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Second quantization theory for many-particles stochastic dynamics on finite transport and storage capacity network

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Abstract

Nella tesi viene studiata la dinamica stocastica di particelle non interagenti su network con capacità di trasporto e immagazzinamento per nodo finite. L'argomento viene affrontato introducendo per il sistema un formalismo di seconda quantizzazione. Dopo avere dimostrato l'effettiva conservazione del numero totale di particelle e che per il sistema vale una relazione di bilancio dettagliato, vengono derivate le relazioni di Onsager per il caso di un network con capacità di trasporto finita. Infine, viene ricavata l'espressione esplicita della distribuzione stazionaria di probabilità per il caso di un network con capacità finita di immagazzinamento per nodo.

Contents

Introduction

The introduction of the statistical mechanics point of view to study the behaviour of systems with a very large number of elements could be seen as one of the great contributions of physics to scientific knowledge. Statistical mechanics models the dynamic evolution of the macroscopic variables of the system, providing a connection between the microscopic and the macroscopic dynamics. Although the price to obtain handable and useful equations can be the unavoidable simplification of the problems at stake, the advantage is the effectiveness in finding and explaining large scale and collective phenomena. This kind of phenomena, due to the simplification procedure they come from, reveals universal features depending on the topology and dimensionality of the system, rather than on the specific nature of the microscopic processes occurring in it. Seeing these considerations, the progress constituted by the introduction of graph theory into statistical mechanics to represent the network of interaction occurring in the systems results clear.

The origin of graph theory has to be dated back to a real world network, with the Königsberg bridges problem solved by Euler in 1735. Although studied in the early years of its history as a branch of mathematics, the concept of network began to be applied with success in almost all the natural and human sciences, providing a way to represent real world systems that entails the emergence of effects otherwise unaccountable. Moreover, graphs may also be regarded as a sort of more complicated lattices upon which certain dynamics can have place; this is indeed the case e.g. of the random walks on network, a topic which has a very broad ranges of research and applications.

In this thesis we study a system of many classicle particles performing random walks on a network whose nodes have both a finite transportation capacity (FTC) and finite storage capacity (FSC), meaning that only a finite number of particles can be sent from one node to another connected node at a time and that up to a finite number of particle can stack on the same node at the same time. The network we work with is a generally good network, being conncted and undirected and, once given, does not change during the evolution of the system; it acts simply as a background upon which particles move. Our main achievement is the development of a suitable field theory formalism to describe this kind of double treshold classical systems. We take advantages of the operatorial commutation rules provided by the formalism to account of the non-commutativity of particle exchanges on the network. Although in the presented models we assume particle conservation; however the extension of the theory to non conservative processes is straightforward and the second quantization formalism, in order to work with variable number of particles, seems to be even more convenient.

Chapter 1

An overview of random walks on networks

In this chapter we introduce the topics that constitute the background layer behind the thesis: random walks and networks. We give a brief overview of the principal definitions in graph theory and random walks and underline the main features of interest in the subject made by the union of both: the random walks on graphs. Indeed, random walks and graph theory are deeply related fields, since, as we shall see, many of the properties of the random walk on a graph can be expressed using results of the spectral graph analysis applied to the transition matrix of the process.

Throughout this chapter, we will follow mainly [1], [2], [3] and [4].

1.1 On networks

Usually represented by means of diagrams, networks are ensembles of points, called *nodes*, connected by lines, or *links*. In order to introduce networks as formally defined mathematical structures, we shall write in terms of *graph*, *vertices* and *edges* rather than networks, nodes and links.

Let $\mathscr{G}$ be a finite set. The *adjacency* is a binary relation on $\mathscr{G}$:

$$i \longleftrightarrow j,$$

with $i \in V$, $j \in U$ and $V, U \in \mathscr{G}$. Thus, adjacency relation defines a collection of ordered pairs $E \subseteq V \times U$. If $V \subseteq \mathscr{G}$ is the set of identical elements called vertices and $E \subseteq V \times V$ is a collection of couple of elements called edges defined by adjancency relation, we identify the graph as $G \equiv G(V, E)$, where V therefore denotes the set of vertices and E the set of edges.

The complement $\overline{G}$ of a graph G is the graph defined on the same set of vertices with the set of edges defined as the edges not present in G.

Graphs can be naturally represented by matrices; to every graph one can associate an adjancency operator $\mathcal{A}$. Let $F(V) \equiv \{ f \colon V \to \mathbb{R} \}$ be the vector space of real functions on V and $\{ e_1, e_2, \ldots, e_M \}$ its canonical orthonormal basis, where $|V| = M$ is the number of vertices. The inner product of f and $g \in F(V)$ is defined as

$$(f, g) \equiv \sum_{i \in V} f(i) g(i).$$

The *adjacency matrix* $\mathbb{A}$ is a $M \times M$ matrix which gives a representation , with respect to the canonical basis, to the adjacency operator $\mathcal{A}$ defined by

$$(\mathcal{A} f)(i) = \sum_{(j,i)} f(j),$$

where $f \in F(\mathcal{A})$ and $(j, i) \in E$. Once the nodes of G are enumerated, $\mathcal{A}$ and $\mathbb{A}$ are uniquely defined up to permutation of rows and columns.

The *connection degree* of the i-th node is the number of links attached to it and it is formally defined as

$$d_i \equiv \sum_{j=1}^{M} \mathbb{A}_{ij}.$$

Prior to go further introducing the concept of Markov chains, we shall mention the features of certain peculiar kind of networks one often works with:

- In a *connected* graph there are not isolated vertices i.e. nodes without links attached to them, meaning that one can go from any node to any other node of the network through existing links.

- In a *simple* graph there can be soley single edges between nodes; multiple edges between a couple of nodes are forbidden, as well as nodes connected to themselves in loops. Therefore, the adiancency matrix of a simple graph has all its diagonal entries equal to 0: $\mathbb{A}_{jj} = 0$.

- In an *undirected* graph the nodes are connected by links without any orientation i.e. in a double direction; in the opposite case of an *oriented* network, one may e.g. jump from j-th node to the k-th but the opposite move is not guaranteed. The adjacency matrix of an undirected graph is simmetric: $\mathbb{A}_{ij} = \mathbb{A}_{ji}$.

- In a *weighted* graph the elements of the adjacency matrix are real-valued functions $\omega\colon E \to \mathbb{R}$ assigning to every link (i,j) a weight ω_{ij}. Connection degree of a weighted graph is given by the sum of the weights of all the links it is attached to:

$$d_i = \sum_{j=1}^{M} \omega_{ij}.$$

However, in a simple and *non-weighted* network, all the adjacency matrix entries differing from 0 are equal to 1: $\mathbb{A}_{ij} \in \{ 0, 1 \}$.

- In a *regular* graph all nodes have exactly the same number of links attached to them, that means $d_1 = d_2 = \cdots = d_M = d$ constant making the network similar to a true lattice. Of course, such a network is also connected.

Concerning our work, we are going to deal with *good* networks, i.e. networks which are simple, connected, undirected and non-weighted. In such a case, the adjacency matrix $\mathbb{A}$ is symmetric and its elements are written as

$$\mathbb{A}_{ij} \equiv 1_{ij} = \begin{cases} 1 & \text{if } (i,j) \in E, \\ 0 & \text{otherwise.} \end{cases}$$

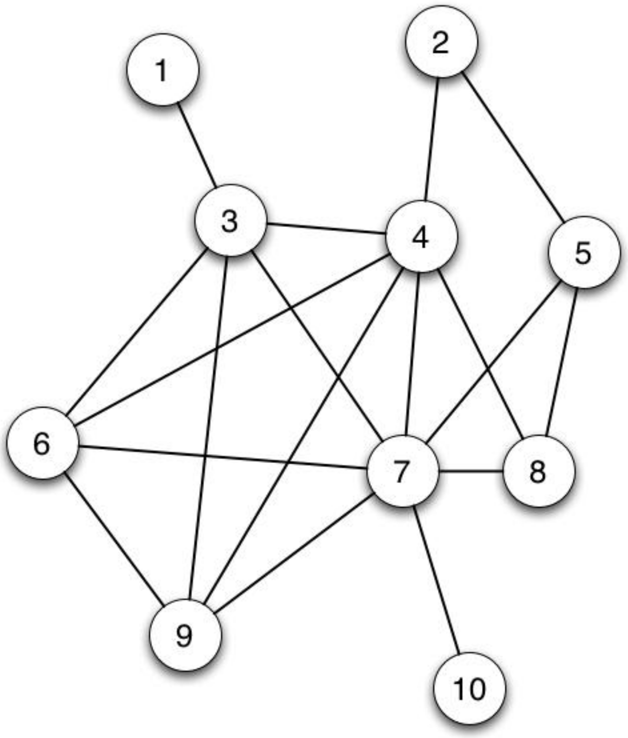
1.2 On markov chains

A random walk may be represented as a Markov chain i.e. a stochastic processes whose evolution depends solely on the present state and not on the past.
Given a probability space E, a measurable space X and a totally ordered set I, a stochastic process is a collection of X-valued random variables on E labelled by I:

$$\{ x_t \mid x_t \in X, t \in I \}.$$

If the set X is finite the stochastic process is said to be finite, and the X-valued random variables can take only a finite number of values. The index t is the time of the process, that evolves assigning different values to x_t and x_{t+1} from the set of states X according to some probability distribution. The stochastic process assigns a transition probability to every possible change of variable value. We write the transition probability for the system to evolve from the state l to the state k as the element $\mathbb{P}_{kl}$ of the matrix $\mathbb{P}$, called *transition matrix*. We have a Markov chain if

$$\begin{aligned} \mathbb{P}_{kl} &= \Pr(x_{t+1} = k | x_t = l) \\ &= \Pr(x_{t+1} = k | x_t = l, x_{t-1} = l_{t-1}, \ldots, x_{t_0} = l_0), \end{aligned}$$



A diagram depicting a small graph. Despite having only ten nodes, it is a valuable exemple of how a good graph is: simple, connected, undirected and non-weighted.

where $k, l, l_t{-}1, \ldots, l_0 \in X$. As it seems from the former equality, the conditional probabilities $\mathbb{P}_{kl}$ do not involve $l_0, \ldots, l_{t-1}$, that represents the absence of memory of the process. If the transition probabilities do not depend on t the Markov chain is said to be *homogeneous*. If N is the number of possible states in X i.e. the number of states the system can be found in, our transition matrix $\mathbb{P}$ therefore is, by construction, a $N \times N$ matrix that comes out to be a *stochastic matrix*, i.e. a matrix whose elements satisfy the properties:

$$\mathbb{P}_{kl} \geq 0, \quad \forall\, k, s \in X, \qquad \text{and} \qquad \sum_{k=1}^{N} \mathbb{P}_{kl} = 1.$$

We say that a state k is accessible from the state l if

$$\exists\, n \geq 1 \in \mathbb{N}\colon (\mathbb{P}^n)_{kl} > 0.$$

The time evolution of a Markov chain described by the transition matrix is ruled by the Chapman-Kolmogorov equation:

$$\mathbb{P}_{ij} = \sum_{k=1}^{N} (\mathbb{P}^{n-t})_{ik} (\mathbb{P}^t)_{kj}, \quad t \in \{\, 1, 2, \ldots, n_1 \,\}\,. \tag{1.1}$$

We will employ now on the Dirac notation, representing a column vector $\vec{a}$ with the ket symbol $|a\rangle$ and a row $\vec{b}$ vector with the bra symbol $\langle b|\,\cdot$; the inner product in the vector space is then represented by the braket contraction between ket and bra, as $\langle b\,|\,a\rangle$. The probability distribution of x_t can be arranged in a column vector as

$$|p(t)\rangle \equiv \begin{pmatrix} p_1(t) \\ p_2(t) \\ \vdots \\ p_N(t) \end{pmatrix} = \begin{pmatrix} \Pr(x_t = l_1) \\ \Pr(x_t = l_2) \\ \vdots \\ \Pr(x_t = l_N) \end{pmatrix},$$

and it evolves according to $\mathbb{P}$ as:

$$|p(t+1)\rangle = \mathbb{P}\,|p(t)\rangle = \mathbb{P}^t\,|p(0)\rangle\,.$$

We say that a Markov chain is *stationary* if it is homogeneous while having the same distribution p_s for any $t \in \mathbb{Z}$. In matrix notation this is equivalent to say that the distribution p_s is the right eigenvector of the transition matrix $\mathbb{P}$ with eigenvalue 1:

$$\mathbb{P}\,|p_s\rangle = 1\,|p_s\rangle\,.$$

Being $\mathbb{P}$ a stochastic matrix, it always has an eigenvalue 1. Indeed

$$\sum_{i=1}^{N} \mathbb{P}_{ij} = 1 \qquad \Longrightarrow \qquad \langle 1|\,\mathbb{P} = \langle 1|\,,$$

where $\langle 1|$ is a row vector with all entries equal to 1. Unfortunately, the positivity if the right eigenvector is not guaranteed.

1.3 Mixing them up: random walks on networks

Let $G \equiv G(V,E)$ be a simple, connected, undirected and unweighted graph with M nodes and m links. Consider a random walk on this good graph. Supposing to lie, at the start, on the node i, to whom we may assign the label v_0 writing $i = v_0$. We suppose then to randomly choose one of the nodes adjacent to v_0, with $d(v_0)$ different but equally probable choices, and jump on it, say the j-th node, giving to it the label $j = v_1$. Then, as a second time step, we can choose at random another node adjacent to j and so on... If at the t-th step we are at the node labelled v_t, we move to a node adjacent to it with probability $\frac{1}{d(v_t)}$. Clearly, this sequence of random nodes $\{\, v_t \mid t = 0,1,2,\dots \,\}$ constructed in this way is a Markov chain.

