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

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Abstract

abstract

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Introduction

The traffic jam in the morning, the airport traffic, but also the functioning of the brain can be study as a network problem. A lot of studies are made to analyze the equilibrium point of a network but only few achieve to understand what happen in the not equilibrium point. This work aim to add a piece to the knowledge in this dark topic.

Due to the vast range of applications, 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 [1][2], 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 [3]; he defines the 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.

Chapter 1

Introduction to Network Theory

In this chapter it is introduce the basic concept of the diffusion or random walk over a network and its connection with the density matrix proposed above.

Scientists use network to map the interaction between units. A lot of problem can be address using network like the road in a city, the internet and the social media, but also the interaction in a protein and the communication between neurons in the brain. Initially, the

1.1 Introduction to Graph Theory

The mathematical framework used in Network theory is given by Graph theory.

A graph is defined by a ordinate couple (V, E) where $V = \{1, 2, 3, ..., n\}$ is the set of nodes 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 called $G = (N, M)$ where N and M are respectively the cardinality of V and E.

The graph can be view also via a matrix called Adjacency matrix 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 that are linked to it. It can be compute from the adjacency matrix as

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

We can defined $G' = (V', E')$ a subgraph of $G = (V, E)$ if $V' \subseteq V$ and $E' \subseteq E$.

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

An important concept is the study of the connection between nodes that are not linked together by an edge. As a matter of fact, two nodes can be connected also passing through multiple other nodes. A *walk* of length k from node i to node j its a sequence of nodes $(x_0, x_1, ..., x_k)$ that begins in node $x_0 = i$ and ends in node $x_k = j$ such that $(x_l, x_{l+1}) \in E$, a node can be crossed multiple times. A walk where the nodes are crossed only one time is called path. An important relevance has the *shortest path* or *geodesic*

that is the path that cross the less number of nodes. The number of walks $W_{ij}(k)$ of length k from node i to node j can be found using the adjacency matrix as

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

A graph is said connected if for each couple of distinct nodes i and j exists a walk that connect them. A *component* of a graph $G = (V, E)$ is a connected subgraph $G' = (V', E')$ that is connected to nothing else, that is $(i, j) \notin E$ for each $i \in V'$ and $j \in V \setminus V'$.

1.2 Random Networks

The network theory has a rich of randoms network. They are used to mimic the complex behavior of real network like Internet and the social networks. There are many way to generates randoms network, we explore some below. Each model focuses on a specific like the degree distribution or the mean distance between nodes.

1.2.1 Erdős-Rényi random graph

The Erdős-Rényi random Graph $G(N, M)$ [4], where N and M are respectively the number of nodes and links, is one of the first attempt to generate a random network. The network is build choosing at random M links from all the possible ones. Usually, is used the contraction proposed by Gilbert $G(N, p)$ [5] , 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 as the distribution of the degree of the nodes $P(k)$ is binomial

$$P(k) = \binom{n-1}{k} p^k (1-p)^{n-1-k} \tag{1.4}$$

and, also, if $p > \frac{1}{N}$ then is almost sure that the network presents a giant component. In this work we use the second approach. In figure 1.1 it is shown two example of E-R random graph, one below and one above the giant component threshold.

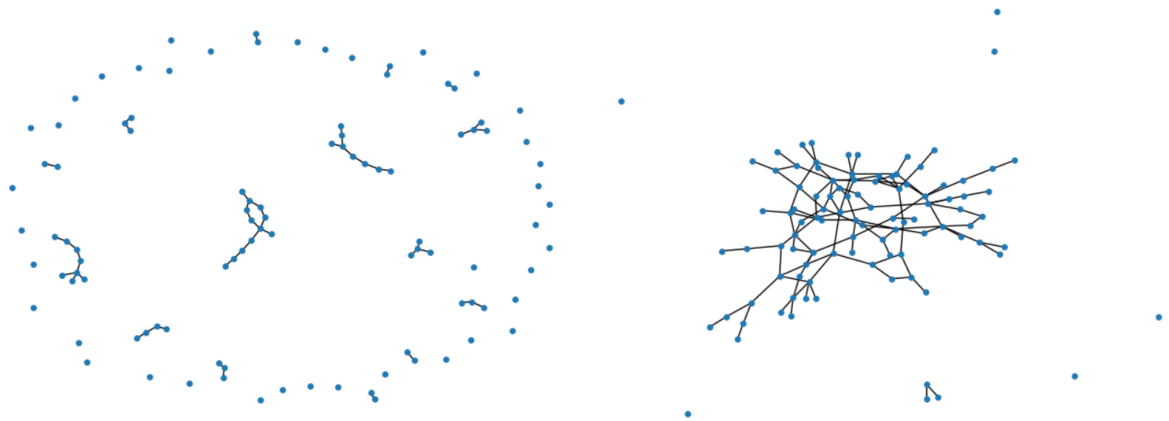

Figure 1.1: Two example of Erdős-Rényi random graphs: on the left, it has 100 nodes and $p = 0.01$; on the right, it has 100 nodes and $p = 0.02$. Overcoming the threshold $p > 0.01$ can be seen the formation of the giant component.

However, the E-R algorithm do not produces network similar to the real ones found in nature, they tend to be more clustered and to have hubs (nodes with very high degree). To simulate this 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 proposed a scale-free Network $G(N, m)$ [6] that mimics the behavior of real graph like the Internet. This type of graph shows some preferential nodes which have a degree order of magnitude higher that the average and present 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 define below:

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.

In figure 1.2 it is shown two example of B-A networks.

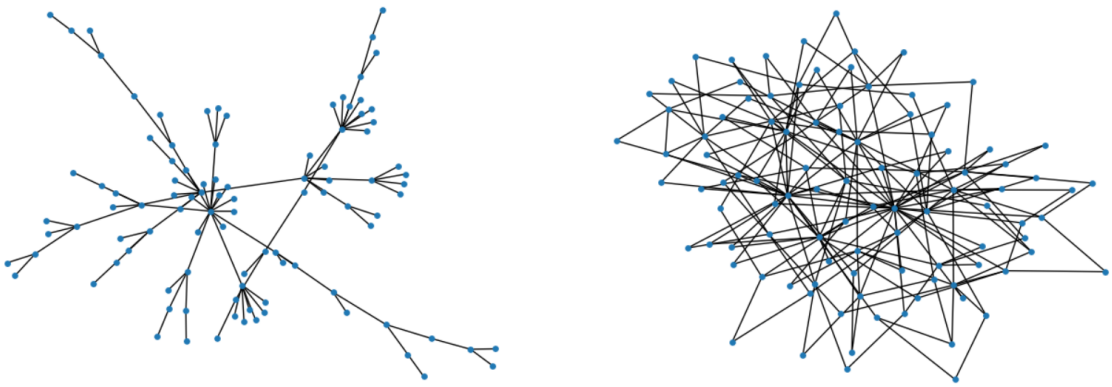

Figure 1.2: Two example of Barabábi-Albert scale-free networks: on the left, it has 100 nodes and $m = 1$; on the right, it has 100 nodes and $m = 2$.

1.2.3 Watts-Strogatz small world network

The Watts-Strogatz small world network $G(N, K, p)$ [7], 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 exhibit high clustering and short average path lengths. The degree distribution is a power law and the network is homogeneous, all nodes have similar degree.

The algorithm is shown below:

1. It is created a ring network with N nodes where each node is connect to the $K/2$ nearest neighbors for each side;
2. For each edge with probability p, the link is removed and another one to node chosen uniformly at random is created, the new link must be a not existing one.

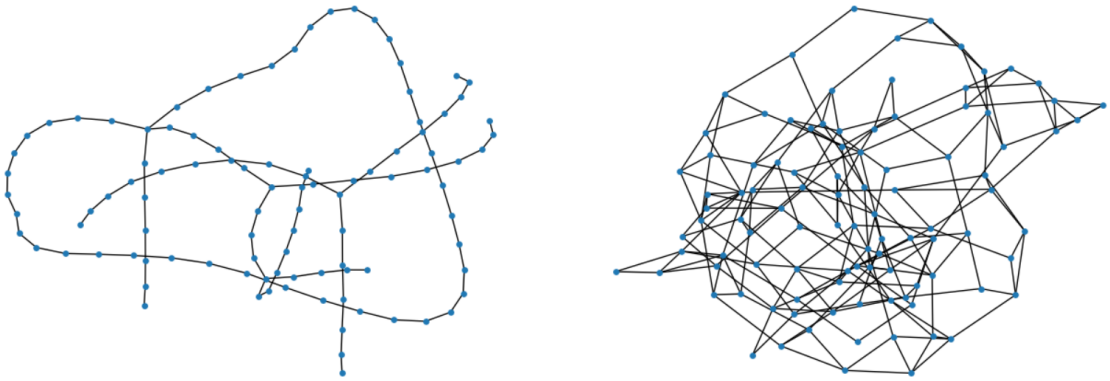

Figure 1.3: Two example of Watts-Strogatz small world networks: on the left, it has 100 nodes, $K = 2$ and $p = 0.1$; on the right, it has 100 nodes, $K = 4$ and $p = 0.3$.

In figure 1.3 it is shown two example of W-S networks.

The B-A and W-S algorithms produce more realistic networks respect to the E-R one, but both focus on their special feature: the B-A network fails to reproduce the high clustering of real network and the W-S one fails to reproduce the hubs characteristic of scale-free networks.

1.3 Random walk on networks

Let consider a network $G(N, E)$ made by N vertices or nodes connected by E links. Consider that in the graph there is a particle and, at each time step, it moves randomly between the nodes, with transition probability P_{ij} to go to the node j starting from the node i; if there is no link between them $P_{ij} = 0$. The dynamics behave as a Markov chain, it has no memory of the previous states. Let be $\rho_i(t)$ the probability to find the particle in the node i at time step n, the discrete time evolution of the system is given by the law

$$\rho_i(n+1) = \sum_j P_{ij}\rho_j(n). \tag{1.5}$$

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

$$\sum_i P_{ij}(\Delta t) = 1. \tag{1.6}$$

The transition probability can be identify with the adjacency matrix of the network

$$P_{ij} = \frac{A_{ij}}{\sum_j A_{ij}}. \tag{1.7}$$

If the system obeys the detail balance, $\pi_{ij}\rho_j^* = \pi_{ji}\rho_i^*$, the system admits a unique stationary solution ρ^* such that

$$\sum_j P_{ij}\rho_j^* = \rho_i^*. \tag{1.8}$$

We can rewrite it in a matrix formalism where Π is the matrix of the transition probability, and $\rho^*(t)$ is the stationary probability vector, as

$$\Pi\rho^* = \rho^*. \tag{1.9}$$

It can be seen that the stationary distribution is the eigenvector with eigenvalue 1.

