag{4.5}$$

The operator $\mathcal{L}^{cl}$ does not mix the diagonal terms with the off-diagonal ones, allowing us to separate the superoperator into two blocks: one for the diagonal element and the another for the off-diagonal ones. Thus, the superoperator $\mathcal{L}^{cl}$ has a diagonal form with spectrum given by $\sigma^{cl} = -(\lambda_1, ..., \lambda_N, 1, ..., 1))$, where λ_i are the eigenvalue of the Laplacian matrix [44]. If the network satisfies the detailed balance condition (1.19), the Laplacian matrix has a zero eigenvalue. Therefore, the superoperator $\mathcal{L}^{cl}$ will also have a zero eigenvalue indicating the presence of a stationary distribution.

4.1.1 Stationary distribution

Following the proof of the stationary distribution in Chapter 3, we can find the stationary density matrix $\hat{\rho}^*$ for the quantum stochastic walk. We will consider only the dissipative dynamics, which decouples the diagonal and off-diagonal terms. The evolution of the diagonal elements is described by:

$$\frac{d}{dt}\rho_{ii} = \sum_j \left[\gamma_{ij}\rho_{jj}(t) - \gamma_{ji}\rho_{ii}(t)\right], \tag{4.6}$$

The stationary distribution must satisfy the detail balance, namely

$$\gamma_{ij}\rho_{jj}(t) = \gamma_{ji}\rho_{ii}. \tag{4.7}$$

Because the damping rates fort this system are symmetric, the diagonal entries must be equal. Instead, considering the vector $|\rho\rangle\rangle$, the block corresponding to the off-diagonal part of $\mathcal{L}$ is already eigenstate with eigenvalue 1. Thus, the off-diagonal terms must be equal to zero. The stationary density matrix can then be expressed as

$$\hat{\rho}^* = \frac{1}{N}\begin{pmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{pmatrix}. \tag{4.8}$$

As discussed in chapter 3.4, the stationary density matrix has maximal von Neumann entropy

$$S\left(\hat{\rho}^*\right) = \ln N. \tag{4.9}$$

The density matrix (4.8) commutes with the Laplacian matrix, confirming that it is indeed the stationary density matrix for the dynamics described by (4.1).

4.2 Quantum Network Master Equation

The previous description of noise in quantum walk lacks of parameter that in thermodynamics correspond to the temperature. Thus, we change picture: instead of considering the noise on the node's basis, we consider the thermal bath interaction in the energy's basis. Let retake the standard Lindblad equation (3.21) with Hamiltonian $\hat{H} = \hat{L}$. We consider the basis $\{|\lambda\rangle\}_\lambda$ such that $\hat{H} = \sum_\lambda \lambda|\lambda\rangle\langle\lambda| = \hat{L}$ is diagonal (the network must hold the detail balance condition (1.19)). We define the jump operator $\hat{J}_{\lambda\mu} = |\lambda\rangle\langle\mu|$

as the jumps from the energy states $|\mu\rangle$ to the energy state $|\lambda\rangle$ obtaining the master equation

$$\frac{d}{dt}\hat{\rho} = -i\left[\hat{L}, \hat{\rho}\right] + \sum_{\lambda\mu} \gamma_{\lambda\mu} \left(\hat{J}_{\lambda\mu} \hat{\rho} \hat{J}^{\dagger}_{\lambda\mu} - \frac{1}{2} \left\{ \hat{J}^{\dagger}_{\lambda\mu} \hat{J}_{\lambda\mu}, \hat{\rho} \right\} \right), \tag{4.10}$$

the coefficients $\gamma_{\lambda\mu}$ indicate the probability to take their respective jumps.

We assume that the dynamics will tend to a stationary distribution in the form of

$$\hat{\rho}^{*} = \frac{e^{-\beta \hat{L}}}{Z}, \tag{4.11}$$

with $Z = \mathrm{Tr}\left[e^{-\beta \hat{L}}\right]$ is the partition function. The master equation for the stationary distribution (4.11) reduces to

$$0 = -i\left[\hat{H}, \frac{e^{-\beta \hat{L}}}{Z}\right] + \sum_{\lambda\mu} \gamma_{\lambda\mu} \left(\hat{J}_{\lambda\mu} \frac{e^{-\beta \hat{L}}}{Z} \hat{J}^{\dagger}_{\lambda\mu} - \frac{1}{2} \left\{ \hat{J}^{\dagger}_{\lambda\mu} \hat{J}_{\lambda\mu}, \frac{e^{-\beta \hat{H}}}{Z} \right\} \right). \tag{4.12}$$

The first term in the r.h.s. vanishes since the commutator is zero. Now, we analyze the terms in the summation independently. The first one can be written as

$$\sum_{\lambda\mu} \gamma_{\lambda\mu} |\lambda\rangle\langle\mu| \frac{e^{-\beta \hat{L}}}{Z} |\mu\rangle\langle\lambda| = \sum_{\lambda\mu} \gamma_{\lambda\mu} \frac{e^{-\beta \epsilon_{\mu}}}{Z} |\lambda\rangle\langle\lambda|. \tag{4.13}$$