The node v_0 may be fixed, but may be drawn from some initial distribution $|p_0\rangle \equiv$

$|p(t_0 = 0)\rangle$ instead. Our random walk induces on the nodes a probability distribution that we represent as a column vector with components $p_i(t)$:

$$|p(t)\rangle = \begin{pmatrix} p_1(t) \\ p_2(t) \\ \vdots \\ p_M(t) \end{pmatrix} = \begin{pmatrix} \Pr(v_t = 1) \\ \Pr(v_t = 2) \\ \vdots \\ \Pr(v_t = M) \end{pmatrix}.$$

Being M the number of nodes of the network, the transition matrix is now a $M \times M$ matrix whose elements are the transition probabilities between different nodes. Dealing with a good graph, at every time step the random walker choose a link of the node to go trough with equal probability. Thus

$$\mathbb{P}_{ij} = \pi_{ij} = \frac{1_{ij}}{d_j},$$

making the transition matrix $\mathbb{P}$ to be related to the adjancency matrix $\mathbb{A}$ of the underlying graph by the relation

$$\mathbb{P} = D^{-1}\mathbb{A}, \tag{1.2}$$

where D is a diagonal matrix having the connections ordinately deployed in its entries as:

$$D \equiv \begin{pmatrix} d_1 & & & 0 \\ & d_2 & & \\ & & \ddots & \\ 0 & & & d_M \end{pmatrix}$$

Thanks to Kolmogorov equation, the evolution of the system is given by

$$|p(t)\rangle = \mathbb{P}^t \, |p(0)\rangle \, .$$

It follows that the probability p^t_{ij} that, starting at j, we reach the i-th node in t time stepsis given by the (i, j)-entry of the transition matrix:

$$p^t_{ij} = (\mathbb{P}^t)_{ij}.$$

The probability distributions at different time $|p_0\rangle$, $|p_1\rangle$, ... are of course generally different. We say that the distribution $|p_0\rangle$ is *stationary*, or a *steady state*, if $|p_t\rangle = |p_0\rangle \equiv |p_s\rangle$ for all $t \geq 0$. A steady distribution, induced by a random walk on the good graph $G(V, E)$ reads

$$|p_s\rangle = \frac{1}{2m} \begin{pmatrix} d_1 \\ d_2 \\ \vdots \\ d_M \end{pmatrix},$$

with $|E| = m$. It is immediate to see that

$$\sum_{j=1}^{M} \pi_{ij} p_s^j = \sum_{j=1}^{M} \frac{1_{ij}}{d_j} \frac{d_j}{2m} = \frac{d_i}{2m} \qquad \Longrightarrow \qquad \mathbb{P}\,|p_s\rangle = |p_s\rangle\,.$$

The steady state satisfies a *detailed balance* condition:

$$\pi_{ij}\, p_s^j = \pi_{ji}\, p_s^i, \qquad \forall\, i, j \in V, \tag{1.3}$$

meaning that the frequency of the passage $j \to i$ is equal to that of the $i \to j$ one. In Markovian terms this is equivalent to the time-reversibility of the stochastic process and in terms of the graphs to the non-weighted connected nature of it. In our work this latter consideration plays an important role to determine the behaviour of an unknown steady state, and therefore we discuss detailed balance in a section dedicated. If the system is in a steady state and we are sitting on an edge and the random walk just passed through it, then the expected number of steps before it passes through it in the same direction again is $2m$. There is a similar facts for nodes: if we are sitting on the node i and the random walk has just visited this node, then the expected number of steps before it returns to it is $\frac{2m}{d_i}$. I G is regular, the return time is just M, the number of nodes.

One of the most important feature of the stationary distribution is that if the graph G is connected and non-bipartite, then the distribution of v_t tends to a stationary distribution as $t \to \infty$. In order to show this feature, we shall outline the analogies between the spectral properties of the transition matrix and the underlying graph.

Let $G(V, E)$ be a graph with $|V| = M$ and $|E| = m$. The *Laplacian* of G is defined to be the matrix whose elements are

$$\mathbb{L}_{ij} \equiv \begin{cases} d_i & \text{if } i = j, \\ -1 & \text{if } i \text{ and } j \text{ are adjacent}, \\ 0 & \text{otherwise.} \end{cases}$$

so that we can write $\mathbb{L} \equiv D - \mathbb{A}$, that is

$$\mathbb{L} = \begin{pmatrix} d_1 & & & 0 \\ & d_2 & & \\ & & \ddots & \\ 0 & & & d_M \end{pmatrix} - \begin{pmatrix} 0 & & & 1_{1j} \\ & 0 & & \\ & & \ddots & \\ 1_{Mj} & & & 0 \end{pmatrix} = \begin{pmatrix} d_1 & & & -1_{1j} \\ & d_2 & & \\ & & \ddots & \\ -1_{Mj} & & & d_M \end{pmatrix}.$$

We now define the *rescaled Laplacian* $\mathbb{L}_R$ as

$$\mathbb{L}_R \equiv D^{-\frac{1}{2}}\, \mathbb{L}\, D^{-\frac{1}{2}},$$

that means

$$\mathbb{L}_R = D^{-\frac{1}{2}}(D - \mathbb{A})D^{-\frac{1}{2}} = \mathcal{I} - D^{-\frac{1}{2}}\mathbb{A}D^{-\frac{1}{2}} = \begin{pmatrix} 1 & & & -\frac{1_{1j}}{\sqrt{d_i d_j}} \\ & 1 & & \\ & & \ddots & \\ -\frac{1_{Mj}}{\sqrt{d_M d_j}} & & & 1 \end{pmatrix}.$$

Being, by construction, D and A symmetric matrices, both $\mathbb{L}$ and $\mathbb{L}_R$ are symmetric too. Thus, $\mathbb{L}_R$ has always M real eigenvalues. These M eigenvalues, say λ_i, are always non-negative: $\lambda_i \geq 0$ for all i. In fact, taking an eigenvector $|k\rangle$ with eigenvalue λ_k:

$$\begin{aligned} \langle k| \mathbb{L}_R |k\rangle &= \lambda_k \langle k \mid k\rangle \\ \langle k| D^{-\frac{1}{2}}\mathbb{L}D^{-\frac{1}{2}} |k\rangle &= \lambda_k \langle k \mid k\rangle \\ \langle v_k| \mathbb{L} |v_k\rangle &= \lambda_k \langle k| D^{\frac{1}{2}}D^{\frac{1}{2}} |k\rangle , \end{aligned}$$

where $|v_k\rangle \equiv D^{-\frac{1}{2}} |k\rangle$ and $\langle v_k| \equiv \langle v_k| D^{-\frac{1}{2}}$. Thus, we can write:

$$\begin{aligned} \lambda_k &= \frac{\langle v_k| \mathbb{L} |v_k\rangle}{\langle k| D^{\frac{1}{2}}D^{\frac{1}{2}} |k\rangle} \\ &= \frac{\sum_{ij}\left\{v_i^k(d_i\delta_{ij})v_j^k - v_i^k(1_{ij})v_j^k\right\}}{\sum_i \left(v_i^k\right)^2 d_i} \\ &= \frac{\sum_i \left(v_i^k\right)^2 d_i \sum_{ij} 2v_i^k v_j^k}{\sum_i \left(v_i^k\right)^2 d_i} \\ &= \frac{\sum_{ij} 2\left(v_i^k\right)^2 d_i - \sum_{ij}\left(v_i^k - v_j^k\right)^2}{\sum_i \left(v_i^k\right)^2 d_i} \\ &= \frac{\sum_{ij}\left(v_i^k - v_j^k\right)^2}{\sum_i \left(v_i^k\right)^2 d_i} \geq 0, \end{aligned}$$

proving that $\lambda_k \geq 0$ for any k. Furthermore $\lambda_k = 0$ is a possible solution, making v_i to be constant:

$$\sum_{ij}\left(v_i^k - v_j^k\right)^2 = 0 \qquad \Longrightarrow \qquad v_i^k = v_j^k, \quad \forall (i,j).$$

Keeping this in mind, we shall re-lebel our real eigenvalues in a non-decreasing order as

$$0 = \lambda_0 \leq \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_{M-1},$$

and write the spectral decomposition

$$\mathbb{L}_R = \sum_{k=0}^{M-1} |k\rangle \langle k| .$$

It is an easly calculation to prove that

$$\sum_{k=0}^{M-1} \lambda_k \leq M,$$

with the equality holding if and only if the graph G has no isolated vertices. Due to this and the fact that $\lambda_0 = 0$, another series of disequalities holds:

$$(M-1)\lambda_1 \leq \sum_{i=1}^{M-1} \lambda_i \leq M,$$

that implies that

$$\lambda_1 \leq \frac{M}{M-1}.$$

Having that

$$(a-b)^2 \leq 2\,(a^2+b^2), \quad \forall\, a,b \in \mathbb{R},$$

means that, summing over the node indeces' couples:

$$\sum_{(ij)} \left(v_i^k - v_j^k\right)^2 \leq 2 \sum_{(ij)} \left[\left(v_i^k\right)^2 + \left(v_j^k\right)^2\right] = 2 \sum_{ij} 1_{ij} \left(v_i^k\right)^2 = 2 \sum_i \left(v_i^k\right)^2 d_i,$$

and thus

$$\lambda_k = \frac{\sum_{ij} \left(v_i^k - v_j^k\right)^2}{\sum_i \left(v_i^k\right)^2 d_i} \leq 2,$$

meaning that $\lambda_k \in [0,2]$ $\forall k \geq 1$ and $\lambda_0 = 0$ or, summing up the results:

$$\begin{cases} \lambda_k \in \mathbb{R} \quad \forall k \in \{\,0,1,2,\ldots,M-1\,\} \\ 0 = \lambda_0 \leq \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_{M-1} \leq 2 \\ \lambda_1 \leq \frac{M}{M-1}. \end{cases}$$

Given that $\mathbb{P} = \mathbb{A}D^{-1}$, we can write

$$\mathbb{P} = D^{\frac{1}{2}}(\mathcal{I} - \mathbb{L}_R)D^{-\frac{1}{2}} \qquad \Longrightarrow \qquad \mathbb{L} = \mathcal{I} - D^{-\frac{1}{2}} P D^{\frac{1}{2}},$$

and try to gather information about $\mathbb{P}$ eigenvalues:

$$\begin{aligned} \langle k|\, \mathbb{L}_R \,|k\rangle \equiv \langle k|\, (\mathcal{I} - D^{-\frac{1}{2}}\, \mathbb{P}\, D^{\frac{1}{2}})\, |k\rangle = \lambda_k \,\langle k \,|\, k\rangle \\ \Longleftrightarrow \qquad \langle k|\, D^{-\frac{1}{2}}\, \mathbb{P}\, D^{\frac{1}{2}}\, |k\rangle = (1-\lambda_k)\, \langle k \,|\, k\rangle \\ \Longleftrightarrow \qquad \langle k|\, D^{-\frac{1}{2}}\, \mathbb{P}\, D^{\frac{1}{2}}\, |k\rangle = (1-\lambda_k)\, \langle k|\, D^{-\frac{1}{2}} D^{\frac{1}{2}}\, |k\rangle\,, \end{aligned}$$

recognizing that it be can written that $|\psi_k\rangle \equiv D^{\frac{1}{2}}|k\rangle$ and $\langle\chi_k| \equiv \langle k| D^{-\frac{1}{2}}$ we thus obtain the equality

$$\langle\chi^k|\,\mathbb{P}\,|\psi^k\rangle = \left(1-\lambda_k\right)\langle\chi^k\,|\,\psi^k\rangle\,,$$

meaning that $\mathbb{P}$ has M real eigenvalues, just as $\mathbb{L}_R$. Named ϕ_k, they appear to satisfy the relations:

$$\begin{cases} \phi_k = 1-\lambda_k \in \mathbb{R}, \\ \lambda_k \leq 2 \implies |\phi_k| \leq 1, \\ 1 = \phi_0 \geq \phi_1 \geq \phi_2 \geq \cdots \geq \phi_{M-1}. \end{cases}$$

Since P is not symmetric its right and left eigenvalues are not just one the trasposted conjugated of the other, and the spectral decomposition reads

$$\mathbb{P} = \sum_{i=0}^{M-1} \phi_i\,|\psi_i\rangle\,\langle\chi_i|\,.$$

The eigenvalue $\phi_0 = 1$ is particulary valuable to us, corresponding to $\lambda_0 = 0$ and to the steady state for the random walk of a single particle. Indeed, when the $M \times M$ matrix $\mathbb{P}$ acts on a M-dimensional vector space (e.g. the vector space of the positions occupied by a single particle undergoing a rondom walk on the network) the components of $|\psi_0\rangle$, the quantities

$$\psi_i^0 \equiv \langle i\,|\,\psi_0\rangle\,,$$

where the vectors $\langle i|$ are the row vector with the i-th entry equal to 1 and the others equal to 0 are the single probabilities of the steady distribution. We can then make use of the normalization condition to write:

$$\sum_{i=0}^{M-1} \psi_i^0 = \sum_{i=0}^{M-1} \langle i\,|\,\psi_0\rangle = 1, \tag{1.4}$$

which, in turn, implies that we can write the ψ_i^0 probabilities as

$$\psi_k^0 = \frac{d_k}{2m}.$$

We are now ready to demonstrate that if the network is both connected and non-bipartite any given probability distribution will converge to the steady one in the long time limit. The two mentioned conditions are verified by checking the Laplacian eigenvalues λ_k:

1. $\lambda_1 > 0$ if the network is connected;
2. $|\lambda_{M-1}| < 2$ if it is non-bipartite.

While, concerning the eigenvalues pf the transition matrix $\mathbb{P}$, the two hypotesis are satisfied if

$$|\phi_i| < 1, \quad \forall\, i > 0.$$

Indeed, given any initial state $|f(0)\rangle$ at time $t = 0$:

$$\begin{aligned}
|f(t)\rangle &= \mathbb{P}^t \, |f(0)\rangle \\
&= \sum_{k=0}^{M-1} \phi_k^t \, |\psi_k\rangle \, \langle \chi_k \,|\, f(0)\rangle \\
&= |\psi_0\rangle \, \langle \chi_0 \,|\, f(0)\rangle + \sum_{k=1}^{M-1} \phi_k^t \, |\psi_k\rangle \, \langle \chi_k \,|\, f(0)\rangle \, .
\end{aligned}$$

Being $|\phi_i| < 1$ if $i > 0$ and $\langle \chi_0 \,|\, f(0)\rangle = \sum_{i=1}^{M} f_i(0) = 1$, it follows immediatly that

$$\lim_{t\to\infty} |f(t)\rangle = |\psi_0\rangle \, . \tag{1.5}$$

This result can be regarded to be very important, as it guarantees the relaxation to steady stade by employing just the spectral properties of the graph.

Moreover, it is possible to relate the relaxing time scale to the second higher eigenvalue of the transition matrix. Indeed:

$$\begin{aligned}
\varepsilon &\equiv |p_s - f(t)| \\
&= \left\| |\psi_0\rangle - \left(|\psi_0\rangle \, \langle \chi_0 \,|\, f(0)\rangle + \sum_{k=1}^{M-1} \phi_k^t \, |\psi_k\rangle \, \langle \chi_k \,|\, f(0)\rangle \right) \right\| \\
&= \left\| \sum_{k=1}^{M-1} \phi_k^t f(\chi_k) \, |\psi_k\rangle \right\| \leq \phi_{\mathrm{max}}^t \left\| \sum_{k=1}^{M-1} f(\chi_k) \, |\psi_k\rangle \right\| \\
&\leq \phi_{\mathrm{max}}^t \simeq e^{-\phi_{max} t},
\end{aligned}$$

where $\phi_{max} \equiv \max\{|\phi_i| \colon i > 1\}$. We can thus extimate the relaxing time scale as

$$\tau_{relax} \sim \ln \phi_{max}.$$

Chapter 2

On the 1-FTC+q-FSC model

Here we show and discuss the main properties of our stochastic dynamical model on a particular double treshold network, i.e. a network where every node can send just one particle per time step (1-FTC) and up to q particles can stack on a node at once (q-FSC). We approach the problem of N particles randomly walking across such a network in an operatorial way, adopting a second quantization formalism to describe movements of the particle on the network as annihilation-creation processes among nodes. We introduce a suitable ansatz to write a stationary state that satisfy an eigenvalue equation unless boundary troubles arose, and derive the corresponding steady probability distribution. Finally, we demonstrate that our dynamics does conserve the overall number of particles.

