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

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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 metric 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

The traffic jam in the morning, the airport traffic, but also the functioning of the brain can be study as a network problem. This kind of problem can be naturally study through network: the vertices indicates the elements and link the interaction between them, for the airport traffic the airport are the vertices and the flights the link, for the brain, instead, the neurons and the synapses.

The first ideas of graph theory was introduce by Euler in 1736 with his famous problem about the Seven Bridges of Königsberg [1]. The dilemma was about the find a route, if it exist, that cross all the seven bridges that connect the two island on the Pregel river with the rest of the city once and only one. Euler solve the problem eliminating all the irrelevant information and focus 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 link. Graph theory was begun. ne of the success of this theory is the proof of the five color problem. It declare that given a plane divided into regions, such as a political map, those regions can be always colored using no more that five different colors, such that two neighboring regions do 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] with their random graphs. This model is widely studied and understood and use a base to for ages. However, due to the increasing our data and computational power, the Erdős-Rényi model starts 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 has not. To answer the new question, in the last 40 years many model has been proposed and studied, each one with their unique properties [5, 6]. The network theory has born.

The natural problem we are facing with the network are dynamical, so we need to add dynamical model to the network. The simplest dynamics we can consider is the random walk, a single particle wandering across the network. Regardless its simplicity, the random walk on network has reveled very powerful and it is used to build several algorithm [7, 8, 9].

With the new 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 the quantum effects, its behavior is different [10]. 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 ech timestep [11]. Otherwise, we consider the time continuos and the evolution

is ruled by the Schrödinger equation with the Laplacian of the network as Hamiltonian [12]. In this dissertation we focus on the second type.

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 [13, 14], 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 [15]. Starting from the Estrada communicability matrix [16], he defines 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 captures the topological features of the network but also its dynamical behavior. In fact, the entropy capture the property of the relaxation on the network. Starting from there, we can expand the information related quantities introducing The Kullback Lieber divergence and the Jensen Shannon divergence. This two quantities can be employ to distinguish between networks [17].

The density matrix introduce by De Domenico is similar to the density matrix of a quantum canonical ensemble with the Laplacian as Hamiltonian. This fact suggests a link between the network entropy and the continuos time random walk. This dissertation used technique borrowed from the study of open quantum system to light up this connection

The aim of this dissertation is to understand physics behind the new formulation for the information theory for complex network and its connection with the relaxation of a dynamics over a network. This 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 in Internet. The theoretical calculations come with numerical simulation made in python.

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 a 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

The mathematical framework used in Network theory is given by 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 viewed also via a $N \times N$ matrix called Adjacency matrix which is defined as

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

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 $W_{ij}(k)$ of length k from node i to node j can be computed using the adjacency matrix as

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

A 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 *irreducible* if 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

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

If it hold, the graph is said *strongly connected*: there exists a path that connect each the nodes to all the other ones.

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.

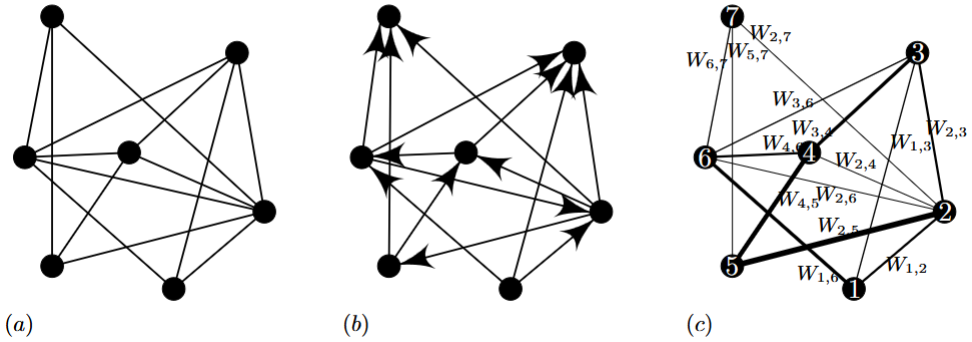

Figure 1.1: Examples of undirected (a), directed (b), weight (c) networks with $N = 7$ and $M = 14$. The arrows indicates the direction of each link. In the weight graph the thickness of the links represents its weight.

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, 18]. 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 approach. 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 produce 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 [5]. This type of graph exhibits some preferential nodes which have a degree order of magnitude higher than the average and it presents a power law as degree distribution. The model works by preferential attachment, where new nodes are more likely to connect to nodes that already have a higher degree.

The algorithm is defined as follow:

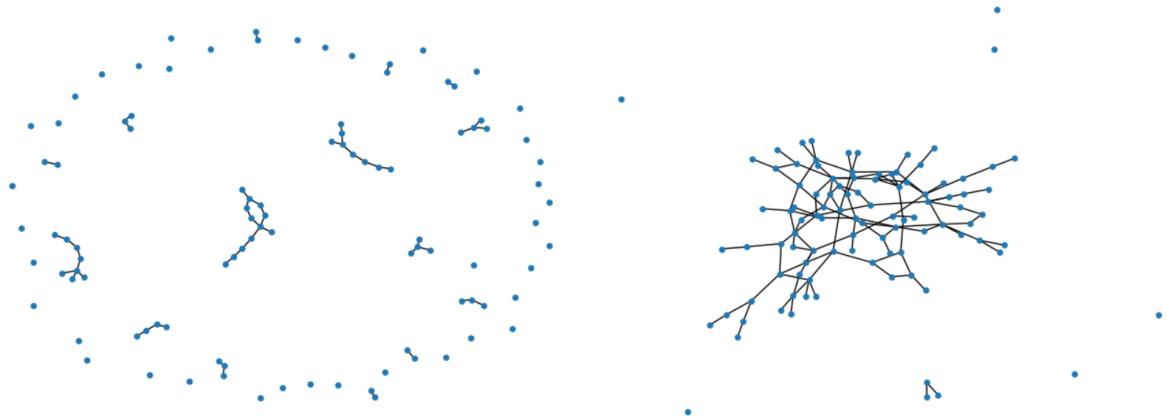

Figure 1.2: Two examples of Erdős-Rényi random graphs: on the left, it has 100 nodes and $p = 0.01$; on the right, it has 100 nodes and $p = 0.02$. Overcoming the threshold $p > 0.01$ can be seen the formation of the giant component.

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.

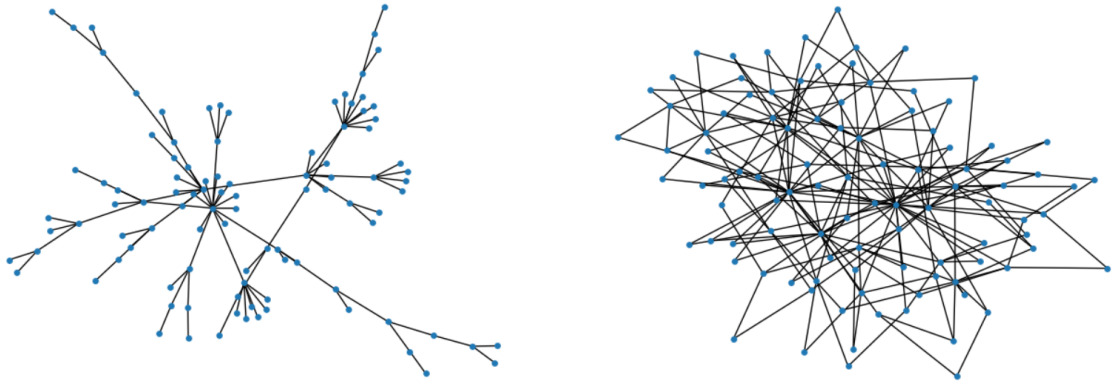

Figure 1.3: Two example of Barabábi-Albert scale-free networks: on the left, it has 100 nodes and $m = 1$; on the right, it has 100 nodes and $m = 2$.

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 [6]. 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.

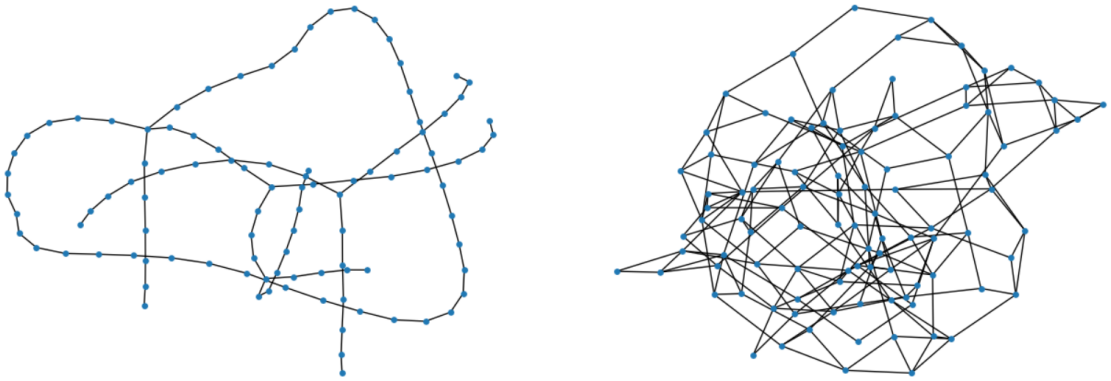

Figure 1.4: Two example of Watts-Strogatz small world networks: on the left, it has 100 nodes, $K = 2$ and $p = 0.1$; on the right, it has 100 nodes, $K = 4$ and $p = 0.3$.

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 [7]

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

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

$$\sum_i L_{ij} = 0. \tag{1.13}$$

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, block for each connected component, each component can be seen as an independent network with their zero eigenvalue.

The solution of master equation (1.12) is

$$\rho(t) = e^{-tL} \rho(0). \tag{1.14}$$

We can prove that

$$\sum_i \dot{\rho}_i(t) = -\sum_i \sum_j L_{ij}\rho_j(t) = -\sum_j \left(\sum_i L_{ij}\right) \rho_j(t) = 0. \tag{1.15}$$

This implies a first integral of motion

$$\sum_i \rho_i(t) = \sum_i \rho_i(0). \tag{1.16}$$

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

$$\sum_j (\pi_{ij}\rho_j^* - \pi_{ji}\rho_i^*) = -\sum_j J_{ij}^* = 0 \tag{1.17}$$

where we introduce the stationary density currents $J_{ij}^* = \pi_{ji}\rho_i^* - \pi_{ij}\rho_j^*$. The stationary density currents J_{ij}^* vanishes and the vector field on the network

$$v_{ij} = \ln \pi_{ij} - \ln \pi_{ji}$$

is exact and it admits a potential V_i such that

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

The stationary distribution can be written in the form

$$\rho_i^* \propto \exp(-V_i) \tag{1.18}$$

and one recovers the MB distribution according to MEP.