While the second becomes

$$\sum_{\lambda\mu} \gamma_{\lambda\mu} \left[\frac{1}{2} |\mu\rangle\langle\lambda \mid \lambda\rangle\langle\mu| \frac{e^{-\beta \hat{L}}}{Z} + \frac{1}{2} \frac{e^{-\beta \hat{L}}}{Z} |\mu\rangle\langle\lambda \mid \lambda\rangle\langle\mu| \right] = \sum_{\lambda\mu} \gamma_{\lambda\mu} \left[\frac{e^{-\beta \epsilon_{\mu}}}{Z} |\mu\rangle\langle\mu| \right]. \tag{4.14}$$

Therefore, inserting the equations (4.13) and (4.14) into the master equation (4.12) we obtain

$$\sum_{\lambda\mu} \left[\gamma_{\lambda\mu} \frac{e^{-\beta\mu}}{Z} - \gamma_{\mu\lambda} \frac{e^{-\beta\lambda}}{Z} \right] |\lambda\rangle\langle\lambda| = 0. \tag{4.15}$$

It is the Kirchhoff's current law that says that the sum of all the currents must vanish. The system should satisfy this request in order to have the Boltzmann distribution. However, fixed β, there are several possible choice for the coefficients $\gamma_{\lambda\mu}$ such that equation (4.15) holds. Each different choice generate a different path to reach the stationary distribution (4.11). We assume a strict condition, the detailed balance condition

We assume that the system must satisfy the maximal entropy production principle: the system should relax to the stationary distribution following the trajectory that has maximal entropy production. The principle is satisfied when the Kirchhoff law (4.15) reduces to the detail balance condition

$$\gamma_{\lambda\mu} \frac{e^{-\beta \epsilon_{\mu}}}{Z} - \gamma_{\mu\lambda} \frac{e^{-\beta \epsilon_{\lambda}}}{Z} = 0, \tag{4.16}$$

which has solution

$$\gamma_{\lambda\mu} = e^{-\frac{\beta}{2}(\epsilon_{\lambda} - \epsilon_{\mu})}. \tag{4.17}$$

Takin the limits $\beta \to \infty$, that is $T \to 0$, the transition rates tends to

$$\gamma_{\lambda\mu} \to \begin{cases} 0 & \lambda > \mu \\ 1 & \lambda = \mu \\ \infty & \lambda < \mu \end{cases} . \tag{4.18}$$

The transition from lower to higher energy state are suppressed, while the opposite one are extremely favorite. Thus, the system is led to the zero energy state that is the stationary state

$$\hat{\rho}^* = |\lambda = 0\rangle\langle\lambda = 0|. \tag{4.19}$$

It is a pure state therefore the von Neumann entropy vanishes.

The opposite limit $\beta \to 0$, that is $T \to \infty$, the transition rates becomes

$$\gamma_{\lambda\mu} \to 1. \tag{4.20}$$

We have the opposite effect, the particle can jump across the different energy state with uniform probability. Thus, the stationary distribution is the maximal entropy state, i.e. the uniform distribution.

$$\hat{\rho}^* = \frac{1}{N}\begin{pmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{pmatrix}. \tag{4.21}$$

It is a maximal entropy state $S = \ln N$.

4.2.1 Return to node's basis

We can go back to the position basis $\{|i\rangle\}_{i<N}$, where $|i\rangle$ indicates the particle in the node i. The jump operators can be expressed in this basis as

$$\hat{J}_{\lambda\mu} = \sum_{ij} \langle i \,|\, \lambda\rangle\langle\mu \,|\, j\rangle \hat{J}_{ij} \tag{4.22}$$

$$\hat{J}^\dagger_{\lambda\mu} = \sum_{ij} \langle j \,|\, \mu\rangle\langle\lambda \,|\, i\rangle \hat{J}^\dagger_{ij} \tag{4.23}$$

where $\hat{J}_{ij} = |i\rangle\langle j|$. Thus, the equation (4.10) becomes

$$\frac{d}{dt}\hat{\rho} = -i\left[\hat{H}, \hat{\rho}\right] + \sum_{ijkl} \gamma_{ij;kl}\left(\hat{J}_{ij}\hat{\rho}\hat{J}^\dagger_{kl} - \frac{1}{2}\left\{\hat{J}^\dagger_{kl}\hat{J}_{ij}, \hat{\rho}\right\}\right), \tag{4.24}$$

with the damping coefficient

$$\gamma_{ij;kl} = \sum_{\lambda\mu} \gamma_{\lambda\mu}\langle i \,|\, \lambda\rangle\langle\lambda \,|\, k\rangle\langle l \,|\, \mu\rangle\langle\mu \,|\, j\rangle. \tag{4.25}$$

The master equation (4.24) is more complicated because its formulate in the general form (3.20). The damping rates are no more diagonal. Inserting the equation (4.17) into (4.25), the damping rates in this basis are

$$\gamma_{ij;kl} = \sum_{\lambda\mu} e^{-\frac{\beta}{2}(\epsilon_\lambda - \epsilon_\mu)}\langle i \,|\, \lambda\rangle\langle\lambda \,|\, k\rangle\langle l \,|\, \mu\rangle\langle\mu \,|\, j\rangle. \tag{4.26}$$

Taking again the two limits, in the extremely hot environment, $\beta \to 0$, the damping rates are

$$\gamma_{ij;kl} = \sum_{\lambda\mu} 1 \langle i \,|\, \lambda\rangle\langle\lambda \,|\, k\rangle\langle l \,|\, \mu\rangle\langle\mu \,|\, j\rangle. \tag{4.27}$$