2.1 Foundations of the model

The *network state* $|\vec{n}\rangle$ of N particles deployed along the M nodes of the network is defined as the tensor product of M base states:

$$|\vec{n}\rangle \equiv |n_1\, n_2\, \dots\, n_k\, \dots\, n_M\rangle \equiv |n_1\rangle \otimes |n_2\rangle \otimes \cdots \otimes |n_k\rangle \otimes \cdots \otimes |n_M\rangle\,.$$

The particles-across-nodes configuration $\vec{n}$ can be quantum-mechanically regarded as a vector lying in a M-dimensional space and having a fixed lenght equal to N:

$$\sum_{i=1}^{M} n_i = N \qquad \Longrightarrow \qquad |\vec{n}| = N,$$

from this time one we shall account for this by writing that $\vec{n} \in \Gamma$, where

$$\Gamma \equiv \left\{ \vec{n} \in \mathbb{Z}^M \;\middle|\; \sum_{i=1}^{M} = N \right\}.$$

The inner product between base states satisfies the orthogonality relation

$$\langle \vec{m} \mid \vec{n} \rangle \equiv \delta_{\vec{m}}^{\vec{n}}, \qquad \forall\, \vec{n}, \vec{m} \in \Gamma,$$

while the completeness relation, also known as decomposition of unity, reads:

$$\sum_{\vec{n}\,\in\,\Gamma} |\vec{n}\rangle \, \langle \vec{n}| \cdot = \mathcal{I}\,.$$

In order to project any generic state $|\varphi\rangle$ on the multiparticle state $|\vec{m}\rangle$, one has to write:

$$\langle \text{projection of}\, \varphi\, \text{state on}\, \vec{m} \rangle \equiv \langle \vec{m} \mid \varphi \rangle \equiv p_{\varphi}(\vec{m}).$$

The expectation value for a generic observable-operator $\mathcal{O}$ while our sistem is in the state ϕ_t is defined to be

$$\begin{aligned}
\big\langle \mathcal{O} \big\rangle_{\phi_t} &\equiv \sum_{\vec{n}\,\in\,\Gamma} \langle \vec{n}|\, \mathcal{O}\, |\phi_t\rangle \\
&= \sum_{\vec{n}\,\in\,\Gamma} \sum_{\vec{m}\,\in\,\Gamma} \langle \vec{n}|\, \mathcal{O}\, |\vec{m}\rangle \, \langle \vec{m} \mid \phi_t \rangle \\
&= \sum_{\vec{n}\,\in\,\Gamma} \sum_{\vec{m}\,\in\,\Gamma} \langle \vec{n}|\, \mathcal{O}\, |\vec{m}\rangle \, p_{\phi_t}(\vec{m}).
\end{aligned}$$

Supposing that any node of the network could send just one particle per time step (1-FTC) and that no more than q particles could stack on each node at a time (q-FSC), we define the peculiar creation and destruction operator $\mathcal{C}_i$ and $\mathcal{B}_j$ by their action on the multiparticle vectors $|\vec{n}\rangle$:

$$\begin{aligned}
\mathcal{B}_j \, |\vec{n}\rangle &= \theta(n_j)\, |\vec{n} - 1_j\rangle \equiv \theta(n_j)\, |n_1, n_2, \ldots, n_{j-1}, n_j - 1, n_{j+1}, \ldots, n_M\rangle\,, \\
\mathcal{C}_i \, |\vec{n}\rangle &= \theta(q - n_i)\, |\vec{n} + 1_i\rangle \equiv \theta(q - n_i)\, |n_1, n_2, \ldots, n_{i-1}, n_i + 1, n_{i+1} \ldots, n_M\rangle\,.
\end{aligned}$$

The commutator operation between $\mathcal{C}_i$ and $\mathcal{B}_j$ reads:

$$\begin{aligned}
&\big[\mathcal{C}_i, \mathcal{B}_j\big]\, |\vec{n}\rangle \equiv \mathcal{C}_i\, \mathcal{B}_j\, |\vec{n}\rangle - \mathcal{B}_j\, \mathcal{C}_i\, |\vec{n}\rangle \\
&\quad = \mathcal{C}_i\, \theta(n_j)\, |\vec{n} - 1_j\rangle - \mathcal{B}_j\, \theta(q - n_i)\, |\vec{n} + 1_i\rangle \\
&\quad = \begin{cases} \theta(q - n_i)\theta(n_j)\, |\vec{n} + 1_i - 1_j\rangle - \theta(q - n_i)\theta(n_j)\, |\vec{n} + 1_i - 1_j\rangle = 0 & \text{if } i \neq j \\ \theta(n_j)\theta(q - n_j + 1)\, |\vec{n}\rangle - \theta(n_j + 1)\theta(q - n_j)\, |\vec{n}\rangle & \text{if } i = j \end{cases} \\
&\quad = \delta_{ij} \Big\{ \theta(n_j)\theta(q - n_j + 1) - \theta(n_j + 1)\theta(q - n_j) \Big\}\, |\vec{n}\rangle \\
&\Longrightarrow \; \big[\mathcal{C}_i, \mathcal{B}_j\big]\, |\vec{n}\rangle = \delta_{ij} \Big\{ \theta(n_j)\theta(q - n_j + 1) - \theta(n_j + 1)\theta(q - n_j) \Big\}\, |\vec{n}\rangle\,.
\end{aligned}$$

We remark that, being Γ a subspace of $\mathbb{Z}^M$, we haven't prevented by axiom the nodes' occupation numbers n_k to reach values greater than q as well as to go down below 0 assuming negative values. These situations will be ruled out by our dynamics. Nevertheless, one could assume from the start to work with physical states (i.e. states $\vec{n}\colon n_k \in [0, q]\,\forall k \in \{\,1, 2, \ldots, M\,\}$) from the very start. If so, the above commutator between $\mathcal{C}_i$ and $\mathcal{B}_j$ reduces to

$$\big[\mathcal{C}_i, \mathcal{B}_j\big]\,|\vec{n}\rangle = \delta_{ij}\Big\{\theta(n_j) - \theta(q - n_j)\Big\}\,|\vec{n}\rangle\,.$$

2.2 The Liouville dynamical equation

Let $\mathbb{P}$ be the *transition matrix* i.e. the stochastic $N_\Gamma \times N_\Gamma$ matrix so that its matrix elements return the conditioned probabilities after a Δt finite time step:

$$\big[\mathbb{P}(\Delta t)\big]_{\vec{n},\vec{m}} = \langle\vec{n}|\,\mathbb{P}(\Delta t)\,|\vec{m}\rangle = p(\vec{n}\mid\vec{m};\,\Delta t),$$

where

$$\sum_{\vec{n}\,\in\,\Gamma}\big[\mathbb{P}(\Delta t)\big]_{\vec{n},\vec{m}} = 1, \qquad \big[\mathbb{P}(\Delta t)\big]_{\vec{n},\vec{m}} \geq 0.$$

The action of $\mathbb{P}$ on a generic state $|\psi(t)\rangle$ is understood to be the finite time step Δt evolution

$$\mathbb{P}(\Delta t)\,|\psi(t)\rangle = |\psi(t+\Delta t)\rangle\,.$$

Since want our dynamical equation to take the quantum-mechanical shape

$$\frac{\partial}{\partial t}\,|\psi(t)\rangle = \mathcal{L}\,|\psi(t)\rangle\,,$$

it follows that, after finite emount of time Δt,

$$|\psi(t+\Delta t)\rangle = \exp\big[\mathcal{L}\Delta t\big]\,|\psi(t)\rangle\,.$$

This leads to the exponential representation of $\mathbb{P}$ by means of the Liouville operator:

$$\mathbb{P}(\Delta t) = \exp\big[\mathcal{L}\Delta t\big],$$

meaning that, in order to let $\mathbb{P}$ be truly stochastic, $\mathcal{L}$ has to be a *Laplacian operator*, i.e.

$$\sum_{\vec{m}\,\in\,\Gamma}\langle\vec{m}|\,\mathcal{L}\,|\vec{n}\rangle = 0 \qquad \Longleftrightarrow \qquad \sum_{\vec{m}\,\in\,\Gamma}\langle\vec{m}|\,\mathbb{P}\,|\vec{n}\rangle = 1.$$

We define our Liouville continuous time evolution operator as

$$\mathcal{L} \equiv \frac{1}{M}\sum_{i=1}^{M}\sum_{j=1}^{M}\pi_{ij}\,\mathcal{C}_i\,\mathcal{B}_j - \frac{1}{M}\sum_{i=1}^{M}\sum_{j=1}^{M}\pi_{ij}\Theta^q_{ij},$$

where the operators Θ_{ij}^{q} are defined by their action on multiparticle network states:

$$\Theta_{ij}^{q}\,|\vec{n}\rangle = \theta(n_j)\theta(q-n_i)\,|\vec{n}\rangle\,.$$

Is this chosen Liouville operator really Laplacian? Or, to write it differently, are we allowed to write the relation

$$\sum_{\vec{m}\,\in\,\Gamma}\langle\vec{m}|\,\mathcal{L}\,|\vec{n}\rangle = 0\,?$$

Let us check the answer by performing some simple computations:

$$\begin{aligned}
&\sum_{\vec{m}\,\in\,\Gamma}\langle\vec{m}|\,\mathcal{L}\,|\vec{n}\rangle\\
&= \frac{1}{M}\sum_{ij}\pi_{ij}\sum_{\vec{m}\,\in\,\Gamma}\langle\vec{m}|\,\mathcal{C}_i\,\mathcal{B}_j\,|\vec{n}\rangle - \frac{1}{M}\sum_{ij}\pi_{ij}\sum_{\vec{m}\,\in\,\Gamma}\langle\vec{m}|\,\Theta_{ij}^{q}\,|\vec{n}\rangle\\
&= \frac{1}{M}\sum_{ij}\pi_{ij}\theta(n_j)\theta(q-n_i)\sum_{\vec{m}\,\in\,\Gamma}\langle\vec{m}\,|\,\vec{n}+1_i-1_j\rangle +\\
&\qquad\qquad - \frac{1}{M}\sum_{ij}\pi_{ij}\theta(n_j)\theta(q-n_i)\sum_{\vec{m}\,\in\,\Gamma}\langle\vec{m}\,|\,\vec{n}\rangle\\
&= \frac{1}{M}\sum_{ij}\pi_{ij}\theta(n_j)\theta(q-n_i)\sum_{\vec{m}\,\in\,\Gamma}\delta^{\vec{m}}_{\vec{n}+1_j-1_i} - \frac{1}{M}\sum_{ij}\pi_{ij}\theta(n_j)\theta(q-n_i)\sum_{\vec{m}\,\in\,\Gamma}\delta^{\vec{m}}_{\vec{n}}\\
&= \frac{1}{M}\sum_{ij}\pi_{ij}\theta(m_j+1)\theta(q-m_i+1) - \frac{1}{M}\sum_{ij}\pi_{ij}\theta(m_j)\theta(q-m_i)\\
&= \frac{1}{M}\sum_{i=1}^{M}\sum_{j=1}^{M}\pi_{ij}\Big\{\theta(n_j+1)\theta(q-n_i+1) - \theta(n_j)\theta(q-n_i)\Big\}.
\end{aligned}$$

To ask the question whether the latter quantity is equal to 0 or not is the same thing as to ask if the two double summations are equal:

$$\sum_{ij}\pi_{ij}\theta(n_j+1)\theta(q-n_i+1) = \sum_{ij}\pi_{ij}\theta(n_j)\theta(q-n_i)\,?$$

The answer is that they comes out to be equal if we take into account the effect that our dynamical bonds rule out the possibility for non-physical states to be dynamically created. An explanation follows: although at a first glance it may seem that the LHS could be equal or greater than the RHS (more relaxed θ conditions meaning more non-zero terms in the summation), every one of those term is balanced by one in the opposite site, being them equal to π_{ij} or 0. Actually, if the k-th node has no particles at all, it means it is impossible to steal a particle from it making both correspective terms equal to 0; the term on the RHS because of $\theta(n_k = 0) = 0$ and the one on the LHS because it would otherwise admitt a non-physical state our dynamics doesn't allow to exist. An analogue remark could be done for the opposite case of already full nodes (e.g. $n_l = q$): the RHS term vanishes being $\theta(q - n_l)$ equal to 0, while the LHS term is related to a non-physical (and thus not allowed) state.

We have thus shown that the Liouville operator is a Laplacian one; this automatically makes $\mathbb{P}$ to be a stochastic matrix:

$$\sum_{\vec{m}\,\in\,\Gamma} \left[\mathcal{L}\right]_{\vec{m},\vec{n}} \equiv \sum_{\vec{m}\,\in\,\Gamma} \langle\vec{m}|\,\mathcal{L}\,|\vec{n}\rangle = 0 \qquad \Longrightarrow \qquad \sum_{\vec{m}\,\in\,\Gamma} \left[\mathbb{P}\right]_{\vec{m},\vec{n}} = 1.$$

2.3 Back to the classical master equation

The Liouville dynamical equation for the time evolution of the state $|\phi(t)\rangle$ is understood to be:

$$\begin{aligned}\frac{\partial}{\partial t}\,|\phi(t)\rangle &= \mathcal{L}\,|\phi(t)\rangle \\ &= \frac{1}{M}\sum_{i=1}^{M}\sum_{j=1}^{M} \pi_{ij}\,\mathcal{C}_i\,\mathcal{B}_j\,|\phi(t)\rangle - \frac{1}{M}\sum_{i=1}^{M}\sum_{j=1}^{M} \pi_{ij}\Theta^q_{ij}\,|\phi(t)\rangle\,.\end{aligned}$$

Projecting both sides on the multiparticle state $|\vec{n}\rangle$, then exploiting the decomposition of unity, we write:

$$
\begin{aligned}
\frac{\partial}{\partial t}\langle \vec{n} \mid \phi(t)\rangle &= \frac{1}{M}\sum_{i=1}^{M}\sum_{j=1}^{M}\pi_{ij}\,\langle \vec{n}|\,\mathcal{C}_i\,\mathcal{B}_j\,|\phi(t)\rangle - \frac{1}{M}\sum_{i=1}^{M}\sum_{j=1}^{M}\pi_{ij}\,\langle \vec{n}|\,\Theta^q_{ij}\,|\phi(t)\rangle \\
\Longleftrightarrow \ \frac{\partial}{\partial t}p_\phi(\vec{n}) &= \frac{1}{M}\sum_{i=1}^{M}\sum_{j=1}^{M}\pi_{ij}\sum_{\vec{m}\in\Gamma}\langle \vec{n}|\,\mathcal{C}_i\,\mathcal{B}_j\,|\vec{m}\rangle\,\langle \vec{m} \mid \phi(t)\rangle + \\
&\quad - \frac{1}{M}\sum_{i=1}^{M}\sum_{j=1}^{M}\pi_{ij}\sum_{\vec{m}\in\Gamma}\langle \vec{n}|\,\Theta^q_{ij}\,|\vec{m}\rangle\,\langle \vec{m} \mid \phi(t)\rangle \\
&= \frac{1}{M}\sum_{ij}\pi_{ij}\sum_{\vec{m}}\theta(m_j)\theta(q-m_i)\,\langle \vec{n} \mid \vec{m}+1_i-1_j\rangle\,p_\phi(\vec{m}) + \\
&\quad - \frac{1}{M}\sum_{ij}\pi_{ij}\sum_{\vec{m}}\theta(m_j)\theta(q-m_i)\,\langle \vec{n} \mid \vec{m}\rangle\,p_\phi(\vec{m}) \\
&= \frac{1}{M}\sum_{ij}\pi_{ij}\sum_{\vec{m}}\theta(m_j)\theta(q-m_i)\delta^{\vec{n}}_{\vec{m}+1_i-1_j}p_\phi(\vec{m}) + \\
&\quad - \frac{1}{M}\sum_{ij}\pi_{ij}\sum_{\vec{m}}\theta(m_j)\theta(q-m_i)\delta^{\vec{n}}_{\vec{m}}p_\phi(\vec{m}) \\
&= \frac{1}{M}\sum_{ij}\pi_{ij}\theta(n_j+1)\theta(q-n_i+1)p_\phi(\vec{n}-1_i+1_j) + \\
&\quad - \frac{1}{M}\sum_{ij}\pi_{ij}\theta(n_j)\theta(q-n_i)p_\phi(\vec{n}).
\end{aligned}
$$

