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Matthieu Vanicat

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THÈSE

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Présentée par

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Préparée au sein du **Laboratoire d'Annecy-le-Vieux de Physique Théorique** et de l'**École doctorale de physique de Grenoble**

Approche intégrabiliste des modèles de physique statistique hors d'équilibre

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Preface

The aim of this thesis is to study out-of-equilibrium statistical physics from the integrable systems point of view. Integrability is used to obtain exact results on models relevant for non-equilibrium physics.

The theory of equilibrium statistical physics has been very successful to describe the properties of systems at thermodynamic equilibrium. Unfortunately, such a theory still eludes us for out-of-equilibrium systems. We lack a theoretical framework and fundamental principles (such as the entropy maximization principle for equilibrium physics) describing the behavior of such systems. We do not know, for instance, how the Boltzmann distribution should be modified. In the last decades, however, there have been promising attempts at constructing generalizations of thermodynamic potentials to out-of-equilibrium systems. The framework of large deviation theory has become very popular and appears particularly efficient to express the out-of-equilibrium properties. It is seen as a possible unifying formalism to deal with statistical physics systems, both in and out of equilibrium. A short introduction to out-of-equilibrium statistical physics can be found in chapter one. We define the framework of Markov chains and introduce the notion of a non-equilibrium stationary state (NESS) in this context. We point out the relevance of the cumulant generating function and the large deviation function for well chosen “dynamic” observables to describe these NESS. We explain how these quantities can be in principle exactly computed with the help of a current-counting deformation of the Markov matrix. We recall also the main tools and properties of the underlying framework, the large deviation theory. The macroscopic fluctuation theory (MFT) uses the large deviation theory to state a general framework to describe non-equilibrium diffusive systems in the thermodynamic limit. An introduction on MFT can be found in chapter five.

In this context, the role of exactly solvable models (integrable models) is central. They can be used as a benchmark to test the predictions of the theories, and they may also help to guess potential fruitful developments. It thus appears important to construct these integrable out-of-equilibrium models, and to develop methods to compute their stationary states and dynamical properties analytically. This manuscript aims to be part of this process. We build on existing techniques to construct several new examples of integrable out-of-equilibrium models. An introduction to integrability in the context of Markov processes can be found in chapter two. The key notions, such as conserved quantities, R and K -matrices, transfer matrices and Bethe ansatz are introduced in the perspective of out-of-equilibrium statistical physics. We detail the periodic boundary condition case as well as the open boundaries condition case. Some techniques for solving the Yang-Baxter and reflection equations are exposed: for example, through the quantum groups framework, and Baxterisation procedures.

To complete the process, it appears highly important to build convenient methods to solve these integrable out-of-equilibrium models and extract exact expressions of physical quantities. In the last few years, the matrix ansatz technique has proven to be very efficient at expressing analytically the stationary state of one dimensional interacting particles systems. It can be seen as a bridge making connection between the non-equilibrium stationary states and the theory of integrable systems. It will play a key role in this manuscript. A review of the state of the art of this method can be found in chapter three. After introducing it on the totally asymmetric simple exclusion process (TASEP), we give its main properties and we show that it often allows us to compute conveniently relevant physical observables, such as the particle currents and densities. We explain how it can be used in integrable models. We compute

exactly the stationary states of some examples in matrix product form and derive analytical expressions for relevant physical quantities. These results allow us to test in particular cases some predictions of the MFT.

The outline of the manuscript is as follows. The first chapter is dedicated to non-equilibrium statistical physics. We try to present concisely the main relevant concepts. We attempt to give a modest new perspective on the Langevin equation on the ring with a non-conservative force, using the rooted trees expansion of the steady state of non-equilibrium Markovian processes.

The second chapter deals with integrability. We review the general theory and provide some new results. First we give an interpretation of the transfer matrices of the periodic and open TASEP as discrete time Markovian processes. Then we introduce new algebraic structures to construct solutions to the Yang-Baxter equation and to the reflection equation through Baxterisation procedures. This yields for instance the determination of integrable boundary conditions for the multi-species asymmetric simple exclusion process (ASEP). We also show how the coordinate Bethe ansatz can be used to find new integrable systems with two species of particles that can react in the bulk. Finally we introduce new integrable out-of-equilibrium models, given by the resolution of the Yang-Baxter and reflection equations: the dissipative symmetric simple exclusion process (DiSSEP), an open boundaries 2-species TASEP and an open boundaries multi-species symmetric simple exclusion process (multi-species SSEP).

Chapter three presents the matrix ansatz technique, which aims to express analytically non-equilibrium stationary states. The connection with the integrable models is explored in detail and suggests a systematic construction of a matrix product steady state in such models. It relies on two key relations: the Zamolodchikov-Faddeev and Ghoshal-Zamolodchikov relations. These general prescriptions are then illustrated by the analytical matrix product construction of the stationary state of the three previously introduced integrable stochastic processes: the DiSSEP, the 2-species TASEP and the multi-species SSEP. It allows us to compute exactly relevant physical quantities in these models, such as particle densities and currents.

Chapter four addresses the problem of the exact computation of the cumulants of the current in the open boundaries ASEP from a new perspective. The current-counting deformation of the Markov matrix is studied through the quantum Knizhnik-Zamolodchikov (q KZ) equations. We provide solutions to these equations in a matrix product form. The connection between the solutions of the q KZ equations and the Koornwinder polynomials is explored. It yields a matrix product expression for certain Koornwinder polynomials. Moreover it suggests an unexpected link between the theory of symmetric polynomials and the cumulant generating function of the current in the stationary state. The latter is conjectured to be obtained as a specific limit of symmetric Koornwinder polynomials.

The last chapter deals with the hydrodynamic limit. We show how the large system size limit can be performed on the physical observables of the three models introduced in chapter three. It yields the mean density and current profiles, but also, depending on the model under consideration, the phase diagram and the relaxation rate (gap). We then present a coarse grained description of the diffusive models studied in the manuscript, called the macroscopic fluctuation theory. This general approach to non-equilibrium systems in the hydrodynamic limit can in principle predict the fluctuations of the particles current and density in the stationary state. We check these predictions for models with evaporation and condensation of particles against the exact results obtained in chapter III for the cumulant of the current in the DiSSEP. We also propose an extension of the theory for multi-species diffusive models based on the analytical results derived for the multi-species SSEP.

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- Crampe, N., Mallick, K., Ragoucy, E., Vanicat, M., *Inhomogeneous discrete-time exclusion processes*, J. Phys. **A 48** (2015) 484002.
- Crampe, N., Ragoucy, E., Rittenberg, V., Vanicat, M., *Integrable dissipative exclusion process: Correlation functions and physical properties*, Phys. Rev. **E 94** (2016) 032102.
- Crampe, N., Evans, M. R., Mallick, K., Ragoucy, E., Vanicat, M., *Matrix product solution to a 2-species TASEP with open integrable boundaries*, J. Phys. **A 49** (2016) 475001.
- Crampe, N., Finn, C., Ragoucy, E., Vanicat, M., *Integrable boundary conditions for multi-species ASEP*, J. Phys. **A 49** (2016), 375201.
- Crampe, N., Frappat, L., Ragoucy, E., Vanicat, M., *3-state Hamiltonians associated to solvable 33-vertex models*, J. Math. Phys. **57** (2016) 093504.
- Crampe, N., Frappat, L., Ragoucy, E., Vanicat, M., *A new braid-like algebra for Baxterisation*, Commun. Math. Phys. **349** (2017) 271.
- Finn, C., Vanicat, M., *Matrix product construction for Koornwinder polynomials and fluctuations of the current in the open ASEP*, J. Stat. Mech. (2017) P023102
- Vanicat, M., *Exact solution to integrable open multi-species SSEP and macroscopic fluctuation theory*, J. Stat. Phys. **166** (2017) 1129.

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Chapter I

Out-of-equilibrium statistical physics

A Equilibrium versus non-equilibrium

1 Physical properties of equilibrium and non equilibrium systems

We start by presenting the properties of systems at thermodynamic equilibrium. We recall briefly the fundamental principles of equilibrium statistical physics. This will help us to gain some intuition about out-of-equilibrium systems and to motivate the different ideas proposed to describe such systems.

a) Equilibrium and entropy maximization

At the macroscopic level, a classical¹ physical system at thermodynamic equilibrium is roughly defined as a system at equilibrium for any physical process we can imagine. For instance it should be at thermal, mechanical, electro-dynamical and chemical equilibrium. In other words this is a state which does not display macroscopic currents of any physical quantities (for example energy, momentum, charges, particles). We know that these states can be completely characterized, or described, by a few macroscopic extensive variables such as the energy, the volume, the number of particles (or their intensive conjugate variables such as the temperature, the pressure, the chemical potential). An example of thermodynamic equilibrium is given by a gas of molecules in a closed room at thermal equilibrium with its environment.

In order to have a more precise description of such states, we need to formalize a bit the discussion. Assume that a system can be in several different configurations \mathcal{C} and denote by \mathfrak{C} the set of these configurations. \mathfrak{C} is sometimes called the *phase space* or the *configuration space* of the system. For instance, if the system is a gas of molecules contained in a fixed closed room, a configuration \mathcal{C} could be the knowledge of the positions and velocities (plus possibly some internal degrees of freedom) of each of the molecules constituting the gas. Another example is the human brain, whose configurations can be simply the knowledge of all the connections between the neurons, or can be chosen to be the knowledge of the precise chemical content of each neuron and synapse.

These examples illustrate that a configuration \mathcal{C} can sometimes be an effective description of the system, which does not necessarily carry all the information about each of its microscopic degrees of freedom. This is explained by some uncertainties we may have on the system (what is the precise composition of a neuron?) or by some assumptions we made to simplify the description (some internal freedom of the molecules may have negligible impact on the behavior of the gas).

This often imposes us to only have a statistical description of the system, trying to model an effective dynamics in this simplified configuration space. This motivates the introduction

¹The discussion focuses here on classical systems but it can be transposed to quantum systems

of a probability $\mathcal{P}(\mathcal{C})$ to observe the system in a configuration \mathcal{C} .

If we assume, for the sake of simplicity, that the set of configurations \mathfrak{C} is finite (we can adapt the discussion below to infinite sets), the entropy associated to the probability distribution \mathcal{P} is defined as²

$$\mathcal{H}(\mathcal{P}) = - \sum_{\mathcal{C} \in \mathfrak{C}} \mathcal{P}(\mathcal{C}) \ln(\mathcal{P}(\mathcal{C})). \quad (\text{I.A.1})$$

The main features of the entropy are the following. A probability being between 0 and 1, it is easy to see that the entropy is always non-negative. The entropy is additive: the entropy associated to the joint probability distribution of two independent random variables is the sum of the entropies associated to the probability distributions of each random variable. In other words, from a physical point of view, if we have two systems that are non-interacting (far from each other for instance), the entropy of the two systems is equal to the sum of the entropies of each system.

The entropy can be intuitively understood as the amount of disorder (or of lack of information) carried by the system. To gain some feeling about this statement, let us consider two extremal cases. If the system is in configuration \mathcal{C} with probability 1 (all the others configurations having vanishing probabilities), *i.e* if we have a full information about the state of the system, the entropy is equal to 0 (it is minimal). Conversely, if we don't know anything about the state of the system, *i.e* if the probabilities of each configuration are equal, the entropy is given by $\ln \Omega$, where Ω is the number of configurations. This value is the maximum of the entropy. Indeed if we want to maximize the entropy under the constraint $\sum_{\mathcal{C} \in \mathfrak{C}} \mathcal{P}(\mathcal{C}) = 1$, we obtain for all $\mathcal{C} \in \mathfrak{C}$ the equation

$$\frac{\partial \mathcal{H}(\mathcal{P})}{\partial \mathcal{P}(\mathcal{C})} - \lambda \frac{\partial}{\partial \mathcal{P}(\mathcal{C})} \left(\sum_{\mathcal{C}' \in \mathfrak{C}} \mathcal{P}(\mathcal{C}') \right) = 0, \quad (\text{I.A.2})$$

where λ is the Lagrange multiplier. It implies that we have for all \mathcal{C} , $\ln \mathcal{P}(\mathcal{C}) + 1 + \lambda = 0$, which proves that the probabilities are all equal and their common value is necessarily $1/\Omega$ (due to the sum to 1 constraint).

This entropy is at the heart of the theory of equilibrium statistical physics. The fundamental law can be stated as follows. A thermodynamic equilibrium is a state (*i.e* a probability distribution) which maximizes the entropy (I.A.1) under a set of constraints [1]. These constraints are determined by the interactions of the system with its environment (*i.e* the reservoirs) and consist in imposing a fixed value for the average of certain physical observables.

They are roughly established by the following procedure³. We have first to identify the physical quantities, which are conserved by the dynamics (for instance the energy, the particle number, the charge) when the system is isolated, *i.e* disconnected from the reservoir. Then, considering the system in contact with the reservoirs again, we have to determine which of these physical quantities are exchanged with the reservoir. The constraints are finally written down by imposing a fixed average value for each of these physical quantities.

For instance, let us consider a gas of particles in a closed room. If the system is completely isolated (no particle or energy exchanges), there is no constraint and the maximization of the entropy yields $\mathcal{P}(\mathcal{C}) = 1/\Omega$. This distribution is commonly called the *microcanonical* distribution.

If the system can exchange energy with the reservoir (heat bath), it imposes a fixed value for the average energy $\langle E \rangle := \sum_{\mathcal{C} \in \mathfrak{C}} \mathcal{P}(\mathcal{C}) E(\mathcal{C})$, where $E(\mathcal{C})$ denotes the energy of the system

²We give here the definition of the entropy used in probability theory. In a more physical context, this definition often involves the Boltzmann constant k , which is set to 1 here.

³Establishing precisely the constraints (for the entropy maximization) can be delicate, particularly in systems, which possess many conserved quantities when they are isolated (typically the integrable systems, see discussion on quenched dynamics in subsection 2 and also chapter II). We consider in such systems Generalized Gibbs Ensembles, see for instance [2, 3]

in configuration \mathcal{C} . The maximization of the entropy yields the equation

$$\frac{\partial \mathcal{H}(\mathcal{P})}{\partial \mathcal{P}(\mathcal{C})} - \lambda \frac{\partial}{\partial \mathcal{P}(\mathcal{C})} \left(\sum_{\mathcal{C}' \in \mathfrak{C}} \mathcal{P}(\mathcal{C}') \right) - \beta \frac{\partial}{\partial \mathcal{P}(\mathcal{C})} \left(\sum_{\mathcal{C}' \in \mathfrak{C}} \mathcal{P}(\mathcal{C}') E(\mathcal{C}') \right) = 0, \quad (\text{I.A.3})$$

where λ and β are the Lagrange multipliers. This implies that

$$\mathcal{P}(\mathcal{C}) = \frac{e^{-\beta E(\mathcal{C})}}{Z}, \quad \text{with} \quad Z(\beta) = \sum_{\mathcal{C} \in \mathfrak{C}} e^{-\beta E(\mathcal{C})}. \quad (\text{I.A.4})$$

This distribution is commonly called the *canonical* distribution (or also the Boltzmann or Gibbs distribution). β is called the inverse temperature.

If the system can in addition exchange particles with the reservoir, the average number of particles $\langle N \rangle := \sum_{\mathcal{C} \in \mathfrak{C}} \mathcal{P}(\mathcal{C}) N(\mathcal{C})$ is also fixed ($N(\mathcal{C})$ denotes the number of particles in the system in configuration \mathcal{C}). A similar computation gives

$$\mathcal{P}(\mathcal{C}) = \frac{e^{-\beta E(\mathcal{C}) - \mu N(\mathcal{C})}}{Z}, \quad \text{with} \quad Z(\beta, \mu) = \sum_{\mathcal{C} \in \mathfrak{C}} e^{-\beta E(\mathcal{C}) - \mu N(\mathcal{C})}. \quad (\text{I.A.5})$$

This distribution is commonly called the *grand-canonical* distribution. μ is called the chemical potential.

Z is called the partition function. It allows us to define the free energy $F = -\ln Z$. The free energy is closely related to the following cumulant generating function⁴

$$\ln \langle e^{\nu E(\mathcal{C})} \rangle = \ln \sum_{\mathcal{C} \in \mathfrak{C}} e^{\nu E(\mathcal{C})} \frac{e^{-\beta E(\mathcal{C})}}{Z} \quad (\text{I.A.6})$$

$$= F(\beta) - F(\beta - \nu). \quad (\text{I.A.7})$$

The free energy thus provides the fluctuations of the energy of the system (average value, variance, and higher order cumulants) by taking successive derivative of $F(\beta)$ with respect to the inverse temperature β .

Note also that the entropy is obtained by the Legendre transform of the free energy (see subsection b) for the definition and properties of Legendre transformation). We have indeed, from previous computations, that

$$\mathcal{H}(\mathcal{P}) = \beta \langle E \rangle - F(\beta), \quad \text{with} \quad \frac{\partial F}{\partial \beta}(\beta) = \langle E \rangle. \quad (\text{I.A.8})$$

The intensive variable β is conjugated to the extensive variable $\langle E \rangle$. Conversely the free energy can be obtained from the Legendre transform of the entropy.

We are now interested in the study of systems which are not at thermodynamic equilibrium. This is the purpose of the next subsection.

b) Non equilibrium and macroscopic currents

An out-of-equilibrium system is basically a system which is not at thermodynamic equilibrium. It can be either relaxing toward a stationary state or in a non-equilibrium stationary state (NESS).

At the macroscopic scale, it translates into the presence of non-vanishing currents of physical quantities (such as energy, particles, charges). A schematic example of such states is given by two particle reservoirs at different densities, connected by a pipe. The high density reservoir will pour into the low density one, establishing a non vanishing macroscopic particle current. In fact, we can find out-of-equilibrium systems everywhere, ranging from the traffic flow on

⁴We present here the case of the canonical distribution but it can be easily adapted to the grand-canonical distribution

a highway, to the development of the human brain, and including propagation of a fire in a forest or dynamics of a group of fish.

Unfortunately, there is no general theory to describe these systems. We do not know what are the relevant variables (like the temperature, pressure, chemical potential or other intensive variables in the thermodynamic equilibrium case) to describe these states. We would like to proceed from a fundamental law, such as an entropy maximization principle, which could provide us some tools, such as the thermodynamic potentials, to describe accurately these systems. We may need to enlarge the configuration space to formulate such maximization entropy principle, considering for instance path histories instead of “static” configurations, and using some kind of action to set the constraints imposed by the environment.

A few promising attempts have been made in the last decades. The discoveries of connections between statistical physics and large deviation theory, could provide an efficient framework to develop a theory for out-of-equilibrium systems. It led for instance to the formulation of the macroscopic fluctuation theory, which has proven to provide a powerful description of non-equilibrium diffusive systems in the hydrodynamic limit (see chapter V).

But a lot remains to be understood. This motivates the study of particular non-equilibrium systems, focusing on the simplest ones, to compute relevant physical quantities and try to infer more universal properties. From this perspective exactly solvable models appear as very powerful tools, and have been used in a wide range of different contexts and frameworks.

We present below a (non-exhaustive) list of mathematical frameworks commonly used to describe out-of-equilibrium systems.

2 Different frameworks for out-of-equilibrium physics

Many different formalisms had been developed to describe out-of equilibrium systems. We present here only a few of them which are widely used in the literature. We try to put, when possible, an emphasis on the role played by integrability and exact solvability in these different frameworks.

We stressed at the beginning of this chapter, that a system involving a huge number of components and with uncertainties on the exact relevant microscopic content and dynamics, is likely to be described by some effective state and some effective dynamics. This motivates the fact of introducing a probability distribution (on the configuration set of the system) to describe the statistical properties of the system. The next thing to do is to determine how this probability distribution evolves with time, *i.e.* what is the effective dynamics chosen to model the time evolution of the system. In the thermodynamic equilibrium case, the precise choice of this dynamics has basically no impact on the long time behavior of the system, which reaches the Boltzmann distribution. But in the non-equilibrium case the choice of the framework used to encode the time evolution of the probability distribution is important to model the relaxation toward equilibrium or the non-equilibrium stationary state. The formalisms presented below correspond to different ways to describe the system dynamics.

Langevin equation A formalism used to describe out-of-equilibrium systems is the Langevin equation. The idea is to add some random component in the force when writing the fundamental law of classical mechanics. The aim is to model some uncertainties in the dynamics at the microscopic scale. If we want for instance to describe the dynamics of a grain of pollen in a bowl of water, we do not know precisely the positions and velocities of each of the molecules of water, which are subject to thermal fluctuations. This will imply random collisions with the grain of pollen and translate into some random component in the force that acts on the pollen. This motivates the following description of the dynamics, where x , v and m are respectively the position, the velocity and the mass of the grain of pollen, γ is a friction coefficient, F is a force and $\xi(t)$ is a Gaussian white noise which satisfies $\langle \xi(t) \rangle = 0$ and $\langle \xi(t)\xi(t') \rangle = \Gamma\delta(t - t')$

$$\begin{cases} m \frac{dv}{dt} = -m\gamma v + F(x) + m\gamma\xi(t) \\ \frac{dx}{dt} = v. \end{cases} \quad (\text{I.A.9})$$

For a high friction coefficient $\gamma \gg 1$, the acceleration can be neglected and the problem reduces to

$$\frac{dx}{dt} = \frac{F(x)}{m\gamma} + \xi(t) \quad (\text{I.A.10})$$

It can be shown that the probability distribution of the process $\mathcal{P}(x, t)$ (*i.e* the probability to find the particle in position x at time t) satisfies the Fokker-Planck equation [4]

$$\frac{\partial}{\partial t} \mathcal{P}(x, t) = -\frac{\partial}{\partial x} \left(\frac{F(x)}{m\gamma} \mathcal{P}(x, t) \right) + \frac{\Gamma}{2} \frac{\partial^2}{\partial x^2} \mathcal{P}(x, t) \quad (\text{I.A.11})$$

The derivation of (I.A.11) from equation (I.A.10) is not straightforward and relies essentially on the use of Itô calculus. We do not provide the details of the computations here. Some consistency checks, on the time evolution of the average value of x for instance, can be nevertheless easily performed.

For the sake of simplicity we can study this Fokker-Planck equation on a ring of perimeter 1, *i.e* imposing periodic boundary condition. The probability distribution has to be consistent with the periodic geometry of the ring, *i.e* $\mathcal{P}(0, t) = \mathcal{P}(1, t)$.

We are looking for the stationary state of the problem, *i.e* a time-independent distribution $\mathcal{S}(x)$ satisfying the Fokker-Planck equation. It is straightforward to deduce that it has to solve the following equation

$$\frac{\Gamma}{2} \frac{d}{dx} \mathcal{S}(x) = \frac{F(x)}{m\gamma} \mathcal{S}(x) + C, \quad (\text{I.A.12})$$

where C is a constant term.

In the case where the force is conservative, *i.e* $\int_0^1 F(u) du = 0$, we can define a potential $V(x) = -\int_0^x F(u) du$ such that $F(x) = -dV/dx$. Note that this potential fulfills the periodicity condition $V(0) = V(1)$ (this would not have been the case for a non-conservative force). In this case the stationary distribution $\mathcal{S}(x)$ is a thermal equilibrium and is given, as expected, by the Boltzmann distribution

$$\mathcal{S}(x) = \frac{1}{Z} \exp\left(-\frac{V(x)}{kT}\right), \quad (\text{I.A.13})$$

with temperature given by $2kT = m\gamma\Gamma$.

In the case where the force is not conservative, $\mathcal{S}(x)$ is not the Boltzmann distribution anymore but a non-equilibrium stationary distribution given (up to a normalization) by

$$\mathcal{S}(x) = \int_0^x du \exp\left(\int_u^x \frac{2F(y)}{\Gamma m\gamma} dy\right) + \int_x^1 du \exp\left(\int_u^1 \frac{2F(y)}{\Gamma m\gamma} dy + \int_0^x \frac{2F(y)}{\Gamma m\gamma} dy\right). \quad (\text{I.A.14})$$

It is indeed straightforward to check that it satisfies (I.A.12) with the constant $C = \frac{\Gamma}{2}(1 - \exp(\int_0^1 \frac{2F(y)}{\Gamma m\gamma} dy))$ and that it fulfills the periodicity condition $\mathcal{S}(0) = \mathcal{S}(1)$. A more intuitive construction of this solution, from a discrete periodic lattice, will be given later in this chapter.

Markov chains Another framework that has become widely used to deal with out-of-equilibrium dynamics is Markov chain theory [5]. It models the system's effective dynamics using the following idea. The system has a given probability $w(\mathcal{C} \rightarrow \mathcal{C}')$ to jump from a given configuration \mathcal{C} to another configuration \mathcal{C}' . The main assumption is that the dynamics is supposed to have no memory: the jump probability depends only on the starting configuration \mathcal{C} and on the target configuration \mathcal{C}' but not on the whole history of the system before arriving in configuration \mathcal{C} . The probability rate can also depend on the time when the jump occurs. Note that the stochastic dynamics of the system has a convenient graphical interpretation: the different configurations of the system are interpreted as the vertices of a graph and the jump probabilities as the oriented edges of the graph, see for instance figures I.1 and I.3.

This description is quite general and can be used to model a wide range of systems and dynamics in very different fields, going from social science, economy, population dynamics to

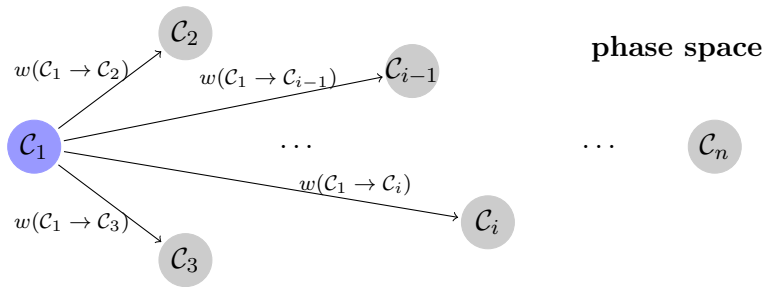


Figure I.1: Graphical representation of a Markov chain

statistical physics, applied mathematics and including chemistry, biophysics, epidemiology and genetics.

The advantage is that, the whole information about the stochastic dynamics of the system can be stored in a single matrix, called the Markov matrix, which contains all the jump probabilities. This allows to recast the time evolution of the probability distribution associated to the system as a linear algebra problem, called the master equation, and use the linear algebra machinery to study it.

Note that the 'no memory' assumption can be partially relaxed (while still using the Markovian formalism) by enlarging the configurations set of the system. If we want for instance the dynamics to depend on the two last configurations of the system (instead of only the last one), we just need to define a Markov chain on 'super configurations', which are defined as a couple of usual configurations of the system. This can be generalized to more complicated dynamics with memory.

This Markov chain framework will be the one used in this manuscript. We will see that integrability can play a key-role to study Markovian processes, because it allows us in some particular cases to compute analytically the stationary state of the model or even to diagonalize exactly the Markov matrix. We will focus on one dimensional interacting particle systems, whose Markov matrices are often closely related to quantum spin chain Hamiltonians, which allows us to use the quantum integrability machinery. In particular we will see that the non-equilibrium stationary states of such models can be often expressed in a matrix product form, with the help of the R -matrix, which is the key object in quantum integrability. This will be discussed in detail in chapter II and chapter III.

Quantum systems: Lindblad equation and quenched dynamics In the last few years the study of out-of-equilibrium quantum systems has become a very active field of research. We present very briefly two approaches frequently used to model such systems.

The first one is the quenched dynamics. The idea can be roughly summarized as follows. We would like to study the thermalization of the system, *i.e* the relaxation of the system toward thermodynamic equilibrium, by pushing it far from equilibrium. This can be achieved by choosing adequately the initial condition or by changing quickly a parameter in the Hamiltonian governing the dynamics. The whole system is decomposed into two subsystems: one could be thought of as playing the role of the environment (*i.e* the reservoir) and the other one as playing the role of a non-isolated system in interaction with the reservoir. The integrable spin chains have a central role in this context. The reason is twofold. Firstly, the quantum Hamiltonian of such models can be diagonalized exactly using Bethe ansatz, which gives theoretically access to the full dynamics of the system and allows us in principle to study analytically the relaxation and equilibrium properties of the system. Secondly, an important feature of integrable models is the fact that they possess a lot of conserved quantities (also called conserved charges). They thus provide toy models to determine what are the relevant charges required in the Boltzmann-like distribution. This led to the development of the notion of *Generalized Gibbs Ensembles* [2,3] and to the discovery of the relevance of quasi-local charges [6].

The second method is the Lindblad equation [7]. This is an equation for the density matrix

of a statistical quantum system. This roughly corresponds to the master equation (I.B.5), which we will encounter in the context of Markov chains. It can for instance describe a quantum system with stochastic interactions with reservoirs. When the system is in contact with two reservoirs at different temperatures (or at different chemical potentials), the density matrix will converge toward a non-equilibrium stationary state (which is not given by a Boltzmann statistics in general). Once again, the integrable quantum spin chains play a privileged role in this context [8–15]. The key object of integrability, the R -matrix, provides an efficient framework, through the RTT algebra (see chapter II for details) to construct the stationary density matrix in a matrix product form.

We now come back to the case of Markov chains, which will be intensively used in this manuscript. We define more precisely this object and present the main tools and properties associated with it.

B Markov chains and stationary states

1 Markov chains

a) Discrete time

We introduced heuristically the concept of Markov chain in the previous section. We now present a more formal mathematical definition.

Definition B.1. *A time-homogeneous discrete time Markov process on a finite state space is a sequence of random variables $(S_n)_{n \geq 0}$ that take values on a finite set \mathfrak{C} and which satisfy the following properties*

$$\forall n \in \mathbb{N}, \forall \mathcal{C}_1, \dots, \mathcal{C}_n \in \mathfrak{C}, \quad \mathbb{P}(S_n = \mathcal{C}_n | S_0 = \mathcal{C}_0, \dots, S_{n-1} = \mathcal{C}_{n-1}) = \mathbb{P}(S_n = \mathcal{C}_n | S_{n-1} = \mathcal{C}_{n-1}), \quad (\text{I.B.1})$$

and

$$\forall n \in \mathbb{N}, \forall \mathcal{C}, \mathcal{C}' \in \mathfrak{C}, \quad \mathbb{P}(S_{n+1} = \mathcal{C} | S_n = \mathcal{C}') = \mathbb{P}(S_n = \mathcal{C} | S_{n-1} = \mathcal{C}'). \quad (\text{I.B.2})$$

To be more explicit, S_n stands for the state of the system at time n . The set \mathfrak{C} represents the configuration space of the system. The quantity $\mathbb{P}(S_n = \mathcal{C})$ denotes the probability for the system to be in the configuration \mathcal{C} at time n . To shorten the notation we introduce

$$P_n(\mathcal{C}) := \mathbb{P}(S_n = \mathcal{C}). \quad (\text{I.B.3})$$

The conditional probability $\mathbb{P}(S_n = \mathcal{C}_n | S_0 = \mathcal{C}_0, \dots, S_{n-1} = \mathcal{C}_{n-1})$ stands for the probability for the system to be in configuration \mathcal{C}_n at time n , knowing that it was in configurations $\mathcal{C}_0, \mathcal{C}_1, \dots, \mathcal{C}_{n-1}$ at time $0, 1, \dots, n-1$ respectively (*i.e* knowing the whole history of the system). The property of no memory of the Markov chain is translated by the fact that the latter conditional probability is equal to $\mathbb{P}(S_n = \mathcal{C}_n | S_{n-1} = \mathcal{C}_{n-1})$ (I.B.1), which is the probability for the system to be in configuration \mathcal{C}_n at time n , knowing only that it was in configuration \mathcal{C}_{n-1} at time $n-1$.

The second property in the definition reflects the fact that the stochastic dynamics is time independent. The probability for the system to be in configuration \mathcal{C} at time n , knowing that it was in configuration \mathcal{C}' at time $n-1$ does not depend on the time n . This allows us to introduce the notation

$$w(\mathcal{C}' \rightarrow \mathcal{C}) := \mathbb{P}(S_n = \mathcal{C} | S_{n-1} = \mathcal{C}') \quad (\text{I.B.4})$$

which stands for the transition probability between configurations \mathcal{C}' and \mathcal{C} .

Proposition B.2. *The probability distribution P_n satisfies the master equation*

$$\forall n \in \mathbb{N}, \forall \mathcal{C} \in \mathfrak{C}, \quad P_{n+1}(\mathcal{C}) = \sum_{\mathcal{C}' \in \mathfrak{C}} w(\mathcal{C}' \rightarrow \mathcal{C}) P_n(\mathcal{C}'). \quad (\text{I.B.5})$$

Proof. We have the equality

$$\begin{aligned} P_{n+1}(\mathcal{C}) &= \sum_{\mathcal{C}' \in \mathfrak{C}} \mathbb{P}(S_{n+1} = \mathcal{C}, S_n = \mathcal{C}') \\ &= \sum_{\mathcal{C}' \in \mathfrak{C}} w(\mathcal{C}' \rightarrow \mathcal{C}) P_n(\mathcal{C}'), \end{aligned}$$

where $\mathbb{P}(S_{n+1} = \mathcal{C}, S_n = \mathcal{C}')$ denotes the probability that the system is in configuration \mathcal{C}' at time n and in configuration \mathcal{C} at time $n + 1$. \blacksquare

The master equation is the key set of equations (there is one equation per configuration \mathcal{C}) which governs the time evolution of the probability distribution. Solving these equations provides the probability distribution of the system at any time. This set of equations is linear in the probabilities $P_n(\mathcal{C})$ for $\mathcal{C} \in \mathfrak{C}$, which suggests to use the linear algebra machinery to recast and study this problem. This leads to the following definition.

Definition B.3. Let \mathcal{V} be the finite dimensional vector space spanned by the basis $\{|\mathcal{C}\rangle, \mathcal{C} \in \mathfrak{C}\}$. For all $n \in \mathbb{N}$, we define $|P_n\rangle \in \mathcal{V}$ by

$$|P_n\rangle = \sum_{\mathcal{C} \in \mathfrak{C}} P_n(\mathcal{C}) |\mathcal{C}\rangle. \quad (\text{I.B.6})$$

We also define the Markov matrix

$$W = \sum_{\mathcal{C}, \mathcal{C}' \in \mathfrak{C}} w(\mathcal{C}' \rightarrow \mathcal{C}) |\mathcal{C}\rangle \langle \mathcal{C}'|, \quad (\text{I.B.7})$$

where $\langle \mathcal{C}'|$ is a vector of the dual space of \mathcal{V} satisfying the scalar product relation $\langle \mathcal{C}'|\mathcal{C}\rangle = \delta_{\mathcal{C}, \mathcal{C}'}$.

We are now equipped to rewrite the time evolution of the probability distribution.

Proposition B.4. For all $n \in \mathbb{N}$, we have the relation

$$|P_{n+1}\rangle = W |P_n\rangle. \quad (\text{I.B.8})$$

This implies that

$$|P_n\rangle = W^n |P_0\rangle. \quad (\text{I.B.9})$$

Proof. This is a direct reformulation of the master equation (I.B.5). \blacksquare

Remark B.5. The transition probabilities $w(\mathcal{C} \rightarrow \mathcal{C}')$ satisfy

$$\sum_{\mathcal{C}' \in \mathfrak{C}} w(\mathcal{C} \rightarrow \mathcal{C}') = 1, \forall \mathcal{C} \in \mathfrak{C}. \quad (\text{I.B.10})$$

This can be reformulated in vector form by introducing the row vector

$$\langle \Sigma| = \sum_{\mathcal{C} \in \mathfrak{C}} \langle \mathcal{C}|. \quad (\text{I.B.11})$$

We have the identity $\langle \Sigma|W = \langle \Sigma|$, which means that the entries of each column of the Markov matrix W sum to 1.

b) Continuous time

We would like to derive a continuous time version of the Markov process presented above. One way to address the problem is to say that each time step of the previous process corresponds to increase an infinitesimal amount of time, which yields the following relabelling of the probability vector $|\mathcal{P}_{ndt}\rangle := |P_n\rangle$. We also need to rescale the transition probabilities by introducing for

$\mathcal{C} \neq \mathcal{C}'$ the transition rate $m(\mathcal{C} \rightarrow \mathcal{C}')$ such that $w(\mathcal{C} \rightarrow \mathcal{C}') = m(\mathcal{C} \rightarrow \mathcal{C}')dt$. The master equation (I.B.8) can be then recast into

$$|\mathcal{P}_{t+dt}\rangle = |\mathcal{P}_t\rangle + dt M |\mathcal{P}_t\rangle, \quad (\text{I.B.12})$$

where the (continuous time) Markov matrix M is defined by

$$M = \sum_{\mathcal{C}, \mathcal{C}' \in \mathfrak{C}} m(\mathcal{C}' \rightarrow \mathcal{C}) |\mathcal{C}\rangle \langle \mathcal{C}'|, \quad (\text{I.B.13})$$

with

$$m(\mathcal{C} \rightarrow \mathcal{C}) = - \sum_{\substack{\mathcal{C}' \in \mathfrak{C} \\ \mathcal{C}' \neq \mathcal{C}}} m(\mathcal{C} \rightarrow \mathcal{C}'). \quad (\text{I.B.14})$$

This yields the following proposition

Proposition B.6. *The time evolution of probability vector $|\mathcal{P}_t\rangle$ obeys the master equation*

$$\frac{d|\mathcal{P}_t\rangle}{dt} = M |\mathcal{P}_t\rangle. \quad (\text{I.B.15})$$

Proof. This equation is obtained by rearranging (I.B.12) as

$$\frac{|\mathcal{P}_{t+dt}\rangle - |\mathcal{P}_t\rangle}{dt} = M |\mathcal{P}_t\rangle \quad (\text{I.B.16})$$

and taking the limit $dt \rightarrow 0$. ■

Remark B.7. *It is easy to check that the sum of the entries of each column of the Markov matrix M is vanishing ($\sum |M = 0$).*

From a more physical perspective, a continuous time Markov process can be interpreted as follows. During an infinitesimal time dt , the system in configuration \mathcal{C} has a probability $m(\mathcal{C} \rightarrow \mathcal{C}') \times dt$ to jump to another configuration \mathcal{C}' .

c) Stationary state

The stationary state is particularly relevant from a physical point of view. This is the probability vector $|\mathcal{S}\rangle = \sum_{\mathcal{C} \in \mathfrak{C}} \mathcal{S}(\mathcal{C}) |\mathcal{C}\rangle$ which contains the probabilities to observe the system in a given configuration after a very long time. This vector should be stable under the dynamics (*i.e* the time evolution) of the process. In the discrete time case it thus satisfies $W|\mathcal{S}\rangle = |\mathcal{S}\rangle$ whereas in the continuous time case it satisfies $M|\mathcal{S}\rangle = 0$. In what follows we will present the results in the continuous time framework (because this framework will be used intensively in this manuscript and the majority of the models studied will be defined in a continuous time setting) but they can be easily transposed to the discrete time framework.

Definition B.8. *A Markovian process is said to be irreducible if for all configurations \mathcal{C} and \mathcal{C}' there exists a sequence of configurations $\mathcal{C}_1, \mathcal{C}_2, \dots, \mathcal{C}_i$ which satisfies*

$$m(\mathcal{C} \rightarrow \mathcal{C}_1)m(\mathcal{C}_1 \rightarrow \mathcal{C}_2) \dots m(\mathcal{C}_i \rightarrow \mathcal{C}') \neq 0. \quad (\text{I.B.17})$$

In other words, the irreducibility condition can be intuitively understood as the fact that there is a non vanishing probability to go from any configuration \mathcal{C} to any other \mathcal{C}' in a finite number of steps. We are now equipped to state the Perron-Frobenius theorem.

Theorem B.9. *If M is the Markov matrix associated to a continuous time⁵ irreducible Markovian process, then M possesses a unique eigenvector with eigenvalue equal to 0 (the stationary state) and all others eigenvalues of M have negative real parts.*

⁵Note that the theorem can be adapted to discrete time Markovian processes.

The Perron-Frobenius theorem implies in particular that the convergence toward the stationary state is exponentially fast.

Nevertheless we will see that when the size of the system, *i.e* the number of configurations in the phase space, tends to infinity, the behavior of the non-vanishing eigenvalue with largest real part is crucial to determine the relaxation properties of large systems.

If this largest real part converges to a non-vanishing value, as the size of the system goes to infinity, the system is said to be *fully gapped*, and the relaxation towards the stationary state in the thermodynamic limit is exponentially fast (the system is sometimes said to be *massive*).

Conversely, if the largest real part converges to zero, the system is said to be *gap-less*. It is then interesting to determine the rate of convergence toward zero of the real part, in function of the system size (it provides the relaxation rates of the system in the thermodynamic limit).

Now that the existence of the stationary state is well established for irreducible Markov chains we address the question of finding an exact expression for this steady state. To do so, let us go back to the master equation. In the continuous time framework, we would like to compute the vector $|\mathcal{S}\rangle$ such that $M|\mathcal{S}\rangle = 0$. This can be written in components as

$$\sum_{\mathcal{C}' \in \mathfrak{C}} m(\mathcal{C}' \rightarrow \mathcal{C}) \mathcal{S}(\mathcal{C}') = 0, \quad \forall \mathcal{C} \in \mathfrak{C} \quad (\text{I.B.18})$$

$$\Leftrightarrow \sum_{\substack{\mathcal{C}' \in \mathfrak{C} \\ \mathcal{C}' \neq \mathcal{C}}} \left(m(\mathcal{C}' \rightarrow \mathcal{C}) \mathcal{S}(\mathcal{C}') - m(\mathcal{C} \rightarrow \mathcal{C}') \mathcal{S}(\mathcal{C}) \right) = 0, \quad \forall \mathcal{C} \in \mathfrak{C}. \quad (\text{I.B.19})$$

The last equality is obtained using the fact that

$$m(\mathcal{C} \rightarrow \mathcal{C}) = - \sum_{\substack{\mathcal{C}' \in \mathfrak{C} \\ \mathcal{C}' \neq \mathcal{C}}} m(\mathcal{C} \rightarrow \mathcal{C}'). \quad (\text{I.B.20})$$

The equation (I.B.19) expresses the fact that the incoming probability flux exactly compensates the outgoing probability flux (this could be viewed as the analogue of Kirchoff's law). Indeed, if we define the probability current from configuration \mathcal{C} to configuration \mathcal{C}' as $j_{\mathcal{C} \rightarrow \mathcal{C}'} = m(\mathcal{C} \rightarrow \mathcal{C}') \mathcal{S}(\mathcal{C}) - m(\mathcal{C}' \rightarrow \mathcal{C}) \mathcal{S}(\mathcal{C}')$, then equation (I.B.19) can be rewritten

$$\sum_{\substack{\mathcal{C}' \in \mathfrak{C} \\ \mathcal{C}' \neq \mathcal{C}}} j_{\mathcal{C} \rightarrow \mathcal{C}'} = 0, \quad \forall \mathcal{C} \in \mathfrak{C}. \quad (\text{I.B.21})$$

2 Thermodynamic equilibrium and detailed balance

One very particular way for the sums in (I.B.19) to vanish is when all the probability currents satisfy $j_{\mathcal{C} \rightarrow \mathcal{C}'} = 0$ independently. This corresponds to the case

$$m(\mathcal{C} \rightarrow \mathcal{C}') \mathcal{S}(\mathcal{C}) = m(\mathcal{C}' \rightarrow \mathcal{C}) \mathcal{S}(\mathcal{C}'), \quad \forall \mathcal{C}, \mathcal{C}' \in \mathfrak{C}. \quad (\text{I.B.22})$$

The latter equation is called detailed balance. It matches exactly the physical description of a thermodynamic equilibrium given previously in this chapter, where it was stressed that this is a state with no macroscopic currents of physical quantities (such as energy, charge, particles) flowing in the system. In the stochastic processes context, these physical macroscopic currents are necessarily produced at the microscopic level by probability currents between configurations.

The previous discussion yields the more formal definition of a thermodynamic equilibrium in the context of Markov chains.

Definition B.10. *The stationary state $|\mathcal{S}\rangle$ of a Markov process is a thermodynamic equilibrium if the detailed balance (I.B.22) is satisfied.*

Remark B.11. *The detailed balance condition involves the expression of the steady state distribution and cannot be checked a priori before knowing this distribution. Nevertheless this*

detailed balance condition can be equivalently recast in a condition depending only on the transition rates $m(\mathcal{C} \rightarrow \mathcal{C}')$. We have indeed for any cycle of configurations, if the detailed balance is satisfied, $\mathcal{C}_1 \rightarrow \mathcal{C}_2 \rightarrow \dots \rightarrow \mathcal{C}_n \rightarrow \mathcal{C}_1$

$$\mathcal{S}(\mathcal{C}_1) = \frac{m(\mathcal{C}_2 \rightarrow \mathcal{C}_1)}{m(\mathcal{C}_1 \rightarrow \mathcal{C}_2)} \mathcal{S}(\mathcal{C}_2) \quad (\text{I.B.23})$$

$$= \frac{m(\mathcal{C}_2 \rightarrow \mathcal{C}_1)}{m(\mathcal{C}_1 \rightarrow \mathcal{C}_2)} \frac{m(\mathcal{C}_3 \rightarrow \mathcal{C}_2)}{m(\mathcal{C}_2 \rightarrow \mathcal{C}_3)} \dots \frac{m(\mathcal{C}_1 \rightarrow \mathcal{C}_n)}{m(\mathcal{C}_n \rightarrow \mathcal{C}_1)} \mathcal{S}(\mathcal{C}_1). \quad (\text{I.B.24})$$

Hence we have

$$m(\mathcal{C}_1 \rightarrow \mathcal{C}_2) m(\mathcal{C}_2 \rightarrow \mathcal{C}_3) \dots m(\mathcal{C}_n \rightarrow \mathcal{C}_1) = m(\mathcal{C}_1 \rightarrow \mathcal{C}_n) \dots m(\mathcal{C}_3 \rightarrow \mathcal{C}_2) m(\mathcal{C}_2 \rightarrow \mathcal{C}_1) \quad (\text{I.B.25})$$

Conversely, if this equality (I.B.25) holds for every cycle, then the detailed balance is satisfied (see next subsection). This can be intuitively interpreted as the equality of the probabilities to go along the cycle in one way or in the reverse way. This sheds some light on the notion of time reversibility which is developed below.

a) Time reversibility

We are now interested in the implications of the detailed balance condition on the time reversibility of the process. More precisely we would like to compare the probability $\mathcal{P}(\{\mathcal{C}(t)\})$, to observe a path history $\{\mathcal{C}(t)\}_{0 \leq t \leq T}$ in the stationary state and the probability to observe the time reversed path $\{\hat{\mathcal{C}}(t)\}_{0 \leq t \leq T}$.

The first thing we need to do is to evaluate $\mathcal{P}(\{\mathcal{C}(t)\})$. We are interested in a path starting at $t = 0$ in configuration \mathcal{C}_1 , exploring successively the configurations $\mathcal{C}_1, \mathcal{C}_2, \dots, \mathcal{C}_n$, with the transition from \mathcal{C}_i to \mathcal{C}_{i+1} occurring between times t_i and $t_i + dt_i$ (where dt_i is infinitesimal), and finishing at $t = T$. For all $1 \leq i \leq n$, the system is thus in configuration \mathcal{C}_i during the time interval $[t_{i-1}, t_i]$ (where t_0 and t_n are defined as $t_0 = 0$ and $t_n = T$). See figure I.2 for an illustration of the path history.

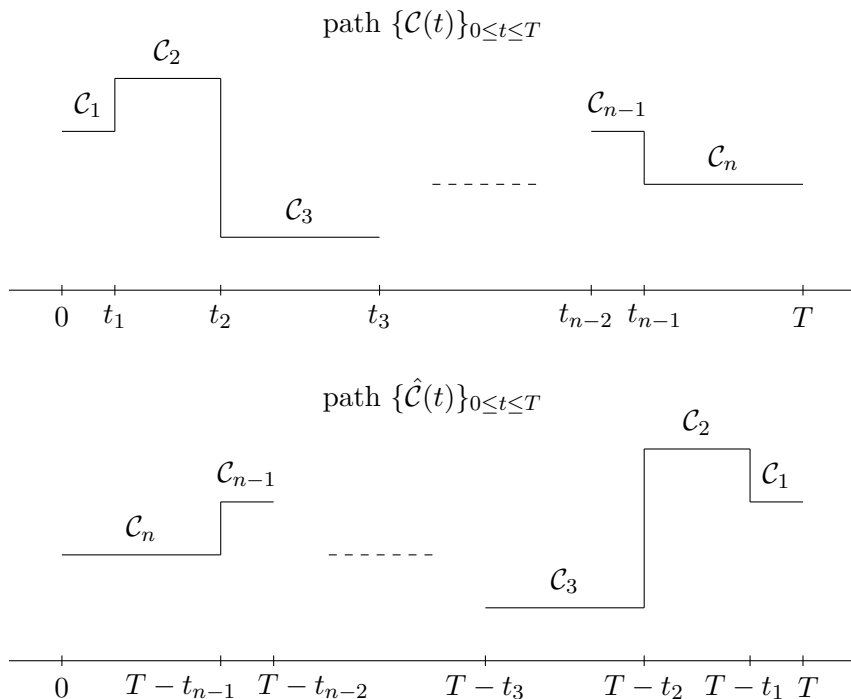


Figure I.2: Graphical representation of the trajectories $\{\mathcal{C}(t)\}_{0 \leq t \leq T}$ and $\{\hat{\mathcal{C}}(t)\}_{0 \leq t \leq T}$

A building block of the probability of the whole path is to compute the probability for the system to stay in a configuration \mathcal{C} during a time interval $[t, t']$. The probability for the system

to stay in \mathcal{C} during the time interval $[t, t + dt]$ is

$$1 - dt \sum_{\substack{\mathcal{C}' \in \mathcal{C} \\ \mathcal{C}' \neq \mathcal{C}}} m(\mathcal{C} \rightarrow \mathcal{C}') = 1 + dt m(\mathcal{C} \rightarrow \mathcal{C}) \quad (\text{I.B.26})$$

Hence the probability for the system to remain in \mathcal{C} during $[t, t']$ can be obtained by multiplying the probabilities that it stays in \mathcal{C} on each infinitesimal intervals $[t + kdt, t + (k + 1)dt]$ which yields for $dt \rightarrow 0$

$$\lim_{dt \rightarrow 0} (1 + dt m(\mathcal{C} \rightarrow \mathcal{C}))^{(t'-t)/dt} = e^{(t'-t)m(\mathcal{C} \rightarrow \mathcal{C})}. \quad (\text{I.B.27})$$

It is then straightforward to deduce that

$$\mathcal{P}(\{\mathcal{C}(t)\}) = \mathcal{S}(\mathcal{C}_1) \left(\prod_{i=1}^{n-1} e^{(t_i - t_{i-1})m(\mathcal{C}_i \rightarrow \mathcal{C}_i)} m(\mathcal{C}_i \rightarrow \mathcal{C}_{i+1}) dt_i \right) e^{(t_n - t_{n-1})m(\mathcal{C}_n \rightarrow \mathcal{C}_n)}. \quad (\text{I.B.28})$$

The time reversed path $\{\hat{\mathcal{C}}(t)\}_{0 \leq t \leq T}$ is defined as $\hat{\mathcal{C}}(t) = \mathcal{C}(T - t)$. Its probability is thus given by

$$\mathcal{P}(\{\hat{\mathcal{C}}(t)\}) = \mathcal{S}(\mathcal{C}_n) \left(\prod_{i=1}^{n-1} e^{(t_i - t_{i-1})m(\mathcal{C}_i \rightarrow \mathcal{C}_i)} m(\mathcal{C}_{i+1} \rightarrow \mathcal{C}_i) dt_i \right) e^{(t_n - t_{n-1})m(\mathcal{C}_n \rightarrow \mathcal{C}_n)}. \quad (\text{I.B.29})$$

We can then compute

$$\frac{\mathcal{P}(\{\mathcal{C}(t)\})}{\mathcal{P}(\{\hat{\mathcal{C}}(t)\})} = \frac{m(\mathcal{C}_{n-1} \rightarrow \mathcal{C}_n) \dots m(\mathcal{C}_2 \rightarrow \mathcal{C}_3) m(\mathcal{C}_1 \rightarrow \mathcal{C}_2) \mathcal{S}(\mathcal{C}_1)}{m(\mathcal{C}_n \rightarrow \mathcal{C}_{n-1}) \dots m(\mathcal{C}_3 \rightarrow \mathcal{C}_2) m(\mathcal{C}_2 \rightarrow \mathcal{C}_1) \mathcal{S}(\mathcal{C}_n)} = 1, \quad (\text{I.B.30})$$

where the last equality is obtained using the detailed balance condition (I.B.22) (which is thus a key property to establish the equality of the path and time reversed path probabilities). Conversely, it is straightforward to show that imposing time reversibility in the stationary state implies the detailed balance (we can take for instance a path with only one jump to prove this fact).

In conclusion the detailed balance condition is equivalent to the time reversibility of the process in the stationary state.

b) Link with the Boltzmann distribution

The last point that remains to be explored concerning the detailed balance condition is its link with the Boltzmann distribution. As stressed previously, when the detailed balance is satisfied, the stationary state describes a physical system at thermodynamic equilibrium by definition. We want to make the connection with the Boltzmann approach presented previously in section A. The system exchanges physical quantities with a single reservoir. For the sake of simplicity, we assume that it only exchanges energy with a reservoir at inverse temperature β which implies that the stationary distribution should be the Boltzmann distribution

$$\mathcal{S}(\mathcal{C}) = \frac{1}{Z} e^{-\beta E(\mathcal{C})}. \quad (\text{I.B.31})$$

To make connection with the Markov process, we have to relate the relevant physical quantities, basically the energy $E(\mathcal{C})$, to the transition rates $m(\mathcal{C} \rightarrow \mathcal{C}')$ defining the stochastic process. The detailed balance implies that we must have

$$\frac{m(\mathcal{C} \rightarrow \mathcal{C}')}{m(\mathcal{C}' \rightarrow \mathcal{C})} = \frac{\mathcal{S}(\mathcal{C}')}{\mathcal{S}(\mathcal{C})} = e^{-\beta \Delta E}, \quad (\text{I.B.32})$$

where $\Delta E = E(\mathcal{C}') - E(\mathcal{C})$.

3 Non-equilibrium stationary states

In this section we are interested in an irreducible Markov process whose stationary state $|\mathcal{S}\rangle$ does not satisfy the detailed balance condition, *i.e.* there exist at least two configurations $\mathcal{C}, \mathcal{C}' \in \mathfrak{C}$ such that

$$m(\mathcal{C} \rightarrow \mathcal{C}')\mathcal{S}(\mathcal{C}) \neq m(\mathcal{C}' \rightarrow \mathcal{C})\mathcal{S}(\mathcal{C}'). \quad (\text{I.B.33})$$

In this case the stationary state is called *non-equilibrium stationary state*. In opposition to the thermal equilibrium case, there are probability currents flowing in the system in the stationary state and the evolution is time irreversible in the stationary state.

The steady state distribution is a priori not of Boltzmann type and cannot be obtained easily. Nevertheless it can be expressed exactly using graph theory. We recall now the basic ingredients.

Definition B.12. A directed graph $G = (\mathfrak{C}, E)$ is a finite set of vertices (or nodes) \mathfrak{C} and a set of directed edges (or arrows) $E \subset \mathfrak{C} \times \mathfrak{C}$. By convention we say that the arrow $(\mathcal{C}', \mathcal{C}) \in E$ is starting from \mathcal{C} and ending at \mathcal{C}' (it will be sometimes denoted as $\mathcal{C} \rightarrow \mathcal{C}'$).

Definition B.13. A rooted tree over the set \mathfrak{C} is a directed graph $T = (\mathfrak{C}, E)$ such that

- the underlying undirected graph is a tree (*i.e.* acyclic and connected⁶).
- there exists a particular node $r(T) \in \mathfrak{C}$ (called the root of T) such that all the arrows are oriented toward $r(T)$ (*i.e.* for any vertex $\mathcal{C} \in \mathfrak{C}$ there exists a unique directed path going from \mathcal{C} to $r(T)$).

For $\mathcal{C} \in \mathfrak{C}$, let $\mathcal{T}(\mathcal{C})$ be the set of rooted trees T over \mathfrak{C} such that $r(T) = \mathcal{C}$.

Examples of directed graphs and rooted trees are given in figure I.3 and in figure I.4 respectively.

Definition B.14. We consider a Markov matrix M over a finite configurations space \mathfrak{C} . The M -weight of a given directed graph $G = (\mathfrak{C}, E)$ is defined by

$$w(G) = \prod_{(\mathcal{C}', \mathcal{C}) \in E} m(\mathcal{C} \rightarrow \mathcal{C}'), \quad (\text{I.B.34})$$

where $m(\mathcal{C} \rightarrow \mathcal{C}')$ for $\mathcal{C}, \mathcal{C}' \in \mathfrak{C}$ are the entries of Markov matrix (see (I.B.13)).

Proposition B.15. The unique stationary measure⁷ $|\mathcal{S}\rangle$ of the irreducible Markov matrix M defined over the finite configurations space \mathfrak{C} is given by

$$\forall \mathcal{C} \in \mathfrak{C}, \quad \mathcal{S}(\mathcal{C}) = \frac{1}{Z} \sum_{T \in \mathcal{T}(\mathcal{C})} w(T),$$

where Z is a normalization constant such that $\sum_{\mathcal{C} \in \mathfrak{C}} \mathcal{S}(\mathcal{C}) = 1$.

Proof. We fix $\mathcal{C}' \in \mathfrak{C}$. For $T \in \mathcal{T}(\mathcal{C}')$ and $\mathcal{C} \in \mathfrak{C} \setminus \{\mathcal{C}'\}$, let \tilde{T} be the directed graph obtained by adding the arrow $(\mathcal{C}, \mathcal{C}')$ to the graph T . \tilde{T} contains exactly one directed cycle $\mathcal{C}' \rightarrow \mathcal{C} \rightarrow \dots \rightarrow \mathcal{C}'' \rightarrow \mathcal{C}'$. Let $\psi(T, \mathcal{C})$ be the graph obtained by removing the edge $(\mathcal{C}', \mathcal{C}'')$ from \tilde{T} .

The application

$$\psi : \mathcal{T}(\mathcal{C}') \times \mathfrak{C} \setminus \{\mathcal{C}'\} \rightarrow \bigcup_{\mathcal{C} \in \mathfrak{C} \setminus \{\mathcal{C}'\}} \mathcal{T}(\mathcal{C}) \quad (\text{I.B.35})$$

is well defined and is bijective.

⁶Acyclic means that there is no cycle, *i.e.* no sequence of consecutive different edges starting and ending at the same vertex. Connected means that any two distinct vertices are linked by a sequence of consecutive edges.

⁷We recall that the stationary measure $|\mathcal{S}\rangle = \sum_{\mathcal{C} \in \mathfrak{C}} \mathcal{S}(\mathcal{C})|\mathcal{C}\rangle$ is defined by the equation $M|\mathcal{S}\rangle = 0$, where the Markov matrix is given in (I.B.13). Written in components it gives (I.B.19).

We indeed observe that $\psi(T, \mathcal{C}) \in \mathcal{T}(\mathcal{C}'')$ (where \mathcal{C}'' was introduced previously while defining $\psi(T, \mathcal{C})$): the underlying undirected graph of $\psi(T, \mathcal{C})$ is connected and acyclic and the arrows are pointing toward \mathcal{C}'' . Then let us prove that ψ is injective. We show that we can reconstruct T from $\psi(T, \mathcal{C})$. The root \mathcal{C}'' of $\psi(T, \mathcal{C})$ is uniquely determined (this is the only node without outgoing arrow). T is obtained by removing the arrow $\mathcal{C}' \rightarrow \mathcal{C}$ from $\psi(T, \mathcal{C})$ and then adding the arrow $\mathcal{C}'' \rightarrow \mathcal{C}'$. Finally the sets $\mathcal{T}(\mathcal{C}') \times \mathcal{E} \setminus \{\mathcal{C}'\}$ and $\bigcup_{\mathcal{C} \in \mathcal{E} \setminus \{\mathcal{C}'\}} \mathcal{T}(\mathcal{C})$ have the same cardinal (because the second set is a disjoint union).

From the definition of the M -weight of a directed graph and of the construction of $\psi(T, \mathcal{C})$, we can see that $w(T)m(\mathcal{C}' \rightarrow \mathcal{C}) = w(\psi(T, \mathcal{C}))m(\mathcal{C}'' \rightarrow \mathcal{C}')$.

We can now complete the proof of the proposition

$$\begin{aligned}
\sum_{\mathcal{C} \in \mathcal{E} \setminus \{\mathcal{C}'\}} m(\mathcal{C}' \rightarrow \mathcal{C}) \mathcal{S}(\mathcal{C}') &= \frac{1}{Z} \sum_{\mathcal{C} \in \mathcal{E} \setminus \{\mathcal{C}'\}} m(\mathcal{C}' \rightarrow \mathcal{C}) \left(\sum_{T \in \mathcal{T}(\mathcal{C}')} w(T) \right) \\
&= \frac{1}{Z} \sum_{\mathcal{C} \in \mathcal{E} \setminus \{\mathcal{C}'\}} \sum_{T \in \mathcal{T}(\mathcal{C}')} w(\psi(T, \mathcal{C})) m(r(\psi(T, \mathcal{C}')) \rightarrow \mathcal{C}') \\
&= \frac{1}{Z} \sum_{\mathcal{C}'' \in \mathcal{E} \setminus \{\mathcal{C}'\}} \sum_{T \in \mathcal{T}(\mathcal{C}'')} w(T) m(\mathcal{C}'' \rightarrow \mathcal{C}') \\
&= \sum_{\mathcal{C}'' \in \mathcal{E} \setminus \{\mathcal{C}'\}} m(\mathcal{C}'' \rightarrow \mathcal{C}') \mathcal{S}(\mathcal{C}'').
\end{aligned}$$

The second equality is obtained using $w(T)m(\mathcal{C}' \rightarrow \mathcal{C}) = w(\psi(T, \mathcal{C}))m(r(\psi(T, \mathcal{C}')) \rightarrow \mathcal{C}')$. The third equality is obtained using the fact that ψ is a bijective map. ■

Example B.16. *In this example we treat the case of a three states Markov chain. This is the simplest situation where we can find a non reversible Markov matrix (i.e for which the detailed balance is broken). The most general Markovian dynamics on three states is illustrated in figure I.3. We compute in this case all the quantities introduced previously. The set of rooted trees*

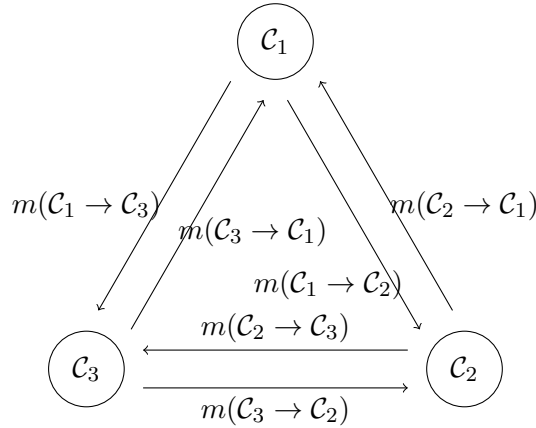


Figure I.3: Graphical representation of a three states Markov chain.

$\mathcal{T}(\mathcal{C}_1)$ contains 3 elements T_1 , T_2 and T_3 which are shown in figure I.4. The M -weight of these trees are respectively

$$\begin{aligned}
w(T_1) &= m(\mathcal{C}_2 \rightarrow \mathcal{C}_1)m(\mathcal{C}_3 \rightarrow \mathcal{C}_1) \\
w(T_2) &= m(\mathcal{C}_3 \rightarrow \mathcal{C}_2)m(\mathcal{C}_2 \rightarrow \mathcal{C}_1) \\
w(T_3) &= m(\mathcal{C}_2 \rightarrow \mathcal{C}_3)m(\mathcal{C}_3 \rightarrow \mathcal{C}_1).
\end{aligned}$$

From that we can compute

$$\sum_{T \in \mathcal{T}(\mathcal{C}_1)} w(T) = m(\mathcal{C}_2 \rightarrow \mathcal{C}_1)m(\mathcal{C}_3 \rightarrow \mathcal{C}_1) + m(\mathcal{C}_2 \rightarrow \mathcal{C}_1)m(\mathcal{C}_3 \rightarrow \mathcal{C}_2) + m(\mathcal{C}_3 \rightarrow \mathcal{C}_1)m(\mathcal{C}_2 \rightarrow \mathcal{C}_3).$$

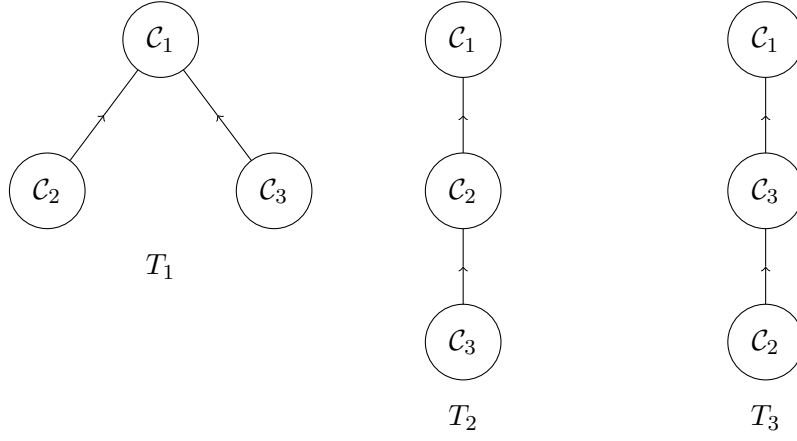


Figure I.4: Elements of $\mathcal{T}(\mathcal{C}_1)$.

The sets $\mathcal{T}(\mathcal{C}_2)$ and $\mathcal{T}(\mathcal{C}_3)$ can be easily deduced from $\mathcal{T}(\mathcal{C}_1)$ by permutations of $\mathcal{C}_1, \mathcal{C}_2, \mathcal{C}_3$ on the rooted trees. This leads to

$$\sum_{T \in \mathcal{T}(\mathcal{C}_2)} w(T) = m(\mathcal{C}_1 \rightarrow \mathcal{C}_2)m(\mathcal{C}_3 \rightarrow \mathcal{C}_2) + m(\mathcal{C}_1 \rightarrow \mathcal{C}_2)m(\mathcal{C}_3 \rightarrow \mathcal{C}_1) + m(\mathcal{C}_3 \rightarrow \mathcal{C}_2)m(\mathcal{C}_1 \rightarrow \mathcal{C}_3).$$

and

$$\sum_{T \in \mathcal{T}(\mathcal{C}_3)} w(T) = m(\mathcal{C}_2 \rightarrow \mathcal{C}_3)m(\mathcal{C}_1 \rightarrow \mathcal{C}_3) + m(\mathcal{C}_2 \rightarrow \mathcal{C}_3)m(\mathcal{C}_1 \rightarrow \mathcal{C}_2) + m(\mathcal{C}_1 \rightarrow \mathcal{C}_3)m(\mathcal{C}_2 \rightarrow \mathcal{C}_1).$$

The normalization factor is thus given by

$$\begin{aligned} Z &= m(\mathcal{C}_2 \rightarrow \mathcal{C}_1)m(\mathcal{C}_3 \rightarrow \mathcal{C}_1) + m(\mathcal{C}_2 \rightarrow \mathcal{C}_1)m(\mathcal{C}_3 \rightarrow \mathcal{C}_2) + m(\mathcal{C}_3 \rightarrow \mathcal{C}_1)m(\mathcal{C}_2 \rightarrow \mathcal{C}_3) \\ &\quad + m(\mathcal{C}_1 \rightarrow \mathcal{C}_2)m(\mathcal{C}_3 \rightarrow \mathcal{C}_2) + m(\mathcal{C}_1 \rightarrow \mathcal{C}_2)m(\mathcal{C}_3 \rightarrow \mathcal{C}_1) + m(\mathcal{C}_3 \rightarrow \mathcal{C}_2)m(\mathcal{C}_1 \rightarrow \mathcal{C}_3) \\ &\quad + m(\mathcal{C}_2 \rightarrow \mathcal{C}_3)m(\mathcal{C}_1 \rightarrow \mathcal{C}_3) + m(\mathcal{C}_2 \rightarrow \mathcal{C}_3)m(\mathcal{C}_1 \rightarrow \mathcal{C}_2) + m(\mathcal{C}_1 \rightarrow \mathcal{C}_3)m(\mathcal{C}_2 \rightarrow \mathcal{C}_1). \end{aligned}$$

In order to give some intuition of the proof given previously, let us show here that the formula of the proposition gives the stationary measure in this particular case

$$\begin{aligned} &\mathcal{S}(\mathcal{C}_1)(m(\mathcal{C}_1 \rightarrow \mathcal{C}_2) + m(\mathcal{C}_1 \rightarrow \mathcal{C}_3)) \\ &= (m(\mathcal{C}_2 \rightarrow \mathcal{C}_1)m(\mathcal{C}_3 \rightarrow \mathcal{C}_1) + m(\mathcal{C}_2 \rightarrow \mathcal{C}_1)m(\mathcal{C}_3 \rightarrow \mathcal{C}_2) + m(\mathcal{C}_3 \rightarrow \mathcal{C}_1)m(\mathcal{C}_2 \rightarrow \mathcal{C}_3)) \\ &\quad \times \frac{1}{Z}(m(\mathcal{C}_1 \rightarrow \mathcal{C}_2) + m(\mathcal{C}_1 \rightarrow \mathcal{C}_3)) \\ &= \frac{1}{Z}[(m(\mathcal{C}_1 \rightarrow \mathcal{C}_2)m(\mathcal{C}_3 \rightarrow \mathcal{C}_2) + m(\mathcal{C}_1 \rightarrow \mathcal{C}_2)m(\mathcal{C}_3 \rightarrow \mathcal{C}_1) + m(\mathcal{C}_3 \rightarrow \mathcal{C}_2)m(\mathcal{C}_1 \rightarrow \mathcal{C}_3))m(\mathcal{C}_2 \rightarrow \mathcal{C}_1) \\ &\quad + (m(\mathcal{C}_2 \rightarrow \mathcal{C}_3)m(\mathcal{C}_1 \rightarrow \mathcal{C}_3) + m(\mathcal{C}_2 \rightarrow \mathcal{C}_3)m(\mathcal{C}_1 \rightarrow \mathcal{C}_2) + m(\mathcal{C}_1 \rightarrow \mathcal{C}_3)m(\mathcal{C}_2 \rightarrow \mathcal{C}_1))m(\mathcal{C}_3 \rightarrow \mathcal{C}_1)] \\ &= m(\mathcal{C}_2 \rightarrow \mathcal{C}_1)\mathcal{S}(\mathcal{C}_2) + m(\mathcal{C}_3 \rightarrow \mathcal{C}_1)\mathcal{S}(\mathcal{C}_3). \end{aligned}$$

The computations for $\mathcal{S}(\mathcal{C}_2)$ and $\mathcal{S}(\mathcal{C}_3)$ work exactly the same way.

Example B.17. To illustrate the stationary distribution formula on a system containing an arbitrary number of configurations, we present here a 'inhomogeneous random walker' on a ring. The configuration space of this model can be described by L integers $1, 2, \dots, L$ denoting the position of the walker on a discrete periodic lattice. We will have by convention $L + 1 \equiv 1$ and $0 \equiv L$. The stochastic dynamics is defined by $m(i \rightarrow i + 1) = p_i$ and $m(i \rightarrow i - 1) = q_i$ for all $1 \leq i \leq L$. All the other transition probabilities are vanishing. It intuitively means that at each time step dt , the walker at position i has a probability $p_i \times dt$ to move forward and a probability $q_i \times dt$ to move backward.

If $p_1 p_2 \dots p_L \neq q_1 q_2 \dots q_L$ then the system does not reach a thermodynamic equilibrium (this can be intuitively understood as the fact that the random walker is subject to a non-conservative force). The stationary distribution⁸ is thus obtained by summing the M -weight of rooted trees. There are very few rooted trees with non vanishing M -weight. They are simply obtained by cutting one bond of the periodic lattice. This yields the expression

$$\mathcal{S}(i) = \left(\prod_{k=i+1}^L q_k \right) \sum_{j=1}^i \left(\prod_{k=j}^{i-1} p_k \right) \times \left(\prod_{k=1}^{j-1} q_k \right) + \left(\prod_{k=1}^{i-1} p_k \right) \sum_{j=i+1}^L \left(\prod_{k=j}^L p_k \right) \times \left(\prod_{k=j-1}^{i+1} q_k \right). \quad (\text{I.B.36})$$

This can be interpreted as the discrete version of the stationary distribution (I.A.14) given in the Langevin equation context.