Using the completeness relation we reach

$$\gamma_{ij;kl} = 1\delta_{ik}\delta_{jl}, \tag{4.28}$$

where δ_{ik} is the Kronecker delta. Thus, the particle travel always through the same link. In this case the position quantum network master equation (4.24) acquires a "symmetric" form

$$\frac{d}{dt}\hat{\rho} = -i\left[\hat{H},\hat{\rho}\right] + \sum_{ij}\left(\hat{J}_{ij}\hat{\rho}\hat{J}_{ij}^{\dagger} - \frac{1}{2}\left\{\hat{J}_{ij}^{\dagger}\hat{J}_{ij},\hat{\rho}\right\}\right). \tag{4.29}$$

Since the relation (4.17) can be modify by a constant, we recover the master equation for the Quantum Stochastic Walk (4.1). The stationary distribution is

$$\hat{\rho}^{*} = \frac{1}{N}\begin{pmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{pmatrix}. \tag{4.30}$$

In contrast, in the extremely cold environment, $\beta \to \infty$, the damping coefficient are

$$\begin{aligned} \gamma_{ij;kl} = {} & \sum_{\lambda\mu} e^{-\frac{\beta}{2}(\epsilon_\lambda - \epsilon_\mu)}\langle i \,|\, \lambda\rangle\langle\lambda \,|\, k\rangle\langle l \,|\, \mu\rangle\langle\mu \,|\, j\rangle\Theta(\lambda-\mu) \\ & + \sum_{\lambda\mu} 1\langle i \,|\, \lambda\rangle\langle\lambda \,|\, k\rangle\langle l \,|\, \mu\rangle\langle\mu \,|\, j\rangle\delta_{\lambda\mu} \\ & + \sum_{\lambda\mu} e^{-\frac{\beta}{2}(\epsilon_\lambda - \epsilon_\mu)}\langle i \,|\, \lambda\rangle\langle\lambda \,|\, k\rangle\langle l \,|\, \mu\rangle\langle\mu \,|\, j\rangle\Theta(\mu-\lambda) \end{aligned} \tag{4.31}$$

The first term cancel out, and the second is a sum of Kronecker delta. Thus, it reduces to

$$\gamma_{ij;kl} = \sum_{\lambda}\langle i \,|\, \lambda\rangle\langle\lambda \,|\, k\rangle\langle l \,|\, \lambda\rangle\langle\lambda \,|\, j\rangle + \sum_{\mu>\lambda}\infty\langle i \,|\, \lambda\rangle\langle\lambda \,|\, k\rangle\langle l \,|\, \mu\rangle\langle\mu \,|\, j\rangle \to \infty \tag{4.32}$$

The stationary distribution (4.19) for the node reduces to

$$\hat{\rho}^{*} = \sum_{ij}\langle i \,|\, \lambda = 0\rangle\langle\lambda = 0 \,|\, j\rangle|i\rangle\langle j| = \sqrt{\rho_i^{*}\rho_j^{*}}|i\rangle\langle j| \tag{4.33}$$

The von Neumann entropy vanishes.

Collegare a overdamped case

4.2.2 Interpretation

The equation (4.10) describes the evolution of a quantum walk in presence of a classic noise, the temperature T determines the noise strength. If we start from the stationary state and we add a perturbation in one node, the spread of the perturbation across the network depends on temperature: higher is the temperature, fewer nodes the perturbation can reach. Thus, the parameter β permits us to analyze the system's dynamics over paths of varying length.

In addition, we can apply a Wick rotation to the quantum dynamics (4.10) returning to a special random walk of classic particle. The rotation connect the stationary distribution at inverse temperature β (4.11) with the propagator at time t (1.15).

$$e^{-\beta\hat{L}} \to e^{-t\hat{L}} \tag{4.34}$$

Thus, cooling down the quantum system is similar to the temporal evolution of the classical one. In fact, the two limits $\beta \to \infty$ and $t \to \infty$ converge to the same distribution: the system will be entirely in the zero eigenstate of the Laplacian. Moreover, the density distribution (4.11) is always in the maximal entropy state, as a consequence, also the distribution for the classical random walk should cross state with maximal entropy.

The complexity of the possible paths is encoded into the von Neumann entropy as explained in chapter 2. The entropy allows us to classify different network based on the dynamical properties of the network itself. We can do it introducing the Kullback-Lieber divergence (2.56) and the Jensen-Shannon divergence (2.57). However, because this quantities employs the trace of a Laplacian's function, the entropy studies only the spectral properties of the system. Therefore, networks with same spectrum but different structure and eigenstate may be indistinguishable with these methods.

4.3 Generalization to other dynamic

Until now, we have examined only the random walk on network, but this framework can be generalize to other more complex dynamics on network [45]. The dynamics should be linear such that the evolution of the observable per node i are

$$\frac{d}{dt}x_i = \sum_j H_{ij}x_j, \tag{4.35}$$

where H_{ij} controls the evolution of the system. For the continuos time random walk the control matrix coincides with the Laplacian. In order to apply the Wick rotation and we obtain the quantum version of the system. Let $G(N, M)$ be a network, we introduce a Hilbert space $\mathcal{H}$ with orthonormal basis $\{|i\rangle\}_{i<N}$, the state $|\psi\rangle$ is defined as

$$|\psi\rangle = \sum_i \sqrt{x_i}|i\rangle \tag{4.36}$$

such that $x_i = |\langle i \mid \psi\rangle|^2$. The evolution follow the Schrödinger equation

$$\frac{d}{dt}|\psi(t)\rangle = -i\hat{H}|\psi(t)\rangle \tag{4.37}$$

where $\hat{H} = \sum_{ij} H_{ij}|i\rangle\langle j|$ is the control operator or the chosen dynamics. To satisfy the Schrödinger equation the control operator must be symmetric. Now we can add thermal noise arriving at quantum master equation (4.10) which has stationary distribution

$$\hat{\rho}^*_H = \frac{1}{Z} e^{-\beta \hat{H}} \tag{4.38}$$

with $Z = \mathrm{Tr}\left[e^{-\beta\hat{H}}\right]$ is the partition function.