Finally, the obtained master equation reads:

$$
\boxed{
\begin{aligned}
\frac{\partial}{\partial t}p_\phi(t) &= \frac{1}{M}\sum_{i=1}^{M}\sum_{j=1}^{M}\pi_{ij}\theta(n_j+1)\theta(q-n_i+1)p_\phi(\vec{n}-1_i+1_j) + \\
&\qquad - \frac{1}{M}\sum_{i=1}^{M}\sum_{j=1}^{M}\pi_{ij}\theta(n_j)\theta(q-n_i)p_\phi(\vec{n}).
\end{aligned}
}
$$

2.4 The steady state and the eigenvalues equation

Let the *steady state* $|\Psi^q_s\rangle$ be defined by this ansatz:

$$
\boxed{|\Psi^q_s\rangle \equiv \sum_{\vec{n}\in\Gamma} C_N^{-1}(\psi)\prod_{k=1}^{M}\psi_k^{n_k}\,\mathcal{C}_k^{n_k}\,|0\rangle\,.}
$$

If we remember that, $\forall k \in \{1, 2, \ldots, M\}$,

$$\begin{aligned}
\mathcal{C}_k^{n_k} |0\rangle &= \underbrace{\mathcal{C}_k\, \mathcal{C}_k \ldots \mathcal{C}_k}_{n_k \text{ times}} |0\rangle\, \theta(q)\theta(q-1_k)\theta(q-2_k)\ldots\theta(q-(n_k-1))\, |0\,0\,\ldots\, n_k\,\ldots\,0\rangle \\
&= \theta(q - n_k + 1)\, |\ldots\, n_k\,\ldots\rangle\,,
\end{aligned}$$

we'll recognize that, adding a $\mathcal{C}_i$ operator to the i-th node:

$$\begin{aligned}
&\mathcal{C}_i \prod_{k=1}^{M} \psi_k^{n_k}\, \mathcal{C}_k^{n_k}\, |0\rangle = \mathcal{C}_i \bigotimes_{k=1}^{M} \psi_k^{n_k} \theta(q - n_k + 1)\, |n_k\rangle \\
&= \bigotimes_{k \neq i} \psi_k^{n_k} \theta(q - n_k + 1)\, |n_k\rangle \otimes \psi_i^{n_i} \theta(q - n_i)\theta(q - n_i + 1)\, |n_i + 1\rangle \\
&= \bigotimes_{k \neq i} \psi_k^{n_k} \theta(q - n_k + 1)\, |n_k\rangle \otimes \psi_i^{n_i} \theta(q - n_i)\, |n_i + 1\rangle\,;
\end{aligned}$$

while, adding a $\mathcal{B}_j$ to the j-th node:

$$\begin{aligned}
&\mathcal{B}_j \prod_{k=1}^{M} \psi_k^{n_k}\, \mathcal{C}_k^{n_k}\, |0\rangle = \mathcal{B}_j \bigotimes_{k=1}^{M} \psi_k^{n_k} \theta(q - n_k + 1)\, |n_k\rangle \\
&= \bigotimes_{k \neq j} \psi_k^{n_k} \theta(q - n_k + 1)\, |n_k\rangle \otimes \psi_j^{n_j} \theta(q - n_j + 1)\theta(n_j)\, |n_j - 1\rangle\,.
\end{aligned}$$

Knowing that

$$\frac{\partial}{\partial t} |\Psi_s^q\rangle = \mathcal{L}\, |\Psi_s^q\rangle = 0 \iff \mathcal{L}_{in}\, |\Psi_s^q\rangle = \mathcal{L}_{out}\, |\Psi_s^q\rangle\,,$$

let us compute and compare both LHS and RHS of the latest equality:

$$
\begin{aligned}
\mathsf{LHS} &= \mathcal{L}_{in}\,|\Psi_s^q\rangle \equiv \frac{1}{M}\sum_{ij}\pi_{ij}\,\mathcal{C}_i\,\mathcal{B}_j\,|\Psi_s^q\rangle \\
&= \frac{1}{M}\sum_{ij}\pi_{ij}\sum_{\vec{n}\,\in\,\Gamma} C_N^{-1}\prod_{k=1}^{M}\psi_k^{n_k}\theta(q-n_k+1)\,\mathcal{C}_i\,\mathcal{B}_j\,|\vec{n}\rangle \\
&= \frac{1}{M}\sum_{ij}\pi_{ij}\sum_{\vec{n}\,\in\,\Gamma} C_N^{-1}\prod_{k=1}^{M}\psi_k^{n_k}\theta(q-n_k+1)\theta(q-n_i)\theta(n_j)\,|\vec{n}-1_j+1_i\rangle \\
&= \frac{1}{M}\sum_{ij}\pi_{ij}\sum_{\vec{n}\,\in\,\Gamma} C_N^{-1}\prod_{k\neq i,j}\psi_k^{n_k}\theta(q-n_k+1)\times \\
&\quad\times\psi_i^{n_i}\theta(q-n_i+1)\theta(q-n_i)\psi_j^{n_j}\theta(q-n_j+1)\theta(n_j)\,|\vec{n}-1_j+1_i\rangle \\
&= \frac{1}{M}\sum_{ij}\pi_{ij}\frac{\psi_j}{\psi_i}\sum_{\vec{n}\,\in\,\Gamma} C_N^{-1}\prod_{k\neq i,j}\psi_k^{n_k}\theta(q-n_k+1)\times \\
&\quad\times\psi_i^{n_i+1}\theta(q-n_i+1)\theta(q-n_i)\psi_j^{n_j-1}\theta(n_j)\theta(q-n_j+1)\theta(q-n_j+2)\,|\vec{n}-1_j+1_i\rangle \\
&= \frac{1}{M}\sum_{ij}\pi_{ij}\frac{\psi_j}{\psi_i}\theta(n_j)\theta(q-n_j+1)\times \\
&\quad\times\sum_{\vec{n}\,\in\,\Gamma} C_N^{-1}\,\psi_i^{n_i+1}\,\theta(q-n_i)\,\psi_j^{n_j-1}\,\theta(q-n_j+2)\prod_{k\neq i,j}\psi_k^{n_k}\theta(q-n_k+1)\,|\vec{n}-1_j+1_i\rangle \\
&= \frac{1}{M}\sum_{ij}\pi_{ij}\theta(n_j)\theta(q-n_j+1)\frac{\psi_j}{\psi_i}\,|\Phi_s^q\rangle\,,
\end{aligned}
$$

where

$$
|\Phi_s^q\rangle = \sum_{\vec{n}\,\in\,\Gamma} C_N^{-1}\psi_i^{n_i+1}\psi_j^{n_j-1}\theta(q-n_i)\theta(q-n_j+2)\prod_{k\neq i,j}\psi_k^{n_k}\theta(q-n_k+1)\,|\vec{n}-1_j+1_i\rangle\,.
$$

On the other hand:

$$\begin{aligned}
\mathsf{RHS} = \mathcal{L}_{out} |\Psi_s^q\rangle &\equiv \frac{1}{M} \sum_{ij} \pi_{ij} \Theta_{ij}^q |\Psi_s^q\rangle \\
&= \frac{1}{M} \sum_{ij} \pi_{ij} \sum_{\vec{n}\,\in\,\Gamma} C_N^{-1} \prod_{k=1}^{M} \psi_k^{n_k} \theta(q - n_k + 1) \Theta_{ij}^q |\vec{n}\rangle \\
&= \frac{1}{M} \sum_{ij} \pi_{ij} \theta(n_j) \theta(q - n_i) \underbrace{\sum_{\vec{n}\,\in\,\Gamma} C_N^{-1} \prod_{k=1}^{M} \psi_k^{n_k} \theta(q - n_k + 1) |\vec{n}\rangle}_{\equiv |\Psi_s^q\rangle} \\
&= \frac{1}{M} \sum_{ij} \pi_{ij} \theta(n_j) \theta(q - n_i) |\Psi_s^q\rangle .
\end{aligned}$$

So, we have found LHS and RHS to be:

$$\begin{aligned}
\mathcal{L}_{in} |\Psi_s^q\rangle &= \frac{1}{M} \sum_{ij} \pi_{ij} \theta(n_j) \theta(q - n_j + 1) \frac{\psi_j}{\psi_i} |\Phi_s^q\rangle , \\
\mathcal{L}_{out} |\Psi_s^q\rangle &= \frac{1}{M} \sum_{ij} \pi_{ij} \theta(n_j) \theta(q - n_i) |\Psi_s^q\rangle .
\end{aligned}$$

It may be easily noticed that:

- if the various $\theta(n_j)$, $\theta(q - n_i)$ and $\theta(q - n_j + 1)$ don't cause any trouble, then both LHS and RHS are equal to $|\Psi_s^q\rangle$ with eigenvalue 1;
- $|\Phi_s^q\rangle = |\Psi_s^q\rangle$ being, by construction, summed over all $\vec{n} \in \Gamma$.

2.5 The steady distribution

Let $p_s^q(\vec{n})$ be the *steady distribution*, i.e. the projection of the steady state $|\Psi_s^q\rangle$ on the state $\vec{n}$. According to our model's formalism:

$$\begin{aligned}
p_s^q(\vec{n}) &\equiv \langle \vec{n} \,|\, \Psi_s^q\rangle \\
&= \sum_{\vec{m}} C_N^{-1} \prod_{k=1}^{M} \psi_k^{m_k} \theta(q - m_k + 1) \langle \vec{n} \mid \vec{m}\rangle \\
&= \sum_{\vec{m}} C_N^{-1} \prod_{k=1}^{M} \psi_k^{m_k} \theta(q - m_k + 1) \delta_{\vec{m}}^{\vec{n}} \\
p_s^q(\vec{n}) &= C_N^{-1} \prod_{k=1}^{M} \psi_k^{n_k} \theta(q - n_k + 1).
\end{aligned}$$

Of course, a good steady distribution has to be, before all else, a physical one. Henceforth, we require the node occupation numbers of a steady distribution to be physical, i.e. non-negative: $n_i \geq 0$ for any i. We may thus re-define $p_s^q(\vec{n})$ as

$$p_s^q(\vec{n})\colon \begin{cases} p_s^q(\vec{n}) = \langle \vec{n} \mid \Psi_s^q \rangle \,, \\ n_k \geq 0, \quad \forall\, k \in \{\, 1, 2, \ldots, M \,\} \,. \end{cases}$$

It will prove to be useful to know how one can correlate the steady distributions for configurations differing solely by the exchange of one particle. We recommend however to pay attention to the requisite for the steady distribution to be physical, e.g. by means of an-added-by-hand $\theta(n_k)$ in the case of particle subtraction from the node k-th. Thus, the distribution for the configuration $\vec{m} - 1_a$ is correlated to that for the configuration $\vec{m}$ as:

$$\begin{aligned}
p_s^q(\vec{m} - 1_a) &\equiv \theta(m_a)\, \langle \vec{m} - 1_a \mid \Psi_s^q \rangle \\
&= \theta(m_a) \sum_{\vec{n}} C_N^{-1} \prod_{k=1}^{M} \psi_k^{n_k} \theta(q - n_k + 1)\, \langle \vec{m} - 1_a \mid \vec{n} \rangle \\
&= \theta(m_a) \sum_{\vec{n}} C_N^{-1} \prod_{k=1}^{M} \psi_k^{n_k} \theta(q - n_k + 1) \delta^{\vec{n}}_{\vec{m} - 1_a} \\
&= \theta(m_a) C_N^{-1} \prod_{k \neq a} \psi_k^{m_k} \theta(q - m_k + 1) \psi_a^{m_a - 1} \underbrace{\theta(q - (m_a - 1) + 1)}_{= \theta(q - m_a + 2)} \\
&= \frac{\theta(m_a)}{\psi_a \theta(q - m_a + 1)} C_N^{-1} \prod_{k=1}^{M} \psi_k^{m_k} \theta(q - m_k + 1) \\
&= \frac{1}{\psi_a\, \theta(q - m_a + 1)} p_s^q(\vec{m}),
\end{aligned}$$

where we have used the equality

$$\theta(q - m_a + 2)\theta(q - m_a + 1) = \theta(q - m_a + 1).$$

In opposite case i.e. if we add a particle to the a-node:

$$
\begin{aligned}
p_s^q(\vec{m}+1_a) \equiv \langle \vec{m}+1_a \mid \Psi_s^q \rangle &= \sum_{\vec{n}} C_N^{-1} \prod_{k=1}^{M} \psi_k^{n_k} \theta(q-n_k+1) \, \langle \vec{m}+1_a \mid \vec{n} \rangle \\
&= \sum_{\vec{n}} C_N^{-1} \prod_{k=1}^{M} \psi_k^{n_k} \theta(q-n_k+1) \delta_{\vec{m}+1_a}^{\vec{n}} \\
&= C_N^{-1} \prod_{k\neq a} \psi_k^{m_k} \theta(q-m_k+1) \psi_a^{m_a+1} \theta(q-(m_k+1)+1) \\
&= C_N^{-1} \prod_{k\neq a} \psi_k^{m_k} \theta(q-m_k+1) \psi_a^{m_a} \psi_a \, \theta(q-m_a) \\
&= \psi_a \, \theta(q-m_a) \, C_N^{-1} \prod_{k=1}^{M} \psi_k^{m_k} \theta(q-m_k+1) = \psi_a \, \theta(q-m_a) \, p_s^q(\vec{m}),
\end{aligned}
$$

where it has been exploited the equality

$$\theta(q-m_a) = \theta(q-m_a) \, \theta(q-m_a+1).$$

We thus have obtained the equalities

$$
\begin{aligned}
p_s^q(\vec{n}+1_a) &= \psi_a \, \theta(q-n_a) \, p_s^q(\vec{n}), \\
p_s^q(\vec{n}-1_b) &= \frac{\theta(n_b)}{\psi_b \, \theta(q-n_b+1)} \, p_s^q(\vec{n});
\end{aligned}
$$

that let us to write the important relation

$$p_s^q(\vec{n}+1_a-1_b) = \frac{\psi_a}{\psi_b} \frac{\theta(n_b)\theta(q-n_a)}{\theta(q-n_b+1)} \, p_s^q(\vec{n}).$$

Being $p_s^q(\vec{n})$ a steady distribution, it must be $\partial_t p_s^q(\vec{n}) = 0$. Imposing this on the master equation, we obtain the equality

$$\boxed{\sum_{i=1}^{M} \sum_{j=1}^{M} \pi_{ij} \frac{\psi_j}{\psi_i} \, \theta(n_i)\theta(n_j+1)\theta(q-n_j) = \sum_{i=1}^{M} \sum_{j=1}^{M} \theta(n_j)\theta(q-n_i).}$$

In facts, if $\partial_t p_s^q(\vec{n}) = 0$, one then has:

$$
\begin{aligned}
&\frac{1}{M} \sum_{ij} \pi_{ij} \theta(n_j+1)\theta(q-n_i+1) p_s^q(\vec{n}-1_i+1_j) = \frac{1}{M} \sum_{ij} \pi_{ij} \theta(n_j)\theta(q-n_i) p_s^q(\vec{n}) \\
\iff &\sum_{ij} \pi_{ij} \theta(n_j+1)\theta(q-n_i+1) \frac{\psi_j}{\psi_i} \frac{\theta(n_i)\theta(q-n_j)}{\theta(q-n_i+1)} p_s^q(\vec{n}) = \sum_{ij} \pi_{ij} \theta(n_j)\theta(q-n_i) p_s^q(\vec{n}) \\
\iff &\sum_{ij} \pi_{ij} \theta(n_i)\theta(n_j+1)\theta(q-n_j) \frac{\psi_j}{\psi_i} = \sum_{ij} \pi_{ij} \theta(n_j)\theta(q-n_i).
\end{aligned}
$$

It is an easy task to notice that, if those θs don't cause troubles, the terms

$$\frac{1}{\psi_i}\sum_{j=1}^{M}\pi_{ij}\psi_j = 1,$$

are equal to 1, meaning that $\mathsf{LHS} = \mathsf{RHS} = M$.

