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Stochastic dynamics on infinite and finite transport capacity networks: an operatorial approach

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Abstract

Nella tesi viene studiata la dinamica stocastica di particelle non interagenti su network con capacità di trasporto finita.

L'argomento viene affrontato introducendo un formalismo operatoriale per il sistema.

Dopo averne verificato la consistenza su modelli risolvibili analiticamente, tale formalismo viene impiegato per dimostrare l'emergere di una forza entropica agente sulle particelle, dovuta alle limitazioni dinamiche del network.

Inoltre viene proposta una spiegazione qualitativa dell'effetto di attrazione reciproca tra nodi vuoti nel caso di processi sincroni.

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Chapter 1

Introduction

The validity of a physical theory is measured on one hand with its capability to predict the behaviour of the studied system, ultimately based on the individuation of the proper quantities to characterize it and of the interaction retained relevant to model their evolution; on the other hand with its generality, that is the abstraction of the theory from the particular features of the model it comes from individuating universal properties to classify it.

The traditional environment of physics is the description of natural phenomena, being its elements more easily understood as following objective rules rather than rational (thus in a certain sense non predictable) behaviours; the final aim is the comprehension of fundamental laws of nature.

Nonetheless physicists have always applied their knowledge to other fields of interest, from natural to human sciences. This is the case of complex system physics, that moves from the purpose of a comprehension of the structural universal properties of the interaction occurring among the elements of a system, rather than the nature of these interactions (that are usually completely different).

A great contribution of physics is the introduction of the statistical mechanics point of view to study the behaviour of systems with very large numbers of elements.

Although the idea of a statistical approach to such a kind of problems was already used (in social science for example), statistical mechanics introduces a way to model the dynamic evolution of the macro variables of the system, providing a connection between the microscopic and the macroscopic dynamics.

The price to obtain handable (i.e. useful) equations can be the unavoidable (over?) simplification of the problems at stake, therefore the comparison with empirical datas remains a fundamental point; but the advantage is the

effectiveness in find and explain large scale and collective phenomena [18], [19].

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.

In light of these considerations results clear the progress constituted by the introduction of graph theory to represent the network of interaction occurring in the systems.

The origin of graph theory has to be dated back to a real world network, with the Königsberg bridges problem solved by Euler (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 otherwise unaccountable effects (by means of trivial topologies such as lattices). Complex networks became in the 90's a large-scale studied topic [10].

The taxonomy of network theory is nowadays impressive and continuously growing, under many approaches.

One of the principal approaches is focused on the network itself and its structures.

The introduction of the concept of random graphs and the idea of networks as dynamical systems themselves, established a first connection with statistical mechanics and ensembles theory. It provides fruitful applications that range from biology (metabolic reaction in cellular networks are modeled by means on directed sparse graph [17]), to genetics (weighted graph [10]), epidemiology (a great improvement in models was achieved by Vespignani using uncorrelated random networks [10]), and many others.

This thesis can be framed in a different approach to connect physics and graph theory: the placement of dynamical systems, free particles or interacting agents, on networks.

The underlying network can be variably relegated to assume a background role, for example in many traffic models or percolation on porous media [16], or a primary one (many models indeed consider agents co-evolving with the network[10]).

It is worth stressing that the distinction of these approaches is far from being sharp, since random walk and graph theory are deeply related already at an abstract level. Fictitious random walks can be employed to explore the

structural properties of a graph, but can equally well represent one-particle processes of real world physical entities.

In this thesis we study the stationary states of random walks on network with a finite transportation capacity of the nodes.

Our main result is to develop an operatorial formalism to describe this kind of classical systems. The operatorial formalism is applied to give a direct proof of the inequality of synchronous and subsequent particle exchanges on the network, and a qualitatively estimate of the effects arising from this inequality.

We work with undirected networks, taken for simplicity connected. The network is given once and does not change during the evolution of the system; in this sense it doesn't have a proper dynamics and acts like a background.

Our focus is on the effects over the stationary distribution determined by changes in dynamics rules: how many particles can move per node and how many particles can move per time-step. In particular we study the steady states of a infinite transport capacity network and of a finite transport capacity network.

This work is based on the definition of a second quantization like formalism.

We take advantages of the operatorial commutation rules provided by the formalism to account of the non-commutativity of particle exchanges on the network.

In the presented models we assume particles conservation; however the extension of the theory to non conservative processes is straightforward and the Fock formalism, in order to work with variable number of particles, seems to be even more convenient.

In the first part of the thesis we define the operatorial formalism defining the network states and the dynamical operators.

We apply the latter to the case of N identical particles performing independent random walks on an infinite transport capacity network. The dynamics is approximated with a single particle exchange among nodes, and the well known steady distribution is correctly recovered.

The same model is then applied to a more realistic finite (one particle) transport capacity network. Again we succeed in recovering the expected steady state; furthermore we understand the shape of the distribution as the effect of an entropic force.

In the second part of the thesis we compare the differences occurring in a dynamics based on subsequent double exchanges of particles among nodes

and in a dynamics based on synchronous double exchanges of particles among nodes, studying the steady states.

In the infinite transport capacity case we find that the steady distribution remains unaltered in both situations, and equal to the single-exchange dynamics.

In the finite transport capacity case we prove that a synchronous dynamics modifies the stationary distribution of the network, as indicated by numerical simulations [1]. In order to pertubatively study the steady state we relate the evolution operator of the synchronous dynamics to the evolution operator of the subsequent dynamics, by means of two operators representing the corrections.

Finally we show that an estimate of the correction effects can explain the over-expression of network states with empty couples of node reported by numerical simulations.

The study developed in the thesis is quite abstract and we do not propose a specific application example.

The initial assumption of non-interacting particles could seem an over simplification proper of a toy model, but many chaotic processes can be well represented as random walks (e.g. routing packets in internet traffic [10]).

The random walks on network may simulate some universal properties of transportation systems from biology [17] to social systems [18], in order to understand the stationary solutions or the rising of critical states like congestion.

In particular, since one of the principal results obtained concernes the enhancement of stationary probabilities for boundary states (i.e. with empty nodes), this suggests an application in traffic models.

Traffic models indeed are interested in the optimization of flows minimizing disutilities (congestion). This kind of systems are naturally implemented on networks, in particular with finite transport capacity limitations [15].

The obtained results for a single step and a double step dynamics is understood as an entropic force acting among empty nodes, and seems to be related to the number of synchronous events occurred in the system.

The extension of the mechanism to more involved models should generate interesting consequences if the number of coupled empty nodes is related to a phase transition (as congestion for example). In such a case the number of synchronous events could be the order parameter of the system.

Chapter 2

Networks and random walks

In this section we introduce the topics that constitute the framework of the thesis: random walk and networks.

We give a brief overview of the principal definitions and define the main parameters of interest in dynamical models described by means of random walk on graph.

In particular we relate this parameters to the spectral properties of the underlying graph, providing in this way a method to perform algebraic calculations to bound the parameters.

We shall prove the principal results that we will employ in the rest of the thesis.

2.1 Markov chains, graphs and random walk on network

A random walk can be represented as a Markov chain: a stochastic process whose evolution depends solely on the present state and not on the past [9].

From a mathematical point of view, given a probability space $\mathcal{E}$, a measurable space $\mathcal{X}$, and a totally ordered set $\mathcal{I}$, a stochastic process is a collection of $\mathcal{X}$-valued random variables on $\mathcal{E}$ labeled by $\mathcal{I}$:

$$\mathcal{P} = \{ x_t \mid x_t \in \mathcal{X}, t \in \mathcal{I} \}$$

If the set $\mathcal{X}$ is finite the stochastic process is said to be finite and its variable can take a finite number of values.

We refer to the index t as the time of the process, that evolves assigning different values to x_t and x_{t+1} from the set of the states $\mathcal{X}$ according to some probability distribution.

The stochastic process assigns a transition probability to every possible change of variable value. We write the transition probability to evolve from the state s to the state k as P_{ks}. We have a Markov chain if:

$$\begin{aligned} &Prob(x_{t+1} = k \,|\, x_t = s, x_{t-1} = s_{t-1} \dots x_{t_0} = s_0) \\ &\quad = Prob(x_{t+1} = k \,|\, x_t = s) \;=\; P_{ks}(t) \\ &\qquad \text{where} \quad k, s, s_{t-1}, \dots, s_0 \in \mathcal{X} \end{aligned}$$

The conditional probabilities $Prob(x_{t+1} = k \,|\, x_t = s)$ do not involve $s_0 \dots s_{t-1}$, that represents the absence of memory of the process.

If transition probabilities do not depend on t the Markov chain is said to be homogeneous.

We can define a $N \times N$ (where N is the number of possible states in $\mathcal{X}$) matrix P, called transition matrix, understanding the indexes of P_{ks} as row and column indexes.

Transition matrix P is a stochastic matrix:

$$\sum_k P_{ks} \;=\; 1 \qquad P_{ks} \geq 0 \qquad \forall k, s \;\in\; \mathcal{X}$$

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

$$\exists\, n \geq 1 \;\in \mathbb{N} \quad : \quad (P^n)_{ks} \;> 0$$

Two states k, s are said to be equivalent iff :

$$\exists\, n, m \geq 1 \;\in \mathbb{N} \quad : \quad (P^n)_{ks} \;> 0 \quad (P^m)_{ks} \;> 0$$

and have all their states in one equivalence class.

An irreducible Markov chain is a Markov chain whose transition matrix is irreducible.

For the time evolution of the Markov chain described by the transition matrix the Chapman-Kolmogorov equation holds

$$(P^n)_{ij} \;=\; \sum_k (P^{n-t})_{ik}\, (P^t)_{kj} \qquad t = 1, \dots, n-1 \tag{2.1.1}$$

In what follow we will use discrete state variables. However, for continuous state variables, fundamental equations of the Markov process read:

$$
\begin{aligned}
Prob(x_2, t_2) &= \int dx_1 P(x_2, t_2|x_1, t_1) Prob(x_1, t_1) \\
P(x_3, t_3|x_1, t_1) &= \int dx_2 P(x_3, t_3|x_2, t_2) P(x_2, t_2|x_1, t_1) \qquad , \quad t_1 < t_2 < t_3
\end{aligned}
$$

Proceeding with matrix notation we will employ now on the Dirac notation, representing column vectors with the *ket* symbol $|\,\rangle$ and row vectors with the *bra* symbol $\langle\,|$. The scalar product of the vector space is represented by the contraction of *bra-ket* $\langle\,|\,\rangle$.

The probability distribution of x_t can be arranged in a column vector (in the literature it is sometimes used the convention of expressing the distribution as a row vector)

$$
\begin{aligned}
|p(t)\rangle &:= \{\, p_i(t) = Prob(x_t = s_i) \,\}_{i \in \mathcal{X}} \\
|p(t+1)\rangle &= P\ |p(t)\rangle = P^t\ |p(0)\rangle
\end{aligned}
$$

We say that Markov chain is stationary iff it is time homogeneous and has 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 transition matrix P with eigenvalue 1 :

$$
P\ |p_s\rangle = 1\ |p_s\rangle \qquad \text{with} \quad \langle i\,|p_s\rangle \geq 0\, \forall i
$$

Since P is a stochastic matrix it always has an eigenvalue 1. Indeed condition $\sum_i P_{ij} = 1$ in matrix notation reads

$$
\langle 1|\ P = \langle 1|
$$

where $\langle 1|$ is a row vector of 1 entries.

Remark: the positivity of the right eigenvector is not guaranteed.

We proceed introducing networks as formally defined mathematical structures [9], using therefore the mathematical term "graph" instead of network.

Let $\mathcal{G}$ be a finite set , *adjacency* is a binary relation on $\mathcal{G}$

$$
v \backsim u \qquad v \in V,\, u \in U \quad V, U \subseteq \mathcal{G}
$$

Adjacency defines a collection of ordered pairs $E \subseteq V \times U$.

We identify the graph as $G(V, E)$, where $V \subseteq \mathcal{G}$ is the set of identical elements called vertices (nodes), and $E \subseteq V \times V$ is a collection of pairs of elements called edges (links), defined by adjacency relation.

Graphs are usually represented by diagrams, drawing vertices as points and edges as lines connecting the points related by adjacency.

It is worth to introduce some further notions and definitions.

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.

The dual graph $\mathcal{L}_G$ of G is a graph created drawing a vertex for every edge of G, and connecting two vertices of $\mathcal{L}_G$ if the corresponding edges in G are incident on the same vertex.

In this thesis we work with undirected graphs, that means relation (2.1) is symmetric. Otherwise graphs are said to be oriented.

moreover we consider only simple graph, which means that no loops (a vertex connected to itself) nor multiple edges are allowed.

A path is an alternating sequence of adjacent vertices and edges with no repeated vertices [10].

Graphs are naturally represented by matrices, indeed to every graph can be associated an adjacency operator $\mathcal{A}$.

Let $\mathcal{F}(V) : V \to \mathbb{R}$ the vector space of real functions on V, and $\{ e_i \}_{i=1}^{M}$ its canonical orthonormal basis , where $|V| = M$ is the number of vertices.

The inner product of $f, g \in \mathcal{F}(V)$ is

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

A is a $M \times M$ square matrix representing, with respect to the canonical basis, the adjacency operator defined by

$$(\mathcal{A}f)(i) = \sum_{(j,i)} f(j) \qquad f \in \mathcal{F}(A), \quad (j, i) \in E$$

Once the vertices of G are enumerated, $\mathcal{A}$ is uniquely defined - and so is A - up to permutation of rows and columns.

The adjacency matrix of a simple graph is a symmetric matrix with entries: $A_{ij} = 1$ if $i \smile j \in E$, 0 otherwise (including $i = j$). In such a case we will write $A_{ij} \equiv 1_{ij}$.

The special case of a complete graph has an adjacency matrix with all 1 off diagonal.

The degree of a vertex i is the number of edges attached to it, formally defined as

$$d_i \;=\; \sum_j A_{ij} \;=\; card\,\{\; j \in V : i \smile j \;\}$$

For a regular graph $d_i = const \quad \forall\, i \in V$.

Let $G(V, E)$ be a graph and create an ordered sequence of nodes as follows: given a starting node i, $v_0 = i$, choose at random one node adjacent to it and assign $v_1 = j$, then choose at random a node adjacent to j, and so on.

This is a random walk on a graph. Clearly a random walk on a graph is a finite Markov chain on the set of nodes of the graph. Moreover every Markov chain can be viewed as a random walk on a graph [3].

The case of interest for our work is the random walk on an undirected graph.

The undirected feature of the graph is related to the time-reversibility of the Markov chain: the random walk considered backwards is a random walks. In terms of the stationary distribution this property corresponds to detailed balance, as we will see in detail.

Most of the fundamental properties of a random walk are determined by the properties of the underlying graph, therefore the spectral analysis of the latter provides a useful tool to obtain quantity and bounds on the main parameters of the walk. We discuss this point in more detail later, following the work of Chung [4] and Lovasz [3].

The random walk induces on the nodes a probability distribution that we represent as a column vector with components

$$p_i(t) \;=\; Prob(v_t = i) \qquad i \;=\; 1 \ldots M$$

The transition probabilities are the entries of the $M \times M$ matrix P where M is the number of the nodes.

We will deal mostly with undirected and connected graphs. In such cases at every time step the random walker chooses a link of the node to go through with equal probability. Therefore

$$(P)_{ij} \;=\; \pi_{ij} \;=\; \frac{1_{ij}}{d_j} \tag{2.1.2}$$

The transition matrix P is related to the adjacency matrix A of the underlying graph by the relation

$$P = D^{-1} A \tag{2.1.3}$$
$$\text{where} \quad D = diag(d_1 \dots d_M) \tag{2.1.4}$$

The graph theory provides also the concept of weighted graph, where adjacency matrix is substituted with affinity matrix W that assign to every edge a weight w_{ij}.

Vertex degree of a weighted graph is

$$d_i = \sum_j w_{ij}$$

and the transition probabilities read

$$(P)_{ij} = \pi_{ij} = \frac{w_{ij}}{d_j} \tag{2.1.5}$$

The introduction of the link weights provides a useful way to describe systems where not all the path are equivalent for the random walker.

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

$$|p(t)\rangle = P^t \, |p(0)\rangle$$

The steady distribution of (2.1.2), induced by a random walk on the undirected connected graph $G(V, E)$, reads

$$p^s(i) = \frac{d_i}{2m} \qquad |E| = m \tag{2.1.6}$$

arranged in the column vector $|p_s\rangle$ of components $p_i = \langle i \, | p \rangle$

Indeed it is immediate to see that

$$\sum_j \pi_{ij} \, p_j^s = \sum_j \frac{1_{ij}}{d_j} \frac{d_j}{2m} = \frac{d_i}{2m} \tag{2.1.7}$$

Furthermore (2.1.6) is unique (being the graph connected).

The system always converges to its steady state as we demonstrate in the next section.

The steady state satisfies a detailed balance condition

$$\pi_{ij}\, p_j^s \;=\; \pi_{ji}\, p_i^s \qquad \forall i,j \;\in\; V \tag{2.1.8}$$

meaning the frequency of the step $i \to j$ is equal to the $j \to i$ one.

In terms of the Markov chain this is equivalent to the time-reversibility of the stochastic process and in terms of the graph to the unweighted connected nature of it.

In our work the 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.

The quantitative study of random walks on graphs usually refers to measures defined as [3]:

- H_{ij} hitting time, written as an $M \times M$ matrix such that its entries represents the expected number of steps to go from j to i
- $\kappa_{ij} \;=\; H_{ij} + H_{ji}$ commute time
- cover time, the expected number of steps to visit every node
- $\mu \;=\; \lim_{t\to\infty} \sup \max_{ij} |\pi_{ij}(t) \;-\; p_s(j)|^{\frac{1}{t}}$, mixing rate

Mixing rate is a measure of the rate of convergence to the steady state in the following sense: $\pi_{ij}(t)$ is the probability to be at node i starting from an arbitrary node j after t steps, thus $|\pi_{ij}(t) \;-\; p_s(j)|$ is the "distance" of this probability from the stationary distribution after t steps.

Many applications of the theory of random walk on graph, in particular in computer science and complex systems, are based on the bounds of these parameters, that for this reason become topics of great interest [11], [12].

In the following section we study the spectral properties of the graph underlying the random walk, reporting in this perspective some remarkable expression for the above defined parameters.

2.2 Spectral properties

Spectral graph theory is a branch of graph theory that, studying the spectra of a graph and its invariants, allows to determine many structural features of the graph itself.

Since its very beginning, this discipline has been developed by mathematicians studing adjacency matrices, in particular those of regular and symmetric graphs, with algebraic methods.

The understanding of many possible interconnections of spectral graph theory with other branches, not only within mathematics (in particular differential geometry [4]), but also in theoretical physics (Hamiltonian systems), chemistry (stability of molecules), computational theory and many other, has been a great stimulus in the develop of this subject beyond its original area.

As sketched above, random walks and graph theory are deeply related subjects, since many of the properties of the random walk can be expressed and bounded using results of the spectral graph analysis applied to transition matrix.

In order to study spectral properties of transition matrices we follow [4] in what concerns the graph spectre, since it uses a "general and normalized form of eigenvalues" suitable for stochastic processes, emphasizing the application to relevant parameters of random walk.

Let $G(V, E)$, with $|V| = M$ and $|E| = m$, be a graph, and let P be the transition matrix of a random walk on G.

As well known, P is in general non-symmetric, nonetheless we can say that its M eigenvalues are all real.

To prove this statement it is useful to resort to the definition of laplacian $\mathcal{L}$ matrix as

$$L = D - A = \begin{pmatrix} d_1 & & \\ & \ddots & \\ & & d_M \end{pmatrix} - \begin{pmatrix} 0 & 1_{1j} & \\ & \ddots & \\ 1_{Mj} & & 0 \end{pmatrix} = \begin{pmatrix} d_1 & -1_{1j} & \\ & \ddots & \\ -1_{Mj} & & d_M \end{pmatrix}$$

$$\mathcal{L} = D^{-\frac{1}{2}} L D^{-\frac{1}{2}} = I - D^{-\frac{1}{2}} A D^{-\frac{1}{2}} = \begin{pmatrix} 1 & & -\frac{1_{1j}}{\sqrt{d_1 d_j}} \\ & \ddots & \\ -\frac{1_{Mj}}{\sqrt{d_M d_j}} & & 1 \end{pmatrix} \tag{2.2.1}$$

D is a diagonal matrix and the connection matrix A is symmetric , so clearly are L and $\mathcal{L}$. Now since $P = AD^{-1}$ follow the relations :

$$\begin{aligned} P &= D^{\frac{1}{2}}(I - \mathcal{L})D^{-\frac{1}{2}} \\ \mathcal{L} &= I - D^{-\frac{1}{2}} P D^{\frac{1}{2}} \end{aligned} \tag{2.2.2}$$

The strategy is to work with the symmetric matrix $\mathcal{L}$ and its eigenvalues, applying then the obtained results to P.

Being $\mathcal{L}$ symmetric it has M real eigenvalues. Taking an eigenvector $|v\rangle$ with λ eigenvalue:

$$\begin{aligned}
\langle v|\mathcal{L}|v\rangle &= \lambda\langle v|v\rangle \\
\langle v|D^{-\frac{1}{2}}\, L\, D^{-\frac{1}{2}}\,|v\rangle &= \lambda\langle v|v\rangle \\
\langle f|L|f\rangle &= \lambda\langle D^{\frac{1}{2}}v|D^{\frac{1}{2}}v\rangle \quad \text{where} |f\rangle = D^{-\frac{1}{2}}|v\rangle \\
\lambda = \frac{\sum_{ij}\{f_i(d_i\delta_{ij})f_j - f_i(1_{ij})f_j\}}{\sum_i f_i^2 d_i} &= \frac{\sum_i f_i^2 d_i \,-\, \sum_{(i,j)} 2f_i f_j}{\sum_i f_i^2 d_i} = \\
\frac{\sum_{(i,j)} 2f_i^2 d_i \,-\sum_{(i,j)}(f_i - f_j)^2}{\sum_i f_i^2 d_i} &= \frac{\sum_{(i,j)}(f_i - f_j)^2}{\sum_i f_i^2 d_i}
\end{aligned} \tag{2.2.3}$$

Equation (2.2.3) proofs that $\lambda \geq 0$. Furthermore is easy to see that $\lambda = 0$ is a solution of the equation, with $f_i = const$. So we can label eigenvalues as $0 = \lambda_0 \leq \lambda_1 \cdots \leq \lambda_{M-1}$, and we write the spectral decomposition

$$\mathcal{L} = \sum_k \lambda_k |v^k\rangle\langle v^k| \tag{2.2.4}$$

If the graph is connected it holds

$$\lambda_0 < \lambda_1 \tag{2.2.5}$$

It is immediate from the computation of $\mathcal{L}$ trace to prove that

$$\sum_i \lambda_i \,\leq\, M \tag{2.2.6}$$

with the equality holding iff the graph has no isolated vertices.