We cqn go in the continuum limit obtaining the master equation equation [8]

$$\dot{\rho}_i(t) = \sum_j \pi_{ij}\rho_j(t) - \pi_{ji}\rho_i(t) = -\sum_j L_{ij}\rho_j(t), \tag{1.10}$$

where $\pi_{ij} = A_{ij}$ is the transition rate, namely the transition probability per units of time, and $L_{ij} = \sum_k \pi_{kj}\delta_{ij} - \pi_{ij}$ is the Laplacian matrix. The first term indicates that a particle is coming in the node i from j and the second one, instead, indicates that a particle is going into node j from i.

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

$$\sum_i L_{ij} = 0. \tag{1.11}$$

The eigenvalue of the Laplacian matrix has always a not negative real part. Its spectrum has at least one zero eigenvalue, therefore it is not invertible [9]. The multiplicity of the zero eigenvalue is equal to the number of connected component of the network; it derived from the fact that if the network is not connected the Laplacian should be a block matrix, one for each connected component, and each block should have its zero eigenvalue, since each block can be seen as an independent network.

The master equation (1.10) has a solution

$$\rho(t) = e^{-tL}\rho(0). \tag{1.12}$$

The master equation, in the matrix formalism, for the stationary distribution reduces to

$$\dot{\rho}^*(t) = -L\rho^*(t) = 0. \tag{1.13}$$

As a matter of fact the stationary distribution is the eigenvector with eigenvalue 0 of the Laplacian matrix. The other eigenvalues are connected to the Ljapunov exponent and to the time that the occurs to converge to ρ^*.

We can prove that

$$\sum_i \dot{\rho}_i(t) = -\sum_i \sum_j L_{ij}\rho_j(t) = -\sum_j \left(\sum_i L_{ij}\right)\rho_j(t) = 0. \tag{1.14}$$

Therefore we have a first integral of motion

$$\sum_i \rho_i(t) = \sum_i \rho_i(0). \tag{1.15}$$

Let suppose that the network satisfy the detail condition, namely

$$\pi_{ij}p_j^* = \pi_{ji}p_i^*, \tag{1.16}$$

then exist a hyperplane Σ_0 that is orthogonal to the stationary distribution is an invariant subspace for the dynamics. Let be $w \in \Sigma_0$, this subspace is identify by the relation

$$\sum_i w_i = 0 \tag{1.17}$$

As a matter of fact, let $w(t) \in \Sigma_0$ then

$$\sum_i w_i(t+1) = \sum_{ij} \pi_{ij} w_j(t) = \sum_j \underbrace{\left(\sum_i \pi_{ij} \right)}_{1} w_j = \sum_j w_j(t) = 0. \tag{1.18}$$

Therefore is possible to decompose any probability vector as a direct sum of the stationary state and the invariant subspace. Let $w(t) \in \Sigma_0$ and $c = \sum_i v_i = 1$ then

$$\rho(t) = \rho^* + w(t) \tag{1.19}$$

Besides, if the detail condition holds, the stationary distribution is

$$\rho^* = \frac{1}{N} (1, 1, \cdots, 1, 1) . \tag{1.20}$$

1.4 Quantum Walk

Instead of studying the diffusion of a classic particle in a network, we can extent the diffusion model to quantum particles. They must follow the Schrödinger equation with the Laplacian operator as Hamiltonian. It can be written as

$$\frac{d}{dt}|\psi\rangle = -i\frac{1}{2}L|\psi\rangle. \tag{1.21}$$

The ket state $|\psi\rangle$ is define as

$$|\psi\rangle = \sum_i \sqrt{\rho_i(t)}|i\rangle, \tag{1.22}$$

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 to be in the state i.

This model is called "continuos time quantum walk" [10]. The formula (1.21) requires that $\hat{L}$ is hermitian; therefore, the network must hold the detail balance.

The equation (1.21) has a solution in the from of

$$|\psi(t)\rangle = \hat{U}(t,0)|\psi(0)\rangle = e^{-\frac{i}{2}\hat{L}t}|\psi(0)\rangle, \tag{1.23}$$

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

However, the system does not converge to the stationary distribution ρ^*. Despite that, it is possible to define a limiting distribution of a quantum walk as follow: suppose we start form node $|a\rangle$, we measure the system after a time t, random variable uniformly distributed over the interval $t \in [0,T]$ [11]. The probability of transition from node a to b is given by

$$\begin{aligned}
\rho_{a\to b}(T) &= \frac{1}{T}\int_0^T |\langle a|e^{-i\frac{t}{2}\hat{L}}|b\rangle|^2 dt \\
&= \frac{1}{T}\int_0^T \sum_{\lambda,\lambda'} \langle a|e^{-i\frac{t}{2}\hat{L}}|\lambda\rangle\langle\lambda \,|\, b\rangle\langle b|e^{-i\frac{t}{2}\hat{L}}|\lambda'\rangle\langle\lambda' \,|\, a\rangle dt \\
&= \sum_{\lambda,\lambda'} \langle a \,|\, \lambda\rangle\langle\lambda \,|\, b\rangle\langle b \,|\, \lambda'\rangle\langle\lambda' \,|\, a\rangle \frac{1}{T}\int_0^T e^{-i(\lambda-\lambda')\frac{t}{2}} dt \\
&= |\langle a \,|\, \lambda\rangle\langle\lambda \,|\, b\rangle|^2 + 2\sum_{\lambda\neq\lambda'} \langle a \,|\, \lambda\rangle\langle\lambda \,|\, b\rangle\langle b \,|\, \lambda'\rangle\langle\lambda' \,|\, a\rangle \frac{1 - e^{-i(\lambda-\lambda')\frac{T}{2}}}{i(\lambda-\lambda')T},
\end{aligned} \tag{1.24}$$

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

$$\rho_{a\to b}(T) \xrightarrow[T\to\infty]{} |\langle a \,|\, \lambda\rangle\langle\lambda \,|\, b\rangle|^2. \tag{1.25}$$

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

$$\hat{\rho} = |\psi\rangle\langle\psi| = \sum_{ij} \sqrt{\rho_i}\sqrt{\rho_j}|i\rangle\langle j|, \tag{1.26}$$

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

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

$$\left\langle \hat{O} \right\rangle = \mathrm{Tr}\left[\hat{O}\hat{\rho}\right]. \tag{1.27}$$

The observable for the probability to be in the node a can be express using the operator $\hat{P}_a = |a\rangle\langle a|$ such that

$$\begin{aligned}
\mathrm{Tr}\left[\hat{P}_a\hat{\rho}(t)\right] &= \sum_i \langle i \,|\, a\rangle\langle a \,|\, \psi\rangle\langle\psi \,|\, i\rangle \\
&= \sum_{ijk} \langle i \,|\, a\rangle\langle a|\sqrt{\rho_j}|j\rangle\langle k|\sqrt{\rho_k}|i\rangle \\
&= \sum_{ijk} \delta_{i,a}\delta_{a,j}\delta_{k,i}\sqrt{\rho_j}\sqrt{\rho_k} \\
&= \sqrt{\rho_a}\sqrt{\rho_a} = \rho_a
\end{aligned} \tag{1.28}$$

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

$$\begin{aligned}
\frac{d}{dt}\hat{\rho}(t) &= \frac{d}{dt}\left(|\psi(t)\rangle\langle\psi(t)|\right) = \\
&= -\frac{i}{2}\hat{L}|\psi(t)\rangle\langle\psi(t)| + |\psi(t)\rangle\langle\psi(t)|\frac{i}{2}\hat{L} \\
&= -\frac{i}{2}\left[\hat{L}, \rho\right]
\end{aligned} \tag{1.29}$$

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

$$\hat{\rho}(t) = \hat{U}(t,0)\hat{\rho}(0)\hat{U}^\dagger(t,0) = e^{-\frac{i}{2}t\hat{L}}\hat{\rho}e^{\frac{i}{2}t\hat{L}}. \tag{1.30}$$

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

If we have uncertainty about the real distribution upon the network 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, $\sum_k^K p_k = 1$, then the mixed density matrix is define as

$$\hat{\rho} = \sum_{k=1}^{K} p_k\hat{\rho}_k \qquad \hat{\rho}_k = |\psi_k\rangle\langle\psi_k|. \tag{1.31}$$

The temporal evolution of the operator is define as in eq. (1.29); the probability to be at node a at time t is the same as in eq. (1.28). 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 happen.

To measure how mixed the density matrix is we can use the Von Neumann entropy $S[\hat{\rho}] = -\operatorname{Tr}[\hat{\rho}\ln\hat{\rho}]$.

Moreover, the Von Neumann entropy is a time invariance since the evolution operator does not change how mixed are the state [12].

1.4.1 1-D quantum random walk

Let consider a toy model: the random walk over a line [10]. The probability to go left or right is $\frac{1}{2}$. To analyze this model 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

$$\hat{L}|j\rangle = 2|j\rangle - |j-1\rangle - |j+1\rangle. \tag{1.32}$$

Therefore,

$$\begin{aligned}\langle j|\hat{L}|p\rangle &= \langle j\,|\,p\rangle - \frac{1}{2}\langle j-1\,|\,p\rangle - \frac{1}{2}\langle j+1\,|\,p\rangle \\ &= e^{ijp} - \frac{1}{2}e^{i(j-1)p} - \frac{1}{2}e^{i(j+1)p} \\ &= e^{ijp}(\cos(p)-1) = (\cos(p)-1)\langle j\,|\,p\rangle\end{aligned} \tag{1.33}$$

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

$$\begin{aligned}\langle j|e^{-i\frac{t}{2}\hat{L}}|k\rangle &= \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-i\frac{t}{2}(\cos(p)-1)}\langle j\,|\,p\rangle\langle p\,|\,k\rangle dp \\ &= \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-ip(j-k)-i\frac{t}{2}(\cos(p)-1)} \\ &= e^{i\frac{t}{2}}(-i)^{k-j}J_{k-j}\left(\frac{t}{2}\right),\end{aligned} \tag{1.34}$$

where $J_n(x)$ is the Bessel function of the first kind of order n. Applying the Wick rotation we obtain

$$\left|\langle j|e^{-i\frac{t}{2}\hat{L}}|k\rangle\right|^2 = e^{-t}\left(I_{k-j}\left(\frac{t}{2}\right)\right)^2, \tag{1.35}$$

where $I_n(x) = i^n J_n(ix)$ is the modified Bessel function of the first kind. In the limit $t >> 1$ it tends to a gaussian centered in the origin and variance $\sqrt{t}$, in accordance with the classical model [13].