Therefore, the network entropy for network under the dynamics (4.35) is

$$S_H(\beta) = -\,\mathrm{Tr}\left[\hat{\rho}^*_H \ln \hat{\rho}^*_H\right]. \tag{4.39}$$

Based on the considered dynamics the network will have a different entropy's value.

4.4 Symmetry breaking

Until now, we have considered the network holding the detail balance condition and, therefore, be mapped in a symmetric matrix; but the majority of the networks do not satisfy this condition.

To deal with them, we modify slightly the Lindblad master equation (4.1). As a matter of fact, in the chapter 3 we have analyzed also the case where the interaction with the environment is not symmetric (3.17). Thus, taking the dissipative part of the equation (3.18) in the Schrödinger picture with the coefficients $\Gamma_{ij} = L_{ij}$ and the jump operators $J_{ij} = |i\rangle\langle j|$ we obtain

$$\frac{d\hat{\rho}(t)}{dt} = \sum_{ij} \Gamma_{ij}\left[\hat{J}_j\hat{\rho}(t), \hat{J}_i^\dagger\right] + \Gamma^\dagger_{ji}\left[\hat{J}_j, \hat{\rho}(t)\hat{J}_i^\dagger\right]. \tag{4.40}$$

Isolating the symmetric and antisymmetric part of the Laplacian, respectively $\gamma_{ij} = (L_{ij} + L_{ji})$ and $\pi_{ij} = \frac{-i}{2}(L_{ij} - L_{ji})$ such that $\Gamma_{ij}(\omega) = \frac{1}{2}\gamma_{ij}(\omega) + i\pi_{ij}(\omega)$, we arrive to the equation

$$\frac{d\hat{\rho}(t)}{dt} = \sum_{ij} \gamma_{ij}\hat{J}_j\hat{\rho}(t)\hat{J}_i^\dagger - \frac{\gamma_{ij}}{2}\left\{\hat{J}_i^\dagger\hat{J}_j, \hat{\rho}(t)\right\} + i\pi_{ij}\left[\hat{J}_i^\dagger\hat{J}_j, \hat{\rho}(t)\right], \tag{4.41}$$

where $[\cdot,\cdot]$ and $\{\cdot,\cdot\}$ are respectively the commutator and anticommutator.

Let define a new Hamiltonian $\hat{H}_A = \sum_{ij} \pi_{ij}\hat{J}_i^\dagger\hat{J}_j$ that encodes the dynamics of the not symmetric part. It give origin to a coherent dynamics that follow the Von Neumann equation. As a matter of fact the total dynamics can be written as

$$\frac{d\hat{\rho}(t)}{dt} = i\left[\hat{H}_A, \hat{\rho}(t)\right] + \sum_{ij} \gamma_{ij}\hat{J}_j\hat{\rho}(t)\hat{J}_i^\dagger - \frac{\gamma_{ij}}{2}\left\{\hat{J}_i^\dagger\hat{J}_j, \hat{\rho}(t)\right\}. \tag{4.42}$$

The dynamics (4.42) does not converge no more to a stationary state due to the Von Neumann part. We can generalize as in the (4.1)

$$\frac{d}{dt}\hat{\rho} = -i\left[\hat{H} + \hat{H}_A, \hat{\rho}\right] + \sum_{ij} \gamma_{ij}\left[\hat{J}_{ij}\hat{\rho}\hat{J}_{ij}^\dagger - \frac{1}{2}\left\{\hat{J}_{ij}^\dagger\hat{J}_{ij}, \hat{\rho}\right\}\right]. \tag{4.43}$$

where $\hat{H}$ is the hermitian part of the Laplacian operator.

The quantum walk on network with a not hermitian Hamiltonian has a evolution operator that is not unitary. It can be split between the hermitian $\hat{H}_S$ and anti-hermitian $\hat{H}_A$ components as

$$U(t,0) = e^{-it\hat{H}_S} e^{-t\hat{H}_A} \tag{4.44}$$

with

$$\hat{H}_S = \frac{1}{2}\left(\hat{H} + \hat{H}^\dagger\right) \qquad \hat{H}_A = \frac{-i}{2}\left(\hat{H} - \hat{H}^\dagger\right) \tag{4.45}$$

If the Hamiltonian $\hat{H}$ is positive defined, the second exponential of the equation (4.44) dissipate energy. The system can be viewed as a quantum open system in exchanging energy with a thermal bath [46]. Thus, we can study it with Lindblad master equation (3.21) in the form

$$\frac{d}{dt}\hat{\rho} = -i\left[\hat{H}_S, \hat{\rho}\right] + \sum_k \gamma_k \left(\hat{J}_k \hat{\rho} \hat{J}_k^\dagger - \frac{1}{2}\left\{\hat{J}_k^\dagger \hat{J}_k, \hat{\rho}\right\}\right). \tag{4.46}$$

The jumps operators must reproduce the same dissipation as the anti-hermitian operator $\hat{H}_A$.