From the latter and keeping in mind the labeling order of λ_i and $\lambda_0 = 0$ follows

$$(M-1)\,\lambda_1 \,\leq\, \sum_{i=1}^{M-1} \lambda_i \,\leq\, M \,\Rightarrow\, \lambda_1 \leq \frac{M}{M-1} \tag{2.2.7}$$

Furthermore equation (2.2.3) fixes the upper bound

$$\lambda_{M-1} \leq 2 \tag{2.2.8}$$

indeed in general $(f(x)-f(y))^2 \leq 2(f(x)^2+f(y)^2$, and properly treating the sum over links

$$\begin{aligned} \sum_{(i,j)}(f_i-f_j)^2 \;\leq\; 2\sum_{(i,j)}(f_i^2+f_j^2) \;=\; 2\sum_i\sum_j 1_{ij}\, f_i^2 \;=\; 2\sum_i f_i^2 d_i \\ \text{thus} \quad \frac{\sum_{(i,j)}(f_i^k-f_j^k)^2}{\sum_i (f_i^k)^2 d_i} \;=\; \lambda_k \;\leq\; \lambda_{M-1} \;\leq\; 2 \end{aligned} \tag{2.2.9}$$

We proceed employing relation (2.2.2) to obtain information about P eigenvalues :

$$\begin{aligned} \langle v^k|\mathcal{L}|v^k\rangle &= \lambda_k\langle v^k|v^k\rangle \\ \langle v^k|I-\; D^{-\frac{1}{2}}\, P\, D^{\frac{1}{2}}|v^k\rangle &= \lambda_k\langle v^k|v^k\rangle \\ \langle v^k|D^{-\frac{1}{2}}\, P\, D^{\frac{1}{2}}|v^k\rangle &= (1-\lambda_k)\langle v^k|v^k\rangle \\ \langle D^{-\frac{1}{2}}v^k|P|D^{\frac{1}{2}}v^k\rangle &= (1-\lambda_k)\langle D^{-\frac{1}{2}}v^k|D^{\frac{1}{2}}v^k\rangle \\ \langle \chi^k|P|\psi^k\rangle &= (1-\lambda_k)\langle \chi^k|\psi^k\rangle \end{aligned} \tag{2.2.10}$$

Thus P has M real eigenvalues

$$\begin{aligned} \phi_k &= 1-\lambda_k \\ |\phi_k| &\leq 1 \quad \text{due to (2.2.8)} \\ \text{with} \quad 1 &= \phi_0 \geq \phi_1 \cdots \geq \phi_{V-1} \end{aligned} \tag{2.2.11}$$

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

$$P = \sum_k \phi_k\, |\psi^k\rangle\langle\chi^k| \tag{2.2.12}$$

Remark: in case of an isolated node we take $(D)_{ii}^{-1}=0$ to avoid problems.

Of particular interest is the maximum eigenvalue $1=\phi_0$, which corresponds to the steady state for the random walk of a single particle. Indeed ϕ_0 corresponds to $\lambda_0=0$ and:

$$f_i^0 = const \quad v_i^0 \propto \sqrt{d_i} \quad \psi_i^0 \propto d_i \quad \chi_i^0 = const \tag{2.2.13}$$

When P acts on a M-dimensional vector space, that is the case of the random walk of a single particle on the network, the entries $\psi_i^0 = \langle i|\psi^0\rangle$

are the probabilities of the steady distribution. In such a case we can use normalization condition to write:

$$\begin{aligned} \sum_i \psi_i^0 = 1 \Rightarrow \psi_i^0 = \frac{d_i}{2m} \\ \sum_i (P)_{ij} = 1 \Rightarrow \chi_i = 1 \end{aligned} \tag{2.2.14}$$

For an ergodic network any initial probability distribution converges to the steady state, in the long time limit.

Necessary and sufficient conditions for ergodicity are to be connected and non bipartite. These can be written for the laplacian eigenvalues as :

1. $\lambda_1 > 0$
2. $|\lambda_{M-1}| < 2$

and for the eigenvalues of transition matrix as:

$$\max_{i>0} |\phi_i| \ < \ 1 \tag{2.2.15}$$

To proof the convergence to stationary distribution we employ the eigenvectors as a base of the $M - dimensional$ vector space, $I = \sum_k \phi_k |\psi_k\rangle\langle\chi_k|$, thus we have for any initial state $|f(0)\rangle$:

$$\begin{aligned} |f(t)\rangle = \quad & P^t \, |f(0)\rangle = \sum_{k=0}^{M-1} \phi_k^t \, |\psi_k\rangle\langle\chi_k|f(0)\rangle \\ = \quad & |\psi_0\rangle\langle\chi_0|f(0)\rangle + \sum_{k=1}^{M-1} \phi_k^t \, |\psi_k\rangle\langle\chi_k|f(0)\rangle \quad \overset{t\to\infty}{\longrightarrow} \quad |\psi_0\rangle \end{aligned} \tag{2.2.16}$$

where we have used that $|\phi_{i\neq 0}| < 1$ and that $\langle\chi_0|f(0)\rangle = \sum_{i=1}^{M} f_i(0) = 1$ since it is a probability distribution.

This result is of great relevance in dynamical models on network, since it guarantees the relaxation to steady state from the spectral properties of the graph.

Moreover, we can relate the relaxing time scale to the second eigenvalue of the transition matrix.

Writing the "distance" from the steady state as:

$$\begin{aligned}\epsilon \;=\; |p_s - f(t)| \;=\; ||\,|\psi_0\rangle \;-\; (|\psi_0\rangle\langle\chi_0|f(0)\rangle \;+\; \sum_{k=1}^{M-1} \phi_k^t\,|\psi_k\rangle\langle\chi_k|f(0)\rangle)\,|| \;= \\ = \;||\sum_{k=1}^{V-1} \phi_k^t\, f(\chi_k)\,|\psi_k\rangle\,|| \;\leq\; |\phi_1|^t\,||\sum_{k=1}^{M-1} f(\chi_k)\,|\psi_k\rangle\,|| \\ \leq\; |\phi_1|^t \;\simeq\; e^{-\phi_1 t}\end{aligned} \tag{2.2.17}$$

where $\phi_1 \;=\; \max\{|\phi_1|, |\phi_k|\}$. We can estimate the relaxing time scale as $\tau_r \sim -log\,\phi_1$.

From its very definition mixing rate is therefore ϕ_1.

An interesting result of stochastic matrices theory is that we are able to write a matrix that transforms P into a symmetric P' [1].

Indeed if we consider the transformation matrix $D^{-\frac{1}{2}}$ we obtain

$$\begin{aligned}|v'\rangle \;&=\; D^{-\frac{1}{2}}\,|v\rangle \\ P' \;&=\; D^{-\frac{1}{2}}\,P\,D^{\frac{1}{2}} \;=\; I \;-\; \mathcal{L}\end{aligned} \tag{2.2.18}$$

Remark: $D^{-\frac{1}{2}}$ matrix is symmetric (diagonal) but not unitary, so what we obtain on the scalar product is:

$$\langle v'|v'\rangle \;=\; \langle v|D\,v\rangle \equiv \langle v| * |v\rangle \tag{2.2.19}$$

It is clear that P' has the same eigenvalues as P, and the same right eigenvectors.

However P' is symmetric and its left eigenvectors are just the transposed of rights one.

Symmetry property of P', that corresponds to symmetry property of $\mathcal{L}$, is connected to the satisfaction of detailed balance condition by P.

To see this let S be a generic stochastic matrix, we define the adjoint operator S^* of S respect the $*$ scalar product as

$$\begin{aligned}S^* \;&=\; (D^{-1}\,S\,D)^T \\ \langle u| * |S\,v\rangle \;&=\; \langle S^* u| * |v\rangle\end{aligned} \tag{2.2.20}$$

and S self-adjoint means $S \;=\; D\,S^T\,D^{-1}$.

Then any random dynamics associated to stochastic matrix S satisfies detailed balance condition iff S is self-adjoint.

Indeed S^* has the same steady state $|v\rangle$ of S (this is true even if S not self-adjoint), with $v_i = D_{ii}$, and

$$S_{ij}\, v_j \;=\; S_{ji}\, v_i \qquad \Longleftrightarrow \qquad v_i^{-1}\, S_{ij}\, v_j \;=\; S_{ji} \tag{2.2.21}$$

Back to the transition matrix of an unweighted network this transformation in explicit form reads

$$\begin{aligned} (P')_{ij} \;&= (D^{-\frac{1}{2}}\, P\, D^{\frac{1}{2}})_{ij} \;=\; \pi_{ij}\sqrt{\frac{d_j}{d_i}} \;=\; \frac{1_{ij}}{\sqrt{d_i d_j}} \\ \langle v^k|\, P'\, |v^k\rangle \;&=\; \phi_k \;=\; \langle \chi^k|P|\psi^k\rangle \\ &\text{with} \quad v_i^k = \frac{1}{\sqrt{d_i}}\, \phi_i^k \end{aligned} \tag{2.2.22}$$

and spectral decomposition of P' reads

$$P' = \sum_k \phi_k\, |v^k\rangle\langle v^k| \tag{2.2.23}$$

Since P' is symmetric can be written as a diagonal matrix with eigenvalues as entries using a transformation matrix U built with eigenvectors:

$$\begin{aligned} \Pi &= \begin{pmatrix} \psi_0 & & \\ & \ddots & \\ & & \psi_M \end{pmatrix} = U^{-1} P' U \\ U &= |v^1\rangle \otimes \cdots \otimes |v^V\rangle = \begin{pmatrix} v_1^1 & v_1^2 & \cdots \\ v_2^1 & v_2^2 & \cdots \\ \vdots & & \end{pmatrix} \end{aligned} \tag{2.2.24}$$

Spectral decomposition of P' is used by Lovasz to write a spectral version of hitting and commute time, that is

$$\begin{aligned} H_{st} \;&=\; 2m \sum_{k=2}^{M} \frac{1}{1-\phi_k} \left(\frac{(v_t^k)^2}{d_t} \;-\; \frac{v_s^k v_t^k}{\sqrt{d_s d_t}}\right) \\ \kappa_{st} \;&=\; 2m \sum_{k=2}^{M} \frac{1}{1-\phi_k} \left(\frac{v_t^k}{\sqrt{d_t}} \;-\; \frac{v_s^k}{\sqrt{d_s}}\right)^2 \end{aligned} \tag{2.2.25}$$

First formula allows to simply demonstrate that "more distant target are more difficult to reach" [3].

Furthermore using (2.2.11) to write $\frac{1}{2} \leq \frac{1}{1-\phi_k} \leq \frac{1}{1-\phi_1}$ and $\langle v^k | \, | v^p \rangle = \delta_{kp}$ the second spectral formula provides an upper and a lower bound for the commute time

$$m(\frac{1}{d_s} + \frac{1}{d_t}) \leq \kappa_{st} \leq \frac{2m}{1-\phi_1}(\frac{1}{d_s} + \frac{1}{d_t})$$

We recognize in the latter the quantity $\phi_0 - \phi_1 = 1 - \phi_1$, called spectral gap, that is also related to relaxation time of the system ($\log(\phi_1) \simeq (1 - \phi_1)^{-1}$)) and therefore assumes a particular importance in spectral theory.

The bounds of the mixing rate with the spectral gap is one of the most employed results of eigenvalue connection with the relevant parameters of random walk on networks.

The advantage of this approach is the possibility to obtain quantitative information on the dynamics by means of algebraic calculus.

Nonetheless, it is worth mentioning the difficulty in eigenvalue computation for exponential large graphs, a fact that shows the possible applicative limits of this method and requires different approaches [3].

Chapter 3

Non-interacting particles on infinite transport capacity networks

In this section we define the operatorial formalism that will be employed to describe the system and its dynamics.

In order to prove its consistency we apply it to the analytically solvable situation of N random walks on an infinite transport capacity networks, recovering the expected steady state.

Finally, we see how the stationary distribution can also be obtained from a maximal entropy principle (in the Gibbs sense).

We are interested in the stochastic dynamics on networks, where at this stage we consider the underlying network as a good graph (connected and undirected), thinking about applications to physical systems or other kinds of applicative tasks.

From this point of view we prefer to speak of particles, understood as random walkers, and to use terminology of network theory rather than the graph one.

To our scopes we have to extend the theory of a single particle performing a random walk on the network to N particles performing independent random walks.

We approach the problem in an operatorial way, adopting many-body quantum mechanical formalism to describe steps of the particle on the network as annihilation-creation processes among nodes.

Our definition of Hilbert space and ladder operators coincide with the Doi-Peliti formalism [6],[5].

Doi developed the idea to describe birth-death processes in classical many-body system using quantum mechanical Fock space, in particular applied with perturbative techniques to molecular dynamics of chemical reaction.

Peliti proposed a rigorous mapping of stochastic processes with discrete states space into a path integrals representation; the passage from a Master equation to an effective action opens the possibility to treat perturbatively a wide range of birth-death markovian processes, in particular those out of equilibrium.

Doi-Peliti formalism in birth- death processes take advantage of the suitable description given by Fock space of states with different dimensions.

In this work we deal with conservative processes, i.e. with fixed particle number. Therefore what we emphasize of the operatorial formalism are the commutation rules of ladder operators, that accounts of the non-commutative feature of processes depending on the degree of freedom of the particles involved.

Furthermore the point view imposed by Fock formalism is focused on a state of the whole network, and not on the particles, resulting the correct approach to study the effects on the dynamics of network transport limitations.

3.1 Network state

We study the case of N particles on a network $G(V, E)$, $|V| = M$, $|E| = m$ using a second quantization formalism to describe a classical system.

This formalism automatically gives us the indistinguishable nature of particles, is strictly connected to matrix formulation of the problem and, due to commutation rules of operators, allows to naturally point out the differences arising in the synchronous movements of particles.

Ladder operators $a_i, a_i^\dagger$ are defined for every node i of the network with usual commutation relation

$$[a_i, a_j^\dagger] = \delta_{ij} \qquad [a_i, a_j] = 0 = [a_i^\dagger, a_j^\dagger] \tag{3.1.1}$$

These operators can be thought as acting on the vectors of an infinite dimensional Fock space.

As usual we build it assuming the existence of an empty normalized state:

$$|0\rangle \equiv |0 \dots 0\rangle \qquad \text{so that} \qquad a_i|0\rangle = 0 \qquad \forall i \tag{3.1.2}$$

and then iterating the application of creation operator to vacuum:

$$(a_i^\dagger)^{n_i}|0\rangle = |n_i\rangle \quad \text{and} \quad \langle 0|(a_i)^{n_i} = \langle n_i| \tag{3.1.3}$$

This is the canonical base , centered on the single nodes of the network and on their occupation numbers.

For states representing independent particles and infinite transport capacity of the nodes the normalization is suitably defined to describe the dynamics of the network, as explicit shown further.

The action of creation/destruction on basis vectors is:

$$\begin{aligned} a_i|n_i\rangle &= n_i|n_i-1\rangle \qquad a_i^\dagger|n_i\rangle = |n_i+1\rangle \\ \langle n_i|a_i^\dagger &= n_i\langle n_i-1| \qquad \langle n_i|a_i = \langle n_i+1| \end{aligned} \tag{3.1.4}$$

Orthogonality of vectors is ensured by commutation relations. On the other hand normalization requires a little digression.

Present definition of states leads to $\langle n|n\rangle = n!\langle 0|0\rangle$, and returns a clear physical meaning. This is exactly the statistical weight of the network state, which arises from the different microscopic ways to realize the state by identical independent particles.

This weight term is the one entering in the entropy definition.

When the features of the system change (interactions, queues in nodes, etc.) this term must disappear.

Decomposition of identity reads

$$I = \sum_{\vec{n}} \frac{|\vec{n}\rangle\langle\vec{n}|}{\langle\vec{n}|\vec{n}\rangle} \tag{3.1.5}$$

where we read the normalized projector on the node occupation number base.

One of the advantages of Fock base is the existence of a number operator with number of particles as eigenvalue. To recover the correct meaning of such an operator, normalization has to be considered in expectation values, and we can use this as an example for consistency of our unusual normalization:

$$
\begin{aligned}
\frac{\langle\vec{n}|\hat{N}|\vec{n}\rangle}{\langle\vec{n}|\vec{n}\rangle} =& \frac{\langle\vec{n}|\sum_i a_i^\dagger a_i|\vec{n}\rangle}{\langle\vec{n}|\vec{n}\rangle} = \sum_i n_i \\
\text{indeed} \quad \frac{\langle n_i|a_i^\dagger a_i|n_i\rangle}{\langle n_i|n_i\rangle} =& n_i \frac{\langle n_i|a_i^\dagger|n_i-1\rangle}{\langle n_i|n_i\rangle} = n_i \frac{\langle n_i|n_i\rangle}{\langle n_i|n_i\rangle} \\
\text{or} \quad \frac{\langle n_i|a_i^\dagger a_i|n_i\rangle}{\langle n_i|n_i\rangle} =& n_i \frac{\langle n_i-1|a_i|n_i\rangle}{\langle n_i|n_i\rangle} = n_i \frac{\langle n_i|n_i\rangle}{\langle n_i|n_i\rangle} \\
\text{or} \quad \frac{\langle n_i|a_i^\dagger a_i|n_i\rangle}{\langle n_i|n_i\rangle} =& n_i^2 \frac{\langle n_i-1|n_i-1\rangle}{\langle n_i|n_i\rangle} = n_i^2 \frac{(n_i-1)!}{n_i!} \\
\text{or} \quad \frac{\langle n_i|(a_i a_i^\dagger-1)|n_i\rangle}{\langle n_i|n_i\rangle} =& \frac{\langle n_i+1|n_i+1\rangle}{\langle n_i|n_i\rangle} - \frac{\langle n_i|n_i\rangle}{\langle n_i|n_i\rangle} = n_i+1-1
\end{aligned}
\tag{3.1.6}
$$

In general expectation value of observables will obtained using the projection on a bra vector written as

$$
\frac{\langle\vec{n}|}{\langle\vec{n}|\,\vec{n}\rangle} \;=\; \frac{1}{\vec{n}!}\,\langle\vec{n}| \tag{3.1.7}
$$

where we introduce the notation $\vec{n}! \equiv n_1! n_2! \ldots n_M!$.

A generic network state can be expanded on the Fock base

$$
\begin{aligned}
&|state\rangle = \sum_{\vec{n}} \frac{|\vec{n}\rangle\langle\vec{n}|state\rangle}{\langle\vec{n}|\vec{n}\rangle} \\
&= \sum_{\{n_1 \ldots n_M\}\in\Gamma} S(n_1,\ldots,n_M) \prod_{i=1}^{M} \frac{1}{n_i!}(a_i^\dagger)^{n_i}|0\ldots0\rangle = \sum_{\Gamma} S(n_1,\ldots,n_M) \prod_{i=1}^{M} \frac{1}{n_i!}|\vec{n}\rangle \\
&\text{where} \qquad \Gamma = \{\vec{n} : \sum_{i=1}^{M} n_i = N\}
\end{aligned}
\tag{3.1.8}
$$

Latter change in the range of the sum singles out the restriction of the physical states space respect the entire Fock space, assuming conservation of particles (at this stage).

The meaning we give to the state contraction with a base vector $\langle m_1 \ldots m_V|$ is the probability to observe m_1 particles in node 1, m_2 in 2 etc., in other word to find the system in the $|\vec{m}\rangle$ state.

From this interpretation we get further condition on coefficients for the normalization of probability distribution:

$$
\begin{aligned}
p(\vec{m}) = \frac{\langle \vec{m}|stato\rangle}{\langle \vec{m}|\vec{m}\rangle} = \frac{S(\vec{m})}{\langle \vec{m}|\vec{m}\rangle} \\
\text{with} \quad \sum_{\vec{m}} \frac{|\vec{m}\rangle\langle \vec{m}|state\rangle}{\langle \vec{m}|\vec{m}\rangle} = \sum_{\vec{m}\vec{n}} \frac{S(\vec{n})}{\langle \vec{n}|\vec{n}\rangle} \frac{\langle \vec{m}|\vec{n}\rangle}{\langle \vec{m}|\vec{m}\rangle} = \\
\sum_{\vec{m}\vec{n}} \delta_{\vec{m}\vec{n}} \frac{S(\vec{n})}{\langle \vec{n}|\vec{n}\rangle} = \sum_{\vec{n}} \frac{S(\vec{n})}{\langle \vec{n}|\vec{n}\rangle} = 1
\end{aligned}
\tag{3.1.9}
$$

Latter constraint is analogue to square-integrability condition for quantum mechanical wave functions, and must be preserved by dynamics.

The functional form of $S(\vec{n})$, that is the probability distribution up to the statistical weight, depends on dynamics of particles.

In detailed balance condition S splits into product of $S_i(n_i) = S_i^{n_i}$, that is the product of single particle probability distribution on nodes. Indeed $S_i = \langle 1_i|state\rangle$ is the probability to find one particle in i-node.

A particular case is the independent particles dynamics on ITC networks. In such a case the probability distribution is the product of the steady distribution for a single particle on the network, that is $p_i = \frac{d_i}{2m} = S_i$, with the statistical weight of the configuration.

Thus

$$
p(n_1 \dots n_V) \propto \frac{S(\vec{n})}{\langle \vec{n}|\vec{n}\rangle} = \frac{1}{n_1! \dots n_V!} \prod_i (\frac{d_i}{2m})^{n_i} \tag{3.1.10}
$$

Condition (3.1.9) is then satisfied (after multiplication by $N!$) since

$$
\begin{aligned}
\sum_{\vec{n}} \frac{\langle \vec{n}|state\rangle}{\langle \vec{n}|\vec{n}\rangle} = \sum_{\vec{n}} \frac{S(\vec{n})}{\langle \vec{n}|\vec{n}\rangle} = \sum_{\vec{n}} \frac{N!}{n_1! \dots n_V!} \prod_i (\frac{d_i}{2m})^{n_i} = (\sum_i \frac{d_i}{2m})^N \\
\text{and} \sum_i \frac{d_i}{2m} = 1
\end{aligned}
\tag{3.1.11}
$$

We can give an explicit version of the steady multinomial distribution as a ket vector in the occupation number representation by means of a function generator

$$
\begin{aligned}
\hat{F}(x) &= e^{\sum_i \frac{d_i}{2m} a_i^\dagger x} \\
|multinomial\rangle &= \frac{d^N}{dx^N}\Big|_{x=0} \hat{F}(x)\,|0\rangle
\end{aligned}
\tag{3.1.12}
$$

In this writing we have used the same trick known for the coherent state where is understood the formal develop $e^{\alpha a^\dagger} = \sum_n \frac{(\alpha a^\dagger)^n}{n!}$.

3.2 Dynamics

We want to describe the dynamics of the random walks of N independent particles on the network.

The dynamics will be approximated by single particle exchanges among nodes and the conditional probabilities π_{ij} will be used to build a transition operator $\hat{P}$.

Furthermore the correspondence between Chapman-Kolmogorov equation and Master equation will be written down.

In order to properly describe the evolution of the network multiparticle states we have to build the transition operator $\hat{P}(t)$ in such a way its matrix elements return the conditional probability $p(\vec{n'}, t + \Delta t|\vec{n}, t)$.

At this stage we restrict our discussion to stationary processes, that is there is no dependence on t of the conditional probabilities.

As a matter of principles we should consider $\hat{P}$ as composed by the totality of possible processes $\Delta\vec{n}$,

$$\begin{aligned} \hat{P} &= \sum_{\Delta\vec{n}} \hat{\pi}(\Delta\vec{n}, \Delta t) \\ p(\vec{n'}|\vec{n}, \Delta t) &= \frac{1}{\vec{n'}!}\langle\vec{n'}| \sum_{\Delta\vec{n}} \hat{\pi}(\Delta\vec{n}, \Delta t)|\vec{n}\rangle \end{aligned} \tag{3.2.1}$$

where $\hat{\pi}(\Delta\vec{n}, \Delta t)$ is the operator that performs the change $\vec{n} \to \vec{n'}$, and Δt is the characteristic time of the process.