If Laplacian is symmetric the system admits a unique stationary solution [7]

$$\rho^* = \frac{1}{N}\left(1, 1, \cdots, 1, 1\right). \tag{1.19}$$

such that

$$\sum_j L_{ij}\rho_j^* = 0. \tag{1.20}$$

Thus, the stationary distribution (1.19) is the eigenvector with eigenvalue 0 of the Laplacian matrix.

We can consider a less strict condition for the system known as detailed balance condition

$$\pi_{ij}\rho_j^* = \pi_{ji}\rho_i^*, \tag{1.21}$$

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

$$S_{ij} = \frac{1}{\sqrt{\rho_i^*}} L_{ij} \sqrt{\rho_j^*}, \tag{1.22}$$

so that the eigenvalues are real and the eigenvectors are orthogonal. In particular (1.19) is the zero eigenvector of S_{ij} and the master equation reads

$$\tilde{p}_i = -\sum_j S_{ij}\tilde{p}_j \tag{1.23}$$

where $\tilde{p}_i = p_i\sqrt{\rho_i^*}$.

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Let us now assume the network satisfies the detailed balance condition (1.21), 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

$$\sum_i w_i = 0. \tag{1.24}$$

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

$$\rho(t) = \rho^* + w(t). \tag{1.25}$$

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

$$S(t) = -\sum_i \rho_i(t)\ln\rho_i(t). \tag{1.26}$$

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

The random walk process is a irreversible, the entropy (1.26) increases by time. In fact, the entropy's derivative for the random walk is

$$\dot{S}(t) = -\sum_i \dot{\rho}_i(t)\ln\rho_i(t) = -\sum_{ij} L_{ij}\rho_j(t)\ln\rho_i(t). \tag{1.27}$$

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

$$\dot{S} = -\sum_\lambda \lambda\rho_\lambda(t)\ln\rho_\lambda(t) \geq 0. \tag{1.28}$$

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

Figure 1.5 shows the Shannon entropy (1.26) for a random walk on different networks: 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. The Shannon entropy is a monotonic increasing function and the stationary distribution has maximal entropy.

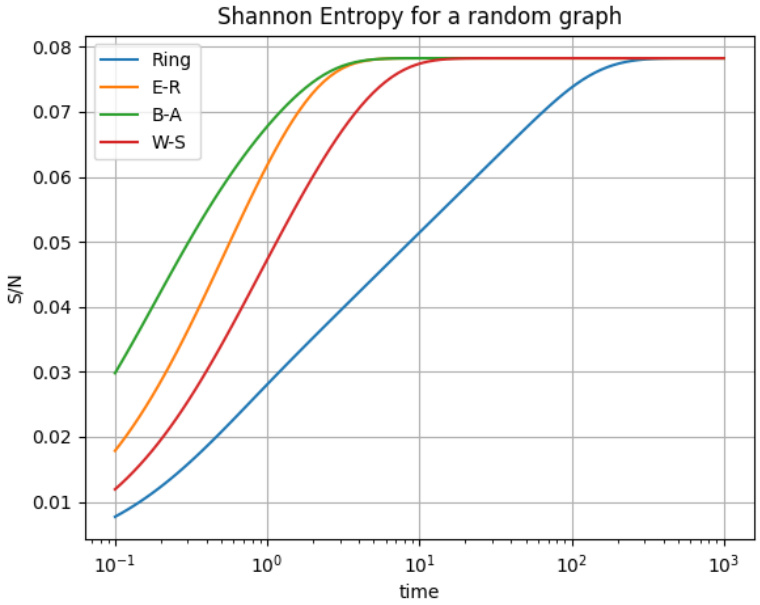

Figure 1.5: Plot of the Shannon entropy as a function of time t for a random walk over different network types with 50 nodes: a ring graph (blue), a Erdős-Rényi (E-R) random graph with connectivity probability 0.7 (orange), a Barabábi-Albert (B-A) scale-free network with parameter m = 3 (green), and 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 $S/N = \ln(50)/50 \approx 0.0782$.

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 equation requires that the Laplacian is hermitian; therefore, the network must hold the detailed balance condition (1.21). This model is known as "continuos time quantum walk" [12, 21]. This model is used to build quantum algorithms [22, 23].

Let us define an orthonormal basis $\{|i\rangle\}$, 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

$$|\psi\rangle = \sum_i \sqrt{\rho_i(t)}|i\rangle, \tag{1.29}$$

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

$$\frac{d}{dt}|\psi\rangle = -i\frac{1}{2}\hat{L}|\psi\rangle. \tag{1.30}$$

where $\hat{L} = \sum_{ij} L_{ij}|i\rangle\langle j|$ is the Laplacian operator. If we apply a Wick rotation into the equation (1.30) we recover the master equation of the classic random walk (1.12).

The solution of the equation (1.30) takes the form

$$|\psi(t)\rangle = \hat{U}(t,0)|\psi(0)\rangle = e^{-\frac{i}{2}\hat{L}t}|\psi(0)\rangle, \tag{1.31}$$

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

It is possible to define a limiting transition probability for a quantum walk as follow: suppose the system starts at node $|a\rangle$, we measure it after a time t, random variable uniformly distributed over the interval $t \in [0,T]$ [21]. The transition probability from node a to b is given by

$$\begin{aligned}
\rho_{a\to b}(T) &= \frac{1}{T}\int_0^T |\langle a|e^{-i\frac{t}{2}\hat{L}}|b\rangle|^2 dt \\
&= \frac{1}{T}\int_0^T \sum_{\lambda,\lambda'} \langle a|e^{i\frac{t}{2}\hat{L}}|\lambda\rangle\langle\lambda\,|\,b\rangle\langle b|e^{-i\frac{t}{2}\hat{L}}|\lambda'\rangle\langle\lambda'\,|\,a\rangle dt \\
&= \sum_{\lambda,\lambda'} \langle a\,|\,\lambda\rangle\langle\lambda\,|\,b\rangle\langle b\,|\,\lambda'\rangle\langle\lambda'\,|\,a\rangle \frac{1}{T}\int_0^T e^{-i(\lambda-\lambda')\frac{t}{2}} dt \\
&= \sum_{\lambda} |\langle a\,|\,\lambda\rangle\langle\lambda\,|\,b\rangle|^2 + 2\sum_{\lambda\neq\lambda'} \langle a\,|\,\lambda\rangle\langle\lambda\,|\,b\rangle\langle b\,|\,\lambda'\rangle\langle\lambda'\,|\,a\rangle \frac{1-e^{-i(\lambda-\lambda')\frac{T}{2}}}{i(\lambda-\lambda')T},
\end{aligned} \tag{1.32}$$

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

$$\rho_{a\to b}(T) \xrightarrow[T\to\infty]{} \sum_{\lambda} |\langle a\,|\,\lambda\rangle\langle\lambda\,|\,b\rangle|^2. \tag{1.33}$$

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

$$\hat{\rho} = |\psi\rangle\langle\psi| = \sum_{ij} \sqrt{\rho_i}\sqrt{\rho_j}|i\rangle\langle j|, \tag{1.34}$$

It is a self-adjoint operator and $\mathrm{Tr}[\hat{\rho}] = 1$ [24].

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

$$\left\langle \hat{O} \right\rangle = \mathrm{Tr}\left[\hat{O}\hat{\rho}\right]. \tag{1.35}$$

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

$$\mathrm{Tr}\left[\hat{P}_k\hat{\rho}(t)\right] = \rho_k. \tag{1.36}$$

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

$$\frac{d}{dt}\hat{\rho}(t) = -\frac{i}{2}\left[\hat{L},\rho\right] \tag{1.37}$$

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

$$\hat{\rho}(t) = \hat{U}(t,0)\hat{\rho}(0)\hat{U}^{\dagger}(t,0) = e^{-\frac{i}{2}t\hat{L}}\hat{\rho}\, e^{\frac{i}{2}t\hat{L}}. \tag{1.38}$$

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

$$\hat{\rho} = \sum_{k=1}^{K} p_k \hat{\rho}_k \qquad \hat{\rho}_k = |\psi_k\rangle\langle\psi_k|. \tag{1.39}$$

The temporal evolution of the operator is defined as in eq. (1.37); the probability to be at node a at time t is the same as in eq. (1.36). All the property 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

$$S[\hat{\rho}] = -\,\mathrm{Tr}[\hat{\rho}\ln\hat{\rho}]. \tag{1.40}$$

It is the quantum counterpart of the Shannon entropy for classical information theory. The Von Neumann entropy (1.40) 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 [12]. 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

$$\hat{L}|j\rangle = 2|j\rangle - |j-1\rangle - |j+1\rangle. \tag{1.41}$$

Therefore, applying this to the momentum state

$$\begin{aligned}\langle j|\hat{L}|p\rangle &= \langle j\,|\,p\rangle - \frac{1}{2}\langle j-1\,|\,p\rangle - \frac{1}{2}\langle j+1\,|\,p\rangle \\ &= e^{ijp} - \frac{1}{2}e^{i(j-1)p} - \frac{1}{2}e^{i(j+1)p} \\ &= e^{ijp}(\cos(p)-1) = (\cos(p)-1)\langle j\,|\,p\rangle\end{aligned} \tag{1.42}$$

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

$$\begin{aligned}\langle j|e^{-i\frac{t}{2}\hat{L}}|k\rangle &= \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-i\frac{t}{2}(\cos(p)-1)}\langle j\,|\,p\rangle\langle p\,|\,k\rangle dp \\ &= \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-ip(j-k)-i\frac{t}{2}(\cos(p)-1)} \\ &= e^{i\frac{t}{2}}(-i)^{k-j}J_{k-j}\left(\frac{t}{2}\right),\end{aligned} \tag{1.43}$$

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

Applying the Wick rotation we obtain

$$\left|\langle j|e^{-i\frac{t}{2}\hat{L}}|k\rangle\right|^2 = e^{-t}\left(I_{k-j}\left(\frac{t}{2}\right)\right)^2, \tag{1.44}$$

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.