From a physical point of view, this formula given in terms of rooted trees does not appear completely satisfactory for several reasons. The first one is that it is not expressed in terms of simple physical quantities (such as the energy in the Boltzmann distribution case). In other words, the link between the probability rates defining the stochastic model and the relevant physical observables of the system is not complete (even if some remarkable progress had been made with the generalized detailed balance, see subsection 1 below).

The second reason is that it is not given together with a maximum entropy principle. Similarly to the thermodynamic equilibrium case, we would like to know if this stationary distribution can be obtained by maximizing an entropy under a set of physical constraints. This would be certainly defined on an enlarged phase space containing typically the path history instead of the static configurations. This is probably intimately linked to the first issue mentioned and may appear as a key to build a general theory to describe non-equilibrium stationary states.

Finally the exact formula of the stationary distribution in terms of rooted trees is often very difficult to use for physical computations. The number of rooted trees is typically increasing exponentially with the number of configurations of the physical system. There are indeed n^{n-2} trees that can be constructed from n vertices. Apart from very particular Markov processes for which the directed graph underlying the Markov matrix is very simple (in the sense that it contains a very small number of edges, as in example B.17), this formula is intractable for computing physical properties in a large system.

One of the main goals of this manuscript is to investigate these non-equilibrium stationary states in some specific cases, where they can be computed exactly in a much simpler form than the rooted trees expansion. The idea is to shed some light on the structure of this steady state in simple out-of-equilibrium models. In chapter III we will see a technique, called matrix ansatz, which allows us to reduce the exponential complexity of the computation to a polynomial complexity, in some particular cases. We hope also to get some intuition from this method about how to relate the non-equilibrium stationary distribution to relevant physical quantities. We will give several new examples of non-equilibrium models for which the matrix ansatz can be efficiently used to compute the stationary state.

C Toward a description of NESS?

In this section, we review very briefly several tools that have been developed to describe out-of-equilibrium systems.

1 Generalized detailed balance and fluctuation theorem

Even if the detailed balance does not hold for a general Markovian process, it is possible to formulate a generalization of it that is always satisfied. For the sake of simplicity, we will

⁸The stationary distribution is unique thanks to the Perron-Frobenius theorem (the Markov chain is obviously irreducible).

consider the particular case where the system is in contact with two reservoirs at different inverse temperatures β_1 and β_2 and can exchange energy with these reservoirs. The discussion below can be adapted to the case of more than two reservoirs and of different physical quantities (such as charges, momentum, particles) exchanged with the reservoirs. The generalized detailed balance relation reads

$$\frac{m(\mathcal{C} \rightarrow \mathcal{C}')}{m(\mathcal{C}' \rightarrow \mathcal{C})} = e^{-\beta_1 \Delta E_1 - \beta_2 \Delta E_2}, \quad (\text{I.C.1})$$

where ΔE_1 (respectively ΔE_2) stands for the energy exchanged with reservoir 1 (respectively 2) during the transition from configuration \mathcal{C} to configuration \mathcal{C}' . We observe that formula (I.C.1) is a generalization of the detailed balance relation (I.B.32), which is easily recovered when $\beta_1 = \beta_2$. Relation (I.C.1) can be physically justified by considering the system and the two reservoirs as an isolated system, whose dynamics should reach the microcanonical distribution. Writing the detailed balance relation for this whole system, and assuming that the energy exchanged is small in comparison to the total energy of the reservoirs, yields the generalized detailed balance condition (see for instance [16,17] for details).

This generalized detailed balance relation can be interpreted as the root of the fluctuation theorem, see subsection 3.

2 Dynamic observables and deformed Markov matrix

In a system at thermodynamic equilibrium, we saw that the stationary distribution is given by the Boltzmann distribution

$$\mathcal{S}(\mathcal{C}) \sim e^{-\beta E(\mathcal{C})} \quad (\text{I.C.2})$$

for a system in contact with a reservoir at inverse temperature β . It allows us to define the free energy, which is simply the cumulant generating function of the energy observable E . This free energy is a very efficient tool to describe the properties of the system. We would like to build the same kind of tool to describe out-of-equilibrium systems and more particularly non-equilibrium stationary states. By analogy with equilibrium systems, the generalized balance condition (I.C.1) suggests to study the fluctuations of the energy exchanged with the reservoirs and to construct the generating function of this observable.

This can be formalized as follows. We are interested in studying an observable \mathcal{O} , whose value $\mathcal{O}(\mathcal{C} \rightarrow \mathcal{C}')$ depends on the transition $\mathcal{C} \rightarrow \mathcal{C}'$ under consideration. It can be for instance the energy exchanged with a particular reservoir during the transition or the number of particles injected at a particular place during the transition. We would like to compute the fluctuations of the observable \mathcal{O} in the stationary state. To give a precise mathematical meaning to this idea, we first need to give a sense to the value of the observable in the stationary state. One way to achieve that is to begin by defining the value of the observable on a whole path history. For the path history $\{\mathcal{C}(t)\}_{0 \leq t \leq T}$ defined in subsection a), which explores successively the configurations $\mathcal{C}_1, \dots, \mathcal{C}_n$ (with transitions occurring at times t_1, \dots, t_{n-1}), we define

$$\mathcal{O}_T(\{\mathcal{C}(t)\}) = \mathcal{O}(\mathcal{C}_1 \rightarrow \mathcal{C}_2) + \dots + \mathcal{O}(\mathcal{C}_{n-1} \rightarrow \mathcal{C}_n). \quad (\text{I.C.3})$$

The value \mathcal{O}_T depends on the time evolution, or path history, of the system (which is governed by the master equation (I.B.15)) on the interval $[0, T]$. It is a random variable. We denote by $\mathcal{P}_T(O)$ the probability that $\mathcal{O}_T = O$. Our goal is to study this probability distribution in the large time T limit. To determine the time evolution of this probability distribution, we have to consider the more precise quantity $\mathcal{P}_T(O, \mathcal{C})$, which denotes the joint probability for the system to be in configuration \mathcal{C} at time T and for the observable \mathcal{O}_T to be equal to O . The value of $\mathcal{P}_T(O)$ will be simply recovered through the relation $\mathcal{P}_T(O) = \sum_{\mathcal{C} \in \mathfrak{C}} \mathcal{P}_T(O, \mathcal{C})$.

Proposition C.1. *The time evolution of $\mathcal{P}_T(O, \mathcal{C})$ is given by*

$$\frac{d\mathcal{P}_T(O, \mathcal{C})}{dT} = \sum_{\substack{\mathcal{C}' \in \mathfrak{C} \\ \mathcal{C}' \neq \mathcal{C}}} m(\mathcal{C}' \rightarrow \mathcal{C}) \mathcal{P}_T(O - \mathcal{O}(\mathcal{C}' \rightarrow \mathcal{C}), \mathcal{C}') - \sum_{\substack{\mathcal{C}' \in \mathfrak{C} \\ \mathcal{C}' \neq \mathcal{C}}} m(\mathcal{C} \rightarrow \mathcal{C}') \mathcal{P}_T(O, \mathcal{C}). \quad (\text{I.C.4})$$

Proof. This equation is derived similarly to what was done for (I.B.5). \blacksquare

This relation can be recast in a more elegant way by introducing the following generating function.

Definition C.2. We define

$$\hat{\mathcal{P}}_T(\mu, \mathcal{C}) = \sum_O e^{\mu O} \mathcal{P}_T(O, \mathcal{C}). \quad (\text{I.C.5})$$

Proposition C.3. The generating function $\hat{\mathcal{P}}_T(\mu, \mathcal{C})$ fulfills the deformed master equation

$$\frac{d\hat{\mathcal{P}}_T(\mu, \mathcal{C})}{dT} = \sum_{\substack{\mathcal{C}' \in \mathfrak{C} \\ \mathcal{C}' \neq \mathcal{C}}} m(\mathcal{C}' \rightarrow \mathcal{C}) e^{\mu \mathcal{O}(\mathcal{C}' \rightarrow \mathcal{C})} \mathcal{P}_T(\mu, \mathcal{C}') - \sum_{\substack{\mathcal{C}' \in \mathfrak{C} \\ \mathcal{C}' \neq \mathcal{C}}} m(\mathcal{C} \rightarrow \mathcal{C}') \mathcal{P}_T(\mu, \mathcal{C}). \quad (\text{I.C.6})$$

Proof. This is established by summing (I.C.4) over O with the factor $e^{\mu O}$. \blacksquare

It can be rewritten in matrix form by introducing the following vector and deformed Markov matrix.

Definition C.4. We define the deformed probability vector

$$|\hat{\mathcal{P}}_T(\mu)\rangle = \sum_{\mathcal{C} \in \mathfrak{C}} \hat{\mathcal{P}}_T(\mu, \mathcal{C}) |\mathcal{C}\rangle, \quad (\text{I.C.7})$$

and the deformed Markov matrix

$$M^\mu = \sum_{\mathcal{C}, \mathcal{C}' \in \mathfrak{C}} m^\mu(\mathcal{C} \rightarrow \mathcal{C}') |\mathcal{C}'\rangle \langle \mathcal{C}|, \quad (\text{I.C.8})$$

with $m^\mu(\mathcal{C} \rightarrow \mathcal{C}') = m(\mathcal{C} \rightarrow \mathcal{C}') e^{\mu \mathcal{O}(\mathcal{C} \rightarrow \mathcal{C}')}$ for $\mathcal{C}' \neq \mathcal{C}$ and $m^\mu(\mathcal{C} \rightarrow \mathcal{C}) = -\sum_{\substack{\mathcal{C}' \in \mathfrak{C} \\ \mathcal{C}' \neq \mathcal{C}}} m(\mathcal{C} \rightarrow \mathcal{C}')$.

A straightforward computation then yields

$$\frac{d|\hat{\mathcal{P}}_T(\mu)\rangle}{dT} = M^\mu |\hat{\mathcal{P}}_T(\mu)\rangle, \quad (\text{I.C.9})$$

which provides the following formal expression

$$|\hat{\mathcal{P}}_T(\mu)\rangle = e^{TM^\mu} |\hat{\mathcal{P}}_0(\mu)\rangle. \quad (\text{I.C.10})$$

We denote by $E_1(\mu), E_2(\mu), \dots$ the eigenvalues of M^μ ordered by decreasing real part, $|\Psi_1\rangle, |\Psi_2\rangle, \dots$ the corresponding right eigenvectors, and $\langle \Phi_1|, \langle \Phi_2|, \dots$ the corresponding left eigenvectors.

The last equation then becomes

$$|\hat{\mathcal{P}}_T(\mu)\rangle = \langle \Phi_1 | \hat{\mathcal{P}}_0(\mu) \rangle e^{TE_1(\mu)} |\Psi_1\rangle + \langle \Phi_2 | \hat{\mathcal{P}}_0(\mu) \rangle e^{TE_2(\mu)} |\Psi_2\rangle + \dots \quad (\text{I.C.11})$$

We now would like to deduce, from these computations, the behavior of the probability distribution $\mathcal{P}_T(O)$ in the long time $T \rightarrow \infty$ limit. This can be studied through the generating function of the cumulant defined as

$$E^T(\mu) := \ln \left(\sum_O e^{\mu O} \mathcal{P}_T(O) \right) = \ln \left(\langle \Sigma | \hat{\mathcal{P}}_T(\mu) \rangle \right), \quad (\text{I.C.12})$$

where we recall that $\langle \Sigma | = \sum_{\mathcal{C} \in \mathfrak{C}} \langle \mathcal{C}|$. We observe, from (I.C.11), that $E^T(\mu)$ behaves asymptotically as a linear function of T . Its long time limit is thus captured by the quantity

$$E(\mu) := \lim_{T \rightarrow \infty} \frac{E^T(\mu)}{T} = E_1(\mu), \quad (\text{I.C.13})$$

which is exactly given by the largest eigenvalue of M^μ .

This cumulant generating function in the stationary state turns out to be an efficient tool to characterize the macroscopic behavior of a physical system in the large size limit (thermodynamic limit, see chapter V), if the observable \mathcal{O} is correctly chosen. In particular the singularities of this function (or of the associated large deviation function, see subsection 4) could determine the phase transitions of the model [18–20].

In this manuscript, we will be interested in interacting particles systems evolving on a one dimensional lattice. A physical quantity of prime interest in such models is the (algebraic) number of particles which cross a particular bond on the lattice during a transition. This observable is indeed representative of the non-equilibrium aspects of these interacting particles systems. It provides a quantitative way to characterize the particles current and its fluctuation in the stationary state, through the computation of the cumulant generating function. In chapter III and chapter IV we will address the problem of computing exactly this generating function for particular models.

This formalism allows also to state an elegant symmetry on the fluctuations of the entropy production, which we present in the subsection below.

3 Gallavotti-Cohen symmetry and fluctuation theorem

Having in mind the generalized balance condition (I.C.1), we now focus on the observable defined by

$$\mathcal{O}(\mathcal{C} \rightarrow \mathcal{C}') = \ln \frac{m(\mathcal{C} \rightarrow \mathcal{C}')}{m(\mathcal{C}' \rightarrow \mathcal{C})}. \quad (\text{I.C.14})$$

This can be interpreted as the entropy production during the transition $\mathcal{C} \rightarrow \mathcal{C}'$ [21]. The associated deformed Markov matrix M^μ can be easily computed, its entries are given, for $\mathcal{C}' \neq \mathcal{C}$, by

$$m^\mu(\mathcal{C} \rightarrow \mathcal{C}') = m(\mathcal{C} \rightarrow \mathcal{C}')^{1+\mu} m(\mathcal{C}' \rightarrow \mathcal{C})^{-\mu}. \quad (\text{I.C.15})$$

We observe that we have the equality $m^\mu(\mathcal{C} \rightarrow \mathcal{C}') = m^{-1-\mu}(\mathcal{C}' \rightarrow \mathcal{C})$ which translates into

$$M^\mu = (M^{-1-\mu})^t, \quad (\text{I.C.16})$$

where t denotes the matrix transposition. We thus deduce that the spectrum of M^μ and of $M^{-1-\mu}$ are identical. This proves the following equality satisfied by the largest eigenvalue $E(\mu)$ of M^μ

$$E(\mu) = E(-1 - \mu). \quad (\text{I.C.17})$$

This is known as the Gallavotti-Cohen symmetry [21–23]. We proved here the symmetry involving the entropy production (which holds for any Markov chain) but similar relations can also be derived for other physical observables, depending on the model under consideration. For instance, we will encounter such a symmetry in chapter IV while studying the cumulant generating function of the particle current for the asymmetric simple exclusion process.

The symmetry on the generating function translates into a symmetry on the large deviation function of the entropy production (see subsection 4 for definition and details), which can be defined as

$$G(s) = \inf_{\mu} [\mu s - E(\mu)]. \quad (\text{I.C.18})$$

Using the symmetry on the generating function E , we obtain

$$\inf_{\mu} [\mu s - E(\mu)] = \inf_{\mu} [(-1 - \mu) \cdot (-s) - s - E(-1 - \mu)] \quad (\text{I.C.19})$$

$$= \inf_{-1-\mu} [(-1 - \mu) \cdot (-s) - E(-1 - \mu)] - s. \quad (\text{I.C.20})$$

This yields the symmetry for the large deviation function

$$G(s) = G(-s) - s. \quad (\text{I.C.21})$$

This last equality is known as the fluctuation theorem. This relation was first observed in [24] and then proven in [25]. It tells us that the probability $\mathcal{P}_T(s)$ to observe during time interval $[0, T]$ an entropy production equal to Ts satisfies

$$\frac{\mathcal{P}_T(-s)}{\mathcal{P}_T(s)} \underset{T \rightarrow \infty}{\sim} e^{-Ts} \quad (\text{I.C.22})$$

This fluctuation theorem (and its generalization to other physical observables, depending on the model under consideration) has very useful implications. It yields near equilibrium the Einstein fluctuation-dissipation relations, the Onsager reciprocity relations and the Kubo linear response theory, see for instance [26].

4 Large deviation functions

In the last decades, the large deviation theory has proven to be a very efficient framework to deal with equilibrium but also non-equilibrium systems. We present briefly below the main tools (from a statistical physicist point of view) associated to this theory. The reader is invited to read the very useful review [27] for details.

a) Large deviation principle

The large deviation theory can be intuitively introduced as a framework to evaluate the probabilities of rare events. From a mathematical point of view, it could be thought as a refinement of the law of large numbers. From a physical point of view, the large deviation functions are seen as possible generalizations of thermodynamic potentials in the out-of-equilibrium context.

Definition C.5. *We consider (S_n) a sequence of random variables taking real values and an interval $A \subset \mathbb{R}$. The probability $\mathbb{P}(S_n \in A)$ is said to follow a large deviation principle if there exists a real number G_A , called the rate, such that*

$$-\lim_{n \rightarrow \infty} \frac{1}{n} \ln \mathbb{P}(S_n \in A) = G_A. \quad (\text{I.C.23})$$

The large deviation principle roughly means that the probability $\mathbb{P}(S_n \in A)$ vanishes exponentially fast with n :

$$\mathbb{P}(S_n \in A) \sim e^{-nG_A} \quad (\text{I.C.24})$$

From this perspective it can be interpreted as a refinement of the law of large numbers, which states that the properly normalized sum of independent identically distributed random variables converges, with probability 1, to the common expectation value of the variables. Here, we observe that if G_A vanishes, the probability measure concentrates, with probability 1, in the set A . In particular (in the case of the normalized sum of independent identically distributed random variables) if A is chosen to be any interval containing the expectation value of the variable, the large deviation principle provides the result of the law of large number together with the rate of convergence of the probability measure (which explains the denomination 'refinement'). This phenomenon is illustrated in the following example.

Example C.6. *We present here one of the simplest example of large deviation principle. We consider a sequence of binary independent random variables (ϵ_k) , that are equal to 1 with probability 1/2 and equal to 0 with probability 1/2. We define*

$$S_n = \frac{1}{n} \sum_{k=1}^n \epsilon_k. \quad (\text{I.C.25})$$

It is straightforward to establish that S_n follows the binomial distribution

$$\mathbb{P}(S_n = k/n) = \frac{1}{2^n} \binom{n}{k}. \quad (\text{I.C.26})$$

We fix $\rho \in [0, 1]$ and we set $k = \lfloor \rho n \rfloor$. It means intuitively that for n large enough, $k/n \simeq \rho$. We can use the Stirling's formula to estimate the asymptotic behavior of $\mathbb{P}(S_n = k/n)$, when n is large. This yields the relation

$$-\lim_{n \rightarrow \infty} \frac{1}{n} \ln \mathbb{P}(S_n = k/n) = \ln 2 + \rho \ln \rho + (1 - \rho) \ln(1 - \rho) := G(\rho). \quad (\text{I.C.27})$$

$G(\rho)$ is the rate function, also called large deviation function. It is a non-negative convex function of ρ , which is minimum for $\rho = 1/2$ (it vanishes for this value), see figure I.5. It allows us to recover the result of the law of large numbers: the probability measure of S_n concentrates, as $n \rightarrow \infty$, toward the expectation value of the variables ϵ_k , which is equal to $1/2$.

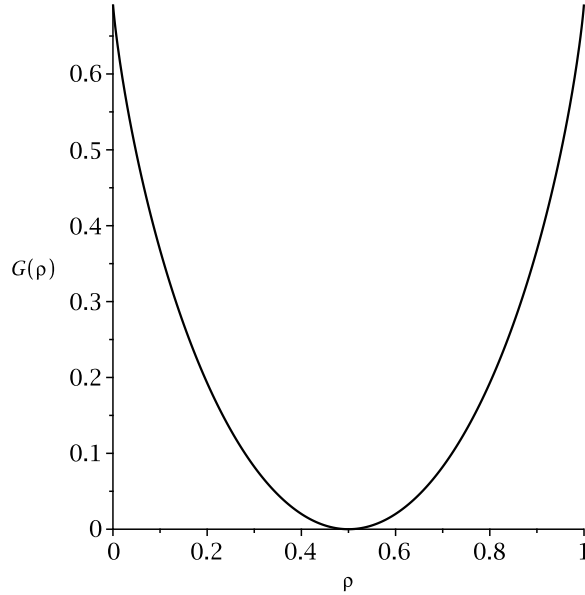


Figure I.5: Plot of the large deviation function $G(\rho)$.

b) Legendre transformation and Gärtner-Ellis theorem

We are now going to see that the large deviation function G is closely related to a quantity, which we already encountered in this manuscript: the cumulant generating function. This connection appears through the Legendre transformation, that we now define.

Definition C.7. If f is a convex function, its Legendre transform g is defined by

$$g(p) = \sup_x (px - f(x)) \quad (\text{I.C.28})$$

If f is everywhere differentiable the previous definition is equivalent to

$$g(p) = px^* - f(x^*), \quad \text{with } x^* \text{ such that } \frac{df}{dx}(x^*) = p. \quad (\text{I.C.29})$$

The inverse transform formula is given by

$$f(x) = \sup_p (px - g(p)), \quad (\text{I.C.30})$$

or if g is everywhere differentiable

$$f(x) = xp^* - g(p^*), \quad \text{with } p^* \text{ such that } \frac{dg}{dp}(p^*) = x. \quad (\text{I.C.31})$$

It means that the Legendre transform is self-inverse (or involutive).

We now define a quantity which will play an important role in this manuscript, the cumulant generating function.

Definition C.8. We consider (S_n) a sequence of real random variables and we define the cumulant generating function of (S_n) by

$$E(\mu) = \lim_{n \rightarrow \infty} \frac{1}{n} \ln \left(\sum_{x \in \mathcal{X}_n} e^{n\mu x} \mathbb{P}(S_n = x) \right), \quad (\text{I.C.32})$$

where \mathcal{X}_n is the discrete⁹ configuration set of the random variable S_n .

It can be shown that the cumulant generating function is always convex (see for instance [27]).

Remark C.9. This function is called cumulant generating function because we can obtain the expectation, variance, and higher order cumulants by taking successive derivatives with respect to the parameter μ . For instance if ϵ_k is a sequence of independent identically distributed random variables with expectation $\langle \epsilon \rangle$ and variance $\text{var}(\epsilon)$, and S_n is given by

$$S_n = \frac{1}{n} \sum_{k=1}^n \epsilon_k, \quad (\text{I.C.33})$$

then it is straightforward to see that

$$E'(0) = \langle \epsilon \rangle, \quad (\text{I.C.34})$$

and

$$E''(0) = \text{var}(\epsilon). \quad (\text{I.C.35})$$

We are now equipped to state the Gärtner-Ellis theorem, which relates the cumulant generating function of a sequence of random variable to its large deviation function.

Theorem C.10. Suppose that the cumulant generating function $E(\mu)$ associated to the sequence of random variable (S_n) is differentiable, then (S_n) satisfies a large deviation principle

$$- \lim_{n \rightarrow \infty} \frac{1}{n} \ln \mathbb{P}(S_n = x) = G(x), \quad (\text{I.C.36})$$

where the large deviation function G is given by the Legendre transform of E

$$G(x) = \sup_{\mu} (\mu x - E(\mu)), \quad (\text{I.C.37})$$

or equivalently

$$G(x) = x\mu^* - E(\mu^*), \quad \text{with } \mu^* \text{ such that } \frac{dE}{d\mu}(\mu^*) = x. \quad (\text{I.C.38})$$

We do not give a rigorous proof of the theorem but we rather propose an argument to convince the reader of its validity. If (S_n) satisfies a large deviation principle with large deviation function G , then we can evaluate

$$\sum_{x \in \mathcal{X}_n} e^{n\mu x} \mathbb{P}(S_n = x) \sim \sum_{x \in \mathcal{X}_n} e^{n\mu x} e^{-nG(x)} = \sum_{x \in \mathcal{X}_n} e^{n(\mu x - G(x))}. \quad (\text{I.C.39})$$

⁹For the sake of simplicity, we consider here random variables S_n taking discrete values $x \in \mathcal{X}_n$ but generalization to continuous random variables is straightforward. We consider also a stochastic process (S_n) parametrized by a discrete variable n but the generalization to stochastic processes (S_t) parametrized by a continuous time t is obvious.

The behavior of the last sum is obtained through a saddle-point analysis, which yields the following expression for the cumulant generating function (I.C.32)

$$E(\mu) = \sup_x (\mu x - G(x)). \quad (\text{I.C.40})$$

The Legendre inverse transform formula gives the desired result.

The Gärtner-Ellis theorem provides a tool to compute large deviation functions through cumulant generating functions. It is commonly used in out-of-equilibrium statistical physics, especially to compute large deviation of particles current in the stationary state in interacting particles systems.

c) Application to out-of-equilibrium statistical physics

We present briefly two relevant utilizations of the large deviation theory in the context of out-of-equilibrium statistical physics. This description is far from being exhaustive. We chose to focus on the applications of the theory which will be used later in this manuscript. The reader is invited to consult the review [27] for a complete description of the role of large deviation theory in statistical physics.

In out-of-equilibrium models, we saw previously that large deviation theory was the correct tool to deal with the fluctuations of dynamic observables in the stationary state. It was indeed stressed that the fluctuations of the dynamic observable were encoded in the quantity (I.C.13), which is exactly defined as the cumulant generating function introduced in the large deviation context (I.C.32), where the time T plays the role of the large deviation parameter. The Legendre transformation then provides the large deviation function associated with this observable. By analogy with equilibrium models, the cumulant generating function may be related to a generalization of the free energy and the large deviation function may be connected to an entropy. These large deviation functions (or cumulant generating functions) are in general difficult to compute exactly: hence it is important to construct models for which such computations are possible. This motivates the study of *integrable systems*, i.e models for which analytical results can be derived. The next chapter is devoted to the presentation of integrability in the context of Markov chains. In chapter III we will compute the first cumulants of the particle current of the dissipative symmetric simple exclusion process. We will explore in chapter IV the connection between the cumulant generating function of the current in the asymmetric simple exclusion process and the theory of symmetric polynomials.

A second application of the large deviation theory in out-of equilibrium physics, which will be of particular interest for us, is the macroscopic fluctuation theory. This is a theory which aims to provide a coarse grained description of diffusive systems. The probability to observe a path history, a time evolution, of properly defined macroscopic variables satisfies a large deviation principle. The large deviation parameter is the size of the system. The rate function can be heuristically interpreted as an action functional. The macroscopic fluctuation theory provides also predictions about fluctuations of the particle current and density in the stationary state. This theory will be presented in details in chapter V. The integrable models also play a central role in this context because they appear as benchmarks to test the predictions of the theory. We will indeed use in chapter V the exact results obtained in chapter III on the dissipative symmetric simple exclusion process and respectively on the open boundaries multi-species symmetric simple exclusion process to check the predictions for dissipative models and respectively to extend the theory to multi-species models.

Chapter II

Integrability

First we introduce classical integrability as motivation, then specific models that will be used as examples throughout, before finally giving the machinery of quantum integrability.

A Introduction, motivations and formalism

1 Conserved quantities

a) Introduction and motivations

The idea behind integrability goes back to the study of classical mechanical systems. It was observed that the conservation of the energy in certain simple systems often permits to solve exactly the equations of motion (basically Newton's law). This idea was precisely formulated by Liouville [28], using the Hamiltonian formalism of the classical dynamics. In this framework a system is described through coordinates of position q_i and momentum p_i ($1 \leq i \leq n$) defining the phase space (of dimension $2n$). The dynamics is encoded with the Hamiltonian $H(p_i, q_i)$ by the equations

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, \quad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}. \quad (\text{II.A.1})$$

The time evolution of a function $F(p_i, q_i)$ of the phase space is obtained by the equation

$$\frac{dF}{dt} = \{H, F\}, \quad (\text{II.A.2})$$

where the Poisson bracket is defined as

$$\{F, G\} = \sum_{i=1}^n \frac{\partial F}{\partial p_i} \frac{\partial G}{\partial q_i} - \frac{\partial G}{\partial p_i} \frac{\partial F}{\partial q_i} \quad (\text{II.A.3})$$

In this framework, a conserved quantity is thus a function F satisfying $\{H, F\} = 0$.

Liouville proved the following theorem.

Theorem A.1. *If the system possesses n independent¹ conserved quantities F_i ($1 \leq i \leq n$), i.e such that $\{H, F_i\} = 0$, in involution*

$$\{F_i, F_j\} = 0, \quad (\text{II.A.4})$$

then the solution of the equations of motion (II.A.1) can be computed through a "quadrature"².

¹The independence has here to be understood as the linear independence of the differential forms dF_i (at a generic point)

²Note that the situation is much less clear when the phase space is infinite dimensional, in classical field theory for instance.

Remark A.2. *The Liouville theorem is proven by performing a change of variables $(p_i, q_i) \rightarrow (F_i, \psi_i)$. The new variables are called the action-angle variables and satisfy the equations*

$$\frac{dF_i}{dt} = 0, \quad \frac{d\psi_i}{dt} = \Omega_i, \quad (\text{II.A.5})$$

where Ω_i are time-independent constants. These equations are easily solved. The coordinates ψ_i are constructed through the relation

$$\psi_i = \frac{\partial S}{\partial F_i}, \quad (\text{II.A.6})$$

where $S(F, q)$ is defined by the quadrature

$$S(F, q) = \int_{q_0}^q \sum_{i=1}^n p_i(F, q) dq_i. \quad (\text{II.A.7})$$

Since this discovery, people have been interested in finding a systematic way to construct Hamiltonians, H , together with the conserved quantities, F_i . This has led to the introduction of different key concepts, like the Lax-pair and the classical r-matrix. The reader may refer to [28] for an introduction to classical integrable systems and a lot of details.

There have been several attempts to adapt and exploit these fundamental concepts in quantum mechanics and statistical physics. This has led to remarkable developments ranging from the discovery of quantum R -matrices and of the Yang-Baxter equation [29], to the quantum inverse scattering method [30, 31], and including the quantum groups [32–34].

These works pointed out the relevance of the conserved quantities in the exact solvability of the quantum Hamiltonians. Unfortunately, we are still lacking a quantum analogue for the Liouville theorem.

In this manuscript, we will make an intensive use of the framework and techniques developed to study the Hamiltonians of quantum spin chains. We will be indeed interested in Markovian processes, defined on a one dimensional lattice, which can be studied within the quantum spin chain framework (the Markov matrix will often be a similarity transform of quantum spin chain Hamiltonian).

b) Markovian case

In the context of Markov matrices, a conserved quantity can be interpreted as an observable whose average value is constant in time. To fix the ideas, let us denote by \mathcal{O} an observable, *i.e* a real valued function $\mathcal{O}(\mathcal{C}) \in \mathbb{R}$ of the configurations \mathcal{C} of the system. The average value of the observable at time t is defined by

$$\langle \mathcal{O} \rangle_t = \sum_{\mathcal{C}} \mathcal{O}(\mathcal{C}) P_t(\mathcal{C}), \quad (\text{II.A.8})$$

where we recall that $P_t(\mathcal{C})$ denotes the probability for the system to be in configuration \mathcal{C} at time t . It will be convenient to reformulate that in a matrix form. We introduce a row vector $\langle \Sigma |$, which stands for the sum of the basis row vectors, and a diagonal matrix O , which encompasses the value of the observable \mathcal{O}

$$\langle \Sigma | = \sum_{\mathcal{C}} \langle \mathcal{C} | \quad \text{and} \quad O = \sum_{\mathcal{C}} \mathcal{O}(\mathcal{C}) |\mathcal{C}\rangle \langle \mathcal{C}|. \quad (\text{II.A.9})$$

The average value of \mathcal{O} at time t can be rewritten

$$\langle \mathcal{O} \rangle_t = \langle \Sigma | O | P_t \rangle = \langle \Sigma | O \exp(tM) | P_0 \rangle, \quad (\text{II.A.10})$$

where we recall that M is the Markov matrix encoding the dynamics of the model (I.B.13) and $|P_t\rangle$ is the probability distribution of the model at time t , see (I.B.15). $|P_0\rangle$ is the initial

probability distribution at time $t = 0$. It is then straightforward to see that, if the matrices O and M commutes, $OM = MO$, then

$$\langle \mathcal{O} \rangle_t = \langle \Sigma | \exp(tM) O | P_0 \rangle = \langle \Sigma | O | P_0 \rangle = \langle \mathcal{O} \rangle_0, \quad (\text{II.A.11})$$

where we used the Markovian property of M , $\langle \Sigma | M = 0$, which implies $\langle \Sigma | \exp(tM) = \langle \Sigma |$. In other words the average value of \mathcal{O} is conserved in time.

Remark A.3. *The observable \mathcal{O} that we studied is a 'static' observable, i.e it depends on the current configuration \mathcal{C} of the system. We can adapt the discussion above to 'dynamic' observables, i.e depending on a transition from a configuration \mathcal{C} to a configuration \mathcal{C}' . We denote by $\mathcal{O}(\mathcal{C} \rightarrow \mathcal{C}')$ the value of the observable associated with this transition. The average value of the observable is now defined as*

$$\langle \mathcal{O} \rangle_t = \sum_{\mathcal{C}, \mathcal{C}'} \mathcal{O}(\mathcal{C} \rightarrow \mathcal{C}') m(\mathcal{C} \rightarrow \mathcal{C}') P_t(\mathcal{C}), \quad (\text{II.A.12})$$

where we recall that $m(\mathcal{C} \rightarrow \mathcal{C}')$ denotes the probability rate from configuration \mathcal{C} to configuration \mathcal{C}' . It can be rewritten by introducing the matrix

$$O = \sum_{\mathcal{C}} \mathcal{O}(\mathcal{C} \rightarrow \mathcal{C}') m(\mathcal{C} \rightarrow \mathcal{C}') |\mathcal{C}'\rangle \langle \mathcal{C}| \quad (\text{II.A.13})$$

in the form $\langle \Sigma | O \exp(tM) | P_0 \rangle$. We thus have the same result as for 'static' observables if $OM = MO$: the average is constant in time.

Remark A.4. *Note that when O commutes with M , they can be diagonalized in the same basis (if they are diagonalizable). In other words they have the same eigenvectors.*

By analogy with classical Newton's dynamics, where it was shown that the presence of conserved quantities is a key property to integrate exactly the equation of motion, we would like to construct Markovian models with 'a lot' of conserved observables. In other words we would like to construct a Markov matrix together with several independent matrices that all commute with each others. In the case of classical Newton's dynamics the number of independent conserved quantities required to exactly solve the equations of motion is precisely known, it depends on the dimension of the phase space. The situation is less clear in the case of Markovian processes. We are lacking a general theorem (as Liouville theorem) that ensures the exact solvability of the model, i.e the exact diagonalization of its Markov matrix, if there are enough conserved quantities.

Nevertheless we will present a framework, taken from quantum integrability, which allows us to produce Markov matrices together with a family of commuting operators, and which provides tools to diagonalize the Markov matrix in some specific cases.

2 Exclusion processes framework

a) The configuration space

The first thing to do, if we want to construct integrable Markov processes, is to define the configuration space of the process, see chapter I. The construction of a Markov matrix commuting with a lot of different operators is a very difficult task and requires to deal with very particular configurations sets. This is the reason we will focus now on what is called *exclusion processes* which provide a fruitful framework to construct integrable Markov processes.

These models are defined on a one dimensional lattice³ composed of L sites that are denoted by the variable $i = 1, 2, \dots, L$. Particles of N different species, labeled $1, 2, \dots, N$, can evolve on this lattice. The term "evolve" is deliberately vague because we focus here on the configuration

³Note that exclusion processes can be also defined on higher dimensional lattices but the one dimensional case reveals to be particularly fruitful in the integrability point of view.

space of the model, we will present the precise stochastic dynamical rules in the next subsection b). The particles are subject to a hard core constraint (exclusion principle), *i.e.* each site is occupied by at most one particle. Note that this constraint could be relaxed to allow several particles to be on the same site, see for instance the generalized exclusion processes [35–37]. A site on the lattice can be in $N + 1$ different states, depending on its content. More precisely for each site i we define a local configuration variable $\tau_i \in \{0, 1, \dots, N\}$, where $\tau_i = 0$ if the site i is empty and $\tau_i = s \geq 1$ if the site i is occupied by a particle of species s . The configuration of the system on the whole lattice are thus in one to one correspondence with the L -uplets $(\tau_1, \dots, \tau_L) \in \{0, \dots, N\}^L$. There are $(N + 1)^L$ configurations.

Following the lines of definition B.3, the goal now is to construct a vector space, with a well chosen vector basis, in order to express the configuration probabilities and the master equation in a concise way. To each configuration $\mathcal{C} = (\tau_1, \dots, \tau_L)$ one can associate a basis vector $|\tau_1, \dots, \tau_L\rangle$. For such a purpose, we associate to a local configuration variable τ_i a basis vector $|\tau_i\rangle$ of \mathbb{C}^{N+1} .

Definition A.5. For $\tau = 0, 1, \dots, N$, the vector $|\tau\rangle$ is defined by

$$|\tau\rangle = \underbrace{(0, \dots, 0)}_{\tau}, 1, \underbrace{(0, \dots, 0)}_{N-\tau}^t, \quad (\text{II.A.14})$$

where t denotes the usual transposition. The vectors $|\tau\rangle$, for $\tau = 0, \dots, N$ constitute a canonical basis of \mathbb{C}^{N+1} .

These vectors $|\tau_i\rangle$ represent the building blocks of the vectors $|\tau_1, \dots, \tau_L\rangle$. The construction is inspired again by quantum spin chains, where the Hilbert space associated to the whole chain is obtained by tensor products of the Hilbert space associated to a single spin.

Definition A.6. For $0 \leq \tau_1, \dots, \tau_L \leq N$, the vector $|\tau_1, \dots, \tau_L\rangle$ is defined by

$$|\tau_1, \dots, \tau_L\rangle = |\tau_1\rangle \otimes |\tau_2\rangle \otimes \dots \otimes |\tau_L\rangle. \quad (\text{II.A.15})$$

The vectors $|\tau_1\rangle \otimes \dots \otimes |\tau_L\rangle$, for $\tau_i = 0, \dots, N$ constitute a canonical basis of $(\mathbb{C}^{N+1})^{\otimes L}$.

In order for the reader to be familiar with the tensor product notation and with the conventions used in this manuscript, we give the following explicit examples.

Example A.7.

$$\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} \otimes \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} = \begin{pmatrix} a_1 b_1 \\ a_1 b_2 \\ a_1 b_3 \\ a_2 b_1 \\ a_2 b_2 \\ a_2 b_3 \\ a_3 b_1 \\ a_3 b_2 \\ a_3 b_3 \end{pmatrix} \quad (\text{II.A.16})$$

and

$$\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \otimes \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \otimes \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} a_1 b_1 c_1 \\ a_1 b_1 c_2 \\ a_1 b_2 c_1 \\ a_1 b_2 c_2 \\ a_2 b_1 c_1 \\ a_2 b_1 c_2 \\ a_2 b_2 c_1 \\ a_2 b_2 c_2 \end{pmatrix} \quad (\text{II.A.17})$$

In words, the tensor product of two vectors of sizes n and m can be seen as a single vector of size $n \times m$ obtained by multiplying each entry of the left vector by the entire right vector. This procedure is used iteratively to construct tensor products of several vectors as a single vector.

We now show how to use this machinery to express in a very compact form the probabilities of the different configurations. We recall that the probability for the system to be in configuration $\mathcal{C} = (\tau_1, \dots, \tau_L)$ at time t is denoted by $P_t(\tau_1, \dots, \tau_L)$.

Definition A.8. We define a vector $|P_t\rangle$ that contains all the configuration probabilities

$$|P_t\rangle = \begin{pmatrix} P_t(0, \dots, 0, 0) \\ P_t(0, \dots, 0, 1) \\ \vdots \\ P_t(N, \dots, N, N) \end{pmatrix} = \sum_{0 \leq \tau_1, \dots, \tau_L \leq N} P_t(\tau_1, \dots, \tau_L) |\tau_1\rangle \otimes \dots \otimes |\tau_L\rangle. \quad (\text{II.A.18})$$

The probabilities of the configurations are stored as the coefficient of a linear expansion. The coefficient in front of a vector $|\tau_1\rangle \otimes \dots \otimes |\tau_L\rangle$ is the probability of the corresponding configuration. This reads formally like the expansion of the wave function of a quantum spin chain system on the Hilbert space basis (the only difference being that the probability of a configuration in the latter case is obtained by absolute value of the coefficient *squared*).

Example A.9. The simplest example we can give of such construction is the case with a single species of particles, i.e for $N = 1$. The local configuration variables τ_i can only take two values in such models: $\tau_i = 0, 1$. We have explicitly

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \text{and} \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad (\text{II.A.19})$$

which span the vector space \mathbb{C}^2 . If we consider the particular case of the basis associated to two sites, we have then

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \quad (\text{II.A.20})$$

corresponding to empty lattice, one particle on the second site, one particle on the first site and the full lattice respectively.

Let us stress that, even though the exclusion condition can appear as a strong restriction on the physical systems that can be well described within this framework, the models that can be constructed in this category display a rich physical phenomenology and capture the essential aspects of non-equilibrium systems [36–38]. The framework of exclusion processes thus enjoy a two-fold interest: on physical side it provides relevant non-equilibrium models and on mathematical side it offers a good laboratory to investigate integrability and exact solvability.

b) Markov matrix

The configurations set of the system being settled, we are now interested in the stochastic dynamics of the model. All the discussion of this subsection will only concern continuous time Markov processes. Nevertheless the machinery that will be developed for the construction of integrable continuous time processes will also provide at the end examples of integrable discrete time processes, see (II.B.29) and (II.C.40) for instance. Once again, it is a hard problem to build a Markov matrix together with a set of commuting operators (which is a strong hint of exact solvability). We have thus to restrict ourself to particular class of stochastic dynamics that has been revealed to be of great interest from the exact solvability point of view. We

will be interested in stochastic dynamics allowing only for local configuration changes on the lattice. The particles can only jump to their direct neighbor sites, exchange or react only with particles on adjacent sites, and can also be created or annihilated locally on a site. The probability rates of such changes depend only on the local configurations on the direct neighbor sites. More precisely we are interested in dynamics encoded by a Markov matrix that can be formally decomposed as a sum of local operators, sometimes called local jump operators, acting non-trivially on two adjacent sites of the lattice (and trivially on the other sites):

$$M = \sum_{i=1}^{L-1} m_{i,i+1}, \quad (\text{II.A.21})$$

with $m_{i,i+1}$ a local jump operator acting on sites i and $i + 1$

$$m_{i,i+1} = \underbrace{\mathbf{1} \otimes \cdots \otimes \mathbf{1}}_{i-1} \otimes m \otimes \underbrace{\mathbf{1} \otimes \cdots \otimes \mathbf{1}}_{L-i-1}, \quad (\text{II.A.22})$$

where m is a Markov matrix of size $(N + 1)^2 \times (N + 1)^2$ acting on two adjacent sites, *i.e.* on the vector space $\mathbb{C}^{N+1} \otimes \mathbb{C}^{N+1}$ and $\mathbf{1}$ is the $(N + 1) \times (N + 1)$ identity matrix. The matrix element $\langle v | \otimes \langle v' | m | \tau \rangle \otimes | \tau' \rangle$, with $(v, v') \neq (\tau, \tau')$, is equal to the probability rate that the system jumps from configuration $(\tau_1, \dots, \tau_{i-1}, \tau, \tau', \tau_{i+2}, \dots, \tau_L)$ to configuration $(\tau_1, \dots, \tau_{i-1}, v, v', \tau_{i+2}, \dots, \tau_L)$. Note that this rate depends only on the local configurations (τ, τ') and (v, v') and not on the states of the other sites.

This class of model can appear very restrictive at first sight but they revealed to be rich enough to encode the essential feature of non equilibrium systems [36–38]. To fix the ideas and show the physical relevance of this framework, we now present examples of such dynamics. The models that we introduce will serve as recurrent examples to illustrate the different concepts exposed throughout this manuscript. Some of them are widely known in the literature.

Example A.10. *The Asymmetric Simple Exclusion Process (ASEP) [39, 40] has become over the last decade a paradigmatic model in out-of-equilibrium statistical physics [36, 41, 42]. It was first introduced in the context of biology and gave rise since then to a lot of interest in different fields. First of all it displays a very rich physical phenomenology with shock waves [43, 44] and boundary induced phase transitions [45–47]. Moreover, from the mathematical point of view, it gave rise to a lot of work in representation theory and combinatorics with the connection to orthogonal polynomials [48, 49], but also in integrability and probability theory with the connection to the Kardar-Parisi-Zhang equation [50, 51].*

The model describes particles of a single species that can diffuse on the lattice. During time dt , a particle has a probability $p \times dt$ (respectively $q \times dt$) to jump to its right (respectively left) neighbor site, provided that it is empty (this is the exclusion constraint, there is at most one particle per site). The asymmetry in the hopping rates mimics a driving force that tends to push the particle in one direction rather than in the other. Note that the ASEP is sometimes defined with a right hopping rate p normalized to 1 (it corresponds to perform a rescaling of the time).

In the vector basis $|0\rangle \otimes |0\rangle$, $|0\rangle \otimes |1\rangle$, $|1\rangle \otimes |0\rangle$, $|1\rangle \otimes |1\rangle$ (ordered this way), the local jump operator m is written

$$m = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -q & p & 0 \\ 0 & q & -p & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (\text{II.A.23})$$

The ASEP admits two limits that are of particular interest. They are presented in the following examples.

Example A.11. *The limit $p = 1$ and $q = 0$ is called the Totally Asymmetric Simple Exclusion Process (TASEP). This model has been widely studied in the literature because it displays*

roughly the same physical behavior as the ASEP but the computations often simplify drastically. We will observe it in the next section for the expression of the stationary state of the model.

In the vector basis $|0\rangle \otimes |0\rangle$, $|0\rangle \otimes |1\rangle$, $|1\rangle \otimes |0\rangle$, $|1\rangle \otimes |1\rangle$ (ordered this way), the local jump operator m is written

$$m = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (\text{II.A.24})$$

Example A.12. The limit $p = 1$ and $q = 1$ is called the Symmetric Simple Exclusion Process (SSEP). There is no more driving force in the bulk, the particles have the same probability rates to jump on the left or on the right. The model thus describes particles diffusing on the lattice with an hard-core constraint. The physics is simpler than in the ASEP case, in the sense that the bulk dynamics tends to converge toward a thermodynamic equilibrium, because there is no driving force. The system can only be driven out-of-equilibrium by interactions with particles reservoirs. We will also observe that the computations of physical quantities are much simpler than for the ASEP. The local jump operator m is written

$$m = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (\text{II.A.25})$$

We observed in the previous examples that the framework is well suited to describe the (driven) diffusion of particle with hard-core repulsion. But it is not limited to this kind of dynamics and can for instance deal with creation/annihilation of particles or reaction between particles. The following example is a simple illustration of this fact.

Example A.13. The Dissipative Symmetric Simple Exclusion Process (DiSSEP) describes particles diffusing in a symmetric way with exclusion constraint (similarly to the SSEP). In addition to that, particle pairs are allowed to condensate or evaporate from the lattice with the same probability rate λ^2 . The local jump operator m is written

$$m = \begin{pmatrix} -\lambda^2 & 0 & 0 & \lambda^2 \\ 0 & -1 & 1 & 0 \\ 0 & 1 & -1 & 0 \\ \lambda^2 & 0 & 0 & -\lambda^2 \end{pmatrix}. \quad (\text{II.A.26})$$

We can also easily define models with several species of particles in interaction. The following example may be thought as one of the simplest case we can imagine.

Example A.14. The 2-species TASEP is a generalization of the TASEP obtained by adding a second species of particles. During an infinitesimal time dt , a particle of first or second species (labeled respectively 1 and 2) can jump to the right with probability dt provided that the neighbor site is empty. A particle of species 2 can also overtake a particle of species 1 with probability dt . In the vector basis $|0\rangle \otimes |0\rangle$, $|0\rangle \otimes |1\rangle$, $|0\rangle \otimes |2\rangle$, $|1\rangle \otimes |0\rangle$, $|1\rangle \otimes |1\rangle$, $|1\rangle \otimes |2\rangle$, $|2\rangle \otimes |0\rangle$, $|2\rangle \otimes |1\rangle$, $|2\rangle \otimes |2\rangle$ (ordered this way), the local jump operator m is written

$$m = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & -1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}. \quad (\text{II.A.27})$$

In all the models presented, we only dealt with the stochastic dynamics in the bulk of the system, never mentioning what is happening on the extremities of the lattice. The boundary conditions are of particular interest in out-of-equilibrium statistical physics because they can influence the macroscopic behavior of the whole system, even if the interactions at the boundaries are very short range. In contrast to equilibrium statistical physics, where the boundary effects are negligible in systems with short range interactions, the system can change phase due to boundary effects. We will focus, in what follows, on two kinds of boundary conditions: the periodic boundary condition and the open boundaries condition.

The periodic boundary condition describes a lattice with a ring shape. The last site L and the first site 1 are neighbors: the first site 1 plays the role of a site $L + 1$ (see figure II.1). The Markov matrix is formally written, in this case,

$$M = \sum_{i=1}^L m_{i,i+1}. \quad (\text{II.A.28})$$

In this equation, it is understood that $L + 1 \equiv 1$.

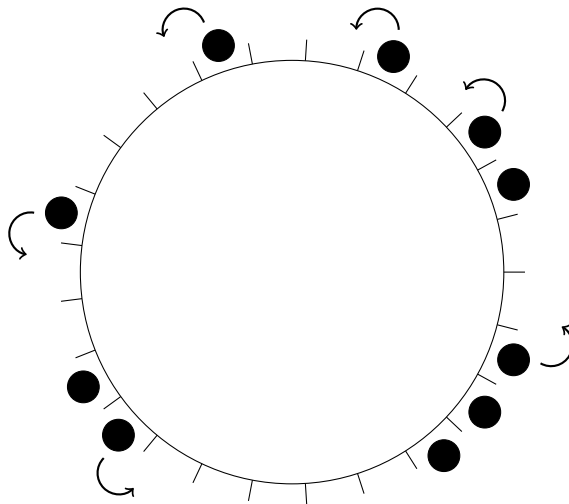


Figure II.1: Dynamical rules of the periodic TASEP.

The open boundaries condition describes a lattice that is coupled with particle reservoirs at its extremities: at the first site, 1, and at the last site, L . Particles of different species can be injected, extracted or exchanged at these two extremities with a probability rate that depends only on the content of the first (respectively last) site, and not on the local configurations on the other sites. In this case the Markov matrix is expressed as

$$M = B_1 + \sum_{i=1}^{L-1} m_{i,i+1} + \bar{B}_L, \quad (\text{II.A.29})$$

with

$$B_1 = B \otimes \underbrace{\mathbf{1} \otimes \cdots \otimes \mathbf{1}}_{L-1}, \quad \text{and} \quad \bar{B}_L = \underbrace{\mathbf{1} \otimes \cdots \otimes \mathbf{1}}_{L-1} \otimes \bar{B}, \quad (\text{II.A.30})$$

where B and \bar{B} are Markov matrices of size $(N + 1) \times (N + 1)$ acting on a single site, *i.e.* on the vector space \mathbb{C}^{N+1} . The matrix element $\langle v | B | \tau \rangle$ (respectively $\langle v | \bar{B} | \tau \rangle$), with $v \neq \tau$, is equal to the probability rate that the system jumps from configuration $(\tau, \tau_2, \dots, \tau_L)$ to configuration $(v, \tau_2, \dots, \tau_L)$ (respectively from $(\tau_1, \dots, \tau_{L-1}, \tau)$ to $(\tau_1, \dots, \tau_{L-1}, v)$). Note that this rate depends only on the local configurations τ and v and not on the states of the other sites.

Example A.15. In the ASEP, we can define the following dynamics at the boundaries. During an infinitesimal time dt , a particle located on site 1 can be absorbed by the left reservoir with probability $\gamma \times dt$, and conversely the left reservoir can inject a particle on the first site, if it is empty, with probability $\alpha \times dt$. Similarly on the site L , the right reservoir can inject a particle (provided that the site is empty) with probability $\delta \times dt$ and remove a particle with probability $\beta \times dt$. In the basis $|0\rangle, |1\rangle$ (ordered this way) the boundary local jump operators B and \bar{B} thus are written

$$B = \begin{pmatrix} -\alpha & \gamma \\ \alpha & -\gamma \end{pmatrix} \quad \text{and} \quad \bar{B} = \begin{pmatrix} -\delta & \beta \\ \delta & -\beta \end{pmatrix} \quad (\text{II.A.31})$$

Note that these boundary local jump operators are also suitable to encode the dynamics with the reservoirs in the case of the SSEP and of the DiSSEP.

Example A.16. In the TASEP case, the dynamics of the system at the boundaries should not be in opposition with the dynamics in the bulk, where particles are only allowed to jump to the right. In other words, the left reservoir can only inject particles on the lattice and the right reservoir can only remove particle from the lattice. This translates into the fact that the boundary rates γ and δ introduced for the ASEP are now vanishing. The boundary local jump operators thus are written

$$B = \begin{pmatrix} -\alpha & 0 \\ \alpha & 0 \end{pmatrix} \quad \text{and} \quad \bar{B} = \begin{pmatrix} 0 & \beta \\ 0 & -\beta \end{pmatrix} \quad (\text{II.A.32})$$

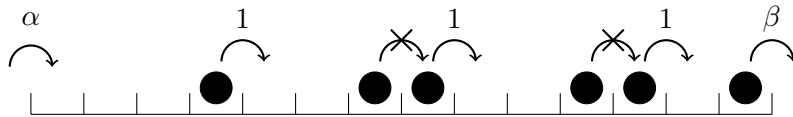


Figure II.2: Dynamical rules of the open TASEP.

We now give an example of boundary jump operators for a multi-species (*i.e.* $N > 1$) model.

Example A.17. For the 2-species TASEP, we do not want the dynamics on the boundaries to be opposite with respect to the dynamics in the bulk (similarly to the single species TASEP). In other words, the left reservoir can only inject particles of both species on the first site (if it is empty) and exchange a particle of species 1 with a particle of species 2, in agreement with the overtake rule in the bulk. Similarly the right reservoir can only remove particles from the last site or exchange particle of species 2 with particles of species 1. An illustration of very specific boundary local jump operators is given (in the basis $|0\rangle, |1\rangle, |2\rangle$) by

$$B = \begin{pmatrix} -1 & \cdot & \cdot \\ 1 - \alpha & -\alpha & \cdot \\ \alpha & \alpha & \cdot \end{pmatrix} \quad \text{and} \quad \bar{B} = \begin{pmatrix} \cdot & \beta & \beta \\ \cdot & -\beta & \cdot \\ \cdot & \cdot & -\beta \end{pmatrix} \quad (\text{II.A.33})$$

We have presented so far the physical framework that we will be interested in throughout this manuscript. We also introduced the main mathematical tools, which we use to define precisely the Markov matrices encoding the stochastic dynamics of the physical systems.

We will now be interested in exactly solvable models. We saw at the beginning of this chapter that the existence of “many” conserved quantities is a strong hint of exact solvability. We see below a systematic way to produce Markov matrices belonging to a set of commuting operators. This construction provides also (at least in specific cases) tools to diagonalize exactly the Markov matrix.

B Integrability for periodic boundary conditions

We start to present the construction of integrable Markov matrices with the case of periodic boundary conditions. The method relies on the construction of a set of commuting operators containing the Markov matrix. This set is conveniently generated by a *transfer matrix*, which depends on a variable called spectral parameter. The Markov matrix is recovered from the transfer matrix by taking the derivative with respect to the spectral parameter. The essential feature of this transfer matrix is that it commutes for different values of the spectral parameter. Similarly to the Markov matrix, which is defined in terms of local jump operators, the transfer matrix will be defined with the help of operators, called R matrices, which also act locally. The R matrix can be thought as a spectral parameter upgrading of the local jump operators m . Moreover the commutation property of the transfer matrix is a direct consequence of a local property satisfied by the R -matrices: the Yang-Baxter equation.

1 R-matrix and transfer matrix

a) R-matrix and Yang-Baxter equation

We introduce in this paragraph the key object of integrability: the R -matrix. It is the building block of the transfer matrix, which generates the Markov matrix together with a set of commuting operators. It is also directly related to the bulk local jump operators m and thus appears as the guarantee of the integrability of the local stochastic rules of the model.

Definition B.1. A matrix $R(z, z')$ of size $(N + 1)^2 \times (N + 1)^2$, i.e acting on $\mathbb{C}^{N+1} \otimes \mathbb{C}^{N+1}$, satisfies the Yang-Baxter equation if

$$R_{1,2}(z_1, z_2) R_{1,3}(z_1, z_3) R_{2,3}(z_2, z_3) = R_{2,3}(z_2, z_3) R_{1,3}(z_1, z_3) R_{1,2}(z_1, z_2). \quad (\text{II.B.1})$$

The Yang-Baxter equation states an equality between products of operators acting on the vector space $\mathbb{C}^{N+1} \otimes \mathbb{C}^{N+1} \otimes \mathbb{C}^{N+1}$. The subscript indices indicate on which copies of \mathbb{C}^{N+1} the operators are acting non trivially. For instance

$$R_{1,2}(z, z') = R(z, z') \otimes \mathbf{1}, \quad R_{2,3}(z, z') = \mathbf{1} \otimes R(z, z'), \quad \dots \quad (\text{II.B.2})$$

We would like to give a pictorial representation of the Yang-Baxter equation. The action of the R -matrix $R_{ij}(z_i, z_j)$ can be represented graphically in figure II.3. The R -matrix is drawn

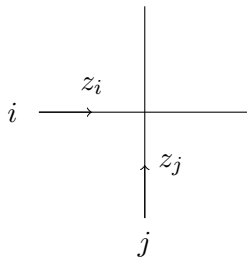


Figure II.3: Graphical representation of the matrix $R_{ij}(z_i, z_j)$.

as a vertex. This vertex is defined by two lines labeled i and j , which correspond to the tensor space component numbers i and j respectively. Each line is oriented by an arrow and carry a spectral parameter. The incoming half line (according to the arrow direction) labeled with i stands for a vector $|\tau\rangle$ of the i -th tensor space component, and can thus be in $N + 1$ different states. Similarly for the incoming half line labeled with j , which stands for a vector $|\tau'\rangle$. The out-going half lines stand for the vectors $\langle v|$, respectively $\langle v'|$, which belong to i -th, respectively j -th tensor space components. When the vectors $|\tau\rangle$, $|\tau'\rangle$ and $\langle v|$, $\langle v'|$ are specified, the vertex represents the matrix element $\langle v|_i \langle v'|_j R_{ij}(z_i, z_j) |\tau\rangle_i |\tau'\rangle_j$.

With this graphical interpretation, we will be able to compute efficiently a matrix element of a product of R matrices acting in different components of the tensor product. It also provides a meaningful illustration of the Yang-Baxter equation, see figure II.4. This pictorial representation of the R -matrix had been widely used in the context of two-dimensional vertex models in equilibrium statistical physics [29].

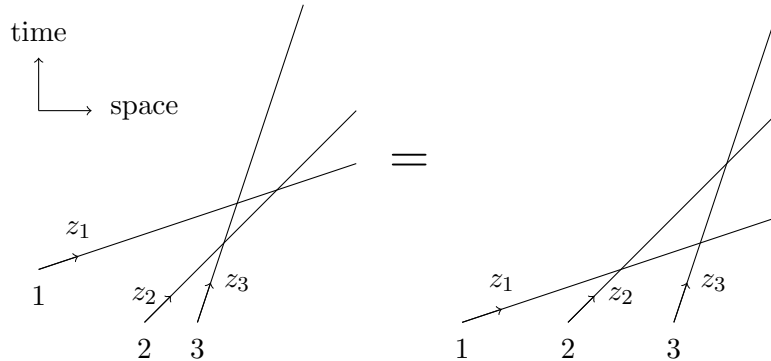


Figure II.4: Graphical representation of the Yang-Baxter equation.

The Yang-Baxter equation has a nice intuitive interpretation (see figure II.4) coming from integrable quantum field theory. In this context the R -matrix $R(z_1, z_2)$ is the diffusion matrix between two particles with rapidities z_1 and z_2 . The integrability is the fact that the diffusion matrix of 3 particles factorizes in this R -matrix (*i.e.* the scattering of three particles can be decomposed into two-particle scatterings). The Yang-Baxter equation is the consistency relation of this factorization, which ensures the independence of the result with respect to the order of the two-particles scatterings.

From a more algebraic side, the R -matrix can be thought as a convenient object to encode the commutation relations of an algebra (see chapter III for instance with the Zamolodchikov-Faddeev relation). The Yang-Baxter relation appears in this case as a consistency relation ensuring the associativity of the algebra.

We would like now to relate the R -matrix to the bulk local jump operator m . To do so, we need one more definition.

Definition B.2. For $R(z, z')$ satisfying the Yang-Baxter equation, we introduce the braided R -matrix

$$\check{R}(z, z') = P.R(z, z'), \quad (\text{II.B.3})$$

where P is the permutation operator in $\mathbb{C}^{N+1} \otimes \mathbb{C}^{N+1}$ that is $P|\tau\rangle \otimes |\tau'\rangle = |\tau'\rangle \otimes |\tau\rangle$, for all $\tau, \tau' = 0, \dots, N$.

Note that the braided matrix $\check{R}(z, z')$ satisfies the braided Yang-Baxter equation

$$\check{R}_{12}(z_1, z_2)\check{R}_{23}(z_1, z_3)\check{R}_{12}(z_2, z_3) = \check{R}_{23}(z_2, z_3)\check{R}_{12}(z_1, z_3)\check{R}_{23}(z_1, z_2). \quad (\text{II.B.4})$$

We are now equipped to state one of the key points of this subsection. It provides a precise definition of integrability for a bulk local jump operator m and relates it to the R -matrix.

Definition B.3. A bulk local jump operator m is said to be integrable if there exists an R -matrix $R(z, z')$ satisfying the Yang-Baxter equation (II.B.1), a constant θ and a complex number z' such that

$$m = \theta \left. \frac{\partial}{\partial z} \check{R}(z, z') \right|_{z=z'}. \quad (\text{II.B.5})$$

In other words, the integrable local jump operators m are obtained by taking the derivative of a braided R -matrix with respect to a spectral parameter. Conversely, we could wonder whether it is possible, starting from a local jump operator m , to upgrade it to a spectral parameter dependent R -matrix. This will be partially answered in subsection c).

We would like to stress that taking the derivative of a braided R -matrix does not provide always a local Markovian matrix. The sum of the entries of each column of the local Markovian matrix should indeed vanish. It is straightforward to check that if the sum of the entries of each column of the R -matrix is equal to 1 then the derivative enjoys the sum to 0 property (but we still have to check that the off-diagonal entries of the derivative are non-negative). This motivates the following definition

Definition B.4. A matrix $R(z, z')$ acting on $\mathbb{C}^{N+1} \otimes \mathbb{C}^{N+1}$ satisfies the Markovian property if

$$\langle \sigma | \otimes \langle \sigma | R(z, z') = \langle \sigma | \otimes \langle \sigma | \quad (\text{II.B.6})$$

where $\langle \sigma |$ defined as $\langle \sigma | = \sum_{v=0}^N \langle v |$ stands for the sum over all the local configurations on one site.

Note that such a R -matrix satisfies the requirement of a discrete time Markovian process, provided that its entries are non-negative. We will see below that it can indeed be used as the building block of discrete time Markov matrices defined on the whole lattice.

We now list a set of properties that will be always satisfied by the R -matrices we will consider. When defining the transfer matrix below, these properties will be essential to ensure its commutation relation and its link with the Markov matrix of the model.

Definition B.5. A matrix $R(z, z')$ acting on $\mathbb{C}^{N+1} \otimes \mathbb{C}^{N+1}$ satisfies the regularity property if

$$R(z, z) = P, \quad (\text{II.B.7})$$

where P is the permutation operator.

The permutation operator P allows us to define the matrix $R_{21}(z, z') := P.R_{12}(z, z').P$. We will often observe in the following that this matrix is closely related to the inverse of the R -matrix. The following definition specifies this connection.

Definition B.6. A matrix $R(z, z')$ acting on $\mathbb{C}^{N+1} \otimes \mathbb{C}^{N+1}$ satisfies the unitarity property if

$$R_{12}(z, z').R_{21}(z', z) = \mathbf{1}. \quad (\text{II.B.8})$$

Note that for a braided R -matrix, it reads $\check{R}(z, z').\check{R}(z', z) = \mathbf{1}$.

In most of the known examples, the dependence of the R -matrix on the two spectral parameters z and z' is simpler than expected, in the sense that it depends only on the ratio z/z' or on the difference $z - z'$. This motivates the following definitions.

Definition B.7. A matrix $R(z, z')$ is said to be multiplicative in the spectral parameters if

$$R(z, z') = R\left(\frac{z}{z'}\right). \quad (\text{II.B.9})$$

It is straightforward to simplify the properties introduced above in this case:

- The Yang-Baxter equation becomes

$$R_{1,2}\left(\frac{z_1}{z_2}\right) R_{1,3}\left(\frac{z_1}{z_3}\right) R_{2,3}\left(\frac{z_2}{z_3}\right) = R_{2,3}\left(\frac{z_2}{z_3}\right) R_{1,3}\left(\frac{z_1}{z_3}\right) R_{1,2}\left(\frac{z_1}{z_2}\right). \quad (\text{II.B.10})$$

- The regularity property becomes $R(1) = P$.
- The unitarity property becomes $R_{12}(z).R_{21}(1/z) = \mathbf{1}$
- The Markovian property becomes $\langle \sigma | \otimes \langle \sigma | R(z) = \langle \sigma | \otimes \langle \sigma |$.

Definition B.8. A matrix $R(z, z')$ is said to be additive in the spectral parameters if

$$R(z, z') = R(z - z'). \quad (\text{II.B.11})$$

It is straightforward to simplify the properties introduced above in this case:

- The Yang-Baxter equation becomes

$$R_{1,2}(z_1 - z_2) R_{1,3}(z_1 - z_3) R_{2,3}(z_2 - z_3) = R_{2,3}(z_2 - z_3) R_{1,3}(z_1 - z_3) R_{1,2}(z_1 - z_2). \quad (\text{II.B.12})$$

- The regularity property becomes $R(0) = P$
- The unitarity property becomes $R_{12}(z).R_{21}(-z) = \mathbf{1}$
- The Markovian property becomes $\langle \sigma | \otimes \langle \sigma | R(z) = \langle \sigma | \otimes \langle \sigma |$.

We now provide examples of such R -matrices, more particularly those related to the stochastic models already introduced in this manuscript.

Example B.9. The R -matrix related to the ASEP is multiplicative in the spectral parameters and is given by

$$R(z) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{(1-z)q}{p-qz} & \frac{z(p-q)}{p-qz} & 0 \\ 0 & \frac{p-q}{p-qz} & \frac{(1-z)p}{p-qz} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (\text{II.B.13})$$

This matrix satisfies the Yang-Baxter equation (II.B.10), the regularity, unitarity and Markovian properties. The link with the bulk local jump operator (II.A.23) is given by $(q-p)\check{R}'(1) = m$, i.e it corresponds to a value $\theta = q - p$.

Example B.10. For the TASEP, the R matrix is obtained by taking the limit $q = 0$ and $p = 1$ on the matrix (II.B.13). It yields to the simple expression

$$R(z) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & z & 0 \\ 0 & 1 & 1-z & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (\text{II.B.14})$$

This matrix satisfies the Yang-Baxter equation (II.B.10), the regularity, unitarity and Markovian properties. The link with the bulk local jump operator (II.A.24) is given by $-\check{R}'(1) = m$, i.e $\theta = -1$.

The R -matrix is graphically represented, as explained previously at the beginning of this subsection, in figure II.5 (in the figure the missing vertices correspond to vanishing matrix elements of the R -matrix of the TASEP). In this particular case of single species models, i.e for $N = 1$, the graphical interpretation can be specified as follows. A dashed incoming line (according to the arrow direction) denotes the vector $|0\rangle$ (or equivalently an empty site), whereas a continuous thick line denotes the vector $|1\rangle$ (or equivalently an occupied site). In a similar way, the out-going lines (after the crossing point) represent the states $\langle 0|$ and $\langle 1|$ on which we are contracting the matrix R . Note that, in models where the number of particles is conserved by the dynamics, the number of incoming continuous thick lines is equal to the number of out-going continuous thick lines.

$$\begin{array}{ccccc} \langle 00 | R_{ij}(\frac{z_1}{z_2}) | 00 \rangle & \langle 10 | R_{ij}(\frac{z_1}{z_2}) | 10 \rangle & \langle 01 | R_{ij}(\frac{z_1}{z_2}) | 10 \rangle & \langle 10 | R_{ij}(\frac{z_1}{z_2}) | 01 \rangle & \langle 11 | R_{ij}(\frac{z_1}{z_2}) | 11 \rangle \\ \begin{array}{c} \text{---} \xrightarrow{z_1} \text{---} \\ \downarrow z_2 \\ \text{---} \\ j \end{array} & \begin{array}{c} \text{---} \xrightarrow{z_1} \text{---} \\ \downarrow z_2 \\ \text{---} \\ j \end{array} & \begin{array}{c} \text{---} \xrightarrow{z_1} \text{---} \\ \downarrow z_2 \\ \text{---} \\ j \end{array} & \begin{array}{c} \text{---} \xrightarrow{z_1} \text{---} \\ \downarrow z_2 \\ \text{---} \\ j \end{array} & \begin{array}{c} \text{---} \xrightarrow{z_1} \text{---} \\ \downarrow z_2 \\ \text{---} \\ j \end{array} \\ 1 & 1 - \frac{z_1}{z_2} & \frac{z_1}{z_2} & 1 & 1 \end{array}$$

Figure II.5: Non-vanishing vertices associated with the R -matrix of the TASEP.

Example B.11. For the SSEP, the R -matrix is additive in the spectral parameters and is given by

$$R(z) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{z}{z+1} & \frac{1}{z+1} & 0 \\ 0 & \frac{1}{z+1} & \frac{z}{z+1} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (\text{II.B.15})$$

This matrix satisfies the Yang-Baxter equation (II.B.12), the regularity, unitarity and Markovian properties. The link with the bulk local jump operator (II.A.25) is given by $\tilde{R}'(0) = m$, i.e $\theta = 1$. Note that the R -matrix can be written concisely as

$$R(z) = \frac{z + P}{z + 1}, \quad (\text{II.B.16})$$

where P is the permutation operator. This writing leads to a straightforward generalization to the multi-species case (see chapter III). The R -matrix of the SSEP can also be obtained from that of the ASEP by taking the limit $p = q = 1$. This limit has to be carefully taken (if not we obtain the permutation matrix) by introducing the following scaling

$$R^{\text{SSEP}}(z) = \lim_{h \rightarrow 0} R^{\text{ASEP}}(e^{hz})|_{q=pe^h}. \quad (\text{II.B.17})$$

This scaling transforms a multiplicative dependence in the spectral parameter into an additive one, as expected.

All the previous examples were related to single species models. We provide here an example of an R -matrix related to a multi-species model.

Example B.12. The R -matrix of the 2-species TASEP is multiplicative in the spectral parameter and is given by

$$R(z) = \begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & z & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & z & \cdot & \cdot \\ \cdot & 1 & \cdot & 1 - z & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & z & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot & 1 - z & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & 1 - z & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix} \quad (\text{II.B.18})$$

This matrix satisfies the Yang-Baxter equation (II.B.10), the regularity, unitarity and Markovian properties. The link with the bulk local jump operator (II.A.27) is given by $-\tilde{R}'(1) = m$, i.e $\theta = -1$.

b) Transfer matrix

We defined previously the integrability of a local jump operator m as being the derivative of some R -matrix. We will justify this definition in this subsection. We will indeed see that in this case it is possible to construct a transfer matrix, which generates a set of commuting operators including the Markov matrix. The R -matrix is the key building block of this transfer matrix as explained in the following definition.

Definition B.13. The inhomogeneous transfer matrix is an operator acting on the whole lattice $(\mathbb{C}^{N+1})^{\otimes L}$ and is given by

$$t(z|z_1, z_2, \dots, z_L) = \text{tr}_0 (R_{0,L}(z, z_L) R_{0,L-1}(z, z_{L-1}) \dots R_{0,1}(z, z_1)). \quad (\text{II.B.19})$$

The parameters z_1, \dots, z_L are called the inhomogeneity parameters, each of them being associated to a particular site of the lattice (see figure II.6). We introduce $\mathbf{z} = (z_1, \dots, z_L)$ to shorten the notation $t(z|\mathbf{z}) = t(z|z_1, \dots, z_L)$.