The damping coefficients do not have to hold the Kirchhoff law. Thus, the system may not converge to a stationary state, some some stationary density currents may persist or the system may not have an attractive distribution to converge.

Conclusion

The aim of this dissertation is to explore the connection between the network's entropy and the random walk, especially the quantum version.

The network's entropy permit us to introduce an information theory for networks, considering not only the topological properties but also the dynamical aspects. In this work, we prove that formulation for the network's entropy can be obtain also starting from a dynamical problem: the quantum walk subjected to thermal noise.

This work is just a first step towards understanding the problem. There are still many obscure aspects of this model as dealing with systems that do not satisfy the detailed balance condition.

Appendix A

Mastubara Green Function

The Matsubara Green function is a way to add the effect of temperature to the QFT formalism [31]. It is base on the analogy of the Boltzmann weight in statistical mechanics and the time evolution operator in quantum mechanics, respectively

$$p(\beta) = \frac{e^{-\beta H}}{Z} \qquad U(t-t') = e^{-i\frac{t-t'}{\hbar}\hat{H}}. \tag{A.1}$$

Kubo observes that the finite temperature can be reformulated via a redefinition of time as $\tau = \frac{it}{\hbar}$ and the density matrix becomes

$$\hat{\rho} \propto e^{-\beta\hat{H}} = U(-i\hbar\beta). \tag{A.2}$$

Matsubara propose that the thermal expectation value of an observable A is equal to

$$\langle A \rangle = \frac{\mathrm{Tr}\left[U(-i\hbar\beta)A\right]}{\mathrm{Tr}\left[U(-i\hbar\beta)\right]}; \tag{A.3}$$

This formulation as a reminiscence of the Gell-Mann and Low formula for the QFT except that the time evolution run over finite time $\tau \in [0, -i\hbar\beta]$

The Matsubara Green Function can be written as

$$G(\beta, t-t') = -\left\langle \hat{T}\psi(t)\psi^\dagger(t')\right\rangle = -\,\mathrm{Tr}\left[e^{-\beta\hat{H}}\psi(t)\psi^\dagger(t')\right] \tag{A.4}$$

For free bosons and fermions it can be computed and gives [31]

$$\begin{aligned} G_\lambda(\beta,\tau) &= -e^{-\epsilon_\lambda t}\left[(1+n(\epsilon_\lambda))\Theta(\tau) + n(\epsilon_\lambda)\Theta(-\tau)\right] \qquad \text{bosons} \\ G_\lambda(\beta,\tau) &= -e^{-\epsilon_\lambda t}\left[(1-f(\epsilon_\lambda))\Theta(\tau) - f(\epsilon_\lambda)\Theta(-\tau)\right] \qquad \text{fermion} \end{aligned} \tag{A.5}$$

where ϵ_λ is the energy level and $n(\epsilon_\lambda)$ and $f(\epsilon_\lambda)$ are respectively the Bose-Einstein distribution and the Fermi-Dirac distribution

$$n(\epsilon_\lambda) = \frac{1}{e^{\beta\epsilon_\lambda}-1} \qquad f(\epsilon_\lambda) = \frac{1}{e^{\beta\epsilon_\lambda}+1}. \tag{A.6}$$

It can be prove that the Matsubara Green function are periodic function with $T = [0, \beta]$ for bosons and $t = [-\beta, \beta]$ for fermions. Indeed

$$\begin{aligned} G(\beta, \beta+\tau) &= -\operatorname{Tr}\left[e^{-\beta\hat{H}}\psi(\beta+\tau)\psi^{\dagger}(0)\right] \\ &= -\operatorname{Tr}\left[e^{-\beta\hat{H}}e^{-(\beta+\tau)\hat{H}}\psi(0)e^{-(\beta+\tau)\hat{H}}\psi^{\dagger}(0)\right] \\ &= -\operatorname{Tr}\left[e^{-\beta\hat{H}}e^{\beta\hat{H}}e^{\tau\hat{H}}\psi(0)e^{-\beta\hat{H}}e^{-\tau\hat{H}}\psi^{\dagger}(0)\right] \\ &= -\operatorname{Tr}\left[e^{-\beta\hat{H}}\psi^{\dagger}(0)e^{\tau\hat{H}}\psi(0)e^{-\tau\hat{H}}\right] \\ &= -\operatorname{Tr}\left[e^{-\beta\hat{H}}\psi^{\dagger}(0)\psi(\tau)\right] = \zeta G(\beta, \tau); \end{aligned} \tag{A.7}$$

where $\zeta = \pm 1$ for bosons or fermions.

As a consequence, the Green function can be expand in a Fourier series and the frequencies are called Matsubara frequencies. They are define as

$$\begin{aligned} \nu_n =& 2\pi n k_B T && \text{bosons} \\ \omega_n =& \pi(2n+1)k_B T && \text{fermions} \end{aligned} \tag{A.8}$$

The propagator for bosons and fermion with the Matsubara frequencies are respectively

$$\mathcal{G}_{\lambda}(i\nu_n) = \frac{1}{i\nu_n - \epsilon_{\lambda}} \qquad \mathcal{G}_{\lambda}(i\omega_n) = \frac{1}{i\omega_n - \epsilon_{\lambda}}. \tag{A.9}$$

Appendix B

Sub-additivity of the network's entropy

In chapter 2 we have claimed that the network's entropy satisfies the sun-additivity property, there is the proof as in [16].