2.6 On particles number conservation

The number operator $\mathcal{N}$

We shall compute the commutator between $\mathcal{L}$ and the operator number of particles $\mathcal{N}$, which is defined as

$$\mathcal{N} \equiv \sum_{k=1}^{M} \mathcal{A}^{\dagger}{}_k\, \mathcal{A}_k\,.$$

If the commutator vanishes, our dynamics will conserve the total number of particles. Indeed, if O is any observable in our theory:

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}O &\equiv \frac{\mathrm{d}}{\mathrm{d}t}\big\langle\mathcal{O}\big\rangle_{\phi_t} \equiv \frac{\mathrm{d}}{\mathrm{d}t}\,\langle\phi_t|\,\mathcal{O}\,|\phi_t\rangle\\
&= \frac{\mathrm{d}}{\mathrm{d}t}\,\langle\phi_0|\,e^{\mathcal{L}^\dagger t}\mathcal{O}e^{\mathcal{L}t}\,|\phi_0\rangle\\
&= \langle\phi_0|\,\mathcal{L}^\dagger e^{\mathcal{L}^\dagger t}\mathcal{O}e^{\mathcal{L}t}\,|\phi_0\rangle +\\
&\qquad + \langle\phi_0|\,e^{\mathcal{L}^\dagger t}\frac{\partial\mathcal{O}}{\partial t}e^{\mathcal{L}t}\,|\phi_0\rangle + \langle\phi_0|\,e^{\mathcal{L}^\dagger t}\mathcal{O}\mathcal{L}e^{\mathcal{L}t}\,|\phi_0\rangle\\
&= \left\langle\frac{\partial}{\partial t}\mathcal{O}\right\rangle_{\phi_t} + \langle\phi_t|\,\mathcal{O}\mathcal{L}\,|\phi_t\rangle - \langle\phi_t|\,\mathcal{L}\mathcal{O}\,|\phi_t\rangle\\
\frac{\mathrm{d}}{\mathrm{d}t}O &\equiv \left\langle\frac{\partial}{\partial t}\mathcal{O}\right\rangle_{\phi_t} + \langle\phi_t|\,\big[\mathcal{L},\mathcal{O}\big]\,|\phi_t\rangle\,.
\end{aligned}$$

Thus, being $\partial_t\mathcal{N} = 0$ and $\mathcal{L} = \mathcal{L}_{in} - \mathcal{L}_{out}$, we get

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{N} = 0 \quad\iff\quad \big[\mathcal{L},\mathcal{N}\big] = 0 \quad\iff\quad \big[\mathcal{L}_{in},\mathcal{N}\big] = \big[\mathcal{L}_{out},\mathcal{N}\big].$$

So, let us to compute and compare the commutators $\big[\mathcal{L}_{in},\mathcal{N}\big]$ and $\big[\mathcal{L}_{out},\mathcal{N}\big]$.

Commutator of $\mathcal{L}_{in}$ and $\mathcal{N}$

Knowing that, if E, F, G and H are operators applied to a generic state,

$$[EF, GH] = E[F,G]H + EG[F,H] + [E,G]HF + G[E,H]F,$$

we can write:

$$\begin{aligned}\big[\mathcal{L}_{in},\mathcal{N}\big]\,|\vec{n}\rangle &= \sum_{ij}\pi_{ij}\sum_{k}\big[\mathcal{C}_i\,\mathcal{B}_j,\mathcal{A}^{\dagger}{}_k\,\mathcal{A}_k\big]\,|\vec{n}\rangle\\
&= \sum_{ij}\pi_{ij}\sum_{k}\Big\{\mathcal{C}_i\big[\mathcal{B}_j,\mathcal{A}^{\dagger}{}_k\big]\,\mathcal{A}_k+\mathcal{C}_i\,\mathcal{A}^{\dagger}\big[\mathcal{B}_j,\mathcal{A}_k\big]+\\
&\quad+\big[\mathcal{C}_i,\mathcal{A}^{\dagger}\big]\,\mathcal{A}_k\,\mathcal{B}_j+\mathcal{A}^{\dagger}{}_k\big[\mathcal{C}_i,\mathcal{A}_k\big]\,\mathcal{B}_j\Big\}\,|\vec{n}\rangle\,.\end{aligned}$$

Commutators between $\mathcal{C}_i$, $\mathcal{B}_j$ and $\mathcal{A}^{\dagger}{}_k$ reads:

$$\begin{aligned}\big[\mathcal{C}_i,\mathcal{A}^{\dagger}{}_j\big]\,|\vec{n}\rangle &\equiv \mathcal{C}_i\,\mathcal{A}^{\dagger}{}_j\,|\vec{n}\rangle-\mathcal{A}^{\dagger}{}_j\,\mathcal{C}_i\,|\vec{n}\rangle\\
&= \mathcal{C}_i\,|\vec{n}+1_j\rangle-\mathcal{A}^{\dagger}{}_j\,\theta(q-n_i)\,|\vec{n}+1_i\rangle\\
&= \delta_{ij}\Big\{\theta(q-n_j-1)-\theta(q-n_j)\Big\}\,|\vec{n}+2_j\rangle\,;\\
\big[\mathcal{B}_i,\mathcal{A}^{\dagger}{}_i\big]\,|\vec{n}\rangle &\equiv \mathcal{B}_i\,\mathcal{A}^{\dagger}{}_j\,|\vec{n}\rangle-\mathcal{A}^{\dagger}{}_i\,\mathcal{B}_i\,|\vec{n}\rangle\\
&= \mathcal{B}_i\,|\vec{n}+1_i\rangle-\mathcal{A}^{\dagger}{}_j\,\theta(n_i)\,|\vec{n}-1_j\rangle\\
&= \delta_{ij}\Big\{\theta(n_j+1)-\theta(n_j)\Big\}\,|\vec{n}\rangle\,;\end{aligned}$$

and those concerning $\mathcal{A}_k$ reads:

$$\begin{aligned}\big[\mathcal{C}_i,\mathcal{A}_j\big]\,|\vec{n}\rangle &\equiv \mathcal{C}_i\,\mathcal{A}_j\,|\vec{n}\rangle-\mathcal{A}_j\,\mathcal{C}_i\,|\vec{n}\rangle\\
&= n_j\,\mathcal{C}_i\,|\vec{n}-n_j\rangle\,\theta(q-n_i)\,\mathcal{A}_k\,|\vec{n}+1_i\rangle\\
&= \delta_{ij}\Big\{n_j\theta(q-n_j+1)-[n_j+1]\theta(q-n_j)\Big\}\,|\vec{n}\rangle\,;\\
\big[\mathcal{B}_i,\mathcal{A}_j\big]\,|\vec{n}\rangle &\equiv \mathcal{B}_i\,\mathcal{A}_j\,|\vec{n}\rangle-\mathcal{A}_j\,\mathcal{B}_i\,|\vec{n}\rangle\\
&= n_j\,\mathcal{B}_i\,|\vec{n}-1_j\rangle-\theta(n_i)\,\mathcal{A}_j\,|\vec{n}-1_i\rangle\\
&= \delta_{ij}\Big\{n_j\theta(n_j-1)-[n_j-1]\theta(n_j)\Big\}\,|\vec{n}-2_j\rangle\,.\end{aligned}$$

Thus:

$$
\begin{aligned}
\big[\mathcal{L}_{\text{in}},\mathcal{N}\big]\,|\vec{n}\rangle = \sum_{ij}\pi_{ij}\sum_{k}\Big\{& n_k\,\mathcal{C}_i\big[\mathcal{B}_j,\mathcal{A}^\dagger{}_k\big]\,|\vec{n}-1_k\rangle + \\
&+\mathcal{C}_i\,\mathcal{A}^\dagger{}_k\big[\mathcal{B}_j,\mathcal{A}_k\big]\,|\vec{n}\rangle + \\
&+\theta(n_j)n_k\big[\mathcal{C}_i,\mathcal{A}^\dagger{}_k\big]\,|\vec{n}-1_j-1_k\rangle + \\
&+\theta(n_j)\,\mathcal{A}^\dagger{}_k\big[\mathcal{C}_i,\mathcal{A}_k\big]\Big\} \\
=\sum ij\pi_{ij}\sum_{k}\Big\{& n_k\delta_{jk}\big\{\theta(n_j)-\theta(n_j-1)\big\}\,\mathcal{C}_i\,|\vec{n}-1_j\rangle + \\
&+\delta_{jk}\big\{n_j\theta(n_j-1)-[n_j-1]\theta(n_j)\big\}\,\mathcal{C}_i\,\mathcal{A}^\dagger{}_k\,|\vec{n}-2_j\rangle + \\
&+n_k\theta(n_j)\delta_{ik}\big\{\theta(q-n_i)-\theta(q-n_i+1)\big\}\,|\vec{n}+1_i-1_j\rangle + \\
&+\theta(n_j)\delta_{ik}\big\{n_i\theta(q-n_i+1)-[n_i+1]\theta(q-n_i)\big\}\,\mathcal{A}^\dagger{}_k\,|\vec{n}-1_j\rangle\Big\} \\
=\sum_{ij}\pi_{ij}\Big\{& n_j\theta(q-n_i)\big\{\theta(n_j)-\theta(n_j-1)\big\}+ \\
&+\theta(q-n_i)\big\{n_j\theta(n_j-1)-[n_j-1]\theta(n_j)\big\}+ \\
&+n_i\theta(n_j)\big\{\theta(q-n_i)-\theta(q-n_i+1)\big\}+ \\
&+\theta(n_j)\big\{n_i\theta(q-n_i+1)-[n_i+1]\theta(q-n_i)\big\}\Big\}\,|\vec{n}+1_i-1_j\rangle \\
=\sum_{ij}\pi_{ij}\Big\{& n_j\theta(q-n_i)\theta(n_j)-n_j\theta(q-n_i)\theta(n_j-1)+ \\
& n_j\theta(q-n_i)\theta(n_j-1)-n_j\theta(n_j)\theta(q-n_i)+\theta(n_j)\theta(q-n_i)+ \\
& n_i\theta(q-n_i)\theta(n_j)-n_i\theta(q-n_i+1)\theta(n_j)+ \\
& n_i\theta(n_j)\theta(q-n_i+1)-n_i\theta(q-n_i)\theta(n_j)-\theta(q-n_i)\theta(n_j)\Big\}\,|\vec{n}+1_i-1_j\rangle \\
=0.&
\end{aligned}
$$

So it has been obtained that $\big[\mathcal{L}_{\text{in}},\mathcal{N}\big]=0$. Let us see the other commutator.

Commutator of $\mathcal{L}_{out}$ and $\mathcal{N}$

I choose to split Θ^q_{ij} operator, in order to make calculations easier:

$$
\Theta^q_{ij}\equiv\Theta^q_i\,\Theta_j\;:\begin{cases}\Theta^q_i\,|\vec{n}\rangle & =\theta(q-n_i)\,|\vec{n}\rangle\,,\\ \Theta_j\,|\vec{n}\rangle & =\theta(n_j)\,|\vec{n}\rangle\,,\end{cases}\qquad \forall i,j\in\{\,1,2,\ldots,M\,\}\,.
$$

The commutator between $\mathcal{L}_{out}$ and the particle number operator now reads:

$$\begin{aligned}
\big[\mathcal{L}_{out}, \mathcal{N}\big] &= \sum_{ij} \pi_{ij} \sum_{k} \big[\Theta_i^q \Theta_j, \mathcal{A}^\dagger{}_k \, \mathcal{A}_k\big] \, |\vec{n}\rangle \\
= \sum_{ij} \pi_{ij} \sum_{k} \Big\{ &\Theta_i^q \big[\Theta_j, \mathcal{A}^\dagger{}_k\big] \, \mathcal{A}_k + \Theta_i^q \, \mathcal{A}^\dagger{}_k \big[\Theta_j, \mathcal{A}_k\big] + \\
&+ \big[\Theta_i^q, \mathcal{A}^\dagger{}_k\big] \, \mathcal{A}_k \, \Theta_j + \mathcal{A}^\dagger{}_k \big[\Theta_i^q, \mathcal{A}_k\big] \Theta_j \Big\};
\end{aligned}$$

Commutators between Θ_i^q, Θ_j and $\mathcal{A}^\dagger{}_k$ give the results:

$$\begin{aligned}
\big[\Theta_i^q, \mathcal{A}^\dagger{}_k\big] \, |\vec{n}\rangle &\equiv \Theta_i^q \, \mathcal{A}^\dagger{}_k \, |\vec{n}\rangle - \mathcal{A}^\dagger{}_k \, \Theta_i^q \, |\vec{n}\rangle \\
&= \Theta_i^q \, |\vec{n} + 1_k\rangle - \theta(q - n_i) \, \mathcal{A}^\dagger{}_k \, |\vec{n}\rangle \\
&= \delta_{ik} \Big\{ \theta(q - n_i - 1) - \theta(q - n_i) \, |\vec{n} + 1_i\rangle \Big\}; \\
\big[\Theta_j, \mathcal{A}^\dagger{}_k\big] \, |\vec{n}\rangle &\equiv \Theta_j \, \mathcal{A}^\dagger{}_k \, |\vec{n}\rangle - \mathcal{A}^\dagger{}_k \, \Theta_j \, |\vec{n}\rangle \\
&= \Theta_j \, |\vec{n} + 1_k\rangle - \theta(n_j) \, \mathcal{A}^\dagger{}_k \, |\vec{n}\rangle \\
&= \delta_{jk} \Big\{ \theta(n_j + 1) - \theta(n_j) \Big\} \, |\vec{n} + 1_j\rangle \, ;
\end{aligned}$$

while those involving $\mathcal{A}_k$ are:

$$\begin{aligned}
\big[\Theta_i^q, \mathcal{A}_k\big] \, |\vec{n}\rangle &\equiv \Theta_i^q \, \mathcal{A}_k \, |\vec{n}\rangle - \mathcal{A}_k \, \Theta_i^q \, |\vec{n}\rangle \\
&= \Theta_i^q n_k \, |\vec{n} - 1_k\rangle - \theta(q - n_i) \, \mathcal{A}_k \, |\vec{n}\rangle \\
&= \delta_{ik} \Big\{ \theta(q - n_i - 1) - \theta(q - n_i) n_i \, |\vec{n} - +1_i\rangle \Big\}; \\
\big[\Theta_j, \mathcal{A}_k\big] \, |\vec{n}\rangle &\equiv \Theta_j \, \mathcal{A}_k \, |\vec{n}\rangle - \mathcal{A}_k \, \Theta_j \, |\vec{n}\rangle \\
&= n_k \Theta_j \, |\vec{n} - 1_k\rangle - \theta(n_j) \, \mathcal{A}_k \, |\vec{n}\rangle \\
&= \delta_{jk} \Big\{ \theta(n_j - 1) - \theta(n_j) \Big\} n_j \, |\vec{n} - 1_j\rangle \, .
\end{aligned}$$