1.4.2 Double tree network

Another important toy modes is the quantum walk over a network that is form by two binary tree with depth n with the ending connected, shown in figure 1.4. We start form one root and we look for the probability to be in the other one [11]. Classically, the probability to cross the network scale exponentially as 2^{-n}, and it is not computable for big n. Instead, using the quantum version it is computable.

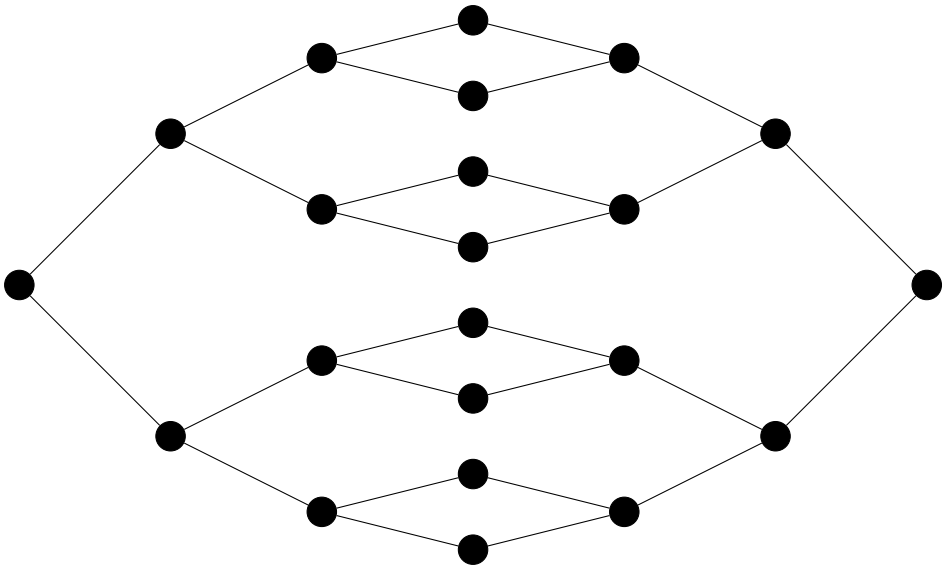

Figure 1.4: The picture of a glued double tree network.

We can introduce a new basis $|\text{col } j\rangle_{j<2n}$ that indicates just the column and not the single node, except for the two border nodes where they coincide, as

$$|\text{col } j\rangle = \frac{1}{\sqrt{N_j}} \sum_{a \in \text{column}} |a\rangle \qquad N_j = \begin{cases} 2^j & 0 \leq j \leq n \\ 2^{2n-j} & n \leq j \leq 2n \end{cases} \tag{1.36}$$

In this basis, the Laplacian act like

$$\langle \text{col } j | \hat{L} | \text{col } j \rangle = 1 \tag{1.37}$$

and

$$\langle \text{col } j \pm 1 | \hat{L} | \text{col } j \rangle = \begin{cases} \dfrac{\sqrt{2}}{2} & j = 0, n, 2, \\ \dfrac{\sqrt{2}}{3} & \text{otherwise} \end{cases} \tag{1.38}$$

Thus, the dynamics along the network reduce to a 1-D quantum walk that is solvable with solution [11]

$$\langle 0 | e^{i\frac{t}{2}\hat{L}} | 2n \rangle = e^{-t} I_{2n}\left(\frac{t}{2}\right), \tag{1.39}$$

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

This chapter introduces this concept of density matrix and entropy for a network. We start form the concept of Communicability matrix defined by Estrada [14] and how it is connected to the correlation in physics, especially for quantum systems. After that we use this matrix to define a possible candidate to the role of density matrix and its features. This approach makes use of quantities and techniques 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 [15]. It must consider

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

$$A_{i,j} = \begin{cases} +1 & \text{if } i \text{ is linked to } j \\ 0 & \text{otherwise} \end{cases} . \tag{2.1}$$

We can define the communicability matrix as

$$G(A) = \sum_{k=1}^{\infty} c_k A^k \tag{2.2}$$

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 [14]

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

We can generalize it adding a constant term β

$$G^E(A) = \sum_{k=1}^{\infty} \frac{\beta A^k}{k!} = e^{\beta A}, \tag{2.4}$$

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 [16]. In this case, it becomes a geometrical series yielding

$$G^R(A) = \sum_{k=1}^{\infty} \alpha^k A^k = (I - \alpha A)^{-1}. \tag{2.5}$$

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 [17].

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

$$EE(A) = \mathrm{Tr}\left[e^{\beta A}\right]. \tag{2.6}$$

In the literature it is called Estrada index [14] 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.

We can define the communicability matrix also with the laplacian matrix $L = D - A$, where D is the degree matrix. Thus, the matrices becomes [15]

$$\begin{aligned} G^E(L) &= \sum_{k=1}^{\infty} \frac{\beta^k L^k}{k!} = e^{\beta L} \\ G^R(L) &= \sum_{k=1}^{\infty} \alpha^k L^k \to \alpha^{-1} \tilde{L}^{-1} \end{aligned} \tag{2.7}$$

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 [18]. Also, the Laplacian Estrada index is define as

$$EE(L) = \mathrm{Tr}\left[e^{\beta L}\right]. \tag{2.8}$$

While the previous quantities using the adjacency matrix focalized over the topological aspects of the network and information spread, the laplacian communicability matrix embodies also the dynamical ones since the laplacian is involved in the random walk over a network.

2.1.1 Hamiltonian system

The formulae (2.7) can be motivated by studying a classic and quantum harmonic oscillator on a network. Consider a set of N harmonic oscillators with coupling matrix $K = A$, 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

$$V(q) = \frac{1}{4}\sum_{i\neq j} K_{ij}(q_i - q_j)^2 = \frac{1}{2}\sum_j K_{jj}q_j^2 - \frac{1}{2}\sum_{i\neq j} K_{ij}q_i q_j, \tag{2.9}$$

where

$$K_{jj} = \sum_{j\neq i} K_{ij}. \tag{2.10}$$

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

$$V(q) = \frac{1}{2}\sum_{i,j} H_{ij}q_i q_j. \tag{2.11}$$

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

$$\mathcal{L} = \frac{1}{2}\sum_{ij} \dot{q}_i G_{ij}\dot{q}_j - \frac{1}{2}\sum_{ij} q_i H_{ij} q_j. \tag{2.12}$$

The equations of motion are

$$\ddot{q}_i = -H_{ij}q_j. \tag{2.13}$$

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

$$\omega^2\phi_i = H_{ij}\phi_j. \tag{2.14}$$

Rewriting it in matrices form

$$|\Omega^2 - H| = |\Omega^2 - H|. \tag{2.15}$$

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

$$H_L = \sum_i \frac{p_i^2}{2} + \sum_{ij}\frac{1}{2}L_{ij}q_i q_j. \tag{2.16}$$

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

$$\begin{aligned} \dot{q}_i &= p_i; \\ \dot{p}_i &= -H_{ij}q_j - \gamma \sum_j (\delta_{ij} - 1_{ij})\, p_j + \sqrt{2T\gamma}\xi_i(t), \end{aligned} \tag{2.17}$$

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

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

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

$$\frac{d}{dt}\sum_i \dot{p}_i = -\gamma \sum_{ij} (\delta_{ij} - 1_{ij})\, p_j + \cancel{\sqrt{2T\gamma} \sum_i \xi_i(t)} = 0. \tag{2.19}$$

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

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

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

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

The distribution $\rho(q, p, t)$ is a Gaussian and satisfies the Fokker-Plank equation [19]

$$\frac{\partial \rho}{\partial t} = -\sum_i p_i \frac{\partial \rho}{\partial q_i} + \sum_{ij} H_{ij} q_j \frac{\partial \rho}{\partial p_i} + \gamma \sum_{ij} (\delta_{ij} - 1_{ij}) \left[\frac{\partial}{\partial p_i} p_j \rho + T \frac{\partial^2 \rho}{\partial p_i \partial p_j} \right]. \tag{2.22}$$

The solution at equilibrium is

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

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

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

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

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

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

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

with partition function

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

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

$$\mathrm{Cov}(q) = \frac{1}{\beta} L^+, \tag{2.28}$$

This is the same result as the Estrada's Communicability matrix $G^R(L)$ (2.7) 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

$$H_L = \sum_i \left(\frac{\hat{p}_i^2}{2} + \frac{K'}{2} \hat{q}_i^2 \right) + \sum_{ij} \frac{1}{2} L_{ij} \hat{q}_i \hat{q}_j. \tag{2.29}$$

We introduce the bosons creation and annihilation operators as

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

and the inverse as

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

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

$$\hat{H}_L = \sum_i \Omega \left(\hat{a}_i \hat{a}_i^\dagger + \frac{1}{2} \right) + \frac{1}{4\Omega} \sum_{ij} \left(\hat{a}_i + \hat{a}_i^\dagger \right) L_{ij} \left(\hat{a}_i + \hat{a}_i^\dagger \right). \tag{2.32}$$

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

$$b_\mu = \sum_j a_j O_{\mu j} \qquad \hat{b}_\mu^\dagger = \sum_j a_j^\dagger O_{\mu j}^T. \tag{2.33}$$

Thus, the new Hamiltonian becomes a sum of independent Hamiltonians

$$\hat{H}_L = \sum_\mu \hat{H}_\mu, \tag{2.34}$$

with

$$\begin{aligned}\hat{H}_\mu &= \Omega\left(\hat{b}_\mu\hat{b}_\mu^\dagger + \frac{1}{2}\right) + \frac{1}{4\Omega}\mu\left(\hat{b}_\mu + \hat{b}_\mu^\dagger\right)^2 \\ &= \Omega\left(\hat{b}_\mu\hat{b}_\mu^\dagger + \frac{1}{2}\right) + \frac{1}{4\Omega}\mu\left[\left(\hat{b}_\mu\right)^2 + \left(\hat{b}_\mu^\dagger\right)^2 + 2\hat{b}_\mu\hat{b}_\mu^\dagger + 1\right] \\ &= \Omega\left[1 + \frac{1}{2\Omega}\mu\right]\left(\hat{b}_\mu\hat{b}_\mu^\dagger + \frac{1}{2}\right) + \frac{1}{4\Omega}\mu\left[\left(\hat{b}_\mu\right)^2 + \left(\hat{b}_\mu^\dagger\right)^2\right].\end{aligned} \tag{2.35}$$