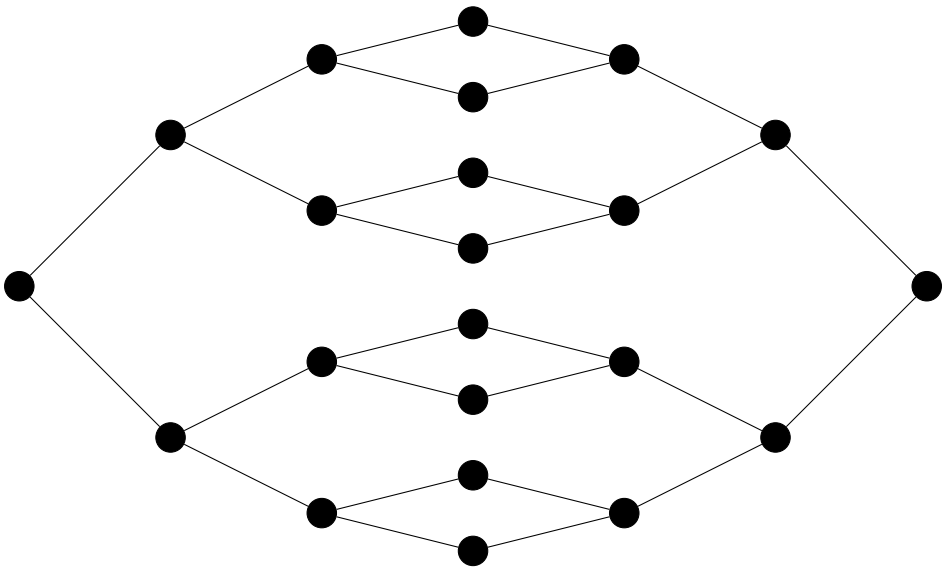

Figure 1.6: The picture of a glued double tree network.

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

$$|\text{col } j\rangle = \frac{1}{\sqrt{N_j}} \sum_{a \in \text{column}} |a\rangle, \tag{1.45}$$

where the renormalization factor N_j is

$$N_j = \begin{cases} 2^j & 0 \leq j \leq n \\ 2^{2n-j} & n \leq j \leq 2n \end{cases}. \tag{1.46}$$

In this basis, the Laplacian act as

$$\begin{aligned} \langle \text{col } j|\hat{L}|\text{col } j\rangle &= 1 \\ \langle \text{col } j \pm 1|\hat{L}|\text{col } j\rangle &= \begin{cases} \frac{\sqrt{2}}{2} & j = 0, n, 2, \\ \frac{\sqrt{2}}{3} & \text{otherwise} \end{cases} \end{aligned} \tag{1.47}$$

Thus, the dynamics along the network reduces to a 1-D quantum walk which has a known computable solution (1.44)

$$\langle 0|e^{i\frac{t}{2}\hat{L}}|2n\rangle = e^{-t} I_{2n}\left(\frac{t}{2}\right), \tag{1.48}$$

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 system one element can be influenced by another ones with which is not directing interacting. For example, considering the city mobility, the road forms the network, closing one road may create traffic in another roads that do not intersect the closed one. To study the correlation between the nodes of a network the communicability matrix was introduced [16]. We call it communicability because correlation as a different meaning in social science, they called in this way the interactions.

Interestingly, this matrix behave as quantum density matrix. Thus, it is a possible candidate to the role of network density matrix and, as a consequence, we can borrow some information quantities as entropy that were introduces for quantum many body and quantum computing, opening a connection between the network theory and quantum realm.

2.1 Estrada's Communicability matrix

Most of the study on complex networks focuses 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 this vision ignores completely the complexity of the network. To overcome that we introduce the communicability matrix, defined to consider also these possible path to go beyond the shortest one [26]. It consider the influence over all the path that cross the choose 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

$$G(A) = \sum_{k=1}^{\infty} c_k A^k \tag{2.1}$$

and 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 and it is heavier

the longer is the path, this is made to give more relevance to the short ones respect to the long ones. It must be chosen such that the series is convergent, they also must penalize long paths to reflect the preference to the shorter one.

An intuitive choice is $c_k = \frac{1}{k!}$, which transforms the communicability into an exponential function [16]

$$G^E(A) = \sum_{k=1}^{\infty} \frac{A^k}{k!} = e^A. \tag{2.2}$$

We can generalize it adding a constant term β

$$G^E(A) = \sum_{k=1}^{\infty} \frac{\beta A^k}{k!} = e^{\beta A}, \tag{2.3}$$

this formulation is similar to the thermal green function for quantum system 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

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

The two formulations for the communicability matrix lead to the same result and conclusion for the network in the limit $\alpha \to \frac{1}{\lambda_N}$ and $\lambda_N - \lambda_{N-1}$ large [28].

From this, we can introduce an global index for the network that consider all the different possible communication as

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

In the literature it is called Estrada index [16] and can be interpreted as the sum of all the self-communication, that is the sum of the paths that end in the same node they have started.

However, the communicability matrices (2.2) and (2.4) study only the network's topology, namely the paths, and ignore the presence of dynamics over the network that may change the way information spreads.

If we consider the simplest dynamics, the random walk, it is governed by the Laplacian matrix L. Thus, the communicability matrices for random walk are [26]

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

where $\tilde{L}^{-1} = \sum_{i=2}^{N} \frac{1}{\mu} v_i^T v_i$ is the Moore-Penrose generalized inverse of the Laplacian. Here, μ are the eigenvalue ordered from the smaller to the bigger such that $\mu_1 < \mu_2 < ... < \mu_N$, and v_i the respective eigenvectors of the Laplacian matrix [29]. Also, the Laplacian Estrada index is define as

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

2.1.1 Hamiltonian formalism

The formulae (2.6) can be motivated by studying a classic and quantum harmonic oscillator on a network. Consider a set of N harmonic oscillators with coupling matrix $K = A$, where A is a symmetric adjacency matrix. In this way, the nodes are considered as particle of mass $m = 1$ connected by springs with constant A_{ij}. 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 are no dumping and no external forces acting in the system besides the thermal fluctuation. Let introduce a set of coordinates q_i that indicates the displacement of the i particle respect the equilibrium position, the elastic elastic potential can be define as

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

where

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

We set $H_{ij} = K_{jj}\delta_{ij} - K_{ij}$, therefore the potential can be written as

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

The H matrix is a laplacian matrix and it is equal to the Laplacian of the network $L = D - A$, where D is the degree matrix. It holds the property $\sum_j H_{ij} = 0$, therefore it has not negative eigenvalues and one must be equal to zero. The zero eigenvalue ensure us that the motion of the center of must is conserved.

We can write the Lagrangian of the system as

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

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

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

Therefore, the spectral signature of the matrix $H = L$ are the same of the harmonic oscillator. In this way we can connect 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 between the eigenvectors.

The Hamiltonian of the system is given by

$$H_L = \sum_i \frac{p_i^2}{2} + \sum_{ij}\frac{1}{2}L_{ij}q_iq_j. \tag{2.15}$$

2.1.2 Network of classic harmonic oscillators

To combine this with the thermodynamics, let consider the presence of a thermal bath in the Hamiltonian formalism using the Langevin equation

$$\begin{aligned} \dot{q}_i &= p_i; \\ \dot{p}_i &= -H_{ij}q_j - \gamma \sum_j (\delta_{ij} - 1_{ij})\, p_j + \sqrt{2T\gamma}\xi_i(t), \end{aligned} \tag{2.16}$$

where γ is the friction coefficient, T is the temperature (Boltzmann constant $K_B = 1$), δ_{ij} the Kronecker delta and 1_{ij} the matrix with all entries equal to 1, $\xi_i(t)$ is white noise, namely

$$\langle \xi_i(t) \rangle = 0 \qquad \langle \xi_i^2(t) \rangle = 1 \tag{2.17}$$

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 derivative of $\sum_i p_i$ is zero, therefore it is an integral of motion,

$$\frac{d}{dt}\sum_i \dot{p}_i = -\gamma \sum_{ij} (\delta_{ij} - 1_{ij})\, p_j + \cancel{\sqrt{2T\gamma} \sum_i \xi_i(t)} = 0. \tag{2.18}$$

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

$$\xi_i(t) = w_i(t) + \frac{1}{N}\sum_k w_k(t). \tag{2.19}$$

The covariance matrix of $\xi_i(t)$ can be written as

$$\langle \xi_i(t)\xi_j(s) \rangle = [\delta_{ij} - 1_{ij}]\, \delta(t-s) \tag{2.20}$$

The distribution $\rho(q, p, t)$ is a Gaussian and satisfies the Fokker-Plank equation [30]

$$\frac{\partial \rho}{\partial t} = -\sum_i p_i \frac{\partial \rho}{\partial q_i} + \sum_{ij} H_{ij} q_j \frac{\partial \rho}{\partial p_i} + \gamma \sum_{ij} (\delta_{ij} - 1_{ij}) \left[\frac{\partial}{\partial p_i} p_j \rho + T \frac{\partial^2 \rho}{\partial p_i \partial p_j} \right]. \tag{2.21}$$

The solution at equilibrium is

$$\rho(q, p) = Z(\beta)^{-1} \exp\left[-\beta \left(\sum_j \frac{p_j^2}{2m_j} + \sum_{ij} \frac{1}{2} q_i H_{ij} q_j \right) \right], \tag{2.22}$$

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

$$Z(\beta) = \int \prod_i dp_i dq_i \ \exp\left[-\beta \left(\sum_j \frac{p_j^2}{2m_j} + \sum_{ij} q_i H_{ij} q_j \right) \right]. \tag{2.23}$$

The marginal distribution on the coordinates is a Maxwell-Boltzmann distribution with the internal energy

$$\rho(q) = Z(\beta)^{-1} e^{-\beta\left(\sum_{ij} q_i H_{ij} q_j\right)}. \tag{2.24}$$

Since there is a sum over the indices i and j we can change the basis of q_i to Q_λ such that the H is diagonal. Therefore, the marginal distribution becomes

$$\rho(q) = Z(\beta)^{-1} e^{-\beta\left(\sum_{\lambda\neq 0} Q_\lambda \lambda Q_\lambda\right)}, \tag{2.25}$$

with partition function

$$Z(\beta) = \int \prod_{\lambda\neq 0} dQ_\lambda e^{-\beta\left(\sum_{\lambda\neq 0} \lambda Q_\lambda^2\right)}. \tag{2.26}$$

The thermal distribution does not involve the zero eigenmode since the thermal bath does not interact with it and, also, 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 expresses also with the Moore-Penrose generalized inverse of the Laplacian

$$\mathrm{Cov}(q) = \frac{1}{\beta} L^+, \tag{2.27}$$

This is the same result as the Estrada's Communicability matrix $G^R(L)$ (2.6) with $\alpha = \beta$. When $T \to 0$ the spread of information drops; and when $T \to +\infty$ it becomes instantaneous.