Hence, commutator between $\mathcal{L}_{out}$ and $\mathcal{N}$ comes out to be:

$$
\begin{aligned}
\big[\mathcal{L}_{out}, \mathcal{N}\big] = \sum_{ij} \pi_{ij} \sum_{k} \Big\{ & n_k \Theta_i^q \big[\Theta_j, \mathcal{A}^\dagger{}_k\big] \left|\vec{n} - 1_k\right\rangle + \\
& \Theta_i^q\, \mathcal{A}^\dagger{}_k \big[\Theta_j, \mathcal{A}_k\big] \left|\vec{n}\right\rangle + \\
& \theta(n_j) n_k \big[\Theta_i^q, \mathcal{A}^\dagger{}_k\big] \left|\vec{n} - 1_k\right\rangle + \\
& \theta(n_j)\, \mathcal{A}^\dagger{}_k \big[\Theta_i^q, \mathcal{A}_k\big] \left|\vec{n}\right\rangle \Big\} \\
= \sum_{ij} \pi_{ij} \sum_{k} \Big\{ & n_k \delta_{jk} \big\{\theta(n_j) - \theta(n_j - 1)\big\} \Theta_i^q \left|\vec{n}\right\rangle + \\
& + n_j \delta_{jk} \big\{\theta(n_j - 1) - \theta(n_j)\big\} \Theta_i^q\, \mathcal{A}^\dagger \left|\vec{n} - 1_j\right\rangle + \\
& \theta(n_j) n_k \delta_{ik} \big\{\theta(q - n_i) - \theta(q - n_i + 1)\big\} \left|\vec{n}\right\rangle + \\
& \theta(n_j) n_i \delta_{ik} \big\{\theta(q - n_i + 1) - \theta(q - n_i)\big\}\, \mathcal{A}^\dagger{}_k \left|\vec{n} - 1_i\right\rangle \Big\} \\
= \sum_{ij} \pi_{ij} \Big\{ & n_j \theta(q - n_i) \big\{\theta(n_j) - \theta(n_j - 1)\big\} + \theta(q - n_i) n_j \big\{\theta(n_j - 1) - \theta(n_j)\big\} + \\
& + n_i \theta(n_j) \big\{\theta(q - n_i) - \theta(q - n_i + 1)\big] + n_i \theta(n_j) \big\{\theta(q - n_+ 1) - \theta(q - n_i)\big\} \Big\} \left|\vec{n}\right\rangle \\
= 0. \quad &
\end{aligned}
$$

We can therefore claim that, in our theory, the dynamics does indeed let the overall number of particles N be conserved:

$$
\big[\mathcal{L}_{in}, \mathcal{N}\big] = 0 = \big[\mathcal{L}_{out}, \mathcal{N}\big] \quad \implies \quad \big[\mathcal{L}, \mathcal{N}\big] = 0.
$$

Chapter 3

On detailed balance property

In this chapter we introduce detailed balance and give an explicit check of the satisfaction of detailed balance condition of our double threshold model.

In the simple case of single particle random walk on a good network (i.e. a network being simple, connected, undirected and non-weighted) every link of a given node has an equal probability to be passed through, dependant only on the connection degree of the departure node. Such a situation provides a first example of detailed balance, since when the steady state is achieved we have

$$\pi_j p_j = \pi_{ji} p_i,$$

meaning an equilibrium condition for every link; i.e. sitting on a link we have the same probability to see the particle passing in a direction or in the other, and we are therefore not able to distinguish a forward time-directed process from a backwards one.

In the context provided by our model, however, what we have to check is a balance term by term in the links among two network states that differs by the exchange of a particle among adjacent nodes. Hence, the detailed balance condition in the network state space reads

$$\left\langle \mathcal{L}_{in} \right\rangle_{\vec{m},\vec{n}} p_s^q(\vec{n}) = \left\langle \mathcal{L}_{in} \right\rangle_{\vec{n},\vec{m}} p_s^q(\vec{m});$$

where

$$\mathcal{L}_{in} \equiv M^{-1} \sum_{ij} \pi_{ij}\, \mathcal{C}_i\, \mathcal{B}_j,$$

$$\pi_{ij} = \frac{1_{ij}}{\psi_j},$$

$$\left|\vec{m}\right\rangle = \left|\vec{n} + 1_a - 1_b\right\rangle.$$

Calculations for the LHS read:

$$\begin{aligned}
\mathsf{LHS} &= \left\langle M\mathcal{L}_{\text{in}}\right\rangle_{\vec{m},\vec{n}} p_s^q(\vec{n}) \\
&\equiv \langle \vec{n}+1_a-1_b| \sum_{ij} \pi_{ij}\, \mathcal{C}_i\, \mathcal{B}_j\, |\vec{n}\rangle\, p_s^q(\vec{n}) \\
&= \sum_{ij} \pi_{ij}\, \langle \vec{n}+1_a-1_b \mid \vec{n}+1_i-1_j\rangle\, \theta(q-n_i)\theta(n_j)p_s^q(\vec{n}) \\
&= \sum_{ij} \pi_{ij}\delta_{ai}\delta_{bj}\theta(q-n_i)\theta(n_j)\, \langle \vec{n}+1_a-1_b \mid \vec{n}+1_a-1_b\rangle\, p_s^q(\vec{n}) \\
&= \pi_{ab}\theta(q-n_a)\theta(n_b)p_s^q(\vec{n}) = \frac{1_{ab}}{\psi_b}\theta(q-n_a)\theta(n_b)p_s^q(\vec{n}).
\end{aligned}$$

While, those for the RHS are:

$$\begin{aligned}
\mathsf{RHS} &= \left\langle M\mathcal{L}_{\text{in}}\right\rangle_{\vec{n},\vec{m}} p_s^q(\vec{m}) \\
&\equiv \langle \vec{n}| \sum_{ij} \pi_{ij}\, \mathcal{C}_i\, \mathcal{B}_j\, |\vec{n}+1_a-1_b\rangle\, p_s^q(\vec{n}+1_a-1_b) \\
&= \sum_{ij} \pi_{ij}\, \langle \vec{n} \mid \vec{n}+1_a+1_i-1_b-1_j\rangle\, \theta(q-n_i)\theta(n_j)p_s^q(\vec{n}+1_a-1_b) \\
&= \sum_{ij} \pi_{ij}\delta_{aj}\delta_{bi}\theta(q-n_i)\theta(n_j)p_s^q(\vec{n}+1_a-1_b) \\
&= \pi_{ba}\theta(q-n_b+1)\theta(n_a+1)p_s^q(\vec{n}+1_a-1_b).
\end{aligned}$$

Knowing that, as a steady distribution

- $n_k \geq 0 \quad \Longrightarrow \quad \theta(n_k+1) = 1, \qquad \forall k \in \{\, 1, 2, \ldots, M \,\},$
- $p_s^q(\vec{n}+1_a-1_b) = \dfrac{\psi_a}{\psi_b}\dfrac{\theta(n_b)\theta(q-n_a)}{\theta(q-n_b+1)}\, p_s^q(\vec{n}).$

we thus write:

$$\begin{aligned}
\mathsf{RHS} &= \pi_{ba}\theta(q-n_b+1)\theta(n_a+1)p_s^q(\vec{n}+1_a-1_b) \\
&= \pi_{ba}\theta(q-n_b+1)\frac{\psi_a}{\psi_b}\frac{\theta(n_b)\theta(q-n_a)}{\theta(q-n_b+1)}p_s^q(\vec{n}) \\
&= \frac{1_{ba}}{\psi_a}\frac{\psi_a}{\psi_b}\theta(n_b)\theta(q-n_a)\, p_s^q(\vec{n}) = \frac{1_{ab}}{\psi_b}\theta(q-n_a)\, p_s^q(\vec{n}).
\end{aligned}$$

It has been found that both sides of the supposed-so equality are actually identical:

$$\begin{aligned}
\mathsf{LHS} &= \frac{1_{ab}}{\psi_b}\, \theta(q-n_a)\theta(n_b)\, p_s^q(\vec{n}), \\
\mathsf{RHS} &= \frac{1_{ab}}{\psi_b}\, \theta(q-n_a)\theta(n_b)\, p_s^q(\vec{n}).
\end{aligned}$$

Hence, a detailed balance condition holds:

$$\left\langle \mathcal{L}_{in} \right\rangle_{\vec{m},\vec{n}} p_s^q(\vec{n}) = \left\langle \mathcal{L}_{in} \right\rangle_{\vec{n},\vec{m}} p_s^q(\vec{m}).$$

This is a very remarkable result, since it means that imposing double treshold bonds to the overall dynamics does not cause an alteration of the microscopic equilibrium of fluxes link by link.

Chapter 4

Towards a h-FTC generalization

Up to this point, we have dealt with situations involving a very limited transportation capacity on the nodes, assuming that only single particles could be transferred in a unit time. Still, it is possible to add further realism to the transport capacity of our model allowing the nodes to send more than one particle at a time, up to a certain number that will be regarded as the new transport threshold. Hence, a double generic threshold dynamical model is proposed. This ultimately leads to a generalization of the results of the previous two sections, being still theoretically possible to obtain an explicit factorized steady distribution that satisfy a microscopic detailed balance condition. Howhever, the problem of the count of the microstates could likely reveal itself to be unsurmountable.

4.1 A new dynamics

In order to account for a more generous transport capacity of the network's nodes, say $h \in \mathbb{N}$, one can replace $\mathcal{B}_k$ destruction operators with new ones defined by this peculiar action on multiparticle states, that is:

$$\mathcal{D}_j \left|\vec{n}\right\rangle \equiv \vartheta_h(n_j) \left|\vec{n} - 1_j\right\rangle ,$$

where

$$\vartheta_h(n_j) \equiv \begin{cases} n_j & \text{if} \quad n_j \leq h, \\ h & \text{if} \quad n_j > h. \end{cases}$$

This choice lets us write the evolution operator as

$$\mathcal{L}^h \equiv \frac{1}{hM} \sum_{i=1}^{M} \sum_{j=1}^{M} \pi_{ij}\, \mathcal{C}_i\, \mathcal{D}_j + \frac{1}{hM} \sum_{i=1}^{M} \sum_{j=1}^{M} \pi_{ij} \Theta_{ij}^{q,h};$$

where a new $\Theta_{ij}^{q,h}$ operator has replaced the old one to act accordingly to

$$\Theta_{ij}^{q,h} \left|\vec{n}\right\rangle = \theta(q - n_i) \vartheta_h(n_j) \left|\vec{n}\right\rangle ,$$

leading to the master equation for the evolution of $p_\varphi(\vec{n})$ distribution:

$$\begin{aligned}
\frac{\partial}{\partial t}\langle\vec{n}\,|\,\varphi_t\rangle &= \frac{1}{hM}\sum_{ij}\langle\vec{n}|\,\mathcal{C}_i\,\mathcal{D}_j\,|\varphi_t\rangle - \frac{1}{hM}\sum_{ij}\langle\vec{n}|\,\Theta_{ij}^{q,h}\,|\varphi_t\rangle \\
\Longleftrightarrow\ \partial_t\phi_\varphi(\vec{n}) &= \frac{1}{hM}\sum_{ij}\pi_{ij}\sum_{\vec{m}\in\Gamma}\langle\vec{n}|\,\mathcal{C}_i\,\mathcal{D}_j\,|\vec{m}\rangle\,p_\varphi(\vec{m})+ \\
&\quad -\frac{1}{hM}\sum_{ij}\pi_{ij}\sum_{\vec{m}\in\Gamma}\langle\vec{n}|\,\Theta_{ij}^{q,h}\,|\vec{m}\rangle\,p_\varphi(\vec{m}) \\
&= \frac{1}{hM}\sum_{ij}\pi_{ij}\sum_{\vec{m}}\vartheta_h(m_j)\theta(q-m_i)\,\langle\vec{n}\,|\,\vec{m}+1_i-1_j\rangle\,p_\varphi(\vec{m})+ \\
&\quad -\frac{1}{hM}\sum_{ij}\pi_{ij}\sum_{\vec{m}}\vartheta_h(m_j)\theta(q-m_i)\,\langle\vec{n}\,|\,\vec{m}\rangle\,p_\varphi(\vec{m}) \\
&= \frac{1}{hM}\sum_{ij}\pi_{ij}\sum_{\vec{m}}\vartheta_h(m_j)\theta(q-m_i)\,\delta^{\vec{n}}_{\vec{m}+1_i-1_j}\,p_\varphi(\vec{m})+ \\
&\quad -\frac{1}{hM}\sum_{ij}\pi_{ij}\sum_{\vec{m}}\vartheta_h(m_j)\theta(q-m_i)\,\delta^{\vec{n}}_{\vec{m}}\,p_\varphi(\vec{m});
\end{aligned}$$

that is

$$\boxed{\begin{aligned}
\frac{\partial}{\partial t}p_\varphi(\vec{n}) &= \frac{1}{hM}\sum_{ij}\pi_{ij}\vartheta_h(n_j+1)\theta(q-n_i+1)p_\phi(\vec{n}-1_i+1_j)+ \\
&\quad +\frac{1}{hM}\sum_{ij}\pi_{ij}\vartheta_h(n_j)\theta(q-n_i)p_\phi(\vec{n}).
\end{aligned}}$$

4.2 A new steady distribution

How may I write the steady distribution in this general h-FTC case? Supposing that the steady state $|\Psi_s^q\rangle$ can be defined to be:

$$|\Psi_s^q\rangle \equiv \sum_{\vec{n}\in\Gamma} C_N^{-1}(\psi)\prod_{k=1}^{M}\frac{\psi_k^{n_k}}{f_h(n_k)}\,\mathcal{C}_k\,|0\rangle\,,$$

the factorizing function f_h being deifned as:

$$f_h(n_i) = \begin{cases} n_i! & \text{if } n_i \le h, \\ h!\,h^{n_i-h} & \text{if } n_i > h. \end{cases}$$

Adding an operator $\mathcal{D}_l$ to the l-th node leads to:

$$\mathcal{D}_l \prod_{k=1}^{M} \frac{\psi_k^{n_k}}{f_h(n_k)} \mathcal{C}_k^{n_k} |0\rangle = \mathcal{D}_j \bigotimes_{k=1}^{M} \frac{\psi_k^{n_k}}{f_h(n_k)} \theta(q - n_k + 1) |n_k\rangle$$
$$= \bigotimes_{k \neq l} \frac{\psi_k^{n_k}}{f_h(n_k)} \theta(q - n_k + 1) |n_k\rangle \otimes \frac{\psi_l^{n_l}}{f_h(n_l)} \theta(q - n_l + 1) \vartheta_h(n_l) |n_l - 1\rangle ,$$

and, thanks to the properties of the f_h functions

$$f_h(n_k + 1) = \vartheta_h(n_k + 1) f_h(n_k) \quad \Longrightarrow \quad \frac{1}{f_h(n_k - 1)} = \frac{\vartheta_h(n_k)}{f_h(n_k)},$$

the eigenvalues equations for $\mathcal{L}_{in} |\Psi_s^q\rangle$ and $\mathcal{L}_{out} |\Psi_s^q\rangle$ read

$$\mathcal{L}_{in} |\Psi_s^q\rangle = \frac{1}{hM} \sum_{ij} \pi_{ij} \vartheta_h(n_i + 1) \theta(q - n_j + 1) \frac{\psi_j}{\psi_i} |\Psi_s^q\rangle ,$$
$$\mathcal{L}_{out} |\Psi_s^q\rangle = \frac{1}{hM} \sum_{ij} \pi_{ij} \vartheta_h(n_j) \theta(q - n_i) |\Psi_s^q\rangle .$$