Let G, H and I be networks such that $G = H + I$ and $\hat{\rho}$, $\hat{\sigma}$ and $\hat{\rho}$ their density matrix respectively. Consider the KL divergence between G and H

$$\begin{aligned} D(\hat{\rho}||\hat{\sigma}) &= -S(\hat{\rho}) - \mathrm{Tr}\left[\hat{\rho} \ln \hat{\sigma}\right] \\ &= -S(\hat{\rho}) + \beta \, \mathrm{Tr}\left[L_H \hat{\rho}\right] + \ln Z_H . \end{aligned} \tag{B.1}$$

Similar for the KL divergence between G and I. Because both the Laplacian and the density matrices are positive defined, the following inequality holds

$$\beta \, \mathrm{Tr}\left[L_H \hat{\rho}\right] \geq 0. \tag{B.2}$$

Thus, the following equation is just a summation of positive term

$$D(\hat{\rho}||\hat{\sigma}) + D(\hat{\rho}||\hat{\tau}) + \beta \, \mathrm{Tr}\left[L_H \hat{\sigma}\right] + \beta \, \mathrm{Tr}\left[L_I \hat{\tau}\right] + \ln Z_H + \ln Z_I \geq 0. \tag{B.3}$$

Inserting equation (B.1) into (B.3), we reach

$$\begin{aligned} -S(\hat{\rho}) + \beta \, \mathrm{Tr}\left[L_H \hat{\rho}\right] + \ln Z_H - S(\hat{\rho}) + \beta \, \mathrm{Tr}\left[L_I \hat{\rho}\right] + \ln Z_I \\ + \beta \, \mathrm{Tr}\left[L_H \hat{\sigma}\right] + \beta \, \mathrm{Tr}\left[L_I \hat{\tau}\right] + \ln Z_H + \ln Z_I \geq 0. \end{aligned} \tag{B.4}$$

We can rearrange it using the fact the $S(\hat{\rho}) = \beta \, \mathrm{Tr}\left[L \hat{\rho}\right] + \ln Z$ and that $L_H + L_I = L_G$ we obtain

$$S(\hat{\sigma}) + S(\hat{\tau}) - S(\hat{\rho}) \geq 0, \tag{B.5}$$

which is the sub additivity property.

Appendix C

Mathematical method to solve differential equation from matrix

In the chapter 4.1 we study the time evolution of the density matrix transforming it into a vector. In this chapter we explain how it works.

First of all, we start with a differential equation in the form

$$\frac{d}{dt}X = AXB, \tag{C.1}$$

where X, A and B are 2×2 matrix. We can solve the differential equation transforming the matrix X into a vector $|X\rangle\rangle = (x_{11}, x_{12}, x_{21}, x_{22})^T$, thus, the differential equation becomes

$$\frac{d}{dt}|X\rangle\rangle = C|X\rangle\rangle, \tag{C.2}$$

C is a matrix that derives from A and B.

As a matter of fact, considering the evolution of each element of X we obtain

$$\begin{cases} \dfrac{dx_{11}}{dt} = a_{11}x_{11}b_{11} + a_{11}x_{12}b_{21} + a_{12}x_{21}b_{11} + a_{12}x_{22}b_{21} \\ \dfrac{dx_{12}}{dt} = a_{11}x_{11}b_{12} + a_{11}x_{12}b_{22} + a_{12}x_{21}b_{12} + a_{12}x_{22}b_{22} \\ \dfrac{dx_{21}}{dt} = a_{21}x_{11}b_{11} + a_{21}x_{12}b_{21} + a_{22}x_{21}b_{11} + a_{22}x_{22}b_{21} \\ \dfrac{dx_{22}}{dt} = a_{21}x_{11}b_{12} + a_{21}x_{12}b_{22} + a_{22}x_{21}b_{12} + a_{22}x_{22}b_{22} \end{cases} \tag{C.3}$$

We can rearrange them in a vectorial form

$$\frac{d}{dt}\begin{pmatrix} x_{11} \\ x_{12} \\ x_{21} \\ x_{22} \end{pmatrix} = \begin{pmatrix} a_{11}b_{11} & a_{11}b_{21} & a_{12}b_{11} & a_{12}b_{21} \\ a_{11}b_{12} & a_{11}b_{22} & a_{12}b_{12} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{21} & a_{22}b_{11} & a_{22}b_{21} \\ a_{21}b_{12} & a_{21}b_{22} & a_{22}b_{12} & a_{22}b_{22} \end{pmatrix} \begin{pmatrix} x_{11} \\ x_{12} \\ x_{21} \\ x_{22} \end{pmatrix} = C|X\rangle\rangle \tag{C.4}$$

The matrix C in equation (C.4) is the tensorial product

$$C = A \otimes B^T = \begin{pmatrix} A_{11}B^T & A_{12}B^T \\ A_{21}B^t & A_{22}B^T \end{pmatrix}. \tag{C.5}$$

where B^T is the transpose of matrix B.

With similar procedure, we can vectorize also the differential equation

$$\frac{d}{dt}X = AX + XB \rightarrow \frac{d}{dt}|X\rangle\rangle = \left(A \otimes \mathbb{I} + \mathbb{I} \otimes B^T\right)|X\rangle\rangle \tag{C.6}$$

where $\mathbb{I}$ is the identity matrix.