We can think to write $\Delta\vec{n}$ as a sum of contributions Δn_{ij}, movement of particles from node j to i. In such an operation we have to be careful : indeed every term Δn_{ij} must be compatible with the others, in such a way that

$$\begin{aligned} \Delta\vec{n} = \vec{n'} - \vec{n} \qquad & \sum_j \Delta n_{ij} - \Delta n_{ji} = \Delta n_i \,, \\ \text{with the costraints} \quad & \Delta n_{ij} \geq 0 \,, \\ & \sum_i \Delta n_i = 0 \end{aligned} \tag{3.2.2}$$

In some way the exchanges on the links are coupled with each others. Neglecting this coupling we can write

$$\hat{P} = \sum_{\Delta\vec{n}} \hat{\pi}(\Delta\vec{n}, \Delta t) \simeq \sum_{ij} \hat{\pi}_{ij}(\Delta n_{ij}, \Delta t) \tag{3.2.3}$$

The problem of this constraint will be overcome in the depression of multiple exchanges due to continuous limit and in the detailed balance of equilibrium states.

In order to achieve an usable form of $\hat{\pi}_{ij}$ we introduce a further simplification.

At this stage $\hat{\pi}_{ij}(\Delta n_{ij}, \Delta t)$ includes contributions of single particle movements, double particle movements, etc. For identical and non interacting particles we treat multiple, e.g. double, exchange as composed of two single particle movements. Thus

$$\begin{aligned} \pi_{ij}(\Delta n = 2) &= \pi_{ij}(\Delta n = 1, \Delta t)\pi_{ij}(\Delta n = 1, \Delta t) \sim O(\Delta t^2) \\ \hat{P} &= \sum_k \frac{1}{k!}(\sum_{ij} \pi_{ij}(\Delta n = 1))^k (\Delta t)^k \end{aligned} \tag{3.2.4}$$

and in the continuous limit $\Delta t \to 0$ we take care just of single particle contributions neglecting other events.

This assumption is stronger than the request of regularity of the process, that is the existence of the limit

$$\lim_{\Delta t \to 0} \frac{\pi_{ij}^{\Delta t} - \delta_{ij}}{\Delta t} \tag{3.2.5}$$

and is what we will use to establish the correspondence between discrete time evolution of Kolmogorov equation and continuous time evolution of Master equation.

Remark: the problem of decomposing the dynamics into single particle fundamental operations lies in the empty node case, when invariant order of operations is broken.

Knowing the probability distribution of the system we can evaluate the adequacy of this approximation, estimating the relevance of the empty node case.

In the case of the multinomial distributions for example

$$p(n_i = 0) = N! \sum_{\vec{n}} \prod_{k \neq i} \frac{p_k^{n_k}}{n_k!} = (1 - p_i)^N = (1 - \frac{p_i}{N} N)^N = (1 - \frac{\bar{n}_i}{N})^N \simeq e^{-\bar{n}_i} \tag{3.2.6}$$

thus we can see that the latter is exponential vanishing as $\bar{n}_i$ increases, but when $\bar{n}_i$ is small, as for $\frac{N}{M}$ small, $p(n_i = 0)$ matters.

Under all these considerations we are finally ready to write down $\hat{\pi}$ ($\Delta n = 1$ understood) using creation/destruction operators as the sum of one body operators acting on single particle spaces, as usual in second quantization notation.

$$\hat{\pi} = \sum_{ij} \hat{\pi}_{ij} = \sum_{ij} \pi_{ij} a_i^\dagger a_j \tag{3.2.7}$$

The $\hat{\pi}_{ij}$ component changes a state $|\dots n_i \dots n_j \dots\rangle$ to $|\dots (n_i{+}1) \dots (n_j{-}1) \dots\rangle$, and the corresponding matrix element (proportional to π_{ij}) can be interpreted as probability of the process.

Writing the explicit correspondence with classical formalism:

$$\begin{aligned} p(i \leftarrow j) &\propto \frac{\langle \dots n_i + 1 n_j - 1 \dots | \hat{\pi} | \dots n_i n_j \dots \rangle}{\langle \vec{n} + 1_i - 1_j | \vec{n} + 1_i - 1_j \rangle} \\ &= \frac{\langle \dots n_i + 1 n_j - 1 \dots | \sum_{mn} \pi_{mn} a_m^\dagger a_n | \dots n_i n_j \dots \rangle}{\langle \vec{n} + 1_i - 1_j | \vec{n} + 1_i - 1_j \rangle} \\ &= \frac{\sum_{mn} \pi_{mn} n_n \langle \dots n_i + 1 n_j - 1 \dots | \dots n_i n_j + 1_m - 1_n \dots \rangle}{\langle \vec{n} + 1_i - 1_j | \vec{n} + 1_i - 1_j \rangle} \\ &= \sum_{mn} \pi_{mn} n_n \delta_{mi} \delta_{nj} = \pi_{ij} n_j \end{aligned} \tag{3.2.8}$$

With this notation the matrix elements are not normalized as probabilities, since

$$\sum_{\vec{m}} \frac{\langle \vec{m} | \, \hat{\pi} \, | n \rangle}{\langle \vec{m} | \, \vec{m} \rangle} = \sum_{ij} \pi_{ij} n_j = N \tag{3.2.9}$$

Therefore, in order to properly understand the process as a Markov one a $\frac{1}{N}$ normalization added by hand is required. Anyway until we work with conservative processes this is not a big deal, since the number of particle is fixed in the formulation of the problem.

Remark: now is clear the reason of chosen normalization of occupation number states, since it gives the extra n_j term above, expected from classical probability. This is the direct consequence of infinite transport capacity feature: we understand the application of destruction operator $\hat{a}_j$ as the departure of a particle from the node; when we compute the probability of

such a process every particle contributes to it since the nodes has unlimited transportation capacity.

Conditions on the stochastic transition matrix are transferred on the transition matrix elements: $\sum_i \pi_{ij} = 1$, $\pi_{ij} \geq 0$.

Furtheremore we observe that we can write $\hat{\pi}$ as

$$\begin{pmatrix} a_1^\dagger & \dots & a_M^\dagger \end{pmatrix} \quad \begin{pmatrix} P \end{pmatrix} \quad \begin{pmatrix} a_1 \\ \vdots \\ a_M \end{pmatrix} \tag{3.2.10}$$

and we recover the familiar P transition matrix for a one particle random walk, establishing a correspondence between operatorial and matrix formalism and allowing this way to use all the results demonstrated in 2.2.

In particular is interesting remark that resorting to (2.2.22) we could write a self-adjoint evolution operator.

Indeed, since we know how to transform P into symmetric P', we can write a transformation matrix (it is (2.2.24)), say U, using the eigenvectors of P', and U is a transformation to get new ladder operators

$$\begin{aligned} \hat{\Pi} &= \sum_k \phi_k \, b_k^\dagger b_k \\ \begin{pmatrix} b_1 \\ \vdots \\ b_M \end{pmatrix} &= U^{-1} \begin{pmatrix} a_1 \\ \vdots \\ a_M \end{pmatrix} \end{aligned} \tag{3.2.11}$$

Is worth remarking that such a transformation would requires the complete resolution of P spectre.

Occupation number representation is suitable to see that $\hat{\pi}$ conserves particle number (i.e. it commutes with number operator)

$$\begin{aligned} [\hat{\pi}, \hat{N}] &= \sum_{i,j,k} \pi_{ij} [a_i^\dagger a_j, a_k^\dagger a_k] = \sum_{i,j,k} \pi_{ij} (a_k^\dagger [a_i^\dagger, a_k] a_j + a_i^\dagger [a_j, a_k^\dagger] a_k) = \\ &= \sum_{i,j,k} \pi_{ij} (-\delta_{ik} a_k^\dagger a_j + a_i^\dagger \delta_{jk} a_k) = 0 \end{aligned} \tag{3.2.12}$$

As already said $\hat{P}$ rules the evolution of network states in the Schrödinger representation

$$|\psi(t+\Delta t)\rangle = \hat{P}|\psi(t)\rangle = \hat{P}^t|\psi(0)\rangle \tag{3.2.13}$$

where $|\psi(0)\rangle$ is the initial condition.

Looking for probability distribution at the first order in the discrete time develop we have the Kolmogorov equation

$$\begin{aligned}
p(\vec{n'}, t+1) &= \frac{\langle n'_1 \dots n'_V|\psi(t+1)\rangle}{\langle \vec{n'}|\vec{n'}\rangle} = \frac{\langle n'_1 \dots n'_V|\hat{\pi}|\psi(t)\rangle}{\langle \vec{n'}|\vec{n'}\rangle} \\
&= \frac{1}{N}\sum_{ij}\pi_{ij}\frac{\langle n'_1 \dots n'_V|a_i^\dagger a_j|\psi(t)\rangle}{\langle \vec{n'}|\vec{n'}\rangle} \\
&= \frac{1}{N}\sum_{\vec{n}\in\Gamma}\sum_{ij}\pi_{ij}\frac{\langle n'_1 \dots n'_V|a_i^\dagger a_j|n_1 \dots n_V\rangle}{\langle \vec{n'}|\vec{n'}\rangle}\frac{\psi(\vec{n},t)}{\langle \vec{n}|\vec{n}\rangle} \\
&= \sum_{\vec{n}\in\Gamma}\delta_{\vec{n}'\vec{n}-1_j+1_i}\sum_{ij}\frac{\pi_{ij}n_j}{N}p(\vec{n},t) = \sum_{ij}\frac{\pi_{ij}(n'_j+1)}{N}p(\vec{n}'-1_i+1_j,t)
\end{aligned} \tag{3.2.14}$$

where this transition amplitude is non-null for states connected by exchange of one particle between connected nodes $\vec{n'} = \vec{n} - \hat{e_j} + \hat{e_i}$, according to previous assumption of discard multiple exchanges in the limit of short time step.

3.3 Steady eigenstate

Now we can write eigenvalue equation for the steady state (3.1.10) in order to verify that it holds employing node occupation number representation.

We remark that the dual bra eigenvector can be written as a coherent state with $\alpha_i = 1$ eigenvalue

$$\begin{aligned}
\langle\chi_0| \;&=\; \sum_{\vec{n}} \langle\vec{n}| \;\frac{1}{\vec{n}!} \;=\; \langle 0|\; e^{\sum_i a_i} \\
\text{where we understand} \quad \langle 0|\; e^{\sum_i a_i} \;&=\; (e^{\sum_i a_i^\dagger}\;|0\rangle)^\dagger
\end{aligned} \tag{3.3.1}$$

Eigenvalue equation for the steady state in the occupation number representation reads

$$
\begin{aligned}
\langle\chi_0|\hat{\pi}|\psi_0\rangle &= N\langle\chi_0|\psi_0\rangle \\
\sum_{\vec{n},\vec{n'}} \frac{\langle\chi_0|\vec{n}\rangle}{\langle\vec{n}|\vec{n}\rangle}\langle\vec{n}|\hat{\pi}|\vec{n'}\rangle\frac{\langle\vec{n'}|\psi_0\rangle}{\langle\vec{n'}|\vec{n'}\rangle} &= N\sum_{\vec{m}}\frac{\langle\chi_0|\vec{m}\rangle\langle\vec{m}|\psi_0\rangle}{\langle\vec{m}|\vec{m}\rangle} \\
\sum_{\vec{n},\vec{n'}} \frac{\chi_0(\vec{n})}{\langle\vec{n}|\vec{n}\rangle}\langle\vec{n}|\sum_{ij}\pi_{ij}a_i^\dagger a_j|\vec{n'}\rangle\frac{\psi_0(\vec{n'})}{\langle\vec{n'}|\vec{n'}\rangle} &= N\sum_{\vec{m}}\chi_0(\vec{m})\frac{\psi_0(\vec{m})}{\langle\vec{m}|\vec{m}\rangle} \\
\sum_{\vec{n},\vec{n'}}\sum_{ij}\pi_{ij}\,n'_j\,\chi_0(\vec{n})\,\frac{\langle\vec{n}|\vec{n'}-1_j+1_i\rangle}{\langle\vec{n}|\vec{n}\rangle}\,p_s(\vec{n'}) &= N\sum_{\vec{m}}\chi_0(\vec{m})\,p_s(\vec{m}) \\
\sum_{\vec{n},\vec{n'}}\sum_{ij}\pi_{ij}\,n'_j\,\chi_0(\vec{n})\,\delta(\vec{n},\,\vec{n'}-1_j+1_i)\,p_s(\vec{n'}) &= N\sum_{\vec{m}}\chi_0(\vec{m})\,p_s(\vec{m}) \\
\sum_{\vec{n}}\sum_{ij}\pi_{ij}\,(n_j+1)\,\chi_0(\vec{n})\,p_s(\vec{n}+1_j-1_i) &= N\sum_{\vec{m}}\chi_0(\vec{m})\,p_s(\vec{m}) \\
\text{inserting}\quad p_s(\vec{n}) = N!\prod_i\frac{(p_i)^{n_i}}{n_i!}\quad \text{with}\, p_i=\psi_i=\frac{d_i}{2m}\qquad &\text{and}\quad \pi_{ij}=\frac{1_{ij}}{d_j} \\
\sum_{\vec{n}}\chi_0(\vec{n})\sum_{ij}\pi_{ij}\,(n_j+1)\,\frac{p_j}{n_j+1}\frac{n_i}{p_j}\prod_i\frac{(p_i)^{n_i}}{n_i!} &= N\sum_{\vec{m}}\chi_0(\vec{m})\prod_i\frac{(p_i)^{m_i}}{m_i!} \\
\sum_{\vec{n}}\chi_0(\vec{n})\sum_{ij}\frac{1_{ij}}{d_j}\,n_i\frac{d_j}{d_i}\prod_i\frac{(p_i)^{n_i}}{n_i!} &= N\sum_{\vec{m}}\chi_0(\vec{m})\prod_i\frac{(p_i)^{m_i}}{m_i!} \\
\sum_{\vec{n}}\chi_0(\vec{n})\sum_i\frac{n_i}{d_i}\sum_j 1_{ij}\prod_i\frac{(p_i)^{n_i}}{n_i!} &= N\sum_{\vec{m}}\chi_0(\vec{m})\prod_i\frac{(p_i)^{m_i}}{m_i!} \\
\sum_{\vec{n}}\chi_0(\vec{n})\sum_i n_i\prod_i\frac{(p_i)^{n_i}}{n_i!} &= N\sum_{\vec{m}}\chi_0(\vec{m})\prod_i\frac{(p_i)^{m_i}}{m_i!}
\end{aligned}
\tag{3.3.2}
$$

We have an eigenvalue N for the steady state since $\sum_{\vec{n}}\frac{\langle\vec{n}|\hat{\pi}|m\rangle}{\langle\vec{n}|\vec{n}\rangle}=N$. When $N=1$ we recover the familiar result.

3.4 Master equation

The definition of a continuous time limit for a Markov process entails the passage to a continuous time evolution of the probability distributions described by a Master equation.

Let consider a regular Markov chain with a Chapman-Kolmogorov equation

$$p(n+\Delta n, t+\Delta t) = \sum_{\Delta n} p(n+\Delta n, t+\Delta t|n,t)\, p(n,t) \tag{3.4.1}$$

The condition of regular process means we can write

$$p(n+\Delta n, t+\Delta t|n,t) \;=\; \pi(\Delta n)\Delta t \;+\; o(\Delta t) \tag{3.4.2}$$

where $\pi(\Delta n)\Delta t$ is the transition rate, that satisfies

$$\sum_{\Delta n} \pi(\Delta n) = 1 \quad \Rightarrow \pi(0) = 1 - \sum_{\Delta n \neq 0} \pi(\Delta n) \tag{3.4.3}$$

Inserting in (3.4.1)

$$\begin{aligned} p(n+\Delta n, t+\Delta t) &= \sum_{\Delta n} \pi(\Delta n)\Delta t\, p(n,t) + \; o(\Delta t) \;= \\ &= \sum_{\Delta n \neq 0} \pi(\Delta n)\Delta t\, p(n,t) + (1 - \sum_{\Delta n \neq 0} \pi(\Delta n)\Delta t)\, p(n-\Delta n, t)\, o(\Delta t) \end{aligned} \tag{3.4.4}$$

Now we can perform the continuous time limit of the incremental ratio defining the time derivative:

$$\frac{p(n,t+\Delta t) \;-\; p(n,t)}{\Delta t} \;=\; \sum_{\substack{\Delta n \\ \Delta n \neq 0}} \pi(\Delta n) p(n-\Delta n, t) \;-\; \sum_{\substack{\Delta n \\ \Delta n \neq 0}} \pi(\Delta n) p(n,t) \;\stackrel{\Delta t \to 0}{=}\; \partial_t p(n,t) \tag{3.4.5}$$

Aiming to write the continuous time evolution equation for the operatorial formalism we begin remarking our decomposition of the dynamics into single particle exchanges entails a regularity condition that reads

$$\hat{P} \;=\; \sum_{ij} \hat{\pi}_{ij} \Delta t + o(\Delta t) \tag{3.4.6}$$

To repeat the procedure used below we have to use normalized operator according to (3.2.9).

Defining

$$\begin{aligned} \pi_{ij} &\propto 1_{ij} \\ \pi_{jj} &= 1 - \sum_i \pi_{ij} \end{aligned} \tag{3.4.7}$$

we have in occupation number representation

$$\hat{P} = \sum_{ij} [\frac{\pi_{ij}}{N} - \frac{\delta_{ij}}{N} (1 - \sum_k \pi_{kj})] \, a_i^\dagger a_j \, \Delta t + o(\Delta t) \tag{3.4.8}$$

thus

$$\frac{\partial}{\partial t} |\phi(t)\rangle = \frac{(\hat{P} - \hat{I}) \, |\phi(t)\rangle}{\Delta t \to 0} = \mathcal{L} \, |\phi(t)\rangle \tag{3.4.9}$$

and we have introduced the Laplacian linear evolution operator (also called Liouvillian for birth-death models [5])

$$\mathcal{L} = \sum_{ij} \{ \, \pi_{ij} - \delta_{ij} \sum_k \pi_{kj}) \, \} a_i^\dagger a_j \tag{3.4.10}$$

We can write the formal solution of (3.4.9)

$$|\phi(t)\rangle = e^{\mathcal{L}t} \, |\phi(0)\rangle \tag{3.4.11}$$

Looking for the expectation values of the states (the probability distribution) what we recover is the Master equation

$$\begin{aligned} \partial_t \frac{\langle \vec{n} | \phi(t) \rangle}{\langle \vec{n} | \vec{n} \rangle} &= \frac{\langle \vec{n} | \sum_{ij} (\, \pi_{ij} - \delta_{ij} \sum_k \pi_{kj}) \, a_i^\dagger a_j \, |\phi(t)\rangle}{\langle \vec{n} | \vec{n} \rangle} \\ \partial_t \, p^\phi(\vec{n}, t) &= \sum_{ij} \sum_{\vec{m}} \pi_{ij} \frac{m_j}{N} \, \delta_{\vec{n}, \, \vec{m} - 1_j + 1_i} \frac{\phi(\vec{m})}{\langle \vec{m} | \vec{m} \rangle} \quad - \sum_{kj} \pi_{kj} \frac{n_j}{N} \frac{\phi(\vec{n})}{\langle \vec{n} | \vec{n} \rangle} \\ \partial_t \, p^\phi(\vec{n}, t) &= \sum_{ij} \frac{\pi_{ij}(n_j + 1)}{N} \, \frac{\phi(\vec{n} + 1_j - 1_i)}{\langle \vec{n} + 1_j - 1_i) | \vec{n} + 1_j - 1_i) \rangle} \quad - \sum_{kj} \pi_{ki} \frac{n_j}{N} p^\phi(\vec{n}) \\ \partial_t \, p^\phi(\vec{n}, t) &= \sum_{ij} \pi_{ij} \frac{(n_j + 1)}{N} \, p^\phi(\vec{n} + 1_j - 1_i) \quad - \sum_{kj} \pi_{kj} \frac{n_j}{N} \, p^\phi(\vec{n}) \end{aligned} \tag{3.4.12}$$

One of the very useful advantages of Master equation is that we do not have to impose the normalization of operator $\hat{\pi}$ to a Markov operator, since the two right hand terms balance each other.

Only when we ask to Master equation to return a number that we want to represent a probability we have to recover proper normalization.

This feature will be fundamental in the finite transport case, when the introduction of non linear interactions among particles unable us to properly normalize the transition operator. Master equation allows us to bypass the problem.

If we think about the meaning of expectation values in node occupation representation we could also write a slightly different form of operatorial Master equation.

Indeed the time variation of the probability of a state is determined by the difference of incoming and outgoing fluxes of probability of the states. This reads

$$\begin{aligned} \partial_t \frac{\langle \vec{n}| \phi\rangle}{\langle \vec{n}|\vec{n}\rangle} &= \sum_{\vec{m}} \frac{\langle \vec{n}| \hat{\pi} |\vec{m}\rangle}{\langle \vec{n}| \vec{n}\rangle} \frac{\langle \vec{m}| \phi\rangle}{\langle \vec{m}|\vec{m}\rangle} - \sum_{\vec{m}} \frac{\langle \vec{m}| \hat{\pi} |\vec{n}\rangle}{\langle \vec{m}| \vec{m}\rangle} \frac{\langle \vec{n}| \phi\rangle}{\langle \vec{n}|\vec{n}\rangle} \\ &= \Phi_{in}(\vec{n}) \quad - \quad \Phi_{out}(\vec{n}) \end{aligned} \tag{3.4.13}$$

Assuming independence of the nodes, since we are dealing with independent particles, we can consider the distribution for every node identifying the incoming and outgoing fluxes of particles in it.

We proceed using the master equation to verify that (3.1.10) is the steady solution of (3.4.12).

$$0 = \sum_j [\sum_k \pi_{jk}(n_k + 1) p_s(\vec{n} - 1_j + 1_k, t) - \sum_i \pi_{ij} n_j p_s(\vec{n}, t)] \tag{3.4.14}$$

We can show that this holds for the multinomial distribution:

$$\frac{\langle \vec{n}|\psi_0\rangle}{\langle \vec{n}|\vec{n}\rangle} = N! \prod_i \frac{\psi_i^{n_i}}{n_i!} \tag{3.4.15}$$

Indeed

$$
\begin{aligned}
\frac{\langle \vec{n} - 1_j + 1_i | \sum_i \hat{\pi}_{ij} | \psi_0 \rangle}{\langle \vec{n'} | \vec{n'} \rangle} &= \frac{\langle \vec{n} | \sum_k \hat{\pi}_{jk} | \psi_0 \rangle}{\langle \vec{n} | \vec{n} \rangle} \\
\sum_{\vec{m}} \sum_i \frac{\langle \vec{n} - 1_j + 1_i | \vec{m} + 1_i - 1_j \rangle}{\langle \vec{n'} | \vec{n'} \rangle} \frac{1_{ij}}{d_j} (m_j) \langle \vec{m} | \psi_0 \rangle &= \sum_{\vec{m}} \sum_k \frac{\langle \vec{n} | \vec{m} - 1_k + 1_j \rangle}{\langle \vec{n} | \vec{n} \rangle} \frac{1_{jk}}{d_k} (m_k) \langle \vec{m} | \psi_0 \rangle \\
\sum_{\vec{m}} \sum_i \dots \delta_{n_i+1 m_i+1} \delta_{n_j 1 m_j - 1} \frac{1_{ij}}{d_j} (m_j) \prod_l \frac{\psi_l^{m_l}}{m_l!} &= \sum_{\vec{m}} \sum_k \dots \delta_{n_j m_j + 1} \delta_{n_k m_k - 1} \frac{1_{jk}}{d_k} (m_k) \prod_l \frac{\psi_l^{m_l}}{m_l!} \\
\sum_i \frac{1_{ij}}{d_j} (n_j) &= \sum_k \frac{1_{jk}}{d_k} (n_k + 1) \frac{\psi_k}{\psi_j} \frac{n_j}{n_k + 1} \\
\text{taking} \qquad \psi_i &= \frac{d_i}{2m} \\
(n_j) \sum_i \frac{1_{ij}}{d_j} &= \frac{n_j}{d_j} \sum_k 1_{jk} \\
d_j &= \sum_k 1_{jk}
\end{aligned}
\tag{3.4.16}
$$

Where we have introduced the explicit form for the probabilities $\pi_{ij} = \frac{1_{ij}}{d_j}$ of a non weighted undirected network. 1_{ij} are the entries of the adjacency matrix.