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

$$\begin{aligned}G_{ij}^L(\beta, \tau > 0) &= \frac{\mathrm{Tr}\left[e^{-\beta\hat{H}_L}\hat{a}_i(\tau)\hat{a}_j^\dagger\right]}{\mathrm{Tr}\left[e^{-\beta\hat{H}_L}\right]} \\ &= \sum_{\mu\nu} O_{\mu i}\frac{\mathrm{Tr}\left[(\tau)e^{-\beta\hat{H}_L}\hat{b}_\mu\hat{b}_\nu^\dagger\right]}{\mathrm{Tr}\left[e^{-\beta\hat{H}_L}\right]}O_{j\nu} \\ &= \sum_\mu O_{i\mu}\left\{-e^{-\mu\tau}\left[\left(1 - f\left(\Omega + \frac{1}{2\Omega^2}\mu\right)\right)\Theta(\tau)\right]\right\}O_{j\mu} \\ &= \sum_\mu O_{i\mu}\left\{\frac{e^{-\mu\tau}}{e^{-\beta\left[\Omega + \frac{1}{2\Omega^2}\mu\right]} + 1}\right\}O_{j\mu}\end{aligned} \tag{2.36}$$

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

$$G^L(\beta) = \sum_\mu O_{i\mu}e^{\beta\left[\Omega + \frac{1}{2\Omega^2}\mu\right]}O_{\mu i}, \tag{2.37}$$

that can be written as

$$G_{ij}^L(\beta) = e^{\beta\Omega}e^{\frac{\beta\omega^2}{2\Omega}L}. \tag{2.38}$$

Comparing it with the eq. (2.7), choosing $2\Omega = \omega^2$ the two equations are related as

$$G^R(L) = e^{-\beta\Omega}G^L(\beta). \tag{2.39}$$

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

$$\hat{\rho}(\beta) = \frac{1}{Z} e^{-\beta \hat{L}} \qquad \text{with} \qquad Z(\beta) = \mathrm{Tr}[e^{-\beta \hat{L}}], \tag{2.40}$$

where Z is the partition function and it is equal to the Laplacian Estrada index of the network (2.8). 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

$$S(\hat{\rho}) = -\mathrm{Tr}[\hat{\rho} \ln \hat{\rho}]. \tag{2.41}$$

The entropy is not negative and it is equal to zero if and oly if the $\hat{\rho}$ is a pure state. It has a higher bound $S \leq \ln(N)$ [12].

Figure 2.1 shows the entropy (2.41) for different types of networks[1]: a ring graph, an Erdős-Rényi (E-R) random graph, a Barabási-Albert (B-A) scale-free graph, and a Watts-Strogatz (W-S) small-sworld graph.

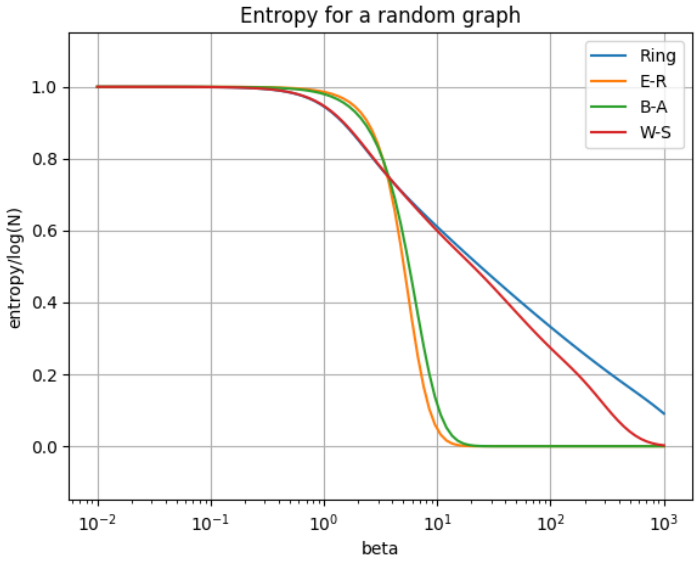

Figure 2.1: Plot of the Von Neumann entropy as a function of β for different network types with 50 nodes: a ring graph (blue), a Erdős-Rényi (E-R) random graph with connectivity probability 0.7 (orange), a Barabási-Albert (B-A) scale-free graph with parameter $m = 3$ (green), and a Watts-Strogatz (W-S)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

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

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

A possible interpretation of this density matrix is given by De Domenico [20]. 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 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

$$\partial_t|\psi(t)\rangle = -\hat{L}|\psi(t)\rangle, \tag{2.42}$$

with the solution

$$|\psi(t)\rangle = \hat{G}(t,0)|\psi(0)\rangle \tag{2.43}$$

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

$$\hat{G}(t,0) = \sum_\lambda e^{-t\lambda}|v_\lambda\rangle\langle v_\lambda| = \sum_\lambda e^{-t\lambda}\hat{\sigma}_\lambda, \tag{2.44}$$

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

$$|\psi(t)\rangle = G(t,0)|\psi(0)\rangle = |\psi_0\rangle + G(t,0)|\Delta\psi\rangle = |\psi_0\rangle + |\Delta\psi(t)\rangle \tag{2.45}$$

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

$$\langle j \,|\, \Delta\psi(t)\rangle = \langle j|e^{-t\hat{L}}|\Delta\psi\rangle = \sum_\lambda \langle j|e^{-t\lambda}\hat{\sigma}_\lambda|\Delta\psi\rangle = \sum_i\sum_\lambda \Delta_i e^{-t\lambda}\langle j|\hat{\sigma}_\lambda|i\rangle. \tag{2.46}$$

We have used equation (2.44) 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

$$T = \sum_i\sum_\lambda \Delta_i e^{-t\lambda}\langle i|\hat{\sigma}_\lambda|i\rangle \tag{2.47}$$

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

$$T = \Delta\sum_i e^{-t\lambda}\langle i|\hat{\sigma}_\lambda|i\rangle = \Delta\,\mathrm{Tr}[\hat{G}(t,0)] \tag{2.48}$$

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

$$\hat{\rho}_t = \frac{1}{T}\Delta e^{-t\hat{L}} = \frac{1}{Z}e^{-t\hat{L}}, \tag{2.49}$$

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 [20].

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.

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

$$D(\hat{\rho}||\hat{\sigma}) = \mathrm{Tr}\left[\hat{\rho}\ln\left(\frac{\hat{\sigma}}{\hat{\rho}}\right)\right]. \tag{2.50}$$

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

$$\mathcal{D}(\hat{\rho}||\hat{\sigma}) = D(\hat{\rho}||\hat{\mu}) + D(\hat{\sigma}||\hat{\mu}) = S(\hat{\mu}) - \frac{1}{2}\left[S(\hat{\rho}) + S(\hat{\sigma})\right], \tag{2.51}$$

where $\hat{\mu} = \frac{1}{2}(\hat{\rho}+\hat{\sigma})$. It is a metric: it is symmetric, positive define, and hold the triangular inequality [21]. It has been use successfully to measure the distance between the layer of a multilayer network [22].

Chapter 3

Lindblad master equation

Before exploring the following chapter it is useful to introduce the Lindblad master equation, called also Gorini-Kossakowski-Sudarshan-Lindblad equation, [23, 24]. This equation was introduced to explain the behavior of a quantum open system, namely a quantum system in contact with the environment. This is important because the Schrödinger equation study only closed system that are not real system: 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 with a Markovian environment, the interaction has no memory. The Schrödinger equation requires an unitary time operator that does not allow decays; instead the time operator of Lindblad master equation allows the system to dissipate energy with the surrounding. Despite that, the Lindblad dynamics is still trace preserving and completely positive.

3.1 Derivation of the formula

We show the derivation of the Lindblad formula as in [25]. First, let $\mathcal{H}_T$ be the Hilbert space of the system and the environment combined, that can be divide 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 just in the dynamics without the environment, we can trace out the degree of freedom derived from it obtaining $\hat{\rho}(t) = \mathrm{Tr}_E[\hat{\rho}_T]$. The total Hamiltonian can be separate 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 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 (3.3) is 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 by the total density matrix. To proceed, we make two more assumption. 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 is true if the system is just put in contact with the environment or the correlation between the system and the environment is short-lived. This is called Born approximation. Second, we consider the environment in a thermal state $\hat{\rho}_E(0) = e^{-\hat{H}_E/T} \,\mathrm{Tr}\left[e^{-\hat{H}_E/T}\right]$, where T is the temperature (the Boltzmann constant $k_B = 1$). Moreover, without loss of generality, we can write the interacting Hamiltonian in the form

$$\hat{H}_I(t) = \sum_i \hat{S}_I \otimes \hat{E}_i, \tag{3.7}$$

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 $\mathcal{H}$. After this assumption, the equation (3.6) becomes

$$\begin{aligned}\frac{d\tilde{\rho}}{dt} =& -i\alpha \sum_i \left(\tilde{S}_i(t)\tilde{\rho}(0)\,\mathrm{Tr}_E\left[\tilde{E}_i(t)\tilde{\rho}_E(0)\right] - \tilde{\rho}(0)\tilde{S}_i(t)\,\mathrm{Tr}_E\left[\tilde{\rho}_E(0)\tilde{E}_i(t)\right]\right) \\ & - \alpha^2 \int_0^t ds \,\mathrm{Tr}_E \left[\tilde{H}_I(t), \left[\tilde{H}_I(s), \tilde{\rho}(t) \otimes \tilde{\rho}_E(t)\right]\right].\end{aligned} \tag{3.8}$$

The first term of the r.h.s. vanish because $\mathrm{Tr}_E\left[\tilde{E}_i(t)\tilde{\rho}_E(0)\right] = \langle E_i(t)\rangle$ can be consider as zero. It may seem strange, but if the 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 do not modify the Von Neumann equation. Instead, The second term needs more stringent assumption: since α is small, the system and the environment should not be correlated during all the time evolution, namely the timescale of the correlation is much smaller 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 we change the integral variable to $t - s$, we arrive to

$$\frac{d\tilde{\rho}(t)}{dt} = -\alpha^2 \int_0^\infty ds \,\mathrm{Tr}_E \left[\tilde{H}_I(t), \left[\tilde{H}_I(t-s), \tilde{\rho}(t) \otimes \tilde{\rho}_E(t)\right]\right]. \tag{3.9}$$

This is called Redfield equation [26]. This is the Markov approximation and 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 [27].