We have introduced in the definition of the transfer matrix an auxiliary space \mathbb{C}^{N+1} , labeled by 0, which gets traced out. See figure II.6 for a graphical illustration.

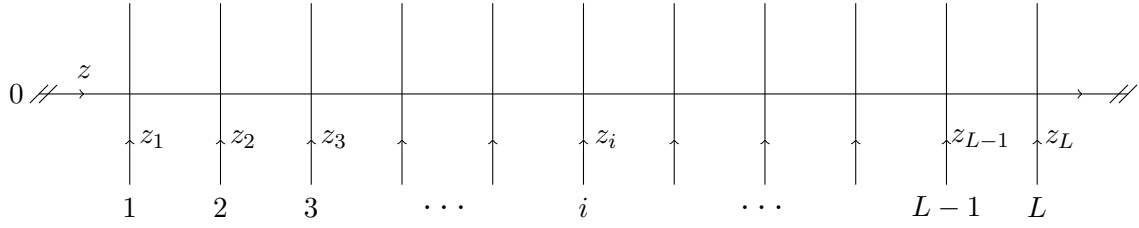


Figure II.6: Graphical representation for $t(z|\mathbf{z})$. Due to the trace in the definition of the transfer matrix, the two double slash should be considered as linked.

Note that when the R -matrix is multiplicative in the spectral parameter, the inhomogeneous transfer matrix is given by

$$t(z|\mathbf{z}) = \text{tr}_0 \left(R_{0,L} \left(\frac{z}{z_L} \right) R_{0,L-1} \left(\frac{z}{z_{L-1}} \right) \dots R_{0,1} \left(\frac{z}{z_1} \right) \right). \quad (\text{II.B.20})$$

We now state the main property of this inhomogeneous transfer matrix.

Proposition B.14. *If the matrix $R(z, z')$ satisfies the Yang-Baxter equation and the unitarity property, the inhomogeneous transfer matrix satisfies the commutation relation*

$$[t(z|\mathbf{z}), t(z'|\mathbf{z})] = 0 \quad (\text{II.B.21})$$

Proof. We compute explicitly

$$\begin{aligned} t(z|\mathbf{z})t(z'|\mathbf{z}) &= \text{tr}_0 \left(R_{0,L} \left(\frac{z}{z_L} \right) \dots R_{0,1} \left(\frac{z}{z_1} \right) \right) \text{tr}_{0'} \left(R_{0',L} \left(\frac{z'}{z_L} \right) \dots R_{0',1} \left(\frac{z'}{z_1} \right) \right) \\ &= \text{tr}_{0,0'} \left(R_{0,L} \left(\frac{z}{z_L} \right) R_{0',L} \left(\frac{z'}{z_L} \right) \dots R_{0,1} \left(\frac{z}{z_1} \right) R_{0',1} \left(\frac{z'}{z_1} \right) \right) \\ &= \text{tr}_{0,0'} \left(R_{0,0'} \left(\frac{z}{z'} \right)^{-1} R_{0,0'} \left(\frac{z}{z'} \right) \times \right. \\ &\quad \left. R_{0,L} \left(\frac{z}{z_L} \right) R_{0',L} \left(\frac{z'}{z_L} \right) \dots R_{0,1} \left(\frac{z}{z_1} \right) R_{0',1} \left(\frac{z'}{z_1} \right) \right) \\ &= \text{tr}_{0,0'} \left(R_{0,0'} \left(\frac{z}{z'} \right)^{-1} \times \right. \\ &\quad \left. R_{0',L} \left(\frac{z'}{z_L} \right) R_{0,L} \left(\frac{z}{z_L} \right) \dots R_{0',1} \left(\frac{z'}{z_1} \right) R_{0,1} \left(\frac{z}{z_1} \right) R_{0,0'} \left(\frac{z}{z'} \right) \right) \\ &= \text{tr}_{0,0'} \left(R_{0',L} \left(\frac{z'}{z_L} \right) R_{0,L} \left(\frac{z}{z_L} \right) \dots R_{0',1} \left(\frac{z'}{z_1} \right) R_{0,1} \left(\frac{z}{z_1} \right) \right) \\ &= t(z'|\mathbf{z})t(z|\mathbf{z}). \end{aligned}$$

■

This property tells us that, expanding the transfer matrix as a polynomial (up to an overall normalization) in the spectral parameter provides operators which commute with each other. The next step will be to see that the Markov matrix is one of these operators. This is the purpose of the following proposition.

Proposition B.15. *The Markov matrix is related to the transfer matrix in the following way*

$$\theta \frac{d \ln t(z)}{dz} \Big|_{z=1} = \theta t'(1)t(1)^{-1} = \sum_{k=1}^L m_{k,k+1} = M, \quad (\text{II.B.22})$$

where $t(z)$ is the homogeneous transfer matrix defined as $t(z) = t(z|1, 1, \dots, 1)$ (this is the inhomogeneous transfer matrix where all the inhomogeneity parameters are set to 1).

Proof. A straightforward computation yields the equality

$$\left. \frac{d \ln t(z)}{dz} \right|_{z=1} = t(1)^{-1} t'(1). \quad (\text{II.B.23})$$

The first step is thus to evaluate

$$\begin{aligned} t(1) &= \text{tr}_0(P_{0,L} \dots P_{0,2} P_{0,1}) \\ &= \text{tr}_0(P_{0,1} P_{1,L} \dots P_{1,2}) \\ &= \text{tr}_0(P_{0,1}) P_{1,L} \dots P_{1,2} \\ &= P_{1,L} \dots P_{1,2}. \end{aligned}$$

so that $t(1)^{-1} = P_{1,2} \dots P_{1,L}$. This is also possible to show that $t(1) = P_{L,L-1} \dots P_{L,1}$, playing with $P_{0,L}$ instead of $P_{0,1}$. This yields the other expression $t(1)^{-1} = P_{L,1} \dots P_{L,L-1}$.

We need also to calculate

$$\begin{aligned} t'(1) &= \sum_{k=2}^L \text{tr}_0(P_{0,L} \dots P_{0,k+1} R'_{0,k}(1) P_{0,k-1} \dots P_{0,1}) + \text{tr}_0(P_{0,L} \dots P_{0,2} R'_{0,1}(1)) \\ &= \sum_{k=2}^L P_{1,L} \dots P_{1,k+1} R'_{1,k}(1) P_{1,k-1} \dots P_{1,2} + P_{L,L-1} \dots P_{L,2} R'_{L,1}(1). \end{aligned}$$

Using the first expression of $t(1)^{-1}$ that we derived for the sum over k and the second expression of $t(1)^{-1}$ for the last term in the previous equation, we obtain

$$\theta t(1)^{-1} t'(1) = \theta \sum_{k=2}^L P_{k-1,k} R'_{k-1,k}(1) + \theta P_{L,1} R'_{L,1}(1) = M. \quad (\text{II.B.24})$$

■

Refinement with twist The transfer matrix defined on a periodic lattice can be modified to 'twist' the periodic boundary conditions. This can be intuitively understood as the fact that the site $L+1$ is not identified with site 1 anymore (usual periodic condition $\tau_{L+1} = \tau_1$) but imposing instead for instance $\tau_{L+1} \equiv \tau_1 + 1$ modulo N , or a more complicated relation.

This twist is achieved by adding an operator $\mathcal{T}(z)$, that may or may not depend on a spectral parameter z , in the expression of the transfer matrix. This twist operator $\mathcal{T}(z)$ has to be carefully chosen in order not to break the integrability of the model, *i.e* the commutation property of the transfer matrix. This yields the definitions below.

Definition B.16. *An integrable twist operator $\mathcal{T}(z)$ is an invertible $(N+1) \times (N+1)$ matrix that satisfies the relation*

$$\check{R}(z_1, z_2) \mathcal{T}(z_1) \otimes \mathcal{T}(z_2) = \mathcal{T}(z_2) \otimes \mathcal{T}(z_1) \check{R}(z_1, z_2). \quad (\text{II.B.25})$$

Note that this relation is a particular (one dimensional or scalar) representation of the so called RTT relation defined later.

Definition B.17. *A twisted transfer matrix is defined as*

$$t_{\mathcal{T}}(z|\mathbf{z}) = \text{tr}_0 \left(R_{0,L} \left(\frac{z}{z_L} \right) R_{0,L-1} \left(\frac{z}{z_{L-1}} \right) \dots R_{0,1} \left(\frac{z}{z_1} \right) \mathcal{T}_0(z) \right). \quad (\text{II.B.26})$$

where $\mathcal{T}(z)$ is an integrable twist operator.

Note that taking $\mathcal{T}(z) = 1$ fulfills the relation (II.B.25) and allows us to recover the usual expression of the non-twisted transfer matrix.

Proposition B.18. *A twisted transfer matrix defines a family of commuting operators*

$$[t_{\mathcal{T}}(z|\mathbf{z}), t_{\mathcal{T}}(z'|\mathbf{z})] = 0. \quad (\text{II.B.27})$$

Proof. This is done in a exactly similar way as for the non-twisted transfer matrix, using in addition the exchange relation (II.B.25) ■

From the out-of-equilibrium physics point of view, the interest of such a twist deformation of the transfer matrix is the possibility (often restricted by integrability) to modify the local stochastic dynamics of the model on the particular sites 1 and L . This is formalized by the following property.

Proposition B.19. *We have the relation*

$$\theta \left. \frac{d \ln t_{\mathcal{T}}(z)}{dz} \right|_{z=1} = \theta t'_{\mathcal{T}}(1) t_{\mathcal{T}}(1)^{-1} = \sum_{k=1}^{L-1} m_{k,k+1} + \mathcal{T}_L(1)^{-1} m_{L,1} \mathcal{T}_L(1) + \theta \mathcal{T}_L(1)^{-1} \mathcal{T}'_L(1). \quad (\text{II.B.28})$$

Proof. The derivation of this formula is done in a similar way as for the untwisted case. ■

Transfer matrix as discrete time Markov matrix We stressed in the previous paragraphs that the transfer matrix can be used to define (through its derivative) continuous time Markov matrices. We are now going to see that the transfer matrix (or a closely related operator) can be used itself in some particular cases to define a discrete time Markov matrix. Rather than generic considerations, we will focus on a particular example related to the transfer matrix of the TASEP.

From the R-matrix associated to the TASEP(II.B.14), we build the inhomogeneous periodic transfer matrix (II.B.20). The homogeneous case (*i.e.* $z_i = 1$) was studied (from the discrete time Markovian process point of view) in [52]. We now introduce the following operator

$$\begin{aligned} M(z|\mathbf{z}) &= t(z|\mathbf{z}) t(z_1|\mathbf{z})^{-1} \\ &= \text{tr}_0 \left[R_{0,L} \left(\frac{z}{z_L} \right) R_{0,L-1} \left(\frac{z}{z_{L-1}} \right) \dots R_{0,1} \left(\frac{z}{z_1} \right) \right] R_{2,1} \left(\frac{z_2}{z_1} \right) \dots R_{L,1} \left(\frac{z_L}{z_1} \right). \end{aligned} \quad (\text{II.B.29})$$

Note that we have normalized $t(z|\mathbf{z})$ using $t(z_1|\mathbf{z})$, but a different choice $t(z_j|\mathbf{z})$, $j = 2, 3, \dots, L$ leads to a similar rotated matrix $M(z|\mathbf{z})$. Obviously $M(z|\mathbf{z})$ commutes with $t(z'|\mathbf{z})$ and has the same eigenvectors. We choose below to use the “normalized matrix” $M(z|\mathbf{z})$ instead of $t(z|\mathbf{z})$ because it allows one to construct easily local jump operators. A direct computation yields indeed that $-M'(1|1, \dots, 1)$, where the derivative is taken with respect to the spectral parameter z , is the Markov matrix of the continuous time TASEP.

From expression (II.B.29) and fig. II.5 we can deduce a graphical representation for $M(z|\mathbf{z})$. The starting point is the lattice illustrated in fig. II.7 that one has to fill according to the matrix element one wants to compute. Instead of explaining it in full generality, we take below a concrete example.

As an example we take $L = 4$ and use the graphical interpretation to compute the transition rate between the initial configuration $(1, 1, 1, 0)$ and the final configuration $(1, 1, 0, 1)$. The initial (resp. final) configuration fixes the form of the incoming (resp. out-going) external lines (dashed or thick) as in fig. II.8. Then, we look for drawings of the form given in fig. II.8 where the remaining thin lines have to be replaced by thick or dashed lines in such a way that the weights (as given in fig.II.5) of all the vertices do not vanish. The total weight of a given possible drawing is then the product of all these weights. It is easy to see that there are only two possible drawings, given in fig. II.9 together with their corresponding weights. Finally the weight of $\langle 1101 | M(z|\mathbf{z}) | 1110 \rangle$ is the sum of the weights of the possible drawings.

Using this graphical interpretation, we are able to compute all the possible rates between any two configurations. We remark in particular that the number of particles is conserved (as

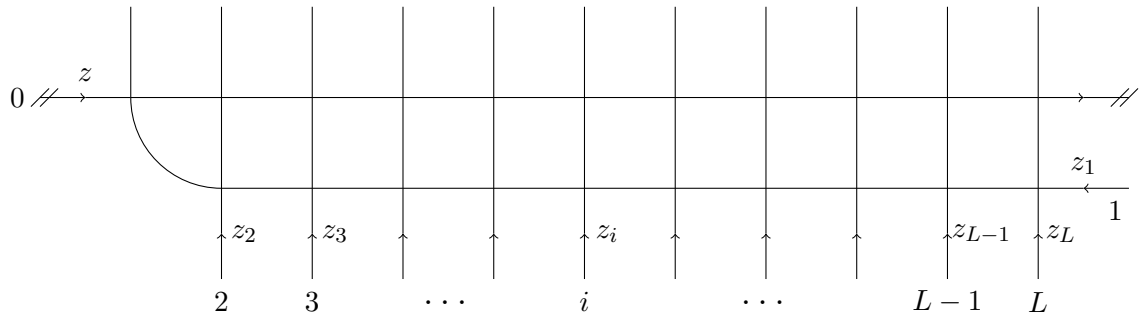


Figure II.7: Graphical representation for $M(z|\mathbf{z})$. Due to the trace in the definition of the transfer matrix, the two double slash should be considered as linked.

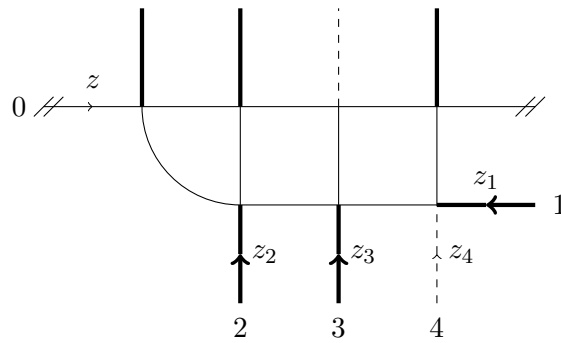


Figure II.8: Starting point for the computation of $\langle 1101|M(z|\mathbf{z})|1110\rangle$.

mentioned previously each non-vanishing vertex preserves the number of particles). Therefore, we restrict ourselves to a given sector with a fixed number of particles. We can also show that all the rates starting from a given configuration (with at least one particle) sum to one which proves that $M(z|\mathbf{z})$ can be used as a discrete time Markov matrix. We have to impose also

$$0 \leq \frac{z_i}{z_1} \leq 1 \quad \text{and} \quad 0 \leq \frac{z}{z_i} \leq 1, \quad i = 1, 2, \dots, L, \quad (\text{II.B.30})$$

so that the probabilities are positive and less than 1. The sector with no particles is special: its dimension is 1 and the matrix $M(z|\mathbf{z})$ is reduced to the scalar $1 + \prod_{i=1}^L (1 - z/z_i)$. Therefore, it cannot be considered as a Markov matrix in the empty sector. From now, we consider only the cases with at least one particle.

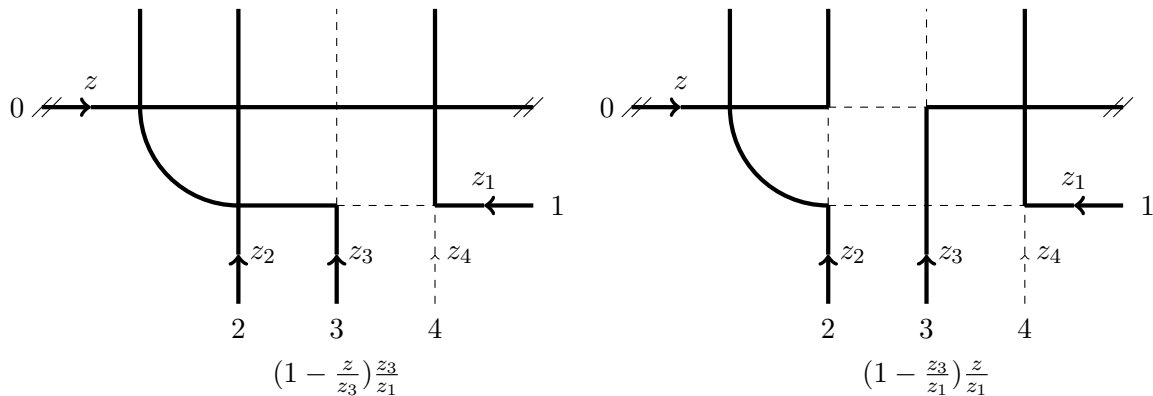


Figure II.9: The two different drawings involved in the computation of the transition rate $\langle 1101|M(z|\mathbf{z})|1110\rangle$ with their respective weights.

The Markov process given by $M(z|\mathbf{z})$ can be interpreted as a discrete time process with

sequential update. The configuration at the time $t + 1$ is obtained from the one at time t by the following dynamics:

- Particle update: starting from right to left (i.e. from the site L to the site $L - 1$ and so on), a particle at the site i jumps to the right on the neighboring site with a probability $1 - z_i/z_1$ provided this site is empty. The particle does not jump with the probability z_i/z_1 . We remind that we are on a periodic lattice, so that the site on the right of the site L is the site 1. Note that a particle located on site 1 does not move.
- Hole update: once the particle update is done, one performs the hole update. Contrary to the particle update, we do not necessarily start and finish at the sites 1 or L . Let r be the site number of a particle (we recall that we restrict ourselves to the case with at least one particle). Starting from the site r , we go from left to right up to the site $r - 1$, using periodicity and knowing that the site on the right of the site L is the site 1. A hole at the site i jumps to the left on the neighboring site with the probability $1 - z/z_{i-1}$ provided the site is occupied. The hole may stay at site i with probability z/z_{i-1} . By convention, we set $z_0 = z_L$.

As mentioned previously, we would like to emphasize that, due to the inhomogeneities in the transfer matrix, the rates depend on the site where the particle or the hole is situated. All the probabilities are positive and less than 1 thanks to (II.B.30). Let us also mention that for the homogeneous case, the update simplifies. Indeed, the first step becomes trivial: the particles do not move.

These rules are illustrated in figure II.10 for a chain with 4 sites in the configuration $(1, 1, 1, 0)$ at time t . We deduce from this figure the different possible rates between the

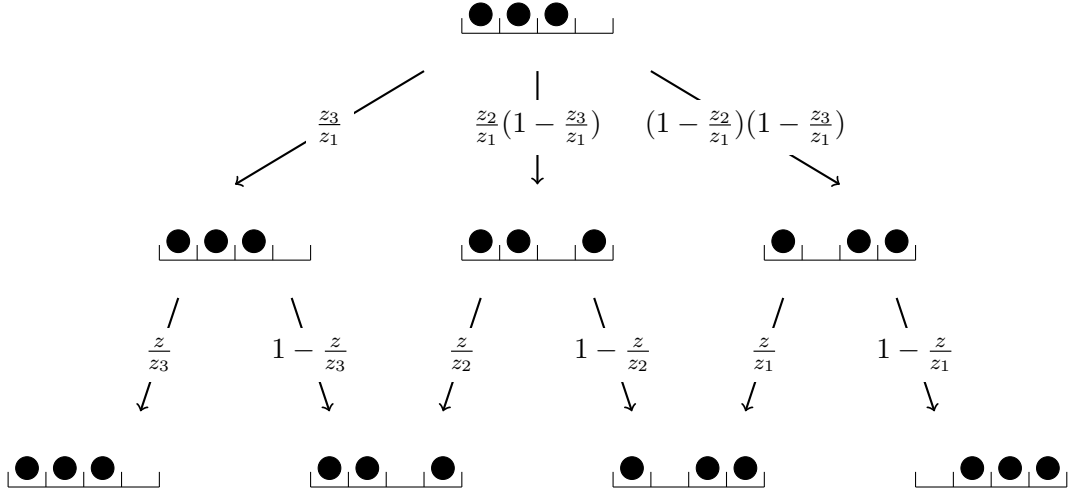


Figure II.10: An example of sequential update corresponding to the Markov matrix $M(z|\mathbf{z})$. The first line is the configuration at time t and the third line shows the possible configurations at time $t + 1$. The second line corresponds to the intermediate configurations after the update of the particles and the hole update still to be done. The label of the arrows provides the rate of the corresponding change of configurations.

configurations which correspond to the entries of $M(z|\mathbf{z})$. One gets

$$M(z|\mathbf{z})((1, 1, 0, 1), (1, 1, 1, 0)) = \langle 1101|M(z|\mathbf{z})|1110\rangle = \left(1 - \frac{z}{z_3}\right) \frac{z_3}{z_1} + \left(1 - \frac{z_3}{z_1}\right) \frac{z}{z_1} \quad (\text{II.B.31})$$

in accordance with the calculation done previously (see figure II.9).

Justification of the sequential up-date: The sequential update described above can be easily identified when considering the Markov matrix $M(z|\mathbf{z})$ at the special point $z = z_j$. Indeed, we

write $M(z_j|\mathbf{z}) = \left(t(z_j|\mathbf{z})\mathfrak{P} \right) \left(\mathfrak{P}^{-1}t(z_1|\mathbf{z})^{-1} \right)$ where \mathfrak{P} is the cyclic permutation. Then, from the explicit expressions

$$t(z_j|\mathbf{z}) = R_{j,j-1}\left(\frac{z_j}{z_{j-1}}\right) \cdots R_{j,1}\left(\frac{z_j}{z_1}\right) R_{j,L}\left(\frac{z_j}{z_L}\right) \cdots R_{j,j+1}\left(\frac{z_j}{z_{j+1}}\right) \quad (\text{II.B.32})$$

$$t(z_1|\mathbf{z})^{-1} = R_{2,1}\left(\frac{z_2}{z_1}\right) R_{3,1}\left(\frac{z_3}{z_1}\right) \cdots R_{L,1}\left(\frac{z_L}{z_1}\right) \quad (\text{II.B.33})$$

it is easy to see that $\mathfrak{P}^{-1}t(z_1|\mathbf{z})^{-1}$ corresponds to the particle update, while $t(z_j|\mathbf{z})\mathfrak{P}$ corresponds to the hole update at $z = z_j$.

Let us remark that such a simple sequential update is specific to the totally asymmetric exclusion process. For the partially asymmetric case, it would be much more involved.

Some properties of the stationary state of the Markov chain defined by $M(z|\mathbf{z})$ will be investigated in chapter III.

2 How to find R-matrices?

We stressed, all along this section, that the R -matrix and the Yang-Baxter equation are the cornerstone of integrability. The R -matrix is the building block⁴ of the transfer matrix. The Yang-Baxter equation ensures the commutation property of the transfer matrix. In order to produce integrable Markovian processes, it thus appears essential to determine R -matrix solutions to the Yang-Baxter equation. This equation is very hard to solve because it involves cubic relations in the entries of the R -matrix. It attracted a lot of attention over the last decades and several solutions have been constructed in specific cases [53–57]. But we are still lacking a general classification of the solutions of this equation.

However different methods have been developed, relying often on algebraic structures hidden behind the Yang-Baxter equation, and providing solutions in some particular situations. We present three of the most commonly used below.

a) Direct resolution of the Yang-Baxter equation

We present a method developed by Baxter to compute the R -matrix of the six-vertex and eight-vertex models. The main idea could be summarized as follows. We would like to isolate some constraints satisfied by the entries of the R -matrix, which are implied by the Yang-Baxter equation. In other words, the $(N+1)^2 \times (N+1)^2$ entries of the R -matrix are lying on some manifold. The spectral parameter parametrizes the manifold: a given spectral parameter corresponds to one point on the manifold and the manifold is spanned when the spectral parameter varies.

Nothing is better than an example to see how it works. We reproduce briefly here the solution of Baxter for the eight-vertex model [29] (in the Markovian case).

Let us define

$$R = \begin{pmatrix} a & 0 & 0 & d \\ 0 & b & c & 0 \\ 0 & c & b & 0 \\ d & 0 & 0 & a \end{pmatrix} \quad (\text{II.B.34})$$

We also introduce the matrix R' (respectively the matrix R'') which is equal to the matrix R but with entries a, b, c, d replaced by a', b', c', d' (respectively by a'', b'', c'', d''). We would like to solve the Yang-Baxter equation

$$R_{12}R'_{13}R''_{23} = R''_{23}R'_{13}R_{12}. \quad (\text{II.B.35})$$

The matrix R intuitively corresponds to $R(z_1/z_2)$, the matrix R' to $R(z_1/z_3)$ and the matrix R'' to $R(z_2/z_3)$ (equation (II.B.35) thus appears as some kind of generalization of (II.B.10)).

⁴In full generality the building block of the transfer matrix is a Lax operator satisfying the RTT relation (II.B.83) and which can be chosen more generally than just equal to R .

Writing equation (II.B.35) in components, we can show that it is equivalent to the following set of equations

$$ac'a'' + da'd'' = bc'b'' + ca'c'' \quad (\text{II.B.36})$$

$$ab'c'' + dd'b'' = ba'c'' + cc'b'' \quad (\text{II.B.37})$$

$$cb'a'' + bd'd'' = ca'b'' + bc'c'' \quad (\text{II.B.38})$$

$$ad'b'' + db'c'' = bd'a'' + cb'd'' \quad (\text{II.B.39})$$

$$aa'd'' + dc'a'' = bb'd'' + cd'a'' \quad (\text{II.B.40})$$

$$da'a'' + ac'd'' = db'b'' + ad'c'' \quad (\text{II.B.41})$$

Following the lines of [29], we observe that these equations are linear in a'' , b'' , c'' , d'' . If we want these equations to have non vanishing solutions, the determinant of any linear system composed of four of these equations should be equal to zero. For instance the determinant of the linear system defined by equations (II.B.36), (II.B.38), (II.B.39) and (II.B.41) is given by

$$(cda'b' - abc'd')[(a^2 - b^2)(c'^2 - d'^2) + (c^2 - d^2)(a'^2 - b'^2)] \quad (\text{II.B.42})$$

To decide which of these two factors should be equal to zero, we consider the case where $a = a'$, $b = b'$, $c = c'$ and $d = d'$. It corresponds intuitively to the case $z_2 = z_3$ in the equation (II.B.10). In this case, we expect from the regularity condition that $R'' = R(z_2/z_3) = R(1) = P$ so that equation (II.B.35) becomes trivial. Indeed we observe in this case that the condition (II.B.42) is satisfied because the first factor vanishes. For continuity reasons, this factor should thus also vanish in the general case $a \neq a'$, $b \neq b'$, $c \neq c'$ and $d \neq d'$. This yields the condition

$$\frac{ab}{cd} = \frac{a'b'}{c'd'} \quad (\text{II.B.43})$$

When this condition is satisfied, we can solve for a'' , b'' , c'' , d'' . Substituting back in the remaining equations (II.B.37) and (II.B.40) yields to the unique constraint

$$\frac{a^2 + b^2 - c^2 - d^2}{ab} = \frac{a'^2 + b'^2 - c'^2 - d'^2}{a'b'} \quad (\text{II.B.44})$$

Following Baxter's work [29], we introduce the following quantities

$$\Delta = \frac{a^2 + b^2 - c^2 - d^2}{2(ab + cd)} \quad (\text{II.B.45})$$

and

$$\Gamma = \frac{ab - cd}{ab + cd} \quad (\text{II.B.46})$$

We can also define Δ' and Γ' (respectively Δ'' and Γ'') where the parameters a, b, c, d replaced by a', b', c', d' (respectively by a'', b'', c'', d''). We can show that the constraints (II.B.43) and (II.B.44) are equivalent to

$$\Delta = \Delta' \quad \text{and} \quad \Gamma = \Gamma'. \quad (\text{II.B.47})$$

When these constraints are satisfied, we recall that we can solve for a'' , b'' , c'' , d'' . It is then straightforward to check that

$$\Delta = \Delta' = \Delta'' \quad \text{and} \quad \Gamma = \Gamma' = \Gamma''. \quad (\text{II.B.48})$$

The equations (II.B.45) and (II.B.46) thus define the manifold on which are lying the entries of the R -matrix. The remaining part of the work is to find a parametrization of the manifold with the help of spectral parameters. The hard part is to determine a parametrization which is additive or multiplicative in the spectral parameter (see the computations below). Baxter succeeded to find one for this eight-vertex model with the help of elliptic functions.

To simplify the computation and also to be consistent with the purpose of this manuscript, we will be interested in the Markovian case, *i.e.* when $d = 1 - a$ and $c = 1 - b$ (and same conditions for the prime and double prime variables), so that the entries of each column of the R -matrix sum to 1. In this particular case, the constraints (II.B.45) and (II.B.46) reduce to

$$\Delta = \Gamma = \frac{a + b - 1}{2ab - a - b + 1} = \frac{a' + b' - 1}{2a'b' - a' - b' + 1} = \frac{a'' + b'' - 1}{2a''b'' - a'' - b'' + 1}. \quad (\text{II.B.49})$$

This can be easily solved in b , b' and b''

$$b = \frac{(\Delta + 1)(a - 1)}{\Delta(2a - 1) - 1}, \quad (\text{II.B.50})$$

and similarly b' and b'' . The equation (II.B.35) is then solved by expressing a'' in function of a and a'

$$a'' = \frac{\Delta(2aa' - a - a' + 1) - a - a' + 1}{\Delta(2aa' - 2a' + 1) - 2a + 1}. \quad (\text{II.B.51})$$

Keeping in mind that we want to find a parametrization with “multiplicative” spectral parameter, we would like to find a function f such that

$$f(a'') = \frac{f(a')}{f(a)}. \quad (\text{II.B.52})$$

This is achieved by the function

$$f : a \rightarrow \frac{a(\lambda - 1) + 1}{a(\lambda + 1) - 1}, \quad (\text{II.B.53})$$

where λ is defined by the relation

$$\Delta = \frac{1 - \lambda^2}{1 + \lambda^2}. \quad (\text{II.B.54})$$

We are now equipped to introduce the spectral parameters $z_1 = f(a)$, $z_2 = f(a')$ and $z_3 = f(a'')$. This allows us to write $R = R(z_1/z_2)$, $R' = R(z_1/z_3)$ and $R'' = R(z_2/z_3)$ where $R(z)$ is defined by

$$R(z) = \begin{pmatrix} \frac{z+1}{\lambda(z-1)+z+1} & 0 & 0 & \frac{\lambda(z-1)}{\lambda(z-1)+z+1} \\ 0 & \frac{z-1}{\lambda(z+1)+z-1} & \frac{\lambda(z+1)}{\lambda(z+1)+z-1} & 0 \\ 0 & \frac{\lambda(z+1)}{\lambda(z+1)+z-1} & \frac{z-1}{\lambda(z+1)+z-1} & 0 \\ \frac{\lambda(z-1)}{\lambda(z-1)+z+1} & 0 & 0 & \frac{z+1}{\lambda(z-1)+z+1} \end{pmatrix} \quad (\text{II.B.55})$$

It satisfies the Yang-Baxter equation (II.B.10), the unitarity, regularity and Markovian properties. It is the R -matrix associated to the DiSSEP. We have indeed

$$2\lambda\check{R}'(1) = m \quad (\text{II.B.56})$$

where m is the bulk local jump operator of the DiSSEP introduced in (II.A.26).

b) Quantum groups

Quantum groups are the theoretical algebraic framework behind the R -matrices. We will briefly define this algebraic structure and then argue on how it can be used to generate solutions to the Yang-Baxter equation.

We first briefly introduce the notion of Hopf algebra, starting from the basics to fix the notations. The reader is invited to refer to [32] for details

Definition B.20. An algebra \mathcal{A} over the field \mathbb{C} is a \mathbb{C} -vector space equipped with two linear maps $\mu : \mathcal{A} \otimes \mathcal{A} \rightarrow \mathcal{A}$, called the multiplication, and $\iota : \mathbb{C} \rightarrow \mathcal{A}$, called the unit, such that the following consistency relations hold⁵

$$\mu(a \otimes \iota(z)) = \mu(\iota(z) \otimes a) = z \cdot a, \quad \forall a \in \mathcal{A}, \forall z \in \mathbb{C} \quad (\text{II.B.57})$$

$$\mu(a_1 \otimes \mu(a_2 \otimes a_3)) = \mu(\mu(a_1 \otimes a_2) \otimes a_3), \quad \forall a_1, a_2, a_3 \in \mathcal{A}. \quad (\text{II.B.58})$$

The last property is usually called associativity of the algebra.

An algebra is said to be commutative if $\mu(a_1 \otimes a_2) = \mu(\sigma(a_1 \otimes a_2))$, for all $a_1, a_2 \in \mathcal{A}$, where σ is the permutation operator, i.e $\sigma(a_1 \otimes a_2) = a_2 \otimes a_1$.

If \mathcal{A} and \mathcal{B} are two algebras, an homomorphism of algebras is a linear map $\psi : \mathcal{A} \rightarrow \mathcal{B}$ satisfying $\psi \circ \mu^{\mathcal{A}} = \mu^{\mathcal{B}} \circ (\psi \otimes \psi)$ and $\iota^{\mathcal{B}} \circ \psi = \iota^{\mathcal{A}}$ where $\mu^{\mathcal{A}}$ and $\iota^{\mathcal{A}}$ (respectively $\mu^{\mathcal{B}}$ and $\iota^{\mathcal{B}}$) denote the multiplication and the unit in \mathcal{A} (respectively in \mathcal{B}).

This definition can appear a bit trivial but we put it here to stress the symmetry with the following definition.

Definition B.21. A coalgebra \mathcal{A} over the field \mathbb{C} is a \mathbb{C} -vector space equipped with two linear maps $\Delta : \mathcal{A} \rightarrow \mathcal{A} \otimes \mathcal{A}$, called the comultiplication, and $\epsilon : \mathcal{A} \rightarrow \mathbb{C}$, called the counit, such that the following consistency relations hold⁶

$$(\mathbb{I} \otimes \epsilon)(\Delta(a)) = (\epsilon \otimes \mathbb{I})(\Delta(a)) = a, \quad \forall a \in \mathcal{A} \quad (\text{II.B.59})$$

$$(\mathbb{I} \otimes \Delta)(\Delta(a)) = (\Delta \otimes \mathbb{I})(\Delta(a)), \quad \forall a \in \mathcal{A}. \quad (\text{II.B.60})$$

The last property is usually called coassociativity of the coalgebra.

A coalgebra is said to be cocommutative if $\Delta(a) = \sigma(\Delta(a))$, for all $a \in \mathcal{A}$.

If \mathcal{A} and \mathcal{B} are two coalgebras, an homomorphism of coalgebras is a linear map $\psi : \mathcal{A} \rightarrow \mathcal{B}$ satisfying $(\psi \otimes \psi) \circ \Delta^{\mathcal{A}} = \Delta^{\mathcal{B}} \circ \psi$ and $\epsilon^{\mathcal{B}} \circ \psi = \epsilon^{\mathcal{A}}$ where $\Delta^{\mathcal{A}}$ and $\epsilon^{\mathcal{A}}$ (respectively $\Delta^{\mathcal{B}}$ and $\epsilon^{\mathcal{B}}$) denote the comultiplication and the counit in \mathcal{A} (respectively in \mathcal{B}).

Definition B.22. A Hopf algebra \mathcal{A} over the field \mathbb{C} is a \mathbb{C} -vector space satisfying the following properties

- \mathcal{A} is simultaneously an algebra and a coalgebra (over the field \mathbb{C});
- the multiplication $\mu : \mathcal{A} \otimes \mathcal{A} \rightarrow \mathcal{A}$ and the unit $\iota : \mathbb{C} \rightarrow \mathcal{A}$ are both homomorphisms of coalgebras;
- the comultiplication $\Delta : \mathcal{A} \rightarrow \mathcal{A} \otimes \mathcal{A}$ and the counit $\epsilon : \mathcal{A} \rightarrow \mathbb{C}$ are both homomorphisms of algebras;
- there exists a linear map $S : \mathcal{A} \rightarrow \mathcal{A}$, called the antipode, such that the following relations hold

$$\mu \circ (S \otimes \mathbb{I})(\Delta(a)) = \mu \circ (\mathbb{I} \otimes S)(\Delta(a)) = \iota \circ \epsilon(a), \quad \forall a \in \mathcal{A}. \quad (\text{II.B.61})$$

Example B.23. If \mathfrak{g} is a Lie algebra, we can define a Hopf structure on its universal enveloping algebra $U(\mathfrak{g})$ (which is defined as the quotient of $\bigoplus_{n \geq 0} \mathfrak{g}^{\otimes n}$ by the ideal generated by the relations $x \otimes y - y \otimes x - [x, y]$, see for instance [32] for details). The universal enveloping algebra is intuitively understood as the algebra generated by all the polynomial relations in the Lie algebra generators. It is thus sufficient to give the definition of the structure maps on the Lie algebra \mathfrak{g} solely (the definition of these maps on elements of $U(\mathfrak{g})$ can be deduced immediately using the homomorphism property)

$$\Delta(g) = g \otimes 1 + 1 \otimes g, \quad S(g) = -g, \quad \epsilon(g) = 0, \quad \forall g \in \mathfrak{g}. \quad (\text{II.B.62})$$

Note that this defines a cocommutative Hopf algebra.

⁵ \circ in the first equation denotes the external composition law of the \mathbb{C} -vectorial space \mathcal{A} .

⁶ To be fully rigorous $z \otimes a$ and $a \otimes z$ are identified with $z \cdot a$, for all $a \in \mathcal{A}$ and $z \in \mathbb{C}$ in the first relation

Definition B.24. We call almost cocommutative a Hopf algebra \mathcal{A} for which there exists an invertible element $\mathcal{R} \in \mathcal{A} \otimes \mathcal{A}$ satisfying

$$\sigma \circ \Delta(a) = \mathcal{R}\Delta(a)\mathcal{R}^{-1}, \quad \forall a \in \mathcal{A}. \quad (\text{II.B.63})$$

If \mathcal{R} satisfies in addition⁷

$$(\Delta \otimes \mathbb{I})(\mathcal{R}) = \mathcal{R}_{13}\mathcal{R}_{23}, \quad (\text{II.B.64})$$

$$(\mathbb{I} \otimes \Delta)(\mathcal{R}) = \mathcal{R}_{13}\mathcal{R}_{12}, \quad (\text{II.B.65})$$

then \mathcal{A} is said to be quasitriangular and \mathcal{R} is called the universal R-matrix.

Proposition B.25. If \mathcal{A} is a quasitriangular Hopf algebra with universal R-matrix \mathcal{R} then

$$\mathcal{R}_{12}\mathcal{R}_{13}\mathcal{R}_{23} = \mathcal{R}_{23}\mathcal{R}_{13}\mathcal{R}_{12} \quad (\text{II.B.66})$$

$$(\epsilon \otimes \mathbb{I})(\mathcal{R}) = (\mathbb{I} \otimes \epsilon)(\mathcal{R}) = 1 \quad (\text{II.B.67})$$

$$(S \otimes \mathbb{I})(\mathcal{R}) = (\mathbb{I} \otimes S^{-1})(\mathcal{R}) = \mathcal{R}^{-1} \quad (\text{II.B.68})$$

$$(S \otimes S)(\mathcal{R}) = \mathcal{R} \quad (\text{II.B.69})$$

The first relation (II.B.66) of the proposition is at the root of the construction of solutions to the Yang-Baxter equation. We sketch here the general idea in order to motivate the discussion below. We recall that a representation $\pi : \mathcal{A} \rightarrow \text{End}(V)$ of an algebra \mathcal{A} over a vector space V is an homomorphism of algebras between \mathcal{A} and the algebra of matrices acting on V , denoted $\text{End}(V)$. The irreducible representations⁸ of the quasitriangular Hopf algebras usually depend (at least for the well-known examples of deformation of affine Lie algebras presented briefly below) on a spectral parameter z . If we denote by π_z this irreducible representation, we can define $R(z, z') := \pi_z \otimes \pi_{z'}(\mathcal{R})$. Applying the representation $\pi_{z_1} \otimes \pi_{z_2} \otimes \pi_{z_3}$ to the equality (II.B.66) yields the Yang-Baxter relation for the matrix $R(z, z')$

$$R_{12}(z_1, z_2)R_{13}(z_1, z_3)R_{23}(z_2, z_3) = R_{23}(z_2, z_3)R_{13}(z_1, z_3)R_{12}(z_1, z_2). \quad (\text{II.B.70})$$

It thus appears very important, from the integrable systems point of view, to construct quasitriangular Hopf algebras and study their representation theory. Jimbo [33] and Drinfeld [34] made a remarkable breakthrough in finding a whole class of examples of non-commutative and non-cocommutative quasitriangular Hopf algebras (only very few examples were known before their work). Their idea can be roughly summarized as follows. They discovered how to deform the commutation relations of an affine Lie algebra $\hat{\mathfrak{g}}$, which is co-commutative Hopf algebra, to obtain a non co-commutative Hopf algebra.

We now present very briefly one of the main deformations of an affine Lie algebra $\hat{\mathfrak{g}}: U_q(\hat{\mathfrak{g}})$. Rather than general considerations we will deal with a case of particular interest: the affine Lie algebra \hat{sl}_{N+1} .

We recall that \hat{sl}_{N+1} is generated by e_i, f_i and h_i , for $i \in \mathbb{Z}/(N+1)\mathbb{Z}$, which are subject to the relations

$$[h_i, h_j] = 0, \quad [h_i, e_j] = C_{i,j}e_j, \quad [h_i, f_j] = -C_{i,j}f_j, \quad [e_i, f_j] = \delta_{i,j}h_i, \quad (\text{II.B.71})$$

and the Serre relations. $C_{i,j} = 2\delta_{i,j} - \delta_{i,j-1} - \delta_{i,j+1}$ are the entries of the Cartan matrix and $\delta_{i,j}$ is equal to 1 if $i - j \in (N+1)\mathbb{Z}$ and 0 otherwise.

The algebra⁹ $U_{t^{1/2}}(\hat{sl}_{N+1})$ is obtained by deforming these commutation relations (with a deformation parameter $t^{1/2}$). More precisely, it is generated by e_i, f_i and $k_i^{\pm 1}$ for $i \in$

⁷The relations hold in $\mathcal{A} \otimes \mathcal{A} \otimes \mathcal{A}$, the subscript on $\mathcal{R} \in \mathcal{A} \otimes \mathcal{A}$ indicate on which tensor spaces it belongs, for instance $\mathcal{R}_{12} = \mathcal{R} \otimes 1, \mathcal{R}_{23} = 1 \otimes \mathcal{R} \dots$

⁸An irreducible representation $\pi : \mathcal{A} \rightarrow \text{End}(V)$ is a representation which has no non-trivial stable subspace, i.e subspace $W \neq \{0\}$ strictly included in V such that for all $a \in \mathcal{A}, \pi(a)(W) \subseteq W$.

⁹We use here a deformation parameter denoted by $t^{1/2}$ instead the usual notation q to ease with forthcoming computations

$\mathbb{Z}/(N+1)\mathbb{Z}$, which are subject to the relations

$$\begin{aligned} k_i k_i^{-1} &= k_i^{-1} k_i = 1, & [k_i, k_j] &= 0, \\ k_i e_j &= t^{C_{i,j}/2} e_j k_i, & k_i f_j &= t^{-C_{i,j}/2} f_j k_i, & [e_i, f_j] &= \delta_{i,j} \frac{k_i - k_i^{-1}}{t^{1/2} - t^{-1/2}}, \end{aligned}$$

and the Serre relations. Note that to recover the non-deformed algebra, we have to set $k_i = t^{h_i/2}$ and take the limit $t \rightarrow 1$.

This algebra can be endowed with a Hopf structure by defining the coproduct

$$\Delta k_i^{\pm 1} = k_i^{\pm 1} \otimes k_i^{\pm 1}, \quad \Delta e_i = 1 \otimes e_i + e_i \otimes k_i, \quad \Delta f_i = f_i \otimes 1 + k_i^{-1} \otimes f_i. \quad (\text{II.B.72})$$

This defines a non cocommutative algebra.

The algebra $U_{t^{1/2}}(\hat{sl}_{N+1})$ admits finite dimensional irreducible representations depending on a spectral parameter z and labeled by an integer l (see for instance [58, 59] for a review in context of non-equilibrium statistical mechanics). We first need to define the associated representation space V_l . For such a purpose we introduce

$$I_l = \{\boldsymbol{\rho} = (\rho_0, \dots, \rho_N) \in \mathbb{N}^{N+1} \mid \rho_0 + \dots + \rho_N = l\}. \quad (\text{II.B.73})$$

For each $\boldsymbol{\rho} \in I_l$ we associate a vector $|\boldsymbol{\rho}\rangle$ and we define

$$V_l = \bigoplus_{\boldsymbol{\rho} \in I_l} \mathbb{C} |\boldsymbol{\rho}\rangle. \quad (\text{II.B.74})$$

The irreducible representation $\pi_z^{(l)} : U_q(\hat{sl}_{N+1}) \rightarrow \text{End}(V_l)$ is given by

$$\pi_z^{(l)}(e_i) |\boldsymbol{\rho}\rangle = z^{\delta_{i,0}} \frac{t^{\rho_i/2} - t^{-\rho_i/2}}{t^{1/2} - t^{-1/2}} |\boldsymbol{\rho} - \mathbf{i}\rangle \quad (\text{II.B.75})$$

$$\pi_z^{(l)}(f_i) |\boldsymbol{\rho}\rangle = z^{-\delta_{i,0}} \frac{t^{\rho_{i+1}/2} - t^{-\rho_{i+1}/2}}{t^{1/2} - t^{-1/2}} |\boldsymbol{\rho} + \mathbf{i}\rangle \quad (\text{II.B.76})$$

$$\pi_z^{(l)}(k_i) |\boldsymbol{\rho}\rangle = z^{\rho_{i+1} - \rho_i} |\boldsymbol{\rho}\rangle, \quad (\text{II.B.77})$$

where $\mathbf{i} \in \mathbb{Z}^{N+1}$ has vanishing entries except the i -th which is equal to 1 and the $i+1$ -th which is equal to -1 (we recall that the indices have to be understood modulo $N+1$). We set by convention $|\boldsymbol{\rho} \pm \mathbf{i}\rangle = 0$ if $\boldsymbol{\rho} \pm \mathbf{i}$ has some negative entry.

It allows us to define the matrix $R^{(l),(l')}(z, z') := \pi_z^{(l)} \otimes \pi_{z'}^{(l')}(\mathcal{R})$. It was shown that it depends in fact only on the ratio of the spectral parameters z and z' : $R^{(l),(l')}(z, z') = R^{(l),(l')}(z/z')$. By taking irreducible representations of different dimension on each of the tensor space components in (II.B.66), we obtain a whole class of generalized (they involve different R -matrices) Yang-Baxter equations

$$R_{12}^{(l),(m)}(z_1/z_2) R_{13}^{(l),(n)}(z_1/z_3) R_{23}^{(m),(n)}(z_2/z_3) = R_{23}^{(m),(n)}(z_2/z_3) R_{13}^{(l),(n)}(z_1/z_3) R_{12}^{(l),(m)}(z_1/z_2). \quad (\text{II.B.78})$$

Example B.26. We give example of such matrices in the particular case $N = 1$. To be consistent with the purpose of this manuscript, the matrices are given after a similarity transformation, discovered in [58], which provides them the Markovian property. For $l = l' = 1$, we have

$$R^{(1),(1)}(z) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1-z}{t-z} & \frac{z(t-1)}{t-z} & 0 \\ 0 & \frac{t-1}{t-z} & \frac{(1-z)t}{t-z} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad (\text{II.B.79})$$

If we set $t = p/q$, we recover the R -matrix associated to the ASEP (II.B.13). For $l = 1$ and $l' = 2$, we have

$$R^{(1),(2)}(z) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{t^{1/2}-z}{t^{3/2}-z} & 0 & \frac{z(t^2-1)}{t^{3/2}-z} & 0 & 0 \\ 0 & 0 & \frac{t^{-1/2}-z}{t^{3/2}-z} & 0 & \frac{z(t-1)}{t^{3/2}-z} & 0 \\ 0 & \frac{t^{1/2}(t-1)}{t^{3/2}-z} & 0 & \frac{(t^{-1/2}-z)t^2}{t^{3/2}-z} & 0 & 0 \\ 0 & 0 & \frac{t^{-1/2}(t^2-1)}{t^{3/2}-z} & 0 & \frac{(t^{1/2}-z)t}{t^{3/2}-z} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \quad (\text{II.B.80})$$

For $l = 2$ and $l' = 1$, we have

$$R^{(2),(1)}(z) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{t^{-1/2}-z}{t^{3/2}-z} & \frac{z(t-1)}{t^{3/2}-z} & 0 & 0 & 0 \\ 0 & \frac{t^{-1/2}(t^2-1)}{t^{3/2}-z} & \frac{t(t^{1/2}-z)}{t^{3/2}-z} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{t^{1/2}-z}{t^{3/2}-z} & \frac{z(t^2-1)}{t^{3/2}-z} & 0 \\ 0 & 0 & 0 & \frac{t^{1/2}(t-1)}{t^{3/2}-z} & \frac{(t^{-1/2}-z)t^2}{t^{3/2}-z} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \quad (\text{II.B.81})$$

Finally for $l = l' = 2$, we have $R^{(2),(2)}(z) =$

$$\begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \frac{1-z}{t^2-z} & \cdot & \frac{z(t^2-1)}{t^2-z} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \frac{(1-z)(1-tz)}{t(t-z)(t^2-z)} & \cdot & \frac{z(1-z)(t-1)}{(t-z)(t^2-z)} & \cdot & \frac{z^2(t-1)(t^2-1)}{(t-z)(t^2-z)} & \cdot & \cdot & \cdot \\ \cdot & \frac{t^2-1}{t^2-z} & \cdot & \frac{(1-z)t^2}{t^2-z} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \frac{(1-z)(t+1)(t^2-1)}{t(t-z)(t^2-z)} & \cdot & \frac{t^3z+(1-2z)t^2+z(z-2)t+z}{(t-z)(t^2-z)} & \cdot & \frac{z(1-z)(t+1)(t^2-1)t}{(t-z)(t^2-z)} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \frac{1-z}{t^2-z} & \cdot & \frac{z(t^2-1)}{t^2-z} & \cdot \\ \cdot & \cdot & \frac{(t-1)(t^2-1)}{(t-z)(t^2-z)} & \cdot & \frac{(1-z)(t-1)t^2}{(t-z)(t^2-z)} & \cdot & \frac{(1-z)(1-tz)t^3}{(t-z)(t^2-z)} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \frac{t^2-1}{t^2-z} & \cdot & \frac{(1-z)t^2}{t^2-z} & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix}. \quad (\text{II.B.82})$$

Remark B.27. Applying the representation $\pi_{z_1}^{(l)} \otimes \pi_{z_2}^{(l)} \otimes \mathbb{I}$, where $\pi_z^{(l)}$ is the fundamental representation (the irreducible representation of smallest dimension) of the Hopf algebra, to the relation (II.B.66), yields the so-called RTT relation

$$R_{12}^{(l),(l)}(z_1, z_2)T_1(z_1)T_2(z_2) = T_2(z_2)T_1(z_1)R_{12}^{(l),(l)}(z_1, z_2), \quad (\text{II.B.83})$$

where $T_1(z_1) = \pi_{z_1}^{(l)} \otimes \pi_{z_2}^{(l)} \otimes \mathbb{I}(\mathcal{R}_{13})$ and $T_2(z_2) = \pi_{z_1}^{(l)} \otimes \pi_{z_2}^{(l)} \otimes \mathbb{I}(\mathcal{R}_{23})$. The matrix $T(z)$ can be seen as a $(l+1) \times (l+1)$ matrix with entries living in the Hopf algebra \mathcal{A} . The RTT relation can be interpreted as a way to encode the commutation relations of the elements of \mathcal{A} . If the generators of \mathcal{A} are correctly stored in the matrix $T(z)$, the RTT relation is then equivalent to the defining relations of the algebra. This provides a very elegant presentation of the algebra, sometimes called the FRT presentation [60]. This gives also a convenient way to define the coproduct of the algebra

$$\Delta(T(z)) = T(z) \dot{\otimes} T(z), \quad (\text{II.B.84})$$

where $\dot{\otimes}$ denotes the usual matrix product between the matrices $T(z)$ and $T(z)$ but taking tensor product of the algebraic entries. For instance

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \dot{\otimes} \begin{pmatrix} e & f \\ g & h \end{pmatrix} = \begin{pmatrix} a \otimes e + b \otimes g & a \otimes f + b \otimes h \\ c \otimes e + d \otimes g & c \otimes f + d \otimes h \end{pmatrix} \quad (\text{II.B.85})$$

The counit is given by

$$\epsilon(T(z)) = \mathbb{I}, \quad (\text{II.B.86})$$

and the antipode is given by

$$S(T(z)) = T(z)^{-1}. \quad (\text{II.B.87})$$

This presentation is often used to define the commutation relations of another deformation of a (affine) Lie algebra \mathfrak{g} : the Yangian $Y(\mathfrak{g})$. The reader can for instance refer to [61] for details.

c) Baxterization

A particularly interesting technique to construct solution to the Yang-Baxter equation was proposed by V.F.R. Jones [62] in a framework of knot theory, which is known as Baxterisation. It allows one to obtain solutions of the YBE with spectral parameter from representations of the braid group or quotients thereof. Important cases are the ones of the Hecke algebra, the Temperley–Lieb algebra or the Birman–Murakami–Wenzl algebra [63, 64]. Since then, many authors tried to generalize or produce other suitable formulae that may lead to solutions of the Yang-Baxter equation, see e.g. [57, 65–70].

Hecke algebra In this paragraph we introduce the Hecke algebra and its Baxterisation. The Hecke algebra has found a lot of applications in integrable systems (see below), in combinatorics [71] and in knot theory [72].

Definition B.28. For any integer $n \geq 1$, and complex $\omega \in \mathbb{C}$, $\mathcal{H}_n(\omega)$ is the unital associative algebra over \mathbb{C} with generators $\sigma_1, \dots, \sigma_{n-1}$ and subject to the relations

$$\sigma_i \sigma_{i+1} \sigma_i = \sigma_{i+1} \sigma_i \sigma_{i+1}, \quad i = 1, \dots, n-2 \quad (\text{II.B.88})$$

$$[\sigma_i, \sigma_j] = 0, \quad |i - j| > 1 \quad (\text{II.B.89})$$

$$\sigma_i \sigma_i^{-1} = \sigma_i^{-1} \sigma_i = 1 \quad (\text{II.B.90})$$

$$\sigma_i^2 = \omega \sigma_i + 1. \quad (\text{II.B.91})$$

Remark B.29. The Hecke algebra can be seen as the quotient of the group algebra build on the Artin's braid group \mathfrak{B}_n by the relation (II.B.91). The Artin's braid group, which is at the heart of the construction of knot invariants, is indeed defined by the relations (II.B.88), (II.B.89) and (II.B.90).

Remark B.30. The Hecke algebra appears as a deformation of the group algebra build from the permutation group \mathfrak{S}_n . For $\omega = 0$, the defining relations of the Hecke algebra coincide indeed with those of the permutation group (where σ_i stands for the permutation of i and $i + 1$). We have in particular $\sigma_i^2 = 1$.

One of the most important feature of the Hecke algebra (at least in the context of integrable systems) lies in the fact that it produces solutions to the (spectral parameter dependent) braided Yang-Baxter equation. The construction is exposed in the following theorem

Theorem B.31. If σ_i satisfy the relations of $\mathcal{H}_n(\omega)$ and t is such that $\omega = t^{-1/2} - t^{1/2}$, then

$$\check{R}_i(z) = \frac{(z-1)\sigma_i + t^{-1/2} - t^{1/2}}{zt^{-1/2} - t^{1/2}}, \quad (\text{II.B.92})$$

satisfies the braided Yang–Baxter equation

$$\check{R}_i(z_1)\check{R}_{i+1}(z_1 z_2)\check{R}_i(z_2) = \check{R}_{i+1}(z_2)\check{R}_i(z_1 z_2)\check{R}_{i+1}(z_1). \quad (\text{II.B.93})$$

Moreover the following properties hold:

$$- \text{unitarity } \check{R}_i(z)\check{R}_i(1/z) = 1, \quad (\text{II.B.94})$$

$$- \text{regularity } \check{R}_i(1) = 1, \quad (\text{II.B.95})$$

$$- \text{locality } \check{R}_i(z)\check{R}_j(z') = \check{R}_j(z')\check{R}_i(z) \quad \text{for } |i - j| > 1. \quad (\text{II.B.96})$$

Proof. The regularity and locality properties are obvious.

The unitarity and the braided Yang–Baxter equation are established through a direct computation, using the relations (II.B.88) and (II.B.91). \blacksquare

Example B.32. We can show that the bulk local jump operator m of the ASEP (II.A.23) provides an explicit representation of the Hecke algebra $\mathcal{H}_n(\omega)$ with $\omega = \sqrt{\frac{q}{p}} - \sqrt{\frac{p}{q}}$ in the tensor space $\text{End}(\mathbb{C}^2)^{\otimes n}$

$$\begin{aligned}\mathcal{H}_n(\omega) &\rightarrow \text{End}(\mathbb{C}^2)^{\otimes n} \\ \sigma_i &\mapsto \mathbb{I}^{\otimes i-1} \otimes S \otimes \mathbb{I}^{\otimes n-i-1}\end{aligned}\quad (\text{II.B.97})$$

where S is a 4×4 matrix (acting on $\mathbb{C}^2 \otimes \mathbb{C}^2$) given by

$$S = \frac{1}{\sqrt{pq}}(m + q), \quad (\text{II.B.98})$$

Then the Baxterised R -matrix

$$\check{R}(z) = \frac{(z-1)S + t^{-1/2} - t^{1/2}}{zt^{-1/2} - t^{1/2}} \quad (\text{II.B.99})$$

corresponding to (II.B.92) with $t^{1/2} = \sqrt{\frac{p}{q}}$ coincides with the expression of the R -matrix of the ASEP given in (II.B.13) (up to the multiplication by the permutation operator to obtain the non-braided R -matrix).

This representation remains valid for the homogeneous N -species ASEP which is defined by the bulk local jump operator m acting on $\mathbb{C}^{N+1} \otimes \mathbb{C}^{N+1}$

$$m = \sum_{0 \leq i < j \leq N} \left[(q|j\rangle\langle i| \otimes |i\rangle\langle j| - q|i\rangle\langle i| \otimes |j\rangle\langle j|) \right] \quad (\text{II.B.100})$$

$$+ \left(p|i\rangle\langle j| \otimes |j\rangle\langle i| - p|j\rangle\langle j| \otimes |i\rangle\langle i| \right) \quad (\text{II.B.101})$$

It provides through the Baxterisation procedure the expression of the R -matrix of the N -species ASEP

$$\check{R}(z) = \sum_{0 \leq i < j \leq N} \left[\left(\frac{(1-z)q}{p-qz} |j\rangle\langle i| \otimes |i\rangle\langle j| + \frac{p-q}{p-qz} |i\rangle\langle i| \otimes |j\rangle\langle j| \right) \right] \quad (\text{II.B.102})$$

$$+ \left(\frac{(1-z)p}{p-qz} |i\rangle\langle j| \otimes |j\rangle\langle i| + \frac{z(p-q)}{p-qz} |j\rangle\langle j| \otimes |i\rangle\langle i| \right). \quad (\text{II.B.103})$$

To summarize, the idea of the Baxterisation is to get a solution of the Yang–Baxter equation (*i.e.* an R -matrix depending on a spectral parameter) from a representation of the Hecke algebra. This idea has been intensively used and generalized to try to classify the solutions of the Yang–Baxter equation [V1, 65–69]. We will see below some of these generalizations.

This procedure strongly motivates the study of the representations in tensor space¹⁰ of the Hecke algebra because they produce integrable models.

We present here the classification of such representations in the particular case $N = 1$, *i.e.*

$$\begin{aligned}\mathcal{H}_n(\omega) &\rightarrow \text{End}(\mathbb{C}^2)^{\otimes n} \\ \sigma_i &\mapsto \mathbb{I}^{\otimes i-1} \otimes S \otimes \mathbb{I}^{\otimes n-i-1}\end{aligned}\quad (\text{II.B.104})$$

where S is acting on $\mathbb{C}^2 \otimes \mathbb{C}^2$. The matrix S has thus to be invertible and to satisfy the relations

$$S_{12}S_{23}S_{12} = S_{23}S_{12}S_{23} \quad (\text{II.B.105})$$

$$S^2 = \omega S + 1. \quad (\text{II.B.106})$$

¹⁰Note that representation in non-tensor spaces play also a very important role, *e.g.* the Temperley–Lieb algebra (which is a quotient of the Hecke algebra) produces integral loop models.

The classification of the constant braided Yang–Baxter equation (II.B.105) for $N = 1$ was done in [73] (to be precise the unbraided relation was classified there but we just need to multiply the solutions on the left by the permutation matrix P to obtain the desired classification). We just need to pick up the 4×4 matrices satisfying also the relation (II.B.106).

The classification of [73] provides 23 solutions, up to transformations

$$S \mapsto \lambda g \otimes g S g^{-1} \otimes g^{-1} \quad ; \quad S \mapsto S^{t_1 t_2} \quad \text{and} \quad S \mapsto P S P, \quad (\text{II.B.107})$$

where λ is a complex non-zero parameter, g is any invertible 2×2 matrix and P is the permutation matrix. Among these solutions, only 9 are also solution to (II.B.106) and this supplementary relation imposes (in general) constraints on their parameters. Using the notations of [73], these solutions are (up to the transformations (II.B.107)):

Matrix	Constraints on the parameters	Value of ω
$R_{H3,1}$	$pq = 1, \quad k^2 = 1, \quad s^2 = 1$	0
$R_{H2,1}$	$k^2 pq = 1$	$k^2 - pq$
$R_{H2,2}$	$k^2 pq = 1$	$k^2 - pq$
$R_{H2,3}$	$k^2 = 1, \quad p + q = 0, \quad 2ks + p^2 + q^2 = 0$	0
$R_{H1,1}$	$4p^2 q^2 = 1$	$2(p^2 - q^2)$
$R_{H1,2}$	$pq = 1$	$p - q$
$R_{H1,3}$	$k^4 = 1$	0
$R_{H1,4}$	$pq = 1, \quad k^2 = 1$	0
$R_{H0,3}$	no constraint	0

(II.B.108)

After imposing these constraints, the previous matrices are not independent anymore: they can be all obtained from the 7 matrices $R_{H2,1}$, $R_{H2,2}$, $R_{H1,1}$, $R_{H1,2}$, $R_{H1,3}$, $R_{H1,4}$, $R_{H0,3}$ (subjected to the constraints given in (II.B.108)).

They are explicitly given by

$$R_{H1,1} = \begin{pmatrix} \sinh(\theta) + \varepsilon & 0 & 0 & \sinh(\theta) \\ 0 & \sinh(\theta) & \cosh(\theta) & 0 \\ 0 & \cosh(\theta) & \sinh(\theta) & 0 \\ \sinh(\theta) & 0 & 0 & \sinh(\theta) - \varepsilon \end{pmatrix} ;$$

$$R_{H1,2} = \begin{pmatrix} a & 0 & 0 & b \\ 0 & 0 & a^{-1} & 0 \\ 0 & a & a - a^{-1} & 0 \\ 0 & 0 & 0 & -a^{-1} \end{pmatrix} ; \quad R_{H1,3} = \varepsilon \begin{pmatrix} 1 & b & -b & ab \\ 0 & 0 & 1 & -a \\ 0 & 1 & 0 & a \\ 0 & 0 & 0 & 1 \end{pmatrix} ; \quad (\text{II.B.109})$$

$$R_{H2,1/H2,2} = \begin{pmatrix} a & 0 & 0 & 0 \\ 0 & 0 & b^{-1} & 0 \\ 0 & b & a - a^{-1} & 0 \\ 0 & 0 & 0 & \varepsilon a^\varepsilon \end{pmatrix} ; \quad R_{H1,4} = \begin{pmatrix} 0 & 0 & 0 & a \\ 0 & 0 & \varepsilon & 0 \\ 0 & \varepsilon & 0 & 0 \\ a^{-1} & 0 & 0 & 0 \end{pmatrix}$$

$$R_{H0,3} = \mathbb{I}_4,$$

where a , b and θ are free complex parameters and $\varepsilon = \pm 1$ that are expressed in terms of p , q and k through the change of variables:

$$R_{H1,1} : \exp \theta = 2p^2 \quad \text{and} \quad q = \frac{\varepsilon}{2p} \quad (\text{II.B.110})$$

$$R_{H1,2} : a = p, \quad q = \frac{1}{a} \quad \text{and} \quad k = b \quad (\text{II.B.111})$$

$$R_{H1,3} : \varepsilon = k^2, \quad a = \varepsilon k q \quad \text{and} \quad b = \varepsilon k p \quad (\text{II.B.112})$$

$$R_{H2,1/H2,2} : a = k^2 \quad \text{and} \quad k p = b \quad (\text{II.B.113})$$

$$R_{H1,4} : a = p. \quad (\text{II.B.114})$$

\mathcal{S}_n and \mathcal{T}_n algebras Here, we introduce new braid-like algebras \mathcal{S}_n and \mathcal{T}_n . We produce, as the main result of this paragraph a new Baxterisation formula that leads to R-matrices depending genuinely on two spectral parameters. The obtained R-matrices satisfy the usual properties of unitarity, regularity and locality. Moreover, we show that the matrix representations of \mathcal{S}_n are determined only by the defining relations of \mathcal{S}_3 . A classification thereof in terms of 4×4 matrices is given together with the expressions of the corresponding R-matrices. We also get the corresponding Hamiltonians. In the general case, a particular $m \times m$ representation is exhibited, that appears to be linked to some generalizations of the multi-species Totally Asymmetric Simple Exclusion Process (TASEP). The results presented here are extracted from the work [V1].

Definition B.33. For any integer $n \geq 1$, \mathcal{S}_n is the unital associative algebra over \mathbb{C} with generators $\sigma_1, \dots, \sigma_{n-1}$ and subject to the relations

$$[\sigma_{i+1} \sigma_i, \sigma_i + \sigma_{i+1}] = 0, \quad i = 1, \dots, n-2 \quad (\text{II.B.115})$$

$$[\sigma_i, \sigma_j] = 0, \quad |i - j| > 1 \quad (\text{II.B.116})$$

where $[\cdot, \cdot]$ stands for the commutator.

Let us stress that the definition of the algebra \mathcal{S}_n does not need the existence of the inverse generators σ_i^{-1} : there are interesting realizations of this algebra where represented generators are non-invertible (see e.g. proposition B.42 below). For $n = 1$, one has $\mathcal{S}_1 \simeq \mathbb{C}$.

Relation (II.B.115) can be written equivalently as

$$\sigma_i \sigma_{i+1} \sigma_i - \sigma_{i+1} \sigma_i^2 = \sigma_{i+1} \sigma_i \sigma_{i+1} - \sigma_{i+1}^2 \sigma_i, \quad (\text{II.B.117})$$

which can be seen as a modification¹¹ of the defining relations of the braid group \mathcal{B}_n (however without the inverse generators). This justifies the terminology we used for the algebra \mathcal{S}_n as a braid-like algebra. Let us also mention that \mathcal{S}_n , like \mathcal{B}_n , is infinite dimensional.

Proposition B.34. Let $\gamma \in \mathbb{C}$ be such that the generators $1 + \gamma \sigma_i$ are invertible $\forall i$ with its inverse understood as the the following formal series:

$$(1 + \gamma \sigma_i)^{-1} = \sum_{k=0}^{\infty} (-\gamma \sigma_i)^k. \quad (\text{II.B.118})$$

Then, the Möbius map

$$\mathbf{m}_{\alpha, \beta, \gamma} : \begin{array}{ccc} \mathcal{S}_n & \rightarrow & \mathcal{S}_n \\ \sigma_i & \mapsto & (\alpha + \beta \sigma_i) (1 + \gamma \sigma_i)^{-1} \end{array} \quad (\text{II.B.119})$$

with $\alpha, \beta \in \mathbb{C}$ is an algebra homomorphism.

Proof. Remark that $\gamma = 0$ ensures the existence of at least one parameter γ such that the condition on the invertibility of $1 + \gamma \sigma_i$ is fulfilled. We divide the proof into two parts, depending on whether γ is null or not.

When $\gamma = 0$, one gets $\mathbf{m}_{\alpha, \beta, 0} = \mathfrak{s}_{\alpha, \beta}$, where $\mathfrak{s}_{\alpha, \beta}(\sigma) = \alpha + \beta \sigma$. It is straightforward to show that $[\mathfrak{s}_{\alpha, \beta}(\sigma_{i+1}) \mathfrak{s}_{\alpha, \beta}(\sigma_i), \mathfrak{s}_{\alpha, \beta}(\sigma_i) + \mathfrak{s}_{\alpha, \beta}(\sigma_{i+1})] = 0$. Thus $\mathfrak{s}_{\alpha, \beta}$ is an homomorphism of \mathcal{S}_n .

For $\gamma \neq 0$, the Möbius transformation is the composition of two maps:

$$\mathbf{m}_{\alpha, \beta, \gamma} = \mathfrak{s}_{\beta/\gamma, \alpha - \beta/\gamma} \circ \mathfrak{s}_{1, \gamma}^{-1} \quad (\text{II.B.120})$$

where $\mathfrak{s}_{1, \gamma}^{-1}(\sigma) = (1 + \gamma \sigma)^{-1}$, as given by the expansion (II.B.118). To prove that $\mathfrak{s}_{1, \gamma}^{-1}$ is also an homomorphism, we start from (II.B.115) written for $\mathfrak{s}_{1, \gamma}(\sigma)$ and multiply this relation on the right by $\mathfrak{s}_{1, \gamma}(\sigma_i)^{-1} \mathfrak{s}_{1, \gamma}(\sigma_{i+1})^{-1} \mathfrak{s}_{1, \gamma}(\sigma_i)^{-1}$ and on the left by $\mathfrak{s}_{1, \gamma}(\sigma_{i+1})^{-1} \mathfrak{s}_{1, \gamma}(\sigma_i)^{-1} \mathfrak{s}_{1, \gamma}(\sigma_{i+1})^{-1}$.

¹¹Unfortunately, we cannot implement a free parameter in this relation and keep the baxterisation procedure. Then, \mathcal{S}_n cannot be viewed as a deformation of the braid group.

This shows that $\mathfrak{s}_{1,\gamma}(\sigma_i)^{-1}$ also verifies (II.B.115). Note that $\mathfrak{s}_{1,\gamma}(\sigma)$ is an invertible element by hypothesis. Then $\mathfrak{m}_{\alpha,\beta,\gamma}$ is an homomorphism since it is a composition of homomorphisms. ■

We also introduce another algebra \mathcal{T}_n , defined as follows

Definition B.35. For any integer $n \geq 1$, \mathcal{T}_n is the unital associative algebra over \mathbb{C} with generators $\tau_1, \dots, \tau_{n-1}$ and subject to the relations

$$[\tau_i \tau_{i+1}, \tau_i + \tau_{i+1}] = 0, \quad i = 1, \dots, n-2 \quad (\text{II.B.121})$$

$$[\tau_i, \tau_j] = 0, \quad |i - j| > 1. \quad (\text{II.B.122})$$

This algebra is closely related to \mathcal{S}_n as stated in the following proposition:

Proposition B.36.

$$\text{The map } \phi : \begin{cases} \mathcal{S}_n & \rightarrow \mathcal{T}_n \\ \sigma_i & \mapsto \tau_{n-i} \end{cases} \text{ is an algebra isomorphism.} \quad (\text{II.B.123})$$

Proof. The isomorphism is proved by direct computations. ■

The following theorem contains the main result of this paragraph and justifies the introduction of the algebra \mathcal{S}_n .