It is easy to see that in the steady state a continuity equation holds for the local fluxes of particles on each node, ensuring particle conservation without the need of imposing a constraint by hand; we can see an analogy with a canonical equilibrium system.

Furthermore we can also see that a detailed balance condition holds, as we will treat in detail later.

3.5 Entropy

We can study the system from a statistical mechanics point of view to show that, in the real free particles case, steady distribution can be derived from a principle of maximal entropy in the Gibbs sense [1].

Provide a maximal entropy principle will be useful in order to explain the mutual attraction of empty nodes in finite transport double step synchronous dynamics.

Gibbs entropy reads

$$\mathcal{S}_G[p] \;=\; -\sum_{\vec{n}} p(\vec{n})\,\log(p(\vec{n})) \tag{3.5.1}$$

we introduce a set of Lagrange multipliers μ_i fixing the average number of particle per node and we vary the functional in p to obtain the maximum

$$\begin{aligned}\delta\mathcal{S}_G[p] \;&=\; -\sum_{\vec{n}} \delta\{\, p(\vec{n})\,\log(p(\vec{n})\frac{n_1!\ldots n_M!}{N!}) \;-\; \sum_i \mu_i\, n_i\, p(\vec{n})\,\} \\ &=\; -\sum_{\vec{n}} \delta p(\vec{n})\{\;\log(p(\vec{n})(n_1!\ldots n_M!) \;-\; \sum_i \mu_i\, n_i\,\} \;=\; 0\end{aligned} \tag{3.5.2}$$

where we have used $\sum_{\vec{n}} p(\vec{n}) \;= 1$ thus $\sum_{\vec{n}} \delta p(\vec{n}) \;= 0$.

It is interesting to remark that the statistical weight associated to the network state $\vec{n}$, that is the number of realization of such a state by identical particles, is the multiplicity factor that results in the contraction of bra-ket occupation representation states: $\langle\vec{n}|\,|\vec{n}\rangle \;=\; \vec{n}!$

We see that the extremal condition reads

$$\begin{aligned}\log(p(\vec{n})) \;&=\; -\log(\prod_i n_i!) \;-\; \sum_i \mu_i\, n_i \\ p(\vec{n}) \;&\propto\; \frac{1}{\prod_i n_i!}\;\exp(-\sum_i \mu_i n_i)\end{aligned} \tag{3.5.3}$$

identifying $\mu_i \;=\; -\log(\psi_i)$ we recover (3.1.10).

In the equilibrium state of the system we can also approach the argument using Boltzmann entropy.

We give to μ_i the meaning of a node potential, understanding an internal system energy $E \;=\; \sum_i \mu_i n_i$.

It is straightforward to see that the configuration $\vec{n}^*$ that maximizes entropy is

$$\begin{aligned}0 \;&=\; \sum_i \frac{\partial}{\partial n_i}\,(\,\log(n_i!)) \;+\; n_i\mu_i\,) \\ &\simeq\; \sum_i \frac{\partial}{\partial n_i}\,(\,n_i\log(n_i)) \;-\, n_i \;+\; n_i\mu_i\,)\end{aligned} \tag{3.5.4}$$

thus imposing that $\sum_i n_i \;=\; N$

$$n_i^* \;=\; N\,\exp(-\mu_i) \tag{3.5.5}$$

we find the maximum microstates configuration.

Chapter 4

Finite transport capacity

In this section we introduce the non-trivial case of a finite transport capacity network.

We see that the stationary solution is the exponential distribution of a system subjected to an entropic force.

The magnitude of the force depends on the number of empty nodes of the states, and the effect is to promote network boundary states.

This is a first result of the thesis.

4.1 1-FTC

Until now we have dealt with networks with infinite transport capacity (ITC).

The practical effect of this feature is the presence of the particles number of the departure node when we compute the transition probabilities among nodes.

In real world networks is reasonable to expect finite transport capacity (FTC), thus we have to adapt our theory to such a situation.

We study the case of a network where every node can send just one particle per time step (1-FTC), that means we have to change the dynamics on the network accordingly.

The transition probability now reads

$$p(i \leftarrow j) \;=\; \pi_{ij}\,\theta(n_j) \tag{4.1.1}$$

where θ is the Heaviside step functions which is 1 when its argument is positive and 0 otherwise.

We introduce a new destruction operator $\hat{b}$ in such a way :

$$\begin{aligned} b_i\ |\vec{n}\rangle\ &=\ |\vec{n}-1_i\rangle \\ \text{and}\quad b_i\,|0\rangle\ &=\ 0 \end{aligned} \tag{4.1.2}$$

thus

$$\frac{\langle \vec{n}+1_i-1_j|\ \pi_{ij}a_i^\dagger b_j\ |\vec{n}\rangle}{\langle \vec{n}+1_i-1_j|\,\vec{n}+1_i-1_j\rangle}\ =\pi_{ij}\,\theta(n_j) \tag{4.1.3}$$

We remark that the role of the step function is executed by the action of $\hat{b}$ destruction operator, that returns a 0 when acts on the vacuum state.

As a matter of principle we can express $\hat{b}$ as a function of $\hat{a}$: $\hat{b} = b(\hat{a})$, even if we can't give an explicit expression of this functional dependence.

Commutation rules with $\hat{a}^\dagger$ are understood with application to an occupation number state and read

$$\begin{aligned} [b_i, a_j^\dagger]\,|\vec{n}\rangle\ =\ \delta_{ij}(\theta(n_i+1)-\theta(n_i))\ =\ \delta_{ij}\,(1-\theta(n_i)) \\ \text{where}\quad n_i \geq 0 \end{aligned} \tag{4.1.4}$$

The new finite transport dynamics is implemented simply substituting $\hat{a}$ destruction operators with $\hat{b}$ in all the dynamic operators.

Thus

$$\begin{aligned} \hat{\pi}\ &=\ \sum_{ij}\ \pi_{ij}\,a_i^\dagger b_j \\ \hat{\mathcal{L}}\ &=\ \sum_{ij}\ \pi_{ij}\,(a_i^\dagger b_j\ -\ a_j^\dagger b_j) \end{aligned} \tag{4.1.5}$$

Does this new dynamics conserve particle number?

I.e. $[\hat{\mathcal{L}}, \hat{N}] \stackrel{?}{=} 0$.

To answer this question we evaluate separately incoming and outgoing part of the Laplacian

$$
\begin{aligned}
[\hat{\mathcal{L}}_{in}, \hat{N}]\ |\vec{n}\rangle \ &= \sum_{ijk} \pi_{ij}\, [a_i^\dagger b_j, a_k^\dagger a_k]\ |\vec{n}\rangle \ = \sum_{ijk} \pi_{ij}\, \{\, a_i^\dagger\, [b_j, a_k^\dagger]\, a_k \ + \ a_k^\dagger\, [a_i^\dagger, a_k]\, b_j \}\ |\vec{n}\rangle \\
&= \sum_{ijk} \pi_{ij}\, \{\, a_i^\dagger\, a_k\, \delta_{jk}(1-\theta(n_j)) - \ a_k^\dagger\, b_j\, \delta_{ik}\, \}\ |\vec{n}\rangle \\
&= \sum_{ij} \pi_{ij}\, \{\, a_i^\dagger\, a_j\, (1-\theta(n_j)) - \ a_i^\dagger\, b_j\, \}\ |\vec{n}\rangle \\
&= \sum_{ij} \pi_{ij}\, \{\, n_j\, (1-\theta(n_j)) - \ \theta(n_j)\, \}\ |\vec{n} + 1_i - 1_j\rangle \\
[\hat{\mathcal{L}}_{out}, \hat{N}]\ |\vec{n}\rangle \ &= \sum_{ijk} \pi_{ij}\, [a_j^\dagger b_j, a_k^\dagger a_k]\ |\vec{n}\rangle \ = \sum_{ijk} \pi_{ij}\, \{\, a_j^\dagger\, [b_j, a_k^\dagger]\, a_k \ + \ a_k^\dagger\, [a_j^\dagger, a_k]\, b_j \}\ |\vec{n}\rangle \\
&= \sum_{ijk} \pi_{ij}\, \{\, a_j^\dagger\, a_k\, \delta_{jk}(1-\theta(n_j)) - \ a_k^\dagger\, b_j\, \delta_{jk}\, \}\ |\vec{n}\rangle \\
&= \sum_{ij} \pi_{ij}\, \{\, a_j^\dagger\, a_j\, (1-\theta(n_j)) - \ a_j^\dagger\, b_j\, \}\ |\vec{n}\rangle \\
&= \sum_{ij} \pi_{ij}\, \{\, n_j\, (1-\theta(n_j)) - \ \theta(n_j)\, \}\ |\vec{n}\rangle
\end{aligned}
\tag{4.1.6}
$$

Thus we see that even if the incoming and outgoing components of the dynamics don't commute with number operator and their commutators are different, when we evaluate their action on the vector their contributions balance each other.

Therefore we can state that this dynamics conserves particles number.

Finite transport $\hat{\pi}$ produces a Markov process iff

$$
\sum_{\vec{m}} \frac{\langle \vec{m}|\, \hat{\pi}\, |\vec{n}\rangle}{\langle \vec{m}|\, \vec{m}\rangle} = \sum_{ij} \pi_{ij}\, \theta(n_j) \ = \ 1 \tag{4.1.7}
$$

that would require a normalization $A(\vec{n}) = \textit{number of non-empty nodes}$, thus dependent on the state.

This impossibility to properly define $\hat{\pi}$ as a Markov process means we are not able to find the steady state as the eigenvector of unitary eigenvalue.

Furthermore the non vanishing commutator with number operator suggests that the occupation number representation is not the appropriate one to express $\hat{\pi}$ eigenvector.

Our evolution equation in Schrödinger representation now is

$$\frac{\partial}{\partial t}\,|\phi(t)\rangle \;=\; \mathcal{L}\;|\phi(t)\rangle \;=\; \{\sum_{ij}(\pi_{ij} \;-\; \delta_{ij}\sum_{k}\pi_{kj})a_i^\dagger b_j\,\}\;|\phi(t)\rangle \tag{4.1.8}$$

with the usual formal solution (3.4.11).

Equation (4.1.8) encloses all the equation for the probability distribution of the possible network states. By contraction with a vector basis we recover classical master equation (see [1])

$$\begin{aligned}
\partial_t p^\phi(\vec{n}) \;&=\; \frac{\partial}{\partial t}\frac{\langle\vec{n}|\,\phi(t)\rangle}{\langle\vec{n}|\,\vec{n}\rangle} \;=\; \frac{\langle\vec{n}|\sum_{ij}(\,\pi_{ij} \;-\; \delta_{ij}\;\sum_k \pi_{kj})\,a_i^\dagger b_j\,|\phi(t)\rangle}{\langle\vec{n}|\vec{n}\rangle} \\
&= \sum_{ij}\sum_{\vec{m}}\pi_{ij}\theta(m_j)\,\delta_{\vec{n},\,\vec{m}-1_j+1_i}\frac{\phi(\vec{m})}{\langle\vec{m}|\vec{m}\rangle} \quad - \sum_{kj}\pi_{kj}\,\theta(n_j)\,\frac{\phi(\vec{n})}{\langle\vec{n}|\vec{n}\rangle} \\
&= \sum_{ij}\pi_{ij}\,\theta(n_j+1)\,\theta(n_i)\,\frac{\phi(\vec{n}+1_j-1_i)}{\langle\vec{n}+1_j-1_i)|\vec{n}+1_j-1_i)\rangle} \quad - \sum_{kj}\pi_{kj}\,\theta(n_j)\,p^\phi(\vec{n}) \\
&= \sum_{ij}\pi_{ij}\theta(n_j+1)\,\theta(n_i)\,p^\phi(\vec{n}+1_j-1_i) \quad - \sum_{kj}\pi_{kj}\theta(n_j)\,p^\phi(\vec{n})
\end{aligned} \tag{4.1.9}$$

Remark: when we solve the Kronecker delta $\sum_{\vec{m}}\delta_{\vec{n},\,\vec{m}-1_j+1_i}$ imposing $\vec{n}+1_j-1_i,=\vec{m}$ we write a $\theta(n_i)$. If we extend the support of our probability function on negative integers setting $p(\dots n_i<0\dots)\equiv 0$ this is not strictly necessary, but when we write $p(\vec{n}-1_i) \;=\; \frac{1}{\psi_i}p(\vec{n})$ as we are going to do it is.

Thus $p(\vec{n}-1_i) \;=\; \frac{\theta(n_i)}{\psi_i}p(\vec{n})$

This remark is valid also in the ITC case, nonetheless the multinomial distribution lead to $p(\vec{n}-1_i) \;=\; \frac{n_i}{\psi_i}p(\vec{n})$ due to the multinomial coefficients, and the presence of n_i makes $\theta(n_i)$ redundant.

We try to write the stationary solution of (4.1.9) as $p_s(\vec{n}) \;\propto\; \prod_k \psi_k^{n_k}$ where $\sum_k n_k = N$, and

$$\sum_j \pi_{ij}\psi_j \;=\; \psi_i \tag{4.1.10}$$

Imposing (3.1.9) we have

$$
\begin{aligned}
p_s(\vec{n}) &= C_N(\psi)^{-1} \prod_k \psi_k^{n_k} \\
C_N(\psi) &= \sum_{\vec{n}} \frac{1}{N!} \frac{d^N}{dx^N}\Big|_{x=0} \prod_k \frac{1}{1-x\psi_k}
\end{aligned}
\tag{4.1.11}
$$

Inserting (4.1.11) in (4.1.9)

$$
\begin{aligned}
0 = \sum_{ij} \pi_{ij}\theta(n_j+1)\, p_s(\vec{n}+1_j-1_i) \quad &- \sum_{kj} \pi_{kj}\theta(n_j)\, p_s(\vec{n}) \\
\sum_{ij} \pi_{ij}\theta(n_j+1)\theta(n_i)\frac{\psi_j}{\psi_i}\, p_s(\vec{n}) \quad &= \sum_{kj} \pi_{kj}\theta(n_j)\, p_s(\vec{n}) \\
\sum_{ij} \pi_{ij}\theta(n_j+1)\theta(n_i)\frac{\psi_j}{\psi_i} &= \sum_{kj} \pi_{kj}\theta(n_j) \\
\sum_i \frac{\theta(n_i)}{\psi_i} \sum_j \pi_{ij}\psi_j &= \sum_{kj} \pi_{kj}\theta(n_j)
\end{aligned}
\tag{4.1.12}
$$

we see that given (4.1.10) in order to check last equality we have to be careful in the evaluation of the boundary state effects where $\theta(n_i)$ counts, i.e. for $\{\, |\vec{n}\rangle \,:\, \exists\, n_i = 0 \,\}$.

With infinite transport dynamics we didn't face this problem because of the presence of the number of particle in the nodes instead of the step function.

We can see that equality holds on the boundaries with an explicit example

$$
\begin{aligned}
\sum_{ij} \pi_{ij} p(n_1, n_2, 0, -1_i + 1_j) &= \sum_{kj} \pi_{kj}\theta(n_j)\, p(n_1, n_2, 0) \\
\sum \begin{cases} \pi_{12}p(n_1-1, n_2+1, 0) \\ \pi_{13}p(n_1-1, n_2, 1) \\ \pi_{21}p(n_1+1, n_2-1, 0) \\ \pi_{23}p(n_1, n_2-1, 1) \\ \pi_{31}p(n_1+1, n_2, -1) \\ \pi_{32}p(n_1, n_2+1, -1) \end{cases} \quad \text{forbidden} &= \sum_j \theta(n_j) p(n_1, n_2, 0) \\
\pi_{12}\frac{\psi_2}{\psi_1} + \pi_{13}\frac{\psi_3}{\psi_1} + \pi_{21}\frac{\psi_1}{\psi_2} + \pi_{23}\frac{\psi_3}{\psi_2} + \pi_{31}\frac{\psi_1}{\psi_3} + \pi_{32}\frac{\psi_2}{\psi_3} &= M - (\#\text{ of empty nodes}) \\
1 + 1 &= 3 - 1
\end{aligned}
\tag{4.1.13}
$$

In the latter we observe the problem of normalizing the process to a Markov one, indeed $\frac{1}{M}$ doesn't work on the boundaries.

Nonetheless by working with Master equation we bypass this issue balancing it in the incoming and outgoing fluxes, and we obtain a correct description of the evolution of the network state even on the boundaries.

The steady state as a vector of the Hilbert space can be explicit written in the occupation number representation as

$$|\psi_0\rangle = \sum_{\vec{n}} C_N(\psi)^{-1} \prod_i (\psi_i a_i^\dagger)^{n_i} |0\rangle \tag{4.1.14}$$

and it is straightforward recover (4.1.11) contracting with $\frac{\langle \vec{m}|}{\vec{m}!}$.

In (4.1.14) the sum runs over all $\{\vec{n} : |\vec{n}| = N\}$, because we are working with conservative random walks.

Another option would be to write the ket states as expanded on the whole infinite dimensional occupation number base, implementing then by-hand in the bra projector the selection of physical N-particle states.

As sketched before we expect that (4.1.14) is eigenstate of (4.1.8) only in the approximation of neglecting the boundary states effects.

Under this condition we find the M eigenvalue of $\hat{\mathcal{L}}_{in} |\psi_0\rangle = \hat{\pi} |\psi_0\rangle$, that corresponds to eigenstate of the normalized markovian operator with 1 eigenvalue.

Indeed

$$\begin{aligned}
\hat{\pi} |\psi_0\rangle &= M |\psi_0\rangle \\
\sum_{ij} \pi_{ij} a_i^\dagger b_j \sum_{\vec{n}} C_N(\psi)^{-1} \prod_k (\psi_k a_k^\dagger)^{n_k} |0\rangle &= M \sum_{\vec{m}} C_N(\psi)^{-1} \prod_k \psi_k^{m_k} |\vec{m}\rangle \\
\sum_{\vec{n}} C_N(\psi)^{-1} \sum_{ij} \pi_{ij} \theta(n_j) \frac{\psi_j}{\psi_i} \frac{\psi_j^{n_j-1}}{\psi_i^{n_i+1}} \prod_{k\neq i,j} \psi_k^{n_k} |\vec{n} + 1_i - 1_j\rangle &= M \sum_{\vec{m}} C_N(\psi)^{-1} \prod_k \psi_k^{m_k} |\vec{m}\rangle \\
\sum_i \frac{1}{\psi_i} \sum_j \pi_{ij} \psi_j \theta(n_j) \sum_{\vec{n}} C_N(\psi)^{-1} \prod_k \psi_k^{n'_k} |\vec{n'}\rangle &= M \sum_{\vec{m}} C_N(\psi)^{-1} \prod_k \psi_k^{m_k} |\vec{m}\rangle \\
\sum_i \frac{1}{\psi_i} \sum_j \pi_{ij} \psi_j \theta(n_j) &\sim M
\end{aligned} \tag{4.1.15}$$

Example of the boundary problem

$$\sum_{ij} \pi_{ij} a_i^\dagger b_j \left|p(n_1, n_2, 0, -1_i + 1_j)\right\rangle = M(\vec{n}) \left|p(n_1, n_2, 0)\right\rangle$$

$$\sum \begin{cases} \pi_{12} a_1^\dagger b_2 \left|p(n_1 - 1, n_2 + 1, 0)\right\rangle \\ \pi_{13} a_1^\dagger b_3 \left|p(n_1 - 1, n_2, 1)\right\rangle \\ \pi_{21} a_2^\dagger b_1 \left|p(n_1 + 1, n_2 - 1, 0)\right\rangle \\ \pi_{23} a_2^\dagger b_3 \left|p(n_1, n_2 - 1, 1)\right\rangle \\ \left.\begin{array}{l} \pi_{31} a_3^\dagger b_1 \left|p(n_1 + 1, n_2, -1)\right\rangle \\ \pi_{32} a_3^\dagger b_2 \left|p(n_1, n_2 + 1, -1)\right\rangle \end{array}\right\} \text{ forbidden} \end{cases} = M(\vec{n}) \left|p(n_1, n_2, 0)\right\rangle$$

$$\pi_{12}\frac{\psi_2}{\psi_1} + \pi_{13}\frac{\psi_3}{\psi_1} + \pi_{21}\frac{\psi_1}{\psi_2} + \pi_{23}\frac{\psi_3}{\psi_2} + \pi_{31}\frac{\psi_1}{\psi_3} + \pi_{32}\frac{\psi_2}{\psi_3} = M - (\#\text{ empty nodes}) \tag{4.1.16}$$

With the same approximation we can write

$$\begin{aligned} \hat{\mathcal{L}}_{out} \left|\psi_0\right\rangle &\sim M \left|\psi_0\right\rangle \\ \sum_{ij} \pi_{ij} a_j^\dagger b_j \left|\psi_0\right\rangle &= \sum_j a_i^\dagger b_j \sum_{\vec{n}} C_N(\psi)^{-1} \prod_k (\psi_k a_k^\dagger)^{n_k} \left|0\right\rangle = \\ \sum_{\vec{n}} C_N(\psi)^{-1} \sum_j \theta(n_j) \prod_k \psi_k^{n_k} \left|\vec{n}\right\rangle &= \sum_j \theta(n_j) \sum_{\vec{n}} C_N(\psi)^{-1} \prod_k \psi_k^{n_k} \left|\vec{n}\right\rangle \\ &= \sum_j \theta(n_j) \left|\psi_0\right\rangle \end{aligned} \tag{4.1.17}$$

Thus we see that just like the classical case the master equation approach allows to safely drop the boundary states effects, since the incoming fluxes balances the outgoing ones.

4.2 Comparison of infinite and finite transport capacity

The network states space is formed by physical and non-physical (with negative occupation number) states, and these parts of the space can't talk each other.

Every state is connected to others following the rules of particles dynamics, when we give to it the operatorial formalism operatorials rules have to

reflect constraints that avoid connection among physical and non-physical states.

This is exactly the advantage of employ Fock base and ladder (with modified normalization) operators.