The equation (3.9) can generate negative density matrix. To exclude this possibility, we consider a superoperator $\mathbb{H}A = [H, A]$, with A a general operator. The eigenvector 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

$$\mathbb{H}\hat{S}_i(\omega) = -\omega\hat{S}_i(\omega) \qquad \mathbb{H}\hat{S}_i^\dagger(\omega) = \omega\hat{S}_i^\dagger(\omega) \tag{3.10}$$

Thus, we can decompose the operators S_i as $\hat{S}_i = \sum_\omega \hat{S}_i(\omega)$. To apply this decompose in (3.9) we need to go back in 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

$$\tilde{H}_i(t) = \sum_{i\omega} e^{-i\hat{H}t}\hat{S}_i(\omega) \otimes \tilde{E}_i(t) = \sum_{i\omega} e^{i\hat{H}t}\hat{S}_i^\dagger(\omega) \otimes \tilde{E}_i(t) \tag{3.11}$$

After having expanded the commutators in (3.9), we can substitute the decomposition for $\hat{S}_k(\omega)$. Using the ciclic property of the trace and the fact that $\mathrm{Tr}[\hat{H}_e, \hat{\rho}_E(0)] = 0$, with some algebra we arrive to the result

$$\frac{d\tilde{\rho}(t)}{dt} = \sum_{\omega,\omega',i,j} e^{i(\omega-\omega')t}\Gamma_{ij}\left[\hat{S}_j(\omega)\tilde{\rho}(t), \hat{S}_i^\dagger(\omega')\right] + e^{-i(\omega-\omega')t}\Gamma_{ji}^\dagger\left[\hat{S}_j(\omega), \tilde{\rho}(t)\hat{S}_i^\dagger(\omega')\right], \tag{3.12}$$

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

$$\Gamma_{ij}(\omega) = \int_0^\infty ds e^{i\omega s}\,\mathrm{Tr}\left[\tilde{E}_i^\dagger(t)\tilde{E}_j(t-s)\hat{\rho}_E(0)\right] \tag{3.13}$$

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 pictures. It does not depend by time since the environment is in the stationary state and the correlations function of the environment decay extremely fast.

Now, we make the last assumption: we consider the system in the rotating wave approximation. The term proportional to $|\omega - \omega'| >> \alpha^2$ will oscillate much faster that 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 (3.12) reduces to

$$\frac{d\tilde{\rho}(t)}{dt} = \sum_{\omega,i,j} \Gamma_{ij}\left[\hat{S}_j(\omega)\tilde{\rho}(t), \hat{S}_i^\dagger(\omega)\right] + \Gamma_{ji}^\dagger\left[\hat{S}_j(\omega), \tilde{\rho}(t)\hat{S}_i^\dagger(\omega)\right]. \tag{3.14}$$

The operators $\Gamma_{ij}(\omega)$ are not force to be 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

$$\begin{aligned}
\gamma_{ij}(\omega) &= \Gamma_{ij}(\omega) + \Gamma_{ij}^\dagger(\omega) = \int_{-\infty}^\infty ds e^{i\omega s}\,\mathrm{Tr}\left[\left\{\tilde{E}_i^\dagger(t), \tilde{E}_j(t-s)\right\}\hat{\rho}_E(0)\right] \\
\pi_{ij}(\omega) &= \frac{-i}{2}\left(\Gamma_{ij}(\omega) - \Gamma_{ij}^\dagger(\omega)\right)\int_{-\infty}^\infty ds e^{i\omega s}\,\mathrm{Tr}\left[\left[\tilde{E}_i^\dagger(t), \tilde{E}_j(t-s)\right]\hat{\rho}_E(0)\right]
\end{aligned} \tag{3.15}$$

Inserting them in the equation (3.14) and going back to the Schrödinger picture, we obtain

$$\frac{d}{dt}\hat{\rho} = -i\left[\hat{H} + \hat{H}_{LS}, \hat{\rho}\right] + \sum_{i,j,\omega} \gamma_{ij}(\omega)\left(\hat{S}_i(\omega)\hat{\rho}\hat{S}_j^\dagger(\omega) - \frac{1}{2}\left\{\hat{S}_i^\dagger(\omega)\hat{S}_j(\omega), \hat{\rho}\right\}\right), \tag{3.16}$$

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 with the interaction of the environment. The equation (3.16) 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.

However, if the matrix $\gamma(\omega)$ can be diagonalize, 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

$$\frac{d}{dt}\hat{\rho} = \mathcal{L}\left[\hat{\rho}\right] = -i\left[\hat{H} + \hat{H}_{LS}, \hat{\rho}\right] + \sum_k \gamma_k\left(\hat{J}_k\hat{\rho}\hat{J}_k^\dagger - \frac{1}{2}\left\{\hat{J}_k^\dagger\hat{J}_k, \hat{\rho}\right\}\right). \tag{3.17}$$

The operator $\hat{J}_k = \sum_j O_{ki}\hat{S}_i$ are called jump operators, the superoperator $\mathcal{L}$ is called Lindblad superoperator and γ_i are the damping rates. In the limit $\gamma_i = 0$ 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 map $\phi_t\left(\hat{\rho}\right) = e^{\mathcal{L}t}\hat{\rho}(0)$ on the space of density matrix such that

$$\hat{\rho}(t) = \phi_t\left(\hat{\rho}(0)\right). \tag{3.18}$$

This maps have the semigroup property, that is

$$\phi_s\left(\phi_t\left(\hat{\rho}(0)\right)\right) = \phi_{t+s}\left(\hat{\rho}(0)\right) \tag{3.19}$$

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 be found also starting from this assumption [27].

The Lindblad master equation is invariant under the following transformation [27]:

- unitary transformation of the Lindblad operator:

$$\sqrt{\gamma_i}\hat{J}_i \to \sqrt{\gamma_i'}\hat{J}_i' = \sum_j u_{ij}\sqrt{\gamma_j}\hat{J}_j \tag{3.20}$$

  where u_{ij} is an unitary matrix.

- inhomogeneous transformation:

$$\begin{aligned} \hat{J}_i &\to \hat{J}_i' = \hat{J}_i + a_i \\ \hat{H}_I &\to \hat{H}' = \hat{H} + \frac{1}{2i}\sum_j \gamma_j\left(a_j^*\hat{J}_j - a_j\hat{J}_j^\dagger\right) \end{aligned} \tag{3.21}$$

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

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

Lastly, we can prove that the dynamics (3.22) conserve $\mathrm{Tr}[\hat{\rho}]$. As a matter of fact, the derivative along time of it is

$$\frac{d}{dt}\mathrm{Tr}[\hat{\rho}] = \mathrm{Tr}\left[-i\left(\hat{H}\hat{\rho} - \hat{\rho}\hat{H}\right) + \hat{J}_k\hat{\rho}\hat{J}_k^\dagger - \frac{1}{2}\left(\hat{L}\hat{\rho} + \hat{\rho}\hat{L}\right)\right] = 0, \tag{3.22}$$

proved using the cyclic property of the trace. But it does not conserve the purity $\mathrm{Tr}\left[\hat{\rho}^2\right]$ that decreases [25].

3.3 Stationary distribution

The Lindblad distribution allows a stationary distribution that satisfies the condition

$$\mathcal{L}\hat{\rho} = 0. \tag{3.23}$$

It can be proven that the stationery distribution is equal to the Gibbs states [27]

$$\hat{\rho}^* = \frac{e^{-\beta\hat{H}}}{\mathrm{Tr}\left[e^{-\beta\hat{H}}\right]}. \tag{3.24}$$

In the previous section we assume that the environment is in a Gibbs state, now consider that the dump parameter satisfies the relation

$$\gamma_{ij}(-\omega) = e^{-\beta\omega}\gamma_{ij}(\omega), \tag{3.25}$$

it is called KMS condition [27].

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

$$P(n,t) = \langle n|\hat{\rho}(t)|n\rangle \tag{3.26}$$

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

$$\frac{dP(n,t)}{dt} = \sum_m \left[W(n|m)P(m,t) + W(m|n)P(n,t)\right] \tag{3.27}$$

with time independent transition rate

$$W(n|m) = \sum_{ij}\gamma_{ij}(\epsilon_n - \epsilon_m)\langle n|\hat{J}_i(t)|m\rangle\langle m|\hat{J}_j(t)|n\rangle. \tag{3.28}$$

Using the equation (3.25) and considering the l.h.s. of the equation (3.27) , we obtain the Fermi Golden rule

$$W(n|m)e^{-\beta\epsilon_n} = W(m|n)e^{-\beta\epsilon_m} \tag{3.29}$$

which is nothing else that a detail balance condition with stationary distribution

$$\hat{\rho} = \frac{1}{Z}e^{-\beta\hat{H}} \tag{3.30}$$

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

3.4 Entropy production

3.5 Caldeira-Leggett model

The Caldeira-Leggett model was proposed in 1983 to reproduce the Brownian motion via a quantum process. It study the dynamics of a particle in contact with a thermal bath made by a set of harmonic oscillator. However, the model present the Markovian propery only in the high temperature weak coupling limit and a not Markovian one in otherwise.

The free Hamiltonian of the particle is

$$H_S = \frac{\hat{p}^2}{2m} + V(\hat{q}), \tag{3.31}$$

where $\hat{p}$ is the momentum operator and $V(\hat{q})$ is the potential.

The particle is in contact with the bath composed by N harmonic oscillator. The Hamiltonian is

$$H_E = \sum \Omega_n (\hat{b}_n^\dagger \hat{b}_n + \frac{1}{2}) = \sum_n \left(\frac{p_n^2}{2m_n} + \frac{1}{2} m_n \Omega_n^2 q_n^2 \right). \tag{3.32}$$

where $\hat{b}_n^\dagger$ and $\hat{b}_n$ are respectively the creation and annihilation operators of the bath, and p_n and q_n the momentum and position operator of the oscillators of bath.