Theorem B.37. If σ_i satisfy the relations of \mathcal{S}_n , then

$$\check{R}_i^\sigma(x, y) = \Sigma_i(y) \Sigma_i(x)^{-1} \quad \text{where } \Sigma_i(x) = 1 - x\sigma_i \quad (\text{II.B.124})$$

satisfy the braided Yang–Baxter equation

$$\check{R}_i(x, y) \check{R}_{i+1}(x, z) \check{R}_i(y, z) = \check{R}_{i+1}(y, z) \check{R}_i(x, z) \check{R}_{i+1}(x, y), \quad (\text{II.B.125})$$

and also the locality, unitarity and regularity properties.

Proof. The unitarity, regularity and locality properties are obvious.

To prove the braided Yang–Baxter equation (II.B.125), let us remark that, after multiplication on the right by $\Sigma_i(y)$ and on the left by $\Sigma_{i+1}(y)$, it is equivalent to

$$A_i(y) A_i(x)^{-1} A_i(z) = A_i(z) A_i(x)^{-1} A_i(y) \quad (\text{II.B.126})$$

where $A_i(x) = \Sigma_{i+1}(x) \Sigma_i(x)$. Relation (II.B.126) is equivalent to

$$[A_i(x), A_i(y)] = 0. \quad (\text{II.B.127})$$

Indeed, setting $z = 0$ in (II.B.126) leads to (II.B.127), which obviously implies (II.B.126). Let us notice now that

$$A_i(x) = 1 - x(\sigma_i + \sigma_{i+1}) + x^2 \sigma_{i+1} \sigma_i \quad (\text{II.B.128})$$

Therefore, the defining relation (II.B.115) of \mathcal{S}_n implies relation (II.B.127) and then the braided Yang–Baxter equation. ■

We want to emphasize that the Baxterisation introduced here depends *separately* on the two spectral parameters. This is a new feature in comparison to the previous Baxterisations [62–64].

Theorem B.37 gives a sufficient condition to obtain the braided Yang–Baxter equation. The following proposition proves that it is also a necessary condition.

Proposition B.38. If $\check{R}_i^\sigma(x, y)$ given by (II.B.124) satisfies the braided Yang–Baxter equation (II.B.125) and the locality property, then the generators σ_i satisfy \mathcal{S}_n .

Proof. We have already seen that the braided Yang–Baxter equation implies (II.B.127). The different coefficients of (II.B.127) w.r.t. x and y imply (II.B.115). The locality implies (II.B.116) which concludes the proof. ■

Until now, we used the algebra \mathcal{S}_n to get a solution of the braided Yang–Baxter equation, but we can use similarly the algebra \mathcal{T}_n :

Theorem B.39. *The generators τ_i satisfy the algebra \mathcal{T}_n if and only if*

$$\check{R}_i^\tau(x, y) = \mathfrak{T}_i(x)\mathfrak{T}_i(y)^{-1} \quad \text{where} \quad \mathfrak{T}_i(x) = 1 - x\tau_i \quad (\text{II.B.129})$$

are unitary, regular and local solutions of the braided Yang–Baxter equation.

Proof. Direct consequence of theorem B.37 and proposition B.38, using the isomorphism of proposition B.36. \blacksquare

Let us stress that there is a flip between the spectral parameters in definitions (II.B.124) and (II.B.129).

We are now interested in some matrix representations of \mathcal{S}_n and in particular the ones useful in the context of integrable systems, *i.e.* representations of \mathcal{S}_n in $\text{End}(\mathbb{C}^m)^{\otimes n}$.

More precisely, we look for representations of the following type

$$\begin{aligned} \mathcal{S}_n &\rightarrow \text{End}(\mathbb{C}^m)^{\otimes n} \\ \sigma_i &\mapsto \mathbb{I}^{\otimes i-1} \otimes S \otimes \mathbb{I}^{\otimes n-i-1} \end{aligned} \quad (\text{II.B.130})$$

where \mathbb{I} is the identity of $\text{End}(\mathbb{C}^m)$ and $S \in \text{End}(\mathbb{C}^m) \otimes \text{End}(\mathbb{C}^m)$. We use the following notation $S_{j,j+1} = \mathbb{I}^{\otimes j-1} \otimes S \otimes \mathbb{I}^{\otimes n-j-1}$: the indices in $S_{j,j+1}$ label the copies of $\text{End}(\mathbb{C}^m)$ in which the operator S acts non-trivially. To look for such matrix representations of \mathcal{S}_n ($n \geq 3$), it is necessary and sufficient to find S satisfying the single relation of \mathcal{S}_3 :

$$[S_{23} S_{12}, S_{12} + S_{23}] = 0. \quad (\text{II.B.131})$$

We give below a classification of the solutions of this equation for $m = 2$ and some solutions for any m .

Before that, let us remark that proposition B.34 implies that if S is a solution of (II.B.131), then so is $\mathfrak{m}_{\alpha,\beta,\gamma}(S)$. We have loosely used the same notation for the Möbius map acting on the algebra and the ones acting on the representation.

Using the Baxterisation introduced in theorem B.37 and the realization of \mathcal{S}_n given by (II.B.130), the matrix

$$\check{R}(x, y) = (\mathbb{I} - yS)(\mathbb{I} - xS)^{-1} \quad (\text{II.B.132})$$

is a solution of the braided Yang–Baxter equation

$$\check{R}_{i,i+1}(x, y)\check{R}_{i+1,i+2}(x, z)\check{R}_{i,i+1}(y, z) = \check{R}_{i+1,i+2}(y, z)\check{R}_{i,i+1}(x, z)\check{R}_{i+1,i+2}(x, y), \quad (\text{II.B.133})$$

where the indices stand for the spaces on which the matrix $\check{R}(x, y)$ acts non-trivially.

Similarly, one gets matrix representations for \mathcal{T}_n . Indeed, we look for representations of the following type

$$\begin{aligned} \mathcal{T}_n &\rightarrow \text{End}(\mathbb{C}^m)^{\otimes n} \\ \tau_i &\mapsto \mathbb{I}^{\otimes i-1} \otimes T \otimes \mathbb{I}^{\otimes n-i-1} \end{aligned} \quad (\text{II.B.134})$$

In this case, one has to solve the equation

$$[T_{12} T_{23}, T_{12} + T_{23}] = 0 \quad (\text{II.B.135})$$

the associated R -matrix being now

$$\check{R}(x, y) = (\mathbb{I} - xT)(\mathbb{I} - yT)^{-1}. \quad (\text{II.B.136})$$

Relation (II.B.131) is difficult to solve in general: there are $(m^3)^2$ cubic relations in terms of the $(m^2)^2$ entries of the matrix S . However, for $m = 2$, using symmetry transformations and a direct resolution with a formal mathematical software, we are able to compute all the solutions which are presented in the following theorem. Note that we do not impose a priori that S is invertible and indeed some particular cases of the solutions are not, see for instance remark B.41. It could be interesting to study if the finite dimensional representations found by 'brute force' computations below arise as natural quotients of the algebra \mathcal{S}_n .

Theorem B.40. *The whole set of representations of \mathcal{S}_n of type (II.B.130), for $m = 2$, is obtained by applying the following transformations*

- $S \mapsto S^{-1}$, when S is invertible,
- $S \mapsto S_{21}^{t_1 t_2}$, where $(\cdot)^{t_1 t_2}$ is the transposition in the space $\text{End}(\mathbb{C}^m) \otimes \text{End}(\mathbb{C}^m)$,
- $S \mapsto Q_1 Q_2 S Q_2^{-1} Q_1^{-1}$, where Q is any invertible element of $\text{End}(\mathbb{C}^m)$.

or Möbius transformation to the seven matrices below:

- two 4-parameter matrices

$$S^{(1)} = \begin{pmatrix} 0 & \cdot & \cdot & \cdot \\ b & c & \cdot & \cdot \\ d & \cdot & 0 & \cdot \\ \cdot & a & \cdot & 0 \end{pmatrix}, \quad S^{(2)} = \begin{pmatrix} 0 & b-c & b+c & d \\ \cdot & 0 & \cdot & a+b \\ \cdot & \cdot & 0 & b-a \\ \cdot & \cdot & \cdot & 0 \end{pmatrix} \quad (\text{II.B.137})$$

- four 3-parameter matrices

$$S^{(3)} = \begin{pmatrix} 0 & \cdot & \cdot & \cdot \\ b & \frac{ab}{c} & \cdot & \cdot \\ c & \cdot & a & \cdot \\ \cdot & \cdot & \cdot & 0 \end{pmatrix}, \quad S^{(4)} = \begin{pmatrix} 0 & \cdot & \cdot & \cdot \\ \cdot & b & \cdot & \cdot \\ \cdot & c & 0 & \cdot \\ \cdot & \cdot & \cdot & a \end{pmatrix}, \quad (\text{II.B.138})$$

$$S^{(5)} = \begin{pmatrix} a & \cdot & \cdot & \cdot \\ \cdot & b & \cdot & \cdot \\ \cdot & \cdot & c & \cdot \\ \cdot & \cdot & \cdot & 0 \end{pmatrix}, \quad S^{(6)} = \begin{pmatrix} 0 & \cdot & \cdot & \cdot \\ b & c & \cdot & a \\ \cdot & \cdot & 0 & \cdot \\ \cdot & -b & b & 0 \end{pmatrix}, \quad (\text{II.B.139})$$

- one 2-parameter matrix

$$S^{(7)} = \begin{pmatrix} -a & \cdot & \cdot & \cdot \\ b & 0 & a & \cdot \\ \cdot & \cdot & -a & \cdot \\ \cdot & \cdot & \cdot & 0 \end{pmatrix}, \quad (\text{II.B.140})$$

where a, b, c, d are free complex parameters.

Proof. The proof consists in finding all the 4×4 matrices S solution of equation (II.B.131). We use a technique introduced in [73] to classify the constant 4×4 solutions of the Yang–Baxter equation. Let s_{ij} (for $i, j = 1, 2, 3, 4$) be the entries of S . Using the transformations exposed in the theorem B.40, we can always look for solution of the equation with $s_{41} = 0$. Indeed if S is a solution with $s_{41} \neq 0$, then S is related through a transformation to a solution S^{new} with $s_{41}^{new} = 0$. More precisely if $s_{14} = 0$ we set $S^{new} = (S_{21})^t$ and we have $s_{41}^{new} = 0$ because the transformation exchanges s_{41} and s_{14} . If $s_{14}s_{41} \neq 0$, we set $S^{new} = Q \otimes Q S Q^{-1} \otimes Q^{-1}$, with

$$Q = \begin{pmatrix} 1 & 0 \\ B & 1 \end{pmatrix}. \quad (\text{II.B.141})$$

We have $s_{41}^{new} = s_{14}B^4 + (s_{24} + s_{34} - s_{12} - s_{13})B^3 + (s_{44} - s_{22} - s_{23} - s_{32} - s_{33} + s_{11})B^2 + (s_{21} + s_{31} - s_{42} - s_{43})B + s_{41}$. Since we are in the case $s_{14} \neq 0$, it is always possible to find B such that $s_{41}^{new} = 0$. Therefore, without loss of generality, we can now set $s_{41} = 0$.

At this stage, we use a computer software to solve (II.B.131) with $s_{41} = 0$. Then, using the transformations given above in theorem B.40, we select the solutions which are not related by transformations and get the seven solutions presented in the theorem. \blacksquare

Remark B.41. *The solution $S^{(4)}$ provides the TASEP Markovian matrix as a subcase:*

$$S^{(4)} \Big|_{a=0; c=1; b=-1} = \begin{pmatrix} 0 & \cdot & \cdot & \cdot \\ \cdot & -1 & \cdot & \cdot \\ \cdot & 1 & 0 & \cdot \\ \cdot & \cdot & \cdot & 0 \end{pmatrix}. \quad (\text{II.B.142})$$

As explained previously in this chapter, each S is an integrable Hamiltonian. Then, from any 4×4 integrable Hamiltonian h obtained in this classification, we can construct new ones by action of the group of transformations generated by

$$h \mapsto Q \otimes Q h (Q \otimes Q)^{-1}; \quad h \mapsto h^{t_1 t_2}; \quad h \mapsto P h P; \quad h \mapsto (\alpha + \beta h)(1 + \gamma h)^{-1} \quad (\text{II.B.143})$$

These transformations are indeed symmetry transformations for the relation (II.B.131) or map a solution of (II.B.131) to a solution of (II.B.135).

Using theorem B.37 and the previous classification theorem B.40, we get a set of solutions to the braided Yang–Baxter equation. The braided R -matrices are easily computed using (II.B.124). One has to keep in mind that one can construct other R -matrices from these ones by using the symmetry transformations described previously.

As explained previously, the resolution of equation (II.B.131) is complicated and a complete classification for any m seems impossible. However, it is still possible to find some solutions. In the following proposition, we present particular non-trivial matrix representations for any m :

Proposition B.42. *Let E_{ij} be the canonical basis of $\text{End}(\mathbb{C}^m)$ and let ρ_i and $\mu_{i,j}$, $1 \leq i < j \leq m$ be some complex numbers. We define*

$$S = \sum_{1 \leq i < j \leq m} \rho_i E_{ii} \otimes E_{jj} + \mu_{i,j} E_{ji} \otimes E_{ij} \quad (\text{II.B.144})$$

Then, the map $\sigma_i \mapsto S_{i,i+1}$ is an homomorphism of algebra $\mathcal{S}_n \rightarrow \text{End}((\mathbb{C}^m)^{\otimes n})$.

Proof. We prove by direct computations that S given by (II.B.144) verifies (II.B.131). \blacksquare

Remark that S is non-invertible. Obviously, the use of the transformations given in theorem B.40 provides new representations isomorphic to (II.B.144).

There is a similar type of representation for \mathcal{T}_n .

Proposition B.43. *Let E_{ij} be the canonical basis of $\text{End}(\mathbb{C}^m)$ and let ζ_j and $\nu_{i,j}$, $1 \leq i < j \leq m$ be some complex numbers. We define*

$$T = \sum_{1 \leq i < j \leq m} \zeta_j E_{ii} \otimes E_{jj} + \nu_{i,j} E_{ji} \otimes E_{ij}, \quad (\text{II.B.145})$$

Then, the map $\tau_i \mapsto T_{i,i+1}$ is an homomorphism of algebra $\mathcal{T}_n \rightarrow \text{End}((\mathbb{C}^m)^{\otimes n})$.

Remark B.44. *The representation given above, when restricted to the Markovian condition $\zeta_j = -\nu_{ij}$, $\forall i, j$, corresponds to the Markov matrix studied in [74]. Hence, the R -matrix $\check{R}^\zeta(x, z)$ constructed here provides an R -matrix for this model. Note that the T -matrix (II.B.145) does not obey the Hecke algebra except when all ζ_j are equal. To deal with genuine inhomogeneous hopping rates, the Hecke algebra is not sufficient: one needs the \mathcal{T}_n algebra introduced in this paper.*

From S (resp. T) given by (II.B.144) (resp. (II.B.145)), one gets an R -matrix using Baxterisation (II.B.132) (resp. (II.B.136)). Surprisingly enough, from these two R -matrices, we can obtain another one, as stated in the following theorem.

Theorem B.45. *Let us define the matrix*

$$\check{R}(x, z) = \check{R}^\rho(x, z)\check{R}^\zeta(x, z), \quad (\text{II.B.146})$$

where $\check{R}^\rho(x, y) = (\mathbb{I} - yS)(\mathbb{I} - xS)^{-1}$ and $\check{R}^\zeta(x, y) = (\mathbb{I} - xT)(\mathbb{I} - yT)^{-1}$ are respectively the Baxterisations of S given by (II.B.144) and of T given by (II.B.145).

If the relations $\rho_i\nu_{i,j} = \mu_{i,j}\zeta_j$ for $1 \leq i < j \leq m$ hold, $\check{R}(x, z)$ satisfies the braided Yang-Baxter equation and is unitary.

Proof. It is proven by direct computations. ■

Let us remark that the relations $\rho_i\nu_{i,j} = \mu_{i,j}\zeta_j$ are equivalent to $[T, S] = 0$.

The R -matrix introduced in the theorem B.45 is a generalization of the matrix introduced in [75] to study the multi-species totally asymmetric exclusion process with different hopping rates. More explicitly, setting $\mu_{i,j} = -\rho_i$ and $\nu_{i,j} = -\zeta_j$, the corresponding R -matrix provided by the theorem B.45 gives the integrable local jump operator of the multi-species totally asymmetric exclusion process with different hopping rates:

$$\left. \frac{\partial \check{R}(x, z)}{\partial x} \right|_{x=z=0} = m = \sum_{1 \leq i < j \leq m} (\rho_i - \zeta_j) E_{ii} \otimes E_{jj} - (\rho_i - \zeta_j) E_{ji} \otimes E_{ij}. \quad (\text{II.B.147})$$

It describes a Markovian model with m species of particles, where the local exchange rules are given by

$$ij \xrightarrow{\rho_i - \zeta_j} ji, \quad \text{if } i < j. \quad (\text{II.B.148})$$

The R -matrix was already presented in [75], but without the factorization provided by the theorem B.45. Using the property $[T, S] = 0$, it can be rewritten as

$$\check{R}(x, y) = \Sigma(x, y) \Sigma(y, x)^{-1} \text{ with } \Sigma(x, y) = (\mathbb{I} - yS)(\mathbb{I} - xT). \quad (\text{II.B.149})$$

To conclude this paragraph, we can mention that numerous questions are still open. The Hecke algebra has been a very useful tool in different contexts: *e.g.* it is the centralizer of the quantum group $\mathcal{U}_q(\mathfrak{gl}_N)$ [63] or it permits to construct link invariants [76]. We believe that the algebra \mathcal{S}_n we have introduced here should have similar fields of applications. We think that the classification of its irreducible representations should be also interesting. The defining relations of the algebra \mathcal{S}_n look also very similar to the ones of the braid group: the connections between these two algebras should also be explored.

In theorem B.45, we show that the product of two R -matrices based on \mathcal{S}_n and \mathcal{T}_n provides a new R -matrix if a simple condition on the parameters holds. It would be interesting to understand if this feature is associated to the special representation used in the theorem or if it is still true at the algebraic level.

Finally, the list of R -matrices provided in this paragraph may be used to introduce also new models in the context of quantum mechanics (spin chains) or 2D-statistical models (loop or vertex models). The knowledge of their associated R -matrix may allow one to solve them using, for example, the algebraic Bethe ansatz [77] or the matrix ansatz [42, 46] (see chapter III).

\mathcal{M}_n algebra

Definition B.46. *For any integer $n \geq 1$, \mathcal{M}_n is the unital associative algebra over \mathbb{C} with generators $\sigma_1, \dots, \sigma_{n-1}$ and subject to the relations*

$$\sigma_i \sigma_{i+1} \sigma_i - \sigma_{i+1} \sigma_i \sigma_{i+1} = \lambda(\sigma_{i+1}^2 - \sigma_i^2) + \mu(\sigma_{i+1} - \sigma_i), \quad i = 1, \dots, n-2 \quad (\text{II.B.150})$$

$$\sigma_i \sigma_{i+1}^2 = \sigma_i^2 \sigma_{i+1}, \quad \sigma_{i+1} \sigma_i^2 = \sigma_{i+1}^2 \sigma_i \quad (\text{II.B.151})$$

$$[\sigma_i, \sigma_j] = 0, \quad |i - j| > 1. \quad (\text{II.B.152})$$

The following theorem contains the main result of this paragraph and justifies the introduction of the algebra \mathcal{M}_n .

Theorem B.47. *If σ_i satisfy the relations of \mathcal{M}_n , then*

$$\check{R}_i(x, y) = \Sigma_i(x, y)\Sigma_i(y, x)^{-1} \quad \text{where} \quad \Sigma_i(x, y) = 1 - \mu xy - (x + \lambda xy)\sigma_i \quad (\text{II.B.153})$$

satisfy the braided Yang–Baxter equation

$$\check{R}_i(x, y)\check{R}_{i+1}(x, z)\check{R}_i(y, z) = \check{R}_{i+1}(y, z)\check{R}_i(x, z)\check{R}_{i+1}(x, y). \quad (\text{II.B.154})$$

and also the locality, unitarity and regularity properties.

Note that the inverse $\Sigma_i(y, x)^{-1}$ in the definition of \check{R} has to be understood as the formal series

$$\Sigma_i(y, x)^{-1} = \sum_{k=0}^{+\infty} (\mu xy + (y + \lambda xy)\sigma_i)^k. \quad (\text{II.B.155})$$

Proof. The first step is to establish the relation

$$\sigma_i^n \sigma_{i+1} \sigma_i - \sigma_{i+1} \sigma_i \sigma_{i+1}^n = \lambda(\sigma_{i+1}^{n+1} - \sigma_i^{n+1}) + \mu(\sigma_{i+1}^n - \sigma_i^n), \quad (\text{II.B.156})$$

for any integer $n \geq 1$. This can be done by induction: the $n = 1$ case is nothing else but the algebraic relation (II.B.150). Then if we assume that the relation holds for a given $n \geq 1$, we have that

$$\begin{aligned} & \sigma_i^{n+1} \sigma_{i+1} \sigma_i = \sigma_i \sigma_{i+1} \sigma_i \sigma_{i+1}^n + \lambda(\sigma_i \sigma_{i+1}^{n+1} - \sigma_i^{n+2}) + \mu(\sigma_i \sigma_{i+1}^n - \sigma_i^{n+1}) \\ &= \left[\sigma_{i+1} \sigma_i \sigma_{i+1} + \lambda(\sigma_{i+1}^2 - \sigma_i^2) + \mu(\sigma_{i+1} - \sigma_i) \right] \sigma_{i+1}^n + \lambda(\sigma_i \sigma_{i+1}^{n+1} - \sigma_i^{n+2}) + \mu(\sigma_i \sigma_{i+1}^n - \sigma_i^{n+1}) \\ &= \sigma_{i+1} \sigma_i \sigma_{i+1}^{n+1} + \lambda(\sigma_{i+1}^{n+2} - \sigma_i^{n+2}) + \mu(\sigma_{i+1}^{n+1} - \sigma_i^{n+1}), \end{aligned}$$

where the last equality is obtained by pushing all the powers to the left using the relations

$$\sigma_i^p \sigma_{i+1}^q = \sigma_i^{p+q-1} \sigma_{i+1}, \quad \sigma_{i+1}^p \sigma_i^q = \sigma_{i+1}^{p+q-1} \sigma_i, \quad \text{for } p, q \geq 1. \quad (\text{II.B.157})$$

These last equations are directly derived from (II.B.151).

Equations (II.B.156) and (II.B.157) immediately imply that

$$\sigma_i^p \sigma_{i+1}^q \sigma_i^r - \sigma_{i+1}^r \sigma_i^q \sigma_{i+1}^p = \lambda(\sigma_{i+1}^{p+q+r-1} - \sigma_i^{p+q+r-1}) + \mu(\sigma_{i+1}^{p+q+r-2} - \sigma_i^{p+q+r-2}), \quad \text{for } p, q, r \geq 1$$

This is equivalent to the relation

$$\begin{aligned} & \frac{\sigma_i}{1 - X\sigma_i} \cdot \frac{\sigma_{i+1}}{1 - Y\sigma_{i+1}} \cdot \frac{\sigma_i}{1 - Z\sigma_i} - \frac{\sigma_{i+1}}{1 - Z\sigma_{i+1}} \cdot \frac{\sigma_i}{1 - Y\sigma_i} \cdot \frac{\sigma_{i+1}}{1 - X\sigma_{i+1}} \quad (\text{II.B.158}) \\ &= \frac{\lambda\sigma_{i+1}^2 + \mu\sigma_{i+1}}{(1 - X\sigma_{i+1})(1 - Y\sigma_{i+1})(1 - Z\sigma_{i+1})} - \frac{\lambda\sigma_i^2 + \mu\sigma_i}{(1 - X\sigma_i)(1 - Y\sigma_i)(1 - Z\sigma_i)} \quad (\text{II.B.159}) \end{aligned}$$

and the relation (II.B.157) can be equivalently rewritten as

$$\frac{\sigma_i}{1 - X\sigma_i} \cdot \frac{\sigma_{i+1}}{1 - Y\sigma_{i+1}} = \frac{\sigma_i}{1 - Y\sigma_i} \cdot \frac{\sigma_{i+1}}{1 - X\sigma_{i+1}}. \quad (\text{II.B.160})$$

We are now ready to prove the Yang-Baxter equation. It will be convenient to write

$$\check{R}_i(x, y) = 1 + \frac{(y - x)\sigma_i}{\Sigma_i(y, x)}. \quad (\text{II.B.161})$$

We can then expand

$$\begin{aligned} & \check{R}_i(x, y)\check{R}_{i+1}(x, z)\check{R}_i(y, z) - \check{R}_{i+1}(y, z)\check{R}_i(x, z)\check{R}_{i+1}(x, y) \quad (\text{II.B.162}) \\ &= (y - x)(z - x)(z - y) \left[\frac{\sigma_i}{\Sigma_i(y, x)} \cdot \frac{\sigma_{i+1}}{\Sigma_{i+1}(z, x)} \cdot \frac{\sigma_i}{\Sigma_i(z, y)} - \frac{\sigma_{i+1}}{\Sigma_{i+1}(z, y)} \cdot \frac{\sigma_i}{\Sigma_i(z, x)} \cdot \frac{\sigma_{i+1}}{\Sigma_{i+1}(y, x)} \right] \\ &+ (y - x)(z - y) \left[\frac{\sigma_i}{\Sigma_i(y, x)} \cdot \frac{\sigma_i}{\Sigma_i(z, y)} - \frac{\sigma_{i+1}}{\Sigma_{i+1}(z, y)} \cdot \frac{\sigma_{i+1}}{\Sigma_{i+1}(y, x)} \right] + (z - x) \left[\frac{\sigma_{i+1}}{\Sigma_{i+1}(z, x)} - \frac{\sigma_i}{\Sigma_i(z, x)} \right] \\ &+ (y - x) \left[\frac{\sigma_i}{\Sigma_i(y, x)} - \frac{\sigma_{i+1}}{\Sigma_{i+1}(y, x)} \right] + (z - y) \left[\frac{\sigma_i}{\Sigma_i(z, y)} - \frac{\sigma_{i+1}}{\Sigma_{i+1}(z, y)} \right]. \end{aligned}$$

Using relation (II.B.158), we are left to prove that

$$\begin{aligned} & (y-x)(z-x)(z-y) \frac{\lambda\sigma_i^2 + \mu\sigma_i}{\Sigma_i(y,x)\Sigma_i(z,x)\Sigma_i(z,y)} \\ &= (y-x)(z-y) \frac{\sigma_i^2}{\Sigma_i(y,x)\Sigma_i(z,y)} + (y-x) \frac{\sigma_i}{\Sigma_i(y,x)} + (z-y) \frac{\sigma_i}{\Sigma_i(z,y)} - (z-x) \frac{\sigma_i}{\Sigma_i(z,x)}, \end{aligned} \quad (\text{II.B.163})$$

as well as the same equation for σ_{i+1} . This is done by a direct computation (all the quantities involved commute with each other). \blacksquare

Remark B.48. *Note that contrary to Hecke and BMW algebras, the defining relations for the \mathcal{M}_n , \mathcal{S}_n , \mathcal{T}_n algebras do not imply necessarily the existence of a minimal polynomial for σ_i . Moreover the Baxterisation of the latter algebras depends on two spectral parameters.*

3 Diagonalization of the transfer matrix

We presented in the previous sections the construction of integrable Markov matrix. The integrability was defined as the fact that the Markov matrix enters a set of commuting operators, generated by a transfer matrix. We stressed that this strong property translates into a lot of conserved quantities and is thus a hint for an exact solvability of the model. This also means that the Markov matrix and the transfer matrix share common eigenvectors (these eigenvectors are independent of the spectral parameter). This justifies the following definition.

Definition B.49. *We denote by $\{|\Psi_i\rangle\}_{1 \leq i \leq 2^L}$ (respectively $\{E_i(z)\}_{1 \leq i \leq 2^L}$) the eigenvectors (respectively the eigenvalues) of the transfer matrix $t(z)$*

$$t(z)|\Psi_i\rangle = E_i(z)|\Psi_i\rangle. \quad (\text{II.B.164})$$

We thus have for the Markov matrix

$$M|\Psi_i\rangle = \theta E_i'(1)|\Psi_i\rangle. \quad (\text{II.B.165})$$

Remark B.50. *We are dealing here with models defined on a periodic lattice. In practice we will encounter a lot of systems for which the stochastic dynamics conserves the number of particles of each species on the periodic lattice (in simple models the particles are often only allowed to jump from site to site but not to appear or disappear). We define*

$$\mathcal{N}(\tau) = \sum_{i=1}^L n_i(\tau), \quad (\text{II.B.166})$$

where $n_i(\tau)$ is a diagonal $(N+1) \times (N+1)$ matrix acting non-trivially on site i (and trivially on other sites) as $\text{diag}(\underbrace{0, \dots, 0}_{\tau}, \underbrace{1, 0, \dots, 0}_{N-\tau})$. The operator $\mathcal{N}(\tau)$ is constructed to count the

number of particles of species τ . Then we have for all τ, τ'

$$[t(z), \mathcal{N}(\tau)] = 0, \quad \text{and} \quad [\mathcal{N}(\tau), \mathcal{N}(\tau')] = 0. \quad (\text{II.B.167})$$

The commutation properties stated just above proves that for such systems the action the transfer matrix is block diagonal (one block corresponds to a fixed number of particles of each species that we call sometimes sector) and that the diagonalization can be performed independently on each sector.

We would like to determine the complete set of eigenvectors of the Markov matrix. Several methods can be used to diagonalize the Markov matrix (they have been historically developed to deal with quantum Hamiltonians). We present below two of them: the coordinate Bethe ansatz and the algebraic Bethe ansatz and illustrate them on examples. We briefly introduce in a second time other diagonalization techniques.

Note that we focus here on the diagonalization of the homogeneous transfer matrix (or equivalently of the Markov matrix) but some of the methods presented below can be also transposed to the case of inhomogeneity parameters.

a) Coordinate Bethe ansatz

The problem of finding the eigenvectors of a Markov matrix is very similar (at least for the models studied here) to the case of quantum Hamiltonians. Stochastic models defined on a one dimensional lattice are indeed often related through a similarity transformation to one dimensional quantum spin chains.

The analytical computation of the eigenvectors and eigenvalues of a quantum Hamiltonian is a rather difficult question, that is even usually impossible to achieve. However, in [78], H. Bethe succeeded in computing exactly the spectrum of the one-dimensional Heisenberg quantum spin chain [79], introducing a method that is now called after him: the coordinate Bethe ansatz (CBA). This technique can be thought as a generalized Fourier transform and opened basically a new field of research. Since then the method had been widely used in different contexts (quantum spin chains, quantum systems, Markovian processes). We point out the pioneering works [80–86].

We begin to present the coordinate Bethe ansatz in systems involving a single species of particle, *i.e.* $N = 1$ in our notation (we recall that in this particular case the occupation variables τ_i take only two values 0 for holes and 1 for particles). A more involved case with two-species of particles will be studied below. We are interested in models where the stochastic dynamics encoded in the Markov matrix conserves the number of particles. The discussion on the block diagonal decomposition of the Markov matrix suggests the following definition.

Definition B.51. For $1 \leq x \leq L$ we introduce the vector

$$|\{x\}\rangle = \underbrace{|0\rangle \otimes \cdots \otimes |0\rangle}_{x-1} \otimes |1\rangle \otimes \underbrace{|0\rangle \otimes \cdots \otimes |0\rangle}_{L-x} \quad (\text{II.B.168})$$

and more generally for $1 \leq x_1 < x_2 < \cdots < x_r \leq L$ we introduce the vector

$$|\{x_1, x_2, \dots, x_r\}\rangle = \underbrace{|0\rangle \otimes \cdots \otimes |0\rangle}_{x_1-1} \otimes |1\rangle \otimes \underbrace{|0\rangle \otimes \cdots \otimes |0\rangle}_{x_2-x_1-1} \otimes |1\rangle \otimes \cdots \otimes |1\rangle \otimes \underbrace{|0\rangle \otimes \cdots \otimes |0\rangle}_{L-x_r}. \quad (\text{II.B.169})$$

Proposition B.52. The vectors $|\{x_1, x_2, \dots, x_r\}\rangle$ define a basis of the sector with r particles (*i.e.* of the eigenspace associated to the eigenvalue r of the operator $\mathcal{N}(1)$ introduced in (II.B.166)). For each vector $|\Psi\rangle$ living in this sector (*i.e.* satisfying $\mathcal{N}(1)|\Psi\rangle = r|\Psi\rangle$) we have the expansion

$$|\Psi\rangle = \sum_{1 \leq x_1 < x_2 < \cdots < x_r \leq L} a(x_1, x_2, \dots, x_r) |\{x_1, x_2, \dots, x_r\}\rangle. \quad (\text{II.B.170})$$

The coordinate Bethe ansatz consists in assuming the following Fourier-like decomposition of the coefficient $a(x_1, x_2, \dots, x_r)$

$$a(x_1, x_2, \dots, x_r) = \sum_{\sigma \in \mathfrak{S}_r} A_\sigma u_{\sigma(1)}^{x_1} u_{\sigma(2)}^{x_2} \cdots u_{\sigma(r)}^{x_r} \quad (\text{II.B.171})$$

\mathfrak{S}_r denotes the permutation group of the elements $\{1, 2, \dots, r\}$. The parameters u_1, u_2, \dots, u_r are called the Bethe roots and are expected to satisfy a set of polynomial algebraic relations called the Bethe equations (see examples below). The coefficients A_σ are expected to be determined by exchange or scattering relations $A_{\sigma t_i} = \check{S}(u_{\sigma(i)}, u_{\sigma(i+1)}) A_\sigma$, where t_i is the permutation $i \leftrightarrow i+1$ (this last relation is sufficient to express any coefficient A_σ in function of the coefficient A_{Id} since the permutations t_1, t_2, \dots, t_{r-1} generate the group \mathfrak{S}_r).

The example of the ASEP The ASEP is a stochastic process whose Markov matrix has been defined in (II.A.21), with the local jump operator m given in (II.A.23). We argued previously that it raised a lot of interest in both physical and mathematical community. On the physical side it is one of the simplest out-of-equilibrium model that can be defined on a ring. On a mathematical side it is integrable and give rise to exact computations. We present the exact diagonalization of this model using CBA.

Example B.53. As a warm-up we begin to expose the method in the sector with 1 particle. The eigenvalue equation $M|\Psi\rangle = E|\Psi\rangle$, where M is the Markov matrix encoding the dynamics of the ASEP and $|\Psi\rangle = \sum_{x=1}^L a(x)|\{x\}\rangle$, can be written in components as

$$Ea(x) = pa(x-1) + qa(x+1) - (p+q)a(x), \quad \text{for } x = 1, \dots, L \quad (\text{II.B.172})$$

where we have assumed the periodicity constraints $a(L+1) = a(1)$ and $a(0) = a(L)$ for this equation to hold also for $x = 1$ and $x = L$. Plugging the Bethe ansatz $a(x) = Au^x$ in this last equation yields

$$E Au^x = pAu^{x-1} + qAu^{x+1} - (p+q)Au^x. \quad (\text{II.B.173})$$

Dividing by Au^x provides the expression of the eigenvalue

$$E = \frac{p}{u} + qu - (p+q). \quad (\text{II.B.174})$$

The periodicity imposes $a(x+L) = a(x)$ which translates into the Bethe equation $u^L = 1$. The Bethe equation admits L different solutions (Bethe roots) which provide for each one an eigenvector of the Markov matrix in the sector with 1 particle. This sector being of dimension L , we thus have diagonalized completely the Markov matrix in this subspace.

In order to get used to the Bethe ansatz and to understand the general structure we present now the case of the 2 particles sector. This is the simplest situation where the coefficients A_σ play an important role.

Example B.54. For $1 \leq x_1 < x_2 \leq L$ and x_1, x_2 not nearest neighbors on the ring, i.e. $x_2 \neq x_1 + 1$ and $(x_1, x_2) \neq (1, L)$ (this particular case is studied below), the eigenvalue equation reads

$$E a(x_1, x_2) = pa(x_1 - 1, x_2) + pa(x_1, x_2 - 1) + qa(x_1 + 1, x_2) + qa(x_1, x_2 + 1) - 2(p+q)a(x_1, x_2). \quad (\text{II.B.175})$$

where we have assumed the periodicity constraints $a(x_1, L+1) = a(1, x_1)$ and $a(0, x_2) = a(x_2, L)$. The ansatz $a(x_1, x_2) = A_{12} u_1^{x_1} u_2^{x_2} + A_{21} u_2^{x_1} u_1^{x_2}$ (note that we made a slight abuse of notation by writing for clarity and convenience A_{12} instead of A_{1d} and A_{21} instead of A_{t_1}) fulfills the eigenvalue equation provided that the eigenvalue is equal to

$$E = p \left(\frac{1}{u_1} + \frac{1}{u_2} \right) + q(u_1 + u_2) - 2(p+q). \quad (\text{II.B.176})$$

When x_1 and x_2 are close together, i.e. when $x_2 = x_1 + 1$, the eigenvalue equation takes a slightly different form

$$E a(x_1, x_2) = pa(x_1 - 1, x_2) + qa(x_1, x_2 + 1) - (p+q)a(x_1, x_2). \quad (\text{II.B.177})$$

Subtracting this equation to (II.B.175) (which holds for every x_1, x_2 thanks to the ansatz and the eigenvalue being fixed to (II.B.176)) yields the 'boundary' condition

$$pa(x_1, x_1) + qa(x_1 + 1, x_1 + 1) - (p+q)a(x_1, x_1 + 1) = 0. \quad (\text{II.B.178})$$

This latter equation is solved if the coefficients A_{12} and A_{21} satisfy

$$A_{21} = -\frac{p + qu_1u_2 - (p+q)u_2}{p + qu_1u_2 - (p+q)u_1} A_{12}. \quad (\text{II.B.179})$$

The periodicity constraints $a(x_1, L+1) = a(1, x_1)$ and $a(0, x_2) = a(x_2, L)$ imply the Bethe equations

$$u_1^L = \frac{A_{12}}{A_{21}} = -\frac{p + qu_1u_2 - (p+q)u_1}{p + qu_1u_2 - (p+q)u_2} \quad (\text{II.B.180})$$

and

$$u_2^L = \frac{A_{21}}{A_{12}} = -\frac{p + qu_1u_2 - (p+q)u_2}{p + qu_1u_2 - (p+q)u_1}. \quad (\text{II.B.181})$$

The problem of diagonalizing the Markov matrix in the 2 particles sector is thus reduced to the resolution of these two polynomial equations of degree $L + 2$. This is still a hard task but this reduction is a huge step forward because the direct diagonalization of the Markov matrix in this sector requires to find the roots of the characteristic polynomial of degree $L(L - 1)/2$ (which grows much faster than L for L large).

Although the 3 particles case could appear as a straightforward generalization of the 2 particles case, it is in fact a crucial step to check toward the validity of the ansatz for a general sector with a given number of particles. It is indeed necessary to verify that the 'three-body interaction' (see details below) does not bring new constraints and factorizes into two-body interactions.

Example B.55. For $1 \leq x_1 < x_2 < x_3 \leq L$ far from each other, the eigenvalue equation can be written in components as

$$\begin{aligned} Ea(x_1, x_2, x_3) &= p[a(x_1 - 1, x_2, x_3) + a(x_1, x_2 - 1, x_3) + a(x_1, x_2, x_3 - 1)] \\ &\quad + q[a(x_1 + 1, x_2, x_3) + a(x_1, x_2 + 1, x_3) + a(x_1, x_2, x_3 + 1)] \\ &\quad - 3(p + q)a(x_1, x_2, x_3) = 0 \end{aligned}$$

The ansatz for the expression of $a(x_1, x_2, x_3)$ given by the general formula (II.B.171) contains $3! = 6$ terms and imposes the following expression for the eigenvalue

$$E = p \left(\frac{1}{u_1} + \frac{1}{u_2} + \frac{1}{u_3} \right) + q(u_1 + u_2 + u_3) - 3(p + q). \quad (\text{II.B.182})$$

The two-body interaction, given by the case $x_2 = x_1 + 1$ and x_3 far from x_1 and x_2 , yields the 'boundary' condition

$$pa(x_1, x_1, x_3) + qa(x_1 + 1, x_1 + 1, x_3) - (p + q)a(x_1, x_1 + 1, x_3) = 0. \quad (\text{II.B.183})$$

This equation is solved if

$$\begin{aligned} \frac{A_{213}}{A_{123}} &= -\frac{p + qu_1u_2 - (p + q)u_2}{p + qu_1u_2 - (p + q)u_1}, & \frac{A_{132}}{A_{312}} &= -\frac{p + qu_1u_3 - (p + q)u_1}{p + qu_1u_3 - (p + q)u_3}, \\ \frac{A_{321}}{A_{231}} &= -\frac{p + qu_2u_3 - (p + q)u_3}{p + qu_2u_3 - (p + q)u_2}. \end{aligned}$$

Once again we used the notation $A_{\sigma(1)\sigma(2)\sigma(3)}$ instead of A_σ for $\sigma \in \mathfrak{S}_3$. Similarly, the two-body interaction, given by the case $x_3 = x_2 + 1$ and x_1 far from x_2 and x_3 , yields the 'boundary' condition

$$pa(x_1, x_2, x_2) + qa(x_1, x_2 + 1, x_2 + 1) - (p + q)a(x_1, x_2, x_2 + 1) = 0. \quad (\text{II.B.184})$$

This equation is again solved if

$$\begin{aligned} \frac{A_{132}}{A_{123}} &= -\frac{p + qu_2u_3 - (p + q)u_3}{p + qu_2u_3 - (p + q)u_2}, & \frac{A_{321}}{A_{312}} &= -\frac{p + qu_1u_2 - (p + q)u_2}{p + qu_1u_2 - (p + q)u_1}, \\ \frac{A_{213}}{A_{231}} &= -\frac{p + qu_1u_3 - (p + q)u_1}{p + qu_1u_3 - (p + q)u_3}. \end{aligned}$$

The three-body interaction given by the case $x_2 = x_1 + 1$ and $x_3 = x_1 + 2$ yields the boundary equation

$$\begin{aligned} &q[a(x_1 + 1, x_1 + 1, x_1 + 2) + a(x_1, x_1 + 2, x_1 + 2)] \\ &+ p[a(x_1, x_1, x_1 + 2) + a(x_1, x_1 + 1, x_1 + 1)] - 2(p + q)a(x_1, x_1 + 1, x_1 + 2) = 0 \end{aligned}$$

This appears to be exactly the sum of the equations (II.B.183) and (II.B.184) given by the two-body interactions and hence it does not bring any new constraint and it is automatically fulfilled.

The periodicity constraints $a(0, x_2, x_3) = a(x_2, x_3, L)$ and $a(x_1, x_2, L + 1) = a(1, x_1, x_2)$ impose the Bethe equations

$$u_1^L = \frac{A_{123}}{A_{231}} = \frac{A_{123}}{A_{213}} \cdot \frac{A_{213}}{A_{231}} = \frac{p + qu_1u_2 - (p + q)u_1}{p + qu_1u_2 - (p + q)u_2} \cdot \frac{p + qu_1u_3 - (p + q)u_1}{p + qu_1u_3 - (p + q)u_3} \quad (\text{II.B.185})$$

and similarly

$$u_2^L = \frac{p + qu_1u_2 - (p + q)u_2}{p + qu_1u_2 - (p + q)u_1} \cdot \frac{p + qu_2u_3 - (p + q)u_2}{p + qu_2u_3 - (p + q)u_3} \quad (\text{II.B.186})$$

and

$$u_3^L = \frac{p + qu_1u_3 - (p + q)u_3}{p + qu_1u_3 - (p + q)u_1} \cdot \frac{p + qu_2u_3 - (p + q)u_3}{p + qu_2u_3 - (p + q)u_2}. \quad (\text{II.B.187})$$

We can now move to the general case.

Proposition B.56. *In the r particles sector, the eigenvectors of the Markov matrix M are given by*

$$|\Psi\rangle = \sum_{1 \leq x_1 < x_2 < \dots < x_r \leq L} \sum_{\sigma \in \mathfrak{S}_r} A_\sigma u_{\sigma(1)}^{x_1} u_{\sigma(2)}^{x_2} \dots u_{\sigma(r)}^{x_r} | \{x_1, x_2, \dots, x_r\} \rangle, \quad (\text{II.B.188})$$

where the Bethe roots u_1, \dots, u_r satisfy the Bethe equations

$$u_i^L = (-1)^{r-1} \prod_{\substack{j=1 \\ j \neq i}}^r \frac{p + qu_iu_j - (p + q)u_i}{p + qu_iu_j - (p + q)u_j} \quad (\text{II.B.189})$$

and the coefficients A_σ are determined (up to an overall normalization) by the relations

$$A_{\sigma \circ \tau_i} = - \frac{p + qu_{\sigma(i)}u_{\sigma(i+1)} - (p + q)u_{\sigma(i+1)}}{p + qu_{\sigma(i)}u_{\sigma(i+1)} - (p + q)u_{\sigma(i)}} A_\sigma. \quad (\text{II.B.190})$$

The associated eigenvalue is given by

$$E = \sum_{i=1}^r \left(\frac{p}{u_i} + qu_i - (p + q) \right). \quad (\text{II.B.191})$$

Proof. This can be proved by showing that the r -body interaction reduces to the sum of two-body interactions (similarly to what was done previously for the three-body interaction). It has been done in details for the XXZ spin chain [80] which is known to be similar, up to a gauge transformation, to the Markov matrix of the ASEP. ■

We stress that the diagonalization problem has been reduced to the resolution a set of algebraic equation of degree $L + 2(r - 1)$ (that has to be put in contrast with finding the roots of the characteristic polynomial of the Markov matrix which is of degree $\binom{L}{r}$ in this sector). This is still a very hard task that we cannot handle in general. However, several methods have been developed to study the Bethe equations in the thermodynamic limit [29, 87–89] and allow exact computations in this limit. Moreover this set of equations can be efficiently studied with numerical methods.

The CBA as a tool to construct integrable models The goal of this paragraph is to show how the CBA can be used to construct exactly solvable models. It presents the main results of [V2]

Since the work of Bethe [78], the classification of solvable one-dimensional systems has been the heart of a lot of researches. General methods are now known but involve huge computations which, in general, do not permit to provide a classification of solvable models. See subsection 2 for details.

In this section, we are interested in finding Markov matrix M such that the following eigenvalue problem

$$M\Psi = E\Psi \quad (\text{II.B.192})$$

can be solved exactly. The Markov matrices under consideration correspond to one-dimensional lattice gases with nearest neighbor interactions [35, 38, 90], and are written as follows

$$M = \sum_{\ell=1}^L m_{\ell, \ell+1} \quad (\text{II.B.193})$$

where we assume periodic boundary conditions (by convention $L + 1 \equiv 1$) and the indices $\ell, \ell + 1$ indicate on which sites the local operator m acts. This type of problem also appears in the context of two-dimensional equilibrium statistical models or one-dimensional spin chains. The archetypes of such models are respectively the 6-vertex model [29] or the Heisenberg spin chain [79]. Here, we focus on the case where m is a 9×9 matrix which means that each site may take three different values.

The cases when M commutes with some charges of the following type

$$\mathcal{N} = \sum_{\ell=1}^L n_{\ell} \quad (\text{II.B.194})$$

are of particular interest. In the context of out-of-equilibrium models, the number of conserved charges corresponds to the number of conserved species of particles (one of the value is for the empty site).

When M commutes with two different charges, the number of non vanishing elements of m is reduced to 15 (in the context of statistical mechanics, it is called the 15-vertex model). In out-of-equilibrium statistical physics, it corresponds to models where there are two classes of conserved particles (such as two species ASEP).

When M commutes with only one charge, they are several possibilities depending on the degeneracy of the eigenvalues of n . One usually takes n with three different eigenvalues: the local jump operator m has then 19 non vanishing entries. Such solvable models have been classified and studied previously in [57, 91–94]. They correspond to out-of-equilibrium models with only one species of particle, but where two particles can occupy the same site.

We concentrate here on Markov matrices M commuting with one charge that has one eigenvalue degenerated twice: m has then 33 non vanishing entries. Usually, the denomination 33-vertex model is dedicated to integrable models whose R -matrix has 33 non-vanishing entries. However, it appears that for the models solvable by CBA, when an R -matrix can be constructed, its non-vanishing entries coincide with the ones of m , see construction in [V1, 57]. Although this property has not been proven in full generality, but only checked case by case, we will call our Markov matrices, 33-vertex Markov matrices. These models may be interpreted, in the context of out-of-equilibrium model, as diffusing particles possessing two internal degrees of freedom. Let us emphasize that such models have been also introduced to study mRNA translation in [95, 96]. Therefore, we hope that the solvable models introduced here may be helpful in this context or to describe other phenomena.

Let us remark that the three cases described above exhaust all the non trivial cases when M possesses conserved charge(s). To fix the notations, we use the canonical basis

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |2\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \quad (\text{II.B.195})$$

The vector $|0\rangle$ will correspond to the empty site whereas $|1\rangle$ and $|2\rangle$ correspond to a particle in different internal states. In this context, the most general Markov matrices which preserve the number of particles are the ones which commute with the charge (II.B.194) with

$$n = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (\text{II.B.196})$$

Therefore the local Hamiltonian m takes the following form

$$m = \begin{pmatrix} m_{11} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & m_{22} & m_{23} & m_{24} & 0 & 0 & m_{27} & 0 & 0 \\ 0 & m_{32} & m_{33} & m_{34} & 0 & 0 & m_{37} & 0 & 0 \\ 0 & m_{42} & m_{43} & m_{44} & 0 & 0 & m_{47} & 0 & 0 \\ 0 & 0 & 0 & 0 & m_{55} & m_{56} & 0 & m_{58} & m_{59} \\ 0 & 0 & 0 & 0 & m_{65} & m_{66} & 0 & m_{68} & m_{69} \\ 0 & m_{72} & m_{73} & m_{74} & 0 & 0 & m_{77} & 0 & 0 \\ 0 & 0 & 0 & 0 & m_{85} & m_{86} & 0 & m_{88} & m_{89} \\ 0 & 0 & 0 & 0 & m_{95} & m_{96} & 0 & m_{98} & m_{99} \end{pmatrix}. \quad (\text{II.B.197})$$

Note that the 15-vertex model is a sub-case of the problem studied here in opposition to the 19-vertex model that exhibits different non vanishing entries.

The goal of this paragraph consists in classifying all such models which are solvable by Coordinate Bethe Ansatz. The main result is exposed right below. The proof is then detailed in several parts. In a first time we perform the first step of the CBA (i.e. the nesting), which leads to a reduced problem dealing with 4×4 R -matrices possessing a specific form. In a second time we classify these R -matrices, solutions of a braided Yang–Baxter equation with spectral parameters.

Main result : We present the final result, after gathering the different constraints that should satisfy the parameters (the computations are detailed below). We obtain the following classification of 33-vertex Markov matrices. The jump operator (II.B.197) is solvable by CBA if and only if its entries obey the following constraints:

(i) We must have:

$$\begin{aligned} m_{23} + m_{47} = 0 & \quad ; & \quad m_{32} + m_{74} = 0 & \quad ; & \quad m_{27} = m_{34} = m_{43} = m_{72} = 0 \\ m_{24} = m_{37} & \quad ; & \quad m_{42} = m_{73} & \quad ; & \quad m_{22} + m_{44} = m_{33} + m_{77}, \end{aligned} \quad (\text{II.B.198})$$

(ii) The matrix

$$T = \begin{pmatrix} t_{55} & t_{56} & t_{58} & t_{59} \\ t_{65} & t_{66} & t_{68} & t_{69} \\ t_{85} & t_{86} & t_{88} & t_{89} \\ t_{95} & t_{96} & t_{98} & t_{99} \end{pmatrix} \quad (\text{II.B.199})$$

where

$$\begin{aligned} t_{55} &= m_{55} + m_{11} - m_{22} - m_{44} ; & t_{58} &= m_{58} + m_{23} ; & t_{85} &= m_{85} + m_{32} ; & t_{59} &= m_{59} \\ t_{66} &= m_{66} + m_{11} - m_{33} - m_{44} ; & t_{69} &= m_{69} + m_{23} ; & t_{96} &= m_{96} + m_{32} ; & t_{68} &= m_{68} \\ t_{88} &= m_{88} + m_{11} - m_{22} - m_{77} ; & t_{56} &= m_{56} - m_{23} ; & t_{65} &= m_{65} - m_{32} ; & t_{86} &= m_{86} \\ t_{99} &= m_{99} + m_{11} - m_{33} - m_{77} ; & t_{89} &= m_{89} - m_{23} ; & t_{98} &= m_{98} - m_{32} ; & t_{95} &= m_{95} \end{aligned} \quad (\text{II.B.200})$$

must be a representation of one of these three algebras:

(a) *Hecke algebras*

$$T_{12}T_{23}T_{12} - m_{24}m_{42}T_{12} = T_{23}T_{12}T_{23} - m_{24}m_{42}T_{23} \quad \text{and} \quad T^2 = \mu T \quad (\text{II.B.201})$$

(b) \mathcal{T}_n *algebras*

$$T_{12}T_{23}T_{12} + T_{12}(T_{23})^2 = T_{23}T_{12}T_{23} + (T_{12})^2T_{23} \quad (\text{II.B.202})$$

(c) \mathcal{S}_n *algebras*

$$T_{12}T_{23}T_{12} + (T_{23})^2T_{12} = T_{23}T_{12}T_{23} + T_{23}(T_{12})^2 \quad (\text{II.B.203})$$

Fortunately, the 4×4 solutions to relations (II.B.201), (II.B.202) or (II.B.203) have been classified: all the possible expressions of T can be then recovered from these classifications. For Hecke algebras, the classification of 4×4 matrices is given in (II.B.109) and for \mathcal{S}_n and \mathcal{T}_n algebras the classification is given in theorem B.40.

We present now the proofs of this result. Constraint (i) is found while performing the first step of the CBA whereas the constraint (ii) is obtained by solving the Yang-Baxter equation for the reduced problem.

Coordinate Bethe ansatz : As mentioned above, we now focus on jump operators (II.B.197) that commute with \mathcal{N} , defined by (II.B.194) and (II.B.196). The basis (II.B.195) allows us to introduce the following elementary states

$$|x_1, i_1; x_2, i_2; \dots; x_r, i_r\rangle = |0\rangle^{\otimes x_1-1} \otimes |i_1\rangle \otimes |0\rangle^{\otimes x_2-x_1-1} \otimes |i_2\rangle \cdots \otimes |i_r\rangle \otimes |0\rangle^{\otimes L-x_r} \quad (\text{II.B.204})$$

where $i_k = 1, 2$ and $x_k = 1, 2, \dots, L$. In words, the state $|x_1, i_1; x_2, i_2; \dots; x_r, i_r\rangle$ stands for the configuration where the particles are in positions x_1, x_2, \dots, x_r with internal states i_1, i_2, \dots, i_r respectively¹².

Notice that $|x_1, i_1; x_2, i_2; \dots; x_r, i_r\rangle$ is an eigenvector of \mathcal{N} with eigenvalue r whatever the values of x_k 's and i_k 's are. In fact, the set of states $|x_1, i_1; x_2, i_2; \dots; x_r, i_r\rangle$ spans the vector space with r particles. Therefore, an Markov matrix eigenstate Ψ_r in a given sector with r particles can be written as a linear combination of the elementary states (II.B.204) with coefficients $a(x_1, \dots, x_r)$, which are complex-valued functions to be determined:

$$\Psi_r = \sum_{1 \leq x_1 < \dots < x_r \leq L} \sum_{i_1, i_2, \dots, i_r=1,2} a_{i_1, i_2, \dots, i_r}(x_1, x_2, \dots, x_r) |x_1, i_1; x_2, i_2; \dots; x_r, i_r\rangle. \quad (\text{II.B.205})$$

The coordinate Bethe ansatz [78] consists in assuming a plane wave decomposition for the functions $a_{i_1, i_2, \dots, i_r}(x_1, x_2, \dots, x_r)$:

$$a_{i_1, i_2, \dots, i_r}(x_1, x_2, \dots, x_r) = \sum_{\sigma \in \mathfrak{S}_r} A_{\sigma}^{(i_1, i_2, \dots, i_r)} \prod_{k=1}^r u_{\sigma(k)}^{x_k}, \quad (\text{II.B.206})$$

where \mathfrak{S}_r is the permutation group of r elements. The unknowns $A_{\sigma}^{(i_1, i_2, \dots, i_r)}$ are functions on the symmetric group algebra depending on the parameters u_1, u_2, \dots, u_r called rapidities and which are solutions of the Bethe equations determined below. To simplify the following computations, we encompass the 2^r different unknowns $A_{\sigma}^{(i_1, i_2, \dots, i_r)}$ for a given σ in the following vector

$$\mathbf{A}_{\sigma} = \sum_{i_1, i_2, \dots, i_r=1,2} A_{\sigma}^{(i_1, i_2, \dots, i_r)} |\bar{i}_1\rangle \otimes |\bar{i}_2\rangle \otimes \cdots \otimes |\bar{i}_r\rangle \quad (\text{II.B.207})$$

where

$$|\bar{1}\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |\bar{2}\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (\text{II.B.208})$$

As usual, we project the eigenvalue problem (II.B.192) on the different elementary states, the eigenvector having the form (II.B.205) with (II.B.206). We do not detail the calculations, since they are similar to the nested coordinate Bethe ansatz developed in [81, 82, 85] based on the ideas of [78]. The computations are divided into two main steps:

- we reduce the original eigenvalue problem with L sites allowing three different states, to an eigenvalue problem for a system with a smaller number of sites, that allow only two different states (this system is called the reduced problem);
- we determine (and classify) when the reduced problem is integrable.

¹²We remind that $|0\rangle$ stands for an empty site.

In the following, we sketch these two steps and give the main results.

First step : Performing the CBA on the position of the particles (and not looking at their internal states), we get a first set of constraints on the parameters of the local Hamiltonian. This corresponds to the constraints (II.B.198) given previously. This first step allows us to determine the energy of the state Ψ_r :

$$E_r = L m_{11} + \sum_{k=1}^r \epsilon(u_k) \quad \text{with} \quad \epsilon(u) = m_{22} + m_{44} - 2m_{11} + \frac{m_{24}}{u} + m_{42} u \quad (\text{II.B.209})$$

provided the coefficients \mathbf{A}_σ are related by

$$\mathbf{A}_{\sigma \mathbf{t}_j} = \check{S}_{j,j+1}(u_{\sigma(j)}, u_{\sigma(j+1)}) \mathbf{A}_\sigma \quad (\text{II.B.210})$$

$$\check{S}(z_1, z_2) = -\frac{z_2}{z_1} \Lambda(z_1, z_2) \Lambda(z_2, z_1)^{-1}, \quad (\text{II.B.211})$$

where $\mathbf{t}_j \in \mathfrak{S}_r$ denotes the transposition $(j, j+1)$ and

$$\Lambda(z_1, z_2) = T - \left(m_{42} z_1 + \frac{m_{24}}{z_2} \right) \mathbb{I}_4. \quad (\text{II.B.212})$$

T is the 4×4 constant matrix (II.B.199) whose entries depend on the entries of m , as stated in (II.B.200).

Let us describe more precisely the meaning of the indices of $\check{S}_{j,j+1}$ in (II.B.210): they indicate in which spaces the 4×4 matrix \check{S} acts non trivially in the tensor product $(\mathbb{C}^2)^{\otimes r}$ spanned by $\{|\bar{i}_1\rangle \otimes |\bar{i}_2\rangle \otimes \cdots \otimes |\bar{i}_r\rangle \mid i_k = 1, 2\}$. Explicitly, we get

$$\check{S}_{j,j+1}(z_1, z_2) = \mathbf{1}_2^{\otimes j-1} \otimes \check{S}(z_1, z_2) \otimes \mathbf{1}_2^{\otimes L-j-1}. \quad (\text{II.B.213})$$

Due to the defining relations of the permutation group \mathfrak{S}_r

$$\mathbf{t}_j^2 = id, \quad [\mathbf{t}_j, \mathbf{t}_k] = 0, \quad |k-j| > 1, \quad \mathbf{t}_j \mathbf{t}_{j+1} \mathbf{t}_j = \mathbf{t}_{j+1} \mathbf{t}_j \mathbf{t}_{j+1},$$

relations (II.B.210) gives constraint on \check{S} :

$$\begin{aligned} \check{S}_{j,j+1}(z_j, z_{j+1}) \check{S}_{j,j+1}(z_{j+1}, z_j) = 1 \quad , \quad [\check{S}_{j,j+1}(z_j, z_{j+1}), \check{S}_{k,k+1}(z_k, z_{k+1})] = 0 \\ \check{S}_{12}(z_1, z_2) \check{S}_{23}(z_1, z_3) \check{S}_{12}(z_2, z_3) = \check{S}_{23}(z_2, z_3) \check{S}_{12}(z_1, z_3) \check{S}_{23}(z_1, z_2). \end{aligned} \quad (\text{II.B.214})$$

The first two relations are trivially satisfied by (II.B.211). The third one (II.B.214), called braided Yang–Baxter equation, holds only if supplementary constraints on the entries of T are satisfied. We postpone the study of these constraints and suppose from now on that they are indeed satisfied.

Because of the periodicity of the model, the rapidities u_j are quantified and must obey the first set of Bethe equations

$$u_j^L \mathbf{A}_{id} = S_{j+1,j}(u_{j+1}, u_j) \cdots S_{r,j}(u_r, u_j) S_{1,j}(u_1, u_j) \cdots S_{j-1,j}(u_{j-1}, u_j) \mathbf{A}_{id}, \quad j = 1, \dots, r. \quad (\text{II.B.215})$$

where

$$S(x, y) = P \check{S}(x, y) \quad \text{and} \quad P = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad (\text{II.B.216})$$

This set of eigenvalue problems is the reduced problem. The matrix S is a 4×4 matrix.

Second step (nesting) : The matrix $S(x, y)$ is obviously regular, $S(x, x) = -P$, so that the set of eigenvalue problems (II.B.215) can be recasted using a transfer matrix

$$t(z; \{u_1, \dots, u_r\}) = \text{tr}_0 \left(S_{10}(u_1, z) \cdots S_{M0}(u_r, z) \right). \quad (\text{II.B.217})$$

This is the transfer matrix introduced in (II.B.19) where the Bethe roots play the role of inhomogeneity parameters. We recall that because of the Yang–Baxter equation (II.B.214), the transfer matrix commute for different values of z :

$$[t(z; \{u_1, \dots, u_r\}), t(z'; \{u_1, \dots, u_r\})] = 0. \quad (\text{II.B.218})$$

Therefore, the Bethe equations (II.B.215) reduced to

$$u_j^L \mathbf{A}_{id} = -t(u_j; \{u_1, \dots, u_r\}) \mathbf{A}_{id} \quad (\text{II.B.219})$$

are compatible since we can diagonalize simultaneously all the $t(u_j; \{u_1, \dots, u_r\})$. Let us remark that the transfer matrix (II.B.217) may be used to define a new integrable system.

To finish the computations, we should solve the reduced problem using, for example, the Bethe ansatz once again. However, in the cases treated here, the reduced problem has no conserved charge and the resolution becomes much harder. How to apply the Bethe ansatz in these cases is still an open question. However, let us mention that new methods appeared recently in order to solve similar problems where there is no conserved charge due to the boundary conditions (generalization of the CBA [97, 98], Onsager approach [99], separation of variables [100], inhomogeneous Bethe equation [101], modified algebraic Bethe ansatz [102–104]). A generalization of these methods may be possible to deal with the eigenvalue problem (II.B.215). In the case of Markovian processes, the matrix ansatz developed in [46] with its link with integrability [V3, 105] may be also helpful for the resolution of this eigenvalue problem.

Braided Yang–Baxter equation :

This part is devoted to the classification of the matrices T such that the braided Yang–Baxter equation (II.B.214) holds. We split the problem into three subcases: *i*) $m_{24}m_{42} \neq 0$, then *ii*) $m_{42} = 0, m_{24} \neq 0$ and *iii*) $m_{24} = 0, m_{42} \neq 0$. The case $m_{24} = m_{42} = 0$ is excluded since it corresponds to an energy (II.B.209) which does not depend on the rapidities (there is no diffusion of particles).

• *Case $m_{24} m_{42} \neq 0$* By taking different expansions w.r.t. z_1, z_2 and z_3 in (II.B.214) and after algebraic manipulations, we find that the braided Yang–Baxter equation (II.B.214) holds if and only if T satisfies:

$$\begin{aligned} T_{12}T_{23}T_{12} - m_{24}m_{42}T_{12} &= T_{23}T_{12}T_{23} - m_{24}m_{42}T_{23}, \\ (T_{12})^2 T_{23} &= T_{12} (T_{23})^2, \\ (T_{23})^2 T_{12} &= T_{23} (T_{12})^2. \end{aligned} \quad (\text{II.B.220})$$

This is a particular case of the algebra \mathcal{M}_n introduced in (II.B.150). Note that these relations come directly from the form (II.B.211) of the S -matrix, and do not depend on the size of T . In general, classifying the solutions of equations (II.B.220) is a difficult task. However, in the case of 4×4 matrices treated here, it is possible to use formal mathematical software to deal with them. Firstly, we prove that all the solutions of (II.B.220) verify

$$T^2 = \mu T. \quad (\text{II.B.221})$$

Secondly, we perform the following transformation

$$T = \tau \tilde{T} + \rho \quad (\text{II.B.222})$$

with ρ solution of $\rho^2 - \mu\rho + m_{24}m_{42} = 0$ and $\tau = \pm\sqrt{\rho^2 + m_{24}m_{42}}$. The matrix \tilde{T} satisfies the relations of the Hecke algebra

$$\tilde{T}_{12}\tilde{T}_{23}\tilde{T}_{12} = \tilde{T}_{23}\tilde{T}_{12}\tilde{T}_{23} \quad , \quad (\text{II.B.223})$$

$$\tilde{T} - \tilde{T}^{-1} = \frac{\mu - 2\rho}{\tau} \equiv \tilde{\mu}. \quad (\text{II.B.224})$$

The classification of the 4×4 matrices satisfying these relations was given in (II.B.109).

The value of μ in (II.B.221) is reconstructed from these data. Indeed, simple algebraic manipulations show that

$$\mu^2 = \frac{m_{24} m_{42}}{x^2(1-x^2)}, \quad \rho = \mu x^2, \quad \tau = x\mu \quad \text{where } x \text{ is a solution of } 2x^2 + \tilde{\mu}x - 1 = 0. \quad (\text{II.B.225})$$

Finally, we remark that for any previous solutions of the Hecke algebra, the matrix \check{S} verifies the Yang–Baxter equation (II.B.214). Performing the change of variable

$$z_j = \frac{\mu(1-x_j) + \delta(1+x_j)}{2m_{42}(1-x_j)}, \quad \text{with } \delta = \sqrt{\mu^2 - 4m_{24}m_{42}}, \quad (\text{II.B.226})$$

one can verify that $\check{S}(z_1, z_2)$ depends only on the ratio $\frac{x_1}{x_2}$ (up to a normalisation factor). In fact, in terms of the variables x_j , equation (II.B.211) is equivalent to the usual Baxterization of the Hecke algebra recalled in (II.B.92).

• *Case $m_{24} = 0$ and $m_{42} \neq 0$.* Now, the different expansions w.r.t. z_1, z_2 and z_3 in (II.B.214), lead to the sole relation:

$$T_{12}T_{23}T_{12} + T_{12}(T_{23})^2 = T_{23}T_{12}T_{23} + (T_{12})^2 T_{23} \quad (\text{II.B.227})$$

One recognizes in (II.B.227) the algebra \mathcal{T}_3 defined in (II.B.121). The 4×4 solutions have been classified in theorem B.40.

• *Case $m_{42} = 0$ and $m_{24} \neq 0$*

This case can be deduced from the case $m_{24} = 0, m_{42} \neq 0$ in the following way. From any solution $\check{S}(z_1, z_2)$ to the braided Yang–Baxter equation, one can construct a new one

$$\check{\Sigma}(z_1, z_2) = \check{S}^{t_1 t_2}(1/z_2, 1/z_1), \quad (\text{II.B.228})$$

where $(\cdot)^{t_j}$ denotes the transposition in space j . Then, starting from

$$\check{S}(z_1, z_2) = -\frac{z_2}{z_1} \Lambda(z_1, z_2) \Lambda(z_2, z_1)^{-1} \quad \text{with } \Lambda(z_1, z_2) = T - \frac{m_{24}}{z_2} \mathbb{I}_4 \quad (\text{II.B.229})$$

we get

$$\check{\Sigma}(z_1, z_2) = -\frac{z_2}{z_1} \bar{\Lambda}(z_1, z_2) \bar{\Lambda}(z_2, z_1)^{-1} \quad \text{with } \bar{\Lambda}(z_1, z_2) = T^{t_1 t_2} - m_{24} z_1 \mathbb{I}_4. \quad (\text{II.B.230})$$

It is clear that, up to a replacement $m_{24} \leftrightarrow m_{42}$, $\check{\Sigma}(z_1, z_2)$ corresponds to the expression of the S-matrix (II.B.211) with $m_{24} = 0$. Therefore, any solution $\check{S}(z_1, z_2)$ of the Yang–Baxter equation for $m_{42} = 0$ is obtained from a solution $\check{\Sigma}(z_1, z_2)$ for $m_{24} = 0$ (classified in the previous paragraph).

For the case $m_{42} = 0$, the condition on T reads

$$T_{12}T_{23}T_{12} + (T_{23})^2 T_{12} = T_{23}T_{12}T_{23} + T_{23}(T_{12})^2 \quad (\text{II.B.231})$$

which is deduced from relation (II.B.227) by transposition, as expected. One recognizes now in (II.B.231) the defining relations of the algebra \mathcal{S}_3 , see (II.B.115).

b) Algebraic Bethe ansatz

We now present another method to diagonalize the Markov matrix (or equivalently the transfer matrix) of an integrable process. This method is called algebraic Bethe ansatz (ABA) [77, 106, 107] and relies heavily on the algebraic structure associated to the integrable model. The main idea is to use the so-called RTT relation that we recall now the key features. Once again we treat here the simple case of single species models (*i.e* $N = 1$), but generalizations to multi-species models have been developed through the nesting procedure [108, 109].

Definition B.57. We define a 2×2 matrix

$$T(z) = \begin{pmatrix} A(z) & B(z) \\ C(z) & D(z) \end{pmatrix}, \quad (\text{II.B.232})$$

with entries $A(z), B(z), C(z), D(z)$ depending on a spectral parameter z and belonging to a non-commutative algebra \mathcal{A} defined with the help of a R -matrix (satisfying the braided Yang-Baxter equation) through the relation

$$\check{R} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} T(z_1) \otimes T(z_2) = T(z_2) \otimes T(z_1) \check{R} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}. \quad (\text{II.B.233})$$

Note that the associativity of the algebra is ensured by the Yang-Baxter equation (see chapter III for details about a similar statement).

Example B.58. For the single species ASEP, the R -matrix is defined in (II.B.13) and the associated RTT relation is equivalent to

$$\begin{aligned} A(z_1)A(z_2) &= A(z_2)A(z_1), & B(z_1)B(z_2) &= B(z_2)B(z_1), \\ C(z_1)C(z_2) &= C(z_2)C(z_1), & D(z_1)D(z_2) &= D(z_2)D(z_1), \\ A(z_1)B(z_2) &= f \begin{pmatrix} z_2 \\ z_1 \end{pmatrix} B(z_2)A(z_1) + g \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} B(z_1)A(z_2), \\ D(z_1)B(z_2) &= f \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} B(z_2)D(z_1) - g \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} B(z_1)D(z_2), \\ C(z_1)A(z_2) &= f \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} A(z_2)C(z_1) - g \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} A(z_1)C(z_2), \\ C(z_1)D(z_2) &= f \begin{pmatrix} z_2 \\ z_1 \end{pmatrix} D(z_2)C(z_1) + g \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} D(z_1)C(z_2), \\ B(z_1)C(z_2) &= \frac{p}{q}C(z_2)B(z_1) + \frac{p}{q}\frac{z_1}{z_2}g \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} [A(z_1)D(z_2) - A(z_2)D(z_1)], \\ D(z_1)A(z_2) &= A(z_2)D(z_1) - \frac{p}{q}g \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \left[C(z_2)B(z_1) - \frac{z_1}{z_2}C(z_1)B(z_2) \right], \end{aligned}$$

with

$$f(z) = \frac{p - qz}{p(1 - z)}, \quad g(z) = \frac{p - q}{p(1 - z)}. \quad (\text{II.B.234})$$

We stress that a representation of the RTT algebra on the vector space $(\mathbb{C}^2)^{\otimes L}$ can always be obtained with the help of the R -matrix.