2.1.3 Network of quantum harmonic oscillators

Instead, for the quantum case ($\hbar = 1$), 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 $[\hat{q}_i, \hat{p}_j] = i\delta_{ij}$.

We need to add a new term; it should be considered as additional springs with constant K' that connect each node to the ground: it prevent the the center of mass from moving. So the Hamiltonian becomes

$$H_L = \sum_i \left(\frac{\hat{p}_i^2}{2} + \frac{K'}{2} \hat{q}_i^2 \right) + \sum_{ij} \frac{1}{2} L_{ij} \hat{q}_i \hat{q}_j. \tag{2.28}$$

We introduce the bosons creation and annihilation operators as

$$\hat{a}_i = \frac{1}{\sqrt{2}} \left(\sqrt{\Omega} \hat{q}_i + \frac{i}{\sqrt{\Omega}} \hat{p}_i \right) \qquad \hat{a}_i^\dagger = \frac{1}{\sqrt{2}} \left(\sqrt{\Omega} \hat{q}_i - \frac{i}{\sqrt{\Omega}} \hat{p}_i \right), \tag{2.29}$$

and the inverse as

$$\hat{q}_i = \sqrt{\frac{1}{2\Omega}} \left(\hat{a}_i + \hat{a}_i^\dagger \right) \qquad \hat{p}_i = i\sqrt{\frac{\Omega}{2}} \left(\hat{a}_i - \hat{a}_i^\dagger \right), \tag{2.30}$$

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

$$\hat{H}_L = \sum_i \Omega \left(\hat{a}_i \hat{a}_i^\dagger + \frac{1}{2} \right) + \frac{1}{4\Omega} \sum_{ij} \left(\hat{a}_i + \hat{a}_i^\dagger \right) L_{ij} \left(\hat{a}_i + \hat{a}_i^\dagger \right). \tag{2.31}$$

Since The network is undirected, L is symmetric and, therefore, we can diagonalize it. The diagonalized laplacian is written in the form $\Lambda = OLO^T$. This generates a new pair of bosons creation and annihilation operators respect the eigenvalue μ of the Laplacian

$$b_\mu = \sum_j a_j O_{\mu j} \qquad \hat{b}_\mu^\dagger = \sum_j a_j^\dagger O_{\mu j}^T. \tag{2.32}$$

Thus, the new Hamiltonian becomes a sum of independent Hamiltonians

$$\hat{H}_L = \sum_\mu \hat{H}_\mu, \tag{2.33}$$

with

$$\begin{aligned} \hat{H}_\mu &= \Omega \left(\hat{b}_\mu \hat{b}_\mu^\dagger + \frac{1}{2} \right) + \frac{1}{4\Omega} \mu \left(\hat{b}_\mu + \hat{b}_\mu^\dagger \right)^2 \\ &= \Omega \left(\hat{b}_\mu \hat{b}_\mu^\dagger + \frac{1}{2} \right) + \frac{1}{4\Omega} \mu \left[\left(\hat{b}_\mu \right)^2 + \left(\hat{b}_\mu^\dagger \right)^2 + 2 \hat{b}_\mu \hat{b}_\mu^\dagger + 1 \right] \\ &= \Omega \left[1 + \frac{1}{2\Omega} \mu \right] \left(\hat{b}_\mu \hat{b}_\mu^\dagger + \frac{1}{2} \right) + \frac{1}{4\Omega} \mu \left[\left(\hat{b}_\mu \right)^2 + \left(\hat{b}_\mu^\dagger \right)^2 \right]. \end{aligned} \tag{2.34}$$

We now consider the system as fermionic so the modes do not excite beyond the first excitation state. In this way we can restrict the Hilbert state of a mode to the span of the ground state $|g\rangle$ and the first excited state $|e_\mu\rangle = b_\mu^\dagger |g\rangle$. A consequence of it is that the second term in the Hamiltonian cancel out.

Now, we can compute the thermal Green function or Matsubara Green function for fermions G. This quantity describes the probability amplitude for the particle to travel from one state to the other in a given time τ (more detail in the Appendix A). For $\tau > 0$ it is

$$\begin{aligned} G_{ij}^L(\beta, \tau > 0) &= \frac{\mathrm{Tr}\left[e^{-\beta \hat{H}_L} \hat{a}_i(\tau) \hat{a}_j^\dagger \right]}{\mathrm{Tr}\left[e^{-\beta \hat{H}_L} \right]} \\ &= \sum_{\mu\nu} O_{\mu i} \frac{\mathrm{Tr}\left[(\tau) e^{-\beta \hat{H}_L} \hat{b}_\mu \hat{b}_\nu^\dagger \right]}{\mathrm{Tr}\left[e^{-\beta \hat{H}_L} \right]} O_{j\nu} \\ &= \sum_\mu O_{i\mu} \left\{ -e^{-\mu\tau} \left[\left(1 - f\left(\Omega + \frac{1}{2\Omega^2} \mu \right) \right) \Theta(\tau) \right] \right\} O_{j\mu} \\ &= \sum_\mu O_{i\mu} \left\{ \frac{e^{-\mu\tau}}{e^{-\beta\left[\Omega + \frac{1}{2\Omega^2}\mu\right]} + 1} \right\} O_{j\mu} \end{aligned} \tag{2.35}$$

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

$$G^L(\beta) = \sum_\mu O_{i\mu} e^{\beta\left[\Omega + \frac{1}{2\Omega^2}\mu\right]} O_{\mu i}, \tag{2.36}$$

that can be written as

$$G^L_{ij}(\beta) = e^{\beta\Omega} e^{\frac{\beta\omega^2}{2\Omega}L}. \tag{2.37}$$

Comparing it with the eq. (2.6), choosing $2\Omega = \omega^2$ the two equations are related as

$$G^R(L) = e^{-\beta\Omega} G^L(\beta). \tag{2.38}$$

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.

2.2 Density matrix and entropy for complex network

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 ensure that it does not only consider the topological features of the network but also the dynamics. Taking the exponential communicability matrix as a reference, we can define a density matrix as

$$\hat{\rho}(\beta) = \frac{1}{Z} e^{-\beta\hat{L}} \qquad \text{with} \qquad Z(\beta) = \mathrm{Tr}[e^{-\beta\hat{L}}], \tag{2.39}$$

where Z is the partition function and it is equal to the Laplacian Estrada index of the network (2.7). It is a hermitian and positive defined matrix with trace equal to unity. It can be seen that $e^{-\beta L}$ is the propagator for diffusion equation in a network at time $t = \beta$.

From this, we can define the Von Neumann entropy as

$$S(\hat{\rho}) = -\mathrm{Tr}[\hat{\rho}\ln\hat{\rho}]. \tag{2.40}$$

The entropy is not negative and it is equal to zero if and only if the $\hat{\rho}$ is a pure state. It has a higher bound $S \leq \ln(N)$ [24].

Figure 2.1 shows the entropy (2.40) 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-sword graph.

Using the density matrix, we can introduce also other thermodynamics quantities like the Helmoltz free energy $F = -\frac{1}{\beta}\ln Z$.

A possible interpretation of this density matrix is given by De Domenico [31]. Consider a network composed of N nodes, encoded in the adjacency matrix A. Each node can be associated with a value n_i representing a property of the network, like the number of

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

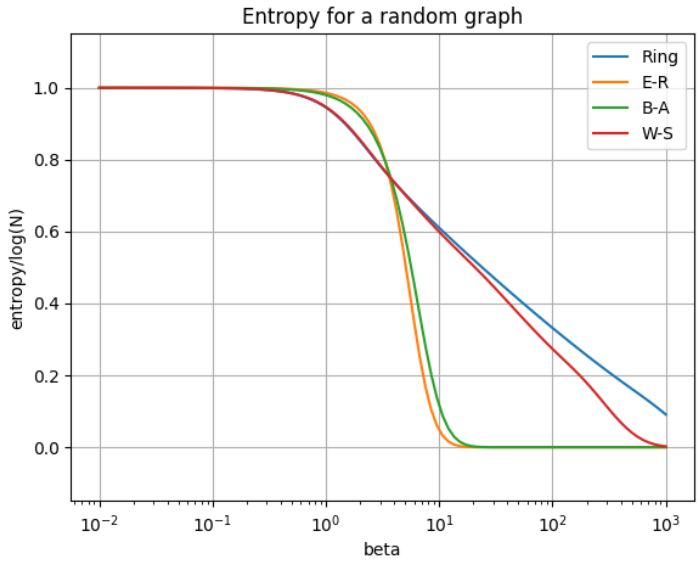

Figure 2.1: Plot of the Von Neumann entropy as a function of β for different network types with 50 nodes: a ring graph (blue), a Erdős-Rényi (E-R) random graph with connectivity probability 0.7 (orange), a Barabási-Albert (B-A) scale-free graph with parameter $m = 3$ (green), and a Watts-Strogatz (W-S) small world graph with parameter $K = 3$ and rewire probability 0.2 (red). The x-axis has a logarithmic scale.

particles in the node in a diffusion model. The evolution of these variables is governed by the control operator $\hat{L}$.