The interaction Hamiltonian is given by

$$H_I = \hat{q} \sum_n k_n \hat{q}_n = -\hat{B}\hat{q} = \hat{q} \sum_n k_n \frac{1}{\sqrt{2m_n\Omega_n}} \left(\hat{b} + \hat{b}^\dagger \right) \tag{3.33}$$

where $\hat{B}$ is the bath operator.

We need to add a counterterm

$$H_C = \sum_n \frac{\hat{q}^2}{2m_n\Omega_n^2}. \tag{3.34}$$

Starting from equation (3.9) in the Schrödinger pictures

$$\frac{d\rho(t)}{dt} = i \left[\hat{H}_S + \hat{H}_C, \hat{\rho}(t) \right] - \int_0^\infty ds \, \mathrm{Tr}_E \left[\hat{H}_I(t), \left[\hat{H}_I(t-s), \hat{\rho}(t) \otimes \hat{\rho}_E(t) \right] \right], \tag{3.35}$$

We can rewrite it using the correlation relations of the bath

$$D(s) = i \left\langle \left[\hat{B}, \hat{B}^\dagger(t-s) \right] \right\rangle \qquad D'(s) = \left\langle \left\{ \hat{B}, \hat{B}^\dagger(t-s) \right\} \right\rangle \tag{3.36}$$

into the formula

$$\frac{d\rho(t)}{dt} = -i \left[\hat{H}_S + \hat{H}_C, \hat{\rho}(t) \right] - \int_0^\infty ds \frac{i}{2} D(s) \left[\hat{q}, \{ \hat{q}(-s), \hat{\rho}(t) \} \right] - \frac{1}{2} D'(s) \left[\hat{q}, [\hat{q}(-s), \hat{\rho}(t)] \right] \tag{3.37}$$

Using the spectral density

$$J(\Omega) = \sum_n \frac{k_n^2}{2m_n\Omega} \delta(\Omega - \Omega_n) \tag{3.38}$$

we can rewrite the correlation as

$$D(s) = 2 \int_0^\infty d\Omega J(\Omega) \sin \Omega s \qquad D'(s) = 2 \int_0^\infty d\Omega J(\Omega) \coth \left(\frac{\Omega}{2k_B T} \right) \cos \Omega s. \tag{3.39}$$

We can simplify further the equation (3.37) looking at the $\hat{q}(-s)$, indeed, it can be written as

$$\hat{q}(-s) = e^{-i\hat{H}_S s}\hat{q}e^{i\hat{H}_S s} \approx \hat{q} - i\left[\hat{H}_S, \hat{q}\right] s = \hat{q} - \frac{\hat{p}}{m}s \tag{3.40}$$

Inserting it into (3.37) we obtain

$$\begin{aligned}\frac{d\rho(t)}{dt} =& -i\left[\hat{H}_S + \hat{H}_C, \hat{\rho}(t)\right] - \frac{i}{2}\int_0^\infty dsD(s)\left[\hat{q}, \{\hat{q}, \hat{\rho}(t)\}\right] \\ &+ \frac{i}{2m}\int_0^\infty ds\, sD(s)\left[\hat{q}, \{\hat{p}, \hat{\rho}(t)\}\right] - \frac{1}{2}\int_0^\infty dsD'(s)\left[\hat{q}, [\hat{q}, \hat{\rho}(t)]\right] \\ &+ \frac{1}{2m}\int_0^\infty ds\; sD'(s)\left[\hat{q}, [\hat{p}, \hat{\rho}(t)]\right].\end{aligned} \tag{3.41}$$

Then, we solve the integral in the high temperature limit: the first term give us the exactly the counter term $-i\left[\hat{H}_C, \hat{\rho}\right]$, the second becomes $-\frac{i\gamma}{2}\left[\hat{q}, \{\hat{p}, \hat{\rho}(t)\}\right]$, the third becomes $2m\gamma k_B T\left[\hat{q}, [\hat{q}, \hat{\rho}(t)]\right]$ and the last give us $\frac{2\gamma k_B T}{\Omega}\left[\hat{q}, [\hat{p}, \hat{\rho}]\right]$ which is negligible in the limit $\Omega \to \infty$ that we are dealing with.

We have reached the Caldeira-Leggett master equation

$$\frac{d\hat{\rho}}{dt} = -i\left[\hat{H}_S, \hat{\rho}(t)\right] - \frac{i\gamma}{2}\left[\hat{q}, \{\hat{p}, \hat{\rho}(t)\}\right] - 2m\gamma k_B T\left[\hat{q}, [\hat{q}, \hat{\rho}(t)]\right]. \tag{3.42}$$

The Caldeira-Leggett master equation reminds of the Langevin equation where the second term is the dissipative one and the third describes the fluctuations.

Chapter 4

Quantum Stochastic Walk

In chapter 1 we have introduced two possibility for a random walk: one using classic particles, the other using quantum ones. But they have different properties that distinguish them self In this chapter, we propose a way to unify the two approach using the Lindblad master equation. This new approach generates a more general random walk on network that include the properties of both the system [28]

4.1 Quantum master equation

Let we consider a quantum system in contact with a thermal bath that randomly interact with; the density matrix of the system $\hat{\rho}$ should follow the Lindblad master equation (3.22)

$$\frac{d}{dt}\hat{\rho} = \mathcal{L}\left[\hat{\rho}\right] = -i\left[\hat{H},\hat{\rho}\right] + \sum_i \gamma_i \left(\hat{J}_i\hat{\rho}\hat{J}_i^\dagger - \frac{1}{2}\left\{\hat{J}_i^\dagger\hat{J}_i,\hat{\rho}\right\}\right), \tag{4.1}$$

where $[\cdot,\cdot]$ and $\{\cdot,\cdot\}$ are respectively the commutator and anticommutator; $\hat{H}$ is the Hamiltonian; $\{\hat{J}_i\}_i$ are the jump operators which describe the interaction with the thermal bath and they are dissipative part of the dynamics; γ_i are the dumping rates, they must be non negative and real, when $\gamma_i = 0$ we recover the Von Neumann equation (1.29). $\mathcal{L}\left[\hat{\rho}\right]$ is a superoperator that act in the space of the density matrix.

The equation (4.1) is composed by two distinct terms: the first term, also called coherent dynamics, $\mathcal{L}^{qm}\left[\hat{\rho}(t)\right] = -i\left[H,\hat{\rho}\right]$ is equal to the quantum walk dynamics; instead, the second $\mathcal{L}^{cl}\left[\hat{\rho}(t)\right] = \sum_i \gamma_i \left(\hat{J}_i\hat{\rho}\hat{J}_i^\dagger - \frac{1}{2}\left\{\hat{J}_i^\dagger\hat{J}_i,\hat{\rho}\right\}\right)$, called decoherent dynamics, encodes the dissipation. As in the quantum random walk, the Hamiltonian $\hat{H}$ is the Laplacian operator $\hat{L}$. We can define a set of jump operator $\{\hat{J}_{ij}\}_{i,j=0}^N$ as general measurement and a set of coefficients $\{\gamma_{ij}\}_{i,j=0}^N$ that behave as the Adjacency matrix, namely $\gamma_{ij} = A_{ij}$ and $\hat{J}_{ij} = |i\rangle\langle j|$. From that, we obtain a master equation that contains both the quantum and classical aspect of a diffusion over a network as

$$\frac{d}{dt}\hat{\rho} = -i(1-\omega)\left[\hat{H},\hat{\rho}\right] + \omega\sum_{ij}\gamma_{ij}\left[\hat{J}_{ij}\hat{\rho}\hat{J}_{ij}^\dagger - \frac{1}{2}\left\{\hat{J}_{ij}^\dagger\hat{J}_{ij},\hat{\rho}\right\}\right]. \tag{4.2}$$

The parameter $\omega \in [0,1]$ allow us to switch between the coherent and dissipative phenomena.

The classical random walk behavior emerges considering the evolution of the diagonal element of the density matrix for just $\mathcal{L}^{cl}$, that is in the limit $\omega = 1$

$$\begin{aligned}\mathcal{L}^{cl}|a\rangle\langle a| &= \sum_{ij}\gamma_{ij}\left[\hat{J}_{ij}|a\rangle\langle a|\hat{J}_{ij}^{\dagger} - \frac{1}{2}\left\{\hat{J}_{ij}^{\dagger}\hat{J}_{ij}, |a\rangle\langle a|\right\}\right] \\ &= \sum_{i}\left[A_{ia}|i\rangle\langle i| - A_{ia}|a\rangle\langle a|\right] \\ &= \sum_{i}A_{ai}|i\rangle\langle i| - d_a|a\rangle\langle a| = -\sum_{i}L_{ai}|i\rangle\langle i|.\end{aligned} \tag{4.3}$$

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

Considering now the off-diagonal terms, they evolve as

$$\begin{aligned}\mathcal{L}^{cl}|a\rangle\langle b| &= \sum_{ij}\gamma_{ij}\left[\hat{J}_{ij}|a\rangle\langle b|\hat{J}_{ij}^{\dagger} - \frac{1}{2}\left\{\hat{J}_{ij}^{\dagger}\hat{J}_{ij}, |a\rangle\langle b|\right\}\right] \\ &= \sum_{ij}\left[\sqrt{A_{ij}}|i\rangle\langle j\,|\,a\rangle\langle b\,|\,j\rangle\langle i|\sqrt{A_{ij}} - \frac{1}{2}|i\rangle\sqrt{A_{ia}}\langle j\,|\,j\rangle\sqrt{A_{ia}}\langle i\,|\,a\rangle\langle b|\right. \\ &\quad \left. -\frac{1}{2}|a\rangle\langle b\,|\,i\rangle\sqrt{A_{ia}}\langle j\,|\,j\rangle\sqrt{A_{ia}}\langle i|\right] \\ &= \sum_{j}\left[-\frac{1}{2}A_{ja}|a\rangle\langle b| - \frac{1}{2}A_{ja}|a\rangle\langle b|\right] \\ &= -\frac{1}{2}(d_a + d_b)|a\rangle\langle b|.\end{aligned} \tag{4.4}$$

$\mathcal{L}^{cl}$ 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 [29].

4.2 Time evolution

Following the resolution proposed by Fujii [30] 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 [25].