Proposition B.59. The matrix defined by

$$T(z) = R_{0,L}(z)R_{0,L-1}(z) \dots R_{0,1}(z), \quad (\text{II.B.235})$$

provides a representation of the RTT algebra defined in (II.B.233) on the vector space $(\mathbb{C}^2)^{\otimes L}$.

Proof. This is shown by direct computation using the Yang-Baxter equation and the relation between the braided and non-braided R matrices: $\check{R}(z) = PR(z)$, where P is the permutation operator. \blacksquare

Note that $T(z)$ is then seen as a 2×2 matrix in tensor component space labeled by 0 with entries $A(z), B(z), C(z), D(z)$ (as defined in (II.B.232)) which are operators on the vector space $(\mathbb{C}^2)^{\otimes L}$. The interest of this explicit representation relies mainly on the following fact.

Lemma B.60. The transfer matrix for a periodic model $t(z)$ defined in (II.B.20) (with the inhomogeneity parameters $z_i = 1$) is obtained from the representation (II.B.235) through the relation

$$t(z) = \text{tr}_0 T(z) = A(z) + D(z). \quad (\text{II.B.236})$$

The idea of the ABA is to express the eigenvectors of the transfer matrix as

$$|\Psi\rangle = B(u_1)B(u_2)\dots B(u_r)|\Omega\rangle, \quad (\text{II.B.237})$$

where $|\Omega\rangle$ is chosen to be an eigenvector of $A(z)$ and $D(z)$ and to satisfy $C(z)|\Omega\rangle = 0$ (it is sometimes called the highest weight vector of the representation). The parameters u_1, u_2, \dots, u_r are called Bethe roots and are solution to a set of algebraic equations (the Bethe equations). The details of the construction depend on the model under consideration. To fix the ideas on a concrete example, we present now the case of the single species ASEP on a periodic lattice.

Proposition B.61. *The eigenvectors of the transfer matrix $t(z)$ of the ASEP in the sector with r particles are given by*

$$|\Psi\rangle = B(u_1)B(u_2)\dots B(u_r)|\Omega\rangle, \quad (\text{II.B.238})$$

where $B(z)$ is constructed from the representation (II.B.235) and

$$|\Omega\rangle = \underbrace{|0\rangle \otimes |0\rangle \otimes \dots \otimes |0\rangle}_{L \text{ times}}. \quad (\text{II.B.239})$$

The Bethe roots are solutions to the Bethe equations

$$\left(\frac{p(1-u_i)}{p-qu_i}\right)^L = (-1)^{r-1} \prod_{\substack{j=1 \\ j \neq i}}^r \frac{pu_i - qu_j}{pu_j - qu_i}. \quad (\text{II.B.240})$$

The associated eigenvalue is given by

$$E(z) = \prod_{j=1}^r \frac{pz - qu_j}{p(z - u_j)} + \left(\frac{p(1-z)}{p-qz}\right)^L \prod_{j=1}^r \frac{pu_j - qz}{p(u_j - z)}. \quad (\text{II.B.241})$$

Proof. First note that $C(z)|\Omega\rangle = 0$ and

$$A(z)|\Omega\rangle = |\Omega\rangle, \quad D(z)|\Omega\rangle = \left(\frac{p(1-z)}{p-qz}\right)^L |\Omega\rangle. \quad (\text{II.B.242})$$

The next step is to compute the action of $A(z)$ on $|\Psi\rangle$ using the commutation relation between $A(z)$ and $B(u_i)$

$$A(z)B(u_i) = \frac{pz - qu_i}{p(z - u_i)} B(u_i)A(z) - \frac{u_i(p - q)}{p(z - u_i)} B(z)A(u_i), \quad (\text{II.B.243})$$

which allows us to push $A(z)$ completely to the right through all the $B(u_i)$. Because of the relation $B(u_i)B(u_j) = B(u_j)B(u_i)$ the vector $A(z)|\Psi\rangle$ is completely symmetric with respect to the Bethe roots. This allows us to write

$$\begin{aligned} A(z)|\Psi\rangle &= A(z)B(u_1)\dots B(u_r)|\Omega\rangle \\ &= \prod_{j=1}^r \frac{pz - qu_j}{p(z - u_j)} |\Psi\rangle - \sum_{i=1}^r \frac{u_i(p - q)}{p(z - u_i)} \prod_{\substack{j=1 \\ j \neq i}}^r \frac{pu_i - qu_j}{p(u_i - u_j)} B(u_1)\dots B(u_{i-1})B(z)B(u_{i+1})\dots B(u_r)|\Omega\rangle. \end{aligned} \quad (\text{II.B.244})$$

Note that the result is split between a 'wanted' part (proportional to $|\Psi\rangle$ as expected) and an 'unwanted' part (where a parameter u_i has been replaced by z in the expression of $|\Psi\rangle$). All the game be to cancel this last part using the action of $D(z)$ on $|\Psi\rangle$. This can be computed using the commutation relation between $D(z)$ and $B(u_i)$

$$D(z)B(u_i) = \frac{pu_i - qz}{p(u_i - z)} B(u_i)D(z) - \frac{u_i(p - q)}{p(u_i - z)} B(z)D(u_i), \quad (\text{II.B.245})$$

which allows us to push $D(z)$ completely to the right through all the $B(u_i)$. This yields

$$D(z)|\Psi\rangle = D(z)B(u_1)\dots B(u_r)|\Omega\rangle = \left(\frac{p(1-z)}{p-qz}\right)^L \prod_{j=1}^r \frac{pu_j - qz}{p(u_j - z)} |\Psi\rangle \quad (\text{II.B.246})$$

$$- \sum_{i=1}^r \frac{u_i(p-q)}{p(u_i - z)} \left(\frac{p(1-u_i)}{p-qu_i}\right)^L \prod_{\substack{j=1 \\ j \neq i}}^r \frac{pu_j - qu_i}{p(u_j - u_i)} B(u_1)\dots B(u_{i-1})B(z)B(u_{i+1})\dots B(u_r)|\Omega\rangle,$$

where we observe again a 'wanted' part and an 'unwanted' part. It is then direct to see that $|\Psi\rangle$ is an eigenvector of $A(z) + D(z)$ if and only if the 'unwanted' parts in (II.B.244) and (II.B.246) cancel one with each other, *i.e* if the Bethe equations hold

$$\left(\frac{p(1-u_i)}{p-qu_i}\right)^L = (-1)^{r-1} \prod_{\substack{j=1 \\ j \neq i}}^r \frac{pu_i - qu_j}{pu_j - qu_i}. \quad (\text{II.B.247})$$

The associated eigenvalue is then given by

$$E(z) = \prod_{j=1}^r \frac{pz - qu_j}{p(z - u_j)} + \left(\frac{p(1-z)}{p-qz}\right)^L \prod_{j=1}^r \frac{pu_j - qz}{p(u_j - z)}. \quad (\text{II.B.248})$$

■

Remark B.62. We recall that the Markov matrix M of the ASEP is obtained from the transfer matrix $t(z)$ through the relation

$$M = (q-p)t'(1)t(1)^{-1} = (q-p) \left. \frac{d \ln t(z)}{dz} \right|_{z=1}. \quad (\text{II.B.249})$$

The vector $|\Psi\rangle$ is thus an eigenvector of M with eigenvalue

$$E = (q-p) \frac{E'(1)}{E(1)} = (q-p)^2 \sum_{i=1}^r \frac{u_i}{(1-u_i)(p-qu_i)}. \quad (\text{II.B.250})$$

Remark B.63. The Bethe roots u_1, \dots, u_r are directly related to the ones introduced in the coordinate Bethe ansatz through the change of variables

$$u_i = \frac{p(1-\tilde{u}_i)}{p-q\tilde{u}_i}. \quad (\text{II.B.251})$$

The parameters $\tilde{u}_1, \dots, \tilde{u}_r$ satisfy indeed the equations

$$\tilde{u}_i^L = (-1)^{r-1} \prod_{\substack{j=1 \\ j \neq i}}^r \frac{p + q\tilde{u}_i\tilde{u}_j - (p+q)\tilde{u}_i}{p + q\tilde{u}_i\tilde{u}_j - (p+q)\tilde{u}_j}, \quad (\text{II.B.252})$$

which are exactly the Bethe equations obtained in the coordinate Bethe ansatz (II.B.189). The eigenvalue of the Markov matrix is expressed in these new variables as

$$E = \sum_{i=1}^r \left(\frac{p}{\tilde{u}_i} + q\tilde{u}_i - (p+q) \right), \quad (\text{II.B.253})$$

in exact agreement with the expression derived from the coordinate Bethe ansatz (II.B.191). The precise link between the two methods (ABA and CBA) has been investigated in [110, 111].

Note that the algebraic Bethe ansatz provides also a fruitful framework to compute physical observables, such as correlation functions. We can mention the works [112–116].

c) Other methods

We present briefly here other methods, which have been successfully developed to diagonalize exactly models with periodic boundary conditions.

While solving the six-vertex and eight-vertex models, Baxter noticed that the eigenvalues of the transfer matrices satisfied some simple functional relations [29]. These functional difference equation gave basically rise to a new angle to study the integrable models: the functional Bethe ansatz [117]. It provides another interpretation of the Bethe equations, which appear in this context as a necessary condition to ensure the vanishing of unwanted residues.

Baxter interpreted these functional relation at the algebraic level [29] through the construction of the Q-operator. The idea is to build an operator having convenient algebraic relations with the transfer matrix, called the t-Q relations. In the last few years this Q-operator was understood to as being some particular transfer matrix with infinite dimensional auxiliary space. It is constructed in a matrix product form (often with q-deformed oscillators) using infinite dimensional representation of RTT algebras [118–120].

The deep algebraic structure carried by the integrable systems was also exploited to diagonalize quantum Hamiltonians through the vertex operators [121] and compute the correlation functions [122, 123]. The connection between this approach and the matrix product method presented in chapters III and IV, which are both related to the Knizhnik-Zamolodchikov equations, remains to be fully understood.

Another method was also introduced to diagonalize models with periodic boundary conditions: the separation of variables (SoV) [124]. This method aims to give an unifying framework for the resolution of classical and quantum integrable systems.

C Integrability for open systems

We present in this section the construction of integrable Markov matrices in the case of open boundary conditions. Similarly to the periodic case, the method relies on the construction of a set of commuting operators (containing the Markov matrix). This set is also generated by a transfer matrix which commutes for different values of the spectral parameter. The Markov matrix is again recovered by taking the derivative of this transfer matrix with respect to the spectral parameter. The transfer matrix is build from two key operators, which act locally on the lattice : the R -matrix, which guarantees the integrability of the bulk dynamics, and the K -matrices, which ensure the integrability of the boundary dynamics with the reservoirs. We have indeed already seen that the R -matrix is directly related to the bulk local jump operator m . We will point out a similar connection between the K -matrices and the boundary local jump operators B and \bar{B} . The commutation property of the transfer matrix is a direct consequence of two local properties: the Yang-Baxter equation, satisfied by the R -matrix, and the reflection equation [125], satisfied by the K -matrices.

1 Reflection matrices and transfer matrix

a) K-matrices and reflection equation

The R -matrix and its properties had already been introduced in the previous section to deal with models defined on the periodic lattice. All along this subsection, the R -matrix $R(z)$ stands for a matrix satisfying the Yang-Baxter equation (II.B.10), the unitarity, regularity and Markovian properties. We will also assume that $R(z)$ is related to a bulk local jump operator through the relation (II.B.5).

We present here the key object to deal with the integrability of the boundary dynamics: the K -matrix. It will be together with $R(z)$ the building block of the transfer matrix.

Definition C.1. *A matrix $K(z)$ of size $(N + 1) \times (N + 1)$, i.e acting on \mathbb{C}^{N+1} , satisfies the*

reflection equation if

$$R_{1,2} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} K_1(z_1) R_{2,1}(z_1 z_2) K_2(z_2) = K_2(z_2) R_{1,2}(z_1 z_2) K_1(z_1) R_{2,1} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}. \quad (\text{II.C.1})$$

The reflection equation states an equality between product of operators acting in $\mathbb{C}^{N+1} \otimes \mathbb{C}^{N+1}$. We recall that the subscript indices indicate on which copies \mathbb{C}^{N+1} of the tensor space the operators are acting non-trivially. For instance

$$K_1(z) = K(z) \otimes \mathbf{1}, \quad K_2(z) = \mathbf{1} \otimes K(z). \quad (\text{II.C.2})$$

We would like to give a pictorial representation of the reflection equation. The action of the K -matrix $K_i(z_i)$ can be represented graphically in figure II.11. The K -matrix is drawn as

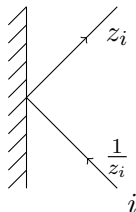


Figure II.11: Graphical representation of the matrix $K_i(z_i)$.

the reflection of a line labeled i , which corresponds to the tensor space component number i , on the boundary. The line is oriented by an arrow and carries a spectral parameter z_i . The incoming half line (according to the arrow direction) stands for a vector $|\tau\rangle$ of the i -th tensor space component, and can thus be in $N + 1$ different states. The out-going half line stands for the vector $\langle v|$, which belongs to the i -th tensor space component. When the vectors $|\tau\rangle$ and $\langle v|$ are specified, the left-reflection diagram represents the matrix element $\langle v|K(z_i)|\tau\rangle$.

For instance, in the particular case of single species models, *i.e.* for $N = 1$, this graphical interpretation can be specified as follows. A dashed line corresponds to the vector $|0\rangle$ (or equivalently to an empty site), whereas a continuous thick line corresponds to $|1\rangle$ (or equivalently to an occupied site). In a similar way, the out-going lines (after the reflection point) represent the state of the vector with which we are contracting to the left the matrix K : dashed line for $\langle 0|$ and continuous thick line for $\langle 1|$. Example of such graphical representation is given explicitly for the TASEP in fig. II.13.

As for the Yang-Baxter equation, there exists a nice intuitive interpretation for the reflection equation coming from quantum field theory (see figure II.12): the K -matrix $K(z)$ is the scattering matrix of a particle with rapidity z on the boundary. The integrability is the fact that the simultaneous scattering of 2 particles on the boundary factorizes in this K -matrix (*i.e.* the scattering of two particles on the boundary can be decomposed into single-particle scatterings on the boundary). The reflection equation is the consistency relation for this factorization, which ensures the independence of the result with respect to the order of the different events (scatterings between the two particles or scatterings on the boundary).

We now present the connection of the K -matrix with the boundary local jump operator B .

Definition C.2. A boundary local jump operator B is said to be integrable if there exists a K -matrix $K(z)$ satisfying the reflection equation (II.C.1) such that

$$B = \frac{\theta}{2} K'(1), \quad (\text{II.C.3})$$

where the constant θ is defined in (II.B.5).

In other words, the integrable boundary local jump operators B are obtained by taking the derivative of a K -matrix with respect to the spectral parameter. Conversely, we could wonder

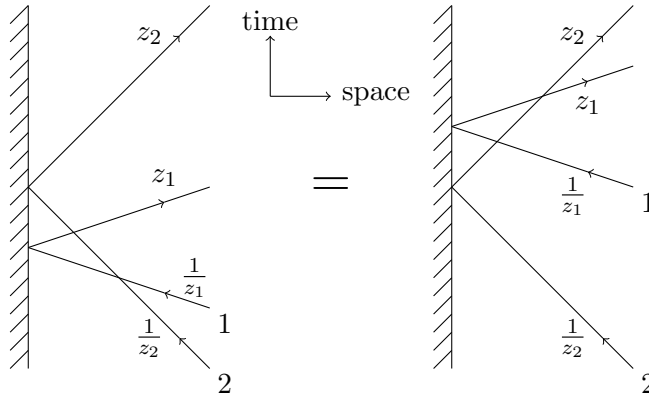


Figure II.12: Graphical representation of the reflection equation.

how is it possible, starting from a local jump operator B , to upgrade it to a spectral parameter dependent K -matrix. This will be partially answered with the Baxterisation procedure presented in subsection b). We would like to stress that taking the derivative of a K -matrix does not provide always a local Markovian matrix. The sum of the entries of each column of the local Markovian matrix should indeed vanish. It is straightforward to check that if the sum of the entries of each column of the K -matrix is equal to 1 then the derivative enjoys the sum to 0 property (but we still have to check that the off-diagonal entries of the derivative are non-negative). This motivates the following definition

Definition C.3. A matrix $K(z)$ acting on \mathbb{C}^{N+1} satisfies the Markovian property if

$$\langle \sigma | K(z) = \langle \sigma |, \quad (\text{II.C.4})$$

where we recall that $\langle \sigma | = \sum_{v=0}^N \langle v |$ achieves the sum over all the local configurations on one site.

Note that a such K -matrix satisfies the requirement of a discrete time Markovian process (provided that its entries are non-negative). We will see below that it can indeed be used as the building block (together with the R -matrix) of discrete time Markov matrices defined on the whole lattice with open boundaries.

We now list a set of properties that can be satisfied by a K -matrix. The usefulness of these properties will make sense while defining the transfer matrix below. They will be essential to connect the transfer matrix to the Markov matrix of the model.

Definition C.4. A matrix $K(z)$ acting on \mathbb{C}^{N+1} satisfies the regularity property if

$$K(1) = \mathbf{1}. \quad (\text{II.C.5})$$

Definition C.5. A matrix $K(z)$ acting on \mathbb{C}^{N+1} satisfies the unitarity property if

$$K(z).K(1/z) = \mathbf{1}. \quad (\text{II.C.6})$$

Remark C.6. We chose to introduce all the definition with R -matrix and K -matrix which are 'multiplicative' in the spectral parameter. We can write similar definition for matrices which are 'additive' in the spectral parameter. In this case a matrix $K(z)$ satisfies the reflection equation if

$$R_{1,2}(z_1 - z_2)K_1(z_1)R_{2,1}(z_1 + z_2)K_2(z_2) = K_2(z_2)R_{1,2}(z_1 + z_2)K_1(z_1)R_{2,1}(z_1 - z_2). \quad (\text{II.C.7})$$

It satisfies the regularity property if $K(0) = \mathbf{1}$ and the unitarity property if $K(z).K(-z) = \mathbf{1}$.

Up to now, we dealt only with the integrability of the left boundary local jump operator B . We can study in a similar way the right boundary local jump operator \bar{B} . This motivates the following definitions.

Definition C.7. A matrix $\overline{K}(z)$ of size $(N+1) \times (N+1)$, i.e acting on \mathbb{C}^{N+1} , satisfies the reversed reflection equation if

$$R_{1,2} \left(\frac{z_1}{z_2} \right)^{-1} \overline{K}_1(z_1) R_{2,1}(z_1 z_2)^{-1} \overline{K}_2(z_2) = \overline{K}_2(z_2) R_{1,2}(z_1 z_2)^{-1} \overline{K}_1(z_1) R_{2,1} \left(\frac{z_1}{z_2} \right)^{-1}, \quad (\text{II.C.8})$$

which can be rewritten without inverse on the R -matrix using the unitarity property $R_{2,1}(z)^{-1} = R_{1,2}(1/z)$.

Definition C.8. A right boundary local jump operator \overline{B} is said to be integrable if there exists a K -matrix $\overline{K}(z)$ satisfying the reversed reflection equation (II.C.8) such that

$$\overline{B} = -\frac{\theta}{2} \overline{K}'(1), \quad (\text{II.C.9})$$

where the constant θ is defined in (II.B.5).

The unitarity, regularity and Markovian properties are defined for $\overline{K}(z)$ in the exact same way as for $K(z)$.

We now provides examples of such K -matrices, more particularly those related to the stochastic models already introduced in this manuscript.

Example C.9. The K -matrices related to the ASEP are multiplicative in the spectral parameter. The matrix $K(z)$ is given by

$$K(z) = \begin{pmatrix} \frac{z(z(\gamma-\alpha)+\alpha-\gamma+q-p)}{\gamma z^2+z(\alpha-\gamma+q-p)-\alpha} & \frac{(z^2-1)\gamma}{\gamma z^2+z(\alpha-\gamma+q-p)-\alpha} \\ \frac{(z^2-1)\alpha}{\gamma z^2+z(\alpha-\gamma+q-p)-\alpha} & \frac{\gamma-\alpha+z(\alpha-\gamma+q-p)}{\gamma z^2+z(\alpha-\gamma+q-p)-\alpha} \end{pmatrix}. \quad (\text{II.C.10})$$

It satisfies the reflection equation (II.C.1) and the unitarity, regularity and Markovian properties. It is related to the left boundary local jump operator B defined in (II.A.31) through the relation

$$\frac{q-p}{2} K'(1) = B, \quad (\text{II.C.11})$$

which corresponds to a value $\theta = q - p$. The right matrix $\overline{K}(z)$ is given by

$$\overline{K}(z) = \begin{pmatrix} \frac{z(z(\beta-\delta)+\delta-\beta+p-q)}{\beta z^2+z(\delta-\beta+p-q)-\delta} & \frac{(z^2-1)\beta}{\beta z^2+z(\delta-\beta+p-q)-\delta} \\ \frac{(z^2-1)\delta}{\beta z^2+z(\delta-\beta+p-q)-\delta} & \frac{\beta-\delta+z(\delta-\beta+p-q)}{\beta z^2+z(\delta-\beta+p-q)-\delta} \end{pmatrix}. \quad (\text{II.C.12})$$

It satisfies the reversed reflection equation (II.C.8) and the unitarity, regularity and Markovian properties. It is related to the right boundary local jump operator \overline{B} defined in (II.A.31) through the relation

$$-\frac{q-p}{2} \overline{K}'(1) = \overline{B}. \quad (\text{II.C.13})$$

Example C.10. For the TASEP, it will appear convenient to introduce the parameters a and b related to the injection/extraction rates α and β through the relations

$$a = \frac{1-\alpha}{\alpha}, \quad b = \frac{1-\beta}{\beta}. \quad (\text{II.C.14})$$

The K -matrices can be then expressed as

$$K(z) = \begin{pmatrix} \frac{z(z+a)}{za+1} & 0 \\ \frac{1-z}{za+1} & 1 \end{pmatrix} \quad (\text{II.C.15})$$

It satisfies the reflection equation (II.C.1) and the unitarity, regularity and Markovian properties. It is connected to the left boundary local jump operator B introduced in (II.A.32) by

$$-\frac{1}{2} K'(1) = B, \quad (\text{II.C.16})$$

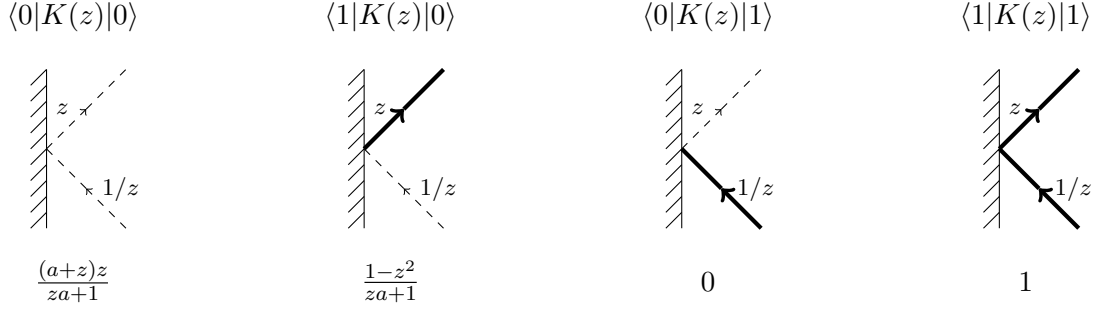


Figure II.13: Graphical representation of the K -matrix of the TASEP.

which corresponds to a value $\theta = -1$. A graphical representation of this K -matrix is given in figure II.13.

The matrix $\bar{K}(z)$ is given by

$$\bar{K}(z) = \begin{pmatrix} 1 & \frac{z^2-1}{z(z+b)} \\ 0 & \frac{zb+1}{z(z+b)} \end{pmatrix} \quad (\text{II.C.17})$$

It satisfies the reversed reflection equation (II.C.8) and the unitarity, regularity and Markovian properties. It is related to the right boundary local jump operator \bar{B} defined in (II.A.32) through the relation

$$\frac{1}{2}\bar{K}'(1) = \bar{B}. \quad (\text{II.C.18})$$

These K -matrices can be obtained from the ones of the ASEP by setting $p = 1$, $q = 0$, $\gamma = 0$ and $\delta = 0$.

Example C.11. In the case of the SSEP, the K -matrices are additive in the spectral parameter. The left boundary matrix $K(z)$ reads

$$K(z) = \begin{pmatrix} \frac{z(\gamma-\alpha)+1}{z(\alpha+\gamma)+1} & \frac{2z\gamma}{z(\alpha+\gamma)+1} \\ \frac{2z\alpha}{z(\alpha+\gamma)+1} & \frac{z(\alpha-\gamma)+1}{z(\alpha+\gamma)+1} \end{pmatrix}. \quad (\text{II.C.19})$$

It satisfies the reflection equation (II.C.7) and the unitarity, regularity and Markovian properties. It is related to the left boundary local jump operator B defined in (II.A.31) through the relation

$$\frac{1}{2}K'(0) = B, \quad (\text{II.C.20})$$

which corresponds to the value $\theta = 1$. The right boundary matrix $\bar{K}(z)$ reads

$$\bar{K}(z) = \begin{pmatrix} \frac{z(\beta-\delta)-1}{z(\beta+\delta)-1} & \frac{2z\beta}{z(\beta+\delta)-1} \\ \frac{2z\delta}{z(\beta+\delta)-1} & \frac{z(\delta-\beta)-1}{z(\beta+\delta)-1} \end{pmatrix} \quad (\text{II.C.21})$$

It satisfies the reversed reflection equation and the unitarity, regularity and Markovian properties. It is related to the right boundary local jump operator \bar{B} defined in (II.A.31) through the relation

$$-\frac{1}{2}\bar{K}'(0) = \bar{B}. \quad (\text{II.C.22})$$

The K -matrices of the SSEP are obtained from the ones of the ASEP by the scaling limit

$$K^{\text{SSEP}}(z) = \lim_{h \rightarrow 0} K^{\text{ASEP}}(e^{hz})|_{q=e^h, p=1}, \quad (\text{II.C.23})$$

and similarly for $\bar{K}(z)$. This scaling transforms a multiplicative dependence in the spectral parameter into an additive one, as expected.

All the previous examples were related to single species models. We provide here an example of R-matrix related to a multi-species model.

Example C.12. A K -matrix for the 2-species TASEP is given by

$$K(z) = \begin{pmatrix} z^2 & 0 & 0 \\ -\frac{az(z^2-1)}{za+1} & \frac{z(a+z)}{za+1} & 0 \\ -\frac{z^2-1}{za+1} & -\frac{z^2-1}{za+1} & 1 \end{pmatrix} \quad (\text{II.C.24})$$

It satisfies the reflection equation (II.C.1) and the unitarity, regularity and Markovian properties. It is connected to the left boundary local jump operator B introduced in (II.A.33) by

$$-\frac{1}{2}K'(1) = B, \quad (\text{II.C.25})$$

which corresponds to a value $\theta = -1$.

b) Transfer matrix

We defined previously the integrability of the boundary local jump operators B and \bar{B} as being the derivative of some K -matrices. This definition will make sense in this subsection. We will indeed see that in this case it is possible to construct a transfer matrix, which generates a set of commuting operators including the Markov matrix. The K -matrices, together with the R -matrix, are the key building blocks of this transfer matrix as explained in the following definition.

Definition C.13. The inhomogeneous transfer matrix for a system with open boundaries is an operator acting on the whole lattice $(\mathbb{C}^{N+1})^{\otimes L}$ and is given by

$$t(z|\mathbf{z}) = \text{tr}_0 \left(\tilde{K}_0(z) R_{0,L} \left(\frac{z}{z_L} \right) \dots R_{0,1} \left(\frac{z}{z_1} \right) K_0(z) R_{1,0}(zz_1) \dots R_{L,0}(zz_L) \right), \quad (\text{II.C.26})$$

where¹³

$$\tilde{K}_1(z) = \text{tr}_0 \left(\bar{K}_0 \left(\frac{1}{z} \right) \left((R_{0,1}(z^2)^{t_1})^{-1} \right)^{t_1} P_{0,1} \right), \quad (\text{II.C.27})$$

or equivalently

$$\bar{K}_1(z) = \text{tr}_0 \left(\tilde{K}_0 \left(\frac{1}{z} \right) R_{01} \left(\frac{1}{z^2} \right) P_{01} \right). \quad (\text{II.C.28})$$

Remark C.14. The matrix $\tilde{K}(z)$ satisfies the dual reflection equation

$$\tilde{K}_2(z_2) (R_{21}^{t_1}(z_1 z_2)^{-1})^{t_1} \tilde{K}_1(z_1) R_{21} \left(\frac{z_2}{z_1} \right) = R_{12} \left(\frac{z_2}{z_1} \right) \tilde{K}_1(z_1) (R_{12}^{t_2}(z_1 z_2)^{-1})^{t_2} \tilde{K}_2(z_2). \quad (\text{II.C.29})$$

A pictorial representation of the transfer matrix with open boundaries is given in figure II.15.

The main feature of the inhomogeneous transfer matrix is that it generates a set of commuting operators. This is expressed in the following proposition

Proposition C.15. The inhomogeneous transfer matrix satisfies the commutation relation

$$[t(z|\mathbf{z}), t(z'|\mathbf{z})] = 0. \quad (\text{II.C.30})$$

¹³We recall that \cdot^{t_i} denotes the usual matrix transposition in the i -th tensor space component

Proof. Let us define

$$\mathcal{K}_0(z) = R_{0,L} \left(\frac{z}{z_L} \right) \dots R_{0,1} \left(\frac{z}{z_1} \right) K_0(z) R_{1,0}(zz_1) \dots R_{L,0}(zz_L). \quad (\text{II.C.31})$$

It is straightforward to check that this dressed K -matrix satisfies the reflection equation

$$R_{0,0'} \left(\frac{z}{z'} \right) \mathcal{K}_0(z) R_{0',0}(zz') \mathcal{K}_{0'}(z') = \mathcal{K}_{0'}(z') R_{0,0'}(zz') \mathcal{K}_0(z) R_{0',0} \left(\frac{z}{z'} \right). \quad (\text{II.C.32})$$

We then follow the lines of [126] to compute

$$\begin{aligned} t(z|\mathbf{z})t(z'|\mathbf{z}) &= \text{tr}_0 \left(\tilde{K}_0(z) \mathcal{K}_0(z) \right) \text{tr}_{0'} \left(\tilde{K}_{0'}(z') \mathcal{K}_{0'}(z') \right) \\ &= \text{tr}_0 \left(\tilde{K}_0(z)^{t_0} \mathcal{K}_0(z)^{t_0} \right) \text{tr}_{0'} \left(\tilde{K}_{0'}(z') \mathcal{K}_{0'}(z') \right) \\ &= \text{tr}_{0,0'} \left(\tilde{K}_0(z)^{t_0} \tilde{K}_{0'}(z') \mathcal{K}_0(z)^{t_0} \mathcal{K}_{0'}(z') \right) \\ &= \text{tr}_{0,0'} \left(\tilde{K}_0(z)^{t_0} \tilde{K}_{0'}(z') \times (R_{0',0}(zz')^{t_0})^{-1} (R_{0',0}(zz')^{t_0}) \times \mathcal{K}_0(z)^{t_0} \mathcal{K}_{0'}(z') \right) \\ &= \text{tr}_{0,0'} \left(\left(\tilde{K}_{0'}(z') \left((R_{0',0}(zz')^{t_0})^{-1} \right)^{t_0} \tilde{K}_0(z) \right)^{t_0} (\mathcal{K}_0(z) R_{0',0}(zz') \mathcal{K}_{0'}(z'))^{t_0} \right) \\ &= \text{tr}_{0,0'} \left(\left(\tilde{K}_{0'}(z') \left((R_{0',0}(zz')^{t_0})^{-1} \right)^{t_0} \tilde{K}_0(z) R_{0',0} \left(\frac{z'}{z} \right) \right) \right. \\ &\quad \left. \times \left(R_{0,0'} \left(\frac{z}{z'} \right) \mathcal{K}_0(z) R_{0',0}(zz') \mathcal{K}_{0'}(z') \right) \right), \end{aligned}$$

where the last equality is obtained by applying the transposition \cdot^{t_0} in auxiliary space 0 and then by inserting the unitarity relation

$$R_{0',0} \left(\frac{z'}{z} \right) R_{0,0'} \left(\frac{z}{z'} \right) = 1. \quad (\text{II.C.33})$$

We observe that we are now in position to use the reflection equation (II.C.32) and respectively the dual reflection equation (II.C.29) to exchange the positions of the matrices $\mathcal{K}_0(z)$ and $\mathcal{K}_{0'}(z')$ and respectively of the matrices $\tilde{K}_0(z)$ and $\tilde{K}_{0'}(z')$. Then we repeat the whole sequence of transformations in reverse order to finally obtain $t(z'|\mathbf{z})t(z|\mathbf{z})$. ■

The previous proposition tells us that, the set of commuting operators can be obtained by expanding the transfer matrix with respect to the spectral parameter.

Remark C.16. *In the case where the R -matrix and the K -matrices are additive in the spectral parameter, the inhomogeneous transfer matrix is defined by*

$$t(z|\mathbf{z}) = \text{tr}_0 \left(\tilde{K}_0(z) R_{0,L}(z - z_L) \dots R_{0,1}(z - z_1) K_0(z) R_{1,0}(z + z_1) \dots R_{L,0}(z + z_L) \right), \quad (\text{II.C.34})$$

with

$$\tilde{K}_1(z) = \text{tr}_0 \left(\bar{K}_0(-z) \left((R_{0,1}(2z)^{t_1})^{-1} \right)^{t_1} P_{0,1} \right), \quad (\text{II.C.35})$$

or equivalently

$$\bar{K}_1(z) = \text{tr}_0 \left(\tilde{K}_0(-z) R_{01}(-2z) P_{01} \right). \quad (\text{II.C.36})$$

We are now equipped to state the connection between the transfer matrix and the Markov matrix of the model.

Proposition C.17. *The Markov matrix is related to the transfer matrix in the simple following way*

$$\frac{\theta}{2} t'(1) = B_1 + \sum_{k=1}^{L-1} m_{k,k+1} + \bar{B}_L = M, \quad (\text{II.C.37})$$

where the homogeneous transfer matrix is defined as $t(z) = t(z|1, \dots, 1)$.

Proof. Using the regularity property of the matrix R and K , we have

$$\begin{aligned}
t'(1) &= \text{tr}_0(\tilde{K}_0(1)P_{0L} \dots P_{01} \cdot K'_0(1) \cdot P_{10} \dots P_{L0}) \\
&+ \sum_{k=1}^{L-1} \left(\text{tr}_0(\tilde{K}_0(1)P_{0L} \dots P_{0,k+1}R'_{0k}(1)P_{0,k-1} \dots P_{01} \cdot 1 \cdot P_{10} \dots P_{L0}) \right. \\
&\quad \left. + \text{tr}_0(\tilde{K}_0(1)P_{0L} \dots P_{01} \cdot 1 \cdot P_{10} \dots P_{k-1,0}R'_{k0}(1)P_{k+1,0} \dots P_{L0}) \right) \\
&+ \text{tr}_0(\tilde{K}_0(1)R'_{0L}(1)P_{0,L-1} \dots P_{01} \cdot 1 \cdot P_{10} \dots P_{L0}) \\
&+ \text{tr}_0(\tilde{K}_0(1)P_{0L} \dots P_{01} \cdot 1 \cdot P_{10} \dots P_{L-1,0}R'_{L0}(1)) \\
&+ \text{tr}_0(\tilde{K}'_0(1)P_{0L} \dots P_{01} \cdot 1 \cdot P_{10} \dots P_{L0}) \\
&= \text{tr}_0(\tilde{K}_0(1))K'_1(1) + 2 \sum_{k=1}^{L-1} \text{tr}_0(\tilde{K}_0(1))\check{R}'_{k,k+1}(1) \\
&\quad - \frac{d}{dz} \text{tr}_0 \left(\tilde{K}_0 \left(\frac{1}{z} \right) R_{0L} \left(\frac{1}{z^2} \right) P_{0L} \right) \Big|_{z=1} \\
&= K'_1(1) + 2 \sum_{k=1}^{L-1} \check{R}'_{k,k+1}(1) - \overline{K}'_L(1).
\end{aligned}$$

The last equality is obtained thanks to the regularity property of \overline{K}

$$\text{tr}_0(\tilde{K}_0(1)) = \overline{K}(1) = 1. \quad (\text{II.C.38})$$

The relations (II.C.3), (II.C.9) and (II.B.5) allow us to conclude the proof. \blacksquare

Example C.18. For the single species TASEP, the matrix $\tilde{K}(z)$ is given by

$$\tilde{K}(z) = \begin{pmatrix} \frac{1}{zb+1} & \frac{1}{zb+1} \\ 0 & \frac{zb}{zb+1} \end{pmatrix} \quad (\text{II.C.39})$$

The graphical representation for the matrix \tilde{K} is given in fig. II.14.

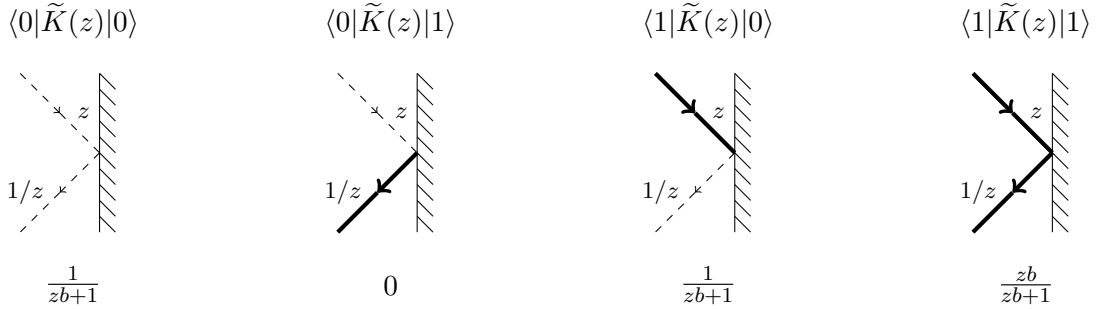


Figure II.14: Graphical representation of the \tilde{K} -matrix of the TASEP.

Transfer matrix as discrete time Markov matrix We showed in the previous paragraphs how the transfer matrix can be used to define (through its derivative) continuous time Markov matrix. We are now going to see on the particular case of the single species open TASEP that the inhomogeneous transfer matrix can be used itself to define a discrete time Markov matrix.

The building blocks of the transfer matrix for the open case are the R matrix defined in (II.B.14) and the boundary matrices K and \tilde{K} defined in (II.C.15) and (II.C.39). They enter the construction of the inhomogeneous open transfer matrix $t(z|\mathbf{z})$ defined in (II.C.26).

We use the operator $t(z|\mathbf{z})$ to define the following discrete time Markov process

$$|P_{t+1}\rangle = t(z|\mathbf{z})|P_t\rangle. \quad (\text{II.C.40})$$

The parameters must satisfy the following constraints

$$0 \leq zz_i \leq 1, \quad 0 \leq \frac{z}{z_i} \leq 1 \quad \text{and} \quad az, bz \geq 0 \quad (\text{II.C.41})$$

to ensure that the entries of $t(z|\mathbf{z})$ are probabilities. We can also show that the entries on each column of $t(z|\mathbf{z})$ sum to one, which guarantees the conservation of the probability $|P_t\rangle$.

We now draw diagrams to represent the action of the transfer matrix. The general picture is displayed in fig. II.15.

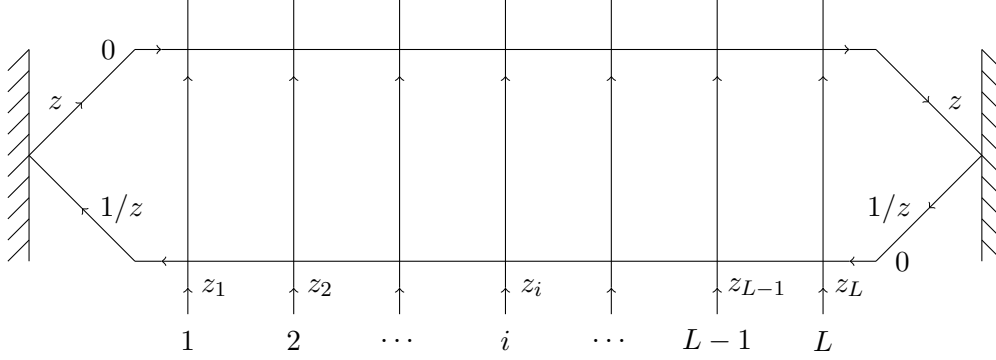


Figure II.15: Graphical representation of the transfer matrix of the open TASEP.

As an example we can compute graphically for $L = 1$ the transition rate $\langle 0|t(z|\mathbf{z})|1\rangle$ between the initial configuration (1) and the final configuration (0) (see fig. II.16). The sum of both contributions drawn in fig. II.16 gives

$$\langle 0|t(z|\mathbf{z})|1\rangle = \frac{z(a+z)(1-zz_1)}{(az+1)(bz+1)} + \frac{zz_1(1-\frac{z}{z_1})}{bz+1} = (1-z^2) \frac{z(a+z_1)}{(az+1)(bz+1)}. \quad (\text{II.C.42})$$

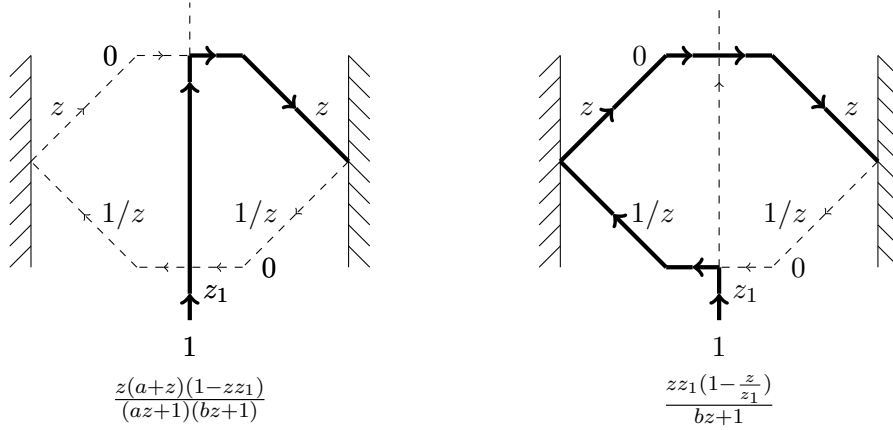


Figure II.16: Graphical computation of the transition rate $\langle 0|t(z|\mathbf{z})|1\rangle$ for $L = 1$. The two different contributions are represented with their respective weights.

The transfer matrix $t(z|\mathbf{z})$ defines a discrete time Markov process on the finite size lattice with open boundaries. The corresponding stochastic dynamics can be described explicitly using a sequential update: starting from a given configuration at time t , the configuration at time $t + 1$ is obtained by the following stochastic rules

- *Initialisation:*

- The left boundary is replaced by an additional site (the site 0 with inhomogeneity parameter 1) occupied by a particle with probability $\frac{1}{az+1}$ and unoccupied with probability $\frac{az}{az+1}$.

- The right boundary is replaced by an additional site (the site $L + 1$ with inhomogeneity parameter 1) occupied by a particle with probability $\frac{bz}{bz+1}$ and unoccupied with probability $\frac{1}{bz+1}$.
- *Particle update:* starting from right to left (from site L to site 0), a particle at site i can jump to the right on the site $i + 1$ (provided that the site is empty) with probability $1 - zz_i$ and stay at the same place with probability zz_i .
- *Hole update:* once arrived at site 0, we go the other way starting from left to right (from site 1 to site $L + 1$): a hole at site i can jump to the left on the site $i - 1$ (provided that the site is occupied) with probability $1 - \frac{z}{z_{i-1}}$ and stay at the same place with probability $\frac{z}{z_{i-1}}$.
- *Summation:* Then we have to drop the additional sites 0 and $L + 1$ and to sum the weights corresponding to the same final configuration.

An example of such sequential update is given in fig. II.17 for $L = 1$. From this figure we can compute the transition rates

$$\begin{aligned} \langle 0|t(z|\mathbf{z})|1\rangle &= \frac{az}{(az+1)(bz+1)} \left[zz_1 \left(1 - \frac{z}{z_1} \right) + 1 - zz_1 \right] \\ &\quad + \frac{1}{(az+1)(bz+1)} \left[(1 - zz_1)z^2 + zz_1 \left(1 - \frac{z}{z_1} \right) \right] \end{aligned} \quad (\text{II.C.43})$$

$$= (1 - z^2) \frac{z(a + z_1)}{(az+1)(bz+1)}, \quad (\text{II.C.44})$$

$$\langle 1|t(z|\mathbf{z})|1\rangle = \frac{z(z+b)}{bz+1} + \frac{(1-z^2)(1-zz_1)}{(az+1)(bz+1)}. \quad (\text{II.C.45})$$

The equation (II.C.44) is, of course, identical to the expression (II.C.42) derived using the graphical representation in fig. II.16.

2 How to find K-matrices?

a) Direct resolution of the reflection equation

Written in components, the reflection equation (II.C.1) gives equations that are quadratic in the entries of the K -matrix. In practice it is thus much simpler to solve than the Yang-Baxter equation (which gives cubic equations in the entries of the R -matrix). However there is so far no general method to systematically solve this reflection equation and it has to be studied case by case. Several classification have been provided for particular models, see for instance [127, 128], and the reader can find in these references a bench of methods to help solving this reflection equation. We present below example of solutions of the reflection equation for the DiSSEP and for the multi-species SSEP. These K -matrices were derived with a technique that is roughly summarized as follows: we performed elementary algebraic manipulations on the quadratic equations (given by (II.C.1)) to obtain an equality between something depending only on the spectral parameter z_1 on the left hand side and something depending only on the spectral parameter z_2 on the right hand side (which proves that the two terms are constant).

Example C.19. *The K -matrices associated to the DiSSEP are multiplicative in the spectral parameter. The left matrix reads*

$$K(z) = \begin{pmatrix} \frac{(z^2+1)((z^2-1)(\gamma-\alpha)+4z\lambda)}{2z((z^2-1)(\alpha+\gamma)+2\lambda(z^2+1))} & \frac{(z^2-1)((z^2+1)(\gamma-\alpha)+2z(\alpha+\gamma))}{2z((z^2-1)(\alpha+\gamma)+2\lambda(z^2+1))} \\ \frac{(z^2-1)((z^2+1)(\alpha-\gamma)+2z(\alpha+\gamma))}{2z((z^2-1)(\alpha+\gamma)+2\lambda(z^2+1))} & \frac{(z^2+1)((z^2-1)(\alpha-\gamma)+4z\lambda)}{2z((z^2-1)(\alpha+\gamma)+2\lambda(z^2+1))} \end{pmatrix} \quad (\text{II.C.46})$$

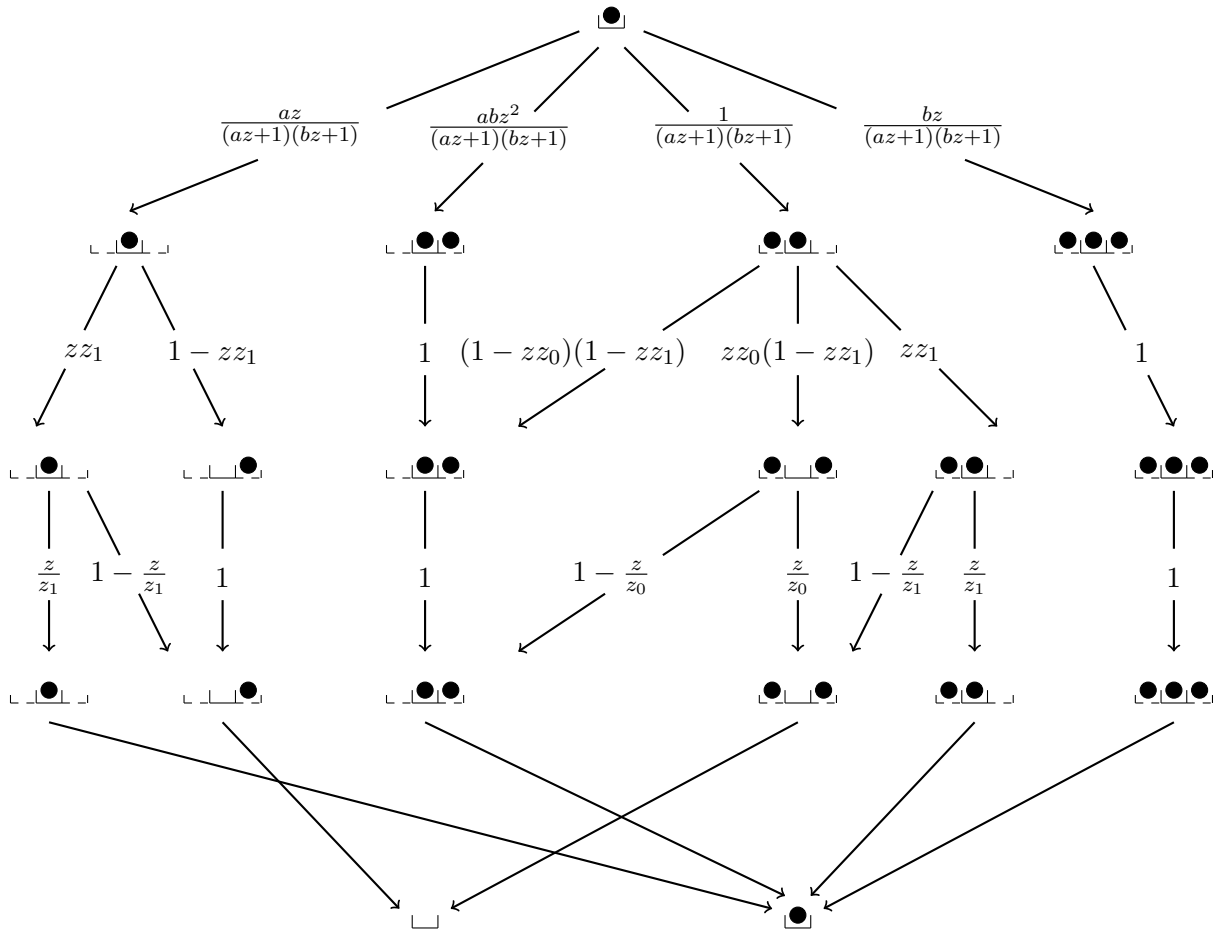


Figure II.17: An example of sequential update corresponding to the Markov matrix $t(z|\mathbf{z})$. The first line is the configuration at time t . The second line represents the possible configurations after adding the two supplementary sites corresponding to the boundaries. The third line corresponds to the intermediate configurations after the updates of the particles. The fourth line represents the possible configurations after the updates of the holes. The label of the arrows provides the rate of the corresponding change of configurations. The last line represents the final configurations at time $t + 1$ after the summation step.

which satisfies the reflection equation, the regularity, unitarity and Markovian properties. It generates the left boundary local jump operator B through the relation

$$\lambda K'(1) = B \quad (\text{II.C.47})$$

which corresponds to a value $\theta = 2\lambda$. The right matrix reads

$$\bar{K}(z) = \begin{pmatrix} \frac{(z^2+1)((z^2-1)(\delta-\beta)+4z\lambda)}{2z((1-z^2)(\beta+\delta)+2\lambda(z^2+1))} & \frac{(z^2-1)((z^2+1)(\delta-\beta)-2z(\beta+\delta))}{2z((1-z^2)(\beta+\delta)+2\lambda(z^2+1))} \\ \frac{(z^2-1)((z^2+1)(\beta-\delta)-2z(\beta+\delta))}{2z((1-z^2)(\beta+\delta)+2\lambda(z^2+1))} & \frac{(z^2+1)((z^2-1)(\beta-\delta)+4z\lambda)}{2z((1-z^2)(\beta+\delta)+2\lambda(z^2+1))} \end{pmatrix} \quad (\text{II.C.48})$$

which satisfies the reversed reflection equation, the regularity, unitarity and Markovian properties. It generates the right boundary local jump operator \bar{B} as follows

$$-\lambda \bar{K}'(1) = \bar{B}. \quad (\text{II.C.49})$$

Example C.20. We are interested in the integrable stochastic boundaries associated to the multi-species SSEP. The multi-species SSEP is a multi-species generalization of the SSEP, whose bulk local jump operator m is given by $m = P - \mathbb{I}$, where P is the permutation matrix acting on $\mathbb{C}^{N+1} \otimes \mathbb{C}^{N+1}$. A more physical description of the dynamics will be given in chapter III. The bulk dynamic is integrable : the R -matrix is given by

$$R(z) = \frac{z + P}{z + 1}. \quad (\text{II.C.50})$$

It is additive in the spectral parameter and satisfies the Yang-Baxter equation (II.B.12), the regularity, unitarity and Markovian properties. The local jump operator m can be recovered through the relation $m = \check{R}'(0)$.

The solutions of the reflection equation (associated with this R -matrix) have been classified in [128]. We present here, without proof, classes of integrable stochastic boundaries B and \bar{B} among this classification. We divide the $N + 1$ species (and holes) into p distinct families F_1, \dots, F_p of non-vanishing cardinalities f_1, \dots, f_p at the left boundary and into q distinct families G_1, \dots, G_q of non-vanishing cardinalities g_1, \dots, g_q at the right boundary. We hence have two different partitions $\{0, \dots, N\} = \bigsqcup_{k=1}^p F_k = \bigsqcup_{k=1}^q G_k$. We define $2(N + 1)$ non negative numbers $\alpha_0, \dots, \alpha_N$ for the left boundary and β_0, \dots, β_N for the right boundary with the constraints

$$\text{for all } 1 \leq k \leq p, \quad \sum_{s \in F_k} \alpha_s = 1, \quad (\text{II.C.51})$$

and

$$\text{for all } 1 \leq k \leq q, \quad \sum_{s \in G_k} \beta_s = 1. \quad (\text{II.C.52})$$

The left boundary conditions are given by

$$B|s'\rangle = -\frac{1}{a}|s'\rangle + \sum_{s \in F_k} \frac{\alpha_s}{a}|s\rangle, \quad 1 \leq s' \leq N. \quad (\text{II.C.53})$$

k in (II.C.53) is such that $s' \in F_k$. Remark that in the particular case where the family of s' contains only one species, i.e. $F_k = \{s'\}$, we get from the constraints that $\alpha_{s'} = 1$ and hence $B|s'\rangle = 0$.

In the same way, the right boundary conditions are given by

$$\bar{B}|s'\rangle = -\frac{1}{b}|s'\rangle + \sum_{s \in G_k} \frac{\beta_s}{b}|s\rangle, \quad 1 \leq s' \leq N, \quad (\text{II.C.54})$$

with k such that $s' \in G_k$. Note that when we have a single family on the left and a single family on the right, i.e. when $p = q = 1$, then the boundary conditions reduce to the one studied in

details in chapter III of this manuscript. To illustrate these boundary conditions, we give some examples in the case $N = 3$ for the left boundary:

$$B = \frac{1}{a} \begin{pmatrix} \alpha_0 - 1 & \alpha_0 & 0 & \alpha_0 \\ \alpha_1 & \alpha_1 - 1 & 0 & \alpha_1 \\ 0 & 0 & 0 & 0 \\ \alpha_3 & \alpha_3 & 0 & \alpha_3 - 1 \end{pmatrix}, \quad \text{with } \alpha_0 + \alpha_1 + \alpha_3 = 1, \quad (\text{II.C.55})$$

$$B = \frac{1}{a} \begin{pmatrix} \alpha_0 - 1 & \alpha_0 & 0 & 0 \\ \alpha_1 & \alpha_1 - 1 & 0 & 0 \\ 0 & 0 & \alpha_2 - 1 & \alpha_2 \\ 0 & 0 & \alpha_3 & \alpha_3 - 1 \end{pmatrix}, \quad \text{with } \alpha_0 + \alpha_1 = 1 \text{ and } \alpha_2 + \alpha_3 = 1, \quad (\text{II.C.56})$$

$$B = \frac{1}{a} \begin{pmatrix} \alpha_0 - 1 & 0 & \alpha_0 & 0 \\ 0 & \alpha_1 - 1 & 0 & \alpha_1 \\ \alpha_2 & 0 & \alpha_2 - 1 & 0 \\ 0 & \alpha_3 & 0 & \alpha_3 - 1 \end{pmatrix}, \quad \text{with } \alpha_0 + \alpha_2 = 1 \text{ and } \alpha_1 + \alpha_3 = 1, \quad (\text{II.C.57})$$

$$B = \frac{1}{a} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \alpha_1 - 1 & \alpha_1 & 0 \\ 0 & \alpha_2 & \alpha_2 - 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \text{with } \alpha_1 + \alpha_2 = 1, \quad (\text{II.C.58})$$

Examples of right boundaries in the case $N = 3$ are obtained by replacing α_i by β_i and a by b in the matrices (II.C.55)-(II.C.58) above.

Coming back to the general multi-species case $N \geq 1$, the K -matrices associated to the boundary local jump operators B and \bar{B} are given by

$$K(z) = \mathbb{I} + \frac{2zaB}{z+a} \quad \text{and} \quad \bar{K}(z) = \mathbb{I} + \frac{2zb\bar{B}}{z-b}. \quad (\text{II.C.59})$$

They satisfy the reflection equation, as well as the regularity, unitarity and Markovian properties. Note the similarity of these expressions with the one of the R -matrix. We have the relations

$$B = \frac{1}{2}K'(0) \quad \text{and} \quad \bar{B} = -\frac{1}{2}\bar{K}'(0). \quad (\text{II.C.60})$$

b) Baxterization

We have seen in the previous section the construction of solutions to the Yang-Baxter equation starting from a local jump operator satisfying specific algebraic relations. This procedure has been extended to the reflection equation [129] through the boundary Hecke algebra [130, 131], that we now introduce.

Boundary Hecke algebra

Definition C.21. For $n \geq 1$, the boundary Hecke algebra $b\mathcal{H}_n(\omega, \omega_0)$ is the unital associative algebra over \mathbb{C} with generators $\sigma_0, \sigma_1, \dots, \sigma_{n-1}$, where $\sigma_1, \dots, \sigma_{n-1}$ satisfy the defining relations (II.B.88), (II.B.89), (II.B.90) and (II.B.91) of the Hecke algebra $\mathcal{H}(\omega)$ and subject to the additional relations

$$\sigma_0 \sigma_1 \sigma_0 \sigma_1 = \sigma_1 \sigma_0 \sigma_1 \sigma_0, \quad (\text{II.C.61})$$

$$\sigma_0 \sigma_i = \sigma_i \sigma_0, \quad i > 1, \quad (\text{II.C.62})$$

$$\sigma_0 \sigma_0^{-1} = \sigma_0^{-1} \sigma_0 = 1, \quad (\text{II.C.63})$$

$$\sigma_0^2 = \omega_0 \sigma_0 + 1, \quad (\text{II.C.64})$$

where ω_0 is a complex number not necessarily equal to ω .

One of the main interest of this algebra, in the context of integrable systems, is the fact that it produces solution to the (spectral parameter dependent) braided reflection equation through the following Baxterisation procedure.

Theorem C.22. *If σ_i satisfy the relations of the boundary Hecke algebra, then*

$$K_0(z) = \frac{(z^2 - 1)\sigma_0 + z(u_0^{-1/2} - u_0^{1/2}) + t_0^{-1/2} - t_0^{1/2}}{z^2 t_0^{-1/2} + z(u_0^{-1/2} - u_0^{1/2}) - t_0^{1/2}}, \quad (\text{II.C.65})$$

where t_0 is such that $\omega_0 = t_0^{-1/2} - t_0^{1/2}$ and u_0 is a free complex parameter, satisfies the braided reflection equation

$$\check{R}_1(z_1/z_2)K_0(z_1)\check{R}_1(z_1z_2)K_0(z_2) = K_0(z_2)\check{R}_1(z_1z_2)K_0(z_1)\check{R}_1(z_1/z_2). \quad (\text{II.C.66})$$

Moreover the following properties hold:

$$- \text{unitarity } K_0(z)K_0(1/z) = 1, \quad (\text{II.C.67})$$

$$- \text{regularity } K_0(1) = 1, \quad (\text{II.C.68})$$

$$- \text{locality } K_0(z)\check{R}_i(z') = \check{R}_i(z')K_0(z) \quad \text{for } i > 1. \quad (\text{II.C.69})$$

Proof. The regularity and locality properties are obvious.

The unitarity and the braided Yang–Baxter equation are established through a direct computation, using the relations (II.C.61), (II.B.91) and (II.C.64). \blacksquare

Example C.23. *We can show that the bulk local jump operator m (II.A.23) and the boundary local jump operator B (II.A.31) of the ASEP provide an explicit representation of the boundary Hecke algebra $b\mathcal{H}_n(\omega, \omega_0)$ with $\omega = \sqrt{\frac{q}{p}} - \sqrt{\frac{p}{q}}$ and $\omega_0 = \sqrt{\frac{\gamma}{\alpha}} - \sqrt{\frac{\alpha}{\gamma}}$ in the tensor space $\text{End}(\mathbb{C}^2)^{\otimes n}$*

$$b\mathcal{H}_n(\omega, \omega_0) \rightarrow \text{End}(\mathbb{C}^2)^{\otimes n}$$

$$\sigma_i \mapsto \mathbb{I}^{\otimes i-1} \otimes S \otimes \mathbb{I}^{\otimes n-i-1} \quad (\text{II.C.70})$$

$$\sigma_0 \mapsto W \otimes \mathbb{I}^{\otimes n-1} \quad (\text{II.C.71})$$

where S is a 4×4 matrix (acting on $\mathbb{C}^2 \otimes \mathbb{C}^2$) given by

$$S = \frac{1}{\sqrt{pq}}(m + q), \quad (\text{II.C.72})$$

and is W a 2×2 matrix (acting on \mathbb{C}^2) given by

$$W = \frac{1}{\sqrt{\alpha\gamma}}(B + \gamma) \quad (\text{II.C.73})$$

Then the Baxterised K -matrix

$$K(z) = \frac{(z^2 - 1)W + z(u_0^{-1/2} - u_0^{1/2}) + t_0^{-1/2} - t_0^{1/2}}{z^2 t_0^{-1/2} + z(u_0^{-1/2} - u_0^{1/2}) - t_0^{1/2}} \quad (\text{II.C.74})$$

corresponding to (II.C.65), with $t_0^{1/2} = \sqrt{\frac{\alpha}{\gamma}}$ and u_0 such that $u_0^{1/2} - u_0^{-1/2} = \frac{p-q+\gamma-\alpha}{\sqrt{\alpha\gamma}}$, coincides with the expression of the K -matrix of the ASEP given in (II.C.10).

Remark C.24. *The Baxterization procedure presented in theorem C.22 can be extended to a more general boundary Hecke algebra, called cyclotomic algebra, where the relation (II.C.64) is generalized to*

$$\sum_{k=0}^r a_k (\sigma_0)^k = 0 \quad (\text{II.C.75})$$

for some fixed $r = 2, 3, \dots$ and a_0, \dots, a_r free parameters. For an introduction to cyclotomic algebras, see e.g. [132]. Then, a K -matrix can be constructed as a polynomial in σ_0 [133]. When $r = 2$, the cyclotomic Hecke algebra is just the boundary Hecke algebra.

Generalization of the boundary algebra We present in this paragraph a generalization of the cyclotomic Hecke algebra, introduced in [134], where the relation related to the minimal polynomial is not required. We present also the Baxterization of this algebra given in [134].

Definition C.25. We consider a generalization of the boundary Hecke algebra, called $\tilde{b}\mathcal{H}_n(\omega)$, which is a unital associative algebra over \mathbb{C} with generators $\sigma_0, \sigma_1, \dots, \sigma_{n-1}$, where $\sigma_1, \dots, \sigma_{n-1}$ satisfy the defining relations (II.B.88), (II.B.89), (II.B.90) and (II.B.91) of the Hecke algebra $\mathcal{H}(\omega)$ and subject to the additional relations

$$\sigma_0 \sigma_1 \sigma_0 \sigma_1 = \sigma_1 \sigma_0 \sigma_1 \sigma_0, \quad (\text{II.C.76})$$

$$\sigma_0 \sigma_i = \sigma_i \sigma_0, \quad i > 1, \quad (\text{II.C.77})$$

$$\sigma_0 \sigma_0^{-1} = \sigma_0^{-1} \sigma_0 = 1. \quad (\text{II.C.78})$$

The previous algebra is the boundary Hecke algebra where the relation (II.C.64) has been taken out. More precisely, the boundary Hecke algebra or the cyclotomic Hecke algebras are quotients of this algebra obtained by imposing a polynomial relation (II.C.75). We present below a Baxterisation procedure of $\tilde{b}\mathcal{H}_n(\omega)$.

Theorem C.26. If σ_i satisfy the relations of $\tilde{b}\mathcal{H}_n(\omega)$, then

$$K_0(z) = (1 - z\sigma_0) \left(1 - \frac{1}{z}\sigma_0\right)^{-1}, \quad (\text{II.C.79})$$

satisfies the braided reflection equation

$$\check{R}_1(z_1/z_2)K_0(z_1)\check{R}_1(z_1z_2)K_0(z_2) = K_0(z_2)\check{R}_1(z_1z_2)K_0(z_1)\check{R}_1(z_1/z_2). \quad (\text{II.C.80})$$

Moreover the following properties hold:

$$\text{– unitarity } K_0(z)K_0(1/z) = 1, \quad (\text{II.C.81})$$

$$\text{– regularity } K_0(1) = 1, \quad (\text{II.C.82})$$

$$\text{– locality } K_0(z)\check{R}_i(z') = \check{R}_i(z')K_0(z) \quad \text{for } i > 1. \quad (\text{II.C.83})$$

Proof. The unitarity, regularity and locality properties are obvious.

The braided Yang–Baxter equation will be established below with theorem C.27 and proposition C.29. \blacksquare

We present now another generalization of the boundary Hecke algebra, introduced in [V4], which will be very useful to deal with the multi-species ASEP.

Theorem C.27. Let σ_i ($i = 1, \dots, L - 1$) be the generators of the Hecke algebra satisfying (II.B.88), (II.B.91) and $\check{R}_i(x)$ the associated braided R -matrices (II.B.92). Let us also define

$$K_0(z) = (1 - (z - 1)\sigma_0) \left(1 - \left(\frac{1}{z} - 1\right)\sigma_0\right)^{-1} \quad (\text{II.C.84})$$

with σ_0 a supplementary generator. The inverse in (II.C.84) is understood as the formal series

$$\left(1 - \left(\frac{1}{z} - 1\right)\sigma_0\right)^{-1} = z \left(1 - (1 - z)(\sigma_0 + 1)\right)^{-1} = (y + 1) \sum_{n=0}^{\infty} (-y)^n (\sigma_0 + 1)^n, \quad (\text{II.C.85})$$

where $y = z - 1$.

Then $K_0(x)$ is a solution of the braided reflection equation

$$\check{R}_1(z_1/z_2)K_0(z_1)\check{R}_1(z_1z_2)K_0(z_2) = K_0(z_2)\check{R}_1(z_1z_2)K_0(z_1)\check{R}_1(z_1/z_2) \quad (\text{II.C.86})$$

if and only if the supplementary generator σ_0 satisfies

$$\sigma_1 \sigma_0 \sigma_1 \sigma_0 - \sigma_0 \sigma_1 \sigma_0 \sigma_1 = \omega (\sigma_0^2 \sigma_1 \sigma_0 - \sigma_0 \sigma_1 \sigma_0^2). \quad (\text{II.C.87})$$

Moreover the operator $K_0(z)$ is unitary:

$$K_0(z)K_0(1/z) = 1, \quad (\text{II.C.88})$$

and satisfies the regularity property

$$K_0(1) = 1. \quad (\text{II.C.89})$$

We denote by $\bar{b}\mathcal{H}_n(\omega)$ the algebra generated by $\sigma_0, \sigma_1, \dots, \sigma_{L-1}$

Proof. We multiply both sides of the braided reflection equation (II.C.86) on the left and on the right by

$$\frac{z_2}{z_1} \left(1 - \left(\frac{1}{z_2} - 1 \right) \sigma_0 \right) = \frac{1}{z_1} (1 + (z_2 - 1)(\sigma_0 + 1)) \quad (\text{II.C.90})$$

and use (II.B.92), (II.C.84) to get the following equivalent relation

$$\begin{aligned} & (1 + y_2(\sigma_0 + 1)) ((z_1 - z_2)\sigma_1 + \omega z_2) \frac{1}{z_1} \check{K}(z_1) ((z_1 z_2 - 1)\sigma_1 + \omega) (1 - y_2\sigma_0) \\ &= (1 - y_2\sigma_0) ((z_1 z_2 - 1)\sigma_1 + \omega) \frac{1}{z_1} \check{K}(z_1) ((z_1 - z_2)\sigma_1 + \omega z_2) (1 + y_2(\sigma_0 + 1)) \end{aligned} \quad (\text{II.C.91})$$

where $y_i = z_i - 1$. Then, we use the expansion (II.C.85) of $\frac{1}{z_1} \check{K}(z_1)$ in terms of y_1 . The coefficient of $y_1 y_2^3$ in (II.C.91) provides relation (II.C.87), which proves that (II.C.86) implies (II.C.87).

To prove the reverse implication, we use the following lemma:

Lemma C.28. *Relation (II.C.87) implies, for $k = 0, 1, 2, \dots$,*

$$\sigma_1 \sigma_0 \sigma_1 \sigma_0^k - \sigma_0^k \sigma_1 \sigma_0 \sigma_1 = \omega (\sigma_0^{k+1} \sigma_1 \sigma_0 - \sigma_0 \sigma_1 \sigma_0^{k+1}), \quad (\text{II.C.92})$$

$$\begin{aligned} \sigma_1 \sigma_0^k \sigma_1 \sigma_0 - \sigma_0 \sigma_1 \sigma_0^k \sigma_1 &= \omega (\sigma_0^{k+1} \sigma_1 \sigma_0 - \sigma_0 \sigma_1 \sigma_0^{k+1}) \\ &+ \sigma_0^k \sigma_1 \sigma_0 - \sigma_0 \sigma_1 \sigma_0^k, \end{aligned} \quad (\text{II.C.93})$$

$$\begin{aligned} \sigma_1 (\sigma_0 + 1)^k \sigma_1 \sigma_0 - \sigma_0 \sigma_1 (\sigma_0 + 1)^k \sigma_1 &= \omega ((\sigma_0 + 1)^{k+1} \sigma_1 \sigma_0 \\ &- \sigma_0 \sigma_1 (\sigma_0 + 1)^{k+1}), \end{aligned} \quad (\text{II.C.94})$$

$$\begin{aligned} \sigma_1 \sigma_0 (\sigma_0 + 1)^k \sigma_1 \sigma_0 - \sigma_0 \sigma_1 \sigma_0 (\sigma_0 + 1)^k \sigma_1 &= \omega (\sigma_0 (\sigma_0 + 1)^{k+1} \sigma_1 \sigma_0 \\ &- \sigma_0 \sigma_1 \sigma_0 (\sigma_0 + 1)^{k+1}). \end{aligned} \quad (\text{II.C.95})$$

The first relation of the lemma (II.C.92) is proven by recursion using (II.C.87). Relation (II.C.93) is proven also by recursion with (II.C.92), (II.B.88) and (II.B.91). The third and the fourth are proven by expanding $(\sigma_0 + 1)^k$ and using (II.C.93).

The lemma allows us to prove that

$$\sigma_1 K(z) \sigma_1 \sigma_0 - \sigma_0 \sigma_1 K(z) \sigma_1 = \omega ((\sigma_0 + 1)K(z) \sigma_1 \sigma_0 - \sigma_0 \sigma_1 (\sigma_0 + 1)K(z)). \quad (\text{II.C.96})$$

Finally, by expanding (II.C.91) and by using relation (II.C.96), we prove that equation (II.C.87) implies (II.C.86) which concludes the proof of the theorem. \blacksquare

The connection between the Baxterisations presented in theorems C.26 and C.27 is detailed in the following proposition.