The steady distribution appears indeed to be

$$p_s^{q,h}(\vec{m}) \equiv \langle \vec{m} \mid \Psi_s^q \rangle = C_N^{-1} \prod_{k=1}^{M} \frac{\psi_k^{m_k}}{f_h(m_k)} \theta(q - m_k + 1),$$

while adding a particle to the i-th node whilst destroying a particle on the j-th node makes the stationary distribution shift as:

$$p_s^{q,h}(\vec{n} + 1_i - 1_j) = \frac{\psi_i}{\psi_j} \frac{\theta(q - n_i)}{\vartheta_h(n_i + 1)} \frac{\vartheta_h(n_j)}{\theta(q - n_j + 1)} p_s^{q,h}(\vec{n}).$$

The condition for the probability distribution to be stationary, applied to the previously obtained master equation, reads:

$$\sum_{i=1}^{M} \sum_{j=1}^{M} \pi_{ij} \frac{\psi_j}{\psi_i} \theta(q - n_j) \vartheta_h(n_i) = \sum_{i=1}^{M} \sum_{j=1}^{M} \pi_{ij} \theta(q - n_i) \vartheta_h(n_j).$$

4.3 Does a detailed balance relation hold?

The detailed balance condition

$$\left\langle \mathcal{L}_{\text{in}}^h \right\rangle_{\vec{m}\vec{n}} p_s^q(\vec{n}) = \left\langle \mathcal{L}_{\text{in}}^h \right\rangle_{\vec{n}\vec{m}} p_s^q(\vec{m}),$$

where

$$\mathcal{L}^h_{\rm in} \equiv \frac{1}{hM}\sum_{i=1}^{M}\sum_{j=1}^{M}\pi_{ij}\,\mathcal{C}_i\,\mathcal{D}_j,$$

$$\pi_{ij} = \frac{1_{ij}}{\psi_j},$$

$$|\vec{m}\rangle \equiv |\vec{n} + 1_a - 1_b\rangle\,,$$

is checked and satisfied:

$$\begin{aligned}\mathsf{LHS} &= \left\langle hM\mathcal{L}^h_{\rm in}\right\rangle_{\vec{m}\vec{n}} p^q_s(\vec{n}) = \frac{1_{ab}}{\psi_b}\theta(q-n_a)\vartheta_h(n_b)\,p^q_s(\vec{n});\\ \mathsf{RHS} &= \left\langle hM\mathcal{L}^h_{\rm in}\right\rangle_{\vec{n}\vec{m}} p^q_s(\vec{m}) = \frac{1_{ab}}{\psi_b}\theta(q-n_a)\vartheta_h(n_b)\,p^q_s(\vec{n}).\end{aligned}$$

meaning that we still have a microscropic detailed balance on links.

Chapter 5

On the Onsager relations for the 1-FTC model

The Onsager relations may be derived from the hypotheses of the detailed balance, either by using the Einsten theory of fluctuations or alternatively the Boltzmann equation. In fact, it is shown in this chapter that similar relations follow directly from the Master equation for a time homogeneous Markov system with a finite number of states. We consider the case of the 1-FTC stochastic model of N particles that perfom random walks on a network whose nodes can send only one particle at a time, still allowing for any number of particles to stack on the same node. Using a quadratic approximate form of entropy, we derive the Onsager relations by expressing the time evolution of the system in terms of the fluctuations around the equilibrium values of certain observable physical quantities.

5.1 The quadratic approximate form of the entropy

The master equation obtained from the 1-FTC model [2] reads

$$\begin{aligned}
\partial_t p^\phi &= \sum_{i=1}^{M}\sum_{j=1}^{M} \pi_{ij}\theta(n_j+1)\theta(n_i)p^\phi(\vec{n}+1_j-1_i) - \sum_{k=1}^{M}\sum_{j=1}^{M} \pi_{kj}\theta(n_j)p^\phi(\vec{n}) \\
&= \sum_{i=1}^{M}\sum_{j=1}^{M} \Big[\pi_{ij}\theta(n_j+1)\theta(n_i)p^\phi(\vec{n}+1_j-1_i) - \pi_{ij}\theta(n_j)p^\phi(\vec{n})\Big],
\end{aligned}$$

where

$$\vec{n} \in \left\{ \vec{n} \in \mathbb{Z}^M \;\middle|\; \sum_{i=1}^{M} = N \right\}.$$

Let θ be any observable generically dependant on time. The average value of θ when computed on the probability distribution p_ϕ is

$$\left\langle \theta \right\rangle_{p_\phi} = \sum_{\vec{n}\,\in\,\Gamma}\sum_{\vec{m}\,\in\,\Gamma} \langle \vec{n}|\, \theta \,|\vec{m}\rangle \, p_\phi(\vec{m}),$$

e.g. in order to know the amount of the average number of particle stacking on the j-th node at time t one would have to write:

$$\left\langle n_j(t) \right\rangle_{p_\phi} = \sum_{\vec{n}\,\in\,\Gamma} n_j(\vec{n},t) p_\phi(\vec{n},t).$$

But how does the average value of a generic observable evolve with time?

The Gibbs entropy, in this case, reads [2] [9] [11]

$$S_G\big[p\big] = -\sum_{\vec{n}\,\in\,\Gamma} p(\vec{n},t)\ln\big[p(\vec{n},t)\big].$$

If our system is near to equilibrium we can write:

$$p(\vec{n}) = p_{eq}(\vec{n}) + \delta(\vec{n}),$$

$$\frac{\delta(\vec{n})}{p(\vec{n})} \ll 1,$$

$$\sum_{\vec{n}\,\in\,\Gamma} p(\vec{n}) = 1 \Rightarrow \sum_{\vec{n}\,\in\,\Gamma} \delta(\vec{n}) = 0.$$

Once written in the near-to-equilibrium distribution in this way, we shall expand the entropy S_G around equilibrium distribution p_{eq} in powers of $\delta_{\vec{n}}$ up to the second order, aiming to achieve a quadratic form:

$$
\begin{aligned}
S_G[p] &= -\sum_{\vec{n}} \Big(p_{eq} + \delta_{\vec{n}}\Big) \qquad \underbrace{\ln\Big(p_{eq} + \delta_{\vec{n}}\Big)}_{=\ln p_{eq} + \frac{\delta_{\vec{n}}}{p_{eq}} - \frac{\delta^2_{\vec{n}}}{p^2_{eq}} + \frac{1}{3!}\frac{\delta^3_{\vec{n}}}{p^3_{eq}} - \dots} \\
&= -\sum_{\vec{n}} \Big(p_{eq} + \delta_{\vec{n}}\Big)\Big(\ln p_{eq} + \frac{\delta_{\vec{n}}}{p_{eq}} - \frac{\delta^2_{\vec{n}}}{2p^2_{eq}} + \dots\Big) \\
&= -\sum_{\vec{n}} \Big(p_{eq}\ln p_{eq} + \delta_{\vec{n}} + \delta_{\vec{n}} + \frac{\delta^2_{\vec{n}}}{p_{eq}} - \frac{\delta^2_{\vec{n}}}{2p_{eq}} - \frac{\delta^3_{\vec{n}}}{2p_{eq}} + \dots\Big) \\
&\simeq -\sum_{\vec{n}} \Big[p_{eq}\ln p_{eq} + \delta_{\vec{n}}\ln p_{eq} + \delta_{\vec{n}} + \frac{\delta^2_{\vec{n}}}{2p_{eq}}\Big] \\
&= -\mathcal{N}_{ms} p_{eq}\ln p_{eq} - \ln p_{eq} \underbrace{\sum_{\vec{n}} \delta_{\vec{n}}}_{=0} - \underbrace{\sum_{\vec{n}} \delta_{\vec{n}}}_{=0} - \frac{1}{2p_{eq}} \sum_{\vec{n}\,\in\,\Gamma} \delta^2_{\vec{n}} \\
&= \Big\{\mathcal{N}_{ms} p_{eq}\ln p_{eq} + \frac{1}{2p_{eq}} \sum_{\vec{n}} \delta^2_{\vec{n}}\Big\} \equiv S^{\mathrm{II}}_a\big[\delta_{\vec{n}}\big].
\end{aligned}
$$

It may be easilty noticed that this approximate expression of S^{II}_a is concave, thus showing a relative maximum. This is perfectly consistent with the system's tendency to reach equilibrium.

5.2 The Onsager relations

If $q^A(\vec{n})$ if the extact value of the observable $\mathcal{Q}^A$ when the system is in the configuration $\vec{n}$, its average value reads

$$\langle q^A \rangle = \sum_{\vec{n}\,\in\,\Gamma} \mathcal{Q}^A(\vec{n})p(\vec{n}).$$

Being $p(\vec{n}) = p_{eq} + \delta(\vec{n})$ we can write the fluctuation of q^A around its equilibrium value as

$$y^A = \sum_{\vec{n}\,\in\,\Gamma} \mathcal{Q}^A(\vec{n})\delta(\vec{n}).$$

So, in order to write the variations of y^A with time as a function of the values q^A in a relatively simple manner, we would like to reduce the summations $\sum_{ij} \pi_{ij}\theta(n_i)\theta(n_j+1)$ and $\sum_{ij} \pi_{ij}\theta(n_j)$ in a symmetric form. Is it possible? It appears to be so as we recall that, being near to equilibrium, we are free to require distribution $p(\vec{n})$ we are working with

1. to be physical;
2. to satisfy detailed balance relations among links.

From the first property, it follows that $n_k \geq 0 \implies \theta(n_k+1) \geq 0$ for any k. Thus, we have to obtain a symmetry between the terms $\sum_{ij} \pi_{ij}\theta(n_i)$ and $\sum_{ji} \theta(n_i)$, that we can rewrite, after a proper reallocation of indexes, as

$$\sum_{ij} \pi_{ij}\theta(n_i), \qquad \text{and} \qquad \sum_{ji} \pi_{ji}\theta(n_i).$$

Now the request for detailed balance property come in play, allowing us to write, term by term, the detailed balance relation

$$\frac{\pi_{ij}\theta(n_i)}{\pi_{ji}\theta(n_i)} = \frac{\pi_{ij}}{\pi_{ji}} = \frac{p_i}{p_j} = \frac{d_i}{d_j},$$

that allows us to perform the transformation

$$\pi_{ij} \longrightarrow \tilde{\pi}_{ij} = \left(D^{-\frac{1}{2}}\pi D^{\frac{1}{2}}\right)_{ij} = \frac{1_{ij}}{d_j}\sqrt{\frac{d_j}{d_i}} = \frac{1_{ij}}{\sqrt{d_i d_j}},$$

wich makes the new matrix $\tilde{\pi}$ to be symmetric: $\tilde{\pi}_{ji} = \tilde{\pi}_{ij}$. Hence, we can write the evolution of fluctuations whit time as

$$\frac{\mathrm{d}}{\mathrm{d}t}y^A = \frac{\mathrm{d}}{\mathrm{d}t}\langle q^A\rangle = \sum_{ij} \delta(\vec{n})\tilde{\pi}_{ij}\Big\{q^A(\vec{n}) - q^A(\vec{n} - 1_i + 1_j)\Big\}.$$

We now wants the approximated entropy S_a^{II} to take the shape

$$\frac{\mathrm{d}}{\mathrm{d}t}S_a^{\mathrm{II}} = \sum_A \gamma_A \frac{\partial}{\partial t}y^A,$$

i.e. to be proportional to the time derivatives of the fluctuations y^A of the observables q^A. The proportionality constant γ^A will be called *thermodynamic forces*. We thus write

$$\frac{\mathrm{d}}{\mathrm{d}t}S_a^{\mathrm{II}} = \sum_A \sum_{\vec{n}\,\in\,\Gamma} \gamma^A q^A(\vec{n})\frac{\mathrm{d}}{\mathrm{d}t}\delta(\vec{n}).$$

But, since the approximated entropy is

$$S_a^{\mathrm{II}} = -\mathcal{N}_\Gamma p_{eq}\ln p_{eq} - \frac{1}{2p_{eq}}\sum_{\vec{n}\,\in\,\Gamma}\delta(\vec{n})^2,$$

then its time derivative reads

$$\frac{\mathrm{d}}{\mathrm{d}t} S_a^{\mathrm{II}} = -\frac{1}{p_{eq}} \sum_{\vec{n} \in \Gamma} \delta(\vec{n}) \frac{\mathrm{d}}{\mathrm{d}t} \delta(\vec{n}),$$

and we therefore obtain the equality

$$-\frac{1}{p_{eq}} \sum_{\vec{n} \in \Gamma} \delta(\vec{n}) \frac{\mathrm{d}}{\mathrm{d}t} \delta(\vec{n}) = \sum_{A} \sum_{\vec{n} \in \Gamma} \gamma^A q^A(\vec{n}) \frac{\mathrm{d}}{\mathrm{d}t} \delta(\vec{n});$$

that lets us write the $\delta(\vec{n})$ as functions of the thermodynamic forces γ^A:

$$\delta(\vec{n}) = -p_{eq} \sum_{A} \gamma^A q^A(\vec{n}) + \lambda,$$

λ being a constant determined by the condition $\sum_{\vec{n}} \delta(\vec{n}) = 0$. Thus, the evolution equation of the thermodynamic forces results to be:

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t} y^A &= \sum_{ij} \delta(\vec{n}) \tilde{\pi}_{ij} \Big\{ q^A(\vec{n}) - q^A(\vec{n} - 1_i + 1_j) \Big\} \\
&= \sum_{ij} p_{eq} \sum_{B} \gamma^B q^B(\vec{n}) \tilde{\pi}_{ij} \theta(n_j) \Big\{ q^A(\vec{n} - 1_i + 1_j) - q^A(\vec{n}) \Big\} \\
&= \sum_{B} \gamma^B \mathscr{L}^{B,A},
\end{aligned}$$

where

$$\mathscr{L}^{B,A} = p_{eq} \sum_{i=1}^{M} \sum_{j=1}^{M} \tilde{\pi}_{ij} \Big\{ q^B(\vec{n}) q^A(\vec{n} - 1_i + 1_j) - q^B(\vec{n}) q^A(\vec{n}) \Big\}.$$

Being $\tilde{\pi}_{ij}$ symmetric, so are the $\mathscr{L}^{A,B}$ functions:

$$\mathscr{L}^{A,B} = p_{eq} \sum_{i=1}^{M} \sum_{j=1}^{M} \tilde{\pi}_{ij} \Big\{ q^A(\vec{n}) q^B(\vec{n} - 1_i + 1_j) - q^A(\vec{n}) q^B(\vec{n}) \Big\} = \mathscr{L}^{B,A}.$$

I finally record that the equilibrium distribution p_{eq} is the 1-FTC steady distribution p_s [2]:

$$p_{eq}(\vec{n}) = p_s(\vec{n}) = C_N^{-1} \prod_{i=1}^{M} \psi_i^{n_i}.$$

Chapter 6

Derivation of the steady distribution for the q-FSC model via entropic principles

In this chapter we show how to derive the explicit form of the steady distribution p_s *in the case of the single treshold q-FSC model. This will be achieved trough a request for the Gibbs entropy to be at its relative maximum when the system is at its equilibrium steady state. Besides, the network state* $\vec{n}*$ *which maximizes the Boltzmann entropy will be given.*