The follow operation can be vectorize as

$$\hat{A}\hat{\rho}\hat{B} \to (\hat{A}\otimes\hat{B})|\rho\rangle\rangle \qquad \hat{A}\hat{\rho} + \hat{\rho}\hat{B} \to \left(\hat{A}\otimes\mathbb{I} + \mathbb{I}\otimes\hat{B}\right)|\rho\rangle\rangle, \tag{4.5}$$

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

$$\hat{A}\otimes\hat{B} = \begin{pmatrix} A_{11}\hat{B} & \cdots & A_{1N}\hat{B} \\ \vdots & \ddots & \vdots \\ A_{n1}\hat{B} & \cdots & A_{NN}\hat{B}\end{pmatrix}. \tag{4.6}$$

More detail are shown in the Appendix B.

In this space the Lindblad equation (4.2) becomes

$$\frac{d}{dt}|\rho(t)\rangle\rangle = \tilde{\mathcal{L}}|\rho(t)\rangle\rangle, \tag{4.7}$$

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

$$\tilde{\mathcal{L}} = -i(1-\omega)\left[\hat{H}\otimes\mathbb{I} - \mathbb{I}\otimes\hat{H}\right] + \omega\sum_{ij}\gamma_{ij}\left[\hat{J}_{ij}\otimes\hat{J}_{ij}^{\dagger} + \hat{J}_{ij}^{\dagger}\hat{J}_{ij}\otimes\mathbb{I} + \mathbb{I}\otimes\hat{J}_{ij}^{\dagger}\hat{J}_{ij}\right]. \tag{4.8}$$

The solution equation (4.7) can be written as

$$|\rho(t)\rangle\rangle = \hat{U}(t,\omega)|\rho(0)\rangle\rangle, \tag{4.9}$$

where $U(t,\omega)$ is the evolution operator [31]

$$\begin{aligned}\hat{U}(t,\omega) = \exp\Big\{&-i\,(1-\omega)\,t\left(\hat{H}\otimes\mathbb{I} - \mathbb{I}\otimes\hat{H}\right)\\ &+ \omega t\sum_{ij}\gamma_{ij}\left[\hat{J}_{ij}\otimes\hat{J}_{ij}^{\dagger} - \frac{1}{2}\hat{J}_{ij}\hat{J}_{ij}^{\dagger}\otimes\mathbb{I} - \frac{1}{2}\mathbb{I}\otimes\hat{J}_{ij}\hat{J}_{ij}^{\dagger}\right]\Big\}\end{aligned} \tag{4.10}$$

The evolution operator is not unitary.

4.3 Entropy production

We can compute also the Von Neumann entropy for the network. Looking at its derivative $\dot{S}(\hat{\rho}(t))$, we can consider just the dissipative part, since the unitary one does not change entropy. Knowing that the dynamics is trace preserving, namely $\mathrm{Tr}\left[\frac{d\hat{\rho}}{dt}\right] = 0$, we obtain

$$\dot{S}(\hat{\rho}) = -\,\mathrm{Tr}\left[\frac{d\hat{\rho}}{dt}\ln\hat{\rho}\right] = -\,\mathrm{Tr}\left[\sum_{ij}\gamma_{ij}\left[\hat{J}_{ij}\hat{\rho}\hat{J}_{ij}^{\dagger} - \frac{1}{2}\left\{\hat{J}_{ij}^{\dagger}\hat{J}_{ij},\hat{\rho}\right\}\right]\ln\hat{\rho}\right]. \tag{4.11}$$

We expand the commutator

$$\dot{S}(\hat{\rho}) = -\sum_{ij}\gamma_{ij}\,\mathrm{Tr}\left[\hat{J}_{ij}\hat{\rho}\hat{J}_{ij}^{\dagger}\ln\hat{\rho} - \frac{1}{2}\hat{J}_{ij}^{\dagger}\hat{J}_{ij}\hat{\rho}\ln\hat{\rho} - \frac{1}{2}\hat{\rho}\hat{J}_{ij}^{\dagger}\hat{J}_{ij}\ln\hat{\rho}\right] \tag{4.12}$$

Since $\ln\hat{\rho}$ and $\hat{\rho}$ commute, the second and third terms can be summed. Thus, substituting $\gamma_{ij} = A_{ij}$ we arrive to

$$\dot{S}(\hat{\rho}) = -\sum_{ij}A_{ij}\,\mathrm{Tr}\left[\hat{J}_{ij}\hat{\rho}\hat{J}_{ij}^{\dagger}\ln\hat{\rho} - \hat{J}_{ij}^{\dagger}\hat{J}_{ij}\hat{\rho}\ln\hat{\rho}\right]. \tag{4.13}$$

Reordering the terms we obtain

$$\dot{S}(\hat{\rho}) = -\sum_{ij}A_{ij}\left(\mathrm{Tr}\left[\hat{J}_{ij}\hat{\rho}\hat{J}_{ij}^{\dagger}\ln\hat{\rho}\right] - \mathrm{Tr}\left[\hat{J}_{ij}^{\dagger}\hat{J}_{ij}\hat{\rho}\ln\hat{\rho}\right]\right) \tag{4.14}$$

The equation (4.14) is always positive, the proof is in the appendix C.

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

4.4 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 case $\omega = 1$, thus, only the dissipative term survive. The dynamics decouples the diagonal and off-diagonal terms. The first follow the evolution

$$\frac{d}{dt}\rho_{ii} = \sum_j \left[W(i|j)\rho_{jj}(t) - W(j|i)\rho_{ii}(t)\right], \tag{4.15}$$

with transition rate

$$W(i|j) = \sum_{lm} \gamma_{lm}\langle i|J_{lm}|j\rangle\langle i|J_{lm}^\dagger|j\rangle = W(j|i). \tag{4.16}$$

Since the stationary distribution must satisfy the detail balance, namely

$$W(i|j)\rho_{jj}(t) = W(j|i)\rho_{ii}. \tag{4.17}$$

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

$$\hat{\rho}^* = \frac{1}{N}\begin{pmatrix} 1 & & \\ & \ddots & \\ & & 1 \end{pmatrix}. \tag{4.18}$$

4.5 Kirchhoff

Let take for this chapter the standard Lindblad equation (4.1) with Hamiltonian $\hat{H} = \hat{L}$

$$\frac{d}{dt}\hat{\rho} = \mathcal{L}[\hat{\rho}] = -i\left[\hat{H}, \hat{\rho}\right] + \sum_{ij}\gamma_{ij}\left(\hat{J}_{ij}\hat{\rho}\hat{J}_{ij}^\dagger - \frac{1}{2}\left\{\hat{J}_{ij}^\dagger\hat{J}_{ij}, \hat{\rho}\right\}\right), \tag{4.19}$$

the jump operator $\hat{J}_{ij} = |i\rangle\langle k|$ indicates the jumps between two node and the coefficient γ_{ij} is not already defined. We can change the basis to $\{|\lambda\rangle\}$ such that $\hat{H} = \sum_\lambda \epsilon_\lambda|\lambda\rangle\langle\lambda|$ is diagonal. The previous equation becomes

$$\frac{d}{dt}\hat{\rho} = -i\left[\hat{H}, \hat{\rho}\right] + \sum_{\lambda\mu}\gamma_{\lambda\mu}\left(\hat{J}_{\lambda\mu}\hat{\rho}\hat{J}_{\lambda\mu}^\dagger - \frac{1}{2}\left\{\hat{J}_{\lambda\mu}^\dagger\hat{J}_{\lambda\mu}, \hat{\rho}\right\}\right), \tag{4.20}$$

with $\hat{J}_{\lambda\mu} = |\lambda\rangle\langle\mu|$ and $\gamma_{\lambda\mu}$ is still not defined. We assume that the dynamics will tend to a stationary distribution in the form of

$$\hat{\rho}^* = \frac{e^{-\beta\hat{H}}}{Z}. \tag{4.21}$$

Thus, the master equation for the stationary distribution is

$$0 = -i\left[\hat{H}, \frac{e^{-\beta\hat{H}}}{Z}\right] + \sum_{\lambda\mu}\gamma_{\lambda\mu}\left(\hat{J}_{\lambda\mu}\frac{e^{-\beta\hat{H}}}{Z}\hat{J}_{\lambda\mu}^\dagger - \frac{1}{2}\left\{\hat{J}_{\lambda\mu}^\dagger\hat{J}_{\lambda\mu}, \frac{e^{-\beta\hat{H}}}{Z}\right\}\right). \tag{4.22}$$

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

$$\sum_{\lambda\mu} \gamma_{\lambda\mu} |\lambda\rangle\langle\mu| \frac{e^{-\beta\hat{H}}}{Z} |\mu\rangle\langle\lambda| = \sum_{\lambda\mu} \gamma_{\lambda\mu} \frac{e^{-\beta\epsilon_\mu}}{Z} |\lambda\rangle\langle\lambda|. \tag{4.23}$$

While the second becomes

$$\sum_{\lambda\mu} \gamma_{\lambda\mu} \left[\frac{1}{2} |\mu\rangle\langle\lambda \,|\, \lambda\rangle\langle\mu| \frac{e^{-\beta\hat{H}}}{Z} + \frac{1}{2} \frac{e^{-\beta\hat{H}}}{Z} |\mu\rangle\langle\lambda \,|\, \lambda\rangle\langle\mu| \right] = \sum_{\lambda\mu} \gamma_{\lambda\mu} \left[\frac{e^{-\beta\epsilon_\mu}}{Z} |\mu\rangle\langle\mu| \right]. \tag{4.24}$$

The master equation (4.22) reduces to

$$\sum_{\lambda\mu} \left[\gamma_{\lambda\mu} \frac{e^{-\beta\epsilon_\mu}}{Z} - \gamma_{\mu\lambda} \frac{e^{-\beta\epsilon_\lambda}}{Z} \right] |\lambda\rangle\langle\lambda|. \tag{4.25}$$

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. The same distribution can be obtain in position space. As a matter of fact, the master equation (4.2) for the distribution (4.21). Let assume that it is the stationary distribution, thus

$$0 = \sum_{\lambda\mu} \gamma_{ij} \left(\hat{J}_{ij} \frac{e^{-\beta\hat{H}}}{Z} \hat{J}_{ij}^\dagger - \frac{1}{2} \left\{ \hat{J}_{ij}^\dagger \hat{J}_{ij}, \frac{e^{-\beta\hat{H}}}{Z} \right\} \right). \tag{4.26}$$

the first term can be written as

$$\sum_{ij} \gamma_{ij} |i\rangle\langle j| \frac{e^{-\beta\hat{H}}}{Z} |j\rangle\langle i| = \sum_{ji} \gamma_{ij} \frac{e^{-\beta H_{jj}}}{Z} |i\rangle\langle i| \tag{4.27}$$