Proposition C.29. *Assume that $\sigma_0 \in \bar{b}\mathcal{H}_n(\omega)$ is such that $\sigma_0 + 1$ is invertible. Then the following map is an algebra morphism*

$$\begin{aligned} \bar{b}\mathcal{H}_n(\omega) &\rightarrow \tilde{b}\mathcal{H}_n(\omega) \\ \sigma_i &\mapsto \sigma_i, \quad 1 \leq i \leq n-1 \end{aligned} \quad (\text{II.C.97})$$

$$\sigma_0 \mapsto \sigma_0(1 + \sigma_0)^{-1}. \quad (\text{II.C.98})$$

Moreover this map transforms the Baxterised K -matrix (II.C.84) into (II.C.79), up to a normalization factor.

Proof. This can be shown by using relation (II.C.87) for σ_0 and lemma C.28. \blacksquare

We now present an application of this algebraic machinery to out-of-equilibrium statistical physics. The algebra $\bar{b}\mathcal{H}_n(\omega)$ is indeed at the root of integrable boundary matrices for the multi-species ASEP. This is detailed in the following paragraph.

Integrable boundary conditions for the multi-species ASEP We wish to give explicit solutions for integrable Markovian boundary matrices B for the multi-species ASEP. These solutions are obtained from K -matrices obeying the braided reflection equation (II.C.86) (with the R -matrix associated to the N -species ASEP (II.B.102) obtained from the Baxterisation (II.B.92)) through the relation

$$B = \frac{q-p}{2}K'(1). \quad (\text{II.C.99})$$

We first present the integrable Markovian boundary conditions B . We will then argue that they belong (up to a shift and normalization) to a $\bar{b}\mathcal{H}_n(\omega)$ algebra. This will provide through the Baxterisation procedure an explicit expression of the associated K -matrices.

The integrable boundary conditions depend on two free real positive parameters (rates) α and γ , and four positive integers s_1 , s_2 , f_1 and f_2 , that label two special slow (s) and two special fast (f) species, with the conditions

$$0 \leq s_1 \leq s_2 < f_2 \leq f_1 \leq N \text{ and } f_1 - f_2 = s_2 - s_1. \quad (\text{II.C.100})$$

The four special species will be essentially created on the boundary, while the remaining species will essentially (but not only) decay onto these four types. Any species in between s_1 and s_2 will be paired with one species in between f_2 and f_1 , allowing a transmutation (on the boundary) between the pairs. Finally, in between s_2 and f_2 , either nothing happens, or the species decay to s_2 and f_2 .

More specifically, integrability is preserved when we have the following rules and rates on the boundary:

- *Class of very slow species:* for species τ with $1 \leq \tau < s_1$, we have:

$$\tau \xrightarrow{\gamma} s_1 \text{ and } \tau \xrightarrow{\alpha} f_1. \quad (\text{II.C.101})$$

- *Class of slow species:* for species τ with $s_1 \leq \tau \leq s_2$, we have:

$$\tau \xrightarrow{\alpha} \bar{\tau} = s_1 + f_1 - \tau = s_2 + f_2 - \tau. \quad (\text{II.C.102})$$

- *Class of intermediate species:* for species τ with $s_2 < \tau < f_2$, we have the two possibilities:

1. $\tau \xrightarrow{0} \tau', \forall \tau'$ (no decay, creation or transmutation).
2. $\tau \xrightarrow{\tilde{\gamma}} s_2$ and $\tau \xrightarrow{\alpha} f_2$.

- *Class of fast species:* for species τ with $f_2 \leq \tau \leq f_1$, we have:

$$\tau \xrightarrow{\tilde{\gamma}} \bar{\tau} = s_1 + f_1 - \tau. \quad (\text{II.C.103})$$

- *Class of very fast species:* for species τ with $f_1 < \tau \leq N$, we have:

$$\tau \xrightarrow{\tilde{\gamma}} s_1 \text{ and } \tau \xrightarrow{\tilde{\alpha}} f_1. \quad (\text{II.C.104})$$

We have introduced the following combination of the rates:

$$\tilde{\alpha} = \frac{(\alpha + \gamma + q - p)\alpha}{\alpha + \gamma}, \quad \tilde{\gamma} = \frac{(\alpha + \gamma + q - p)\gamma}{\alpha + \gamma}. \quad (\text{II.C.105})$$

This implies that α , γ , p , q are constrained such that $\tilde{\alpha}$, $\tilde{\gamma}$ are positive.

obtained from a right reflection matrix $\overline{K}(z)$ which satisfies the reflection equation (II.C.8). Due to the symmetry relation (for the R-matrix of the multi-species ASEP)

$$R_{21}(z) = U_1 U_2 R_{12}(z) U_1 U_2, \quad \text{with } U = \begin{pmatrix} & & 1 \\ & \cdot & \\ 1 & & \end{pmatrix}, \quad (\text{II.C.111})$$

the matrix $\overline{K}(z)$ can be constructed from a solution $K(z)$ of the reflection equation (II.C.1) through the relation

$$\overline{K}(z) = U K(1/z) U. \quad (\text{II.C.112})$$

A right boundary matrix \overline{B} is obtained with the relation

$$\overline{B} = -\frac{q-p}{2} \overline{K}'(1). \quad (\text{II.C.113})$$

Explicitly, the right boundary matrices are deduced from relation (II.C.112) and take the form

$$\overline{B}(\beta, \delta | s'_1, s'_2, f'_1, f'_2) = U B(\beta, \delta | s''_1, s''_2, f''_1, f''_2) U \quad (\text{II.C.114})$$

where U is defined in (II.C.111). The conjugation by U implies $f''_j = N - s'_j$ and $s''_j = N - f'_j$, $j = 1, 2$.

Let us stress that the parameters entering \overline{B} are independent from the ones used in the left boundary B . Altogether we will have four real parameters: α, γ for the left boundary, and β, δ for the right one. In the same way, the labels s'_1, s'_2, f'_1, f'_2 of the four special species in the right boundary are independent from the four special species labels s_1, s_2, f_2, f_1 in the left boundary.

The bijection between right and left boundaries can be seen in the following identity

$$\overline{B}(\beta, \delta | s_1, s_2, f_2, f_1) \equiv B(\delta, \beta | s_1, s_2, f_2, f_1) \Big|_{z \leftrightarrow \tilde{z}} \quad (\text{II.C.115})$$

where $z \leftrightarrow \tilde{z}$ means that we interchange β with $\tilde{\beta}$ and δ with $\tilde{\delta}$. As in the case of left boundaries, we use the notation

$$\tilde{\beta} = \frac{(\beta + \delta + q - p)\beta}{\beta + \delta} \quad \text{and} \quad \tilde{\delta} = \frac{(\beta + \delta + q - p)\delta}{\beta + \delta}. \quad (\text{II.C.116})$$

Example C.33. For the case $N = 1$, we recover the one-species ASEP. We get only one possible choice for s_1, s_2, f_1 and f_2 given by $s_1 = s_2 = 0$ and $f_1 = f_2 = 1$. Then, in the language used in this paragraph, the particle 0 (vacancy) is slow and the particle 1 is fast and the rates at the boundary are given by

$$0 \xrightarrow{\alpha} 1 \quad \text{and} \quad 1 \xrightarrow{\tilde{\gamma}} 0. \quad (\text{II.C.117})$$

One recovers that for the one-species ASEP, the generic boundary is integrable. The boundary matrix has the form

$$B = \begin{pmatrix} -\alpha & \tilde{\gamma} \\ \alpha & -\tilde{\gamma} \end{pmatrix}. \quad (\text{II.C.118})$$

One can use Bethe ansatz method to compute the eigenvalues and compute for example the spectral gap [135].

Conjugation by a diagonal matrix provides the non-Markovian boundary matrix used to compute the cumulant of the current [18]:

$$B(s) = \begin{pmatrix} -\alpha & e^s \tilde{\gamma} \\ e^{-s} \alpha & -\tilde{\gamma} \end{pmatrix}. \quad (\text{II.C.119})$$

It still corresponds to an integrable boundary.

	$s_1 = s_2 = 0$ $f_1 = f_2 = 1$	$s_1 = s_2 = 1$ $f_1 = f_2 = 2$	$s_1 = s_2 = 0$ $s_1 = s_2 = 2$
Type of part.	part. 0 slow part. 1 fast part. 2 very fast	part. 0 very slow part. 1 slow part. 2 fast	part. 0 slow part. 1 intermediate part. 2 fast
Rates	$0 \xrightarrow{\alpha} 1$ $1 \xrightarrow{\tilde{\gamma}} 0$ $2 \xrightarrow{\tilde{\gamma}} 0$ $2 \xrightarrow{\tilde{\alpha}} 1$	$0 \xrightarrow{\tilde{\gamma}} 1$ $0 \xrightarrow{\alpha} 2$ $1 \xrightarrow{\alpha} 2$ $2 \xrightarrow{\tilde{\gamma}} 1$	$0 \xrightarrow{\alpha} 2$ $1 \xrightarrow{\tilde{\gamma}} 0$ $2 \xrightarrow{\tilde{\gamma}} 0$ $0 \xrightarrow{\alpha} 2$ $1 \xrightarrow{\tilde{\gamma}} 0$ $2 \xrightarrow{\tilde{\gamma}} 0$
Name in [V5]	L_1	L_2	L_4 L_3

Table II.1: The four integrable boundaries in the case $N = 2$. The last row corresponds to the names of these boundaries in [V5].

Example C.34. For the case $N = 2$, we obtain the two-species ASEP. There are four possibilities summarized in table II.1. We recover the boundaries found in [V5].

Example C.35. Some of the boundary matrices can be related to former studies of boundary Hecke algebras [136, 137]. In our notation, they correspond to the matrices $B(\alpha, \gamma|0, s_2, N - s_2, N)$ or $B^0(\alpha, \gamma|0, s_2, N - s_2, N)$. Among them, some have been considered: $B^0(\alpha, \gamma|0, 1, N - 1, N)$ was analyzed in [138], and for the two-species ASEP ($N = 2$) $B^0(\alpha, \gamma|0, 0, 2, 2)$ was studied in [139–141].

Proposition C.36. For any matrix $B = B(\alpha, \beta|s_1, s_2, f_2, f_1)$ or $B = B^0(\alpha, \beta|s_1, s_2, f_2, f_1)$, the generators

$$\sigma_0 = \frac{B + \alpha + \gamma + q - p}{p - q} \text{ and } \sigma_1 = (m + q)/\sqrt{pq} \quad (\text{II.C.120})$$

obey relation (II.C.87), where $m \equiv m_{12}$ is given in (II.B.100) and B acts non trivially in space 1.

Proof. The matrices σ_1 and σ_0 given in (II.B.98) and (II.C.120) act on two site multi-species ASEP configurations. For a given start state, $\tau\tau'$, we can find a subset of the particle species $\mathcal{S} = \{\tau, \tau', \tau'', \dots\}$ such that for any polynomial in σ_1 and σ_0 acting on this state, these are the only species involved in the resulting configurations.

For all of the boundary matrices we consider, the subset \mathcal{S} turns out to be small, and related to the different classes of particles we introduced above: the non-diagonal part of σ_1 exchanges particles on sites 1 and 2, as allowed by bulk matrix m ; the non-diagonal part of σ_0 injects and removes particles at site 1 as allowed by the boundary transitions given previously. The idea of the proof is then to project the ‘global’ matrices σ_0, σ_1 down to the smaller number of species in \mathcal{S} . If for every starting state we can show that the resulting projected σ_0, σ_1 satisfy (II.C.87), then this implies that the ‘global’ matrices also satisfy (II.C.87).

At this point, the proof decomposes into different steps:

- We remark that for any start state $\tau\tau'$, the set \mathcal{S} falls into one of three categories:

$$\mathcal{S} = \{\tau, \tau', s_1, s_2, f_1, f_2\}, \quad (\text{II.C.121})$$

$$\mathcal{S} = \{\tau, s_1 + f_1 - \tau, \tau', s_1 + f_1 - \tau'\}, \quad (\text{II.C.122})$$

$$\mathcal{S} = \{\tau, s_1 + f_1 - \tau, \tau', s, f\}, \text{ with } (s, f) = (s_1, f_1) \text{ or } (s_2, f_2) \quad (\text{II.C.123})$$

Note that these sets can be reduced depending on the class of the species τ and τ' . For instance, if τ and τ' are of very slow class, then $\mathcal{S} = \{\tau, \tau', s_1, f_1\}$. Note also that the ordering of the start state does not change \mathcal{S} so τ, τ' are interchangeable in (II.C.123).

- Projecting the boundary matrix, B , corresponding to σ_0 down to the species in \mathcal{S} results in a boundary matrix of size $|\mathcal{S}|$ of type (II.C.106) or (II.C.107). To see this, we perform the projection by ‘deleting’ species from B by removing the corresponding row and column: we use the following operations which preserve the forms (II.C.106) or (II.C.107):
 - Deleting any species in the very slow, intermediate, or very fast class;
 - Deleting a species, $\tilde{\tau}$, in the slow or fast class with $\tilde{\tau} \neq s_1, f_1$ if we also delete the species $s_1 + f_1 - \tilde{\tau}$;
 - Deleting species s_1 and f_1 together, if $s_1 = 1$, $f_1 = N$, and $f_1 - f_2 = s_2 - s_1 > 0$.
 - Deleting species s_2 and f_2 together, if $f_2 = s_2 + 1$, and $f_1 - f_2 = s_2 - s_1 > 0$.

These operations are always sufficient to project down to any subsets \mathcal{S} as defined above. The projected σ_0 is then obtained from the projected B through (II.C.120).

- For the local bulk matrix m (giving σ_1) we can delete any number of species, preserving the form (II.B.100).
- To complete the proof all we need to do is to verify that all boundary matrices in this family give σ_0 matrices which satisfy (II.C.87) for size 2 up to 6 (the maximum $|\mathcal{S}|$). We have done this by a direct computation with a formal mathematical software package.

To illustrate the projection on \mathcal{S} , we consider the following boundary matrix

$$B = \left(\begin{array}{c|c|c|c|c|c} -\sigma & & & & & \\ \hline \gamma & -\alpha & & & \tilde{\gamma} & \tilde{\gamma} \\ \hline & & -\alpha & \tilde{\gamma} & \tilde{\gamma} & \\ \hline & & & -\sigma' & & \\ \hline & & \alpha & \alpha & -\tilde{\gamma} & \\ \hline \alpha & \alpha & & & -\tilde{\gamma} & \tilde{\alpha} \\ \hline & & & & & -\tilde{\sigma} \end{array} \right) \quad (\text{II.C.124})$$

and give some examples of start state (τ, τ') and the resulting subset \mathcal{S} and corresponding reduced matrix. In the case where $(\tau, \tau') = (0, 3)$, we obtain $\mathcal{S} = \{0, 3, s_1 = 1, s_2 = 2, f_1 = 5, f_2 = 4\}$ and the reduced matrix reads

$$\left(\begin{array}{c|c|c|c|c} -\sigma & & & & \\ \hline \gamma & -\alpha & & & \tilde{\gamma} \\ \hline & & -\alpha & \tilde{\gamma} & \tilde{\gamma} \\ \hline & & & -\sigma' & \\ \hline & & \alpha & \alpha & -\tilde{\gamma} \\ \hline \alpha & \alpha & & & -\tilde{\gamma} \end{array} \right). \quad (\text{II.C.125})$$

In the case where $(\tau, \tau') = (1, 5)$, we obtain $\mathcal{S} = \{1, 5\}$ and the reduced matrix reads

$$\begin{pmatrix} -\alpha & \tilde{\gamma} \\ \alpha & -\tilde{\gamma} \end{pmatrix}. \quad (\text{II.C.126})$$

Finally, in the case where $(\tau, \tau') = (2, 3)$, we obtain $\mathcal{S} = \{2, 3, 4\}$ and the reduced matrix reads

$$\begin{pmatrix} -\alpha & \tilde{\gamma} & \tilde{\gamma} \\ 0 & -\sigma' & 0 \\ \alpha & \alpha & -\tilde{\gamma} \end{pmatrix}. \quad (\text{II.C.127})$$

From theorem C.27, we can now give an expression for the Baxterised K -matrices of the multi-species ASEP. ■

3 Diagonalization of the transfer matrix

The diagonalization of the transfer matrix in the open case is much harder than in the periodic case. The main reason is the fact that the particles number may not be conserved by the dynamics on the boundaries (even if the particles number is conserved by the bulk dynamics). The situation is thus different from the periodic case where the diagonalization had been achieved at fixed number of particles, separately in each sector (we recall that the transfer matrix was block diagonal). The most commonly used methods in the periodic case, the coordinate Bethe ansatz and the algebraic Bethe ansatz cannot be applied directly here.

However the coordinate Bethe ansatz had been modified successfully in some particular cases, such as model with diagonal boundaries [89]. More recently it had been applied to the open single species ASEP [97, 142], providing partial results on the eigenvectors.

The algebraic Bethe ansatz had also been adapted successfully to diagonalize transfer matrices of certain open models, such as the open XXX and XXZ spin chain, first for triangular boundaries [102], and later for general boundaries [103, 104]. It has also been applied to the open single species TASEP [143].

We present in the example below how the results of the algebraic Bethe ansatz for the open XXZ spins chain can be used to compute the spectrum of the DiSSEP with open boundaries.

Example C.39. *We encountered the DiSSEP several times in this manuscript, through the presentation of its local jump operators m in (II.A.26) and B, \bar{B} in (II.A.31), and then through the associated R -matrix (II.B.55) and K -matrices (II.C.46) and (II.C.48). This proved the integrability of the model. The reader may refer to subsection 1 for details about the dynamics and properties of the DiSSEP. The integrability of this model is also revealed through its unexpected connexion with the XXZ spins chain. To be more precise, let us introduce the following quantum Hamiltonian H*

$$H = (\alpha - \gamma)\sigma_1^+ - \frac{\alpha + \gamma}{2}(\sigma_1^z + 1) + (\delta - \beta)\sigma_L^+ - \frac{\delta + \beta}{2}(\sigma_L^z + 1) - \frac{\lambda^2 - 1}{2} \sum_{k=1}^{L-1} \left(\sigma_k^x \sigma_{k+1}^x + \sigma_k^y \sigma_{k+1}^y - \frac{\lambda^2 + 1}{\lambda^2 - 1} (\sigma_k^z \sigma_{k+1}^z - 1) \right) \quad (\text{II.C.135})$$

where $\sigma^{x,y,z,+,-}$ are the Pauli matrices. It corresponds to the open XXZ spins chain with upper triangular boundaries. This Hamiltonian H is conjugated to the Markov matrix M of the DiSSEP defined as usual by

$$M = B_1 + \sum_{k=1}^{L-1} m_{k,k+1} + \bar{B}_L. \quad (\text{II.C.136})$$

Namely, one has

$$H = Q_1 Q_2 \dots Q_L M Q_1^{-1} Q_2^{-1} \dots Q_L^{-1} \quad \text{where} \quad Q = \begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix}. \quad (\text{II.C.137})$$

Let us also mention that the XXZ Model for particular choices of boundaries is conjugated to the Markov matrix of the open ASEP. However, for the boundaries present in (II.C.135), the conjugation provides non-Markovian boundaries (the sum to 0 property is not fulfilled).

We deduce from (II.C.137) that the spectrum of M is identical to the one of H . Moreover, the eigenvalues (but not the eigenvectors) of XXZ spin chain with upper triangular boundaries are the same that the ones for diagonal boundaries and one can use the results of [86, 126, 144]. Note also that for $\lambda^2 = 1$, the bulk Hamiltonian becomes diagonal, and the full Hamiltonian triangular, allowing to get its spectrum easily without Bethe ansatz, in accordance with the results of subsection 1.

The eigenvalues of H with diagonal boundaries can be parametrized in two different ways depending on the choice of the pseudo-vacuum:

- For the pseudo-vacuum with all the spins up and in the notations of the present paper, the eigenvalues of H are given by

$$E = -\alpha - \beta - \gamma - \delta + 4(\phi - 1)^2 \sum_{i=1}^N \frac{u_i}{(u_i - \phi^2)(u_i - 1)} \quad (\text{II.C.138})$$

where $N = 0, 1, \dots, L$ and u_i are the Bethe roots. The Bethe roots must satisfy the following Bethe equations

$$\frac{u_i + a\phi^2}{\phi(au_i + 1)} \frac{u_i + b\phi^2}{\phi(bu_i + 1)} \left(\frac{\phi(u_i - 1)}{u_i - \phi^2} \right)^{2L} = \prod_{\substack{j=1 \\ j \neq i}}^N \frac{\phi^2(\phi^2 u_i - u_j)(u_i u_j - 1)}{(u_i - \phi^2 u_j)(u_i u_j - \phi^4)} \quad (\text{II.C.139})$$

where $i = 1, 2, \dots, N$ and a and b are defined in (III.B.10).

- For the pseudo-vacuum with all the spins down, the eigenvalues of H are given by

$$E = 4(\phi - 1)^2 \sum_{i=1}^N \frac{v_i}{(v_i - \phi^2)(v_i - 1)} \quad (\text{II.C.140})$$

where v_i satisfy the following Bethe equations

$$\frac{av_i + \phi^2}{\phi(v_i + a)} \frac{bv_i + \phi^2}{\phi(v_i + b)} \left(\frac{\phi(v_i - 1)}{v_i - \phi^2} \right)^{2L} = \prod_{\substack{j=1 \\ j \neq i}}^N \frac{\phi^2(\phi^2 v_i - v_j)(v_i v_j - 1)}{(v_i - \phi^2 v_j)(v_i v_j - \phi^4)}. \quad (\text{II.C.141})$$

Let us stress again that, although the spectrum of the XXZ spin chain is the same for diagonal or upper boundaries, the eigenvectors are different. For the XXZ spin chains with upper triangular boundaries, the eigenvectors associated to the parametrization (II.C.138) and (II.C.139) of the eigenvalues were computed only recently by algebraic Bethe ansatz in [145] based on the previous results for the XXX spin chain [102, 103]. The computation of the eigenvectors associated to the parametrization (II.C.140) and (II.C.141) is still an open problem.

In the past few years, other techniques had been used to tackle this diagonalization problem of open systems. In the spirit of functional Bethe ansatz, the Off-diagonal Bethe ansatz was developed and successfully applied to several open models [101, 146].

The Baxter Q-operator idea was adapted, using matrix product expressions obtained through infinite dimensional representations of RTT algebras, to the (current counting deformation) of the open ASEP, in a pioneering work [120].

New ideas also emerged to deal with these open systems. The separation of variables method, inspired from the action-angle variables construction in classical integrable systems, was successfully used to solve several models [100, 147–149], see also [150] for an introduction. This method could provide an unifying framework for the exact resolution of both classical and quantum integrable systems, but a lot remains to be understood.

Finally, the q-Onsager algebra provided another point of view on the exact resolution of open models [151, 152].

All the diagonalization techniques presented in this subsection have proven to be efficient on particular models but may appear difficult to adapt to new models. A somehow hard analysis has to be performed each time. Moreover these methods provide the spectrum of the model parametrized with Bethe roots, which have to satisfy the Bethe equations. We saw previously that these Bethe equations are non-linear coupled algebraic relations, which appear (apart from very particular cases) impossible to solve exactly. These equations can be analyzed for large system sizes, *i.e.* in the thermodynamic limit (see chapter V for details). They have been studied for periodic models, introducing for instance the Bethe roots density [29, 87–89], which yields exact results for physical observables. However, for finite size systems, the exact

computations of physical quantities cannot be performed completely, they are always expressed in terms of Bethe roots.

In the following chapter we present an alternative method, which can be applied to integrable Markovian processes: the matrix ansatz. This method provides the stationary state of the model analytically. Its huge advantage is that it does not require to solve any Bethe equations and gives access to exact expressions of physical observables for finite size systems. Moreover its range of application seems to be quite large and, in some sens, quite model independent: it seems to be possible to use it for any integrable Markovian exclusion process at the price of solving two key relations, the Zamolodchikov-Faddeev and the Ghoshal-Zamolodchikov relations. However this method gives only one eigenvector of the transfer matrix, the stationary state, and does not provide the complete spectrum and eigenvectors of the model. We do not have access to the full dynamics of the model but only to the stationary state. Moreover this method had been applied, so far, only on Markovian models (or on current-counting deformation of the Markovian models) but not on general integrable model like quantum spin chains.

Chapter III

Matrix ansatz for non-equilibrium steady states

A Presentation of the method and link with integrability

The matrix ansatz (also called matrix product state) has become over the last decades an incredibly powerful tool in a lot of different fields. In physics, this method can be roughly described as a way to encode spatial correlations in probability distributions, and thus goes far beyond the mean-field approximation. In mathematics such states could be interpreted as generalized characters associated to representation of various algebras and endorse the role of a keystone at the interplay between combinatorics, representation theory, integrability and stochastic processes. The matrix product states were simultaneously and independently introduced in the context of one dimensional Markovian systems on one side and of one dimensional quantum Hamiltonians on the other side.

In statistical physics of classical systems, the matrix ansatz was developed to express exactly the steady state of stochastic processes describing particles in interaction. It was used for the first time in [46] and led to a rigorous description of phase transitions in an out-of-equilibrium system [47, 153]. This chapter will be devoted to this topic, more details and references about the relevant literature are given in the next section.

At the same time, in quantum physics, the Density Matrix Renormalization Group (DMRG) algorithm [154] has proven to be very efficient in computing, with a high numerical accuracy, the ground state and low energy states of one dimensional Hamiltonian with short range interactions [155, 156]. The convergence and validity of this algorithm has been proven to be directly related to the existence of a matrix product expression for the eigenvectors under consideration [157]. During the same period, on the exact result side, the ground state of several one dimensional Hamiltonians had been analytically expressed with a matrix ansatz [158–160], which permitted exact computation of physical quantities such as correlation lengths. More recently, in statistical physics of open quantum systems, very interesting results have been obtained in the context of the Lindblad equation (that describes a quantum system coupled to reservoirs) where the density matrix has been expressed analytically in a matrix product form [11, 12, 161]. These works also pointed out the link of the matrix ansatz with integrability.

We can also mention that, in integrable models, the eigenvectors obtained with the algebraic Bethe ansatz technique can also be reformulated using matrix product states [162, 163]. It is also important to point out that recent progress have been made in integrable models by computing explicitly Baxter Q operator in a matrix product form [120] and [119]. In these works the Q operator is constructed as a generalized transfer matrix with infinite dimensional auxiliary space.

In representation theory and combinatorics, recent progress has been made in expressing Macdonald polynomials (which form a family of multivariate polynomials, symmetric under permutation of variables, and containing Schur, Hall-Littlewood and Jack polynomials as specializations) in a matrix product form [49]. This led in particular to explicit formulas and

sum rules [164, 165]. This matrix product expression gave also the framework to introduce a new family of polynomials [166], that encompasses the Macdonald polynomials. In a similar way Koornwinder polynomials¹ (which form a family of multivariate Laurent polynomials, symmetric under permutation and inversion of variables) have been expressed in some particular cases in a matrix product form [V6, 141]. All these works shed light on connections and interplay between symmetric polynomials, representation theory of Hecke algebras, quantum Knizhnik-Zamolodchikov equations and integrable stochastic processes. The chapter IV of this manuscript will be devoted to this topic.

Finally, in knot theory the study of the so-called “quantum invariants” initiated by the celebrated Jones polynomial [72] appeared as a small revolution in the field. These knot invariants are polynomials constructed in a matrix product form using representations of the braid group and its quotients (Hecke algebra, Birman-Murakami-Wenzl algebra,...).

In the present chapter we will focus on the role of the matrix ansatz for exact solvability in classical non-equilibrium steady states. We will particularly investigate its link with integrability. The idea of the method will be introduced on the specific example of the TASEP from which we will draw the general framework. Some new examples will be given as an illustration.

1 General idea and example

a) General idea

In the context of exact results in out-of-equilibrium statistical physics, the matrix ansatz is a technique introduced to express analytically the stationary distribution of certain exclusion processes. It was first successfully used in the seminal paper [46] to compute exactly the stationary state of the TASEP. Since this pioneering work, it has been widely used in the context of Markovian dynamics. During the past few years the computation of the stationary distribution of the multi-species (T)ASEP on a periodic lattice has attracted a lot of interest. Initiated in [46] and [167] for respectively two and three species of particles, the steady state was first expressed in the general case in a matrix product form [168–171] by reformulating a pushing procedure. Another matrix product solution was found later by studying the interplay between the steady state of the multi-species ASEP and the Macdonald polynomials [49]. The connection to three dimensional integrability of the multi-species TASEP also gave rise to another matrix product expression [172, 173]. Several works tackled particular multi-species ASEPs with open boundaries, such as [174] for reflexive boundary conditions, or [139, 175, 176] for semi-permeable boundaries and finally [V5, V7] for integrable boundaries for 2-species TASEP. Some generalizations of the multi-species TASEP with inhomogeneous hopping rates have been solved using a matrix ansatz on the periodic lattice [74], and also for very specific boundary conditions [177]. We can also point out here the matrix product solution of the ABC model on the ring with equal densities of each species [178]. In the simpler case of the multi-species SSEP, a matrix product expression of the steady state was recently proposed [V8] for a particular class of integrable boundary conditions. We can also mention some work related to single species ASEP-like models with discrete time dynamics [V9, 179], or deterministic dynamics in the bulk with stochastic boundaries [180] or with impurity [181]. A matrix product expression of the steady state of a cellular automaton coupled with stochastic boundaries was also recently found [182]. In [183] the steady state of an integrable two-species zero range process, introduced in [58] was constructed in a matrix product form, generalizing the well known factorized stationary distribution of the single species zero range process [184]. The matrix ansatz has also been widely used to deal with reaction-diffusion stochastic models. Several coagulation-decoagulation models were solved this way in [185] or in [186] where a classification of such “matrix product” exactly solvable models is provided. Recently a model with pair creation and annihilation of particles was exactly solved using a matrix ansatz in [V10]. The reader may refer to the review [42] for more details about the use of matrix product states in non-equilibrium steady states.

¹these polynomials will be defined in details in chapter IV

The matrix product ansatz arises as a natural generalization of the factorized distribution

$$\mathcal{S}(\tau_1, \tau_2, \dots, \tau_L) = \frac{1}{Z} f(\tau_1) f(\tau_2) \dots f(\tau_L), \quad (\text{III.A.1})$$

where f is a real function and Z is a normalization such that the sum of the weights equals 1.

Remark A.1. *Despite its apparently simple form, the distribution (III.A.1) has found many important applications in non-equilibrium steady states. A paradigmatic example is given by the stationary distribution of the (single species) zero range process on a ring [39]. In this model, there are no constraints on the number of particles lying on each site of the lattice, the particles can hop to the left (respectively right) nearest neighbor site with probability rate qw_n (respectively pw_n), where n denotes the number of particles sitting on the departure site and w_n is a non-negative number, see figure III.1. The essential feature of such models is that the hopping rates depend only on the departure site and not on the target site (in contrast with the exclusion processes). It thus describes a system in which the interactions between the particles have zero range. Several generalization of this model have been proposed: with open boundaries [187], with discrete time dynamics [188, 189], with continuous mass on each site [188, 189], with particle number constrained on each site [190], or with several species of particles [183]. The reader may refer to the review [184] for more details.*

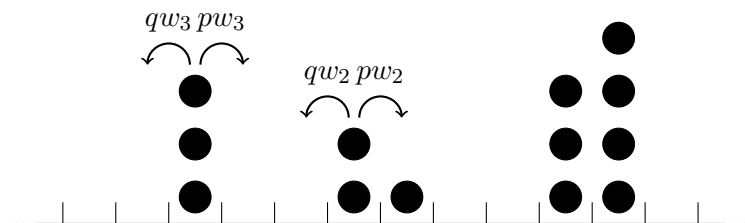


Figure III.1: Dynamical rules of the zero range process.

This distribution (III.A.1) is that of independent and identically distributed random variables τ_1, \dots, τ_L with probability distribution given by the (properly normalized) function f . This framework cannot describe any correlated variables. The fundamental idea of the matrix ansatz is to replace the real valued function f by a matrix valued function. More precisely, to each local configuration variable τ_i is associated a matrix X_{τ_i} . The variable τ_i can take $N + 1$ different values $0, 1, \dots, N$, hence there are $N + 1$ different matrices² X_0, X_1, \dots, X_N . This leads to the following definition.

Definition A.2. *A probability distribution $\mathcal{S}(\tau_1, \tau_2, \dots, \tau_L)$, $0 \leq \tau_i \leq N$, is said to have a matrix product form if there exist matrices X_0, X_1, \dots, X_N and U and a trace operator tr (which satisfies the cyclic property $tr(AB) = tr(BA)$) with non-negative values such that*

$$\mathcal{S}(\tau_1, \tau_2, \dots, \tau_L) = \frac{1}{Z_L} tr(U X_{\tau_1} X_{\tau_2} \dots X_{\tau_L}), \quad (\text{III.A.2})$$

where the normalization Z_L ensures that the sum of the probabilities gives 1. In practice, when the model under consideration is irreducible (it implies in particular that none of the particle species number is conserved by the dynamics, which is often the case for models with open boundaries), Z_L is equal to $tr(UC^L)$, with

$$C = X_0 + X_1 + \dots + X_N. \quad (\text{III.A.3})$$

Remark A.3. *The matrix product expression above encompasses the cases of systems with open boundaries or systems on a ring.*

²Note that this could be generalized to the case where the local configuration τ_i takes continuous values. We have in this case an infinity of matrices X_t , parametrized by a continuous parameter t

For models defined on a lattice with open boundaries, the matrix U is written using a row vector $\langle\langle W|$ and a column vector $|V\rangle\rangle$ in the form $U = |V\rangle\rangle\langle\langle W|$. The distribution then reads

$$\mathcal{S}(\tau_1, \tau_2, \dots, \tau_L) = \frac{1}{Z_L} \langle\langle W|X_{\tau_1}X_{\tau_2} \dots X_{\tau_L}|V\rangle\rangle, \quad (\text{III.A.4})$$

where the normalization Z_L is equal to $\langle\langle W|C^L|V\rangle\rangle$, with

$$C = X_0 + X_1 + \dots + X_N. \quad (\text{III.A.5})$$

For models defined on a periodic lattice, the matrix U is taken equal to the identity matrix. The distribution then reads

$$\mathcal{S}(\tau_1, \tau_2, \dots, \tau_L) = \frac{1}{Z_L} \text{tr}(X_{\tau_1}X_{\tau_2} \dots X_{\tau_L}). \quad (\text{III.A.6})$$

In this case the normalization has often a more subtle expression if the particle number of the species is conserved by the dynamics: we have to sum the weights of the lattice configurations that have a given particle number of each species.

The vectors $\langle\langle W|$ and $|V\rangle\rangle$ (or the trace operator tr) are needed to contract the matrix product to get a real valued probability. We use the notation with a double bracket on the vectors $\langle\langle W|$ and $|V\rangle\rangle$ to distinguish the vector space in which they belong (the vector space on which the matrices X_τ act linearly) from the vector space of physical configurations whose vectors are written with a single bracket (for instance the vector $|\mathcal{S}\rangle\rangle$).

The matrix product form of a distribution can capture correlations between the local configuration variables through the non commutative structure of the algebra generated by X_0, \dots, X_N . The order of the matrices in the product is thus very important. We stress that this matrix product framework can thus be used to deal with systems that do not have Boltzmann statistics and that lie beyond the scope of the central limit theorem (which describes uncorrelated variables). This is for instance well illustrated by the work [191] in which the statistics of a sum of correlated variables (with matrix product distribution) was studied.

In order to express the stationary distribution of an exclusion process using this matrix product formalism, it is of course crucial to carefully choose the matrices X_τ and the vectors $\langle\langle W|$ and $|V\rangle\rangle$ (for systems with open boundaries). It turns out that the algebraic relations that these objects must fulfill are closely related to the Markov matrix of the model. This last point will be discussed in details in the next sections.

The matrix ansatz formulation of the steady state reveals also to be very convenient to express the multi-point correlation functions in the stationary state. If we define the variable $\rho_s^{(i)}$ such that $\rho_s^{(i)} = 1$ if there is a particle of species s on site i and $\rho_s^{(i)} = 0$ otherwise, then the k -point correlation function is by definition equal to the quantity $\langle \rho_{s_1}^{(i_1)} \dots \rho_{s_k}^{(i_k)} \rangle$, where the bracket $\langle \cdot \rangle$ stands for the expectation value in the stationary distribution. The matrix product structure of the steady state allows us to write concisely

$$\langle \rho_{s_1}^{(i_1)} \dots \rho_{s_k}^{(i_k)} \rangle = \frac{1}{Z_L} \langle\langle W|C^{i_1-1}X_{s_1}C^{i_2-i_1-1}X_{s_2} \dots C^{i_k-i_{k-1}-1}X_{s_k}C^{L-i_k}|V\rangle\rangle. \quad (\text{III.A.7})$$

In particular the mean density (one-point correlation function) of particle of species s at site i reads

$$\langle \rho_s^{(i)} \rangle = \frac{1}{Z_L} \langle\langle W|C^{i-1}X_sC^{L-i}|V\rangle\rangle. \quad (\text{III.A.8})$$

Note that in the single species case $N = 1$, that we encountered many times with the examples of the ASEP, TASEP and SSEP along this manuscript, $\tau_i = 0, 1$ and we have always $\rho_1^{(i)} = \tau_i$. In this single species case, to lighten the notations, the multi-point correlation function will be simply written $\langle \tau_{i_1} \dots \tau_{i_k} \rangle$.

We now present the example of the TASEP to fix the ideas and get used to the different notions introduced.

b) Historical example of the TASEP

The stationary distribution of the TASEP with open boundary conditions was analytically expressed using a matrix product form in the pioneering work [46]. We recall that the Markov matrix governing the stochastic dynamics of this model is given in the form

$$M = B_1 + \sum_{k=1}^{L-1} m_{k,k+1} + \bar{B}_L \quad (\text{III.A.9})$$

where m has been introduced in (II.A.24) and B, \bar{B} in (II.A.32). We reproduce hereafter some of the results obtained in [46].

Proposition A.4. *The stationary distribution of the TASEP with open boundary condition (III.A.9) is given by the matrix product expression*

$$\mathcal{S}(\tau_1, \tau_2, \dots, \tau_L) = \frac{1}{Z_L} \langle\langle W | \prod_{i=1}^L (\tau_i D + (1 - \tau_i) E) | V \rangle\rangle, \quad (\text{III.A.10})$$

where the matrices E, D and the boundary vectors $\langle\langle W |$ and $|V\rangle\rangle$ satisfy the algebraic relations

$$DE = D + E, \quad \langle\langle W | E = \frac{1}{\alpha} \langle\langle W |, \quad D |V\rangle\rangle = \frac{1}{\beta} |V\rangle\rangle, \quad (\text{III.A.11})$$

and the normalization is given by $Z_L = \langle\langle W | C^L |V\rangle\rangle$, with $C = D + E$.

Note that in the case studied here of the single species TASEP, the local variables τ_i can only take two values, 0 and 1. The expression (III.A.10) is thus completely equivalent to the one in definition A.2 if we set $X_0 = E$ and $X_1 = D$ (we used the name E and D for the matrices X_0 and X_1 to stick to the notation introduced in [46]). The proof of the proposition A.4 will be given in subsection 2. We now recall an explicit representation of $E, D, \langle\langle W |$ and $|V\rangle\rangle$ as infinite dimensional matrices and vectors respectively. The operators E and D can be expressed as acting linearly on a Fock space, with basis denoted by $\{|k\rangle\rangle\}_{k \geq 0}$

$$E = \sum_{k=0}^{+\infty} [|k\rangle\rangle \langle\langle k| + |k+1\rangle\rangle \langle\langle k|], \quad D = \sum_{k=0}^{+\infty} [|k\rangle\rangle \langle\langle k| + |k\rangle\rangle \langle\langle k+1|]. \quad (\text{III.A.12})$$

In matrix notation it gives explicitly

$$E = \begin{pmatrix} 1 & 0 & 0 & 0 & \dots \\ 1 & 1 & 0 & 0 & \\ 0 & 1 & 1 & 0 & \\ 0 & 0 & 1 & 1 & \\ \vdots & & & & \ddots \end{pmatrix}, \quad D = \begin{pmatrix} 1 & 1 & 0 & 0 & \dots \\ 0 & 1 & 1 & 0 & \\ 0 & 0 & 1 & 1 & \\ 0 & 0 & 0 & 1 & \\ \vdots & & & & \ddots \end{pmatrix}. \quad (\text{III.A.13})$$

The boundary vectors $\langle\langle W |$ and $|V\rangle\rangle$ are represented as

$$\langle\langle W | = \sum_{k=0}^{+\infty} \left(\frac{1-\alpha}{\alpha} \right)^k \langle\langle k|, \quad |V\rangle\rangle = \sum_{k=0}^{+\infty} \left(\frac{1-\beta}{\beta} \right)^k |k\rangle\rangle, \quad (\text{III.A.14})$$

or more explicitly

$$\langle\langle W | = \left(1 \quad \left(\frac{1-\alpha}{\alpha} \right) \quad \left(\frac{1-\alpha}{\alpha} \right)^2 \quad \dots \right), \quad |V\rangle\rangle = \begin{pmatrix} 1 \\ \left(\frac{1-\beta}{\beta} \right) \\ \left(\frac{1-\beta}{\beta} \right)^2 \\ \vdots \end{pmatrix}. \quad (\text{III.A.15})$$

It is straightforward to check that the expressions (III.A.12) and (III.A.14) fulfill the algebraic relations (III.A.11). It proves that these algebraic relations are consistent. Moreover the scalar product $\langle\langle W|V\rangle\rangle = \alpha\beta/(\alpha + \beta - 1)$ is non-vanishing.

The matrix product expression of the stationary state of the open TASEP has proven to be a very powerful tool with which to compute physical quantities and to study the macroscopic behavior of the system. It permitted, in particular, (see chapter V) the rigorous derivation of the phase diagram of the model. We recall here the calculation of the normalization, of the particle current and of the particle density given in [46]. We begin by showing the efficiency of the algebraic relations (III.A.11), to analytically compute the stationary weights, on a particular example:

$$Z_5 \mathcal{S}(0, 1, 0, 1, 1) = \langle\langle W|EDED D|V\rangle\rangle \quad (\text{III.A.16})$$

$$= \frac{1}{\alpha\beta^2} \langle\langle W|DE|V\rangle\rangle \quad (\text{III.A.17})$$

$$= \frac{1}{\alpha\beta^2} \langle\langle W|D + E|V\rangle\rangle \quad (\text{III.A.18})$$

$$= \frac{1}{\alpha\beta^2} \left(\frac{1}{\alpha} + \frac{1}{\beta} \right) \langle\langle W|V\rangle\rangle. \quad (\text{III.A.19})$$

The equality between line 1 and line 2 is obtained using the action of the matrices E and D on the boundary vectors $\langle\langle W|$ and $|V\rangle\rangle$ respectively. We get the third line because of the algebraic relation $DE = D + E$. The last equality is again obtained because of the relations on the boundary vectors.

Proposition A.5. *The normalization Z_L is given in a closed form by*

$$Z_L = \sum_{p=1}^L \frac{p(2L-1-p)! \left(\frac{1}{\beta} \right)^{p+1} - \left(\frac{1}{\alpha} \right)^{p+1}}{L!(L-p)! \frac{1}{\beta} - \frac{1}{\alpha}} \langle\langle W|V\rangle\rangle. \quad (\text{III.A.20})$$

We choose to present now the detailed proof of formula (III.A.20) to illustrate the efficiency of the algebraic relations to compute physical quantities.

Proof. Following the lines of [46], the first step is to prove the relation

$$C^n = \sum_{p=0}^n B_{n,p} \sum_{q=0}^p E^q D^{p-q}, \quad (\text{III.A.21})$$

where $B_{n,p}$ is a combinatorial factor given explicitly by

$$B_{n,p} = \frac{p(2n-1-p)!}{n!(n-p)!}. \quad (\text{III.A.22})$$

This relation is obtained by direct reordering of the matrices E and D in the product $(E+D)^n$. We push E to the left (respectively D to the right) because it behaves conveniently on the left vector $\langle\langle W|$ (respectively on the right vector $|V\rangle\rangle$). This can be achieved thanks to the fact that $DE = D + E$. The relation (III.A.21) is proved by induction.

The case $n = 1$ is easily verified. Assume now that the formula (III.A.21) is established for a given $n \geq 1$. We can then compute

$$C^{n+1} = C^n C = \sum_{p=0}^n B_{n,p} \sum_{q=0}^p E^q D^{p-q} (E + D). \quad (\text{III.A.23})$$

It thus appears that we need to reorder the products of the form $D^k E$. It is straightforward to prove (by induction for instance) that

$$D^k E = D^k + D^{k-1} + \dots + D + E. \quad (\text{III.A.24})$$

Hence, by elementary manipulations on sums, we obtain

$$C^{n+1} = \sum_{p=1}^{n+1} \left(\sum_{l=p-1}^n B_{n,l} \right) \sum_{q=0}^p E^q D^{p-q}. \quad (\text{III.A.25})$$

We thus need to compute

$$\sum_{l=p-1}^n B_{n,l} = B_{n+1,p}. \quad (\text{III.A.26})$$

This last equality can be readily checked using the recursive relation $B_{n+1,p} = B_{n+1,p+1} + B_{n,p-1}$ and the fact that $B_{n,n} = 1 = B_{n+1,n+1}$. At the end we obtain

$$C^{n+1} = \sum_{p=0}^{n+1} B_{n+1,p} \sum_{q=0}^p E^q D^{p-q}, \quad (\text{III.A.27})$$

which ends the induction proof of (III.A.21). We are now in position to contract C^L with the boundary vectors $\langle\langle W|$ and $|V\rangle\rangle$. Using the fact that

$$\langle\langle W|E^q = \frac{1}{\alpha^q} \langle\langle W|, \quad \text{and} \quad D^{p-q}|V\rangle\rangle = \frac{1}{\beta^{p-q}} |V\rangle\rangle, \quad (\text{III.A.28})$$

and the formula

$$\sum_{q=0}^p \frac{1}{\alpha^q} \frac{1}{\beta^{p-q}} = \frac{\frac{1}{\alpha^{p+1}} - \frac{1}{\beta^{p+1}}}{\frac{1}{\alpha} - \frac{1}{\beta}}, \quad (\text{III.A.29})$$

we establish the desired result (III.A.20). ■

Proposition A.6. *The mean particle current between sites i and $i + 1$ is given by*

$$\langle j \rangle = \frac{Z_{L-1}}{Z_L}, \quad (\text{III.A.30})$$

where Z_L is the normalization computed in (III.A.20). Note that the current does not depend on the sites where it is measured, as expected from the particle conservation in the bulk.

Proof. The mean number of particles that cross the bond between sites i and $i + 1$ per unit of time is given by the sum of probabilities for configurations with a particle on site i and a hole on site $i + 1$ (*i.e.* configurations for which it is possible that a particle jumps from site i to $i + 1$ during the next transition). This has then to be multiplied by the 'rate of a jump' which is 1. This gives

$$\langle j \rangle = \sum_{\tau_1, \dots, \tau_{i-1}, \tau_{i+2}, \dots, \tau_L=0,1} \mathcal{S}(\tau_1, \dots, \tau_{i-1}, 1, 0, \tau_{i+2}, \dots, \tau_L) \quad (\text{III.A.31})$$

$$= \frac{\langle\langle W|(E + D) \dots (E + D)DE(E + D) \dots (E + D)|V\rangle\rangle}{Z_L} \quad (\text{III.A.32})$$

$$= \frac{\langle\langle W|C^{i-1}DEC^{L-i-1}|V\rangle\rangle}{Z_L} \quad (\text{III.A.33})$$

$$= \frac{\langle\langle W|C^{i-1}(D + E)C^{L-i-1}|V\rangle\rangle}{Z_L} \quad (\text{III.A.34})$$

$$= \frac{Z_{L-1}}{Z_L}. \quad (\text{III.A.35})$$

Proposition A.7. *The mean density of particle at site i is expressed analytically as*

$$\langle \tau_i \rangle = \sum_{k=1}^{L-i} B_{k,1} \frac{Z_{L-k}}{Z_L} + \frac{Z_{i-1}}{Z_L} \sum_{k=1}^{L-i} B_{L-i,k} \frac{1}{\beta^{k+1}}, \quad (\text{III.A.36})$$

where the combinatorial coefficient $B_{n,p}$ is given in (III.A.22). ■

Note that here and in what follows, the notation $\langle \cdot \rangle$ stands for the expectation with respect to the stationary distribution.

Proof.

$$\langle \tau_i \rangle = \sum_{\tau_1, \dots, \tau_L=0,1} \tau_i \mathcal{S}(\tau_1, \dots, \tau_L) \quad (\text{III.A.37})$$

$$= \sum_{\tau_1, \dots, \tau_{i-1}, \tau_{i+1}, \dots, \tau_L=0,1} \mathcal{S}(\tau_1, \dots, \tau_{i-1}, 1, \tau_{i+1}, \dots, \tau_L) \quad (\text{III.A.38})$$

$$= \frac{\langle\langle W|(E+D)\dots(E+D)D(E+D)\dots(E+D)|V\rangle\rangle}{Z_L} \quad (\text{III.A.39})$$

$$= \frac{\langle\langle W|C^{i-1}DC^{L-i}|V\rangle\rangle}{Z_L}. \quad (\text{III.A.40})$$

The proof relies essentially on the identity

$$DC^n = \sum_{k=0}^{n-1} B_{k+1,1} C^{n-k} + \sum_{k=2}^{n+1} B_{n,k-1} D^k, \quad (\text{III.A.41})$$

which can be proven by induction on n . We thus have

$$\langle\langle W|C^{i-1}DC^{L-i}|V\rangle\rangle = \sum_{k=0}^{L-i-1} B_{k+1,1} \langle\langle W|C^{L-1-k}|V\rangle\rangle + \sum_{k=2}^{L-i+1} \frac{B_{L-i,k-1}}{\beta^k} \langle\langle W|C^{i-1}|V\rangle\rangle \quad (\text{III.A.42})$$

from which it is easy to establish the desired result (III.A.36). \blacksquare

We stress that the results (III.A.20), (III.A.30) and (III.A.36) are exact and valid for any size L of the lattice. These physical observables were computed efficiently using the matrix product formulation of the steady state. We will see in chapter V that the analytical expressions obtained can be studied in the thermodynamic limit (*i.e.* in the large lattice size L limit), to derive asymptotic expressions of the observables and compute rigorously the phase diagram of the system. In particular we will see that the model displays boundary induced phase transitions.

c) Pushing procedure for the open TASEP

We present here (without any proof) a combinatorial interpretation of the stationary weights of the open single species TASEP, called the pushing procedure. This procedure is well known for the multi-species TASEP on the ring [168] and has also been successfully applied to understand the combinatorics of the stationary weights of the single species open TASEP in the particular case $\alpha = \beta = 1$. We start by presenting the method in this particular case and then we generalize to free parameters α and β .

To shorten the notations, a configuration on the lattice can be seen as a binary string of 0 and 1 of length L . For instance the binary string 1010 corresponds to the configuration $\mathcal{C} = (1, 0, 1, 0)$. The stationary weight of a given configuration is obtained by enumerating all the possible binary strings that we get by pushing the 1's to the right through the 0's or by doing nothing. For instance starting from 110 we can obtain 110, 101 and 011. Hence we have the weight 3 for the configuration 110 which is consistent with the matrix product computation

$$\langle\langle W|DDE|V\rangle\rangle = \langle\langle W|D(D+E)|V\rangle\rangle = \langle\langle W|D^2|V\rangle\rangle + \langle\langle W|DE|V\rangle\rangle \quad (\text{III.A.43})$$

$$= \langle\langle W|D^2|V\rangle\rangle + \langle\langle W|D|V\rangle\rangle + \langle\langle W|E|V\rangle\rangle = 3\langle\langle W|V\rangle\rangle, \quad (\text{III.A.44})$$

using the fact that $\langle\langle W|E = \langle\langle W|$ and $D|V\rangle\rangle = |V\rangle\rangle$ because $\alpha = \beta = 1$.

We give another example with the binary string 1010. We can obtain 1010, 1001, 0110, 0101 and 0011. This gives us a weight equal to 5 which is consistent with

$$\begin{aligned}
\langle\langle W|DEDE|V \rangle\rangle &= \langle\langle W|(D+E)(D+E)|V \rangle\rangle = \langle\langle W|(D^2+DE+ED+E^2)|V \rangle\rangle \text{ (III.A.45)} \\
&= \langle\langle W|D^2|V \rangle\rangle + \langle\langle W|D|V \rangle\rangle + \langle\langle W|E|V \rangle\rangle + \langle\langle W|ED|V \rangle\rangle + \langle\langle W|E^2|V \rangle\rangle \\
&= 5\langle\langle W|V \rangle\rangle. \text{ (III.A.46)}
\end{aligned}$$

Pushing procedure for generic α and β We present a generalization of the pushing procedure for the cases where α and β are generic. To the best of our knowledge this generalization was not known up to now.

In addition to the rules given above, the 1's are now allowed to enter the binary string to the left with a weight $a = (1 - \alpha)/\alpha$ (note that $a = 0$ when $\alpha = 1$) and leave the binary string to the right with a weight $b = (1 - \beta)/\beta$ (again $b = 0$ if $\beta = 1$). Note that now, starting from a given binary string, we can access all the other binary strings of same length (by pushing the 1's to the right and making them enter or leave the binary string). Moreover, there are several ways to get a binary string starting from the initial one: we choose the one with the minimal number of 1's leaving or entering the system. This point will be detailed at the end of the paragraph.

Nothing is better than a concrete example to understand the procedure. From the binary string 110, we can obtain 110, 101 and 011 with weight 1. But we can also obtain 100, 010 and 001 with weight b (by making the right most 1 leave the binary string). Making the two 1's leave the binary string we get 000 with weight b^2 . We can also make a new 1 enter the system to obtain 111 with weight a . Summing all these contributions we end up with the stationary weight $3 + 3b + b^2 + a$ for the configuration 110 which is consistent with the matrix product computation

$$\begin{aligned}
\langle\langle W|DDE|V \rangle\rangle &= \langle\langle W|D^2|V \rangle\rangle + \langle\langle W|D|V \rangle\rangle + \langle\langle W|E|V \rangle\rangle \text{ (III.A.47)} \\
&= ((1+b)^2 + (1+b) + (1+a))\langle\langle W|V \rangle\rangle \text{ (III.A.48)} \\
&= (3 + 3b + b^2 + a)\langle\langle W|V \rangle\rangle, \text{ (III.A.49)}
\end{aligned}$$

using the fact that $\langle\langle W|E = \frac{1}{\alpha}\langle\langle W| = (1+a)\langle\langle W|$ and $D|V \rangle\rangle = \frac{1}{\beta}|V \rangle\rangle = (1+b)|V \rangle\rangle$.

We give another example with the configuration 1010. From this binary string we can obtain the string 1010, 1001, 0110, 0101 and 0011 with weight 1. We can also make the right most 1 leave the binary string to get 1000, 0100, 0010 and 0001 with weight b . Pushing the two 1's out of the string gives 0000 with weight b^2 . We can also make a new 1 appear on the left on the string to obtain 1110, 1101, 1011 and 0111 with weight a . If two 1's are injected on the left we get 1111 with weight a^2 . The last binary string 1100 is obtained with weight ab by making a 1 appear on the left and the right most 1 leave on the right. Summing all these contributions gives the total stationary weight $5 + 4b + b^2 + 4a + a^2 + ab$ in agreement with

$$\begin{aligned}
\langle\langle W|DEDE|V \rangle\rangle &= \langle\langle W|D^2|V \rangle\rangle + \langle\langle W|D|V \rangle\rangle + \langle\langle W|E|V \rangle\rangle + \langle\langle W|ED|V \rangle\rangle + \langle\langle W|E^2|V \rangle\rangle \\
&= ((1+b)^2 + (1+b) + (1+a) + (1+a)(1+b) + (1+a)^2)\langle\langle W|V \rangle\rangle \\
&= (5 + 4b + b^2 + 4a + a^2 + ab)\langle\langle W|V \rangle\rangle. \text{ (III.A.50)}
\end{aligned}$$

It is important to recall that in this procedure we always select the simplest path to go from the starting binary string to any other binary string. Simplest path should be understood here as the path whose weight has the minimal powers of a and b (the minimal sum of the powers of a and b to be fully rigorous: a path of weight $a^n b^m$ is preferred against a path of weight $a^{n'} b^{m'}$ if $n + m < n' + m'$). For instance, it is indeed easy to see that there are several possibilities to go from the binary string 1010 to the binary string 0110. We could first choose to make both 1's leave the string on the right and then make two new 1's appear on the left and push them at the correct position, giving a weight $a^2 b^2$. But we saw that it is also possible to just push one step the left most 1 to the right, with weight $1 = a^0 b^0$. Since $0 + 0 < 2 + 2$ we keep the second path (which is manifestly the simplest path).

2 Telescopic relations

In this subsection we will discuss the algebraic constraints that should be satisfied by the matrices X_0, X_1, \dots, X_N and the boundary vectors $\langle\langle W|$ and $|V\rangle\rangle$ in order that the matrix product state (III.A.4) computes correctly the stationary distribution. An efficient formalism to present these algebraic relations is the one of the tensor product. We already encountered this framework when defining the vector basis associated to the physical configurations on the lattice, see chapter II. We will use it here to write the stationary distribution in a concise way.

Proposition A.8. *The matrix product state defined in (III.A.4) can be recast in the form*

$$|\mathcal{S}\rangle = \frac{1}{Z_L} \langle\langle W| \begin{pmatrix} X_0 \\ X_1 \\ \vdots \\ X_N \end{pmatrix} \otimes \begin{pmatrix} X_0 \\ X_1 \\ \vdots \\ X_N \end{pmatrix} \otimes \dots \otimes \begin{pmatrix} X_0 \\ X_1 \\ \vdots \\ X_N \end{pmatrix} |V\rangle\rangle. \quad (\text{III.A.51})$$

Proof. This is a direct consequence of the definition of the tensor product, see for instance example A.7. We thus have

$$\langle\langle W| \begin{pmatrix} X_0 \\ X_1 \\ \vdots \\ X_N \end{pmatrix} \otimes \begin{pmatrix} X_0 \\ X_1 \\ \vdots \\ X_N \end{pmatrix} \otimes \dots \otimes \begin{pmatrix} X_0 \\ X_1 \\ \vdots \\ X_N \end{pmatrix} |V\rangle\rangle = \begin{pmatrix} \langle\langle W|X_0 \dots X_0 X_0|V\rangle\rangle \\ \langle\langle W|X_0 \dots X_0 X_1|V\rangle\rangle \\ \vdots \\ \langle\langle W|X_N \dots X_N X_N|V\rangle\rangle \end{pmatrix}, \quad (\text{III.A.52})$$

in agreement with the matrix product expression III.A.4. ■

We are now equipped to present the root of the algebraic relations involved in the matrix product formulation.

a) Particular example of the TASEP

We begin with the case of the single species open TASEP

Proposition A.9. *The algebraic constraints stated in (III.A.11) are equivalent to the telescopic relations:*

- *in the bulk*

$$DE = D + E \quad \Leftrightarrow \quad m \begin{pmatrix} E \\ D \end{pmatrix} \otimes \begin{pmatrix} E \\ D \end{pmatrix} = \begin{pmatrix} E \\ D \end{pmatrix} \otimes \begin{pmatrix} -1 \\ 1 \end{pmatrix} - \begin{pmatrix} -1 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} E \\ D \end{pmatrix} \quad (\text{III.A.53})$$

- *at the left boundary*

$$\langle\langle W|E = \frac{1}{\alpha} \langle\langle W| \quad \Leftrightarrow \quad \langle\langle W|B \begin{pmatrix} E \\ D \end{pmatrix} = \langle\langle W| \begin{pmatrix} -1 \\ 1 \end{pmatrix} \quad (\text{III.A.54})$$

- *at the right boundary*

$$D|V\rangle\rangle = \frac{1}{\beta} |V\rangle\rangle \quad \Leftrightarrow \quad \bar{B} \begin{pmatrix} E \\ D \end{pmatrix} |V\rangle\rangle = - \begin{pmatrix} -1 \\ 1 \end{pmatrix} |V\rangle\rangle \quad (\text{III.A.55})$$

where m , B and \bar{B} are defined in (II.A.24) and (II.A.32).

Proof. We compute explicitly

$$m \begin{pmatrix} E \\ D \end{pmatrix} \otimes \begin{pmatrix} E \\ D \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} E^2 \\ ED \\ DE \\ D^2 \end{pmatrix} = \begin{pmatrix} 0 \\ DE \\ -DE \\ 0 \end{pmatrix} \quad (\text{III.A.56})$$

and

$$\begin{pmatrix} E \\ D \end{pmatrix} \otimes \begin{pmatrix} -1 \\ 1 \end{pmatrix} - \begin{pmatrix} -1 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} E \\ D \end{pmatrix} = \begin{pmatrix} -E \\ E \\ -D \\ D \end{pmatrix} - \begin{pmatrix} -E \\ -D \\ E \\ D \end{pmatrix} = \begin{pmatrix} 0 \\ E + D \\ -E - D \\ 0 \end{pmatrix}. \quad (\text{III.A.57})$$

We thus obtain the desired result (III.A.53). In the same way for the relation on the left boundary, we compute

$$\langle\langle W|B \begin{pmatrix} E \\ D \end{pmatrix} = \langle\langle W| \begin{pmatrix} -\alpha & 0 \\ \alpha & 0 \end{pmatrix} \begin{pmatrix} E \\ D \end{pmatrix} = \langle\langle W| \begin{pmatrix} -\alpha E \\ \alpha E \end{pmatrix} = \begin{pmatrix} -\alpha \langle\langle W|E \\ \alpha \langle\langle W|E \end{pmatrix} \quad (\text{III.A.58})$$

and

$$\langle\langle W| \begin{pmatrix} -1 \\ 1 \end{pmatrix} = \begin{pmatrix} -\langle\langle W| \\ \langle\langle W| \end{pmatrix}, \quad (\text{III.A.59})$$

which yields the property (III.A.54). The equation (III.A.55) is derived in a very similar way. ■

Note that these relations are called telescopic because of their “divergence like” form. This appellation will also make sense with the proof of the following proposition. At first sight, it may appear a bit complicated to encode single relations in complicated tensor forms, like (III.A.53) instead of $DE = D + E$. However, it allows simple generalization to other models, as well as a nice and simple proof of the stationary measure property (see below).

Proposition A.10. *The matrix product state*

$$|\mathcal{S}\rangle = \frac{1}{Z_L} \langle\langle W| \begin{pmatrix} E \\ D \end{pmatrix} \otimes \begin{pmatrix} E \\ D \end{pmatrix} \otimes \cdots \otimes \begin{pmatrix} E \\ D \end{pmatrix} |V\rangle, \quad (\text{III.A.60})$$

where E , D , $\langle\langle W|$ and $|V\rangle$ satisfy the telescopic relations (III.A.53), (III.A.54) and (III.A.55), is the stationary state of the model, i.e $M|\mathcal{S}\rangle = 0$.

Note that this proposition is strictly equivalent to the proposition A.4. It has just been reformulated using the tensor product formalism.

Proof.

$$\begin{aligned}
& \left(B_1 + \sum_{k=1}^{L-1} m_{k,k+1} + \bar{B}_L \right) \langle\langle W | \left(\frac{E}{D} \right) \otimes \left(\frac{E}{D} \right) \otimes \cdots \otimes \left(\frac{E}{D} \right) | V \rangle\rangle \\
&= \langle\langle W | \left[B \left(\frac{E}{D} \right) \right] \otimes \left(\frac{E}{D} \right) \otimes \cdots \otimes \left(\frac{E}{D} \right) | V \rangle\rangle + \langle\langle W | \left(\frac{E}{D} \right) \otimes \cdots \otimes \left(\frac{E}{D} \right) \otimes \left[\bar{B} \left(\frac{E}{D} \right) \right] | V \rangle\rangle \\
&+ \sum_{k=1}^{L-1} \langle\langle W | \underbrace{\left(\frac{E}{D} \right) \otimes \cdots \otimes \left(\frac{E}{D} \right)}_{k-1} \otimes \left[m \left(\frac{E}{D} \right) \otimes \left(\frac{E}{D} \right) \right] \otimes \underbrace{\left(\frac{E}{D} \right) \otimes \cdots \otimes \left(\frac{E}{D} \right)}_{L-k-1} | V \rangle\rangle \\
&= \langle\langle W | \begin{pmatrix} -1 \\ 1 \end{pmatrix} \otimes \left(\frac{E}{D} \right) \otimes \cdots \otimes \left(\frac{E}{D} \right) | V \rangle\rangle - \langle\langle W | \left(\frac{E}{D} \right) \otimes \cdots \otimes \left(\frac{E}{D} \right) \otimes \begin{pmatrix} -1 \\ 1 \end{pmatrix} | V \rangle\rangle \\
&+ \sum_{k=1}^{L-1} \langle\langle W | \underbrace{\left(\frac{E}{D} \right) \otimes \cdots \otimes \left(\frac{E}{D} \right)}_{k-1} \otimes \left[\left(\frac{E}{D} \right) \otimes \begin{pmatrix} -1 \\ 1 \end{pmatrix} - \begin{pmatrix} -1 \\ 1 \end{pmatrix} \otimes \left(\frac{E}{D} \right) \right] \otimes \underbrace{\left(\frac{E}{D} \right) \otimes \cdots \otimes \left(\frac{E}{D} \right)}_{L-k-1} | V \rangle\rangle \\
&= \sum_{k=1}^L \langle\langle W | \underbrace{\left(\frac{E}{D} \right) \otimes \cdots \otimes \left(\frac{E}{D} \right)}_{k-1} \otimes \begin{pmatrix} -1 \\ 1 \end{pmatrix} \otimes \underbrace{\left(\frac{E}{D} \right) \otimes \cdots \otimes \left(\frac{E}{D} \right)}_{L-k} | V \rangle\rangle \\
&\quad - \sum_{k=1}^L \langle\langle W | \underbrace{\left(\frac{E}{D} \right) \otimes \cdots \otimes \left(\frac{E}{D} \right)}_{k-1} \otimes \begin{pmatrix} -1 \\ 1 \end{pmatrix} \otimes \underbrace{\left(\frac{E}{D} \right) \otimes \cdots \otimes \left(\frac{E}{D} \right)}_{L-k} | V \rangle\rangle \\
&= 0.
\end{aligned}$$

The action of the Markov matrix on the matrix product state leads to a telescopic sum. \blacksquare

b) General case

The previous cancellation scheme is quite general and goes far beyond the single species TASEP case. In fact the algebraic structure defined by the telescopic relations (in the bulk and on the boundaries) appears in all known examples of matrix product expression of the stationary state (of continuous time Markov processes). To be more precise, we consider a stochastic process described by the Markov matrix (II.A.29) where m is a $(N+1)^2 \times (N+1)^2$ matrix, while B and \bar{B} are $(N+1) \times (N+1)$ matrices. We first introduce two key vectors.

Definition A.11. *We introduce two vectors \mathbf{X} and $\bar{\mathbf{X}}$*

$$\mathbf{X} = \begin{pmatrix} X_0 \\ X_1 \\ \vdots \\ X_N \end{pmatrix}, \quad \bar{\mathbf{X}} = \begin{pmatrix} \bar{X}_0 \\ \bar{X}_1 \\ \vdots \\ \bar{X}_N \end{pmatrix}. \quad (\text{III.A.61})$$

For a given bulk local jump operator m , we say that \mathbf{X} and $\bar{\mathbf{X}}$ satisfy the bulk telescopic relation if we have

$$m\mathbf{X} \otimes \mathbf{X} = \mathbf{X} \otimes \bar{\mathbf{X}} - \bar{\mathbf{X}} \otimes \mathbf{X}. \quad (\text{III.A.62})$$

For given boundary local jump operators B and \bar{B} , we say that \mathbf{X} and $\bar{\mathbf{X}}$ satisfy the boundary telescopic relations if there exist two boundary vectors $\langle\langle W |$ and $|V \rangle\rangle$ such that

$$\langle\langle W | B\mathbf{X} = \langle\langle W | \bar{\mathbf{X}}, \quad \bar{B}\mathbf{X}|V \rangle\rangle = -\bar{\mathbf{X}}|V \rangle\rangle. \quad (\text{III.A.63})$$

We are now equipped to state the generalization of proposition A.10.

Proposition A.12. *If the vectors \mathbf{X} and $\overline{\mathbf{X}}$ satisfy the telescopic relations (III.A.62) and (III.A.63), then the matrix product state*

$$|\mathcal{S}\rangle = \frac{1}{Z_L} \langle\langle W | \mathbf{X} \otimes \mathbf{X} \otimes \cdots \otimes \mathbf{X} | V \rangle\rangle \quad (\text{III.A.64})$$

satisfies

$$M|\mathcal{S}\rangle = 0, \quad (\text{III.A.65})$$

where the Markov matrix is given by

$$M = B_1 + \sum_{k=1}^{L-1} m_{k,k+1} + \overline{B}_L. \quad (\text{III.A.66})$$

If $|\mathcal{S}\rangle$ is not vanishing, it thus provides the stationary state³ associated to the Markov matrix.

Proof. The property is proven using exactly the same cancellation scheme as for A.10, replacing the vector $(E, D)^t$ by \mathbf{X} and the vector $(-1, 1)^t$ by $\overline{\mathbf{X}}$. ■

Remark A.13. *In [192] it was proven that for any Markov matrix M that can be decomposed into the sum of operators acting locally on the lattice*

$$M = B_1 + \sum_{k=1}^{L-1} m_{k,k+1} + \overline{B}_L, \quad (\text{III.A.67})$$

it is possible to construct explicitly matrices X_0, \dots, X_N and $\overline{X}_0, \dots, \overline{X}_N$ and vectors $\langle\langle W |$ and $|V \rangle\rangle$ such that the telescopic relations (III.A.62) and (III.A.63) are fulfilled. Thanks to the previous property, we know that the stationary state is given in a matrix product form by (III.A.64) (if it is not vanishing). In practice, the construction of the vector $\langle\langle W |$ in [192] requires the prior knowledge of the stationary distribution of the model... Hence the result of [192] appears more as an existence theorem (the existence of a matrix product expression of the steady state) than as a useful tool for explicit computations of physical quantities. Indeed the algebraic relations given by (III.A.62) and (III.A.63) satisfied by the matrices X_0, \dots, X_N and $\overline{X}_0, \dots, \overline{X}_N$ and the vectors $\langle\langle W |$ and $|V \rangle\rangle$ are not sufficient to fix the value of the stationary weights (we cannot perform in general algebraic computations as we showed in (III.A.16) for the TASEP), the explicit representation is needed (or further algebraic relations, as we will see below).

c) Other examples

We have already seen in the above subsection the matrix product expression of the steady state of the open single species TASEP. We now present the case of the ASEP and of the SSEP. We give the matrix product solution within the developed framework of telescopic relations.

Example A.14. *We recall that the stochastic dynamics of the ASEP is encoded in the local jump operators m defined in (II.A.23) and B, \overline{B} defined in (II.A.31). We define the vector*

$$\mathbf{X} = \begin{pmatrix} E \\ D \end{pmatrix} \quad (\text{III.A.68})$$

where the algebraic elements E and D satisfy the relation $pDE - qED = (p - q)(E + D)$. Similarly to the TASEP case, representation of such operators as infinite matrices exists and will be given in chapter IV. We also introduce the vector

$$\overline{\mathbf{X}} = \begin{pmatrix} q - p \\ p - q \end{pmatrix}, \quad (\text{III.A.69})$$

³If the Markov matrix is irreducible, we know that the stationary state is unique. If it is not irreducible, it provides one or several of the stationary states.

and the boundary vectors $\langle\langle W|$ and $|V\rangle\rangle$ which satisfy

$$\langle\langle W|(\alpha E - \gamma D) = (p - q)\langle\langle W|, \quad \text{and} \quad (\beta D - \delta E)|V\rangle\rangle = (p - q)|V\rangle\rangle. \quad (\text{III.A.70})$$

Representation of $\langle\langle W|$ and $|V\rangle\rangle$ as infinite row and column vectors will also be given in chapter IV.