The troubles in dealing with our complete double treshold model 1-FTC+q-FSC lie in the fact that one should distinguish between the probability of the microstate of the system, defined by the location of each particle, from the probability of the network state $\vec{n}$*. In other words, a usually great number of microstates does correspond to a single network state* $\vec{n}$*. The task of computing that number of corresponding microstates in the case of th double treshold model seems to be a rather impossible one to perform. Nevertheless, this could be done more easily if one accepts to treat a simplified model having the high* q *treshold only i.e. a node can store up to* q *particles only, but the transport capacity of the network is regarded as infinite, thus allowing each node to send any number of its particles at a time.*

6.1 Computing microstates

The Gibbs entropy, functional of the probability distribution $p(\vec{n})$, is defined as

$$S_G\big[p(\vec{n})\big] \equiv -\sum_{\vec{n}\,\in\,\Gamma} p(\vec{n}) \ln\left[\frac{p(\vec{n})}{\omega(\vec{n})}\right],$$

$\omega(\vec{n})$ being the number of microstates correspondig to the configuration state $\vec{n}$ of the network system. If our network has M nodes, N particles and a maximum storage capacity q on each node, then the maximum theoretical storage capacity of the whole network is qM and the overall number of *holes* (i.e. nodes' slots left empty by particles) will be

$$\overline{N} \equiv qM - N.$$

Knowing that $\overline{N}$ is fixed, we shall adopt an antiparticle point of view by writing the state $|\vec{n}\rangle = |n_1, n_2, \ldots, n_M\rangle$ as $|\overline{n_1}, \overline{n_2}, \ldots, \overline{n_M}\rangle$ and considering $\overline{\omega}(\vec{n})$ instead of $\omega(\vec{n})$, where $\overline{\omega}(\vec{n})$ is the number of microstates corresponding to the network state $\vec{n}$ from the holes point of view, given the equalities:

$$n_j + \overline{n_j} = q, \quad \forall j, \qquad \text{and} \qquad \sum_{j=1}^{M} \overline{n_j} = \overline{N} = qM - N.$$

So, how could we arrange our $qM - N$ antiparticles along N nodes? Concerning the first node (any label choice is as good as another, of course), one has $qM - N$ different choices to deploy a first antiparticles, $qM - N - 1$ choices to pick up and deploy a second one, $qM - N - 2$ with the third antiparticle and so on, up to the $\overline{n_1}$-th antiparticle, havig $qM - N - \overline{n_1} + 1$ different ways to choose it among the remnants antiparticles. So, the compute for the first node:

$$\begin{aligned}
\#_{\textit{first node}} &= \frac{(qM-N)(qM-N-1)(qM-N-2)\ldots(qM-N-\overline{n_1}+1)}{\overline{n_1}!} \\
&= \frac{(qM-N)(qM-N-1)\ldots(qM-N-\overline{n_1}+1)(qM-N-\overline{n_1})!}{\overline{n_1}!\,(qM-N-\overline{n_1})!} \\
&= \frac{(qM-N)!}{\overline{n_1}!\,(qM-N-\overline{n_1})!}.
\end{aligned}$$

Dealing with the second node, one has $(qM - N - \overline{n_1})$ different ways to choose the first antiparticle, $(qM - N - \overline{n_1} + 1)$ ways to choose a second one, up to $(qM - N - \overline{n_1} - \overline{n_2} + 1)$ possible choices regarding th $\overline{n_2}$-th antiparticle. By doing similar calculations to those of the first node, one obtains

$$\#_{\textit{second node}} = \frac{(qM-N-\overline{n_1})!}{\overline{n_2}!\,(qM-N-\overline{n_1}-\overline{n_2})!}.$$

Doing calculations for a generic k-th node, will give

$$\#_{\textit{k-th node}} = \frac{\big(qM-N-\sum_{i=1}^{k-1}\overline{n_i}!\big)!}{\overline{n_k}!\,\big(qM-N-\sum_{i=1}^{k}\overline{n_i}!\big)!},$$

up to the last M-th node where, given that $\sum_{i=1}^{M} = qM - N$ and that $0! = 1$, one has:

$$\#_{M\text{-}th\ node} = \frac{\left(qM - N - \sum_{i=1}^{M-1} \overline{n_i}!\right)!}{\overline{n_M}!\left(qM - N - \sum_{i=1}^{M} \overline{n_i}!\right)!} = \frac{\left(qM - N - \sum_{i=1}^{M-1} \overline{n_i}!\right)!}{\overline{n_M}!}.$$

Finally, by multiplying all the single node calculations one obtains

$$\begin{aligned}\overline{\omega}(\vec{n}) &= \#_{\mathit{first\ node}}\#_{\mathit{second\ node}} \cdots \#_{k\text{-}th\ node} \cdots \#_{M\text{-}th\ node}\\ &= \frac{(qM - N)!}{\overline{n_1}!\,(qM - N - \overline{n_1})!} \cdot \frac{(qM - N - \overline{n_1})!}{\overline{n_2}!\,(qM - N - \overline{n_1} - \overline{n_2})!} \cdot \\ &\cdots \frac{\left(qM - N - \sum_{i=1}^{k-1} \overline{n_i}!\right)!}{\overline{n_k}!\left(qM - N - \sum_{i=1}^{k} \overline{n_i}!\right)!} \cdots \frac{\left(qM - N - \sum_{i=1}^{M-1} \overline{n_i}!\right)!}{\overline{n_M}!}.\end{aligned}$$

With $M - 1$ pairs of factors that delete themselves out (the first half-denominator of every term against the numerator of the next one), the compute of the hole microstates comes out to be

$$\overline{\omega}(\vec{n}) = \frac{(qM - N)!}{\overline{n_1}!\,\overline{n_2}!\,\ldots\,\overline{n_M}!},$$

giving to Gibbs entropy the explicit form:

$$S_G\big[p(\vec{n})\big] = -\sum_{\vec{n}\,\in\,\Gamma} p(\vec{n}) \ln\left[\frac{p(\vec{n})}{(qM - N)!} \prod_{i=1}^{M} \overline{n_i}!\right].$$

6.2 Variational calculus for steady distribution

After having added Lagrange multiplier β_i in order to fix the average number of antiparticles on each i-th node, one obtains the functional

$$S_G\big[p(\vec{n})\big] = -\sum_{\vec{n}\,\in\,\Gamma} p(\vec{n}) \ln\left[\frac{p(\vec{n})}{(qM - N)!} \prod_{i=1}^{M} \overline{n_i}!\right] + \sum_{i=1}^{M} \beta_i \sum_{\vec{n}\,\in\,\Gamma} \overline{n_i} p(\vec{n}),$$

then, being $\delta(qM - N)! = 0$ and given that

$$\sum_{\vec{n}\,\in\,\Gamma} p(\vec{n}) = 1 \quad\implies\quad \sum_{\vec{n}\,\in\,\Gamma} \delta p(\vec{n}) = 0,$$

the stationarity of S_G functional along with variations $\delta p(\vec{n})$ reads:

$$\delta S_G\big[p(\vec{n})\big] = \sum_{\vec{n}\,\in\,\Gamma} \delta p(\vec{n}) \left\{ \ln\big[p(\vec{n})\big] + \ln\big[\overline{n_1}!\overline{n_2}! \ldots \overline{n_M}!\big] + \sum_{i=1}^{M} \beta_i \overline{n_i} \right\} = 0,$$

and implies that, since this has to happen $\forall\, \delta p(\vec{n})$ variations:

$$\ln\left[p_s(\vec{n})\prod_{i=1}^{M}\overline{n_i}!\right] = -\sum_{i=1}^{M}\beta\,\overline{n_i}$$
$$\Leftrightarrow\; p_s(\vec{n}) \propto \frac{e^{-\sum_i \beta_i \overline{n_i}}}{\prod_i \overline{n_i}!} = \frac{\prod_i e^{-\beta_i\overline{n_i}}}{\prod_i \overline{n_i}!} = \prod_{i=1}^{M}\frac{e^{-\beta_i\overline{n_i}!}}{\overline{n_i}!}.$$

So, $p_s(\vec{n})$ is factorized as

$$p_s(\vec{n}) = \prod_{i=1}^{M} p_s^i(\overline{n_i}),$$

where the single-node antiparticle distributions p_s^i are, $\forall i \in \{\,1, 2, \ldots, M\,\}$,

$$p_s^i(\overline{n_i}) \propto \frac{e^{-\beta_i\overline{n_i}}}{\overline{n_i}} = K_i\frac{e^{-\beta_i\overline{n_i}}}{\overline{n_i}}.$$

whith K_i being a proportionality constant, to fix whom one can use the normalization request

$$\sum_{\overline{n_i}=0}^{q} p_s^i(\overline{n_i}) = 1,$$

that makes K_i to be

$$K_i^{-1} = \sum_{k=0}^{q}\frac{e^{-k\beta_k}}{k!}.$$

Finally, given that $\overline{n_i} = q - n_i$, one recovers the single-node particle distribution

$$\boxed{p_s^i(n_i) = K_i\frac{e^{\beta_i(n_i-q)}}{(q-n_i)!}.}$$

6.3 Notes about the average number of antiparticles

Since we know that, if θ is any observable generally dependant on time, its average value on the probability distribution p_ϕ is

$$\langle\theta\rangle_{p_\phi} = \sum_{\vec{n}\,\in\,\Gamma}\sum_{\vec{m}\,\in\,\Gamma}\langle\vec{n}|\,\theta\,|\vec{m}\rangle\, p_\phi(\vec{m}),$$

in order to know the average number of particles stackingon the j-th node when the system is in the steady state, one has to write:

$$\langle n_j\rangle_{\Psi_s^q} \equiv \sum_{\vec{n}\,\in\,\Gamma}\langle\vec{n}|\,\mathcal{N}_j\,|\Psi_s^q\rangle = \sum_{\vec{n}\,\in\,\Gamma}\sum_{\vec{m}\,\in\,\Gamma}\langle\vec{n}|\,a_j a_j^\dagger\,|\vec{m}\rangle\, p_s^q(\vec{m})$$
$$= \sum_{\vec{n}\,\in\,\Gamma}\sum_{\vec{m}\,\in\,\Gamma} n_j\,\delta_{\vec{n}}^{\vec{m}}\, p_s^q(\vec{m}) = \sum_{\vec{n}\,\in\,\Gamma} n_j\, p_s^q(\vec{n}).$$

On that account, having written the operator number of antiparticles living on the j-th node as

$$\overline{\mathcal{N}_j} \equiv q - a_j^\dagger a_j,$$

it seems to be perfectly reasonable (and consistent to our formalism), for the sake of our entropic derivation, to have considered the average number of antiparticles on node j as

$$\langle \overline{\mathcal{N}_j} \rangle_{\Psi_s^q} = \sum_{\vec{n} \in \Gamma} \overline{n_j}\, p_s^q(\vec{n}).$$

6.4 On Boltzmann entropy maximization

Given the Boltzmann entropy

$$S_B\big[p(\vec{n})\big] \equiv -\ln\big[p(\vec{n})\big],$$

is straightforward to verify if there is a multiparticle configuration $\vec{n}_*$ which, in a steady probability distribution, maximizes S_B. We have to perform a derivative with respect to the vector $\vec{n}$ and check the configuration $\vec{n}_*$ that makes it to be equal to 0:

$$\vec{n}_* \; : \frac{\partial}{\partial \vec{n}} \ln\big[p_s(\vec{n})\big]\Big|_{\vec{n}=\vec{n}_*} = 0.$$

But, being the steady distribution factorized node-by-node as

$$p(\vec{n}) = \prod_{i=1}^{M} p_i(\overline{n_i}),$$

all we have to do is a collection of M derivatives, all of them have to be put equal to 0:

$$\frac{\partial}{\partial \overline{n_i}} \ln\bigg\{ K_i \frac{e^{-\beta_i \overline{n_i}}}{\overline{n_i}!} \bigg\}\bigg|_{\overline{n_i}=\overline{n_i}^*} = 0, \quad \forall i \in \big\{1, 2, \ldots, M\big\}.$$

So, remembering the Stirling approximate form

$$\ln \overline{n_i}! \simeq \overline{n_i} \ln \overline{n_i} - \overline{n_i},$$

we shall write:

$$\begin{aligned}
& \frac{\partial}{\partial \overline{n_i}} \big\{ \ln K_i - \beta_i \overline{n_i} - \ln \overline{n_i}! \big\}\Big|_{\overline{n_i}=\overline{n_i}^*} = 0 \\
\Longleftrightarrow \quad & \frac{\partial}{\partial \overline{n_i}} \big\{ \ln K_i - \beta_i \overline{n_i} - \overline{n_i} \ln \overline{n_i} + \overline{n_i} \big\}\Big|_{\overline{n_i}=\overline{n_i}^*} = 0 \\
& \Longleftrightarrow \quad -\beta_i - \ln \overline{n_i}^* = 0 \\
& \Longleftrightarrow \quad \overline{n_i}^* \propto e^{-\beta_i} \\
& \Longrightarrow \quad \overline{n_i}^* = C e^{-\beta_i}.
\end{aligned}$$

We can fix the normalizing constant C requiring that $\sum_i \overline{n_i}^* = qM - N$:

$$\sum_{i=1}^{M} \overline{n_i} = \sum_{i=1}^{M} C e^{-\beta_i} = C \sum_{i=1}^{M} e^{-\beta_i} = qM - N \qquad \Longrightarrow \qquad C = \frac{qM - N}{\sum_{k=1}^{M} e^{-\beta_k}}.$$

We therefore obtains

$$\overline{n_i}^* = \frac{qM - N}{\sum_{k=1}^{M} e^{-\beta_k}}\, e^{-\beta_i},$$

or, going back to a particle-centred point of view:

$$\boxed{n_i^* = q - \frac{qM - N}{\sum_{k=1}^{M} e^{-\beta_k}}\, e^{-\beta_i}.} \tag{6.1}$$

Thaks to the extreme cases:

$$\lim_{\beta_i \to 0} n_i = q - C, \quad \text{and} \quad \lim_{\beta_i \to \infty} n_i = q,$$

we shall give to the Lagrange multiplier β_i a meaning similar to that of an attractive node potential.

Conclusive remarks

The random walks on network may perhaps simulate some universal properties of transportation systems from biology to social systems. The application of physical methods to study the dynamical and statistical properties of random walks can help us to explore universal features relevant to understand stationary solutions or the rising of critical statistical states as traffic congestion.

In this thesis we studied the dynamics of N non-interacting particles on a simple, connected, undirected and non-weighted network using a field theory approach. The network state has been described by means of Fock-like states and the dynamics has been represented using suitable ladder operators.

We succeeded in demonstrate that, despite the overall dynamics have been heavily conditioned by the presence of a threshold in the nodes' transport capacity and one in the nodes' storage capacity, a condition of microscopic detailed balance still hold, allowing for the existence of an equilibrium steady distribution. Moreover, in the context of a model with only a finite transport threshold, we showed that the condition of proximity to equilibrium and the detailed balance make possible to write down the Onsager relations. Finally, in the opposite case of a model with only the finite storage capacity in play, we succeeded in computing the number of microstates corresponding to a nework state; this allowed us to write, exploiting a principle of maximum entropy at equilibrium, the explicit form of the factorized steady distribution, whence it can be easily seen the rise of the probability to have a congested node.

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