Thanks to ergodic principle the system, waiting a sufficient long time, explores all the connected states of the space, that are all physical states for a good network and a single step dynamics of particle; the temporal average gives the probability weights for the steady state.

As shown the steady state for infinite transport capacity networks is a multinomial distribution: we are in the true free particles case and all distribution on single nodes are independent, centered in $\overline{n}_i = \psi_i N$.

The transition from infinite to finite transport capacity of the network results ultimately in a passage to non-free particle case, although particles remains non-interacting.

The particles of the system are still indistinguishable, indeed ladder operators are still bosonic. Nonetheless network nodes label them in the moment they decide which one moves, and this explains the necessity to define new destruction operators to describe dynamics and the change of multiplicity weights of states.

The steady distribution on the nodes changes from the multinomial to an exponential, as we lost the multinomial factor.

This transition can be thought as due to the introduction of a friction that pushes the distributions on single nodes to zero.

From the operatorial formalism point of view the core of the issue lies in the impossibility to normalize the transition oparator to unity. Indeed we have seen that natural normalization $\frac{1}{M}$ fails on boundary states where we find $\sum_i \frac{\theta(n_i)}{M} = \frac{M-n(0)}{M}$.

We can explain this situation remarking that in the true free particle case the point of view centered on the particles or on the nodes is the same, since every particle gives its contribution of probability to move. In other words, we normalize the Markov process with the total number of particles.

Finite transport dynamics consists in the possibility for every node to send only one particle, therefore the point of view is necessary centered on the nodes, and that is why the normalization of Markov process requires the number of nodes and is independent on the number of particles on the network.

This is true unless the network is in a boundary state, with an empty node.

The empty state of a node is reflected in a leak of possible moves of the network slowing down its exploration of states space.

Furthermore formal passage from Markov process to continuous time evolution is based on the subtraction of identity; when normalization fails we should change it, that means change time scales.

The net effect is like the introduction of a friction term that slows down the dynamics of the system in such states, and the permanence for a longer time in the state means an enhancement of the probability associated to it.

Chapter 5

Detailed balance

In this section we introduce detailed balance remarking its utility to study equilibrium systems. Then we give an explicit check of the satisfaction of detailed balance condition of the already studied systems.

Detailed balance in statistical mechanics is a powerful tool for the study of equilibrium systems, since it allows to study directly stationary properties even without a complete solution of the dynamics. A detailed balance condition requires not only a macroscopic equilibrium of the system, but an equilibrium at microscopic level of the processes occurring in it.

Ultimately detailed balance can be understood as the symmetry for time reversal of the dynamics, since in equilibrium condition every process should not be sensitive to the forward or backward evolution of time [7]. This indeed is the case of a configuration of the system of extremal entropy, where only reversible processes occur.

When the steady state of a system provides internal currents, although its master equation vanishes, detailed balance is not satisfied since the internal currents, although constant in time, break the time reversibility of the dynamics. This is the case of non equilibrium statistical mechanics, where we are no more able to apply a principle of maximal entropy to study the steady state of the system, and new approaches are required [20].

The simple case of single particle random walk on a network (fully connected and non-directed) assigns to every link of a given node an equal probability to be passed through, dependent only on the connection degree of the departure node.

Such a situation provides a first example of detailed balance, since when steady state is achieved we have:

$$\pi_{ij}\, p_j \;=\; \pi_{ji}\, p_i \tag{5.0.1}$$

that means 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.

5.1 ITC

Extending the theory to N identical non interacting particles if we work with ideal infinite transport capacity networks we expect nothing change, since independence of particles (not affected by network limitations) ensures independence of the N random walks and therefore detailed balance on links.

The point of view of second quantization formalism lead us to consider network state and transition among network states as the sum of all possible exchanges configuration allowed among nodes.

Therefore when we speak of detailed balance condition now we refer to a balance term by term in the links among two states, and no more among two nodes.

Detailed balance condition in the network states space reads

$$< \hat{\pi} >_{\vec{m}\vec{n}} \; p_s(\vec{n}) \; =< \hat{\pi} >_{\vec{n}\vec{m}} \; p_s(\vec{m}) \tag{5.1.1}$$

We verify that (5.1.1) holds in the steady sate of the single step dynamics, that is for (3.2.7) and (3.1.10).

Transition amplitudes are non-vanishing for connected states, in this case for states that differs in the exchange of a particle among adjacent nodes.

$$\frac{\langle \vec{n} + 1_a - 1_b | \sum_{ij} \pi_{ij} \, a_i a_j \; | \vec{n} \rangle}{\langle \vec{n} + 1_a - 1_b | \, \vec{n} + 1_a - 1_b \rangle} \, p_s(\vec{n}) \; = \; \frac{\langle \vec{n} | \sum_{ij} \pi_{ij} \, a_i a_j \; | \vec{n} + 1_a - 1_b \rangle}{\langle \vec{n} | \, \vec{n} \rangle} \, p_s(\vec{n} + 1_a - 1_b) \tag{5.1.2}$$

Right-hand side reads

$$\frac{\langle \vec{n} + 1_a - 1_b | \sum_{ij} \pi_{ij} \, a_i a_j \; | \vec{n} \rangle}{\langle \vec{n} + 1_a - 1_b | \, \vec{n} + 1_a - 1_b \rangle} \, p_s(\vec{n}) \; = \; \sum_{ij} \pi_{ij} \, n_j \, \frac{\langle \vec{n} + 1_a - 1_b | \, \vec{n} + 1_i - 1_j \rangle}{\langle \vec{n} + 1_a - 1_b | \, \vec{n} + 1_a - 1_b \rangle} \, p_s(\vec{n})$$

$$= \sum_{ij} \pi_{ij} \, n_j \delta_{ai} \delta_{bj} \, p_s(\vec{n}) \; = \; \pi_{ab} \, n_b \, p_s(\vec{n})$$

Left-hand side

$$\frac{\langle \vec{n}| \sum_{ij} \pi_{ij}\, a_i a_j \; |\vec{n} + 1_a - 1_b\rangle}{\langle \vec{n}|\, \vec{n}\rangle}\, p_s(\vec{n} + 1_a - 1_b) \; =$$
$$= \sum_{ij} \pi_{ij}\, n_j \, \frac{\langle \vec{n}|\, \vec{n} + 1_a - 1_b + 1_i - 1_j\rangle}{\langle \vec{n}|\, \vec{n}\rangle}\, p_s(\vec{n} + 1_a - 1_b)$$
$$= \sum_{ij} \pi_{ij}\, n_j\, \delta_{bi}\delta_{aj}\, p_s(\vec{n} + 1_a - 1_b) \; = \; \pi_{ba}\,(n_a + 1)\, \frac{\psi_a}{n_a + 1}\frac{n_b}{\psi_b}\, p_s(\vec{n})$$

Thus for $\pi_{ij} = \frac{1_{ij}}{\psi_j}$ and thanks to the symmetry of 1_{ij}, (5.1.1) holds as we recover the detailed balance at the network links level.

We remark that detailed balance is a stricter requirement than the global balance of fluxes entailed in the vanishing condition of Master equation, since it does not allow internal currents.

Its satisfaction is deeply related with the non-directed nature of links (resulting in the symmetry of adjacency matrix) and topological nature of link weights.

5.2 1-FTC

Dealing with FTC networks we lost the real independence of particles, since the possibility of a particle to move is conditioned by the presence of other particles in the nodes, anyway we have independence of nodes and we were able to find a real steady solution of master equation holding even on boundary states.

We verify that (5.1.1) holds in the steady sate of a 1-FTC network and a single step dynamics, that is for (4.1.5) and (4.1.14).

Transition amplitude are non-vanishing for connected states, in this case for states that differs in the exchange of a particle among adjacent nodes.

$$\frac{\langle \vec{n} + 1_a - 1_b| \sum_{ij} \pi_{ij}\, a_i b_j \; |\vec{n}\rangle}{\langle \vec{n} + 1_a - 1_b|\, \vec{n} + 1_a - 1_b\rangle}\, p_s(\vec{n}) \; = \; \frac{\langle \vec{n}| \sum_{ij} \pi_{ij}\, a_i b_j \; |\vec{n} + 1_a - 1_b\rangle}{\langle \vec{n}|\, \vec{n}\rangle}\, p_s(\vec{n} + 1_a - 1_b) \tag{5.2.1}$$

Right-hand side reads

$$\frac{\langle \vec{n} + 1_a - 1_b | \sum_{ij} \pi_{ij}\, a_i b_j \; |\vec{n}\rangle}{\langle \vec{n} + 1_a - 1_b | \, \vec{n} + 1_a - 1_b \rangle}\, p_s(\vec{n}) \;=\; \sum_{ij} \pi_{ij}\, \theta(n_j)\, \frac{\langle \vec{n} + 1_a - 1_b | \, \vec{n} + 1_i - 1_j \rangle}{\langle \vec{n} + 1_a - 1_b | \, \vec{n} + 1_a - 1_b \rangle}\, p_s(\vec{n})$$

$$= \sum_{ij} \pi_{ij}\, \theta(n_j) \delta_{ai} \delta_{bj}\, p_s(\vec{n}) \;=\; \pi_{ab}\, \theta(n_b)\, p_s(\vec{n})$$

Left-hand side

$$\frac{\langle \vec{n} | \sum_{ij} \pi_{ij}\, a_i b_j \; |\vec{n} + 1_a - 1_b\rangle}{\langle \vec{n} | \, \vec{n} \rangle}\, p_s(\vec{n} + 1_a - 1_b) \;=$$

$$= \sum_{ij} \pi_{ij}\, \theta(n_j)\, \frac{\langle \vec{n} | \, \vec{n} + 1_a - 1_b + 1_i - 1_j \rangle}{\langle \vec{n} | \, \vec{n} \rangle}\, p_s(\vec{n} + 1_a - 1_b)$$

$$= \sum_{ij} \pi_{ij}\, \theta(n_j) \delta_{bi} \delta_{aj}\, p_s(\vec{n} + 1_a - 1_b) \;=\; \pi_{ba}\, \theta(n_a + 1)\, \psi_a \frac{\theta(n_b)}{\psi_b}\, p_s(\vec{n})$$

Thus for $\pi_{ij} \;=\; \frac{1_{ij}}{\psi_j}$ and thanks to the symmetry of 1_{ij}, (5.1.1) holds.

Chapter 6

Double exchange dynamics

In this section we discuss the inequality in performing subsequent exchanges of particles among network nodes or synchronous exchanges, obtaining the main results of our work.

The transport limitation of the nodes introduces a non-linear interaction among particles.

We give an explicit proof in the case of a double exchange.

In the model with infinite transport capacity we see that the difference does not change the stationary distribution.

In the model with finite transport capacity the differences introduced by the synchronous implementation of the double exchange modify the stationary distribution and a perturbative approach seems to be necessary.

An estimate of the corrective term introduced shows a promotion in the unknown stationary distribution of states with empty adjacent nodes, differentiating it from the single exchange stationary distribution.

6.1 Double exchange dynamics on ITC networks

In the previous we have written the dynamics as a sequence of elementary single particle exchanges, imposing the rule that just one single particle is allowed to move every time step.

A diametrically opposed picture would be to let all the particles move every updating of the network state.

Since we are working with non interacting particles every single particle random walk should not be sensitive to other particle walks, and we could think that multiparticle synchronous exchange are equivalent to subsequent single particle exchanges.

Ultimately this equivalence is based on the invariance of the order of fundamental single particle processes, and turns out to be not true.

Indeed a particle exchange process is weighted depending on the state of the network. In a synchronous scenario all the exchanges performed per time step are weighted with the same network state. On the other hand a sequence of exchanges upgrade the network state after every process and therefore weights these processes on different network configurations.

In order to show this non equivalence we study the case of double particle synchronous exchange comparing it with a two subsequent single exchange process.

When the exchange of particles concerns different couples of nodes the two dynamics are equivalent. The order invariance is broken when one node both sends and receives a particle in the same process, and this can result in a different probability to observe a network state.

Comparing the two approaches to the dynamics we will find this term of double exchanges on subsequent nodes as a natural consequence of commutation rules.

We can try to visualise this situation as

$$\begin{aligned} \overset{i}{\bullet} \longrightarrow \overset{j}{\bullet} \longrightarrow \overset{l}{\bullet} \qquad &\sim \frac{n_i}{N}\,\pi_{ji}\,\frac{(n_j+1)}{N}\,\pi_{lj} \\ \\ \overset{i}{\bullet} \longrightarrow \overset{j}{\bullet} \qquad &\sim \frac{n_i}{N}\,\pi_{ji}\,\frac{n_j}{N}\,\pi_{lj} \\ \overset{j}{\bullet} \longrightarrow \overset{l}{\bullet} \end{aligned} \tag{6.1.1}$$

We can already remark that in the particular case of node j empty state the difference is stressed, since we have a process that is completely forbidden in the synchronous scenario, but not in the other one.

Similarly when we work with finite transport capacity , e.g. every node can send just one particle per time step, we expect a difference arising just in empty node case.

Let $\hat{\pi}(|\Delta\vec{n}=2|)$ be the operator that performs double particle exchanges among network couples of nodes. We compare it with the second term of the whole operator written as a develop of single exchange operators $\hat{\pi}(\Delta\vec{n}) = \sum_k \frac{(\sum_{ij}\hat{\pi}_{ij})^k}{k!}$.

In the first case we have an operator $\hat{\pi}(|\Delta\vec{n} = 2|)$ that first destroys a couple of particles, then creates a couple of particles. In the second case the operator $(\hat{\pi}(|\Delta\vec{n} = 1|))^2$ destroys a particle, creates a particle and then repeats the operation.

Second quantization formalism allows to point out the difference of these two dynamics using commutation relation.

We write $\hat{\pi}(|\Delta\vec{n} = 2|)$ as a two-body operator in the node-occupation number base.

$$\hat{\pi}(|\Delta\vec{n} = 2|) = \sum_{ijkl} V_{ikjl} a_i^\dagger a_k^\dagger a_j a_l = \sum_{ijkl} \pi_{ij}\pi_{kl} a_i^\dagger a_k^\dagger a_j a_l \tag{6.1.2}$$

where we use the independence of particles to write $V_{ikjl} = \pi_{ij}\pi_{kl}$.

A straightforward calculation of the square of single exchange operator gives, using commutation relations to write it in normal form:

$$\begin{aligned}(\hat{\pi}(|\Delta\vec{n} = 1|))^2 = (\sum_{ij} \hat{\pi}_{ij})^2 = (\sum_{ij} \pi_{ij} a_i^\dagger a_j)(\sum_{kl} \pi_{kl} a_k^\dagger a_l) = \\ \sum_{ijkl} \pi_{ij}\pi_{kl} a_i^\dagger a_j a_k^\dagger a_l = \sum_{ijkl} \pi_{ij}\pi_{kl} a_i^\dagger (a_k^\dagger a_j + \delta_{kj}) a_l = \\ \sum_{ijkl} \pi_{ij}\pi_{kl} a_i^\dagger a_k^\dagger a_j a_l + \sum_{il} a_i^\dagger a_l \sum_j \pi_{ij}\pi_{jl} \\ = \sum_{ijkl} \pi_{ij}\pi_{kl} a_i^\dagger a_k^\dagger a_j a_l + \sum_{il} \Delta_{il} a_i^\dagger a_l\end{aligned} \tag{6.1.3}$$

In the previous we have defined $\sum_j \pi_{ij}\pi_{jl} = \Delta_{il}$ that is the product of two stochastic matrix, so a stochastic matrix itself.

A comparison of the these two operators reads:

$$\begin{aligned}\hat{\pi}(|\Delta\vec{n} = 2|) &= \frac{1}{2}(\hat{\pi}(|\Delta\vec{n} = 1|))^2 - \frac{1}{2}\hat{\Delta} \\ \hat{\Delta} &= \sum_{ij} \Delta_{ij} a_i^\dagger a_j\end{aligned} \tag{6.1.4}$$

In (6.1.3) we see that $\hat{\Delta}$ it is due to the contribution to all possible double exchanges of those among subsequent nodes (this is the meaning of δ_{jk}), i.e. it represents the contribution of processes with different weights in subsequents dynamics respect the synchronous one.

To properly understand the matrix elements of $\hat{\pi}(|\Delta\vec{n}=1|)^2$ as the conditioned probabilities of a Markov process we have to check normalization.

For $\hat{\pi}(\Delta n = 1)$ normalization is $\frac{1}{N}$. By squaring it we expect to have $A = \frac{1}{N^2}$, and it holds. Indeed

$$
\begin{aligned}
1 = A\sum_{\vec{m}} \frac{\langle\vec{m}|\ \hat{\pi}(|\Delta\vec{n}=1|)^2\ |n\rangle}{\langle\vec{m}|\,\vec{m}\rangle} &= A\sum_{\vec{m}} \frac{\langle\vec{m}|\ \sum_{ijkl}\pi_{ij}\pi_{kl}a_i^\dagger a_k^\dagger a_j a_l + \sum_{il}\Delta_{il}a_i^\dagger a_l\ |n\rangle}{\langle\vec{m}|\,\vec{m}\rangle} = \\
= A\sum_{\vec{m}}\{(\sum_{\substack{jl\\ j\neq l}} n_j\, n_l\ + \sum_j n_j(n_j-1)\,)\sum_{ik}\pi_{ij}\pi_{kl}&\frac{\langle\vec{m}|\,|n+1_i+1_k-1_j-1_l\rangle}{\langle\vec{m}|\,\vec{m}\rangle} \quad + \\
\sum_l n_l\sum_i \Delta_{il}\,\frac{\langle\vec{m}|\,|n+1_i-1_l\rangle}{\langle\vec{m}|\,\vec{m}\rangle}\,\} &= \\
= A\,(\sum_{\substack{jl\\ j\neq l}} n_j\, n_l\ + \sum_j n_j(n_j-1)\,)\ + N \quad &= \\
= \quad A\{\quad N^2\ - \sum_l n_l^2\ + \sum_j n_j^2\ - N\ + N\} &= A\,N^2
\end{aligned}
\tag{6.1.5}
$$

In the same way we have to take care of the normalization of $|\Delta\vec{n}=2|$ to have $\sum_{\vec{m}}(\hat{\pi_2})_{\vec{m}\vec{n}} = 1$, and since

$$
\sum_m \langle\hat{\pi}_2\rangle_{mn} = \sum_m \frac{1}{2}\langle(\hat{\pi}_1)^2\rangle_{mn} - \sum_m \frac{1}{2}\langle\hat{\Delta}\rangle_{mn} = \frac{1}{2}N^2 - \frac{1}{2}N \tag{6.1.6}
$$

we find
$A_2 = \frac{1}{2}\frac{1}{N^2-N}$.

One of the advantages of master equation is that we don't have to care about normalization to unity since it allows to individuate incoming and outgoing fluxes of states probability, and this two pieces compensate normalization each other.

Working in Schrödinger representation we came to the formal solution of evolution equation (3.4.9) with the definition of the evolution operator

$$
\hat{U}(t) = e^{\hat{\mathcal{L}}t} \tag{6.1.7}
$$

We can formally expand the exponential

$$e^{\hat{\mathcal{L}}t}\,|\psi_0\rangle \;=\; \sum_{k=0}^{\infty} \frac{1}{k!}\hat{\mathcal{L}}^k t^k\,|\psi_0\rangle \;=\; 0 \tag{6.1.8}$$

Going back to our derivation of single exchange dynamics it was ultimately based on the individuation of the characteristic time Δt of a single particle exchange, realized by $\hat{\mathcal{L}}$; therefore we can understand the Laplacian k-power as the evolution of the state due to k multiple subsequent exchanges of particles (we are using the same argument exposed in (3.2.4)).

It is straightforward to see that the steady state, that has 0 eigenvalue, remains steady at every power of the development.

Double exchange subsequent Laplacian operator reads

$$\begin{aligned}
(\hat{\mathcal{L}})^2 \;&=\; (\sum_{ij}\hat{\pi})^2_{ij} + (\sum_{k}\hat{n}_k)^2 - 2\sum_{ijk}\hat{\pi}_{ij}\hat{n}_k \\
&=\; \sum_{ijkl}\pi_{ij}\pi_{kl}a_i^\dagger a_k^\dagger a_j a_l \;+\; \sum_{ijkl}\pi_{ij}\pi_{kl}a_j^\dagger a_l^\dagger a_j a_l \;-\; 2\sum_{ijkl}\pi_{ij}\pi_{kl}a_i^\dagger a_l^\dagger a_j a_l \\
&+\; \sum_{ijkl}\pi_{ij}\pi_{kl}\delta_{jk}a_i^\dagger a_l \;+\; \sum_{ijkl}\pi_{ij}\pi_{kl}\delta_{jl}a_j^\dagger a_l \\
&\equiv\; \hat{\mathcal{L}}_d \;+\; \hat{\mathcal{L}}_\Delta \\
&\text{where}\quad \hat{\mathcal{L}}_d \;=\; \sum_{ijkl}\pi_{ij}\pi_{kl}a_i^\dagger a_k^\dagger a_j a_l \;+\; \sum_{ijkl}\pi_{ij}\pi_{kl}a_j^\dagger a_l^\dagger a_j a_l \;-\; 2\sum_{ijl}\pi_{ij}a_i^\dagger a_l^\dagger a_j a_l \\
&\text{and}\quad \hat{\mathcal{L}}_\Delta \;=\; \sum_{ijl}\pi_{ij}\pi_{jl}a_i^\dagger a_l \;+\; \sum_{j}a_j^\dagger a_j
\end{aligned} \tag{6.1.9}$$

$\hat{\mathcal{L}}_\Delta$ represent the contribution to the dynamics of those double exchanges on subsequent nodes, indeed it is generated by the commutation rules of creation destruction operators in normal ordering of $(\hat{\mathcal{L}})^2$.