The network can be described using the Dirac notation. Let be $|\psi\rangle = \sum_i n_i |i\rangle$ the state of the system, where $|i\rangle$ is the canonical vector identifying the node i. 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 dynamics can be written as

$$\partial_t |\psi(t)\rangle = -\hat{L}|\psi(t)\rangle, \tag{2.41}$$

with the solution

$$|\psi(t)\rangle = \hat{G}(t,0)|\psi(0)\rangle \tag{2.42}$$

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

Since $\hat{L}$ is Hermitian, the propagator can be diagonalized in the orthogonal basis $\{|v_\lambda\rangle\}_\lambda$ of eigenvectors of the control operator

$$\hat{G}(t,0) = \sum_\lambda e^{-t\lambda} |v_\lambda\rangle\langle v_\lambda| = \sum_\lambda e^{-t\lambda} \hat{\sigma}_\lambda, \tag{2.43}$$

where $\hat{\sigma}_\lambda$ is the projection over the left and right eigenvectors with the λ eigenvalue. The operators do not depend on time, they are constant along the process, only the eigenvalues 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 as $|\Delta\psi_0\rangle = \sum_i \Delta_i |i\rangle$. The time evolution of the state becomes

$$|\psi(t)\rangle = G(t,0)|\psi(0)\rangle = |\psi_0\rangle + G(t,0)|\Delta\psi\rangle = |\psi_0\rangle + |\Delta\psi(t)\rangle \tag{2.44}$$

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

Since the stationary component is constant in time, we focus on the perturbation. The value of the perturbation at node j at time t is

$$\langle j \,|\, \Delta\psi(t)\rangle = \langle j|e^{-t\hat{L}}|\Delta\psi\rangle = \sum_\lambda \langle j|e^{-t\lambda}\hat{\sigma}_\lambda|\Delta\psi\rangle = \sum_i \sum_\lambda \Delta_i e^{-t\lambda}\langle j|\hat{\sigma}_\lambda|i\rangle. \tag{2.45}$$

We have used equation (2.43) and the definition of the perturbation. This equation shows that the perturbation travels through N different streams, one for each σ_λ, with the 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. Sometimes, the dynamics traps part of the perturbation in a specific node. The trapped perturbation's size can be compute as

$$T = \sum_i \sum_\lambda \Delta_i e^{-t\lambda}\langle i|\hat{\sigma}_\lambda|i\rangle \tag{2.46}$$

Assuming maximal uncertainty in the perturbation, obtainable when $\Delta_i = \Delta$, the equation reduces to

$$T = \Delta \sum_i e^{-t\lambda}\langle i|\hat{\sigma}_\lambda|i\rangle = \Delta \,\mathrm{Tr}[\hat{G}(t,0)] \tag{2.47}$$

Since the trapped perturbation regulates the stream's sizes, it can be responsible for the generation of the streams itself. Thus, we can define a density matrix

$$\hat{\rho}_t = \frac{1}{T}\Delta e^{-t\hat{L}} = \frac{1}{Z}e^{-t\hat{L}}, \tag{2.48}$$

where $Z = \mathrm{Tr}[e^{-t\hat{L}}]$ is the partition function. This density matrix can be interpreted as the probability that the perturbation will flow through a specific stream $\hat{\sigma}_l$ in the ensemble of all the possible streams [31].

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

Starting from the concept of entropy, we can also introduce the Kullback-Liebler divergence as

$$D(\hat{\rho}||\hat{\sigma}) = \mathrm{Tr}\left[\hat{\rho}\ln\left(\frac{\hat{\sigma}}{\hat{\rho}}\right)\right]. \tag{2.49}$$

It can be used to make comparisons between networks. Moreover, this concept we can be applied to the reconstruction of network starting from real data using the maximum likelihood estimation.

However the Kullback-Liebler divergence is not symmetric, so can not be use as a metric. But we can symmetrize introducing the Jensen-Shannon divergence as

$$\mathcal{D}(\hat{\rho}||\hat{\sigma}) = D(\hat{\rho}||\hat{\mu}) + D(\hat{\sigma}||\hat{\mu}) = S(\hat{\mu}) - \frac{1}{2}\left[S(\hat{\rho}) + S(\hat{\sigma})\right], \tag{2.50}$$

where $\hat{\mu} = \frac{1}{2}(\hat{\rho}+\hat{\sigma})$. It is a metric: it is symmetric, positive define, and hold the triangular inequality [32]. It has been use successfully to measure the distance between the layer of a multilayer network [17].

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 [33, 34]. This equation was introduced to explain 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 experiment we can build are susceptible to the external environment. In this way we can recover and justify the basic assumption physicists do in quantum statistical mechanics.

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 an unitary time operator that does not allow energy dissipations. In contrast, the time operator of Lindblad master equation permits the system to dissipate energy with the surrounding. 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 [35, 36]. First, let $\mathcal{H}_T$ be the Hilbert space of the system and the environment combined, that can be divided between the Hilbert spaces $\mathcal{H}$ of the proper system and $\mathcal{H}_E$ of the environment. The combined system is a quantum closed system and evolves following the Von Neumann equation $\partial_t \hat{\rho}_T(t) = -i[\hat{H}_T, \hat{\rho}_T(t)]$, where $\hat{H}_T$ is the Hamiltonian of the total universe. Since we are interesting only 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 $H_T = H \otimes \mathbb{I}_E + \mathbb{I}_S \otimes H_E + \alpha H_I$, 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. It is useful to work in the interaction pictures where the operators becomes

$$\tilde{O}(T) = e^{i(\hat{H}+\hat{H}_E)t} \hat{O} e^{-i(\hat{H}+\hat{H}_E)t}, \tag{3.1}$$

and the Von Neumann equation reduces to

$$\frac{d\tilde{\rho}_T(t)}{dt} = -i\alpha \left[\tilde{H}_I(t), \tilde{\rho}_T(t)\right]. \tag{3.2}$$

The solution to (3.2) is

$$\tilde{\rho}_T(t) = \tilde{\rho}_T(0) - i\alpha \int_0^t ds \left[\tilde{H}_I(s), \tilde{\rho}_T(s)\right]. \tag{3.3}$$

Even though the equation (3.3) has an exact solution, it is complicate to compute. To simplify the calculation, we can introduce the (3.3) into the (3.2) giving

$$\frac{d\tilde{\rho}_T(T)}{dt} = -i\alpha \left[\tilde{H}_I(T), \tilde{\rho}_T(0)\right] - \alpha^2 \int_0^t ds \left[\tilde{H}_I(t), \left[\tilde{H}_I(s), \tilde{\rho}_T(s)\right]\right] \tag{3.4}$$

Apply this method again, we obtain

$$\frac{d\tilde{\rho}_T(T)}{dt} = -i\alpha \left[\tilde{H}_I(T), \tilde{\rho}_T(0)\right] - \alpha^2 \int_0^t ds \left[\tilde{H}_I(t), \left[\tilde{H}_I(s), \tilde{\rho}_T(t)\right]\right] + O(\alpha^3) \tag{3.5}$$

Now, we make an approximation: we consider the strength of the interaction α weak, in this way we can neglect the last term. Now we can trace out the environment obtaining

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

However, the equation (3.6) still depends on the total density matrix. To proceed, we make two more assumptions. First, we consider the initial state of the universe as a separable state $\hat{\rho}_T(0) = \hat{\rho}(0) \otimes \hat{\rho}_E(0)$. This holds if the system is 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 to be in a thermal state

$$\hat{\rho}_E(0) = \frac{e^{-\hat{H}_E/T}}{\mathrm{Tr}\left[e^{-\hat{H}_E/T}\right]}, \tag{3.7}$$

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

$$\hat{H}_I(t) = \sum_i \hat{S}_i \otimes \hat{E}_i, \tag{3.8}$$

where $\hat{S}_i$ is an operator acting on $\mathcal{H}$ (is not a spin operator) and $\hat{E}_i$ is an operator acting on $\mathcal{H}_\mathcal{E}$. After this assumption, the equation (3.6) becomes

$$\begin{aligned}\frac{d\tilde{\rho}}{dt} = &- i\alpha \sum_i \left(\tilde{S}_i(t)\tilde{\rho}(0)\,\mathrm{Tr}_E\left[\tilde{E}_i(t)\tilde{\rho}_E(0)\right] - \tilde{\rho}(0)\tilde{S}_i(t)\,\mathrm{Tr}_E\left[\tilde{\rho}_E(0)\tilde{E}_i(t)\right]\right) \\ &- \alpha^2 \int_0^t ds \,\mathrm{Tr}_E \left[\tilde{H}_I(t), \left[\tilde{H}_I(s), \tilde{\rho}(t) \otimes \tilde{\rho}_E(t)\right]\right].\end{aligned} \tag{3.9}$$

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 as 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 more stronger assumption: since α is small, the system and the environment should remain uncorrelated throughout the evolution, that is 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. To add this property, we can extend the upper limit of the integration to infinity with no real change in the outcome. Then, changing the integral variable to $t - s$, we arrive to

$$\frac{d\tilde{\rho}(t)}{dt} = -\alpha^2 \int_0^\infty ds\, \mathrm{Tr}_E\left[\tilde{H}_I(t), \left[\tilde{H}_I(t-s), \tilde{\rho}(t)\otimes\tilde{\rho}_E(t)\right]\right]. \tag{3.10}$$

This is called Redfield equation [37]. 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 sum of approximations made before are called Born-Markov approximation [36].

The equation (3.10) can generate a negative density matrix. To exclude this possibility, we consider a superoperator $\mathbb{H}A = [H, A]$, with A a general operator. The eigenvectors of the superoperator generate a complete basis of the space $\{\hat{S}_i(\omega)\}$ of the bounded operators acting on the Hilbert $\mathcal{H}$, they satisfy the condition

$$\mathbb{H}\hat{S}_i(\omega) = -\omega\hat{S}_i(\omega) \qquad \mathbb{H}\hat{S}_i^\dagger(\omega) = \omega\hat{S}_i^\dagger(\omega). \tag{3.11}$$

Here, ω indicates the energy difference after the operator $\hat{A}_i(\omega)$ has acted. It satisfies the relations

$$\begin{aligned} e^{i\hat{H}_S t}\hat{A}(\omega)e^{-i\hat{H}_S t} &= e^{-i\omega t} \\ e^{i\hat{H}_S t}\hat{A}^\dagger(\omega)e^{-i\hat{H}_S t} &= e^{i\omega t} \end{aligned} \tag{3.12}$$

We can decompose the operators S_i as $\hat{S}_i = \sum_\omega \hat{S}_i(\omega)$. To apply this decomposition in (3.10), 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 in the interacting picture

$$\tilde{H}_i(t) = \sum_{i\omega} e^{-i\hat{H}t}\hat{S}_i(\omega)\otimes\tilde{E}_i(t) = \sum_{i\omega} e^{i\hat{H}t}\hat{S}_i^\dagger(\omega)\otimes\tilde{E}_i(t) \tag{3.13}$$

After expanding the commutators in (3.10), we substitute the decomposition for $\hat{S}_k(\omega)$. 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

$$\frac{d\tilde{\rho}(t)}{dt} = \sum_{\omega,\omega',i,j} e^{i(\omega-\omega')t}\Gamma_{ij}\left[\hat{S}_j(\omega)\tilde{\rho}(t), \hat{S}_i^\dagger(\omega')\right] + e^{-i(\omega-\omega')t}\Gamma_{ji}^\dagger\left[\hat{S}_j(\omega), \tilde{\rho}(t)\hat{S}_i^\dagger(\omega')\right], \tag{3.14}$$