Then it is easy to check that the telescopic relations (III.A.62) and (III.A.63) hold and hence the steady state is given by (III.A.64).

Example A.15. Similar results hold for the SSEP with matrices E , D and boundary vectors $\langle\langle W|$ and $|V\rangle\rangle$ that fulfill

$$DE - ED = E + D, \quad \langle\langle W|(\alpha E - \gamma D) = \langle\langle W|, \quad \text{and} \quad (\beta D - \delta E)|V\rangle\rangle = |V\rangle\rangle. \quad (\text{III.A.71})$$

We have in this case

$$\mathbf{X} = \begin{pmatrix} E \\ D \end{pmatrix}, \quad \text{and} \quad \bar{\mathbf{X}} = \begin{pmatrix} -1 \\ 1 \end{pmatrix} \quad (\text{III.A.72})$$

We will encounter in section B more complex examples where the auxiliary vector $\bar{\mathbf{X}}$ (sometimes called hat vector) contains non scalar operators (*i.e* which do not commute with the matrices X_i), in contrast to what we saw up to now in the examples.

3 Thermodynamic equilibrium case

We now make some remarks about the matrix ansatz for a system that reaches a thermodynamic equilibrium in the long time limit. To fix the ideas we present as usual the example of the SSEP and ASEP.

a) Some examples

Example A.16. The SSEP reaches in the long time limit a thermodynamic equilibrium if and only if the particle densities of the two reservoirs are equal, *i.e*

$$\frac{\alpha}{\alpha + \gamma} = \frac{\delta}{\beta + \delta}. \quad (\text{III.A.73})$$

This condition can be rewritten more concisely $\alpha\beta = \delta\gamma$. This constraint can be derived using the detailed balance condition (that defines rigorously a thermodynamic equilibrium in the Markov chain context, see chapter I). We have indeed

$$\mathcal{S}(0, \dots, 0) = \frac{\gamma}{\alpha} \mathcal{S}(1, 0, \dots, 0) \quad (\text{III.A.74})$$

$$= \frac{\gamma}{\alpha} \mathcal{S}(0, 1, 0, \dots, 0) \quad (\text{III.A.75})$$

$$\dots \quad (\text{III.A.76})$$

$$= \frac{\gamma}{\alpha} \mathcal{S}(0, \dots, 0, 1) \quad (\text{III.A.77})$$

$$= \frac{\gamma\delta}{\alpha\beta} \mathcal{S}(0, \dots, 0), \quad (\text{III.A.78})$$

which proves that $\frac{\gamma\delta}{\alpha\beta} = 1$ is necessary. In this particular case the matrix product formulation of the steady state simplifies drastically:

$$|\mathcal{S}\rangle = \begin{pmatrix} 1-r \\ r \end{pmatrix} \otimes \dots \otimes \begin{pmatrix} 1-r \\ r \end{pmatrix}, \quad (\text{III.A.79})$$

where $r = \frac{\alpha}{\alpha + \gamma} = \frac{\delta}{\beta + \delta}$. We observe that the matrices E and D can thus be chosen as scalars in this case ($E = 1 - r$, $D = r$) and the auxiliary vector $\bar{\mathbf{X}} = 0$. The telescopic relations read indeed

$$B \begin{pmatrix} 1-r \\ r \end{pmatrix} = 0, \quad m \begin{pmatrix} 1-r \\ r \end{pmatrix} \otimes \begin{pmatrix} 1-r \\ r \end{pmatrix} = 0, \quad \bar{B} \begin{pmatrix} 1-r \\ r \end{pmatrix} = 0. \quad (\text{III.A.80})$$

Example A.17. *The ASEP reaches a thermodynamic equilibrium if and only if the parameters $\alpha, \beta, \gamma, \delta$ and q fulfill the constraint*

$$\frac{\gamma\delta}{\alpha\beta} \left(\frac{q}{p}\right)^{L-1} = 1. \quad (\text{III.A.81})$$

This can be intuitively understood as the reservoir densities compensating exactly the driving force in the bulk. Once again this constraint can be determined using the detailed balance condition (that must hold in a thermodynamic equilibrium). We have indeed

$$\mathcal{S}(0, \dots, 0) = \frac{\gamma}{\alpha} \mathcal{S}(1, 0, \dots, 0) \quad (\text{III.A.82})$$

$$= \frac{\gamma q}{\alpha p} \mathcal{S}(0, 1, 0, \dots, 0) \quad (\text{III.A.83})$$

$$\dots \quad (\text{III.A.84})$$

$$= \frac{\gamma q^{L-1}}{\alpha p^{L-1}} \mathcal{S}(0, \dots, 0, 1) \quad (\text{III.A.85})$$

$$= \frac{\gamma\delta}{\alpha\beta} \left(\frac{q}{p}\right)^{L-1} \mathcal{S}(0, \dots, 0), \quad (\text{III.A.86})$$

which proves that $\frac{\gamma\delta}{\alpha\beta} \left(\frac{q}{p}\right)^{L-1} = 1$. In this particular case the stationary state can still be given in matrix product form

$$|\mathcal{S}\rangle = \frac{1}{Z_L} \langle\langle W | \mathbf{X} \otimes \dots \otimes \mathbf{X} | V \rangle\rangle, \quad (\text{III.A.87})$$

with

$$\mathbf{X} = \begin{pmatrix} E \\ D \end{pmatrix} \quad (\text{III.A.88})$$

where the operators E, D and the boundary vectors $\langle\langle W |$ and $|V\rangle\rangle$ satisfy

$$pDE = qED, \quad \langle\langle W | (\alpha E - \gamma D) = 0, \quad (\delta E - \beta D) | V \rangle\rangle = 0. \quad (\text{III.A.89})$$

The vector \mathbf{X} above satisfies the relations $m\mathbf{X} \otimes \mathbf{X} = 0$, $\langle\langle W | B\mathbf{X} = 0$ and $\bar{B}\mathbf{X} | V \rangle\rangle = 0$ which ensure that (III.A.87) is the stationary state of the model. An explicit representation of such matrices and vector can be found on the $L + 1$ dimensional vector space spanned by the basis $\{|k\rangle\rangle\}_{0 \leq k \leq L}$

$$E = \sum_{k=0}^{L-1} |k+1\rangle\rangle \langle\langle k|, \quad D = \sum_{k=0}^{L-1} \frac{\delta}{\beta} \left(\frac{q}{p}\right)^k |k+1\rangle\rangle \langle\langle k|, \quad (\text{III.A.90})$$

and

$$\langle\langle W | = \langle\langle L|, \quad |V\rangle\rangle = |0\rangle\rangle. \quad (\text{III.A.91})$$

In matrix notation it gives explicitly

$$E = \begin{pmatrix} 0 & 0 & 0 & \dots & 0 \\ 1 & 0 & 0 & & \vdots \\ 0 & 1 & 0 & \ddots & \vdots \\ \vdots & & \ddots & \ddots & 0 \\ 0 & \dots & 0 & 1 & 0 \end{pmatrix}, \quad D = \begin{pmatrix} 0 & 0 & 0 & \dots & 0 \\ \frac{\delta}{\beta} & 0 & 0 & & \vdots \\ 0 & \frac{\delta q}{\beta p} & 0 & \ddots & \vdots \\ \vdots & & \ddots & \ddots & 0 \\ 0 & \dots & 0 & \frac{\delta}{\beta} \left(\frac{q}{p}\right)^{L-1} & 0 \end{pmatrix}, \quad (\text{III.A.92})$$

and

$$\langle\langle W | = (0 \quad \dots \quad 0 \quad 1), \quad |V\rangle\rangle = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}. \quad (\text{III.A.93})$$

It is easy to see that this representation works only when the constraint (III.A.81) is satisfied. Indeed the relation $\langle\langle W | (\alpha E - \gamma D) = 0$ is only fulfilled in this case.

Note that the matrix product state (III.A.87) can be rewritten as an inhomogeneous factorized state

$$|\mathcal{S}\rangle = \left(\frac{1}{\frac{\delta}{\beta} \left(\frac{q}{p} \right)^{L-1}} \right) \otimes \cdots \otimes \left(\frac{1}{\frac{\delta}{\beta} \frac{q}{p}} \right) \otimes \left(\frac{1}{\frac{\delta}{\beta}} \right) \quad (\text{III.A.94})$$

or equivalently using the constraint (III.A.81)

$$|\mathcal{S}\rangle = \left(\frac{1}{\frac{\alpha}{\gamma}} \right) \otimes \left(\frac{1}{\frac{\alpha}{\gamma} \frac{p}{q}} \right) \otimes \cdots \otimes \left(\frac{1}{\frac{\alpha}{\gamma} \left(\frac{p}{q} \right)^{L-1}} \right). \quad (\text{III.A.95})$$

The two previous examples both share the feature of having a vanishing auxiliary vector $\bar{\mathbf{X}}$ in the telescopic relations associated to the matrix product formulation of the steady state. This seems to be always the case in systems that reach a thermodynamic equilibrium and whose steady state can be written in matrix product form (although we do not have any general proof of this fact). The relation $m\mathbf{X} \otimes \mathbf{X} = 0$ (telescopic relation with vanishing auxiliary vector) gave in the previous examples commutation relations of the type $X_i X_j = \exp(-\Delta E/kT) X_j X_i$ where $\exp(-\Delta E/kT) = \frac{S(\dots, i, j, \dots)}{S(\dots, j, i, \dots)}$ is the Boltzmann factor obtained when exchanging particles of species i and j lying on adjacent sites on the lattice (see chapter I for details). Similar observations hold also for the relations on the boundary vectors $\langle\langle W |$ and $|V\rangle\rangle$. We will encounter this fact again in the remark below.

b) A new look on the open TASEP stationary distribution

We end up this subsection on matrix product steady states with an intriguing observation. The stationary distribution of the single species open TASEP can be obtained as the marginal of the Boltzmann distribution of a more complex process at thermodynamic equilibrium. To be more precise this process is also defined on a one dimensional lattice with L sites. Each site i of the lattice can be in three different states: $\tau_i = -, 0, +$. The stochastic dynamics of the process is defined as usual locally (on two adjacent sites in the bulk and on the single extremal sites at the boundaries) by the following rules

Left	Bulk	Right
$- \xrightarrow{1} 0$	$0+ \xleftrightarrow{1} +0$	$+ \xrightarrow{1} 0$
$0 \xrightarrow{a} -$	$0- \xleftrightarrow{1} -0$	$0 \xrightarrow{b} +$
	$+- \xleftrightarrow{1} 00$	

(III.A.96)

where the parameters a and b , that appeared previously in the pushing procedure of the TASEP, are given by

$$a = \frac{1 - \alpha}{\alpha}, \quad \text{and} \quad b = \frac{1 - \beta}{\beta}. \quad (\text{III.A.97})$$

In the basis $|--\rangle, |-0\rangle, |-+\rangle, |0-\rangle, |00\rangle, |0+\rangle, |+-\rangle, |+0\rangle, |++\rangle$ ordered this way, the bulk local jump operator m associated to the above dynamical rules reads

$$m = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & -1 & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & -1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & -1 & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & -1 & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot & -1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & -1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}. \quad (\text{III.A.98})$$

In the basis $|-\rangle, |0\rangle, |+\rangle$ ordered like this, the boundary local jump operators read

$$B = \begin{pmatrix} -1 & a & \cdot \\ 1 & -a & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}, \quad \text{and} \quad \bar{B} = \begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & -b & 1 \\ \cdot & b & -1 \end{pmatrix}. \quad (\text{III.A.99})$$

The stationary state of this model can be expressed in a matrix product form. We define e and d two algebraic elements such that $de = 1$ and two boundary vectors $\langle\langle W|$ and $|V\rangle\rangle$ such that $\langle\langle W|e = a\langle\langle W|$ and $d|V\rangle\rangle = b|V\rangle\rangle$. Representation of such algebraic objects are $e = E - 1$ and $d = D - 1$ with E, D given in (III.A.12) and $\langle\langle W|$ and $|V\rangle\rangle$ are the same as the ones given in (III.A.14). We define

$$\mathbf{X} = \begin{pmatrix} X_- \\ X_0 \\ X_+ \end{pmatrix} = \begin{pmatrix} e \\ 1 \\ d \end{pmatrix}. \quad (\text{III.A.100})$$

We then have

$$m\mathbf{X} \otimes \mathbf{X} = m \begin{pmatrix} e^2 \\ e \\ ed \\ e \\ 1 \\ d \\ de \\ d \\ d^2 \end{pmatrix} = \begin{pmatrix} 0 \\ -e + e \\ 0 \\ e - e \\ -1 + de \\ -d + d \\ 1 - de \\ d - d \\ 0 \end{pmatrix} = 0. \quad (\text{III.A.101})$$

We have also

$$\langle\langle W|B\mathbf{X} = \langle\langle W| \begin{pmatrix} -e + a \\ e - a \\ 0 \end{pmatrix} = 0, \quad \text{and} \quad \bar{B}\mathbf{X}|V\rangle\rangle = \begin{pmatrix} 0 \\ -b + d \\ b - d \end{pmatrix} |V\rangle\rangle = 0. \quad (\text{III.A.102})$$

Hence the steady state is given by

$$|\mathcal{S}\rangle = \frac{1}{Z_L} \langle\langle W|\mathbf{X} \otimes \cdots \otimes \mathbf{X}|V\rangle\rangle. \quad (\text{III.A.103})$$

This is a thermodynamic equilibrium, the detailed balance is indeed satisfied. To prove this statement we have to check that the identity $m(\mathcal{C} \rightarrow \mathcal{C}')\mathcal{S}(\mathcal{C}) = m(\mathcal{C}' \rightarrow \mathcal{C})\mathcal{S}(\mathcal{C}')$ holds for every allowed transition $\mathcal{C} \rightarrow \mathcal{C}'$. We have for instance

$$\mathcal{S}(\tau_1, \dots, \tau_{i-1}, 0, +, \tau_{i+2}, \dots, \tau_L) - \mathcal{S}(\tau_1, \dots, \tau_{i-1}, +, 0, \tau_{i+2}, \dots, \tau_L) \quad (\text{III.A.104})$$

$$= \frac{1}{Z_L} \langle\langle W|X_{\tau_1} \dots X_{\tau_{i-1}} (1d - d1) X_{\tau_{i+2}} \dots X_{\tau_L}|V\rangle\rangle \quad (\text{III.A.105})$$

$$= 0, \quad (\text{III.A.106})$$

or

$$\mathcal{S}(\tau_1, \dots, \tau_{i-1}, +, -, \tau_{i+2}, \dots, \tau_L) - \mathcal{S}(\tau_1, \dots, \tau_{i-1}, 0, 0, \tau_{i+2}, \dots, \tau_L) \quad (\text{III.A.107})$$

$$= \frac{1}{Z_L} \langle\langle W|X_{\tau_1} \dots X_{\tau_{i-1}} (de - 1 \cdot 1) X_{\tau_{i+2}} \dots X_{\tau_L}|V\rangle\rangle \quad (\text{III.A.108})$$

$$= 0, \quad (\text{III.A.109})$$

or for transitions involving the boundaries

$$a\mathcal{S}(0, \tau_2, \dots, \tau_L) - \mathcal{S}(-, \tau_2, \dots, \tau_L) \quad (\text{III.A.110})$$

$$= \frac{1}{Z_L} \langle\langle W|(a - e)X_{\tau_2} \dots X_{\tau_L}|V\rangle\rangle \quad (\text{III.A.111})$$

$$= 0. \quad (\text{III.A.112})$$

Similar computations apply also for other allowed transitions.

From the identities $E = 1 + e$ and $D = 1 + d$ it is straightforward to see that the stationary weights of the TASEP are obtained by summing several Boltzmann weights of this process. For instance

$$\langle\langle W|DE|V\rangle\rangle = \langle\langle W|1 \cdot 1|V\rangle\rangle + \langle\langle W|1 \cdot e|V\rangle\rangle + \langle\langle W|d \cdot 1|V\rangle\rangle + \langle\langle W|d \cdot e|V\rangle\rangle. \quad (\text{III.A.113})$$

Each of the term in the last sum is a Boltzmann weight of the '(-, 0, +)' process.

It would be interesting to study if the same kind of approach could be generalized to other non-equilibrium models. This would support the fact that we need to enlarge the configuration space of out-of-equilibrium systems to obtain an efficient description of their stationary distribution. A lot remains to be understood in this direction.

4 Link with integrability

Although the matrix ansatz is often associated with integrable models because of the numerous examples of matrix product stationary states that can be found in this class, it does not seem to exist only in such privileged systems. There are indeed a few example of a matrix product formulation of the steady state in models that are not known to be integrable (but are not proven to be non-integrable...). Among them can be mentioned the ABC model on the ring with equal densities of each particle species [178] or a two species TASEP with open boundaries [176]. However we will argue in this subsection that, for stochastic integrable models, the construction of the steady state in a matrix product form is made easier by the use of the R and K matrices. These key objects play indeed a central role in encoding the algebraic relations that must be satisfied by the matrices and boundary vectors involved in the matrix ansatz.

a) Algebraic setup

The starting point of the construction is to define a vector which depends on the spectral parameter z and that can be seen as an upgrading of the vector \mathbf{X}

$$\mathbf{A}(z) = \begin{pmatrix} A_0(z) \\ A_1(z) \\ \vdots \\ A_N(z) \end{pmatrix} \quad (\text{III.A.114})$$

The entries $A_i(z)$ of this vector belongs to a non-commutative algebra \mathcal{A} and have a finite expansion with respect to the spectral parameter z :

$$A_i(z) = \sum_{k=-p}^q G_{i,k} z^k, \quad \text{with } G_{i,k} \in \mathcal{A}. \quad (\text{III.A.115})$$

We will see that the generators $G_{i,k}$ and their commutation relations play a crucial role in the matrix product construction: they are the building blocks of the matrices X_0, \dots, X_N involved in the matrix ansatz. The number of components $N + 1$ of the vector is directly related to the number of different possible local configurations on a single site (N different species of particles plus the hole). The vector $\mathbf{A}(z)$ can be thought as a spectral parameter dependent generalization of the vector

$$\mathbf{X} = \begin{pmatrix} X_0 \\ X_1 \\ \vdots \\ X_N \end{pmatrix} \quad (\text{III.A.116})$$

involved in the matrix product expression of the steady state. The precise relation between these two vectors will be given in subsection b).

We now give examples of such vectors $\mathbf{A}(z)$ that are relevant in the study of the TASEP, ASEP and SSEP. These three models will be systematically used all along this subsection to illustrate the different notions introduced. They are indeed probably familiar to the reader and will help to fix the ideas.

Example A.18. *The specific expression of the vector $\mathbf{A}(z)$ that is relevant to the matrix product formulation of the stationary state in the TASEP and in the ASEP reads [V3]*

$$\mathbf{A}(z) = \begin{pmatrix} z + e \\ \frac{1}{z} + d \end{pmatrix}. \quad (\text{III.A.117})$$

Note that the commutation relations satisfied by the generators e and d are not the same in the case of the TASEP and of the ASEP, see subsection b).

Example A.19. *In the case of the SSEP, the vector $\mathbf{A}(z)$ takes the explicit form [105]*

$$\mathbf{A}(z) = \begin{pmatrix} -z + E \\ z + D \end{pmatrix}. \quad (\text{III.A.118})$$

We will see in section B more examples of such vectors $\mathbf{A}(z)$ with a richer expansion and a bigger number of components.

b) Zamolodchikov-Faddeev relation

The question that we address now is the one of encoding the commutation relations of the generators entering the definition of the vector $\mathbf{A}(z)$. It was first noticed in [105] and then investigated in [V3] that the Zamolodchikov-Faddeev relation play a central role in the matrix product construction. In the same spirit as the FRT formalism (which permits to present the commutation relations of the generators of the quantum groups out of the associated R -matrix), this relation is a way to efficiently encode the algebraic relations required by the matrix ansatz, with the help of the R -matrix associated to the integrable model.

Definition A.20. *A Zamolodchikov-Faddeev algebra is an algebra generated by the algebraic elements entering the definition of the vector $\mathbf{A}(z)$ subject to the Zamolodchikov-Faddeev (ZF) relation⁴*

$$\check{R} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \mathbf{A}(z_1) \otimes \mathbf{A}(z_2) = \mathbf{A}(z_2) \otimes \mathbf{A}(z_1). \quad (\text{III.A.119})$$

In words, the action of the matrix \check{R} induces an exchange of the spectral parameters z_1 and z_2 . The same kind of idea will appear again in chapter IV, when dealing with the quantum Knizhnik-Zamolodchikov equation. This ZF relation is well-known in the context of integrable quantum field theory. It was first introduced in [193]. It appears as a generalization of the commutation of creation operators of bosons (which corresponds to $\check{R}(z) = 1$) or the anti-commutation of creation operators of fermions (which corresponds to $\check{R}(z) = -1$).

Proposition A.21. *The Zamolodchikov-Faddeev relation (III.A.119) defines an associative algebra if the matrix \check{R} satisfies the braided Yang-Baxter equation.*

Proof. The order of the spectral parameters z_1 , z_2 and z_3 in the product $\mathbf{A}(z_3) \otimes \mathbf{A}(z_2) \otimes \mathbf{A}(z_1)$ can be reversed in two different ways. We can first exchange z_1 and z_2 , then exchange z_1 and z_3 and finally exchange z_2 and z_3 like this

$$\begin{aligned} \mathbf{A}(z_3) \otimes \mathbf{A}(z_2) \otimes \mathbf{A}(z_1) &= \check{R}_2 \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \mathbf{A}(z_3) \otimes \mathbf{A}(z_1) \otimes \mathbf{A}(z_2) \\ &= \check{R}_2 \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \check{R}_1 \begin{pmatrix} z_1 \\ z_3 \end{pmatrix} \mathbf{A}(z_1) \otimes \mathbf{A}(z_3) \otimes \mathbf{A}(z_2) \\ &= \check{R}_2 \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \check{R}_1 \begin{pmatrix} z_1 \\ z_3 \end{pmatrix} \check{R}_2 \begin{pmatrix} z_2 \\ z_3 \end{pmatrix} \mathbf{A}(z_1) \otimes \mathbf{A}(z_2) \otimes \mathbf{A}(z_3), \end{aligned}$$

⁴Note that the ZF algebra is in general defined for a vector $\mathbf{A}(z)$ which is a Laurent series with respect to z . We are interested in this manuscript in a vector $\mathbf{A}(z)$ with a finite expansion with respect to the spectral parameter z , which thus corresponds to a subclass of the general ZF framework.

where we recall that $\check{R}_1 = \check{R} \otimes \mathbf{1}$ and $\check{R}_2 = \mathbf{1} \otimes \check{R}$.

The other way is to first exchange z_2 and z_3 , then exchange z_1 and z_3 and finally exchange z_1 and z_2 :

$$\begin{aligned} \mathbf{A}(z_3) \otimes \mathbf{A}(z_2) \otimes \mathbf{A}(z_1) &= \check{R}_1 \left(\frac{z_2}{z_3} \right) \mathbf{A}(z_2) \otimes \mathbf{A}(z_3) \otimes \mathbf{A}(z_1) \\ &= \check{R}_1 \left(\frac{z_2}{z_3} \right) \check{R}_2 \left(\frac{z_1}{z_3} \right) \mathbf{A}(z_2) \otimes \mathbf{A}(z_1) \otimes \mathbf{A}(z_3) \\ &= \check{R}_1 \left(\frac{z_2}{z_3} \right) \check{R}_2 \left(\frac{z_1}{z_3} \right) \check{R}_1 \left(\frac{z_1}{z_2} \right) \mathbf{A}(z_1) \otimes \mathbf{A}(z_2) \otimes \mathbf{A}(z_3). \end{aligned}$$

The consistency between these two different ways of performing the computation (*i.e* the associativity of the algebra) is ensured by the fact that \check{R} satisfies the braided Yang-Baxter equation. \blacksquare

Remark A.22. Another consistency relation, which arises when applying the ZF relation twice, is ensured by the unitarity (II.B.8) of the matrix \check{R} :

$$\mathbf{A}(z_2) \otimes \mathbf{A}(z_1) = \check{R} \left(\frac{z_1}{z_2} \right) \mathbf{A}(z_1) \otimes \mathbf{A}(z_2) = \check{R} \left(\frac{z_1}{z_2} \right) \check{R} \left(\frac{z_2}{z_1} \right) \mathbf{A}(z_2) \otimes \mathbf{A}(z_1). \quad (\text{III.A.120})$$

Remark A.23. If there exist a vector $v(z)$ (with scalar entries) satisfying $\check{R} \left(\frac{z_1}{z_2} \right) v(z_1) \otimes v(z_2) = v(z_2) \otimes v(z_1)$, (*i.e* which is a scalar representation of the ZF algebra), then it is possible to construct a sub-algebra of the quantum group associated with \check{R} that fulfills the requirement of the ZF algebra (III.A.119). More precisely, if $\mathbf{T}(z)$ is a matrix (with algebraic entries) that satisfies the RTT relation (II.B.83), then the vector defined by $\mathbf{A}(z) = \mathbf{T}(z)v(z)$ satisfies (III.A.119). More generally if we have a representation $\mathbf{A}(z)^{(q)}$ of the ZF algebra on a vector space \mathcal{V}_q and a representation $\mathbf{T}(z)^{(q')}$ of the RTT algebra on a vector space $\mathcal{V}_{q'}$ then we can build a new representation $\mathbf{T}(z)^{(q')} \mathbf{A}(z)^{(q)}$ of the ZF algebra on the vector space $\mathcal{V}_{q'} \otimes \mathcal{V}_q$. See chapter IV and [V3] for more details.

We now turn to a more physical interpretation of the ZF relation and shed some light on its connection with the telescopic relation (III.A.62).

Proposition A.24. Let $\mathbf{A}(z)$ satisfies the ZF relation (III.A.119). Define the vectors $\mathbf{X} = \mathbf{A}(1)$ and $\bar{\mathbf{X}} = \theta \mathbf{A}'(1)$ (where θ is the proportionality coefficient involved in (II.B.5) and \cdot' denotes the derivation with respect to the spectral parameter). Then we have the telescopic relation

$$m\mathbf{X} \otimes \mathbf{X} = \mathbf{X} \otimes \bar{\mathbf{X}} - \bar{\mathbf{X}} \otimes \mathbf{X}. \quad (\text{III.A.121})$$

Proof. The telescopic relation is obtained by taking the derivative with respect to z_1 in the ZF relation (III.A.119) and setting $z_1 = z_2 = 1$. We then need to apply the definition of the vectors \mathbf{X} and $\bar{\mathbf{X}}$ and to use the fact that $m = \theta \check{R}'(1)$. \blacksquare

This precise connection between the ZF relation and the bulk telescopic relation of the matrix ansatz was first stated in [105] for the SSEP and in [V3] for the general case. We now present how this framework can be applied to the TASEP, ASEP and SSEP.

Example A.25. We come back to the TASEP case. We write the ZF relation with the matrix \check{R} , defined in (II.B.14), and the vector $\mathbf{A}(z)$, defined in (III.A.117), to determine the algebraic constraints satisfied by the generators e and d . A direct computation yields

$$\check{R} \left(\frac{z_1}{z_2} \right) \mathbf{A}(z_1) \otimes \mathbf{A}(z_2) = \mathbf{A}(z_2) \otimes \mathbf{A}(z_1) \Leftrightarrow \begin{pmatrix} 0 & & & \\ \frac{z_2 - z_1}{z_2} (de - 1) & & & \\ \frac{z_1 - z_2}{z_2} (de - 1) & & & \\ & & & 0 \end{pmatrix} = 0 \Leftrightarrow de = 1. \quad (\text{III.A.122})$$

The matrices E and D are thus given by

$$\begin{pmatrix} E \\ D \end{pmatrix} = \mathbf{X} = \mathbf{A}(1) = \begin{pmatrix} 1+e \\ 1+d \end{pmatrix}. \quad (\text{III.A.123})$$

We can then recover easily from the relation $de = 1$ that

$$DE = (1+d)(1+e) = 1+e+d+de = 1+e+1+d = E+D, \quad (\text{III.A.124})$$

in agreement with the statement (III.A.11). This framework allows us also to recover the expression of the hat vector

$$\bar{\mathbf{X}} = \theta \mathbf{A}'(1) = - \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}, \quad (\text{III.A.125})$$

where we recall that the value of θ associated to the TASEP is -1 .

Example A.26. In the ASEP case the matrix \check{R} is defined in (II.B.13) and the vector $\mathbf{A}(z)$ in (III.A.117). A straightforward computation allows us to establish that the ZF relation is equivalent to the relation $pde - qed = p - q$. The expressions of the matrices E and D are again derived through

$$\begin{pmatrix} E \\ D \end{pmatrix} = \mathbf{X} = \mathbf{A}(1) = \begin{pmatrix} 1+e \\ 1+d \end{pmatrix}. \quad (\text{III.A.126})$$

The relation $pde - qed = p - q$ implies immediately that

$$pDE - qED = (1+d)(1+e) - q(1+e)(1+d) = (p-q)(1+e+d) + pde - qed = (p-q)(E+D), \quad (\text{III.A.127})$$

in agreement with A.14. We can also derive the expression of the hat vector

$$\bar{\mathbf{X}} = \theta \mathbf{A}'(1) = (q-p) \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \begin{pmatrix} q-p \\ p-q \end{pmatrix}, \quad (\text{III.A.128})$$

where we recall that the value of θ associated to the ASEP is $q-p$.

Example A.27. In the SSEP case, the matrix \check{R} has been introduced in (II.B.15) and the vector $\mathbf{A}(z)$ is given in (III.A.118). We write the ZF relation (with additive spectral parameters, in agreement with the Yang-Baxter equation (II.B.12)), to determine the commutation relation satisfied by the generators E and D . By direct computation we show that

$$\check{R}(z_1 - z_2) \mathbf{A}(z_1) \otimes \mathbf{A}(z_2) = \mathbf{A}(z_2) \otimes \mathbf{A}(z_1) \Leftrightarrow DE - ED = E + D, \quad (\text{III.A.129})$$

which is in agreement with A.15. We can also derive the expression of the hat vector

$$\bar{\mathbf{X}} = \theta \mathbf{A}'(0) = \begin{pmatrix} -1 \\ 1 \end{pmatrix}, \quad (\text{III.A.130})$$

where we recall that the value of θ associated to the SSEP is 1 .

The examples presented above should not mislead the reader to think that the ZF relation is equivalent to the telescopic relation (III.A.62). This is the case only when the hat vector $\bar{\mathbf{X}}$ has scalar entries (as in the three examples presented above). But let us stress that when $\bar{\mathbf{X}}$ is not scalar, the ZF relation often contains far more information than the telescopic relation. In the next section B we will encounter an example in which the telescopic relation does not give enough information to compute efficiently the stationary weights of the model (using only the algebraic relations, as it has been done in (III.A.16) for instance, and not using the explicit representation of the matrices X_i). In such model some additional information given by the ZF relations are needed to simplify the computations (for instance information telling us how to commute an operator X_i with a hat operator \bar{X}_j). Moreover, we will observe in the particular examples of section B, that the ZF relations often provide a change of generator basis that is very convenient for the computation of physical quantities. The reader may refer to section B for more details.

c) Ghoshal-Zamolodchikov relations

The previous sub-section dealt with the encoding of the commutation relations that must be verified by the matrices X_0, \dots, X_N involved in the matrix ansatz. We address here the question of the algebraic relations between the boundary vectors $\langle\langle W|$ and $|V\rangle\rangle$ and the matrices X_i . Similarly to the bulk case, where (for integrable models) the bulk telescopic relation can be upgraded to a spectral parameter dependent relation (the ZF relation) containing more information, the boundary telescopic relations derive also from more general relations: the Ghoshal-Zamolodchikov (GZ) relations. They are intuitively interpreted as the boundary counterparts of the ZF relation. They are expressed using the K matrices associated to the integrable model under consideration.

Definition A.28. For matrices K and \bar{K} satisfying the reflection equations (II.C.1) and (II.C.8), the Ghoshal-Zamolodchikov relations read

$$\langle\langle W| \left(K(z) \mathbf{A} \left(\frac{1}{z} \right) - \mathbf{A}(z) \right) = 0, \quad \left(\bar{K}(z) \mathbf{A} \left(\frac{1}{z} \right) - \mathbf{A}(z) \right) |V\rangle\rangle = 0. \quad (\text{III.A.131})$$

Note that in these relations the vector $|V\rangle\rangle$ (respectively $\langle\langle W|$) is a (possibly infinite dimensional) column vector (row vector respectively). The entries of $\mathbf{A}(z)$ are (possibly infinite dimensional) matrices acting on the vectors $\langle\langle W|$ and $|V\rangle\rangle$ with the usual matrix product.

These relations appeared first in the context of quantum field theory to deal with integrable boundaries [194]. In this context $|V\rangle\rangle$ is interpreted as the vacuum state of the theory. The relevance of these relations for integrable stochastic processes was first noticed in [105] and then investigated in [V3].

Proposition A.29. The two Ghoshal-Zamolodchikov relations (III.A.131) are consistent with the Zamolodchikov-Faddeev relation (III.A.119).

Proof. Starting from the quantity $\langle\langle W| \mathbf{A}(z_2) \otimes \mathbf{A}(z_1)$, there are indeed two different ways to change $z_1 \rightarrow 1/z_1$ and $z_2 \rightarrow 1/z_2$. The first one is to change z_2 to $1/z_2$ using the GZ relation, then exchange $1/z_2$ and z_1 using the ZF relation, and then change z_1 to $1/z_1$ and finally exchange $1/z_1$ and $1/z_2$:

$$\begin{aligned} \langle\langle W| \mathbf{A}(z_2) \otimes \mathbf{A}(z_1) &= K_1(z_2) \langle\langle W| \mathbf{A} \left(\frac{1}{z_2} \right) \otimes \mathbf{A}(z_1) \\ &= K_1(z_2) \check{R}(z_1 z_2) \langle\langle W| \mathbf{A}(z_1) \otimes \mathbf{A} \left(\frac{1}{z_2} \right) \\ &= K_1(z_2) \check{R}(z_1 z_2) K_1(z_1) \langle\langle W| \mathbf{A} \left(\frac{1}{z_1} \right) \otimes \mathbf{A} \left(\frac{1}{z_2} \right) \\ &= K_1(z_2) \check{R}(z_1 z_2) K_1(z_1) \check{R} \left(\frac{z_1}{z_2} \right) \langle\langle W| \mathbf{A} \left(\frac{1}{z_2} \right) \otimes \mathbf{A} \left(\frac{1}{z_1} \right), \end{aligned}$$

where we recall that $K_1(z) = K(z) \otimes \mathbf{1}$.

The other way to perform the transformation is to first exchange z_1 and z_2 , then change z_1 to $1/z_1$, then exchange $1/z_1$ and z_2 and finally change z_2 to $1/z_2$:

$$\begin{aligned} \langle\langle W| \mathbf{A}(z_2) \otimes \mathbf{A}(z_1) &= \check{R} \left(\frac{z_1}{z_2} \right) \langle\langle W| \mathbf{A}(z_1) \otimes \mathbf{A}(z_2) \\ &= \check{R} \left(\frac{z_1}{z_2} \right) K_1(z_1) \langle\langle W| \mathbf{A} \left(\frac{1}{z_1} \right) \otimes \mathbf{A}(z_2) \\ &= \check{R} \left(\frac{z_1}{z_2} \right) K_1(z_1) \check{R}(z_1 z_2) \langle\langle W| \mathbf{A}(z_2) \otimes \mathbf{A} \left(\frac{1}{z_1} \right) \\ &= \check{R} \left(\frac{z_1}{z_2} \right) K_1(z_1) \check{R}(z_1 z_2) K_1(z_2) \langle\langle W| \mathbf{A} \left(\frac{1}{z_2} \right) \otimes \mathbf{A} \left(\frac{1}{z_1} \right). \end{aligned}$$

The consistency between these two different ways of doing the transformation is ensured by the fact that the matrix K satisfies the reflection equation (II.C.1). Similarly there are also two ways to transform z_1 to $1/z_1$ and z_2 to $1/z_2$ in the expression $\mathbf{A}(z_2) \otimes \mathbf{A}(z_1)|V\rangle\rangle$. The consistency is again ensured by the fact that the matrix \bar{K} solves the reversed reflection equation (II.C.8). ■

Remark A.30. *Another consistency relation, which arises when applying a GZ relation twice, is ensured by the unitarity (II.C.6) of the matrices K and \bar{K} :*

$$\langle\langle W|\mathbf{A}(z) = K(z)\langle\langle W|\mathbf{A}\left(\frac{1}{z}\right) = K(z)K\left(\frac{1}{z}\right)\langle\langle W|\mathbf{A}(z), \quad (\text{III.A.132})$$

and

$$\mathbf{A}(z)|V\rangle\rangle = \bar{K}(z)\mathbf{A}\left(\frac{1}{z}\right)|V\rangle\rangle = \bar{K}(z)\bar{K}\left(\frac{1}{z}\right)\mathbf{A}(z)|V\rangle\rangle. \quad (\text{III.A.133})$$

We now turn to a more physical interpretation of the GZ relations and shed some light on their connection with the boundary telescopic relations (III.A.63).

Proposition A.31. *Let $\mathbf{A}(z)$, $\langle\langle W|$ and $|V\rangle\rangle$ satisfying the GZ relations (III.A.131). Define the vectors $\mathbf{X} = \mathbf{A}(1)$ and $\bar{\mathbf{X}} = \theta\mathbf{A}'(1)$ (where θ is the proportionality coefficient involved in (II.B.5), (II.C.3) and (II.C.9)). Then we have the telescopic relations (III.A.63):*

$$\langle\langle W|B\mathbf{X} = \langle\langle W|\bar{\mathbf{X}}, \quad \bar{B}\mathbf{X}|V\rangle\rangle = -\bar{\mathbf{X}}|V\rangle\rangle. \quad (\text{III.A.134})$$

Proof. The telescopic relations are obtained by taking the derivative with respect to z in the GZ relations (III.A.131) and setting $z = 1$. We then need to apply the definition of the vectors \mathbf{X} and $\bar{\mathbf{X}}$ and to use the fact that $B = \frac{\theta}{2}K'(1)$ and $\bar{B} = -\frac{\theta}{2}\bar{K}'(1)$. ■

We now illustrate these GZ relations on the familiar examples that are the TASEP, the ASEP and the SSEP.

Example A.32. *Coming back again to the TASEP case, we write the GZ relations with the boundary matrices K and \bar{K} defined in (II.C.15) and (II.C.17) and the vector $\mathbf{A}(z)$ defined in (III.A.117) to determine the algebraic constraints between by the generators e and d and the boundary vectors $\langle\langle W|$ and $|V\rangle\rangle$. A direct computation yields*

$$\langle\langle W|K(z)\mathbf{A}\left(\frac{1}{z}\right) = \langle\langle W|\mathbf{A}(z) \Leftrightarrow \langle\langle W|\left(\frac{(1-z^2)(\alpha e + \alpha - 1)}{\alpha z - \alpha - z} - \frac{(1-z^2)(\alpha e + \alpha - 1)}{\alpha z - \alpha - z}\right) = 0 \Leftrightarrow \langle\langle W|(\alpha e + \alpha - 1) = 0. \quad (\text{III.A.135})$$

In the same way

$$\bar{K}(z)\mathbf{A}\left(\frac{1}{z}\right)|V\rangle\rangle = \mathbf{A}(z)|V\rangle\rangle \Leftrightarrow \left(\frac{(z^2-1)(\beta d + \beta - 1)}{z(\beta z - \beta + 1)} - \frac{(z^2-1)(\beta d + \beta - 1)}{z(\beta z - \beta + 1)}\right)|V\rangle\rangle = 0 \Leftrightarrow (\beta d + \beta - 1)|V\rangle\rangle = 0. \quad (\text{III.A.136})$$

We can then recover easily, from the relation $\langle\langle W|(\alpha e + \alpha - 1) = 0$ and having in mind the identity $E = 1 + e$, that

$$\langle\langle W|E = \langle\langle W|(1 + e) = \frac{1}{\alpha}\langle\langle W| \quad (\text{III.A.137})$$

in agreement with the statement (III.A.11). Similarly using relation $(\beta d + \beta - 1)|V\rangle\rangle = 0$ we can show

$$D|V\rangle\rangle = (1 + d)|V\rangle\rangle = \frac{1}{\beta}|V\rangle\rangle \quad (\text{III.A.138})$$

which is also in agreement with (III.A.11).

Example A.33. In the ASEP case the matrices K and \bar{K} are defined in (II.C.10) and (II.C.12) and the vector $\mathbf{A}(z)$ in (III.A.117). A straightforward computation allows us to establish that the GZ relations are equivalent to the relations

$$\langle\langle W | (\alpha e - \gamma d) = (\gamma - \alpha + p - q) \langle\langle W | \quad (\text{III.A.139})$$

and

$$(\beta d - \delta e) |V\rangle\rangle = (\delta - \beta + p - q) |V\rangle\rangle. \quad (\text{III.A.140})$$

Using the identities $E = 1 + e$ and $D = 1 + d$ these relations imply immediately that

$$\langle\langle W | (\alpha E - \gamma D) = (p - q) \langle\langle W | \quad (\text{III.A.141})$$

and

$$(\beta D - \delta E) |V\rangle\rangle = (p - q) |V\rangle\rangle \quad (\text{III.A.142})$$

which are in agreement with (III.A.70).

Example A.34. In the SSEP case, the matrices K and \bar{K} have been introduced in (II.C.19) and (II.C.21) and the vector $\mathbf{A}(z)$ is given in (III.A.118). We write the GZ relations (with additive spectral parameters, in agreement with the reflection equation (II.C.7)), to determine the algebraic relations satisfied by the generators E and D and the boundary vectors $\langle\langle W |$ and $|V\rangle\rangle$. By direct computation we show that

$$\langle\langle W | K(z) \mathbf{A}(-z) = \langle\langle W | \mathbf{A}(z) \quad \Leftrightarrow \quad \langle\langle W | (\alpha E - \gamma D) = \langle\langle W | \quad (\text{III.A.143})$$

and

$$\bar{K}(z) \mathbf{A}(-z) |V\rangle\rangle = \mathbf{A}(z) |V\rangle\rangle \quad \Leftrightarrow \quad (\beta D - \delta E) |V\rangle\rangle = |V\rangle\rangle, \quad (\text{III.A.144})$$

in agreement with III.A.71.

5 Ground state of the transfer matrix

a) Inhomogeneous ground state

We stressed in the previous sections the direct relation between the ZF and GZ relations on one hand, and the steady state of the Markov matrix of integrable models on the other hand. We explained in chapter II that the Markov matrix associated to an integrable process belongs to a family of commuting operators generated by the transfer matrix. Because of this commutation property, the whole family of operators shares the same eigenvectors. In particular the steady state of the Markov matrix should be an eigenvector of the transfer matrix. In order to address this problem in full generality, we will be interested in the transfer matrix with inhomogeneity parameters (introduced in chapter II). This motivates the following definition.

Definition A.35. For $\mathbf{A}(z)$, $\langle\langle W |$ and $|V\rangle\rangle$ satisfying the ZF relation (III.A.119) and the GZ relations (III.A.131), we define the inhomogeneous ground state⁵

$$|\mathcal{S}(z_1, z_2, \dots, z_L)\rangle\rangle = \frac{1}{Z_L(z_1, z_2, \dots, z_L)} \langle\langle W | \mathbf{A}(z_1) \otimes \mathbf{A}(z_2) \otimes \dots \otimes \mathbf{A}(z_L) |V\rangle\rangle, \quad (\text{III.A.145})$$

where $Z_L(z_1, z_2, \dots, z_L) = \langle\langle W | C(z_1) C(z_2) \dots C(z_L) |V\rangle\rangle$ with

$$C(z) = A_0(z) + A_1(z) + \dots + A_N(z). \quad (\text{III.A.146})$$

$|\mathcal{S}(z_1, z_2, \dots, z_L)\rangle\rangle$ is a inhomogeneous deformation of the steady state $|\mathcal{S}\rangle\rangle$ (of the Markov matrix obtained by taking the derivative of the transfer matrix with respect to the spectral parameter). The following proposition clarifies this statement.

⁵the notation $|\mathcal{S}(z_1, z_2, \dots, z_L)\rangle\rangle$ should not be confused with the components $\mathcal{S}(\tau_1, \tau_2, \dots, \tau_L)$ of the undeformed steady state. The distinction between these two objects should be clear from the context.

Proposition A.36. $|\mathcal{S}\rangle = |\mathcal{S}(1, 1, \dots, 1)\rangle$ is the steady state of the model, i.e $M|\mathcal{S}\rangle = 0$, where M is given by (II.C.37).

Proof. This derives directly from the propositions A.24, A.31 and A.12. \blacksquare

Proposition A.37. The normalization $Z_L(z_1, z_2, \dots, z_L)$ is symmetric under permutation of variables $z_i \leftrightarrow z_j$ and inversion of variable $z_i \rightarrow 1/z_i$.

This property shed some light on the possible connection of $Z_L(z_1, z_2, \dots, z_L)$ with the theory of symmetric functions. This relation will be clarified and explored in chapter IV.

Proposition A.38. For all $i = 1, \dots, L$ we have

$$t(z_i|z_1, \dots, z_L)|\mathcal{S}(z_1, z_2, \dots, z_L)\rangle = |\mathcal{S}(z_1, z_2, \dots, z_L)\rangle \quad (\text{III.A.147})$$

and

$$t(1/z_i|z_1, \dots, z_L)|\mathcal{S}(z_1, z_2, \dots, z_L)\rangle = |\mathcal{S}(z_1, z_2, \dots, z_L)\rangle. \quad (\text{III.A.148})$$

The specialized transfer matrices

$$\begin{aligned} t(z_i|z_1, \dots, z_L) &= \check{R}_{i-1,i}\left(\frac{z_i}{z_{i-1}}\right) \dots \check{R}_{1,2}\left(\frac{z_i}{z_1}\right) K_1(z_i) \\ &\times \check{R}_{1,2}(z_i z_1) \dots \check{R}_{i-1,i}(z_i z_{i-1}) \check{R}_{i,i+1}(z_i z_{i+1}) \dots \check{R}_{L-1,L}(z_i z_L) \\ &\times \bar{K}_L\left(\frac{1}{z_i}\right) \check{R}_{L-1,L}\left(\frac{z_i}{z_L}\right) \dots \check{R}_{i,i+1}\left(\frac{z_i}{z_{i+1}}\right) \end{aligned}$$

and

$$\begin{aligned} t(1/z_i|z_1, \dots, z_L) &= \check{R}_{i,i+1}\left(\frac{z_{i+1}}{z_i}\right) \dots \check{R}_{L,1,L}\left(\frac{z_L}{z_i}\right) \bar{K}_L(z_i) \\ &\times \check{R}_{L-1,L}\left(\frac{1}{z_i z_L}\right) \dots \check{R}_{i,i+1}\left(\frac{1}{z_i z_{i+1}}\right) \check{R}_{i-1,i}\left(\frac{1}{z_i z_{i-1}}\right) \dots \check{R}_{1,2}\left(\frac{1}{z_i z_1}\right) \\ &\times K_1\left(\frac{1}{z_i}\right) \check{R}_{1,2}\left(\frac{z_1}{z_i}\right) \dots \check{R}_{i-1,i}\left(\frac{z_{i-1}}{z_i}\right) \end{aligned}$$

are sometimes called the scattering matrices. Those matrices will appear again in chapter IV in the context of quantum Knizhnik-Zamolodchikov equations.

Proof. Analyzing the explicit form of $t(z_i|z_1, \dots, z_L)$ we see that when acting on $|\mathcal{S}(z_1, z_2, \dots, z_L)\rangle$ it takes the inhomogeneity parameter z_i and pushes it to the right through all the z_j (by successive permutation because of the ZF relation satisfied by $\mathbf{A}(z)$). It then inverts z_i into $1/z_i$ at the right boundary (because of the GZ relation). $1/z_i$ is then pushed to the left and again inverted at the left boundary, to finally being placed in its initial position, completing in this manner the whole circle. More precisely

$$\begin{aligned} t(z_i|z_1, \dots, z_L)|\mathcal{S}(z_1, \dots, z_L)\rangle &= \check{R}_{i-1,i}\left(\frac{z_i}{z_{i-1}}\right) \dots \check{R}_{1,2}\left(\frac{z_i}{z_1}\right) K_1(z_i) \\ &\times \check{R}_{1,2}(z_i z_1) \dots \check{R}_{i-1,i}(z_i z_{i-1}) \check{R}_{i,i+1}(z_i z_{i+1}) \dots \check{R}_{L-1,L}(z_i z_L) \\ &\times \bar{K}_L\left(\frac{1}{z_i}\right) |\mathcal{S}(z_1, \dots, z_{i-1}, z_{i+1}, \dots, z_L, z_i)\rangle \\ &= \check{R}_{i-1,i}\left(\frac{z_i}{z_{i-1}}\right) \dots \check{R}_{1,2}\left(\frac{z_i}{z_1}\right) K_1(z_i) \\ &\times |\mathcal{S}\left(\frac{1}{z_i}, z_1, \dots, z_{i-1}, z_{i+1}, \dots, z_L\right)\rangle \\ &= |\mathcal{S}(z_1, \dots, z_L)\rangle. \end{aligned}$$

The proof is exactly the same for the scattering matrix $t(1/z_i|z_1, \dots, z_L)$ but the circle is made the other way around. \blacksquare

Remark A.39. Note that the definition A.35 and the propositions A.36, A.37 and A.38 can be easily adapted to the periodic case (we chose not to give them explicitly here to avoid repetitions). The reader may refer to subsection c) where an example of model defined on the periodic lattice is studied in details.

Now, a question arises naturally: is the inhomogeneous ground state $|\mathcal{S}(z_1, z_2, \dots, z_L)\rangle$ an eigenvector of the transfer matrix $t(z|z_1, \dots, z_L)$ for a generic z ? In all the models that we have encountered so far (ASEP, TASEP, SSEP) the answer is yes, but we are still lacking for a general proof of this fact. Indeed in all the models that we have studied, a specific (model dependent) analysis of the degree and symmetries of the transfer matrix was needed to prove this fact. The common way to tackle the problem is to remark that the transfer matrix often has rational entries in the spectral parameter z . Knowing that $|\mathcal{S}(z_1, z_2, \dots, z_L)\rangle$ is an eigenvector of $t(z|z_1, \dots, z_L)$ for $z = z_i^{\pm 1}$ and studying some symmetry of the transfer matrix is often enough to prove by degree considerations that the inhomogeneous ground state is an eigenvector of the transfer matrix for all z . We give below several examples.

b) Some examples

Example A.40. We begin to present the case of the ASEP defined on a lattice with open boundaries. We have for this model

$$t(z|z_1, \dots, z_L)|\mathcal{S}(z_1, \dots, z_L)\rangle = \lambda(z|z_1, \dots, z_L)|\mathcal{S}(z_1, \dots, z_L)\rangle \quad (\text{III.A.149})$$

with

$$\lambda(z|z_1, \dots, z_L) = 1 + (pq)^{L-1} \left(\prod_{i=1}^L \frac{(1 - zz_i)(z_i - z)}{(p - qzz_i)(pz_i - qz)} \right) \\ \times \frac{(1 - z^2)(\delta p^2 + (\beta - \delta + q - p)pqz - \beta q^2 z^2)(\gamma p^2 + (\alpha - \gamma + q - p)pqz - \alpha q^2 z^2)}{(p^2 - q^2 z^2)(\delta z^2 + (\beta - \delta + q - p)z - \beta)(\gamma z^2 + (\alpha - \gamma + q - p)z - \alpha)}.$$

This relation is proved using the symmetry

$$t(z|z_1, \dots, z_L) = (\lambda(z|z_1, \dots, z_L) - 1) t\left(\frac{p}{qz}|z_1, \dots, z_L\right). \quad (\text{III.A.150})$$

More details about this symmetry relation can be found in [V3].

Example A.41. Concerning the SSEP defined on a lattice with open boundaries, the situation is very similar. We have indeed for this model

$$t(z|z_1, \dots, z_L)|\mathcal{S}(z_1, \dots, z_L)\rangle = \lambda(z|z_1, \dots, z_L)|\mathcal{S}(z_1, \dots, z_L)\rangle \quad (\text{III.A.151})$$

with

$$\lambda(z|z_1, \dots, z_L) = 1 + \left(\prod_{i=1}^L \frac{(z - z_i)(z + z_i)}{(z + 1 - z_i)(z + 1 + z_i)} \right) \frac{z((\alpha + \gamma)(z + 1) - 1)((\beta + \delta)(z + 1) - 1)}{(z + 1)((\alpha + \gamma)z + 1)((\beta + \delta)z + 1)}.$$

This relation is proved using the symmetry

$$t(z|z_1, \dots, z_L) = (\lambda(z|z_1, \dots, z_L) - 1) t(-1 - z|z_1, \dots, z_L). \quad (\text{III.A.152})$$

More details about this symmetry relation can be found in [V3].

c) Inhomogeneous periodic TASEP

We study, in this subsection, the ground state of the periodic inhomogeneous transfer matrix. Instead of addressing the problem in full generality (which would have been a bit redundant with the open case), we prefer to present the method through a specific simple example: the periodic TASEP. The inhomogeneous transfer matrix associated to the single species periodic TASEP was introduced in chapter II. It has been proven to be itself the Markov matrix encoding a discrete time process. We are now interested in computing the inhomogeneous ground state of this transfer matrix (note that in this particular case the inhomogeneous ground state can be called stationary state because the associated eigenvalue is equal to 1 thanks to the Markovian property of the transfer matrix). The results presented here are mostly extracted from [V9] and the reader is invited to refer to this paper for the details.

The building block of the stationary state is the following vector

$$v(z) = \begin{pmatrix} z \\ 1 \end{pmatrix}. \quad (\text{III.A.153})$$

It satisfies the Zamolodchikov-Faddeev relation

$$R_{12}(z_1/z_2)v_1(z_1)v_2(z_2) = v_1(z_1)v_2(z_2). \quad (\text{III.A.154})$$

The stationary state of the process $M(z|\mathbf{z})$ (defined in (II.B.29)) is constructed from

$$|\mathcal{S}\rangle = v_1(z_1)v_2(z_2)\dots v_L(z_L). \quad (\text{III.A.155})$$

Recall that the subscripts denote which component of the tensor space the vector v belongs to. To be more precise, since the process conserves the number of particles, there are L independent sectors (as mentioned previously we do not consider the empty sector), each corresponding to a given number m of particles in the system. The stationary state is hence degenerate: there is one stationary state for each sector. Moreover, the exact normalization $Z^{(m)}$ of the stationary state depends on the sector we are considering. Then, each stationary state is given by the components of $|\mathcal{S}\rangle$ corresponding to the sector and correctly normalized.

The following calculation justifies that $|\mathcal{S}\rangle$ given in (III.A.155) is the stationary state of the system. Indeed, for $i = 1, 2, \dots, L$ we have

$$\begin{aligned} t(z_i|\mathbf{z})|\mathcal{S}\rangle &= R_{i,i-1}\left(\frac{z_i}{z_{i-1}}\right)\dots R_{i,1}\left(\frac{z_i}{z_1}\right)R_{i,L}\left(\frac{z_i}{z_L}\right)\dots R_{i,i+1}\left(\frac{z_i}{z_{i+1}}\right)v_1(z_1)\dots v_L(z_L) \\ &= v_1(z_1)v_2(z_2)\dots v_L(z_L) \\ &= |\mathcal{S}\rangle, \end{aligned}$$

where $t(z|\mathbf{z})$ has been introduced in (II.B.20). The first equality is obtained using the regularity property of the R-matrix whereas the second equality is obtained using $L-1$ times the property (III.A.154). Clearly, $t(z|\mathbf{z})$ is a polynomial of degree less or equal to L in z . It is possible to show (using the graphical interpretation for instance) that in the sectors where there is at least one particle, the degree of $t(z|\mathbf{z})$ is in fact at most equal to $L-1$. Hence we can deduce through interpolation arguments that in these sectors, the stationary state is given by the corresponding components of $|\mathcal{S}\rangle$. Note that when we take the homogeneous limit $z_i \rightarrow 1$ we recover the uniform stationary distribution of the continuous time TASEP.

From the knowledge of the stationary distribution, we can calculate various physical quantities. We shall see that some observables can be expressed as symmetric polynomials in the inhomogeneity parameters z_1, \dots, z_L .

The weight of the configuration (τ_1, \dots, τ_L) is readily obtained using (III.A.155):

$$\mathcal{S}(\tau_1, \dots, \tau_L) = \prod_{i=1}^L (\delta_{1,\tau_i} + z_i \delta_{0,\tau_i}). \quad (\text{III.A.156})$$

In the sector with m particles, the normalization factor of the stationary state is obtained by summing the weights of all the configurations with m particles

$$Z^{(m)} = \sum_{\substack{I \subset \{1, \dots, L\} \\ |I|=L-m}} \prod_{i \in I} z_i = e_{L-m}(z_1, \dots, z_L), \quad (\text{III.A.157})$$

where e_{L-m} is the elementary symmetric homogeneous polynomial of degree $L - m$. The normalization factor can be written as a Schur polynomial:

$$Z^{(m)} = s_{1^{L-m}}^A(z_1, \dots, z_L), \quad \text{where } 1^{L-m} = (\underbrace{1, \dots, 1}_{L-m}, \underbrace{0, \dots, 0}_m). \quad (\text{III.A.158})$$

We remind the definition of the Schur polynomial (of type A) associated with a partition $\lambda = (\lambda_1, \dots, \lambda_L)$ with $\lambda_1 \geq \dots \geq \lambda_L \geq 0$:

$$s_\lambda^A(z_1, \dots, z_L) = \frac{\det \left((z_j)^{L-i+\lambda_i} \right)_{i,j}}{\det \left(z_j^{L-i} \right)_{i,j}}. \quad (\text{III.A.159})$$

This expression of the partition function in terms of the Schur polynomial allows us to relate the value of $Z^{(m)}$ in the homogeneous limit ($z_i \rightarrow 1$) with the dimension of the representation $\pi^A(\lambda)$ of $sl(L)$ labeled by the Young tableau $[\lambda]$. Indeed, using the Weyl character formula (see e.g. [195, 196] for a review), we obtain

$$s_\lambda^A(1, \dots, 1) = \prod_{1 \leq j \leq i \leq L} \frac{\lambda_j - \lambda_i + i - j}{i - j} = \dim(\pi^A(\lambda)). \quad (\text{III.A.160})$$

In particular, we have

$$Z^{(m)} \Big|_{z_1 = \dots = z_L = 1} = \dim(\pi^A(1^{L-m})) = \binom{L}{m} \quad (\text{III.A.161})$$

in accordance with a direct computation starting from (III.A.157).

In the sector with m particles, the particle density at site i is obtained by summing the weights of all the configurations with m particles, one of them being at site i

$$\langle \tau_i \rangle = \frac{e_{L-m}(z_1, \dots, z_{i-1}, z_{i+1}, \dots, z_L)}{e_{L-m}(z_1, \dots, z_L)}. \quad (\text{III.A.162})$$

We can show that $\sum_{i=1}^L \langle \tau_i \rangle = m$ as expected.

The higher correlation functions take also a very simple form. The correlations between the sites $i_1 < i_2 < \dots < i_\ell$ is given by

$$\langle \tau_{i_1} \tau_{i_2} \dots \tau_{i_\ell} \rangle = \frac{e_{L-m}(z_1, \dots, z_{i_1-1}, z_{i_1+1}, \dots, z_{i_2-1}, z_{i_2+1}, \dots, z_{i_\ell-1}, z_{i_\ell+1}, \dots, z_L)}{e_{L-m}(z_1, \dots, z_L)}. \quad (\text{III.A.163})$$

For $\ell > m$, the correlation functions vanish as expected since the number of particles is m and the correlation functions for more than m particles has no meaning.

d) Inhomogeneous open TASEP

We now move to the case of the single species open TASEP, whose inhomogeneous transfer matrix had been introduced in chapter II. It has been shown that this transfer matrix defines a discrete time Markov process. The results displayed are taken from [V9].

The stationary state is expressed as a matrix product. Indeed, the probability of the configuration $\mathcal{C} = (\tau_1, \dots, \tau_L)$ can be written as

$$\mathcal{S}(\tau_1, \dots, \tau_L) = \frac{1}{Z_L} \langle\langle W | \prod_{i=1}^L ((1 - \tau_i)E(z_i) + \tau_i D(z_i)) | V \rangle\rangle, \quad (\text{III.A.164})$$

where the normalization factor is $Z_L = \langle\langle W | C(z_1) \dots C(z_L) | V \rangle\rangle$, with $C(z) = E(z) + D(z)$. We recall that the algebraic elements $E(z)$ and $D(z)$ are the entries of the vector

$$\mathbf{A}(z) = \begin{pmatrix} E(z) \\ D(z) \end{pmatrix}. \quad (\text{III.A.165})$$

Using this vector, the stationary state can be written in a more compact way (III.A.145)

The vector $A(z)$ allows us to write easily the exchange relations between $E(z)$ and $D(z)$ through the ZF relation:

$$\check{R}(z_1/z_2)A(z_1) \otimes A(z_2) = A(z_2) \otimes A(z_1). \quad (\text{III.A.166})$$

Written explicitly it gives four relations

$$\begin{cases} [E(z_1), E(z_2)] = 0 \\ [D(z_1), D(z_2)] = 0 \\ \frac{z_1}{z_2} D(z_1) E(z_2) = D(z_2) E(z_1) \\ D(z_1) E(z_2) = \frac{z_2}{z_2 - z_1} [E(z_2) D(z_1) - E(z_1) D(z_2)] \end{cases} \quad (\text{III.A.167})$$

Let us remark that the third relation is implied by the fourth.

The relations between the boundary vectors $\langle\langle W |, |V \rangle\rangle$ and the algebraic elements $E(z)$, $D(z)$ are given by the GZ relations

$$\langle\langle W | K(z) A(1/z) = \langle\langle W | A(z), \quad \bar{K}(z) A(1/z) | V \rangle\rangle = A(z) | V \rangle\rangle. \quad (\text{III.A.168})$$

Written explicitly we obtain four relations

$$\begin{cases} \langle\langle W | E(z) = \langle\langle W | \frac{(a+z)z}{za+1} E(1/z) \\ \langle\langle W | E(z) = \frac{z(a+z)}{z^2-1} \langle\langle W | (D(1/z) - D(z)) \end{cases} \quad \text{and} \quad \begin{cases} D(z) | V \rangle\rangle = \frac{zb+1}{z(b+z)} D(1/z) | V \rangle\rangle \\ D(z) | V \rangle\rangle = \frac{bz+1}{z^2-1} (E(z) - E(1/z)) | V \rangle\rangle \end{cases} \quad (\text{III.A.169})$$

Let us remark that for each boundary, the first relation is implied by the second one.

We now prove that the vector $|\mathcal{S}\rangle$ is the stationary state of the transfer matrix. From proposition A.38 we know that

$$t(z_i | \mathbf{z}) |\mathcal{S}\rangle = |\mathcal{S}\rangle, \quad (\text{III.A.170})$$

and also

$$t(1/z_i | \mathbf{z}) |\mathcal{S}\rangle = |\mathcal{S}\rangle. \quad (\text{III.A.171})$$

We show below, using the graphical representation, that the numerators of the entries of $t(z | \mathbf{z})$ are polynomials of degree less than $L + 2$. Since the equation $t(z | \mathbf{z}) |\mathcal{S}\rangle = |\mathcal{S}\rangle$ is satisfied for $2L$ different values of z ($z = z_1, 1/z_1, \dots, z_L, 1/z_L$), we get through interpolation arguments that for $L \geq 3$, $t(z | \mathbf{z}) |\mathcal{S}\rangle = |\mathcal{S}\rangle$ for all z . For $L < 5$ we checked by computer that this equation is satisfied.

We use the graphical representation given in figures II.5, II.13 and II.14, interpreting the last vertex of fig. II.5 as in fig. III.2. We can see that any matrix element $\langle\langle \mathcal{C}' | t(z | \mathbf{z}) | \mathcal{C} \rangle\rangle$ can be decomposed into continuous thick lines that do not intersect, as illustrated in the figure III.3.

The vertices that do not enter a thick line have degree 0 in z . Thus, the total degree of the matrix element is the sum of the degree of each thick line, plus the degree coming from the boundaries that we look at separately. We first consider lines that are in the 'bulk' (that

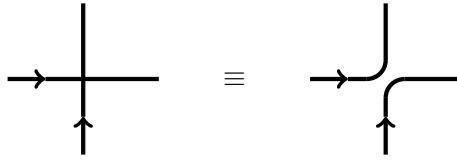


Figure III.2: Vertex with non-intersecting thick lines.

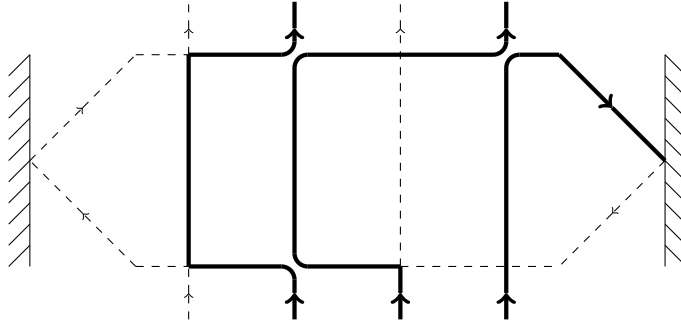


Figure III.3: Decomposition of a matrix element into thick continuous lines.

do not include a boundary). Looking at the weights of the vertices in fig. II.5, one can see that the incoming part of a line always carry a degree 1. Moreover, a line corresponding to a degree n must cross at least n exit lines, the first on the left being always of degree 0. This implies that the bulk part is at most of degree L . Figure II.14 shows that the right boundary does not change this counting. The left boundary can add at most a degree 2, as it can be seen on figure II.13. Altogether, this leads to a total degree $L + 2$.

We now construct an explicit representation of the algebraic elements $E(z)$ and $D(z)$. We introduce the shift operators e and d such that $de = 1$, which are well known in the context of the continuous time open TASEP since they enter the construction of the original matrix ansatz [46]. We define

$$\tilde{E}(z) = z + e \quad \text{and} \quad \tilde{D}(z) = 1/z + d, \quad (\text{III.A.172})$$

and the boundary vectors such that

$$\langle\langle \tilde{W} | e = a \langle\langle \tilde{W} | \quad \text{and} \quad d | \tilde{V} \rangle\rangle = b | \tilde{V} \rangle\rangle. \quad (\text{III.A.173})$$

It is readily verified that the Zamolodchikov-Faddeev relation (III.A.166) and the Ghoshal-Zamolodchikov relations (III.A.168) are satisfied. From the results of [46] giving explicit forms for e , d , $\langle\langle \tilde{W} |$ and $| \tilde{V} \rangle\rangle$, we deduce that $\langle\langle \tilde{W} |$ and $| \tilde{V} \rangle\rangle$ can be chosen such that $\langle\langle \tilde{W} | \tilde{V} \rangle\rangle \neq 0$ which guarantees the non-vanishing of $|\mathcal{S}\rangle$.

The matrix ansatz allows us to calculate the stationary probability of any given configuration. Let $1 \leq j_1 < \dots < j_r \leq L$ be integers and $\mathcal{C}(j_1, \dots, j_r)$ be the configuration (τ_1, \dots, τ_L) with $\tau_i = 1$ if $i = j_k$ and $\tau_i = 0$ otherwise. We define the (non-normalized) weight of the word with $D(j_1), \dots, D(j_r)$ at positions j_1, \dots, j_r as

$$W_L(j_1, \dots, j_r) = Z_L \times \mathcal{S}(\mathcal{C}(j_1, \dots, j_r)) \quad (\text{III.A.174})$$

$$= \langle\langle W | \dots D(z_{j_1}) \dots D(z_{j_2}) \dots D(z_{j_r}) \dots | V \rangle\rangle, \quad (\text{III.A.175})$$

where the dots stand for $E(z_i)$ operators.

The same quantity can be calculated using the explicit representation (III.A.172):

$$\tilde{W}_L(j_1, \dots, j_r) = \langle\langle \tilde{W} | \dots \left(d + \frac{1}{z_{j_1}} \right) \dots \left(d + \frac{1}{z_{j_2}} \right) \dots \left(d + \frac{1}{z_{j_r}} \right) \dots | \tilde{V} \rangle\rangle. \quad (\text{III.A.176})$$

The weight $W_L(j_1, \dots, j_r)$ computed from the relations (III.A.167) and (III.A.169) is proportional to the weight $\tilde{W}_L(j_1, \dots, j_r)$ computed using the explicit representation (thanks to the

uniqueness of the steady-state guaranteed by the Perron-Frobenius theorem). Thus, we have

$$W_L(j_1, \dots, j_r) = f(z_1, \dots, z_L) \widetilde{W}_L(j_1, \dots, j_r). \quad (\text{III.A.177})$$

The multiplicative coefficient is obtained by comparing the weights of the empty configuration:

$$f(z_1, \dots, z_L) = \frac{\langle\langle W|E(z_1) \dots E(z_L)|V \rangle\rangle}{(a+z_1) \dots (a+z_L) \langle\langle W|V \rangle\rangle}; \quad (\text{III.A.178})$$

$f(z_1, \dots, z_L)$ is symmetric under the permutation of the z_i thanks to (III.A.167) but also under the transformation $z_i \mapsto 1/z_i$ thanks to (III.A.169). The group generated by these transformations is denoted by BC_L in reference to the Weyl group of the root system of the Lie algebra $sp(2L)$.

The expression of $\widetilde{W}_L(j_1, \dots, j_r)$ is given by

$$\begin{aligned} \widetilde{W}_L(j_1, \dots, j_r) &= \frac{z_1 \dots z_L}{z_{j_1} \dots z_{j_r}} \sum_{p=0}^r b^p \sum_{q_{r-p}=j_{r-p}}^L \frac{1}{z_{q_{r-p}}} \sum_{q_{r-p-1}=j_{r-p-1}}^{q_{r-p}-1} \frac{1}{z_{q_{r-p-1}}} \dots \sum_{q_1=j_1}^{q_2-1} \frac{1}{z_{q_1}} \\ &\times \prod_{l_0=1}^{j_1-1} \left(1 + \frac{a}{z_{l_0}}\right) \prod_{l_1=q_1+1}^{j_2-1} \left(1 + \frac{a}{z_{l_1}}\right) \dots \prod_{l_{r-p}=q_{r-p}+1}^{j_{r-p+1}-1} \left(1 + \frac{a}{z_{l_{r-p}}}\right) \end{aligned}$$

By convention when $p = r$ in the first sum, there is no summation over the q_i and the formula reduces to $b^r \prod_{l_0=1}^{j_1-1} \left(1 + \frac{a}{z_{l_0}}\right)$. We also set $j_{r+1} = L + 1$ in the last product when $p = 0$. The proof of this formula is obtained by induction on the size L , using the identity

$$\begin{aligned} \widetilde{D}(z_{j_r}) \widetilde{E}(z_{j_r+1}) &= \left(\frac{1}{z_{j_r}} + d\right) (z_{j_r+1} + e) = \frac{1}{z_{j_r}} (z_{j_r+1} + e) + z_{j_r+1} \left(\frac{1}{z_{j_r+1}} + d\right) \\ &= \frac{1}{z_{j_r}} \widetilde{E}(z_{j_r+1}) + z_{j_r+1} \widetilde{D}(z_{j_r+1}). \end{aligned}$$

Another important step is to compute the normalization factor of the probability distribution. We define $C(z) = E(z) + D(z)$ and $\widetilde{C}(z) = \widetilde{E}(z) + \widetilde{D}(z)$. The normalization factors are thus given by $Z_L(z_1, \dots, z_L) = \langle\langle W|C(z_1) \dots C(z_L)|V \rangle\rangle$, and $\widetilde{Z}_L(z_1, \dots, z_L) = \langle\langle \widetilde{W}|\widetilde{C}(z_1) \dots \widetilde{C}(z_L)|\widetilde{V} \rangle\rangle$ for the explicit representation. Thanks to the property (III.A.177), we have

$$Z_L(z_1, \dots, z_L) = f(z_1, \dots, z_L) \widetilde{Z}_L(z_1, \dots, z_L). \quad (\text{III.A.179})$$

Z_L and \widetilde{Z}_L are symmetric under BC_L .