The generalization to $N \times N$ matrix and finite dimensional operator is straightforward.

Bibliography

[1] Euler Leonhard. “Solutio Problematis Ad Geometriam Situs Pertinentis”. In: *Commentarii Academiae Scientiarum Petropolitanae* 8 (1736), pp. 128–140.

[2] P. J. Heawood. “Map-Colour Theorem”. In: *Proceedings of the London Mathematical Society* s2-51.1 (Jan. 1949), pp. 161–175. ISSN: 0024-6115. DOI: `10.1112/plms/s2-51.3.161`.

[3] G. Ringel. *Map Color Theorem*. Grundlehren der mathematischen Wissenschaften. Springer Berlin Heidelberg, 2012. ISBN: 9783642657597. DOI: `10.1007/978-3-642-65759-7`. URL: `https://books.google.it/books?id=EfoOCQAAQBAJ`.

[4] Paul Erdős and Alfréd Rényi. “On the Evolution of Random Graphs”. In: *Publication of the Mathematical Institute of the Hungarian Academy of Sciences* 5.1 (1960), pp. 17–61.

[5] P. Erdős and A Rényi. “On Random Graphs I”. In: *Publicationes Mathematicae* 6 (1959), pp. 290–297.

[6] Albert-László Barabási and Réka Albert. “Emergence of Scaling in Random Networks”. In: *Science* 286.5439 (Oct. 1999), pp. 509–512. ISSN: 1095-9203. DOI: `10.1126/science.286.5439.509`.

[7] Duncan J. Watts and Steven H. Strogatz. “Collective dynamics of ’small-world’ networks”. In: *Nature* 393 (1998), pp. 440–442. DOI: `10.1038/30918`.

[8] Naoki Masuda, Mason A. Porter, and Renaud Lambiotte. “Random walks and diffusion on networks”. In: *Physics Reports* 716-717 (2017), pp. 1–58. DOI: `https://doi.org/10.1016/j.physrep.2017.07.007`.

[9] David F. Gleich. “PageRank Beyond the Web”. In: *SIAM Review* 57.3 (2015), pp. 321–363. DOI: `10.1137/140976649`.

[10] Sergey Brin and Lawrence Page. “The anatomy of a large-scale hypertextual Web search engine”. In: *Computer Networks and ISDN Systems* 30.1 (1998). Proceedings of the Seventh International World Wide Web Conference, pp. 107–117. ISSN: 0169-7552. DOI: `https://doi.org/10.1016/S0169-7552(98)00110-X`.

[11] J Kempe. “Quantum random walks: An introductory overview”. In: *Contemporary Physics* 44.4 (2003), pp. 307–327. DOI: `10.1080/00107151031000110776`.

[12] Y. Aharonov, L. Davidovich, and N. Zagury. “Quantum random walks”. In: *Phys. Rev. A* 48 (2 1993), pp. 1687–1690. DOI: `10.1103/PhysRevA.48.1687`.

[13] Edward Farhi and Sam Gutmann. “Quantum computation and decision trees”. In: *Phys. Rev. A* 58 (2 1998), pp. 915–928. DOI: 10.1103/PhysRevA.58.915.

[14] Kartik Anand and Ginestra Bianconi. “Entropy measures for networks: Toward an information theory of complex topologies”. In: *Phys. Rev. E* 80 (4 2009), p. 045102. DOI: 10.1103/PhysRevE.80.045102.

[15] Ginestra Bianconi. “Entropy of network ensembles”. In: *Phys. Rev. E* 79 (3 2009), p. 036114. DOI: 10.1103/PhysRevE.79.036114.

[16] Manlio De Domenico and Jacob Biamonte. “Spectral Entropies as Information-Theoretic Tools for Complex Network Comparison”. In: *Physical Review X* 6.4 (Dec. 2016). ISSN: 2160-3308. DOI: 10.1103/physrevx.6.041062.

[17] Ernesto Estrada and Naomichi Hatano. “Communicability in complex networks”. In: *Physical Review E* 77.3 (Mar. 2008). DOI: 10.1103/physreve.77.036111.

[18] Manlio De Domenico et al. “Structural reducibility of multilayer networks”. In: *Nature Communications* 6 (2015). DOI: 10.1038/ncomms7864.

[19] E. N. Gilbert. “Random Graphs”. In: *The Annals of Mathematical Statistics* 30.4 (1959), pp. 1141–1144. DOI: 10.1214/aoms/1177706098.

[20] S. Boccaletti et al. “Complex networks: Structure and dynamics”. In: *Physics Reports* 424.4 (2006), pp. 175–308. DOI: https://doi.org/10.1016/j.physrep.2005.10.009.

[21] Andrew M. Childs, Edward Farhi, and Sam Gutmann. “An Example of the Difference Between Quantum and Classical Random Walks”. In: *Quantum Information Processing* 1 (2002), pp. 35, 43. DOI: 10.1023/A:1019609420309.

[22] G. D. Paparo and M. A. Martin-Delgado. “Google in a Quantum Network”. In: *Scientific Reports* 2 (2012). DOI: 10.1038/srep00444.

[23] Jacob Biamonte, Mauro Faccin, and Manlio De Domenico. “Complex networks from classical to quantum”. In: *Communications Physics* 2 (2019). DOI: 10.1038/s42005-019-0152-6.