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

$$\Gamma_{ij}(\omega) = \int_0^\infty ds e^{i\omega s} \operatorname{Tr}\left[\tilde{E}_i^\dagger(t)\tilde{E}_j(t-s)\hat{\rho}_E(0)\right] \tag{3.15}$$

where 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 $|\omega - \omega'| >> \alpha^2$ will oscillate much faster than the timescale of the system; thus, they do not contribute to the evolution of the system. 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 (3.14) reduces to

$$\frac{d\tilde{\rho}(t)}{dt} = \sum_{\omega,i,j} \Gamma_{ij}\left[\hat{S}_j(\omega)\tilde{\rho}(t), \hat{S}_i^\dagger(\omega)\right] + \Gamma_{ji}^\dagger\left[\hat{S}_j(\omega), \tilde{\rho}(t)\hat{S}_i^\dagger(\omega)\right]. \tag{3.16}$$

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

$$\begin{aligned}
\gamma_{ij}(\omega) &= \Gamma_{ij}(\omega) + \Gamma_{ij}^\dagger(\omega) = \int_{-\infty}^\infty ds e^{i\omega s} \operatorname{Tr}\left[\left\{\tilde{E}_i^\dagger(t), \tilde{E}_j(t-s)\right\}\hat{\rho}_E(0)\right] \\
\pi_{ij}(\omega) &= \frac{-i}{2}\left(\Gamma_{ij}(\omega) - \Gamma_{ij}^\dagger(\omega)\right)\int_{-\infty}^\infty ds e^{i\omega s} \operatorname{Tr}\left[\left[\tilde{E}_i^\dagger(t), \tilde{E}_j(t-s)\right]\hat{\rho}_E(0)\right]
\end{aligned} \tag{3.17}$$

Inserting them into the equation (3.16) and returning to the Schrödinger picture, we obtain

$$\frac{d}{dt}\hat{\rho} = -i\left[\hat{H} + \hat{H}_{LS}, \hat{\rho}\right] + \sum_{i,j,\omega}\gamma_{ij}(\omega)\left(\hat{S}_i(\omega)\hat{\rho}\hat{S}_j^\dagger(\omega) - \frac{1}{2}\left\{\hat{S}_i^\dagger(\omega)\hat{S}_j(\omega), \hat{\rho}\right\}\right), \tag{3.18}$$

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 and it adjusts the energy levels due to thee interaction with the environment. The equation (3.18) is the general version of the Markovian master equation. The matrix $\gamma(\omega)$ must be positive define, although the trace preserving 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 $\hat{O}$ a unitary operator, and considering the simplest case of just one frequency ω then we can write the Lindblad-Gorini-Kossakowski-Sudarshan master equation as

$$\frac{d}{dt}\hat{\rho} = \mathcal{L}[\hat{\rho}] = -i\left[\hat{H} + \hat{H}_{LS}, \hat{\rho}\right] + \sum_k \gamma_k\left(\hat{J}_k\hat{\rho}\hat{J}_k^\dagger - \frac{1}{2}\left\{\hat{J}_k^\dagger\hat{J}_k, \hat{\rho}\right\}\right). \tag{3.19}$$

The operator $\hat{J}_k = \sum_i O_{ki}\hat{S}_i$ are called jump operators, the superoperator $\mathcal{L}$ is called Lindblad superoperator and γ_i are the damping rates. In the limit $\gamma_k = 0$ the Von Neumann equation is recovered.

3.2 Properties of the Lindblad equation

The Lindblad master equation satisfies some important properties. The Lindblad master equation defines a set of dynamical maps $\phi_t(\hat{\rho}) = e^{\mathcal{L}t}\hat{\rho}(0)$ on the space of density matrices such that

$$\hat{\rho}(t) = \phi_t(\hat{\rho}(0)). \tag{3.20}$$

These maps have the semigroup property, that is,

$$\phi_s(\phi_t(\hat{\rho}(0))) = \phi_{t+s}(\hat{\rho}(0)) \tag{3.21}$$

The Lindblad master equation is the most general form for the generator of a quantum dynamical system. As a matter of fact, the Lindblad equation can also be derived starting from this assumption [36].

The Lindblad master equation is invariant under the following transformations [36]:

- Unitary transformation of the Lindblad operator:

$$\sqrt{\gamma_i}\hat{J}_i \to \sqrt{\gamma_i'}\hat{J}_i' = \sum_j u_{ij}\sqrt{\gamma_j}\hat{J}_j \tag{3.22}$$

  where u_{ij} is an unitary matrix.

- Inhomogeneous transformation:

$$\begin{aligned} \hat{J}_i &\to \hat{J}_i' = \hat{J}_i + a_i \\ \hat{H}_I &\to \hat{H}' = \hat{H} + \frac{1}{2i}\sum_j \gamma_j\left(a_j^*\hat{J}_j - a_j\hat{J}_j^\dagger\right) \end{aligned} \tag{3.23}$$

  where $a_i \in \mathbf{C}$ and $b \in \mathbf{R}$.

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

Lastly, we can prove that the dynamics (3.24) conserve $\mathrm{Tr}[\hat{\rho}]$. As a matter of fact, the derivative along time of it is

$$\frac{d}{dt}\mathrm{Tr}[\hat{\rho}] = \mathrm{Tr}\left[-i\left(\hat{H}\hat{\rho} - \hat{\rho}\hat{H}\right) + \hat{J}_k\hat{\rho}\hat{J}_k^\dagger - \frac{1}{2}\left(\hat{L}\hat{\rho} + \hat{\rho}\hat{L}\right)\right] = 0, \tag{3.24}$$

proved using the cyclic property of the trace. However, it does not conserve the purity $\mathrm{Tr}[\hat{\rho}^2]$ that decreases [35].

3.3 Time evolution

Following the resolution proposed by Fujii [38] for a quantum harmonic oscillator, we can solve the Lindblad master equation. First of all, 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 called Fock-Liouville space [35].

The follow operation can be vectorize as

$$\hat{A}\hat{\rho}\hat{B} \to (\hat{A}\otimes\hat{B})|\rho\rangle\rangle \qquad \hat{A}\hat{\rho}+\hat{\rho}\hat{B} \to \left(\hat{A}\otimes\mathbb{I}+\mathbb{I}\otimes\hat{B}\right)|\rho\rangle\rangle, \tag{3.25}$$

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

$$\hat{A}\otimes\hat{B} = \begin{pmatrix} A_{11}\hat{B} & \cdots & A_{1N}\hat{B} \\ \vdots & \ddots & \vdots \\ A_{n1}\hat{B} & \cdots & A_{NN}\hat{B} \end{pmatrix}. \tag{3.26}$$

More detail are shown in the Appendix B.

In this space the Lindblad equation (3.19) becomes

$$\frac{d}{dt}|\rho(t)\rangle\rangle = \tilde{\mathcal{L}}|\rho(t)\rangle\rangle, \tag{3.27}$$

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

$$\tilde{\mathcal{L}} = -i\left[\hat{H}\otimes\mathbb{I}-\mathbb{I}\otimes\hat{H}\right]+\sum_k\gamma_k\left[\hat{J}_k\otimes\hat{J}_k^\dagger+\hat{J}_k^\dagger\hat{J}_k\otimes\mathbb{I}+\mathbb{I}\otimes\hat{J}_k^\dagger\hat{J}_k\right]. \tag{3.28}$$

The solution equation (3.27) can be written as

$$|\rho(t)\rangle\rangle = \hat{U}(t)|\rho(0)\rangle\rangle, \tag{3.29}$$

where $U(t)$ is the evolution operator

$$\begin{aligned}\hat{U}(t) = \exp\Big\{&-it\left(\hat{H}\otimes\mathbb{I}-\mathbb{I}\otimes\hat{H}\right)\\ &+t\sum_k\gamma_k\left[\hat{J}_k\otimes\hat{J}_k^\dagger-\frac{1}{2}\hat{J}_k\hat{J}_k^\dagger\otimes\mathbb{I}-\frac{1}{2}\mathbb{I}\otimes\hat{J}_k\hat{J}_k^\dagger\right]\Big\}\end{aligned} \tag{3.30}$$

The evolution operator is not unitary.

3.4 Entropy production

In thermodynamics, the irreversibility is encoded in the entropy function: a process is reversible if and only if the process does not produce entropy, $\Delta S = 0$, otherwise is irreversible. The Lindblad master equation (3.19) should describe irreversible processes of an open quantum system since the thermal fluctuations are not reversible.

Considering the derivative of the Von Neumann entropy

$$\dot{S}\left(\hat{\rho}(t)\right) = -\operatorname{Tr}\left[\frac{d\hat{\rho}}{dt}\ln\hat{\rho}\right]+\operatorname{Tr}\left[\frac{d\hat{\rho}}{dt}\right] \tag{3.31}$$

Knowing that the dynamics is trace preserving, namely $\mathrm{Tr}\left[\frac{d\hat{\rho}}{dt}\right] = 0$, it reduces to

$$\dot{S}\left(\hat{\rho}(t)\right) = -\,\mathrm{Tr}\left[\frac{d\hat{\rho}}{dt}\ln\hat{\rho}\right] \tag{3.32}$$

To prove that the Lindblad dynamics is truly irreversible we can insert it into (3.32). The Von Neumann dynamical part does not produce entropy, thus, we can only consider the dissipative one. We reach the equation

$$\dot{S}(\hat{\rho}) = -\,\mathrm{Tr}\left[\sum_k \gamma_k \left[\hat{J}_k\hat{\rho}\hat{J}_k^\dagger - \frac{1}{2}\left\{\hat{J}_k^\dagger\hat{J}_k,\hat{\rho}\right\}\right]\ln\hat{\rho}\right]. \tag{3.33}$$

We expand the commutator

$$\dot{S}(\hat{\rho}) = -\sum_k \gamma_k\,\mathrm{Tr}\left[\hat{J}_k\hat{\rho}\hat{J}_k^\dagger\ln\hat{\rho} - \frac{1}{2}\hat{J}_k^\dagger\hat{J}_k\hat{\rho}\ln\hat{\rho} - \frac{1}{2}\hat{\rho}\hat{J}_k^\dagger\hat{J}_k\ln\hat{\rho}\right] \tag{3.34}$$

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

$$\dot{S}(\hat{\rho}) = -\sum_k \gamma_k\left(\mathrm{Tr}\left[\hat{J}_k\hat{\rho}\hat{J}_k^\dagger\ln\hat{\rho}\right] - \mathrm{Tr}\left[\hat{J}_k^\dagger\hat{J}_k\hat{\rho}\ln\hat{\rho}\right]\right) \tag{3.35}$$