We give an explicit check of the master equation generated by (6.1.9) for the steady state:

$$\frac{\langle\vec{n}|\;\partial_t\;|\psi_0\rangle}{\langle\vec{n}|\,\vec{n}\rangle} \;=\; \sum_{\vec{m}}\frac{\langle\vec{n}|\;\hat{\mathcal{L}}^2\;|\vec{m}\rangle}{\langle\vec{n}|\,\vec{n}\rangle}\frac{\langle\vec{m}\,|\psi_0\rangle}{\langle\vec{m}|\,\vec{m}\rangle} \;=\; 0$$

Indeed:

$$\frac{\langle \vec{n}|\ \partial_t\ |\psi_0\rangle}{\langle \vec{n}|\,\vec{n}\rangle} = \sum_{\vec{m}} \{\ \frac{\langle \vec{n}|\ \hat{\mathcal{L}}_d\ |\vec{m}\rangle}{\langle \vec{n}|\,\vec{n}\rangle} + \frac{\langle \vec{n}|\ \hat{\mathcal{L}}_\Delta\ |\vec{m}\rangle}{\langle \vec{n}|\,\vec{n}\rangle}\}\frac{\langle \vec{m}\,|\psi_0\rangle}{\langle \vec{m}|\,\vec{m}\rangle} = \tag{6.1.10}$$

Performing an explicit calculation of the addenda we get

$$= \sum_{\vec{m}} \{\ \frac{\langle \vec{n}|\ \sum_{ijkl} \pi_{ij}\pi_{kl} a_i^\dagger a_k^\dagger a_j a_l\ |\vec{m}\rangle}{\langle \vec{n}|\,\vec{n}\rangle} \tag{6.1.11}$$

$$+ \frac{\langle \vec{n}|\ \sum_{jl}\ a_j^\dagger a_l^\dagger a_j a_l\ |\vec{m}\rangle}{\langle \vec{n}|\,\vec{n}\rangle} \tag{6.1.12}$$

$$-2\,\frac{\langle \vec{n}|\ \sum_{ijl}\ a_i^\dagger a_l^\dagger a_j a_l\ |\vec{m}\rangle}{\langle \vec{n}|\,\vec{n}\rangle} \tag{6.1.13}$$

$$+ \frac{\langle \vec{n}|\ \sum_{ijl} \pi_{ij}\pi_{jl} a_i^\dagger a_l\ |\vec{m}\rangle}{\langle \vec{n}|\,\vec{n}\rangle} \tag{6.1.14}$$

$$+ \frac{\langle \vec{n}|\ \sum_j a_j^\dagger a_j\ |\vec{m}\rangle}{\langle \vec{n}|\,\vec{n}\rangle}\ \}\frac{\langle \vec{m}\,|\psi_0\rangle}{\langle \vec{m}|\,\vec{m}\rangle} \tag{6.1.15}$$

$$
\begin{aligned}
(6.1.11) \;&= \sum_{\vec{m}} \Big(\sum_{\substack{ijkl \\ j\neq l}} \pi_{ij}\pi_{kl}\, m_j\, m_l\, \delta_{\vec{n}\vec{m}+1_i-1_j+1_k-1_l} \;+ \sum_{ijk} \pi_{ij}\pi_{kj}(m_j)(m_j-1)\Big) p_s(\vec{m}) \\
&= \sum_{\substack{ijkl \\ j\neq l}} \pi_{ij}\pi_{kl}(n_j+1)(n_l+1)p_s(\vec{n}-1_i+1_j-1_k+1_l) \\
&+ \sum_{ijk} \pi_{ij}\pi_{kj}(n_j+2)(n_j+1)p_s(\vec{n}-1_i+2_j-1_k) \\
&= \Big(\sum_{\substack{ijkl \\ j\neq l \\ i\neq k}} \frac{1_{ij}}{\psi_j}\frac{1_{kl}}{\psi_l}(n_j+1)(n_l+1)\frac{\psi_j}{n_j+1}\frac{\psi_l}{n_l+1}\frac{n_i}{\psi_i}\frac{n_k}{\psi_k} \\
&+ \sum_{\substack{ijl \\ j\neq l}} \frac{1_{ij}}{\psi_j}\frac{1_{kl}}{\psi_l}(n_j+1)(n_l+1)\frac{\psi_j}{n_j+1}\frac{\psi_l}{n_l+1}\frac{n_i}{\psi_i}\frac{n_i-1}{\psi_i} \\
&+ \sum_{\substack{ijk \\ i\neq k}} \frac{1_{ij}}{\psi_j}\frac{1_{kj}}{\psi_j}(n_j+2)(n_j+1)\frac{\psi_j^2}{(n_j+2)(n_j+1)}\frac{n_i}{\psi_i}\frac{n_k}{\psi_k} \\
&+ \sum_{ij} \frac{1_{ij}}{\psi_j}\frac{1_{ij}}{\psi_j}(n_j+2)(n_j+1)\frac{\psi_j^2}{(n_j+2)(n_j+1)}\frac{n_i}{\psi_i}\frac{n_i-1}{\psi_i}\Big)\, p(\vec{n}) \\
&= \Big(\sum_{\substack{ik \\ i\neq k}} \frac{n_i}{\psi_i}\frac{n_k}{\psi_k} \sum_j 1_{ij} \sum_l 1_{kl}(1-\delta_{jl}) \\
&+ \sum_i \frac{n_i(n_i-1)}{\psi_i^2} \sum_j 1_{ij} \sum_l 1_{kl}(1-\delta_{jl}) \\
&+ \sum_i \frac{n_i}{\psi_i} \sum_k \frac{n_k}{\psi_k}(1-\delta_{ik}) \sum_j 1_{ij}1_{kj}
\end{aligned}
$$

$$
\begin{aligned}
&+ \sum_i \frac{n_i(n_i-1)}{\psi_i^2} \sum_j 1_{ij}1_{ij}\,)\,p(\vec{n}) \\
&= (\sum_{\substack{ik \\ i\neq k}} (\, n_i\, n_k \;-\; \frac{n_i}{\psi_i}\,\frac{n_k}{\psi_k} \sum_j 1_{ij}1_{kj}) \;+\; \sum_i n_i(n_i-1) \;-\; \sum_i \frac{n_i(n_i-1)}{\psi_i^2} \sum_j 1_{ij}1_{ij}) \\
&+ \sum_i \frac{n_i}{\psi_i} \sum_k \frac{n_k}{\psi_k} \sum_j 1_{ij}1_{kj} \\
&+ \sum_i \frac{n_i^2}{\psi_i^2} \sum_j 1_{ij}1_{ij} \;-\; \sum_i \frac{n_i}{\psi_i^2} \sum_j 1_{ij}1_{ij}\,)\,p(\vec{n}) \\
&= (\sum_i n_i \sum_k n_k\,(1-\delta_{ki}) \;-\; \sum_{ik} \frac{n_i}{\psi_i}\,\frac{n_k}{\psi_k} \sum_j 1_{ij}1_{kj} \;+\; \sum_i \frac{n_i}{\psi_i^2} \sum_j 1_{ij}1_{ij} \\
&+ \sum_i n_i\,(n_i-1) \;+ \sum_i \frac{n_i}{\psi_i} \sum_k \frac{n_k}{\psi_k} \sum_j 1_{ij}1_{kj} \;-\; \sum_i \frac{n_i}{\psi_i^2} \sum_j 1_{ij}1_{ij}\,)\,p(\vec{n}) \\
&= (N^2 \;-\; N)\,p(\vec{n})
\end{aligned}
$$

$$
\begin{aligned}
(6.1.12) \;&=\; \sum_{\vec{m}} \{ \sum_{\substack{jl \\ j\neq l}} m_j m_l\, \delta_{\vec{n}\vec{m}} \;+\; \sum_j m_j(m_j-1)\,\delta_{\vec{m}\vec{n}}\,\}\,p(\vec{m}) \\
&=\; \{ \sum_j n_j \sum_l n_l\,(1-\delta_{jl}) \;+\; \sum_j n_j^2 \;-\; \sum_j n_j\,\}\,p(\vec{n}) \qquad (6.1.16) \\
&=\; \{\, N^2 \;-\; N\,\}\,p(\vec{n})
\end{aligned}
$$

$$
\begin{aligned}
(6.1.13) \;&=\; \sum_{\vec{m}} -2\,\{ \sum_{\substack{ijl \\ j\neq l}} \pi_{ij}\, m_j m_l\, \delta_{\vec{n}\vec{m}+1_i-1_j} \;+ \sum_{ij} \pi_{ij}\, m_j(m_j-1)\,\}\,p(\vec{m}) \\
&=\; -2\{ \sum_{\substack{ijl \\ j\neq l}} \pi_{ij}\,(n_j+1) n_l \;+\; \sum_{ij} \pi_{ij}\, n_j(n_j+1)\,\}\,p(\vec{n}-1_i+1_j) \\
&=\; -2\,\{ \sum_{\substack{ijl \\ j\neq l}} \frac{1_{ij}}{\psi_j}\,(n_j+1) n_l\,\frac{\psi_j}{n_j+1}\frac{n_i}{\psi_i} \;+\; \sum_{ij} \frac{1_{ij}}{\psi_j}\, n_j(n_j+1)\,\frac{\psi_j}{n_j+1}\frac{n_i}{\psi_i}\,\}\,p(\vec{n}) \\
&=\; -2\{ \sum_{ij} \frac{1_{ij}}{\psi_i}\, n_i \sum_l n_l\,(1-\delta_{jl}) \;+\; \sum_{ij} 1_{ij}\, n_j\, \frac{n_i}{\psi_i}\,\}p(\vec{n}) \\
&=\; -2\,\{ \sum_i n_i \sum_l n_l \;+\; \sum_i \frac{n_i}{\psi_i} \sum_j 1_{ij}\, n_j \;-\; \sum_{ij} 1_{ij}\, n_j \frac{n_i}{\psi_i}\} \, p_{\vec{n}} \\
&=\; -2N^2\, p(\vec{n}) \qquad (6.1.17)
\end{aligned}
$$

$$
\begin{aligned}
(6.1.14) \;&=\; \sum_{\vec{m}} \sum_{ijl} \pi_{ij}\pi_{jl}\, m_l\, \delta_{\vec{n}\vec{m}+1_i-1_l}\, p(\vec{m}) \;=\; \sum_{ijl} \pi_{ij}\pi_{jl}\, (n_l+1)\, p(\vec{n}-1_i+1_l) \\
&= \sum_{ijl} \pi_{ij}\pi_{jl}\, (n_l+1) \frac{\psi_l}{n_l+1} \frac{n_i}{\psi_i}\, p(\vec{n}) \;=\; \sum_i \frac{n_i}{\psi_i} \sum_j \frac{1_{ij}}{\psi_j} \sum_l 1_{jl}\, p(\vec{n}) \\
&= N p(\vec{n})
\end{aligned}
\tag{6.1.18}
$$

$$
(6.1.15) \;=\; \sum_{\vec{m}} \sum_j m_j\, \delta_{\vec{m}\vec{n}}\, p(\vec{m})\, N\, p(\vec{n}) \;=\; N\, p(\vec{n}) \tag{6.1.19}
$$

Putting all together we see that (6.1.10) vanishes.

In order to study the synchronous dynamics we have two ways: we can try to derive it from a continuous time limit using (6.1.2), or we can proceed as follows.

Master equation allows to individuate the incoming and outgoing fluxes of states probability, that is

$$
\begin{aligned}
\partial_t p(\vec{n}) &= \sum_{\vec{m}} \frac{\langle \vec{n}|\, \hat{\Pi}_{in}\, |\vec{m}\rangle}{\langle \vec{n}|\, \vec{n}\rangle} p(\vec{m}) - \sum_{\vec{m}} \frac{\langle \vec{m}|\, \hat{\Pi}_{out}\, |\vec{n}\rangle}{\langle \vec{m}|\, \vec{m}\rangle} p(\vec{n}) \\
&= \Phi_{in}(\vec{n}) \quad - \quad \Phi_{out}(\vec{n})
\end{aligned}
\tag{6.1.20}
$$

In case of single step dynamics as we have already seen

$$
\hat{\Pi}_{in} \;=\; \sum_{ij} \pi_{ij} a_i^\dagger a_j \qquad \hat{\Pi}_{out} \;=\; \sum_j a_j^\dagger a_j
$$

$$
\begin{aligned}
\partial_t p(\vec{n}) &= \sum_{ij} \pi_{ij}(n_j+1) p(\vec{n}+1_j-1_i) - \sum_{kl} \pi_{kl} n_l p(\vec{n}) \\
\Phi_{in}(\vec{n}) \;&=\; \sum_{ij} \pi_{ij}(n_j+1) p(\vec{n}+1_j-1_i) \\
\Phi_{out}(\vec{n}) \;&=\; \sum_{kl} \pi_{kl} n_l p(\vec{n})
\end{aligned}
$$

For the double step synchronous dynamics we move from the operator that performs double exchanges, that is $\hat{\pi}(|\Delta\vec{n}=2|) = \sum_{ijkl} \pi_{ij}\pi_{kl} a_i^\dagger a_k^\dagger a_j a_l$, and in analogy with the single step case we write

$$\hat{\mathcal{L}}_2 \;=\; \sum_{ijkl} \pi_{ij}\pi_{kl} \left\{\, a_i^\dagger a_k^\dagger a_j a_l \;-\; a_j^\dagger a_l^\dagger a_j a_l \,\right\} \tag{6.1.21}$$

Applying (6.1.21) to a network state $|p\rangle$ and taking expectation value we recover the Master equation with the incoming and outgoing fluxes.

$$\begin{aligned} \partial_t p(\vec{n}) &= \sum_{\vec{m}} \frac{\langle\vec{n}|\sum_{ijkl}\frac{1}{2}\pi_{ij}\pi_{kl}a_i^\dagger a_k^\dagger a_j a_l\,|\vec{m}\rangle}{\langle\vec{n}|\,\vec{n}\rangle} p(\vec{m}) - \sum_{\vec{m}} \frac{\langle\vec{m}|\sum_{ijkl}\frac{1}{2}\pi_{ij}\pi_{kl}a_j^\dagger a_l^\dagger a_j a_l\,|\vec{n}\rangle}{\langle\vec{m}|\,\vec{m}\rangle} p(\vec{n}) \\ &= \Phi^2_{in}(\vec{n}) \quad - \Phi^2_{out}(\vec{n}) \end{aligned} \tag{6.1.22}$$

It is immediate to compute the equation for the steady state (3.1.10), indeed it is sufficient to observe that the incoming flux coincides with (6.1.11) and the outgoing (up to the sign) with (6.1.12).

The result is that the double exchange synchronous dynamics has the same steady state than the subsequent and the single exchange one:

$$\frac{\langle\vec{n}|\;\partial_t\;|\psi_0\rangle}{\langle\vec{n}|\,\vec{n}\rangle} \;=\; \sum_{\vec{m}} \frac{\langle\vec{n}|\;\hat{\mathcal{L}}^2\;|\vec{m}\rangle}{\langle\vec{n}|\,\vec{n}\rangle}\frac{\langle\vec{m}\,|\psi_0\rangle}{\langle\vec{m}|\,\vec{m}\rangle} \;=\; N \tag{6.1.23}$$

Although the synchronous and the subsequent dynamics admit the same steady state they are conceptually different.

If we think about the states space of the network a one step process, single or repeated, connects all the physical states of the space.

The double exchange dynamics conversely realizes connections among states that differs for a double exchange of particles, indeed $\Phi^2(\vec{n})$ sums over all contributions of states that differs for two particle exchanges from $\vec{n}$, and therefore, depending on the initial state, accesses only to a half of the whole space, dividing it in an even and in an odd subsets.

Anyway Master equation accounts for probability distribution, and the average on the initial states hides this issue leaving the steady state unchanged.

We observe that the synchronous dynamics essentially differs from the subsequent one in the processes described by $\hat{\mathcal{L}}_\Delta$. We can recognise in it

the transition operator (6.1.4), and studying the dynamics generated by this operator we find that it admits the usual steady state (3.1.10).

Indeed

$$\begin{aligned}
\sum_{il} \frac{1}{2}\Delta_{il}(n_l+1)p(\vec{n}+1_i-1_l) &= \sum_{il}\frac{1}{2}\Delta_{il}n_l p(\vec{n}) \\
\sum_{il}\frac{1}{2}\Delta_{il}(n_l+1)\frac{d_l}{n_l+1}\frac{n_i}{d_i} &= \sum_l \frac{1}{2}n_l\sum_i \Delta_{il} \\
\sum_{il}\frac{n_i}{d_i}d_l\Delta_{il} &= N \\
\sum_{il}\frac{n_i}{d_i}d_l\sum_j\frac{1_{ij}}{d_j}\frac{1_{jl}}{d_l} &= N \\
\sum_i\frac{n_i}{d_i}\sum_j\frac{1_{ij}}{d_j}\sum_l 1_{jl} &= N \\
\sum_i\frac{n_i}{d_i}\sum_j\frac{1_{ij}}{d_j}d_j &= N
\end{aligned} \tag{6.1.24}$$

This not surprising since is easy to see that it is a one step dynamics ruled by the stochastic matrix Δ associated to an adjacency matrix $\mathcal{A}' = \mathcal{A}^2$.

The difference of the two dynamics ultimately lies in assigned probabilities to the situation of a double exchange on subsequent nodes, so it modifies the fluxes in the Master equation and modifies the probability to go from a network state to another.

The unnormalized weight of this contribution is $\frac{N}{2}$.

Nonetheless this is true both for the incoming and outgoing fluxes, and a the two terms balance out. In other words we have a complete time reversibility of the process and the probability that it happens in a verse is equal to the one of the other verse.

Since we have built the subsequent and the synchronous dynamics in two slightly different ways this effect is accounted in different ways as well.

At the operatorial level this difference is reflected in the use of $\hat{\pi}_{ij}$ or $\hat{n}_j$ in the definition of operators that generate incoming and outgoing fluxes, $\hat{\Delta_{in}}$ and $\hat{\Delta_{out}}$.

In $\hat{\mathcal{L}}_2$ we have the contribution of $\hat{\mathcal{L}}_\Delta$ divided in the incoming and outgoing fluxes.

Furthermore we can have an idea of what happens also studying normalizations.

The double exchange synchronous dynamics allows less possible exchanges than the subsequent one, and this is accounted by $\hat{\Delta}$.

Being a one step process $\hat{\Delta}$ would require a normalization $\frac{1}{N}$, but as it comes from the square of a single step process it has a $\frac{1}{N^2}$ resulting in a normalized eigenvalue $\frac{1}{N}$.

With the same argumentation followed for the normalization of the 1-FTC single exchange dynamics we understand it as a slow down of the dynamics due to the reduction of possible movements of the network.

This kind of effect is exasperated in the $1-FTC$ model, where in general we do not see a difference in the weights of subsequent nodes processes but only an inhibition of these when the intermediate node is empty.

Steady state of double step subsequent dynamics is the same than single step, therefore we can check that detailed balance condition for $\hat{\pi}^2$ holds.

Now in the states space the connected states are those with a double particle exchange difference.

$$\begin{aligned}
&\frac{\langle \vec{n}+1_a-1_b+1_c-1_d|\ \sum_{ijkl}\pi_{ij}\pi_{kl}a_i^\dagger a_k^\dagger a_j a_l\ +\ \sum_{ijkl}\pi_{ij}\pi_{kl}\delta_{jk}a_i^\dagger a_l\ |\vec{n}\rangle}{\langle \vec{n}+1_a-1_b+1_c-1_d|\,\vec{n}+1_a-1_b+1_c-1_d\rangle}\,p_s(\vec{n})\\
&=\ \frac{\langle \vec{n}|\ \sum_{ijkl}\pi_{ij}\pi_{kl}a_i^\dagger a_k^\dagger a_j a_l\ +\ \sum_{ijkl}\pi_{ij}\pi_{kl}\delta_{jk}a_i^\dagger a_l\ ,|\vec{n}+1_a-1_b+1_c-1_d\rangle}{\langle \vec{n}|\,\vec{n}\rangle}\\
&p_s(\vec{n}+1_a-1_b+1_c-1_d)
\end{aligned} \tag{6.1.25}$$

Before we proceed, we observe that the first addendum between the bra-ket connects states with two exchanges of difference, whereas the second connects states with a single exchange of difference between nodes 2 links far (this is the net effect of a double step process on subsequent nodes).

Therefore we have to compare this two kind of terms separately.

We compare

$$\begin{aligned}
&\frac{\langle \vec{n}+1_a-1_b+1_c-1_d|\ \sum_{ijkl}\pi_{ij}\pi_{kl}a_i^\dagger a_k^\dagger a_j a_l\ |\vec{n}\rangle}{\langle \vec{n}+1_a-1_b+1_c-1_d|\,\vec{n}+1_a-1_b+1_c-1_d\rangle}\,p_s(\vec{n})\\
&=\sum_{ijkl}\pi_{ij}\pi_{kl}\,n_j\,n_l\,\delta_{\vec{n}+1_a-1_b+1_c-1_d\vec{n}+1_i-1_j+1_k-1_l}\,p_s(\vec{n})\\
&=\sum_{ijkl}\pi_{ij}\pi_{kl}\,n_j\,n_l\,\delta_{ai}\,\delta_{bj}\,\delta_{ck}\,\delta_{dl}\,p_s(\vec{n})\\
&=\ \pi_{ab}\pi_{cd}\,n_b\,n_d\,p_s(\vec{n})
\end{aligned} \tag{6.1.26}$$

with

$$
\begin{aligned}
&\frac{\langle \vec{n}|\, \sum_{ijkl} \pi_{ij}\pi_{kl} a_i^\dagger a_k^\dagger a_j a_l \;|\vec{n}+1_a-1_b+1_c-1_d\rangle}{\langle \vec{n}|\,\vec{n}\rangle}\, p_s(\vec{n}+1_a-1_b+1_c-1_d) \\
&= \sum_{ijkl} \pi_{ij}\pi_{kl}\, n_j\, n_l\, \delta_{\vec{n}\vec{n}+1_a-1_b+1_c-1_d+1_i-1_j+1_k-1_l}\, p_s(\vec{n}+1_a-1_b+1_c-1_d) \\
&= \sum_{ijkl} \pi_{ij}\pi_{kl}\, n_j\, n_l\, \delta_{bi}\, \delta_{aj}\, \delta_{dk}\, \delta_{cl}\, p_s(\vec{n}+1_a-1_b+1_c-1_d) \\
&= \pi_{ba}\pi_{dc}\, (n_a+1)\, (n_c+1)\, \frac{\psi_a}{(n_a+1)}\, \frac{\psi_c}{(n_c+1)}\, \frac{(n_b)}{\psi_b}\, \frac{(n_d)}{\psi_d}\, p_s(\vec{n})
\end{aligned}
\tag{6.1.27}
$$

finding

$$
\frac{1_{ab}}{\psi_b}\frac{1_{cd}}{\psi_d}\, n_b\, n_d\, p_s(\vec{n}) \;=\; \frac{1_{da}}{\psi_a}\frac{1_{dc}}{\psi_c}\, \psi_a\, \psi_c\, \frac{(n_b)}{\psi_b}\, \frac{(n_d)}{\psi_d}\, p_s(\vec{n}) \tag{6.1.28}
$$

Then we compare

$$
\begin{aligned}
&\frac{\langle \vec{n}+1_a-1_b+1_c-1_d|\, \sum_{ijl} \pi_{ij}\pi_{jl}\, a_i^\dagger a_l \;|\vec{n}\rangle}{\langle \vec{n}+1_a-1_b+1_c-1_d|\,\vec{n}+1_a-1_b+1_c-1_d\rangle}\, p_s(\vec{n}) \\
&= \sum_{ijl} \pi_{ij}\pi_{jl}\, n_l\, \delta_{\vec{n}+1_a-1_b+1_c-1_d\vec{n}+1_i-1_l}\, p_s(\vec{n}) \\
&= \sum_{ijl} \pi_{ij}\pi_{jl}\, n_l\, \delta_{ab}\, \delta_{ci}\, \delta_{dl}\, p_s(\vec{n}) \\
&= \delta_{ab} \sum_j \pi_{cj}\pi_{jd}\, n_d\, p_s(\vec{n})
\end{aligned}
\tag{6.1.29}
$$

with

$$
\begin{aligned}
&\frac{\langle \vec{n}| \sum_{ijl} \pi_{ij}\pi_{jl}\, a_i^\dagger b_l \, |\vec{n} + 1_a - 1_b + 1_c - 1_d\rangle}{\langle \vec{n}|\, \vec{n}\rangle}\, p_s(\vec{n} + 1_a - 1_b + 1_c - 1_d) \\
&= \sum_{ijl} \pi_{ij}\pi_{jl}\, n_l\, \delta_{\vec{n}\vec{n}+1_a-1_b+1_c-1_d+1_i-1_l}\, p_s(\vec{n} + 1_a - 1_b + 1_c - 1_d) \\
&= \sum_{ijl} \pi_{ij}\pi_{jl}\, n_l\, \delta_{ab}\, \delta_{di}\, \delta_{cl}\, p_s(\vec{n} + 1_a - 1_b + 1_c - 1_d) \\
&= \delta_{ab} \sum_j \pi_{dj}\pi_{jc}\, (n_c + 1)\, \frac{\psi_c}{(n_c + 1)} \frac{(n_d)}{\psi_d}\, p_s(\vec{n})
\end{aligned}
\tag{6.1.30}
$$

finding

$$
\sum_j \frac{1_{cj}}{\psi_j} \frac{1_{jd}}{\psi_d}\, n_d\, p_s(\vec{n}) \;=\; \sum_j \frac{1_{dj}}{\psi_d} \frac{1_{jc}}{\psi_c}\, \psi_c\, \frac{(n_d)}{\psi_d}\, p_s(\vec{n}) \tag{6.1.31}
$$

We see that under the same considerations of one step dynamics detailed balance is verified.