[24] Michael A. Nielsen and Isaac L. Chuang. *Quantum Computation and Quantum Information: 10th Anniversary Edition*. Cambridge University Press, 2010.

[25] Milton Abramowitz and Irene A. Stegun. *Handbook of Mathematical Functions with Formulas, Graphs and Mathematical Tables*. 1965.

[26] Ernesto Estrada, Naomichi Hatano, and Michele Benzi. “The physics of communicability in complex networks”. In: *Physics Reports* 514.3 (2012), pp. 89–119. ISSN: 0370-1573. DOI: 10.1016/j.physrep.2012.01.006.

[27] Leo Katz. “A new status index derived from sociometric analysis”. In: *Psychometrika* 18 (1953), p. 39.43. DOI: https://doi.org/10.1007/BF02289026.

[28] Michele Benzi and Christine Klymko. “On the Limiting Behavior of Parameter-Dependent Network Centrality Measures”. In: *SIAM Journal on Matrix Analysis and Applications* 36.2 (2015), pp. 686–706. DOI: 10.1137/130950550.

[29] A. D. Fokker. "Die mittlere Energie rotierender elektrischer Dipole im Strahlungsfeld". In: *Annalen der Physik* 348.5 (1914), pp. 810–820. DOI: https://doi.org/10.1002/andp.19143480507.

[30] I. Gutman and W. Xiao. "Generalized inverse of the laplacian matrix and some applications". In: *Bulletin (Académie serbe des sciences et des arts. Classe des sciences mathématiques et naturelles. Sciences mathématiques)* 29 (2004), pp. 15–23. ISSN: 05617332, 24060909. URL: http://www.jstor.org/stable/44095641.

[31] Piers Coleman. *Introduction to Many-Body Physics*. Cambridge University Press, 2015. ISBN: 9781139020916. DOI: https://doi.org/10.1017/CBO9781139020916.

[32] Arsham Ghavasieh, Carlo Nicolini, and Manlio De Domenico. "Statistical physics of complex information dynamics". In: *Phys. Rev. E* 102 (5 2020), p. 052304. DOI: 10.1103/PhysRevE.102.052304.

[33] Solomon Kullback and R. A. Leibler. "On Information and Sufficiency". In: *Annals of Mathematical Statistics* 22 (1951), pp. 79–86. DOI: 10.1214/aoms/1177729694.

[34] A. P. Majtey, P. W. Lamberti, and D. P. Prato. "Jensen-Shannon divergence as a measure of distinguishability between mixed quantum states". In: *Phys. Rev. A* 72 (5 2005), p. 052310. DOI: 10.1103/PhysRevA.72.052310.

[35] Jop Briët and Peter Harremoës. "Properties of classical and quantum Jensen-Shannon divergence". In: *Physical Review A* 79.5 (May 2009). DOI: 10.1103/physreva.79.052311.

[36] Göran Lindblad. "On the generators of quantum dynamical semigroups". In: *Communications in Mathematical Physics* 48 (1976), pp. 119–130. DOI: 10.1007/BF01608499.

[37] Vittorio Gorini, Andrzej Kossakowski, and E. C. G. Sudarshan. "Completely positive dynamical semigroups of N-level systems". In: *Journal of Mathematical Physics* 17.5 (May 1976), pp. 821–825. DOI: 10.1063/1.522979.

[38] Daniel Manzano. "A short introduction to the Lindblad master equation". In: *AIP Advances* 10.2 (Feb. 2020), p. 025106. DOI: 10.1063/1.5115323.

[39] Heinz-Peter Breuer and Francesco Petruccione. *The Theory of Open Quantum Systems*. Oxford University Press, Jan. 2007. ISBN: 9780199213900. DOI: 10.1093/acprof:oso/9780199213900.001.0001.

[40] A. G. Redfield. "On the Theory of Relaxation Processes". In: *IBM Journal of Research and Development* 1.1 (1957), pp. 19–31. DOI: 10.1147/rd.11.0019.

[41] Kazuyuki Fujii. *Quantum Damped Harmonic Oscillator*. 2012. arXiv: 1209.1437 [quant-ph]. URL: https://arxiv.org/abs/1209.1437.

[42] James D. Whitfield, César A. Rodríguez-Rosario, and Alán Aspuru-Guzik. "Quantum stochastic walks: A generalization of classical random walks and quantum walks". In: *Phys. Rev. A* 81 (2 2010), p. 022323. DOI: 10.1103/PhysRevA.81.022323.

[43] Krzysztof Domino et al. “Properties of quantum stochastic walks from the asymptotic scaling exponent”. In: *Quantum Information and Computation* 18 (2018), pp. 181–197. DOI: `10.26421/QIC18.3-4-1`.

[44] M. Bruderer and M. B. Plenio. “Decoherence-enhanced performance of quantum walks applied to graph isomorphism testing”. In: *Phys. Rev. A* 94 (6 2016). DOI: `10.1103/PhysRevA.94.062317`.

[45] Arsham Ghavasieh and Manlio De Domenico. “Generalized network density matrices for analysis of multiscale functional diversity”. In: *Phys. Rev. E* 107 (4 2023), p. 044304. DOI: `10.1103/PhysRevE.107.044304`.

[46] H. J. Korsch. *Lindblad dynamics of the damped and forced quantum harmonic oscillator*. 2019. URL: `https://arxiv.org/abs/1908.01187`.