To ensure that $\dot{S}(\hat{\rho}) > 0$, the system must satisfy the following condition

$$\sum_k \gamma_k\,\mathrm{Tr}\left[\hat{J}_k\hat{\rho}\hat{J}_k^\dagger\ln\hat{\rho}\right] \leq \sum_k \gamma_k\,\mathrm{Tr}\left[\hat{J}_k^\dagger\hat{J}_k\hat{\rho}\ln\hat{\rho}\right], \tag{3.36}$$

that depends on the choice of the γ_k. Assume the positivity of the damping rates, the majority of the processes satisfies this condition, the inequality (3.36) holds if the following inequality is satisfied

$$\mathrm{Tr}\left[\hat{J}_k\hat{\rho}\hat{J}_k^\dagger\ln\hat{\rho}\right] \leq \mathrm{Tr}\left[\hat{J}_k^\dagger\hat{J}_k\hat{\rho}\ln\hat{\rho}\right]. \tag{3.37}$$

It can be proved to be always satisfied. 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 transform also the jump operator in this basis $\hat{\mathcal{J}}_k = \hat{O}\hat{J}_k\hat{O}^\dagger$. The l.h.s. of the inequality (3.37) becomes with some algebra can be reduces to

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

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 r.h.s. 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 just a Kronecker delta. We use the completeness relation $I = \sum_\mu |\mu\rangle\langle\mu|$ obtaining

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

The inequality (3.37) reduces to

$$N \sum_{\lambda\mu} \rho_\lambda \ln \rho_\mu x_{\lambda\mu}^{(k)} \leq N \sum_{\lambda\mu} \rho_\lambda \ln \rho_\lambda x_{\lambda\mu}^{(k)}. \tag{3.42}$$

We can rearrange the term in the two sum as

$$\begin{aligned}\sum_\lambda \sum_{\mu<\lambda} \left(\rho_\lambda \ln \rho_\mu + \rho_\mu \ln \rho_\lambda\right) x_{\lambda\mu}^{(k)} + \sum_\lambda \rho_\lambda \ln \rho_\lambda x_{\lambda\lambda}^{(k)} \leq \\ \sum_\lambda \sum_{\mu<\lambda} \left(\rho_\lambda \ln \rho_\lambda + \rho_\mu \ln \rho_\mu\right) x_{\lambda\mu}^{(k)} + \sum_\lambda \rho_\lambda \ln \rho_\lambda x_{\lambda\lambda}(k)\end{aligned} \tag{3.43}$$

Therefore, it is sufficient that the following equation is satisfied

$$\rho_\lambda \ln \rho_\mu + \rho_\mu \ln \rho_\lambda \leq \rho_\lambda \ln \rho_\lambda + \rho_\mu \ln \rho_\mu. \tag{3.44}$$

Moving all the term in the right hand side we reach

$$\begin{aligned}\rho_\lambda \ln \rho_\mu + \rho_\mu \ln \rho_\lambda - \rho_\lambda \ln \rho_\lambda - \rho_\mu \ln \rho_\mu \leq 0 \\ (\rho_\lambda - \rho_\mu) \ln\left(\frac{\rho_\mu}{\rho_\lambda}\right) \leq 0\end{aligned} \tag{3.45}$$

That is always satisfied. The equality is satisfied for the stationary distribution.

The last result tell us that the dynamics increases the entropy and, thus, change a pure density matrix in a mixed one. As a consequence, the the stationary distribution must have maximum entropy.

3.5 Stationary distribution

The Lindblad equation allows for a stationary distribution that satisfies the condition

$$\mathcal{L}\hat{\rho} = 0. \tag{3.46}$$

In the previous section, we assumed that the environment is in a Gibbs state. Now, consider that the damping parameter satisfies the relation

$$\gamma_{ij}(-\omega) = e^{-\beta\omega}\gamma_{ij}(\omega) \tag{3.47}$$

which is called KMS condition [36]. If this condition is satisfied, it can be proven that the stationary distribution is equal to the Gibbs states [36]

$$\hat{\rho}^* = \frac{e^{-\beta\hat{H}}}{\mathrm{Tr}\left[e^{-\beta\hat{H}}\right]}. \tag{3.48}$$

If the spectrum of the Hamiltonian $H = \sum_n \epsilon_n |n\rangle\langle n|$ is not degenerate, it gives rise to a closed equation for the population

$$P(n,t) = \langle n|\hat{\rho}(t)|n\rangle \tag{3.49}$$

Thus, the dynamics decouple the diagonal and off-diagonal terms. The former are governed by the Pauli master equation

$$\frac{dP(n,t)}{dt} = \sum_m \left[W(n|m)P(m,t) - W(m|n)P(n,t)\right] \tag{3.50}$$

with time independent transition rate

$$W(n|m) = \sum_{ij} \gamma_{ij}(\epsilon_n - \epsilon_m)\langle n|\hat{J}_i(t)|m\rangle\langle m|\hat{J}_j(t)|n\rangle. \tag{3.51}$$

Using the equation (3.47) and considering the l.h.s. of the equation (3.50) , we obtain the Fermi Golden rule

$$W(n|m)e^{-\beta\epsilon_n} = W(m|n)e^{-\beta\epsilon_m} \tag{3.52}$$

which is nothing other that a detailed balance condition with stationary distribution

$$\hat{\rho} = \frac{1}{Z}e^{-\beta\hat{H}} \tag{3.53}$$

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

Chapter 4

Quantum Network Master Equation

In chapter 2 we have introduce the concept of density matrix for a network, based on the communicability matrix. This quantity considers the correlation between the nodes created by the random walk dynamics.

In this chapter we try to unify the two concept taken from the quantum realm: the quantum random walk and the density matrix. In fact, we considering a quantum walk process exposed to thermal noise we obtain a stationaty distribution which coincides with the network's density matrix. The interaction between the quantum system and the thermal noise are considered Markovian, thus, it is studied with the Lindblad master equation.

4.1 Quantum Stochastic Random Walk

One of the firsts approaches to a Open Quantum Walk on network was proposed by Whitfield, Rodríguez-Rosario and Aspuru-Guzik. [39]. They defined a quantum walk on network in contact with a thermal bath, the dynamics is describe by a Lindblad master equation with the jump operators proportional to the Adjacency matrix A_{ij} of the network. The thermal bath act as noise in the dynamics which does not follow strictly the Von Neumann equation (1.37). The system dissipation reminds the classic random walk.

Let we 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. we can describe the its evolution with the Lindblad master equation (3.24): the Laplacian operator $\hat{L}$ is Hamiltonian $\hat{H}$ and the jump operator $\{\hat{J}_k\}_{k<M}$ are the jumps from two node connected by a link. For convenience, we will call the jump operator with two indeces referring to the starting node and the ending node of the jump;therefore, the jumps operator are $\hat{J}_{ij} = |i\rangle\langle j|$. The dumping rates γ_i are the $\gamma_{ij} = A_{ij}$. We obtain the master equation

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

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

equation (4.1) is composed by two distinct terms: the first term, also called coherent dynamics, $\mathcal{L}^{qm}[\hat{\rho}(t)] = -i[H, \hat{\rho}]$ is equal to the quantum walk dynamics; instead, the second $\mathcal{L}^{cl}[\hat{\rho}(t)] = \sum_i \gamma_i \left(\hat{J}_i \hat{\rho} \hat{J}_i^\dagger - \frac{1}{2}\left\{\hat{J}_i^\dagger \hat{J}_i, \hat{\rho}\right\}\right)$, called decoherent dynamics, encodes the dissipation. When $\gamma_{ij} = 0$ we recover the Von Neumann equation for the quantum walk (1.37). $\mathcal{L}[\hat{\rho}]$ is a superoperator that act in the space of the density matrix.

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

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

where the evolution operator is defined as [40]

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

The master equation (4.1) contains both the quantum and classical aspect of a diffusion over a network. As a matter of fact,the classical random walk behavior emerges considering the evolution of the diagonal element of the density matrix under just the dissipative part. Let $\rho = |k\rangle\langle k|$ be the density matrix of a system in node k, it evolves following

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

where d_i is the degree of the node i. We have recovered the dynamics of the classical random walk over a network.

Considering the off-diagonal terms, they evolve as

$$\begin{aligned}\mathcal{L}^{cl}|k\rangle\langle kl| &= \sum_{ij}\gamma_{ij}\left[\hat{J}_{ij}|k\rangle\langle l|\hat{J}_{ij}^\dagger - \frac{1}{2}\left\{\hat{J}_{ij}^\dagger\hat{J}_{ij}, |k\rangle\langle l|\right\}\right] \\ &= \sum_j \left[-\frac{1}{2}A_{jk}|k\rangle\langle l| - \frac{1}{2}A_{jl}|k\rangle\langle l|\right] \\ &= -\frac{1}{2}(d_k + d_l)|a\rangle\langle b|.\end{aligned} \tag{4.5}$$

$\mathcal{L}^{cl}$ do not mixed the diagonal term with the off-diagonal ones. Thus, the superoperator is divide in two block: one for the diagonal element, the other for the off-diagonal ones. The superoperator $\mathcal{L}^{cl}$ has a diagonal form with spectrum $\sigma^{cl} = -(\lambda_1, ..., \lambda_N, \frac{1}{2}(d_1 + d_2), ..., \frac{1}{2}(d_N + d_{N-1}))$, where λ_i are the eigenvalue of the Laplacian matrix [41]. If the network satisfies the detailed balance condition (1.21), the Laplacian matrix has a zero eigenvalue and, therefore, also the superoperator $\mathcal{L}^{cl}$ has a zero eigenvalue and a stationary distribution.

4.1.1 Stationary distribution

Following the prove of the stationary distribution in chapter 3, we can find the stationary density matrix $\hat{\rho}^*$ for the quantum stochastic walk. Let consider the only dissipation dynamics. The dynamics decouples the diagonal and off-diagonal terms. The first follow the evolution

$$\frac{d}{dt}\rho_{ii} = \sum_j \left[W(i|j)\rho_{jj}(t) - W(j|i)\rho_{ii}(t)\right], \tag{4.6}$$

with transition rate

$$W(i|j) = W(j|i) = A_{ij}. \tag{4.7}$$

Since the stationary distribution must satisfy the detail balance, namely

$$W(i|j)\rho_{jj}(t) = W(j|i)\rho_{ii}. \tag{4.8}$$

Thus, the diagonal entries must be equal. Instead, considering the vector $|\rho\rangle\rangle$, the block of corresponding to the off diagonal part of $\mathcal{L}$ is already diagonal with eigenvalue $\frac{1}{2}(d_i + d_j) > 0$. Thus, off diagonal terms must be equal to zero.