Note: in (6.1.26) and (6.1.27) the particular cases of a double departure from a node or a double arrival read slightly different when computed , with a $(n)(n \pm 1)$ instead of $(n)(n')$.

Anyway an explicit calculation shows that nothing special happens and therefore we avoid to treat this case apart.

As a final remark we observe that since the contribution of $\hat{\Delta}$ is balanced apart we can state that detailed balance holds also in the synchronous case.

6.2 Double exchange dynamics on 1-FTC networks

A proper definition of the double exchange dynamics is a hard task if we move from the definition of a Markov operator, since normalization presents difficulties even at the level of single step process. Therefore we bypass the problem employing the Master equation approach to study the evolution of the system.

Like the finite transport case we have $|\psi_0(t)\rangle \;=\; e^{\hat{\mathcal{L}}t}\, |\psi_0\rangle$, where $\partial_t\, |\psi_0(t)\rangle = \hat{\mathcal{L}}\, |\psi_0(t)\rangle = 0$.

We can formally expand the exponential understanding the Laplacian k-power as the evolution of the state due to k multiple subsequent exchanges of particles.

It is straightforward to see that the steady state remains steady.

$$e^{\hat{\mathcal{L}}t}\,|\psi_0\rangle \;=\; \sum_{k=0}^{\infty} \frac{1}{k!}\hat{\mathcal{L}}^k t^k\,|\psi_0\rangle \;=\; 0 \tag{6.2.1}$$

We compute $\hat{\mathcal{L}}^2$ using explicit representation (4.1.8) (the application on the right to a $|\vec{n}\rangle$ vector is understood):

$$\begin{aligned}
\hat{\mathcal{L}}^2 \;&=\; \big(\sum_{ij} \pi_{ij}(a_i^\dagger b_j \;-\; a_j^\dagger b_j)\big)^2 \\
&= \sum_{ijkl} \pi_{ij}\pi_{kl} a_i^\dagger b_j a_k^\dagger b_l \;+\; \sum_{ijkl} \pi_{ij}\pi_{kl} a_j^\dagger b_j a_l^\dagger b_l \;-\; \sum_{ijkl} \pi_{ij}\pi_{kl} a_i^\dagger b_j a_l^\dagger b_l \;-\; \sum_{ijkl} \pi_{ij}\pi_{kl} a_j^\dagger b_j a_k^\dagger b_l \\
&= \sum_{ijkl} \pi_{ij}\pi_{kl} a_i^\dagger a_k^\dagger b_j b_l \;+\; \sum_{ijkl} \pi_{ij}\pi_{kl}\delta_{jk}(1-\theta(n_j)) a_i^\dagger b_l \\
&+ \sum_{ijkl} \pi_{ij}\pi_{kl} a_j^\dagger a_l^\dagger b_j b_l \;+\; \sum_{ijkl} \pi_{ij}\pi_{kl}\delta_{jl}(1-\theta(n_j)) a_j^\dagger b_l \\
&- \sum_{ijkl} \pi_{ij}\pi_{kl} a_i^\dagger a_l^\dagger b_j b_l \;-\; \sum_{ijkl} \pi_{ij}\pi_{kl}\delta_{jl}(1-\theta(n_j)) a_i^\dagger b_l \\
&- \sum_{ijkl} \pi_{ij}\pi_{kl} a_j^\dagger a_k^\dagger b_j b_l \;-\; \sum_{ijkl} \pi_{ij}\pi_{kl}\delta_{jk}(1-\theta(n_j)) a_j^\dagger b_l \\
&= \sum_{ijkl} \pi_{ij}\pi_{kl} a_i^\dagger a_k^\dagger b_j b_l \;+\; \sum_{ijkl} \pi_{ij}\pi_{kl} a_j^\dagger a_l^\dagger b_j b_l \;-\; \sum_{ijkl} 2\pi_{ij}\pi_{kl} a_i^\dagger a_l^\dagger b_j b_l \\
&+ \sum_{ijkl} \pi_{ij}\pi_{kl}\delta_{jk}(1-\theta(n_j)) a_i^\dagger b_l \;+\; \sum_{ijkl} \pi_{ij}\pi_{kl}\delta_{jl}(1-\theta(n_j)) a_j^\dagger b_l \\
&- \sum_{ijkl} \pi_{ij}\pi_{kl}\delta_{jl}(1-\theta(n_j)) a_i^\dagger b_l \;-\; \sum_{ijkl} \pi_{ij}\pi_{kl}\delta_{jk}(1-\theta(n_j)) a_j^\dagger b_l \\
&= \sum_{ijkl} \pi_{ij}\pi_{kl}\{\, a_i^\dagger a_k^\dagger b_j b_l \;+\; a_j^\dagger a_l^\dagger b_j b_l \;-2 a_i^\dagger a_l^\dagger b_j b_l \,\} \\
&+ \{\sum_{il} a_i^\dagger b_l \sum_j (1-\theta(n_j))\,\pi_{ij}\pi_{jl} \;+\; \sum_j (1-\theta(n_j)) a_j^\dagger b_j \sum_{ik} \pi_{ij}\pi_{kj}\,\} \\
&- \{\sum_{ij} \pi_{ij}(1-\theta(n_j)) a_i^\dagger b_j \;+\; \sum_{jl} \pi_{jl}(1-\theta(n_j)) a_j^\dagger b_l\,\} \\
&\equiv \hat{\mathcal{L}}_d \;+\; \hat{\mathcal{L}}_\Delta \;-\; \hat{\mathcal{L}}_\delta
\end{aligned} \tag{6.2.2}$$

$$\text{where} \quad \hat{\mathcal{L}}_d = \sum_{ijkl} \pi_{ij}\pi_{kl}\{\, a_i^\dagger a_k^\dagger b_j b_l \,+\, a_j^\dagger a_l^\dagger b_j b_l \,-2a_i^\dagger a_l^\dagger b_j b_l \,\}$$

$$\hat{\mathcal{L}}_\Delta = \sum_{il} a_i^\dagger b_l \sum_j (1-\theta(n_j))\,\pi_{ij}\pi_{jl} \,+\, \sum_j (1-\theta(n_j)) a_j^\dagger b_j \,\sum_{ik} \pi_{ij}\pi_{kj}$$

$$\hat{\mathcal{L}}_\delta = \sum_{ij} \pi_{ij}(1-\theta(n_j)) a_i^\dagger b_j \,+\, \sum_{jl} \pi_{jl}(1-\theta(n_j)) a_j^\dagger b_l$$

It is worth to spend some words to analyze what we have just found, comparing it with the ITC case.

$\hat{\mathcal{L}}_d$ corresponds to (6.1.2) given the easy rule ($\hat{a} \to \hat{b}$).

We can read in the first two terms the two operators representing the synchronous double particle exchange on a 1-FTC network. We remark the problem to normalize them to a Markov process.

$\hat{\mathcal{L}}_\Delta$ and $\hat{\mathcal{L}}_\delta$ represent the contributions of the commutation rules appeared in the normal ordering operation.

$\hat{\mathcal{L}}_\Delta$ correspond to $\hat{\mathcal{L}}_\Delta$ of ITC, with the differences due to the different dynamics property of the system.

The first addendum, that represent the contribution of double exchanges among subsequent nodes, now entails a $(1-\theta(n_j))$ (it makes sense in the application to a $|\vec{n}\rangle$ vector) : therefore it gives a non-vanishing contribution iff $\exists\, n_j = 0 \,\in \vec{n}$ (i.e. on boundary states), with a relevance proportional to the number of empty nodes in the configuration.

The second addendum is the complementary for the outgoing flux.

We evaluate these terms on the steady state (4.1.14)

$$\begin{aligned}
\frac{\langle \vec{n}|\, \hat{\mathcal{L}}_\Delta\, |\psi_0\rangle}{\langle \vec{n}|\, \vec{n}\rangle} &= \sum_{\vec{m}} \frac{1}{\vec{n}!}\, \langle \vec{n}|\, \sum_{il} \Delta_{il}(\vec{m}) a_i^\dagger b_l \,+\, \sum_j (1-\theta(m_j)) a_j^\dagger b_j \;|\vec{m}\rangle\; p_s(\vec{m}) \\
&= \sum_{\vec{m}} \{ \sum_{il} \Delta_{il}(\vec{m})\theta(m_l)\delta_{\vec{n}\vec{m}+1_i-1_l} \,+\, \sum_j (1-\theta(m_j))\theta(m_j)\delta_{\vec{n}\vec{m}} \,\}\, p_s(\vec{m}) \\
&= \sum_{il} \Delta_{il}(\vec{n}-1_i+1_l)\theta(n_l+1) p_s(\vec{n}-1_i+1_l) \,+\, \sum_j (1-\theta(n_j))\theta(n_j)\, p_s(\vec{n}) \\
&= \{ \sum_{il} \frac{\theta(n_i)}{\psi_i} \psi_l \theta(n_l+1) \sum_j \pi_{ij}\pi_{jl}(1-\theta(n_j)) + \sum_j (1-\theta(n_j))\theta(n_j) \,\}\, p_s(\vec{n}) \\
&= \sum_{il} \frac{\theta(n_i)}{\psi_i} \psi_l \sum_j \pi_{ij}\pi_{jl}(1-\theta(n_j))\, p_s(\vec{n})
\end{aligned} \tag{6.2.3}$$

where we used $(1-\theta(n_j))\theta(n_j)=0$.

Inserting the explicit form $\pi_{ij}=\frac{1_{ij}}{\psi_j}$ we find

$$\sum_{il}\frac{\theta(n_i)}{\psi_i}\psi_l\sum_j\pi_{ij}\pi_{jl}(1-\theta(n_j)) = \sum_{il}\frac{\theta(n_i)}{\psi_i}\psi_l\sum_j\frac{1_{ij}}{\psi_j}\frac{1_{jl}}{\psi_l}(1-\theta(n_j)) =$$
$$\sum_i\frac{\theta(n_i)}{\psi_i}\sum_j(1-\theta(n_j))\frac{1_{ij}}{\psi_j}\sum_l 1_{jl} = \sum_i\frac{\theta(n_i)}{\psi_i}\sum_j(1-\theta(n_j))1_{ij}$$
$$=\sum_i\frac{\theta(n_i)}{\psi_i}\sum_j 1_{ij} - \sum_i\frac{\theta(n_i)}{\psi_i}\sum_j\theta(n_j)1_{ij} = M - n(0) - \sum_i\frac{\theta(n_i)}{\psi_i}\sum_j\theta(n_j)1_{ij} \tag{6.2.4}$$

where

$$\sum_i\frac{\theta(n_i)}{\psi_i}\sum_j\theta(n_j)1_{ij}\sim(\#\text{ empty adjacent nodes of the state})\equiv n(00)$$

Finally $\hat{\mathcal{L}}_\delta$ is interesting since it doesn't have an analogous in ITC (where $[\hat{\pi},\hat{n}]=0$).

We can recast this term in the form

$$\hat{\mathcal{L}}_\delta = \sum_{ij}\pi_{ij}a_i^\dagger b_j(2-\theta(n_i)-\theta(n_j)) \tag{6.2.5}$$

stressing that its contribution vanishes when two adjacent nodes are empty, while it is maximum when they are both non-empty.

We evaluate the expectation value on the steady state (4.1.14)

$$
\begin{aligned}
&\frac{\langle \vec{n}|\, \hat{\mathcal{L}}_\delta\, |\psi_0\rangle}{\langle \vec{n}|\, \vec{n}\rangle} \;= \sum_{\vec{m}} \frac{1}{\vec{n}!}\, \langle \vec{n}|\, \sum_{ij} \pi_{ij} a_i^\dagger b_j (2-\theta(m_i)-\theta(m_j))\; |\vec{m}\rangle\; p_s(\vec{m}) \\
&= \sum_{\vec{m}} \{ \sum_{ij} \pi_{ij} (2-\theta(m_i)-\theta(m_j))\, \theta(m_j) \delta_{\vec{n}\vec{m}+1_i-1_j}\, p_s(\vec{m}) \\
&= \sum_{ij} \pi_{ij} (2-\theta(n_i-1)-\theta(n_j+1))\, \theta(n_j+1)\, p_s(\vec{n}-1_i+1_j) \\
&= \sum_{ij} \pi_{ij} (1-\theta(n_i-1))\, \frac{\theta(n_i)}{\psi_i} \psi_j p_s(\vec{n})
\end{aligned}
\tag{6.2.6}
$$

and using (4.1.10)

$$
\begin{aligned}
&\sum_j \theta(n_i)(1-\theta(n_i-1)) \;=\; (M \;-\; n(0)) \;-\; (M \;-\; n(0) \;-\; n(1)) \\
&= n(1)
\end{aligned}
$$

Steady state of double step subsequent dynamics is the same than single step, therefore we can check detailed balance condition for $\hat{\pi}^2$ holds.

Now in the states space the connected states are those with a double particle exchange difference.

$$
\begin{aligned}
&\frac{\langle \vec{n}+1_a-1_b+1_c-1_d|\, \sum_{ijkl} \pi_{ij}\pi_{kl} a_i^\dagger a_k^\dagger b_j b_l \;+\; \sum_{ijkl} \pi_{ij}\pi_{kl}\delta_{jk}(1-\theta(n_j)) a_i^\dagger b_l\; |\vec{n}\rangle}{\langle \vec{n}+1_a-1_b+1_c-1_d|\, \vec{n}+1_a-1_b+1_c-1_d\rangle}\, p_s(\vec{n}) \\
&= \frac{\langle \vec{n}|\, \sum_{ijkl} \pi_{ij}\pi_{kl} a_i^\dagger a_k^\dagger b_j b_l \;+\; \sum_{ijkl} \pi_{ij}\pi_{kl}\delta_{jk}(1-\theta(n_j)) a_i^\dagger b_l\, , |\vec{n}+1_a-1_b+1_c-1_d\rangle}{\langle \vec{n}|\, \vec{n}\rangle} \\
&p_s(\vec{n}+1_a-1_b+1_c-1_d)
\end{aligned}
\tag{6.2.7}
$$

Before we proceed we remark that the first addendum between the bra-ket connects states with two exchanges of difference, whereas the second connects states with a single exchange of difference between nodes far 2 links (this is the net effect of a double step process on subsequent nodes).

Therefore we have to compare this two kind of terms separately.

We compare

$$
\begin{aligned}
&\frac{\langle \vec{n}+1_a-1_b+1_c-1_d|\ \sum_{ijkl}\pi_{ij}\pi_{kl}a_i^\dagger a_k^\dagger b_j b_l\ |\vec{n}\rangle}{\langle \vec{n}+1_a-1_b+1_c-1_d|\,\vec{n}+1_a-1_b+1_c-1_d\rangle}\,p_s(\vec{n})\\
&=\sum_{ijkl}\pi_{ij}\pi_{kl}\,\theta(n_j)\,\theta(n_l)\,\delta_{\vec{n}+1_a-1_b+1_c-1_d\vec{n}+1_i-1_j+1_k-1_l}\,p_s(\vec{n})\\
&=\sum_{ijkl}\pi_{ij}\pi_{kl}\,\theta(n_j)\,\theta(n_l)\,\delta_{ai}\,\delta_{bj}\,\delta_{ck}\,\delta_{dl}\,p_s(\vec{n})\\
&=\ \pi_{ab}\pi_{cd}\,\theta(n_b)\,\theta(n_d)\,p_s(\vec{n})
\end{aligned}
\tag{6.2.8}
$$

with

$$
\begin{aligned}
&\frac{\langle \vec{n}|\ \sum_{ijkl}\pi_{ij}\pi_{kl}a_i^\dagger a_k^\dagger b_j b_l\ |\vec{n}+1_a-1_b+1_c-1_d\rangle}{\langle \vec{n}|\,\vec{n}\rangle}\,p_s(\vec{n}+1_a-1_b+1_c-1_d)\\
&=\sum_{ijkl}\pi_{ij}\pi_{kl}\,\theta(n_j)\,\theta(n_l)\,\delta_{\vec{n}\vec{n}+1_a-1_b+1_c-1_d+1_i-1_j+1_k-1_l}\,p_s(\vec{n}+1_a-1_b+1_c-1_d)\\
&=\sum_{ijkl}\pi_{ij}\pi_{kl}\,\theta(n_j)\,\theta(n_l)\,\delta_{bi}\,\delta_{aj}\,\delta_{dk}\,\delta_{cl}\,p_s(\vec{n}+1_a-1_b+1_c-1_d)\\
&=\ \pi_{ba}\pi_{dc}\,\theta(n_a+1)\,\theta(n_c+1)\,\psi_a\frac{\theta(n_b)}{\psi_b}\,\psi_c\frac{\theta(n_d)}{\psi_d}\,p_s(\vec{n})
\end{aligned}
\tag{6.2.9}
$$

finding

$$
\frac{1_{ab}}{\psi_b}\frac{1_{cd}}{\psi_d}\,\theta(n_b)\,\theta(n_d)\,p_s(\vec{n})\ =\ \frac{1_{da}}{\psi_a}\frac{1_{dc}}{\psi_c}\,\theta(n_a+1)\,\theta(n_c+1)\,\psi_a\frac{\theta(n_b)}{\psi_b}\,\psi_c\frac{\theta(n_d)}{\psi_d}\,p_s(\vec{n})
\tag{6.2.10}
$$

Then we compare

$$
\begin{aligned}
&\frac{\langle \vec{n}+1_a-1_b+1_c-1_d|\ \sum_{ijl}\pi_{ij}\pi_{jl}(1-\theta(n_j))\,a_i^\dagger b_l\ |\vec{n}\rangle}{\langle \vec{n}+1_a-1_b+1_c-1_d|\,\vec{n}+1_a-1_b+1_c-1_d\rangle}\,p_s(\vec{n})\\
&=\sum_{ijl}\pi_{ij}\pi_{jl}(1-\theta(n_j))\,\theta(n_l)\,\delta_{\vec{n}+1_a-1_b+1_c-1_d\vec{n}+1_i-1_l}\,p_s(\vec{n})\\
&=\sum_{ijl}\pi_{ij}\pi_{jl}(1-\theta(n_j))\,\theta(n_l)\,\delta_{ab}\,\delta_{ci}\,\delta_{dl}\,p_s(\vec{n})\\
&=\delta_{ab}\sum_j\pi_{cj}\pi_{jd}\,(1-\theta(n_j))\,\theta(n_d)\,p_s(\vec{n})
\end{aligned}
\tag{6.2.11}
$$

with

$$\frac{\langle\vec{n}|\,\sum_{ijl}\pi_{ij}\pi_{jl}(1-\theta(n_j))\,a_i^\dagger b_l\;|\vec{n}+1_a-1_b+1_c-1_d\rangle}{\langle\vec{n}|\,\vec{n}\rangle}\,p_s(\vec{n}+1_a-1_b+1_c-1_d)$$
$$=\sum_{ijl}\pi_{ij}\pi_{jl}(1-\theta(n_j))\,\theta(n_l)\,\delta_{\vec{n}\vec{n}+1_a-1_b+1_c-1_d+1_i-1_l}\,p_s(\vec{n}+1_a-1_b+1_c-1_d)$$
$$=\sum_{ijl}\pi_{ij}\pi_{jl}(1-\theta(n_j))\,\theta(n_l)\,\delta_{ab}\,\delta_{di}\,\delta_{cl}\,p_s(\vec{n}+1_a-1_b+1_c-1_d)$$
$$=\delta_{ab}\sum_j\pi_{dj}\pi_{jc}\,(1-\theta(n_j))\,\theta(n_c+1)\,\psi_c\frac{\theta(n_d)}{\psi_d}\,p_s(\vec{n}) \tag{6.2.12}$$

finding

$$\sum_j\frac{1_{cj}}{\psi_j}\frac{1_{jd}}{\psi_d}\,(1-\theta(n_j))\,\theta(n_d)\,p_s(\vec{n})\;=\;\sum_j\frac{1_{dj}}{\psi_d}\frac{1_{jc}}{\psi_c}\,(1-\theta(n_j))\,\theta(n_c+1)\,\psi_c\frac{\theta(n_d)}{\psi_d}\,p_s(\vec{n}) \tag{6.2.13}$$

We see that under the same considerations of one step dynamics detailed balance is verified.

Note: in (6.2.8) and (6.2.9) the particular cases of a double departure from a node or a double arrival read slightly different when computed , with a $\theta(n)\theta(n\pm1)$ instead of $\theta(n)\theta(n')$.

Anyway an explicit calculation shows that nothing special happens and therefore we avoid to treat this case apart.

6.3 Synchronous dynamics on 1-FTC networks

We can write the Laplacian operator of the synchronous double exchange dynamics proceeding as we have done for the ITC case.