Whereas, the second term becomes

$$\sum_{ij} \frac{\gamma_{ij}}{2} |j\rangle\langle j| \frac{e^{-\beta\hat{H}}}{Z} + \frac{\gamma_{ij}}{2} \frac{e^{-\beta\hat{H}}}{Z} |j\rangle\langle j| = \sum_{ijk} \frac{1}{2} \left(\gamma_{ij} \frac{e^{-\beta H_{jk}}}{Z} + \gamma_{ik} \frac{e^{-\beta H_{jk}}}{Z} \right) |j\rangle\langle k| \tag{4.28}$$

We can combine together all the terms obtaining

$$\begin{aligned} \sum_{ji} \left(\gamma_{ji} \frac{e^{-\beta H_{ii}}}{Z} - \gamma_{ij} \frac{e^{-\beta H_{jj}}}{Z} \right) |j\rangle\langle j| = 0 \\ \sum_{jk} \frac{1}{2} \left(\sum_i \gamma_{ij} + \sum_i \gamma_{ik} \right) \frac{e^{-\beta H_{jk}}}{Z} |j\rangle\langle k| = 0 \end{aligned} \tag{4.29}$$

The first equation is again the Kirchhoff's current law, while the second is a condition over the parameter γ.

If the previous condition are satisfy the stationary distribution of the system is the canonical one. In our case it becomes

$$\hat{\rho}^* = \frac{e^{-\beta\hat{L}}}{Z} \qquad Z = \mathrm{Tr}[e^{-\beta\hat{L}}] \tag{4.30}$$

that is the density matrix (2.40) introduced by De Domenico to identify networks.

4.6 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 (4.2). As a matter of fact, in the chapter 3 we have analyzed also the case where the interaction with the environment is not symmetric (3.13). Thus, taking the dissipative part of the equation (3.14) in the Schrödinger picture with the coefficients $\Gamma_{ij} = L_{ij}$ and the jump operators $J_{ij} = |i\rangle\langle j|$ we obtain

$$\frac{d\hat{\rho}(t)}{dt} = \sum_{ij} \Gamma_{ij} \left[\hat{J}_j \hat{\rho}(t), \hat{J}_i^\dagger \right] + \Gamma_{ji}^\dagger \left[\hat{J}_j, \hat{\rho}(t) \hat{J}_i^\dagger \right]. \tag{4.31}$$

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

$$\frac{d\hat{\rho}(t)}{dt} = \sum_{ij} \gamma_{ij} \hat{J}_j \hat{\rho}(t) \hat{J}_i^\dagger - \frac{\gamma_{ij}}{2} \left\{ \hat{J}_i^\dagger \hat{J}_j, \hat{\rho}(t) \right\} + i\pi_{ij} \left[\hat{J}_i^\dagger \hat{J}_j, \hat{\rho}(t) \right], \tag{4.32}$$

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

$$\frac{d\hat{\rho}(t)}{dt} = i \left[\hat{H}_A, \hat{\rho}(t) \right] + \sum_{ij} \gamma_{ij} \hat{J}_j \hat{\rho}(t) \hat{J}_i^\dagger - \frac{\gamma_{ij}}{2} \left\{ \hat{J}_i^\dagger \hat{J}_j, \hat{\rho}(t) \right\}. \tag{4.33}$$

The dynamics (4.33) does not converge no more to a stationary state due to the Von Neumann part. We can generalize as in the (4.2)

$$\frac{d}{dt}\hat{\rho} = -i \left[(1-\omega)\hat{H} + \omega \hat{H}_A, \hat{\rho} \right] + \omega \sum_{ij} \gamma_{ij} \left[\hat{J}_{ij} \hat{\rho} \hat{J}_{ij}^\dagger - \frac{1}{2} \left\{ \hat{J}_{ij}^\dagger \hat{J}_{ij}, \hat{\rho} \right\} \right]. \tag{4.34}$$

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 [32]. 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 [32]

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

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 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

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

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.

Appendix C

Entropy production

In chapter 4 computing the derivative of the entropy for the quantum stochastic walk we reach the result (4.14)

$$\dot{S}(\hat{\rho}) = -\sum_{ij} A_{ij} \left(\mathrm{Tr}\left[\hat{J}_{ij}\hat{\rho}\hat{J}_{ij}^{\dagger} \ln \hat{\rho} \right] - \mathrm{Tr}\left[\hat{J}_{ij}^{\dagger}\hat{J}_{ij}\hat{\rho} \ln \hat{\rho} \right] \right) \tag{C.1}$$

that it is positive ensuring the increasing of the entropy.

To prove the last statement, since $A_{ij}$is always positive, we need to prove the following inequality

$$\mathrm{Tr}\left[\hat{J}_{ij}\hat{\rho}\hat{J}_{ij}^{\dagger} \ln \hat{\rho} \right] \leq \mathrm{Tr}\left[\hat{J}_{ij}^{\dagger}\hat{J}_{ij}\hat{\rho} \ln \hat{\rho} \right]. \tag{C.2}$$

First we diagonalize the density matrix. let be $|\Lambda_i\rangle$ the eigenstate with eigenvalue Λ_i, the density matrix can be written as

$$\hat{\rho} = \sum_k \Lambda_k |\Lambda_k\rangle\langle\Lambda_k|. \tag{C.3}$$

We transform also the jump operator in this basis $\hat{\mathcal{J}}_{ij} = \hat{O}\hat{J}_{ij}\hat{O}^{\dagger}$. The l.h.s. of the inequality (C.2) becomes with some algebra can be reduces to

$$\begin{aligned} \mathrm{Tr}\left[\hat{J}_{ij}\hat{\rho}\hat{J}_{ij}^{\dagger} \ln \hat{\rho} \right] &= \sum_{kl} \mathrm{Tr}\left[\hat{\mathcal{J}}_{ij}\Lambda_k |\Lambda_k\rangle\langle\Lambda_k| \hat{\mathcal{J}}_{ij}^{\dagger} \ln \Lambda_l |\Lambda_l\rangle\langle\Lambda_l| \right] \\ &= \sum_{kl} \Lambda_k \ln \Lambda_l \, \mathrm{Tr}\left[|\langle\Lambda_l|\hat{\mathcal{J}}_{ij}|\Lambda_k\rangle|^2 \right] \\ &= N \sum_{kl} \Lambda_k \ln \Lambda_l x_{kl}^{(ij)} \end{aligned} \tag{C.4}$$

where $x_{kl}^{(ij)} = |\langle\Lambda_l|\hat{\mathcal{J}}_{ij}|\Lambda_k\rangle|^2$ and it is symmetric respect the change $k \leftrightarrow l$.

The r.h.s. becomes

$$\begin{aligned}\mathrm{Tr}\left[\hat{J}_{ij}^{\dagger}\hat{J}_{ij}\hat{\rho}\ln\hat{\rho}\right] &= \sum_{kl}\mathrm{Tr}\left[\hat{J}_{ij}^{\dagger}\hat{J}_{ij}\Lambda_k|\Lambda_k\rangle\langle\Lambda_k|\ln\Lambda_l|\Lambda_l\rangle\langle\Lambda_l|\right]\\ &= \sum_{kl}\Lambda_k\ln\Lambda_l\,\mathrm{Tr}\left[\langle\Lambda_l|\hat{J}_{ij}^{\dagger}\hat{J}_{ij}|\Lambda_k\rangle\langle\Lambda_k\,|\,\Lambda_l\rangle\right]\\ &= \sum_{k}\Lambda_k\ln\Lambda_k\,\mathrm{Tr}\left[\langle\Lambda_k|\hat{J}_{ij}^{\dagger}\hat{J}_{ij}|\Lambda_k\rangle\right]\\ &= \sum_{kl}\Lambda_k\ln\Lambda_k\,\mathrm{Tr}\left[\langle\Lambda_k|\hat{J}_{ij}^{\dagger}|\Lambda_l\rangle\langle\Lambda_l|\hat{J}_{ij}|\Lambda_k\rangle\right]\\ &= N\sum_{kl}\Lambda_k\ln\Lambda_k x_{kl}^{(ij)}.\end{aligned} \tag{C.5}$$

The second braket in the trace is just a Kronecker delta. We use the completeness relation $I=\sum_l|\Lambda_l\rangle\langle\Lambda_l|$ obtaining

$$\begin{aligned}\mathrm{Tr}\left[\hat{J}_{ij}^{\dagger}\hat{J}_{ij}\hat{\rho}\ln\hat{\rho}\right] &= \sum_{kl}\Lambda_k\ln\Lambda_k\,\mathrm{Tr}\left[\langle\Lambda_k|\hat{J}_{ij}^{\dagger}|\Lambda_l\rangle\langle\Lambda_l|\hat{J}_{ij}|\Lambda_k\rangle\right]\\ &= N\sum_{kl}\Lambda_k\ln\Lambda_k x_{kl}^{(ij)}.\end{aligned} \tag{C.6}$$

The inequality (C.2) reduces to

$$N\sum_{kl}\Lambda_k\ln\Lambda_l x_{kl}^{(ij)} \leq N\sum_{kl}\Lambda_k\ln\Lambda_k x_{kl}^{(ij)}. \tag{C.7}$$

We can rearrange the term in the two sum as

$$\begin{aligned}\sum_{k}\sum_{l<k}2\Lambda_k\ln\Lambda_l x_{k,l}^{(ij)}+\sum_{k}\Lambda_k\ln\Lambda_k x_{k,k}^{(ij)} \leq\\ \sum_{k}\sum_{l<k}\left(\Lambda_k\ln\Lambda_k+\Lambda_l\ln\Lambda_l\right)x_{kl}^{(ij)}+\sum_{k}\Lambda_k\ln\Lambda_k x_{kk}\end{aligned} \tag{C.8}$$

Therefore, to prove it it necessary that

$$2\Lambda_k\ln\Lambda_l \leq \Lambda_k\ln\Lambda_k+\Lambda_l\ln\Lambda_l, \tag{C.9}$$

but it can be proved using the triangular inequality.

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