The stationary density matrix will be

$$\hat{\rho}^* = \frac{1}{N}\begin{pmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{pmatrix}. \tag{4.9}$$

As anticipated, the stationary distribution has maximal Von Neumann entropy

$$S\left(\hat{\rho}^*\right) = \ln N. \tag{4.10}$$

4.2 Quantum Network Master Equation

The previous description of noise in quantum walk lack 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 (3.19) with Hamiltonian $\hat{H} = \hat{L}$. We consider the basis $\{|\lambda\rangle\}$ such that $\hat{H} = \sum_\lambda \epsilon_\lambda |\lambda\rangle\langle\lambda| = \hat{L}$ is diagonal (the network must hold the detail balance condition (1.21)). 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

$$\frac{d}{dt}\hat{\rho} = -i\left[\hat{H}, \hat{\rho}\right] + \sum_{\lambda\mu}\gamma_{\lambda\mu}\left(\hat{J}_{\lambda\mu}\hat{\rho}\hat{J}^\dagger_{\lambda\mu} - \frac{1}{2}\left\{\hat{J}^\dagger_{\lambda\mu}\hat{J}_{\lambda\mu}, \hat{\rho}\right\}\right), \tag{4.11}$$

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

$$\hat{\rho}^* = \frac{e^{-\beta\hat{H}}}{Z}, \tag{4.12}$$

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

The master equation for the stationary distribution is

$$0 = -i\left[\hat{H}, \frac{e^{-\beta\hat{H}}}{Z}\right] + \sum_{\lambda\mu}\gamma_{\lambda\mu}\left(\hat{J}_{\lambda\mu}\frac{e^{-\beta\hat{H}}}{Z}\hat{J}^{\dagger}_{\lambda\mu} - \frac{1}{2}\left\{\hat{J}^{\dagger}_{\lambda\mu}\hat{J}_{\lambda\mu}, \frac{e^{-\beta\hat{H}}}{Z}\right\}\right). \tag{4.13}$$

The first term in the r.h.s. vanishes because the commutator is zero. The first term of the sum can be written as

$$\sum_{\lambda\mu}\gamma_{\lambda\mu}|\lambda\rangle\langle\mu|\frac{e^{-\beta\hat{H}}}{Z}|\mu\rangle\langle\lambda| = \sum_{\lambda\mu}\gamma_{\lambda\mu}\frac{e^{-\beta\epsilon_\mu}}{Z}|\lambda\rangle\langle\lambda|. \tag{4.14}$$

While the second becomes

$$\sum_{\lambda\mu}\gamma_{\lambda\mu}\left[\frac{1}{2}|\mu\rangle\langle\lambda\,|\,\lambda\rangle\langle\mu|\frac{e^{-\beta\hat{H}}}{Z} + \frac{1}{2}\frac{e^{-\beta\hat{H}}}{Z}|\mu\rangle\langle\lambda\,|\,\lambda\rangle\langle\mu|\right] = \sum_{\lambda\mu}\gamma_{\lambda\mu}\left[\frac{e^{-\beta\epsilon_\mu}}{Z}|\mu\rangle\langle\mu|\right]. \tag{4.15}$$

Therefore, the master equation (4.13) reduces to

$$\sum_{\lambda\mu}\left[\gamma_{\lambda\mu}\frac{e^{-\beta\epsilon_\mu}}{Z} - \gamma_{\mu\lambda}\frac{e^{-\beta\epsilon_\lambda}}{Z}\right]|\lambda\rangle\langle\lambda| = 0. \tag{4.16}$$

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 canonical distribution. However, there are several possible choice for the coefficients $\gamma_{\lambda\mu}$ such that equation (4.16) holds. Each different choice generate a different path to reach the stationary distribution (4.12). 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 (4.16) reduces to the detail balance condition

$$\gamma_{\lambda\mu}\frac{e^{-\beta\epsilon_\mu}}{Z} - \gamma_{\mu\lambda}\frac{e^{-\beta\epsilon_\lambda}}{Z} = 0, \tag{4.17}$$

which has solution

$$\gamma_{\lambda\mu} = e^{-\frac{\beta}{2}(\epsilon_\lambda - \epsilon_\mu)}. \tag{4.18}$$

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

$$\gamma_{\lambda\mu} \to \begin{cases} 0 & \lambda > \mu \\ 1 & \lambda = \mu \\ \infty & \lambda < \mu \end{cases}. \tag{4.19}$$

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

$$\hat{\rho}^* = |\lambda = 0\rangle\langle\lambda = 0|. \tag{4.20}$$

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

$$\gamma_{\lambda\mu} \to 1. \tag{4.21}$$

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.

$$\hat{\rho}^* = \frac{1}{N} \begin{pmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{pmatrix}. \tag{4.22}$$

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

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

$$\hat{J}^\dagger_{\lambda\mu} = \sum_{ij} \langle j \,|\, \mu\rangle\langle \lambda \,|\, i\rangle \hat{J}^\dagger_{ij} \tag{4.24}$$

where $\hat{J}_{ij} = |i\rangle\langle j|$. Thus, the equation (4.11) becomes

$$\frac{d}{dt}\hat{\rho} = -i\left[\hat{H}, \hat{\rho}\right] + \sum_{ijkl} \gamma_{ij;kl} \left(\hat{J}_{ij}\hat{\rho}\hat{J}^\dagger_{kl} - \frac{1}{2}\left\{ \hat{J}^\dagger_{kl}\hat{J}_{ij}, \hat{\rho} \right\} \right), \tag{4.25}$$

with the dump coefficient

$$\gamma_{ij;kl} = \sum_{\lambda\mu} \gamma_{\lambda\mu} \langle i \,|\, \lambda\rangle\langle \lambda \,|\, k\rangle\langle l \,|\, \mu\rangle\langle \mu \,|\, j\rangle. \tag{4.26}$$

Inserting the equation (4.18) into (4.26) we reach

$$\gamma_{ij;kl} = \sum_{\lambda\mu} e^{-\frac{\beta}{2}(\epsilon_\lambda - \epsilon_\mu)} \langle i \,|\, \lambda\rangle\langle \lambda \,|\, k\rangle\langle l \,|\, \mu\rangle\langle \mu \,|\, j\rangle. \tag{4.27}$$

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

$$\gamma_{ij;kl} = \sum_{\lambda\mu} 1 \langle i \,|\, \lambda\rangle\langle \lambda \,|\, k\rangle\langle l \,|\, \mu\rangle\langle \mu \,|\, j\rangle. \tag{4.28}$$

Using the completeness relation we reach

$$\gamma_{ij;kl} = 1\delta_{ik}\delta_{jl}, \tag{4.29}$$

where δ_{ik} is the Kronecker delta. In this case the position quantum network master equation (4.25) becomes "symmetric"

$$\frac{d}{dt}\hat{\rho} = -i\left[\hat{H}, \hat{\rho}\right] + \sum_{ij}\left(\hat{J}_{ij}\hat{\rho}\hat{J}_{ij}^{\dagger} - \frac{1}{2}\left\{\hat{J}_{ij}^{\dagger}\hat{J}_{ij}, \hat{\rho}\right\}\right). \tag{4.30}$$

The stationary distribution is

$$\hat{\rho}^{*} = \frac{1}{N}\begin{pmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{pmatrix}. \tag{4.31}$$

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

$$\begin{aligned} \gamma_{ij;kl} = &\sum_{\lambda\mu} e^{-\frac{\beta}{2}(\epsilon_\lambda - \epsilon_\mu)}\langle i \,|\, \lambda\rangle\langle\lambda \,|\, k\rangle\langle l \,|\, \mu\rangle\langle\mu \,|\, j\rangle\Theta(\lambda - \mu) \\ &+ \sum_{\lambda\mu} 1\langle i \,|\, \lambda\rangle\langle\lambda \,|\, k\rangle\langle l \,|\, \mu\rangle\langle\mu \,|\, j\rangle\delta_{\lambda\mu} \\ &+ \sum_{\lambda\mu} e^{-\frac{\beta}{2}(\epsilon_\lambda - \epsilon_\mu)}\langle i \,|\, \lambda\rangle\langle\lambda \,|\, k\rangle\langle l \,|\, \mu\rangle\langle\mu \,|\, j\rangle\Theta(\mu - \lambda) \end{aligned} \tag{4.32}$$

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

$$\gamma_{ij;kl} = \sum_{\lambda}\langle i \,|\, \lambda\rangle\langle\lambda \,|\, k\rangle\langle l \,|\, \lambda\rangle\langle\lambda \,|\, j\rangle + \sum_{\mu>\lambda}\infty\langle i \,|\, \lambda\rangle\langle\lambda \,|\, k\rangle\langle l \,|\, \mu\rangle\langle\mu \,|\, j\rangle \to \infty \tag{4.33}$$

4.2.2 Interpretation

The equation (4.11) 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 (4.11) returning to a special random walk of classic particle. The rotation connect the stationary distribution at inverse temperature β (4.12) with the propagator at time t (1.14).

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

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.

The complexity of the possible paths is encoded into the Von Neumann entropy as explained in chapter 2. The entropy allows us to make a distinction between different

network based on the dynamical properties of the network itself. We can do it introducing the Kullback-Lieber divergence (2.49) and the Jensen-Shannon divergence (2.50). 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 [42]. 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 $\{|i\rangle\}_{i<N}$, N is the number of node, be a orthonormal basis for the Hilbert space $\mathcal{H}$, the state $|\psi\rangle$ is defined as

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

such that $x_i = |\langle i \,|\, \psi\rangle|^2$. 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 (4.11) which has stationary distribution

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

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

$$S = -\,\mathrm{Tr}\left[\frac{1}{Z}e^{-\beta\hat{H}}\ln\left(\frac{1}{Z}e^{-\beta\hat{H}}\right)\right]. \tag{4.39}$$

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 (3.15). Thus, taking the dissipative part of the equation (3.16) in the Schrödinger picture with the coefficients $\Gamma_{ij} = L_{ij}$ and the jump operators $J_{ij} = |i\rangle\langle j|$ we obtain

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

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)

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

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

Conclusion

Appendix A

Mastubara Green Function

The Matsubara Green function is a way to add the effect of temperature to the QFT formalism [43]. 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 [43]

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

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

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

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

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

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

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

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

We can rearrange them in a vectorial form

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

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

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

where B^T is the transpose of matrix B.

With similar procedure, we can vectorize also the differential equation

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

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

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

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