Thus

$$\hat{\mathcal{L}}_{sync}\;=\;\sum_{\substack{ijkl\\ j\neq l}}\pi_{ij}\pi_{kl}(a_i^\dagger a_k^\dagger b_j b_l\;-\;a_j^\dagger a_l^\dagger b_j b_l\,) \tag{6.3.1}$$

Expectation value of $\hat{\mathcal{L}}_{sync}$ on the steady single step dynamics state (4.1.14) reads

$$\frac{\langle\vec{n}|}{\vec{n}!}\quad \partial_t\,|\psi_0\rangle \;=\; \frac{\langle\vec{n}|}{\vec{n}!}\sum_{\substack{ijkl\\ j\neq l}}\pi_{ij}\pi_{kl}(a_i^\dagger a_k^\dagger b_j b_l \;-\; a_j^\dagger a_l^\dagger b_j b_l\,)\,|\psi_0\rangle$$

$$=\sum_{\vec{m}}\{\sum_{\substack{ijkl\\ j\neq l}}\pi_{ij}\pi_{kl}\theta(m_j)\theta(m_l)p_s(\vec{m})\delta_{\vec{n}\vec{m}+1_i+1_k-1_j-1_l}\;-\;\sum_{\substack{jl\\ j\neq l}}\theta(n_j)\theta(n_l)p_s(\vec{n})\delta_{\vec{n}\vec{m}}\}$$

$$=\{\sum_{\substack{ijkl\\ j\neq l}}\pi_{ij}\pi_{kl}\theta(n_j+1)\theta(n_l+1)\frac{\theta(n_i)}{\psi_i}\psi_j\frac{\theta(n_k)}{\psi_k}\psi_l\;-\;\sum_{\substack{jl\\ j\neq l}}\theta(n_j)\theta(n_l)\,\}\,p_s(\vec{n}) \tag{6.3.2}$$

using the explicit form $\pi_{ij}=\frac{1_{ij}}{\psi_j}$

$$\sum_{ik}\frac{\theta(n_i)}{\psi_i}\frac{\theta(n_k)}{\psi_k}\sum_{\substack{jl\\ j\neq l}}\frac{1_{ij}}{\psi_j}\frac{1_{kl}}{\psi_l}\psi_j\psi_l \;=\; \sum_{ik}\frac{\theta(n_i)}{\psi_i}\frac{\theta(n_k)}{\psi_k}\sum_l 1_{kl}(\psi_i-1_{il})$$

$$=\;(M-n(0))^2\;-\;\sum_{ik}\frac{\theta(n_i)}{\psi_i}\frac{\theta(n_k)}{\psi_k}\sum_l 1_{kl}1_{il}$$

and

$$\sum_{\substack{jl\\ j\neq l}}\theta(n_j)\theta(n_l)\;=\;\sum_j\theta(n_j)\sum_l(\theta(n_l)-\delta_{jl})\;=\;(M-n(0))^2-(M-n(0)) \tag{6.3.3}$$

and we see that (4.1.14) is no more the steady state.
This is not surprising since if

$$\frac{1}{2}(\hat{\pi}_1)^2\;=\;\sum_{ijkl}\pi_{ij}\pi_{kl}\,a_i^\dagger a_k^\dagger b_j b_l\;+\;\{\sum_{il}a_i^\dagger b_l\sum_j(1-\theta(n_j))\,\pi_{ij}\pi_{jl}\;=\;\hat{\pi}_2\;-\hat{\Delta}_{in} \tag{6.3.4}$$

as in the ITC case but

$$\frac{1}{2}(\hat{n})^2\;=\;\sum_{jl}a_j^\dagger a_l^\dagger b_j b_l\;+\;\sum_j(1-\theta(n_j))a_j^\dagger b_j\sum_{ik}\pi_{ij}\pi_{kj}\;=\;\hat{n}_2\;-\hat{\Delta}_{out} \tag{6.3.5}$$

and its easy to see that $\langle m|\;\hat{\Delta}_{out}\;|n\rangle\sim(1-\theta(n_j))\theta(n_j)$ always vanishes, thus $\hat{\mathcal{L}}_\Delta\;=\;\hat{\Delta}_{in}$.

Therefore we do not have the balance in the incoming and outgoing fluxes of the Master equation.

On the other side now there is a new term as a correction for the outgoing flux of $\hat{\mathcal{L}}^2$ that is $\hat{\mathcal{L}}$, that does not appear in $\hat{\mathcal{L}}_{sync}$, and we can write

$$\hat{\mathcal{L}}_{sync} = \frac{1}{2}\hat{\mathcal{L}}^2 - \frac{1}{2}(\hat{\mathcal{L}}_{\Delta} - \hat{\mathcal{L}}_{\delta}) \tag{6.3.6}$$

6.4 Empty nodes spatial correlation

What we are interested in are the probabilities to have empty adjacent nodes in the different steady states of subsequent and synchronous double steps dynamics.

Numerical simulations [1] indicate that synchronous steady state promotes adjacency of empty nodes, therefore we expect to find a spatial correlation in the probability of two nodes to be empty.

We can give an explanation of the phenomena as follows.

The FTC dynamics doesn't weight processes depending on the number of particles in nodes, therefore double step synchronous dynamics shows only the inhibition of the mixing mechanism in case of an empty node in the middle of the path.

This feature joint with the enhancement of empty nodes probability, that we have seen in the passage from infinite to finite transport capacity networks already at the one step level, leads to an effect of empty node mutual attraction.

In order to see this effect from our model first of all we remark that the analogous of number operator with b reads

$$a_i^\dagger b_i \left|n_i\right\rangle = \begin{cases} 1\left|n_i\right\rangle & \text{if} \quad n_i > 0 \\ 0 \quad \text{if} \quad n_i = 0 \end{cases} \tag{6.4.1}$$

and we define the "slacker inspector" operators

$$\begin{aligned} \hat{\mathcal{S}}_1 &= \sum_i (1 - a_i^\dagger b_i) = \sum_i \hat{s}_i \\ \hat{\mathcal{S}}_2 &= \sum_{ij} 1_{ij}(1 - a_i^\dagger a_j^\dagger b_i b_j) = \sum_{ij} \hat{s}_{ij} \end{aligned} \tag{6.4.2}$$

The action of these operators on a basis vector is:

- $\hat{s}_i$ returns 1 if the node i is empty, 0 otherwise (counts boundaries)
- $\hat{s}_{ij}$ returns 0 if two adjacent nodes are occupied, whereas returns 1 if one or both of the adjacent nodes are empty.

Consequently the expectation value of $\hat{\mathcal{S}}_2$ on a network state is the probability to have one or two adjacent nodes empty.

$$\sum_{\vec{n}} \frac{1}{n!} \langle \vec{n}| \hat{\mathcal{S}}_2 |\phi(t)\rangle = < \mathcal{S}_2(t) >_\phi \tag{6.4.3}$$

The point is

$$< \mathcal{S}_2 >_{sync} \quad \overset{?}{>} \quad < \mathcal{S}_2 >_{sub} \tag{6.4.4}$$

But this requires us to know steady state of subsequent (we almost do) and synchronous (we do not) dynamics.

Equivalently we can study variance of $\hat{\mathcal{S}}_1$

$$< \mathcal{S}_1^2 >_{sync} \quad \overset{?}{>} \quad < \mathcal{S}_1^2 >_{sub} \tag{6.4.5}$$

The lack of knowledge about the steady synchronous state moreover impedes the evaluation of the detailed balance condition.

6.5 Empty nodes spatial correlation from detailed balance

The difficulty in evaluation of the new steady state oblige us to try another approach to overcome this problem.

The idea is to turn back to the Markov process point of view, ignoring the inconsistency of normalization and keeping in mind that the properly defined evolution of the system is given by the Laplacian (where normalizations are balanced), to use detailed balance condition.

As already said for an equilibrium steady state of the network we can reasonably guess detailed balance keeps holding if we switch from a subsequent dynamics of particle to a synchronous one.

We assume that detailed balance is true for the subsequent (as we have proved) and the synchronous (we guess) double step dynamics with the respective steady states.

$$\begin{aligned}(\pi_1)^2_{\vec{m}\vec{n}}\, p_s(\vec{n}) \;&=\; (\pi_1)^2_{\vec{n}\vec{m}}\, p_s(\vec{m}) \\ (\pi_2)_{\vec{m}\vec{n}}\, p_{ss}(\vec{n}) \;&=\; (\pi_2)_{\vec{n}\vec{m}}\, p_{ss}(\vec{m})\end{aligned} \tag{6.5.1}$$

We know $(\pi_1)^2$, p_s and π_2, but we don't know p_{ss}.

If we evaluate e.g.

$$(\pi_2)_{\vec{m}\vec{n}}\, p_s(\vec{n}) \;>\; (\pi_2)_{\vec{n}\vec{m}}\, p_s(\vec{m}) \tag{6.5.2}$$

we can write

$$\frac{p_{ss}(\vec{m})}{p_{ss}(\vec{n})} \;=\; \frac{(\pi_2)_{\vec{m}\vec{n}}}{(\pi_2)_{\vec{n}\vec{m}}} > \frac{(\pi_1)^2_{\vec{m}\vec{n}}}{(\pi_1)^2_{\vec{n}\vec{m}}} \;=\; \frac{p_s(\vec{m})}{p_s(\vec{n})} \tag{6.5.3}$$

We state that, if the equilibrium is unbalanced in a direction by the ratio of transition probabilities then the ratio of the probability distributions will be pushed in the opposite direction to recover balance condition.

We know that the difference between the transition operators are the contribution of the commutator in normal ordering procedure (i.e. exchange among subsequent nodes) and the double sending from the same node

$$\begin{aligned}(\hat{\pi}_1)^2 \;&=\; \sum_{ijkl} \pi_{ij}\pi_{kl} a_i^\dagger a_k^\dagger b_j b_l \;+\; \sum_{ijkl} \pi_{ij}\pi_{kl}\delta_{jk}(1-\theta(n_j)) a_i^\dagger b_l \\ &=\; \sum_{\substack{ijkl \\ j\neq l}} \pi_{ij}\pi_{kl} a_i^\dagger a_k^\dagger b_j b_l \;+\; \sum_{ijk} \pi_{ij}\pi_{kj} a_i^\dagger a_k^\dagger b_j b_j \;+\; \sum_{ijkl} \pi_{ij}\pi_{kl}\delta_{jk}(1-\theta(n_j)) a_i^\dagger b_l \\ &=\; \hat{\pi}_2 \;+\; \hat{\pi}_\delta \;+\; \hat{\Delta}\end{aligned} \tag{6.5.4}$$

inserting in the first of (6.5.1)

$$\begin{aligned}(\hat{\pi}_2 \;+\; \hat{\pi}_\delta \;+\; \hat{\Delta})_{\vec{m}\vec{n}}\, p_s(\vec{n}) \;&=\; (\hat{\pi}_2 \;+\; \hat{\pi}_\delta \;+\; \hat{\Delta})_{\vec{n}\vec{m}}\, p_s(\vec{m}) \\ (\pi_2)_{\vec{m}\vec{n}}\, p_s(\vec{n}) \;-\; (\pi_2)_{\vec{n}\vec{m}}\, p_s(\vec{m}) \;&=\; (\,(\pi_\delta)_{\vec{n}\vec{m}} \;+\; (\Delta)_{\vec{n}\vec{m}}\,)\, p_s(\vec{m}) - (\,(\pi_\delta)_{\vec{m}\vec{n}} \;+\; (\Delta)_{\vec{m}\vec{n}}\,)\, p_s(\vec{n})\end{aligned} \tag{6.5.5}$$

and thus

$$(\,(\pi_\delta)_{\vec{m}\vec{n}} \;+\; (\Delta)_{\vec{m}\vec{n}}\,)\, p_s(\vec{n}) \;<\; (\,(\pi_\delta)_{\vec{n}\vec{m}} \;+\; (\Delta)_{\vec{n}\vec{m}}\,)\, p_s(\vec{m}) \tag{6.5.6}$$

is equivalent to (6.5.2).

Let consider two network states: $\vec{n}(00)$ with a couple of empty adjacent nodes and $\vec{m}$ without.

Numerical simulation [1] suggests the direction of the disequilibrium of balance equation

$$(\pi_2)_{\vec{m}\vec{n}(00)}\, p_s(\vec{n}(00)) \;<\; (\pi_2)_{\vec{n}(00)\vec{m}}\, p_s(\vec{m}) \tag{6.5.7}$$

that agree with our model iff

$$(\,(\pi_\delta)_{\vec{m}\vec{n}(00)} \;+\; (\Delta)_{\vec{m}\vec{n}(00)}\,)\, p_s(\vec{n}(00)) \;>\; (\,(\pi_\delta)_{\vec{n}(00)\vec{m}} \;+\; (\Delta)_{\vec{n}(00)\vec{m}}\,)\, p_s(\vec{m}) \tag{6.5.8}$$

We know all the terms of the latter, indeed

$$\begin{aligned}(\pi_\delta)_{\vec{n}(00)\vec{m}}\, p_s(\vec{m}) \;&=\; \frac{\langle \vec{n}(00)|\, \sum_{ijk} \pi_{ij}\pi_{kj} a_i^\dagger a_k^\dagger b_j b_j \;|\vec{m}\rangle}{\langle \vec{n}(00)|\, \vec{n}(00)\rangle}\, p_s(\vec{m}) \\ &=\; \sum_{ijk} \pi_{ij}\pi_{kj}\, \theta(m_j)\theta(m_j-1)\delta_{\vec{n}(00)\vec{m}+1_i+1_k-2_j}\, p_s(\vec{m})\end{aligned} \tag{6.5.9}$$

$$\begin{aligned}(\pi_\delta)_{\vec{m}\vec{n}(00)}\, p_s(\vec{n}(00)) \;&=\; \frac{\langle \vec{m}|\, \sum_{ijk} \pi_{ij}\pi_{kj} a_i^\dagger a_k^\dagger b_j b_j \;|\vec{n}(00)\rangle}{\langle \vec{m}|\, \vec{m}\rangle}\, p_s(\vec{n}(00)) \\ &=\; \sum_{ijk} \pi_{ij}\pi_{kj}\, \theta(n_j)\theta(n_j-1)\delta_{\vec{m}\vec{n}(00)+1_i+1_k-2_j}\, p_s(\vec{n}(00))\end{aligned} \tag{6.5.10}$$

$$\begin{aligned}(\Delta)_{\vec{n}(00)\vec{m}}\, p_s(\vec{m}) \;&=\; \frac{\langle \vec{n}(00)|\, \sum_{ijkl} \pi_{ij}\pi_{kl}\delta_{jk}(1-\theta(m_j)) a_i^\dagger b_l \;|\vec{m}\rangle}{\langle \vec{n}(00)|\, \vec{n}(00)\rangle}\, p_s(\vec{m}) \\ &=\; \sum_{ijl} \pi_{ij}\pi_{jl}\, (1-\theta(m_j))\theta(m_l)\delta_{\vec{n}(00)\vec{m}+1_i-1_l}\, p_s(\vec{m})\end{aligned} \tag{6.5.11}$$

$$\begin{aligned}(\Delta)_{\vec{m}\vec{n}(00)}\, p_s(\vec{n}(00)) \;&=\; \frac{\langle \vec{m}|\, \sum_{ijkl} \pi_{ij}\pi_{kl}\delta_{jk}(1-\theta(n_j)) a_i^\dagger b_l \;|\vec{n}(00)\rangle}{\langle \vec{m}|\, \vec{m}\rangle}\, p_s(\vec{n}(00)) \\ &=\; \sum_{ijl} \pi_{ij}\pi_{jl}\, (1-\theta(n_j))\theta(n_l)\delta_{\vec{m}\vec{n}(00)+1_i-1_l}\, p_s(\vec{n}(00))\end{aligned} \tag{6.5.12}$$

$\hat{\pi}_\delta$ represents the double sending of a single node and therefore it depends obviously on the occupation state of the node, but it doesn't depend on the occupation state of other nodes. Indeed the θ function arguments of every addendum depends only on one nodes index.

Thus (6.5.9) (6.5.10) are blind to the difference of a (00) couple instead of $(0 \dots 0)$ and are negligible to our purpose.

With a similar argumentation we can discard the terms of (6.5.11) and (6.5.12) with only one θ.

Finally we have to verify the inequality

$$\sum_{ijl} \pi_{ij}\pi_{jl}\,\theta(n_j)\theta(n_l)\delta_{\vec{m}\vec{n}(00)+1_i-1_l}\,p_s(\vec{n}(00)) \;<\; \sum_{ijl} \pi_{ij}\pi_{jl}\,\theta(m_j)\theta(m_l)\delta_{\vec{n}(00)\vec{m}+1_i-1_l}\,p_s(\vec{m}) \tag{6.5.13}$$

$\vec{m}$ and $\vec{n}(00)$ have to be network states that differ for the exchange of one particle, and we can estimate

$$\frac{p_s(\vec{m})}{p_s(\vec{n}(00))} \;=\; \frac{\psi_i}{\psi_j} \;\sim 1 \tag{6.5.14}$$

thus

$$\sum_{ijl} \pi_{ij}\pi_{jl}\,\theta(n_j)\theta(n_l)\delta_{\vec{m}\vec{n}(00)+1_i-1_l} \;<\; \sum_{ijl} \pi_{ij}\pi_{jl}\,\theta(m_j)\theta(m_l)\delta_{\vec{n}(00)\vec{m}+1_i-1_l} \tag{6.5.15}$$

and a rude estimating reads

$$\begin{aligned} &\sum_{ijl} \pi_{ij}\pi_{jl}\,\theta(n_j)\theta(n_l)\delta_{\vec{m}\vec{n}(00)+1_i-1_l} \;\sim\; M \,-\, n(0) \,-\, n(00) \\ &\sum_{ijl} \pi_{ij}\pi_{jl}\,\theta(m_j)\theta(m_l)\delta_{\vec{n}(00)\vec{m}+1_i-1_l} \;\sim\; M \,-\, n(0) \end{aligned} \tag{6.5.16}$$

verifying (6.5.8).

Since inequality is proved we can use (6.5.3) to write

$$\frac{p_{ss}(\vec{n}(00))}{p_{ss}(\vec{m})} \;>\; \frac{p_s(\vec{n}(00))}{p_s(\vec{m})} \tag{6.5.17}$$

Latter comparison shows that in a 1-FTC network with synchronous dynamics the probability to observe a state with a couple of adjacent nodes

empty (normalized with the probability of a generic connected state) is enhanced if compared to a subsequent dynamics system.

As we have shown the probability distribution can be derived from a principle of maximum entropy, in the Gibbs sense.

The found result of enhancement of $n(00)$ states should therefore correspond to a major number of admissible realization of such a state respect $n(0 \dots 0)$

We can try to explain this phenomenon as a problem of volumes exclusion.

In $n(0 \dots 0)$ we exclude two volumes, in $n(00)$ we exclude a single volume, and if the latter leaves a bigger volumes than the two volumes separated, there are more possible configuration to realize $n(00)$.

Since we observe this effect only in FTC case this differences in volumes must be related to the multinomial coefficient of weights.

Chapter 7

Conclusions

The random walks on network may 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 shed light on universal features relevant to understand the stationary solutions or the rising of critical states like congestion. In this thesis we studied the dynamics of N non-interacting particles on a connected and undirected network using an operatorial approach.

The network state has been described by means of Fock-like states and the dynamics has been represented using ladder operators.

The non-interacting condition for the particles corresponds to a free particles dynamics, as naively expected, only assuming an unlimited transport capacity of the network.

In such a case we correctly recover well known results: the probability distribution of a network state is the product of the probabilities distributions induced by the simple random walk of a single free particle, with the statistical weight of the configuration.

But our formalism allows us to consider more general cases when non linear interactions among particles are introduced through the dependence of the transition probabilities from the network state.

A relevant case is when one introduces a limited transportation capacity, that is a natural assumptions for real transportation systems.

Assuming a limited transport capacity of the network, for simplicity 1 particle per node, although particles are non-interacting the dynamics substantially changes, and we can no more speak of free particles.

The new dynamics is described defining unusual destruction operator $\hat{b}$ and establishing the substitution rule $\hat{a} \to \hat{b}$ in transition operators.

The dynamical restriction imposed by the network limitations results in

a differentiation of the particles by means of the node, in the moment it decides which one moves. Therefore fails the equivalence between following the particles or the states of the nodes, and we recognize an account of it in the need to normalize the processes with the number of nodes, instead of the particles.

Consequently the steady state changes, loosing the multinomial coefficient representing the weight of the free particles network state. Nevertheless, for a one-exchange evolution, it is still possible to analytically check that the distribution is an exact solution of the Master equation.

The steady state of the system generates a distribution on the single nodes pushed toward the 0 of occupation number.

From a physical point of view the lack of a universal normalization is equivalent to a slowing down of the evolution time scale for the network states with empty node. This implies an increase of the visiting probability of such nodes that is equivalent to the existence of an entropic force which favours these states.

We succeeded in proving that the stationary distribution is an exponential distribution as expected for a random walk with friction, that can be related to an Entropic principle.

Numerical simulations points out a significant difference from the analytical distribution when one considers synchronous movements in the network. To analyze this problem we took profusely advantage of the defined second quantization formalism, consolidated in the first part of the work, to define a double step evolution of the network.

Our aim is to apply a perturbative approach to understand and quantify the results of numerical simulations.

In particular we pointed out in an easy way the differences occurring between a subsequent and a synchronous exchange process thanks to commutation rules.

As a first general remark, independent from the transport limitation, a slow down of the dynamics occurs in the synchronous scenario, due to the inhibition of a certain number of processes (i.e. lowering the links in the states space).

The difference between a subsequent or a synchronous realization of the particle exchanges emerges in the probability assigned to subsequent nodes processes.

In the infinite transport capacity network case we are able to recast it in a one-step like operator, therefore admitting the steady state as an eigenvector.

To define synchronous Laplacian we followed a derivation based on the individuation of incoming and outoing fluxes. In this way we can observe

a balance of the process weight variations, with the result of an unchanged steady state.

The finite transport network generates a much more involved situation.

The unusual network-state dependent commutation relations for $\hat{b}$, the destruction operator of finite capacity nodes, give a non symmetric contribution to the incoming and outgoing fluxes. Therefore the steady solution of the subsequent dynamics Master equation does not hold in the synchronous scenario.

In order to perturbatively study the new steady state we relate the Laplacian of the synchronous dynamics to the Laplacian of the single exchange dynamics, by means of two operators representing corrective terms.

Finally we attempt to explain a feature that has been pointed out by numerical simulations [1] in the finite transport case: i.e. the overexpression of the state with couples of adjacent empty nodes.

To this purpose we employ the analytical results we have found for the subsequent dynamics and the equation that relates it to the synchronous one.

Our assumptions is that this overexpression is a consequence of a change of the visiting probability of such states with respect to the stationary distribution of the one step process.

In particular for the 1-FTC synchronous dynamics we recognize in the Master equation a corrective term depending on the empty states of adjacent nodes.

Considerations based on the detailed balance condition, assumed satisfied by the unknown steady state, lead us to write an inequality. Under some approximations the inequality suggests to understand the corrective term as an enhancement for the probability of states with adjacent empty nodes.

In this way we succeeded in differentiating the synchronous steady distribution from the single step process one, since the latter is blind to the adjacency of empty nodes.

An interesting perspective for a further development of the topic could be the application of path integrals tools to the problem.

Starting from the work of Peliti the mapping of Master equations into effective actions has been widely used and extended to many stochastic processes.

The main advantage of this method is the possibility to study perturbatively hardly handable systems and, although out of equilibrium, to employ techniques proper of equilibrium statistical mechanics (such as renormalization group [13]).

Peliti itself proposed a simple model of diffusion on a lattice [5]. Starting from a Liouvillian very similar to (3.4.10) he obtained an effective action exactly solved by means of the definition of the discrete version of derivative operator. Ultimately this is based upon the regular topological feature of the lattice, that fails in the passage to a network.

However, the extension of this kind of model to network backgrounds seems to be at least fascinating.

The definition of discrete derivative on network proposed by Bazzani [1] can be applied to attempt an exact solution of an effective action based on (3.4.10), namely something like

$$\begin{aligned} U_\tau(\vec{\eta},\vec{\bar{\eta}}) \;=\; & \int \mathcal{D}\vec{\eta}\mathcal{D}\vec{\bar{\eta}}\, exp\{ - \int_0^\tau dt[\sum_k i\bar{\eta}_k\dot{\eta}_k \\ & - \sum_{kj} \pi_{kj}(i\bar{\eta}_k\eta_j \;-\; i\bar{\eta}_j\eta_j) \;+\; \sum_j i\bar{\eta}_j(\tau)\eta_j(\tau)\} \end{aligned}$$

$$\text{where} \quad \mathcal{D}\vec{\eta} \equiv \prod_{i=1}^{M} \mathcal{D}\eta_i \quad \text{and} \quad \mathcal{D}\eta \equiv \lim_{N\to\infty} \prod_{k}^{N-1} \frac{d\eta_k}{\sqrt{2\pi}}$$

recovering in this way the single exchange on ITC network case.

Then would be straightforward the extension to 1-FTC case, in order to perturbatively study the steady solution of the synchronous dynamics.

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