Our goal is to get an analytic expression for the normalization factor. For this purpose, for any sequence of complex numbers $\mathbf{u} = (u_1, u_2, \dots)$, we define the shifted product by

$$(z|\mathbf{u})^k = \begin{cases} (z - u_1)(z - u_2) \dots (z - u_k), & k > 0, \\ 1 \text{ if } k = 0, \end{cases} \quad (\text{III.A.180})$$

We have the result (the proof can be found in [V9]):

$$\widetilde{Z}_L(z_1, \dots, z_L) = \frac{\det((z_j|\mathbf{v})^{L+2-i} - (1/z_j|\mathbf{v})^{L+2-i})_{i,j}}{\det(z_j^{L+1-i} - (1/z_j)^{L+1-i})_{i,j}} \quad \text{with } \mathbf{v} = (-a, -b, 0, \dots, 0). \quad (\text{III.A.181})$$

When $a, b = 0$, we recognize in the L.H.S. of equation (III.A.181), the expression of the Schur polynomial of type C associated to the partition $1^L = (1, \dots, 1)$. We remind that the Schur polynomial of type C associated with the partition $\lambda = (\lambda_1, \dots, \lambda_L)$ with $\lambda_1 \geq \dots \geq \lambda_L \geq 0$ is defined by:

$$\widetilde{Z}_L(z_1, \dots, z_L) \Big|_{a=b=0} = s_\lambda^C(z_1, \dots, z_L) = \frac{\det((z_j)^{L+1-i+\lambda_i} - (1/z_j)^{L+1-i+\lambda_i})_{i,j}}{\det(z_j^{L+1-i} - (1/z_j)^{L+1-i})_{i,j}}. \quad (\text{III.A.182})$$

As in the periodic case where the normalization factor is linked to the Schur polynomial of type A and to the representation of the Lie algebra $sl(L)$ (see (III.A.160) and (III.A.161)), the normalization factor (III.A.182) is given in terms of the Schur polynomial of type C and is associated to representation of the Lie algebra $sp(2L)$. These observations will allow us to use results of the Lie algebra theory to take the homogeneous limit $z_i \rightarrow 1$.

When a, b are arbitrary, we need to use some generalizations of the Schur polynomial, called *shifted (or factorial) Schur polynomials*. A shifted Schur polynomial of type A , is defined, for any sequence of complex numbers $\mathbf{u} = (u_1, u_2, \dots)$ [197], as follows:

$$s_\lambda^A(z_1, \dots, z_L | \mathbf{u}) = \frac{\det \left((z_j | \mathbf{u})^{L-i+\lambda_i} \right)_{i,j}}{\det \left(z_j^{L-i} \right)_{i,j}}. \quad (\text{III.A.183})$$

Similarly, we define the shifted (or factorial) Schur polynomial of type C as⁶

$$s_\lambda^C(z_1, \dots, z_L | \mathbf{u}) = \frac{\det \left((z_j | \mathbf{u})^{L+1-i+\lambda_i} - (1/z_j | \mathbf{u})^{L+1-i+\lambda_i} \right)_{i,j}}{\det \left(z_j^{L+1-i} - (1/z_j)^{L+1-i} \right)_{i,j}}. \quad (\text{III.A.184})$$

Thus, the normalization factor (III.A.181) is the shifted Schur polynomial of type C associated to the partition 1^L and to the sequence $\mathbf{v} = (-a, -b, 0, 0, \dots)$. For this particular partition, the shifted Schur polynomial of type C can be expanded on the usual type C Schur polynomials as (the proof can be found in [V9])

$$\tilde{Z}_L(z_1, \dots, z_L) = s_{1^L}^C(z_1, \dots, z_L | \mathbf{v}) = \sum_{n=0}^{L+1} \frac{a^n - b^n}{a - b} s_{1^{L+1-n}}^C(z_1, \dots, z_L). \quad (\text{III.A.185})$$

Using the explicit representation, we can also determine the particle density at site i from the stationary measure:

$$\begin{aligned} \langle \tau_i(z_1, \dots, z_L) \rangle &= \left(b + \frac{1}{z_i} \right) \frac{\tilde{Z}_{L-1}(z_1, \dots, z_{i-1}, z_{i+1}, \dots, z_L)}{\tilde{Z}_L(z_1, \dots, z_L)} + \\ (1 - ab) &\times \sum_{k=0}^{L-i-1} \frac{\tilde{Z}_{i-1+k}(z_1, \dots, z_{i-1}, z_{i+1}, \dots, z_{i+k}) \Big|_{b=0} \tilde{Z}_{L-i-1-k}(z_{i+2+k}, \dots, z_L) \Big|_{a=0}}{\tilde{Z}_L(z_1, \dots, z_L)}. \end{aligned}$$

In the homogeneous limit $z_i \rightarrow 1$, $s_{1^{L+1-n}}^C(1, \dots, 1)$ is equal to the dimension of the $sp(2L)$ representation associated to the partition 1^{L+1-n} :

$$s_{1^{L+1-n}}^C(1, \dots, 1) = \frac{n}{L+1} \binom{2L+2}{L+1-n} = \dim(\pi^C(1^{L+1-n})). \quad (\text{III.A.186})$$

This expression is obtained through the general formula (see [196] for instance):

$$\dim(\pi^C(\lambda)) = \prod_{1 \leq i < j \leq L} \left(\frac{\lambda_i - \lambda_j + j - i}{j - i} \frac{\lambda_i + \lambda_j + 2L + 2 - j - i}{2L + 2 - j - i} \right) \prod_{i=1}^L \frac{\lambda_i + L + 1 - i}{L + 1 - i}. \quad (\text{III.A.187})$$

Then from (III.A.185), we get

$$\tilde{Z}_L(1, 1, \dots, 1) = \frac{g_L(a) - g_L(b)}{a - b} \quad \text{with} \quad g_L(x) = \sum_{n=0}^L \frac{n+1}{L+1} \binom{2L+2}{L-n} x^{n+1} \quad (\text{III.A.188})$$

in accordance with the results known for continuous time open TASEP [46]

$$Z_L = \frac{h_L(\frac{1}{\alpha}) - h_L(\frac{1}{\beta})}{\frac{1}{\alpha} - \frac{1}{\beta}} \quad \text{with} \quad h_L(x) = \sum_{p=1}^L \frac{p}{2L-p} \binom{2L-p}{L} x^{p+1}. \quad (\text{III.A.189})$$

⁶It is easy to see that $s_\lambda^C(z_1, \dots, z_L | \mathbf{u})$ is indeed a polynomial in the variables z_1, \dots, z_L .

The equality between these two expressions is ensured by the identity

$$g_L(x-1) = h_L(x) - \frac{1}{L} \binom{2L}{L-1} \quad (\text{III.A.190})$$

and recalling that $a = \frac{1}{\alpha} - 1$ and $b = \frac{1}{\beta} - 1$.

In particular, when $a = b = 0$ (i.e. $\alpha = \beta = 1$), Z_L is equal to the dimension of the representation 1^L , which is the Catalan number $C_{L+1} = \frac{1}{L+2} \binom{2L+2}{L+1}$.

The model considered here has non-diagonal boundary matrices (see (II.C.15)) and cannot be completely diagonalized by the usual integrability methods (like CBA or ABA). In the last few years, various specific techniques have been developed for solving such problems, based on the functional Bethe ansatz [198–200], the coordinate Bethe ansatz [97, 98, 142, 201], the separation of variables [100, 147, 148], the q-Onsager approach [151, 152] and the algebraic Bethe ansatz [102, 103]. Recently, a generalization [101, 146, 202] of the TQ relations expresses the eigenvalues of problems in terms of solutions of a new type of Bethe equations, called inhomogeneous Bethe equations.

In what follows, we shall find an unexpected relation between the ‘partition function’ Z_L and the Baxter Q operator appearing in the TQ -relations.

In [143], the Bethe equations corresponding to the eigenvalues and the eigenvectors of the transfer matrix (II.C.26) associated to the open TASEP have been computed using the modified algebraic Bethe ansatz. In this context, the eigenvalue of the transfer matrix (II.C.26) corresponding to the stationary state $\Lambda(z)$ is given by

$$\Lambda(z) = z^{L+1} \frac{b+z}{bz+1} \prod_{k=1}^L \frac{zu_k-1}{u_k-z} - \frac{(z^2-1)}{(bz+1)} \prod_{j=1}^L \left[(z-z_j) \left(z - \frac{1}{z_j} \right) \right] \prod_{k=1}^L \frac{u_k}{u_k-z}, \quad (\text{III.A.191})$$

where u_k are called Bethe roots and are solutions of the following Bethe equations

$$\prod_{p=1}^L \frac{(u_j - z_p)(u_j z_p - 1)}{u_j z_p} = (u_j + b) \prod_{\substack{k=1 \\ k \neq j}}^L \left(u_j - \frac{1}{u_k} \right), \quad \text{for } j = 1, 2, \dots, L. \quad (\text{III.A.192})$$

Let us stress that here the Bethe roots are the ones corresponding to the steady state. The corresponding Bethe equations (III.A.192) were found in [143] not to depend on the boundary parameter a . The Bethe roots corresponding to other states obey different Bethe equations (see [143], or [203] for the homogeneous case) which involve parameter a . We now introduce the following function:

$$Q(z) = \prod_{k=1}^L \left(\frac{1}{u_k} - \frac{1}{z} \right). \quad (\text{III.A.193})$$

This function (up to a coefficient z^L) is linked to the polynomial Q of Baxter [29]: its zeros are the Bethe roots. The eigenvalue (III.A.191) can be written in terms of the Q function as follows

$$\Lambda(z) = \frac{z(b+z)Q(1/z)}{(bz+1)Q(z)} - \frac{(z^2-1)}{(bz+1)Q(z)} \prod_{j=1}^L \left[(z-z_j) \left(\frac{1}{zz_j} - 1 \right) \right]. \quad (\text{III.A.194})$$

For the steady-state eigenvector, we know that $\Lambda(z) = 1$. Hence $Q(z)$ satisfies

$$z(z+b)Q(1/z) - (1+bz)Q(z) = (z^2-1) \prod_{j=1}^L \left[(z-z_j) \left(\frac{1}{zz_j} - 1 \right) \right]. \quad (\text{III.A.195})$$

This equation, called TQ relation, allows us to compute explicitly the function Q : for a given L , it can be shown that equation (III.A.195) has a unique solution of the form (III.A.193).

For the model studied here, the function Q and the normalization factor $\tilde{Z}(z_1, \dots, z_L)$ are closely related. Namely, we get

$$Q(z) = \tilde{Z}(z_1, \dots, z_L)|_{a \rightarrow -1/z} = \sum_{n=1}^{L+1} \frac{(-1/z)^n - b^n}{-1/z - b} s_{1^{L+1-n}}^C(z_1, \dots, z_L) \quad (\text{III.A.196})$$

$$= \sum_{p=0}^L \left(-\frac{1}{z}\right)^p \sum_{n=0}^{L-p} b^n s_{1^{L-n-p}}^C(z_1, \dots, z_L) \quad (\text{III.A.197})$$

where we have used the explicit form of \tilde{Z} given in (III.A.185). To prove this result, we remark that $Q(x)$ given by (III.A.197) has the form (III.A.193) and we show that it satisfies the TQ relation (III.A.195). We have

$$\begin{aligned} z(z+b)Q(1/z) - (1+bz)Q(z) &= -z \sum_{n=1}^{L+1} ((-z)^n - (-1/z)^n) s_{1^{L+1-n}}^C(z_1, \dots, z_L) \\ &= (z^2 - 1) s_{1^L}^C(z_1, \dots, z_L | z, 1/z, 0, \dots, 0). \end{aligned} \quad (\text{III.A.198})$$

Finally, we readily check that $s_{1^L}^C(z_1, \dots, z_L | z, 1/z, 0, \dots, 0)$ vanishes at the points $z = z_j$ and $z = 1/z_j$ which allows us to conclude that (III.A.198) is equal to the L.H.S. of (III.A.195).

Relation (III.A.196) means that the Bethe roots (zeros of the function Q) are linked to the zeros of the steady-state normalization factor in the complex plane of the transition rate a . These zeros appeared previously (for the homogeneous case) in [204–206] as Lee-Yang zeros and allows the generalization of the Lee-Yang theory for the phase transition of non equilibrium system. Therefore, relation (III.A.196) expresses an unexpected relation between two objects arising from very different contexts.

B Application to integrable models: examples

The goal of this section is to provide several examples of physical systems that can be investigated using the framework presented in this chapter. These systems, comprising reaction diffusion processes or involving several species of particles, will hopefully by their diversity illustrate all the different notions introduced. The study conducted below will mainly concern the matrix product construction of the steady state, taking advantage of the integrability of the models as stressed previously. A particular attention will also be put on the exact computation of physical quantities, in order to stress the efficiency and usefulness of the matrix ansatz for physical applications.

1 A diffusive model with evaporation and condensation

We consider in this subsection a one parameter generalization of the SSEP. The model involves a single species of particle that can diffuse on a one dimensional lattice coupled with two reservoirs at its extremities. In the bulk the particles can jump with equal probability rate to the left or right neighboring site provided that it is empty (exclusion constraint). The injection and extraction rates at the boundaries are asymmetric to model the coupling with the particle reservoirs. In addition to the usual dynamics of the SSEP, we allow the annihilation and creation of particle pairs on two adjacent sites in the bulk, with equal probability rates (provided again that the two target sites are empty when performing a pair creation, to respect the exclusion constraint). This pair creation and annihilation is said to be *dissipative* because it does not conserve the number of particles in the bulk. This explains the name of the model: Dissipative Symmetric Simple Exclusion Process (DiSSEP). This model has been exactly solved on the periodic lattice in [207]. The model with open boundaries has been defined in [V3] and studied in details in [V10]. We present here the main results, following the lines of [V10].

a) Presentation of the model

The precise stochastic dynamics is given as follows. During an infinitesimal time dt , a particle in the bulk can jump to the left or to the right neighboring site with probability dt if it is unoccupied. A pair of neighbor particles can also be annihilated with probability $\lambda^2 \times dt$ and be created on unoccupied neighbor sites with probability $\lambda^2 \times dt$ (see figure III.4). At the two extremities of the lattice the dynamics is modified to take into account the interaction with the reservoirs: at the first site (connected with the left reservoir), during time dt , a particle is injected with probability $\alpha \times dt$ if the site is empty and extracted with probability $\gamma \times dt$ if it is occupied. The dynamics is similar at last site (connected with the right reservoir) with injection rate δ and extraction rate β . The dynamical rules can be summarized in the following table where 0 stands for vacancy and 1 stands for a particle. The transition rates between the configurations are written above the arrows.

Left	Bulk	Right
0 $\xrightarrow{\alpha}$ 1	01 $\xleftrightarrow{1}$ 10	1 $\xrightarrow{\beta}$ 0
1 $\xrightarrow{\gamma}$ 0	00 $\xleftrightarrow{\lambda^2}$ 11	0 $\xrightarrow{\delta}$ 1

(III.B.1)

The Markov matrix encoding the stochastic dynamics of the process is given as usual as the sum of operators acting locally on the lattice:

$$M = B_1 + \sum_{k=1}^{L-1} m_{k,k+1} + \bar{B}_L, \quad (III.B.2)$$

where the local jump operators B , \bar{B} and m are given by

$$B = \begin{pmatrix} -\alpha & \gamma \\ \alpha & -\gamma \end{pmatrix}, \quad m = \begin{pmatrix} -\lambda^2 & 0 & 0 & \lambda^2 \\ 0 & -1 & 1 & 0 \\ 0 & 1 & -1 & 0 \\ \lambda^2 & 0 & 0 & -\lambda^2 \end{pmatrix}, \quad \bar{B} = \begin{pmatrix} -\delta & \beta \\ \delta & -\beta \end{pmatrix}. \quad (III.B.3)$$

We recall that we already encountered these local operators in the examples (II.A.26) and (II.A.31) in chapter II.

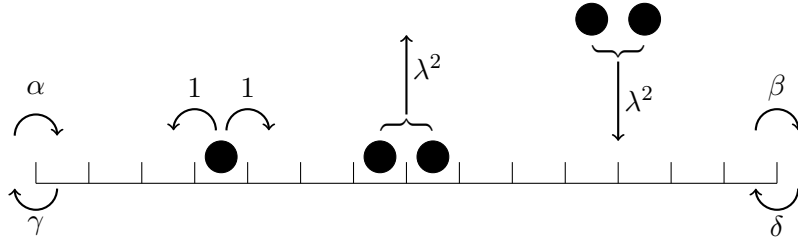


Figure III.4: Dynamical rules of the DisSEP.

We choose the coefficient of condensation and evaporation to be λ^2 and not λ for later convenience. Let us remark that the SSEP is recovered when the creation/annihilation rate λ^2 vanishes. The limit $\lambda^2 \rightarrow \infty$ provides a model with only condensation and evaporation.

The system is driven out of equilibrium by the boundaries. As shown in (III.B.51) and (III.B.53), there are particle currents in the stationary state for generic boundary rates α , β , γ and δ . We will see below (V.A.13) that these choices of rates describe particle reservoirs with densities

$$\rho_l = \frac{\alpha}{\alpha + \gamma}, \quad \text{and} \quad \rho_r = \frac{\delta}{\beta + \delta}. \quad (III.B.4)$$

Remark B.1. *The system will converge in the long time limit to a thermodynamic equilibrium if and only if the densities of the particle reservoirs at the boundaries are both equal to 1/2.*

This translates to $\alpha = \gamma$ and $\beta = \delta$. The detailed balance condition is indeed only satisfied in this case. This can be interpreted by the fact that the system is in some way coupled to a particle reservoir in the bulk because of the evaporation and condensation. This reservoir has a fixed density $1/2$ because the evaporation and condensation processes happen with the same probability rate. The thermodynamic equilibrium can thus occur if and only if the two other particle reservoirs at the boundaries have the same density $1/2$.

Remark B.2. The model displays several symmetries that are listed below:

- The evaporation/condensation probability rate is chosen to be λ^2 , hence all the results should be invariant under the transformation $\lambda \rightarrow -\lambda$.
- The left/right symmetry of the chain is given by the transformations $\alpha \leftrightarrow \delta$, $\gamma \leftrightarrow \beta$ and a change of numbering of the sites $i \rightarrow L + 1 - i$.
- The vacancy-particle symmetry translates into $\alpha \leftrightarrow \gamma$ and $\delta \leftrightarrow \beta$.

The DiSSEP defines an integrable model. We indeed saw in chapter II that there exists an R matrix (II.B.55) satisfying the Yang Baxter equation and such that $m = 2\lambda\check{R}'(1)$. There exist also boundary matrices K and \bar{K} , introduced in (II.C.46) and (II.C.48) respectively, satisfying the reflection equation and such that $B = \lambda K'(1)$ and $\bar{B} = -\lambda\bar{K}'(1)$. Following the lines of chapter II, we can construct a transfer matrix

$$t(z) = \text{tr}_0(\tilde{K}_0(z)R_{0,L}(z) \dots R_{0,1}K_0(z)R_{1,0}(z) \dots R_{L,0}(z)) \quad (\text{III.B.5})$$

where

$$\tilde{K}(z) = \text{tr}_0 \left(\bar{K}_0 \left(\frac{1}{z} \right) \left((R_{0,1}(z^2)^{t_1})^{-1} \right)^{t_1} P_{0,1} \right). \quad (\text{III.B.6})$$

This transfer matrix satisfies the key relation $[t(z), t(z')] = 0$ and is directly related to the Markov matrix M through

$$M = \lambda t'(1). \quad (\text{III.B.7})$$

b) Matrix ansatz

This subsection is devoted to the construction of the steady state of the model in a matrix product form. Following the general procedure developed in this chapter for integrable stochastic processes, we start by introducing a vector $\mathbf{A}(z)$ with algebraic entries and a finite expansion with respect to the spectral parameter z :

$$\mathbf{A}(z) = \begin{pmatrix} G_1 z + G_2 + \frac{G_3}{z} \\ -G_1 z + G_2 - \frac{G_3}{z} \end{pmatrix}. \quad (\text{III.B.8})$$

To determine the commutation relations of the generators G_i 's, we write the ZF relation

$$\check{R} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \mathbf{A}(z_1) \otimes \mathbf{A}(z_2) = \mathbf{A}(z_2) \otimes \mathbf{A}(z_1) \quad \Leftrightarrow$$

$$\frac{z_1^2 - z_2^2}{z_1 z_2} \begin{pmatrix} \frac{\left((z_1 z_2 + 1) \left((\lambda + 1) G_2 G_1 + (\lambda - 1) G_1 G_2 \right) + (z_2 (\lambda - 1) - z_1 (\lambda + 1)) \left(G_1 G_3 - G_3 G_1 \right) \right)}{z_2 (\lambda - 1) - z_1 (\lambda + 1)} \\ \frac{\left((z_1 z_2 - 1) \left((\lambda + 1) G_2 G_1 + (\lambda - 1) G_1 G_2 \right) - (z_1 (\lambda + 1) + z_2 (\lambda - 1)) \left(G_1 G_3 - G_3 G_1 \right) \right)}{z_1 (\lambda + 1) + z_2 (\lambda - 1)} \\ \frac{\left((z_1 z_2 - 1) \left((\lambda + 1) G_2 G_1 + (\lambda - 1) G_1 G_2 \right) + (z_1 (\lambda + 1) + z_2 (\lambda - 1)) \left(G_1 G_3 - G_3 G_1 \right) \right)}{-z_1 (\lambda + 1) - z_2 (\lambda - 1)} \\ \frac{\left((z_1 z_2 + 1) \left((\lambda + 1) G_2 G_1 + (\lambda - 1) G_1 G_2 \right) + (z_1 (\lambda + 1) - z_2 (\lambda - 1)) \left(G_1 G_3 - G_3 G_1 \right) \right)}{z_1 (\lambda + 1) - z_2 (\lambda - 1)} \end{pmatrix} = 0.$$

This can be concisely and equivalently rewritten with the three following relations

$$[G_1, G_3] = 0, \quad G_2 G_1 = \phi G_1 G_2, \quad \text{and} \quad G_3 G_2 = \phi G_2 G_3, \quad \text{with} \quad \phi = \frac{1 - \lambda}{1 + \lambda}. \quad (\text{III.B.9})$$

The relations on the boundaries are obtained by writing the GZ relations. On the left boundary vector we have

$$\begin{aligned} \langle\langle W|K(z)\mathbf{A}\left(\frac{1}{z}\right) = \langle\langle W|\mathbf{A}(z) \Leftrightarrow \\ \langle\langle W|\left(\frac{\left(1-z^4\right)\left((\alpha+\gamma+2\lambda)G_1+(\alpha+\gamma-2\lambda)G_3+(\alpha-\gamma)G_2\right)}{z\left((\alpha+\gamma+2\lambda)z^2-\alpha-\gamma+2\lambda\right)}\right)}{\left(z^4-1\right)\left((\alpha+\gamma+2\lambda)G_1+(\alpha+\gamma-2\lambda)G_3+(\alpha-\gamma)G_2\right)}\right)}{z\left((\alpha+\gamma+2\lambda)z^2-\alpha-\gamma+2\lambda\right)}\rangle\rangle = 0. \end{aligned}$$

On the right boundary the GZ relation reads

$$\begin{aligned} \overline{K}(z)\mathbf{A}\left(\frac{1}{z}\right)|V\rangle\rangle = \mathbf{A}(z)|V\rangle\rangle \Leftrightarrow \\ \left(\frac{\left(1-z^4\right)\left((\beta+\delta+2\lambda)G_3+(\beta+\delta-2\lambda)G_1+(\delta-\beta)G_2\right)}{z\left((\beta+\delta-2\lambda)z^2-\beta-\delta-2\lambda\right)}\right)}{\left(z^4-1\right)\left((\beta+\delta+2\lambda)G_3+(\beta+\delta-2\lambda)G_1+(\delta-\beta)G_2\right)}\right)}{z\left((\beta+\delta-2\lambda)z^2-\beta-\delta-2\lambda\right)}\rangle\rangle = 0. \end{aligned}$$

These two relations are equivalent to

$$\begin{cases} \langle\langle W|(G_1 - c G_2 - a G_3) = 0, \\ (G_3 - b G_1 - d G_2)|V\rangle\rangle = 0 \end{cases} \text{ with } \begin{cases} a = \frac{2\lambda - \alpha - \gamma}{2\lambda + \alpha + \gamma}, & c = \frac{\gamma - \alpha}{2\lambda + \alpha + \gamma}, \\ b = \frac{2\lambda - \delta - \beta}{2\lambda + \delta + \beta}, & d = \frac{\beta - \delta}{2\lambda + \delta + \beta}. \end{cases} \quad (\text{III.B.10})$$

All this construction allows us to express the steady state as the matrix product state

$$|\mathcal{S}\rangle = \frac{1}{Z_L} \langle\langle W|\mathbf{X} \otimes \dots \otimes \mathbf{X}|V\rangle\rangle \quad (\text{III.B.11})$$

where

$$\mathbf{X} = \begin{pmatrix} E \\ D \end{pmatrix} := \mathbf{A}(1). \quad (\text{III.B.12})$$

We define also the auxiliary vector

$$\overline{\mathbf{X}} = \begin{pmatrix} -H \\ H \end{pmatrix} := 2\lambda\mathbf{A}'(1). \quad (\text{III.B.13})$$

We thus have the explicit relations

$$\begin{cases} E = G_1 + G_2 + G_3, \\ D = G_2 - G_1 - G_3, \\ H = 2\lambda(G_3 - G_1). \end{cases} \quad (\text{III.B.14})$$

The commutation relations on the G_i 's (III.B.9) translates into commutation relations on the E, D, H generators:

$$[D, E] = EH + HD, \quad \text{and} \quad [H, E] = [H, D] = \lambda^2(D^2 - E^2). \quad (\text{III.B.15})$$

These relations are equivalent to the very useful telescopic relation

$$w \begin{pmatrix} E \\ D \end{pmatrix} \otimes \begin{pmatrix} E \\ D \end{pmatrix} = \begin{pmatrix} E \\ D \end{pmatrix} \otimes \begin{pmatrix} -H \\ H \end{pmatrix} - \begin{pmatrix} -H \\ H \end{pmatrix} \otimes \begin{pmatrix} E \\ D \end{pmatrix}. \quad (\text{III.B.16})$$

Notice here that, in contrast with the SSEP case (see [16]) where H is a scalar, the commutation relations between H and E , D are not trivial. The action of the generators E , D and H on the boundary vectors $\langle\langle W|$ and $|V\rangle\rangle$ are obtained by direct translation of the action of the generators G_i 's (III.B.10):

$$\langle\langle W|(\alpha E - \gamma D) = \langle\langle W|H, \quad \text{and} \quad (\delta E - \beta D)|V\rangle\rangle = -H|V\rangle\rangle. \quad (\text{III.B.17})$$

It is equivalent to

$$\langle\langle W|B \begin{pmatrix} E \\ D \end{pmatrix} = \langle\langle W| \begin{pmatrix} -H \\ H \end{pmatrix}, \quad \text{and} \quad \bar{B} \begin{pmatrix} E \\ D \end{pmatrix} |V\rangle\rangle = - \begin{pmatrix} -H \\ H \end{pmatrix} |V\rangle\rangle. \quad (\text{III.B.18})$$

Note that the relations satisfied by the generators E , D and H are strictly equivalent to the relations verified by the G_i 's, they just correspond to the change of basis (III.B.14). We gave them in order to make the connection with the usual presentation of the matrix ansatz and to make the comparison with the SSEP easier. Nevertheless we will not use the E , D , H basis in the following and stick with the G_i 's basis because the computations will be more efficient.

The explicit representation of the boundary vectors $\langle\langle W|$ and $|V\rangle\rangle$ and of the generators G_i 's (or equivalently of the generators E , D and H) can be found in [V3]. We do not present it here because it does not simplify the computation of the physical quantities (that can be efficiently done using the algebraic relations (III.B.9) and (III.B.10), see next subsection) and it does not shed any new light on the stationary distribution. Nevertheless the existence of such explicit representation is necessary to prove the existence of the generators and boundary vectors.

Remark B.3. *As previously seen in this chapter (see subsection 5 for details), we can define the inhomogeneous ground state*

$$|\mathcal{S}(z_1, \dots, z_L)\rangle\rangle = \frac{\langle\langle W|\mathbf{A}(z_1) \otimes \dots \otimes \mathbf{A}(z_L)|V\rangle\rangle}{Z_L(z_1, \dots, z_L)}, \quad (\text{III.B.19})$$

where the normalization

$$Z_L(z_1, \dots, z_L) = \langle\langle W|C(z_1) \dots C(z_L)|V\rangle\rangle, \quad \text{with} \quad C(z) = A_0(z) + A_1(z) + A_2(z). \quad (\text{III.B.20})$$

This inhomogeneous deformation of the steady state (we recall that $|\mathcal{S}(1, \dots, 1)\rangle\rangle$ is the steady state) is an eigenvector of the inhomogeneous transfer matrix associated to the model

$$t(z|z_1, \dots, z_L)|\mathcal{S}(z_1, \dots, z_L)\rangle\rangle = \lambda(z|z_1, \dots, z_L)|\mathcal{S}(z_1, \dots, z_L)\rangle\rangle, \quad (\text{III.B.21})$$

where the eigenvalue is equal to

$$\lambda(z|z_1, \dots, z_L) = 1 + \phi^{2L} \frac{(z^4 - 1)(az^2 + \phi^2)(bz^2 + \phi^2)}{(z^4 - \phi^4)(z^2 + a)(z^2 + b)} \prod_{i=1}^L \frac{((zz_i)^2 - 1)(z^2 - z_i^2)}{((zz_i)^2 - \phi^2)(z^2 - (\phi z_i)^2)}. \quad (\text{III.B.22})$$

This can be proven (see subsection 5 for details) using degree consideration and the symmetry property on the transfer matrix

$$t(z|z_1, \dots, z_L) = (\lambda(z|z_1, \dots, z_L) - 1)t\left(\frac{\phi}{z}|z_1, \dots, z_L\right). \quad (\text{III.B.23})$$

c) Computation of physical quantities

We now focus on the computation of physical quantities in the stationary state. We will see that the matrix ansatz algebra, introduced to express the steady state, reveals to be very efficient in computing correlation functions and mean values of the currents. Before studying the general model, we focus on the case $\lambda = 1$ ($\phi = 0$), where the calculations simplify drastically: it corresponds to the free fermion point of the model we introduced.

For $\lambda = 1$, all the eigenvalues and the eigenvectors can be computed easily as shown in the following proposition.

Proposition B.4. For $L \geq 3$, the 2^L eigenvectors are characterized by the set $\epsilon = (\epsilon_1, \epsilon_2, \dots, \epsilon_L)$ with $\epsilon_i = \pm 1$ and are given by

$$\Omega(\epsilon) = v(\epsilon_1, \epsilon_2, \alpha, \gamma) \otimes \begin{pmatrix} 1 \\ \epsilon_2 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ \epsilon_3 \end{pmatrix} \otimes \dots \otimes \begin{pmatrix} 1 \\ \epsilon_{L-1} \end{pmatrix} \otimes v(\epsilon_L, \epsilon_{L-1}, \delta, \beta) \quad (\text{III.B.24})$$

where $v(\epsilon, \epsilon', \mu, \nu) = \begin{pmatrix} \epsilon' + \nu \\ 1 + \mu + f(\epsilon, \epsilon', \mu + \nu) \end{pmatrix}$ and $f(\epsilon, \epsilon', \tau) = \epsilon\epsilon' - 1 - \frac{\tau}{2}(1 - \epsilon)$. The corresponding eigenvalues are

$$\Lambda(\epsilon) = f(\epsilon_1, \epsilon_2, \alpha + \gamma) + \sum_{j=2}^{L-2} (\epsilon_j \epsilon_{j+1} - 1) + f(\epsilon_L, \epsilon_{L-1}, \delta + \beta). \quad (\text{III.B.25})$$

Let us remark that the ASEP on a ring with Langmuir kinetics has been treated similarly in [208].

Proof. This can be checked by a direct computation. ■

Corollary B.5. From the previous results, we deduce that the stationary state is

$$\Omega(+, +, \dots, +) = \frac{1}{Z_L} \begin{pmatrix} 1 + \gamma \\ 1 + \alpha \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 1 \end{pmatrix}^{\otimes L-2} \otimes \begin{pmatrix} 1 + \beta \\ 1 + \delta \end{pmatrix} \quad (\text{III.B.26})$$

where $Z_L = 2^{L-2}(2 + \alpha + \gamma)(2 + \beta + \delta)$ is the normalisation such that the entries be probabilities.

Proof. We have indeed $\Lambda(+, +, \dots, +) = 0$. ■

From this stationary state, we can compute the mean value of the injected current by the left reservoir (resp. by the right reservoir)

$$\langle j_{\text{left}} \rangle = \frac{\alpha - \gamma}{2 + \alpha + \gamma} \quad (\text{resp. } \langle j_{\text{right}} \rangle = \frac{\delta - \beta}{2 + \delta + \beta}). \quad (\text{III.B.27})$$

We see that the current has the sign of $\alpha - \gamma$ (resp. $\delta - \beta$). As expected, it goes to the left when extraction is promoted, and to the right when injection is proeminent. It vanishes for $\alpha = \gamma$. The lattice current in the bulk vanishes.

We can also compute easily the first excited state whose eigenvalue provides the relaxation rate. Indeed, the greatest non vanishing eigenvalue is

$$\begin{cases} G = -4 & \text{if } \alpha + \gamma > 2 \text{ and } \beta + \delta > 2 \\ G = -2 - \beta - \delta & \text{if } \alpha + \gamma > 2 \text{ and } \beta + \delta < 2 \\ G = -2 - \alpha - \gamma & \text{if } \alpha + \gamma < 2 \text{ and } \beta + \delta > 2 \\ G = -\alpha - \gamma - \beta - \delta & \text{if } \alpha + \gamma < 2 \text{ and } \beta + \delta < 2 \end{cases} \quad (\text{III.B.28})$$

These results shall be generalized in the thermodynamic limit in chapter V for any λ using the Bethe equations. The general result displayed on figure V.4 matches the above values of the gap for $\lambda = 1$ ($\phi = 0$).

For this particular choice of λ , it is also possible to get the generating function of the cumulants of the current entering in the system from the left reservoir (the same result is also obtained by symmetry for the right reservoir). For general λ , one obtains the variance in (III.B.73). It is well established (see chapter I for instance) that this generating function is the greatest eigenvalue of the following deformed Markov matrix

$$M = B_1(\mu) + \sum_{k=1}^{L-1} m_{k,k+1} + \bar{B}_L, \quad (\text{III.B.29})$$

where the local jump operator $B(\mu)$ is deformed as follows

$$B(\mu) = \begin{pmatrix} -\alpha & \gamma e^{-\mu} \\ \alpha e^{\mu} & -\gamma \end{pmatrix}. \quad (\text{III.B.30})$$

One can show by direct computation that the greatest eigenvalue is given by⁷

$$E(\mu) = -\frac{2 + \alpha + \gamma}{2} + \frac{1}{2} \sqrt{4 + 4\alpha e^{\mu} + 4\gamma e^{-\mu} + (\alpha + \gamma)^2} \quad (\text{III.B.31})$$

with the eigenvector

$$\Omega(\mu) = \begin{pmatrix} 1 + \gamma e^{-\mu} \\ 1 + \alpha + E(\mu) \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 1 \end{pmatrix}^{\otimes L-2} \otimes \begin{pmatrix} 1 + \beta \\ 1 + \delta \end{pmatrix}. \quad (\text{III.B.32})$$

The rate-function $G(j)$ associated to the current is the Legendre transformation of this generating function of the cumulants:

$$G(j) = \mu^* j - E(\mu^*), \quad \left. \frac{d}{d\mu} E(\mu) \right|_{\mu=\mu^*} = j \quad (\text{III.B.33})$$

Its explicit form can be extracted from the expression of $E(\mu)$ and is given in the following proposition

Proposition B.6.

$$G(j) = 1 + \frac{\alpha + \gamma}{2} - \sqrt{1 + \Delta(j) + \left(\frac{\alpha + \gamma}{2}\right)^2} + j \ln \left(\frac{\Delta(j)}{2\alpha} + \frac{j}{\alpha} \sqrt{1 + \Delta(j) + \left(\frac{\alpha + \gamma}{2}\right)^2} \right) \quad (\text{III.B.34})$$

where

$$\Delta(j) = 2j^2 + \sqrt{4(\alpha\gamma + j^2 + j^4) + j^2(\alpha + \gamma)^2}. \quad (\text{III.B.35})$$

Let us stress that (III.B.34) represents an exact result on the large deviation function of the current on the left boundary. The function $G(j)$ is convex and vanishes when j is equal to the mean value of the current on the left boundary given by (III.B.27) as expected, see figure III.5. Note that it is not Gaussian.

We now come back to the general case $\lambda \neq 1$ ($\phi \neq 0$). We start by stating a formula, giving the value of a general word in the generators G_i 's, that will be of prime utility to compute correlation functions and mean values of particle currents. It thus appears as one of the main analytical result obtained concerning the DiSSEP.

Proposition B.7. *For all integers $p, q, r \geq 0$ we have the equality*

$$\frac{\langle\langle W | G_1^p G_2^q G_3^r | V \rangle\rangle}{\langle\langle W | G_2^{p+q+r} | V \rangle\rangle} = \frac{\prod_{\ell=0}^{p-1} (c \phi^{p-1-\ell} + ad \phi^{q+r+\ell}) \prod_{n=0}^{r-1} (d \phi^{r-1-n} + bc \phi^{q+p+n})}{\prod_{k=q}^{p+q+r-1} (1 - ab \phi^{2k})}, \quad (\text{III.B.36})$$

Note that the value of any word in the generators G_i 's (not necessarily ordered as above) can be easily obtained from this formula because the commutation relations among the G_i 's are very simple (III.B.9). The reordering of the G_i 's makes appear only a power of ϕ .

⁷We recover that $E(0) = 0$ in agreement with the fact that at $\mu = 0$ the greatest eigenvalue is vanishing because of the Markovian property. Note that $E(\mu)$ depends only on the boundary rates of the left reservoir α and γ , and not on the boundary rates of the right reservoir β and δ .

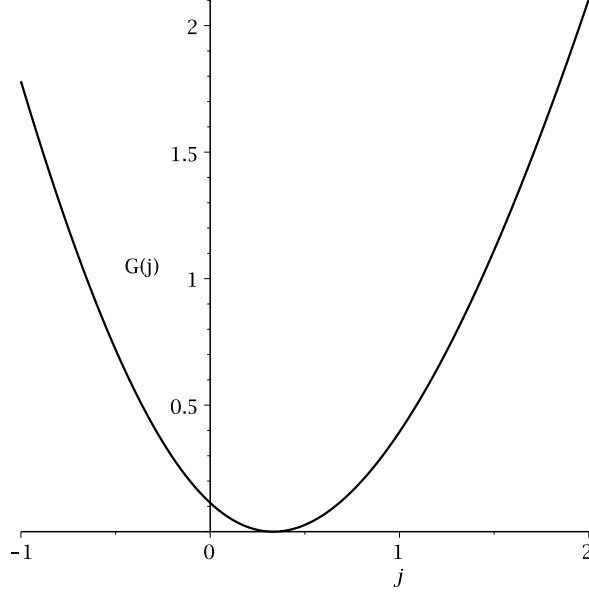


Figure III.5: Example of large deviation function $G(j)$ (on the plot $\alpha = 2, \gamma = 0.5$).

Proof. In order to compute $\langle\langle W|G_1^p G_2^q G_3^r|V\rangle\rangle$, we use a change of generators defined as follows

$$L_i = \frac{G_1}{\phi^i} - aG_3\phi^i, \quad \text{and} \quad R_k = \frac{G_3}{\phi^k} - bG_1\phi^k. \quad (\text{III.B.37})$$

This is built so that L_i and R_k fulfill the following relations (derived straightforwardly from (III.B.9) and (III.B.10))

$$\begin{aligned} G_2^i L_i &= L_0 G_2^i, \quad R_k G_2^k = G_2^k R_0, \quad [L_i, G_1] = [L_i, G_3] = [R_k, G_1] = [R_k, G_3] = 0 \\ \text{and} \quad \langle\langle W|L_0 &= c\langle\langle W|G_2, \quad R_0|V\rangle\rangle = dG_2|V\rangle\rangle. \end{aligned} \quad (\text{III.B.38})$$

The change of generators (III.B.37) can be inverted to get

$$G_1 = \frac{\phi^{k+i}}{1 - ab\phi^{2(k+i)}} \left(\frac{L_i}{\phi^k} + a\phi^i R_k \right), \quad \text{and} \quad G_3 = \frac{\phi^{k+i}}{1 - ab\phi^{2(k+i)}} \left(b\phi^k L_i + \frac{R_k}{\phi^i} \right). \quad (\text{III.B.39})$$

We can now begin the computation

$$\begin{aligned} \langle\langle W|G_1^p G_2^q G_3^r|V\rangle\rangle &= \frac{\phi^q}{1 - ab\phi^{2q}} \langle\langle W| \left(\frac{L_0}{\phi^q} + aR_q \right) G_1^{p-1} G_2^q G_3^r|V\rangle\rangle \\ &= \frac{1}{1 - ab\phi^{2q}} \langle\langle W|cG_2 G_1^{p-1} G_2^q G_3^r|V\rangle\rangle + \frac{1}{1 - ab\phi^{2q}} \langle\langle W|G_1^{p-1} G_2^q G_3^r a d\phi^q G_2|V\rangle\rangle \\ &= \frac{c\phi^{p-1} + ad\phi^{q+r}}{1 - ab\phi^{2q}} \langle\langle W|G_1^{p-1} G_2^{q+1} G_3^r|V\rangle\rangle. \end{aligned}$$

The first equality is obtained using (III.B.39) with $i = 0$ and $k = q$ to transform the leftmost G_1 . The second equality relies on the relations (III.B.38). We get the last one using (III.B.9). This relation provides a recursion for $\langle\langle W|G_1^p G_2^q G_3^r|V\rangle\rangle$ that we can iterate to obtain

$$\langle\langle W|G_1^p G_2^q G_3^r|V\rangle\rangle = \left(\prod_{l=0}^{p-1} \frac{c\phi^{p-1-l} + ad\phi^{r+q+l}}{1 - ab\phi^{2(q+l)}} \right) \langle\langle W|G_2^{q+p} G_3^r|V\rangle\rangle. \quad (\text{III.B.40})$$

Performing similar computations with G_3 we obtain the following recursive relation

$$\begin{aligned} \langle\langle W|G_2^{q+p} G_3^r|V\rangle\rangle &= \frac{\phi^{q+p}}{1 - ab\phi^{2(q+p)}} \langle\langle W|G_2^{q+p} G_3^{r-1} \left(bL_{q+p} + \frac{R_0}{\phi^{q+p}} \right) |V\rangle\rangle \\ &= \frac{d\phi^{r-1} + bc\phi^{q+p}}{1 - ab\phi^{2(q+p)}} \langle\langle W|G_2^{q+p+1} G_3^{r-1}|V\rangle\rangle, \end{aligned}$$

to get

$$\langle\langle W|G_2^{q+p}G_3^r|V\rangle\rangle = \left(\prod_{n=0}^{r-1} \frac{d\phi^{r-1-n} + bc\phi^{q+p+n}}{1 - ab\phi^{2(q+p+n)}} \right) \langle\langle W|G_2^{p+q+r}|V\rangle\rangle. \quad (\text{III.B.41})$$

Recombining (III.B.40) and (III.B.41) together, the desired result (III.B.36) is proved. \blacksquare

Let us stress that since G_1, G_2, G_3 form a basis, the knowledge of all words built on them allows us to reconstruct all words built on E and D using the two first relations of (III.B.14). In particular, we are able to compute exactly physical observables, as it is illustrated below.

Proposition B.8. *The one-point function (i.e the mean particle density) reads for $1 \leq i \leq L$*

$$\langle\tau_i\rangle = \frac{1}{2} \frac{\langle\langle W|G_2^{i-1}(-G_1 + G_2 - G_3)G_2^{L-i}|V\rangle\rangle}{\langle\langle W|G_2^L|V\rangle\rangle} \quad (\text{III.B.42})$$

$$= \frac{1}{2} - \frac{c\phi^{i-1} + ad\phi^{L+i-2} + d\phi^{L-i} + bc\phi^{2L-i-1}}{2(1 - ab\phi^{2L-2})}, \quad (\text{III.B.43})$$

the connected two-point correlation function, for $1 \leq i < j \leq L$, is given by

$$\langle\tau_i\tau_j\rangle_c = \langle\tau_i\tau_j\rangle - \langle\tau_i\rangle\langle\tau_j\rangle \quad (\text{III.B.44})$$

$$= \frac{\langle\langle W|C^{i-1}DC^{j-i-1}DC^{L-j}|V\rangle\rangle}{\langle\langle W|C^L|V\rangle\rangle} - \frac{\langle\langle W|C^{i-1}DC^{L-i}|V\rangle\rangle}{\langle\langle W|C^L|V\rangle\rangle} \frac{\langle\langle W|C^{j-1}DC^{L-j}|V\rangle\rangle}{\langle\langle W|C^L|V\rangle\rangle}$$

$$= \frac{\phi^{L+j-i-3}(1 - \phi^2)(1 + b\phi^{2(L-j)})(1 + a\phi^{2(i-1)})(d + bc\phi^{L-1})(c + ad\phi^{L-1})}{4(1 - ab\phi^{2(L-1)})^2(1 - ab\phi^{2(L-2)})} \quad (\text{III.B.45})$$

and the connected three-point correlation function, for $1 \leq i < j < k \leq L$, is equal to

$$\langle\tau_i\tau_j\tau_k\rangle_c = \langle\tau_i\tau_j\tau_k\rangle - \langle\tau_i\rangle\langle\tau_j\tau_k\rangle - \langle\tau_j\rangle\langle\tau_i\tau_k\rangle - \langle\tau_k\rangle\langle\tau_i\tau_j\rangle + 2\langle\tau_i\rangle\langle\tau_j\rangle\langle\tau_k\rangle \quad (\text{III.B.46})$$

$$= -\frac{\phi^{L+k-i-5}(1 - \phi^2)^2(1 + b\phi^{2(L-k)})(1 + a\phi^{2(i-1)})(d + bc\phi^{L-1})(c + ad\phi^{L-1})}{8(1 - ab\phi^{2(L-1)})^3(1 - ab\phi^{2(L-2)})(1 - ab\phi^{2(L-3)})}$$

$$\times [\phi^{L-j}(d + bc\phi^{L-3})(1 + 2a\phi^{2(j-1)} + ab\phi^{2(L-1)}) + \phi^{j-1}(c + ad\phi^{L-3})(1 + 2b\phi^{2(L-j)} + ab\phi^{2(L-1)})]. \quad (\text{III.B.47})$$

Remark that for generic i, j, k , the two- and three-point correlation functions satisfy both a set of closed linear relations:

$$(1 - \lambda^2) \left(\langle\tau_{i-1}\tau_j\rangle_c + \langle\tau_{i+1}\tau_j\rangle_c + \langle\tau_i\tau_{j-1}\rangle_c + \langle\tau_i\tau_{j+1}\rangle_c \right) = 4(1 + \lambda^2) \langle\tau_i\tau_j\rangle_c \quad (\text{III.B.48})$$

$$(1 - \lambda^2) \left(\langle\tau_{i-1}\tau_j\tau_k\rangle_c + \langle\tau_{i+1}\tau_j\tau_k\rangle_c + \langle\tau_i\tau_{j-1}\tau_k\rangle_c + \langle\tau_i\tau_{j+1}\tau_k\rangle_c + \langle\tau_i\tau_j\tau_{k-1}\rangle_c \right. \\ \left. + \langle\tau_i\tau_j\tau_{k+1}\rangle_c \right) = 6(1 + \lambda^2) \langle\tau_i\tau_j\tau_k\rangle_c \quad (\text{III.B.49})$$

Proposition B.9. *The mean particle lattice current between sites i and $i + 1$ (i.e the mean number of particles, counted algebraically, that jump from site i to site $i + 1$ per unit of time) is given by the exact expression*

$$\langle j_{lat}^{i \rightarrow i+1} \rangle = \frac{\langle\langle W|C^{i-1}(DE - ED)C^{L-i-1}|V\rangle\rangle}{\langle\langle W|C^L|V\rangle\rangle} \quad (\text{III.B.50})$$

$$= \frac{1 - \phi bc\phi^{2L-i-2} + d\phi^{L-i-1} - ad\phi^{L+i-2} - c\phi^{i-1}}{2(1 - ab\phi^{2L-2})}. \quad (\text{III.B.51})$$

Counting positively the pairs of particles which condensate on the lattice and negatively the pairs which evaporate, we get for the mean evaporation-condensation current on sites i and

$i + 1$ (i.e the mean number of particles, counted algebraically, that condensate on sites i and $i + 1$ per unit of time)

$$\langle j_{cond}^{i,i+1} \rangle = 2 \frac{\langle\langle W | C^{i-1} \lambda^2 (E^2 - D^2) C^{L-i-1} | V \rangle\rangle}{\langle\langle W | C^L | V \rangle\rangle} \quad (\text{III.B.52})$$

$$= \frac{(1 - \phi)^2 bc \phi^{2L-i-2} + d \phi^{L-i-1} + ad \phi^{L+i-2} + c \phi^{i-1}}{1 + \phi} \frac{1}{1 - ab \phi^{2L-2}}. \quad (\text{III.B.53})$$

Note that the above expressions behave as expected under the three symmetries:

1. The symmetry $\lambda \rightarrow -\lambda$, that translates into $\phi \rightarrow 1/\phi$, $a \rightarrow 1/a$, $c \rightarrow -c/a$, $b \rightarrow 1/b$ and $d \rightarrow -d/b$, leaves them invariant.
2. The left/right symmetry, that becomes $a \leftrightarrow b$, $c \leftrightarrow d$ and $i \rightarrow L + 1 - i$, changes the sign of the lattice current, keeps the condensation current and the density invariant.
3. The particle-hole symmetry, which reads $a \rightarrow a$, $b \rightarrow b$, $c \rightarrow -c$ and $d \rightarrow -d$, changes the sign of both currents and transforms $\langle n_i \rangle$ into $1 - \langle n_i \rangle$.

The physical quantities computed above are not all independent. The particle conservation law at site i reads

$$\langle j_{lat}^{i-1 \rightarrow i} \rangle - \langle j_{lat}^{i \rightarrow i+1} \rangle + \frac{1}{2} \langle j_{cond}^{i-1,i} \rangle + \frac{1}{2} \langle j_{cond}^{i,i+1} \rangle = 0, \quad (\text{III.B.54})$$

which can be seen on the matrix product ansatz using relations (III.B.15). From the identity $[D, E] = [D, C]$ one then deduces

$$\langle j_{lat}^{i \rightarrow i+1} \rangle = \langle \tau_i \rangle - \langle \tau_{i+1} \rangle, \quad (\text{III.B.55})$$

and using $E^2 - D^2 = C^2 - CD - DC$ one gets

$$\langle j_{cond}^{i,i+1} \rangle = 2\lambda^2 \left(1 - \langle \tau_i \rangle - \langle \tau_{i+1} \rangle \right). \quad (\text{III.B.56})$$

From these three relations, one obtains

$$\langle j_{cond}^{i-1,i} \rangle - \langle j_{cond}^{i,i+1} \rangle + 2\lambda^2 \left(\langle j_{lat}^{i-1 \rightarrow i} \rangle + \langle j_{lat}^{i \rightarrow i+1} \rangle \right) = 0 \quad (\text{III.B.57})$$

$$\langle \tau_{i-1} \rangle + \langle \tau_{i+1} \rangle - 2\langle \tau_i \rangle + \lambda^2 \left(2 - \langle \tau_{i-1} \rangle - \langle \tau_{i+1} \rangle - 2\langle \tau_i \rangle \right) = 0. \quad (\text{III.B.58})$$

Remark B.10. *The one point correlation function verifies a closed set of equation as for the SSEP, in contrast with the ASEP case where the equations couple the one point function and the two points function. This property remains valid for the higher order correlation functions (III.B.48), which allows in principle to compute them. However, for the multi-points correlation functions, solving this set of equation can be very hard. This points out the usefulness of the matrix product ansatz which makes the calculations much easier.*

Fluctuations of the currents As mentioned previously, there are closed linear relations between the two- and three-point correlation functions which allow one to compute the cumulant of the currents. In this section, we present the computations of the second cumulant of the lattice current between sites i and $i + 1$. Let us note that it depends on the site, because of the evaporation-condensation process. As usual for such a purpose, we use the deformed Markovian matrix defined as follows:

$$M^\mu = B_1 + \sum_{k=1}^{i-1} m_{k,k+1} + m_{i,i+1}^\mu + \sum_{k=i+1}^{L-1} w_{k,k+1} + \bar{B}_L \quad \text{with} \quad m^\mu = \begin{pmatrix} -\lambda^2 & 0 & 0 & \lambda^2 \\ 0 & -1 & e^\mu & 0 \\ 0 & e^{-\mu} & -1 & 0 \\ \lambda^2 & 0 & 0 & -\lambda^2 \end{pmatrix}. \quad (\text{III.B.59})$$

Let $|\Psi^\mu\rangle$ be the eigenstate of M^μ with highest eigenvalue

$$M^\mu |\Psi^\mu\rangle = E(\mu) |\Psi^\mu\rangle. \quad (\text{III.B.60})$$

$E(\mu)$ is the generating function for the cumulants of the lattice current between sites i and $i + 1$. We introduce the following notation for vectors

$$\langle\{j\}| = \left(\langle 0| + \langle 1|\right)^{\otimes(j-1)} \otimes \langle 1| \otimes \left(\langle 0| + \langle 1|\right)^{\otimes(L-j)} \quad (\text{III.B.61})$$

$$\langle\{j, k\}| = \left(\langle 0| + \langle 1|\right)^{\otimes(j-1)} \otimes \langle 1| \otimes \left(\langle 0| + \langle 1|\right)^{\otimes(k-j-1)} \otimes \langle 1| \otimes \left(\langle 0| + \langle 1|\right)^{\otimes(L-k)} \quad (\text{III.B.62})$$

⋮

In words, $\langle\{j_1, j_2, \dots, j_M\}|$ represents configurations with one particle at site j_1, j_2, \dots, j_M , and anything else on the other sites. Remark that this definition applies whatever the order on j_1, \dots, j_M , and thus extends the one given in the above equations. By extension, we note $\langle\emptyset| = (\langle 0| + \langle 1|)^{\otimes L}$. Then, we define the components:

$$T_j(\mu) \equiv T_j = \frac{\langle\{j\}|\Psi^\mu\rangle}{\langle\emptyset|\Psi^\mu\rangle}; \quad U_{jk}(\mu) \equiv U_{jk} = \frac{\langle\{j, k\}|\Psi^\mu\rangle}{\langle\emptyset|\Psi^\mu\rangle} \quad \text{and} \quad V_{jkl}(\mu) \equiv V_{jkl} = \frac{\langle\{j, k, l\}|\Psi^\mu\rangle}{\langle\emptyset|\Psi^\mu\rangle}. \quad (\text{III.B.63})$$

Note that by construction, U and V are symmetric, e.g. $U_{jk} = U_{kj}$. Now, projecting equation (III.B.60) on $\langle\emptyset|$, we get

$$E(\mu) = (e^{-\mu} - 1)(T_{i+1} - U_{i,i+1}) + (e^\mu - 1)(T_i - U_{i,i+1}). \quad (\text{III.B.64})$$

We also project equation (III.B.60) on $\langle\{j\}|$ for $j = 1$, $1 < j < i$ and $i + 1 < j < L$, $j = i$, $j = i + 1$, and $j = L$. We get respectively:

$$E(\mu) T_1 = \alpha(1 - T_1) - \gamma T_1 + \lambda^2(1 - T_1 - T_2) + T_2 - T_1 + (e^{-\mu} - 1)(U_{1,i+1} - V_{1,i,i+1}) + (e^\mu - 1)(U_{1,i} - V_{1,i,i+1}), \quad (\text{III.B.65})$$

$$E(\mu) T_j = \lambda^2(2 - 2T_j - T_{j+1} - T_{j-1}) + T_{j+1} - 2T_j + T_{j-1} + (e^{-\mu} - 1)(U_{j,i+1} - V_{j,i,i+1}) + (e^\mu - 1)(U_{j,i} - V_{j,i,i+1}), \quad (\text{III.B.66})$$

$$E(\mu) T_i = \lambda^2(2 - 2T_i - T_{i+1} - T_{i-1}) + T_{i+1} - 2T_i + T_{i-1} + (e^{-\mu} - 1)(T_{i+1} - U_{i,i+1}), \quad (\text{III.B.67})$$

$$E(\mu) T_{i+1} = \lambda^2(2 - 2T_{i+1} - T_{i+2} - T_i) + T_{i+2} - 2T_{i+1} + T_i + (e^\mu - 1)(T_i - U_{i,i+1}), \quad (\text{III.B.68})$$

$$E(\mu) T_L = \delta(1 - T_L) - \beta T_L + \lambda^2(1 - T_L - T_{L-1}) + T_{L-1} - T_L + (e^{-\mu} - 1)(U_{i+1,L} - V_{i,i+1,L}) + (e^\mu - 1)(U_{i,L} - V_{i,i+1,L}). \quad (\text{III.B.69})$$

These equations are solved iteratively, expanding all quantities as series in μ . We set

$$\begin{aligned} E(\mu) &= E^{(0)} + \mu E^{(1)} + \frac{\mu^2}{2} E^{(2)} + o(\mu^2), \\ T_j(\mu) &= T_j^{(0)} + \mu T_j^{(1)} + o(\mu), \\ U_{j,k}(\mu) &= U_{j,k}^{(0)} + \mu U_{j,k}^{(1)} + o(\mu). \end{aligned}$$

In the above expansions, $E^{(0)} = 0$ is the greatest eigenvalue of the undeformed Markov matrix and $E^{(1)} = \langle j_{lat}^{i \rightarrow i+1} \rangle$ is the mean value of the lattice current measured between the site i and $i + 1$, where the deformation occurs. We recall that $\langle j_{lat}^{i \rightarrow i+1} \rangle$ has been computed in (III.B.51). The value of $T_j^{(0)} = \langle \tau_j \rangle$ has also been already calculated, see (III.B.43). Similarly, $U_{j,k}^{(0)}$ is linked to the two-points correlation function, see (III.B.45).

We wish to compute $E(\mu)$ up to order 2, which corresponds to the variance of the lattice current. We get it through the expansion of (III.B.64) up to order 2:

$$E^{(1)} = T_i^{(0)} - T_{i+1}^{(0)}, \quad (\text{III.B.70})$$

$$E^{(2)} = 2\left(T_i^{(1)} - T_{i+1}^{(1)}\right) + T_i^{(0)} + T_{i+1}^{(0)} - 2U_{i,i+1}^{(0)}. \quad (\text{III.B.71})$$

Equation (III.B.70) just reproduces the relation (III.B.55) between the mean values of the lattice current and of the density.

To get $T_j^{(1)}$, one considers equations (III.B.65)-(III.B.69) at first order in μ . They only involve $T_j^{(1)}$, $T_j^{(0)}$ and $U_{jk}^{(0)}$, and can be solved recursively in $T_j^{(1)}$. We get

$$\begin{pmatrix} T_{i+1}^{(1)} \\ T_i^{(1)} \end{pmatrix} = \frac{\phi^L}{1 - ab\phi^{2L-2}} \begin{pmatrix} \frac{b\phi^{L-i-1} + \phi^{i+1-L}}{\phi^2 - 1} & \frac{a\phi^i + \phi^{-i}}{\phi^2 - 1} \\ \frac{b\phi^{L-i} + \phi^{i-L}}{\phi^2 - 1} & \frac{a\phi^{i-1} + \phi^{1-i}}{\phi^2 - 1} \end{pmatrix} \begin{pmatrix} \sum_{l=0}^{i-1} (a\phi^l + \phi^{-l}) I_{l+1} \\ \sum_{l=0}^{L-i-1} (b\phi^l + \phi^{-l}) I_{L-l} \end{pmatrix}$$

with

$$I_j = \frac{(\phi + 1)^2}{4\phi} \times \begin{cases} E^{(1)} T_i^{(0)} + T_{i+1}^{(0)} - U_{i,i+1}^{(0)}, & \text{for } j = i \\ E^{(1)} T_{i+1}^{(0)} - T_i^{(0)} + U_{i,i+1}^{(0)}, & \text{for } j = i + 1 \\ E^{(1)} T_j^{(0)} + U_{j,i+1}^{(0)} - U_{j,i}^{(0)}, & \text{otherwise} \end{cases} \quad (\text{III.B.72})$$

Plugging these values into (III.B.71), we get the analytical expression of the variance of the lattice current:

$$E^{(2)} = T_i^{(0)} + T_{i+1}^{(0)} - 2U_{i,i+1}^{(0)} \quad (\text{III.B.73})$$

$$+ \frac{2}{1 + \phi} \left\{ \frac{\phi^i (b\phi^{2L-2i-1} - 1)}{1 - ab\phi^{2L-2}} \sum_{\ell=0}^{i-1} (a\phi^\ell + \phi^{-\ell}) I_{\ell+1} - \frac{\phi^{L-i} (a\phi^{2i-1} - 1)}{1 - ab\phi^{2L-2}} \sum_{\ell=0}^{L-i-1} (b\phi^\ell + \phi^{-\ell}) I_{L-\ell} \right\}.$$

Using the explicit form of I_j , one can compute the sums in (III.B.73) to perform the thermodynamic limit for $E^{(2)}$, see chapter V. Let us conclude this subsection by mentioning that the higher cumulants may be computed in principle by similar methods. However, the computations become much harder and are beyond the scope of this manuscript.

Comparison with SSEP As mentioned previously the DiSSEP is a deformation of the SSEP which can be easily recovered when taking $\lambda = 0$. This limit already reveals at the level of the matrix product ansatz algebra: the commutation relations between E , D and H (III.B.15) become simpler when $\lambda = 0$. We have indeed $[H, E] = [H, D] = 0$. Hence H can be chosen equal to the identity. In this case we recover the well known relation $[D, E] = D + E$, relevant in the construction of the steady state of the SSEP. Remark that the generators G_1 , G_2 and G_3 in contrast “diverge” when taking the limit $\lambda \rightarrow 0$ (this can be seen by inverting the change of basis (III.B.14)).

We can also take the limit $\lambda \rightarrow 0$ at the level of the physical observables. For the one and two points correlation function we get

$$\lim_{\lambda \rightarrow 0} \langle \tau_i \rangle = \frac{\rho_l (L + B - i) + \rho_r (i - 1 + A)}{L + A + B - 1}, \quad \text{with } A = \frac{1}{\alpha + \gamma}, \quad B = \frac{1}{\beta + \delta}$$

and

$$\lim_{\lambda \rightarrow 0} \langle \tau_i \tau_j \rangle_c = -\frac{(i - 1 + A) (B + L - j) (\rho_l - \rho_r)^2}{(L + A + B - 1)^2 (L + A + B - 2)},$$

which are in agreement with the known expressions for the SSEP [16, 209]. For the lattice and evaporation-condensation currents we get

$$\lim_{\lambda \rightarrow 0} \langle j_{lat}^{i \rightarrow i+1} \rangle = \frac{\rho_l - \rho_r}{L + A + B - 1} \quad \text{and} \quad \lim_{\lambda \rightarrow 0} \langle j_{cond}^{i, i+1} \rangle = 0,$$

also in agreement with the SSEP results.

We can also take carefully the limit of the expression (III.B.73) to recover the variance of the lattice current for the SSEP model [209]

$$E_{SSEP}^{(2)} = \frac{\rho_l + \rho_r}{L + A + B - 1} + \frac{(A - 3A^2 + 2A^3 + B - 3B^2 + 2B^3)(\rho_l - \rho_r)^2}{3(L + A + B - 1)^3(L + A + B - 2)} \\ - \frac{(\rho_l - \rho_r)^2}{3(L + A + B - 1)^2(L + A + B - 2)} + \frac{\rho_l^2 + \rho_r^2}{(L + A + B - 1)(L + A + B - 2)} - \frac{2(\rho_l^2 + \rho_l \rho_r + \rho_r^2)}{3(L + A + B - 2)}.$$

To summarize, the DiSSEP is an integrable one parameter generalization of the SSEP, where particles pairs are allowed to condensate and evaporate with the same probability rates. From a physical point of view, it provides an example of exclusion process in which the lattice current is not conserved along the lattice but depends on the place it is measured. It appears as a toy model for which a lot of physical quantities can be exactly computed but it displays also an interesting phenomenology, with non-trivial density profiles. From a more mathematical point of view, it provides a simple example of matrix product expression for the stationary state, which involves non-scalar 'hat operators'. It also points out the usefulness of the ZF and GZ relations to select an efficient generators basis and a convenient change of parameters. It also stresses the fact that the computations of physical observables can be achieved using only the algebraic relations between the generators and not necessarily using an explicit representation. We will come back to this model in chapter V to study its properties in the thermodynamic limit.

2 An open two species TASEP

We now turn to a detailed study of another example of stochastic model that we already encountered several times in this manuscript, through its local jump operators and its R and K matrices. This model is called the two-species totally asymmetric exclusion process (2-TASEP) with open boundaries and was first introduced and studied in [V5]. The integrable boundaries associated to the two species ASEP were classified there and the matrix product structure of the stationary state was investigated on a particular example. An explicit matrix product representation of the steady state of the models was given in [V7] together with the rigorous derivation of the phase diagrams and the exact computation of physical quantities. Following the lines of [V5] and [V7], we present here the main results.

a) Presentation of the model

The model is a Markov process that enters the framework of exclusion process introduced in chapter II. It describes two species of particles in stochastic evolution on a one-dimensional lattice comprising L sites and coupled with two reservoirs at the boundaries. Each site $i = 1, \dots, L$ can be in one of three states $\tau_i = 0, 1$ or 2 . As usual, state 0 may be considered as an empty site or hole. State 1 is interpreted as a species of heavy, slow particles (sometimes called second class particles). State 2 corresponds to a species of light, fast particles (sometimes called first class particles). At each pair of nearest neighbor sites in the bulk, the exchange rates read

$$1\ 0 \xrightarrow{1} 0\ 1 \quad , \quad 2\ 0 \xrightarrow{1} 0\ 2 \quad , \quad 2\ 1 \xrightarrow{1} 1\ 2. \quad (\text{III.B.74})$$

(Note that several other labelling conventions for the three particle species have been employed in the literature e.g. [169].) The sites 1 and L are in contact with boundary reservoirs and particles are exchanged at different rates at the boundaries. For generic values of these boundary

rates, the system is not integrable (in contrast with the 1-species TASEP, which is integrable for arbitrary boundary rates). Finding in this general case an exact solution looks hopeless. However, in [V5], using a systematic procedure (the resolution of the reflection equation), all possible boundary rates for the 2-species TASEP that preserve integrability were classified. Amongst such models, some had been studied earlier: the first open two-species matrix product solutions were derived in [210]; in [211] the boundary conditions for which the stationary state may be expressed using the matrices D , E , A of [46] and [212] were deduced; in [175, 176] the restricted class of *semi-permeable* boundaries, in which second class particles can neither enter nor leave the system was studied. In all of these cases a matrix product representation of the stationary state was found involving the quadratic algebra used by Derrida, Evans, Hakim and Pasquier [46] in their exact solution of the 1-species exclusion process with open boundaries.

In the present example, we construct a matrix ansatz for integrable 2-TASEP with open boundaries that allow all species of particles to enter and leave the system. The algebraic structures required will be much more involved than the fundamental quadratic algebra of [46].

We shall study two classes of 2-species TASEP models with the following boundary rates

$$\begin{array}{ccc}
 & \text{left boundary} & \text{right boundary} \\
 (M_1) : & \begin{array}{l} 2 \xrightarrow{\alpha} 1 \\ 0 \xrightarrow{\alpha} 1 \\ 0 \xrightarrow{1-\alpha} 2 \end{array} & \begin{array}{l} 2 \xrightarrow{\beta} 0 \\ 1 \xrightarrow{\beta} 0 \\ 1 \xrightarrow{1-\beta} 2 \end{array} \\
 & & \text{(III.B.75)}
 \end{array}$$

or

$$\begin{array}{ccc}
 & \text{left boundary} & \text{right boundary} \\
 (M_2) : & \begin{array}{l} 2 \xrightarrow{\alpha} 1 \\ 0 \xrightarrow{\alpha} 1 \\ 0 \xrightarrow{1-\alpha} 2 \end{array} & \begin{array}{l} 2 \xrightarrow{\beta} 0 \\ 1 \xrightarrow{\beta} 0 \end{array} \\
 & & \text{(III.B.76)}
 \end{array}$$

Hereafter, the two different models will be denoted by (M_1) and (M_2) . Note that in the classification of [V5] the left boundary conditions were referred to as L_2 and the right hand boundary conditions for (M_1) or (M_2) were referred to as R_2 and R_3 respectively. It is a simple matter to translate our results for (M_2) to the case of right boundary R_2 and left boundary L_3 . The final case of right boundary R_3 and left boundary L_3 leaves the stationary state devoid of holes and thus reduces to a one-species TASEP.

The physical interpretation of the boundary conditions is as follows. In both models (M_1) , (M_2) the left-hand boundary conditions correspond to a boundary reservoir containing only first and second class particle with densities α and $1 - \alpha$ respectively, with no holes. In model (M_1) the right-hand boundary conditions correspond to a reservoir containing second-class particles and holes with densities $1 - \beta$ and β respectively, with no first-class particles. In model (M_2) the right-hand boundary conditions correspond to a reservoir containing first-class particles and holes with densities $1 - \beta$ and β respectively, with no second-class particles.

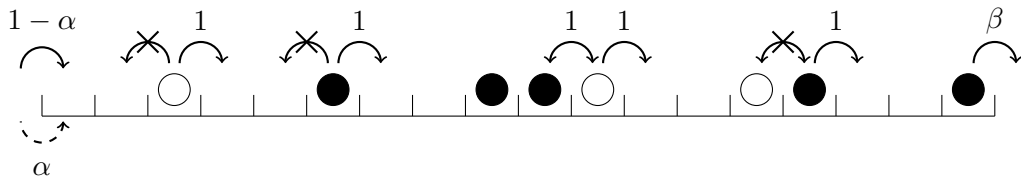


Figure III.6: Dynamical rules of the 2-species TASEP. The empty sites stands for species 0, circles for species 1 and bullets for species 2. On the left boundary the continuous line means injection of bullets whereas the dashed line means injection of circles.

The 2-TASEP is a finite Markov process that reaches a unique steady-state in the long time limit, in which each configuration has the stationary probability (or weight) $\mathcal{S}(\tau_1, \tau_2, \dots, \tau_L)$.

The column-vector $|\mathcal{S}\rangle$ of length 3^L , whose components are the probabilities $\mathcal{S}(\tau_1, \tau_2, \dots, \tau_L)$, satisfies the stationary master equation

$$M^{(3)}|\mathcal{S}\rangle = 0, \quad (\text{III.B.77})$$

where $M^{(3)}$ is the $3^L \times 3^L$ Markov matrix for the 2-TASEP system. It can be decomposed as

$$M^{(3)} = B_1^{(3)} + \sum_{\ell=1}^{L-1} m_{\ell, \ell+1}^{(3)} + \bar{B}_L^{(3)}, \quad (\text{III.B.78})$$

with the local bulk update operator acting on nearest neighbor sites

$$m^{(3)} = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & -1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} \quad (\text{III.B.79})$$

where the points in the matrix stand for vanishing entries. The boundary operators read

$$B^{(3)} = \begin{pmatrix} -1 & 0 & 0 \\ 1 - \alpha & -\alpha & 0 \\ \alpha & \alpha & 0 \end{pmatrix}, \quad \hat{B}^{(3)} = \begin{pmatrix} 0 & \beta & \beta \\ 0 & -\beta & 1 - \beta \\ 0 & 0 & -1 \end{pmatrix}, \quad \check{B}^{(3)} = \begin{pmatrix} 0 & \beta & \beta \\ 0 & -\beta & 0 \\ 0 & 0 & -\beta \end{pmatrix}. \quad (\text{III.B.80})$$

These operators are written as usual in the local state basis $(0, 1, 2)$ which is the natural choice corresponding to increasing order of priority in the update rules. We recall that in equation (III.B.78), the subscripts indicate on which sites of the lattice the local operators act non-trivially, and the right boundary matrix $\bar{B}^{(3)}$ corresponds to $\hat{B}^{(3)}$ for the processes (M_1) and $\check{B}^{(3)}$ for (M_2) . As a rule, the superscripts in (III.B.78) (and later in (III.B.107)) indicate the number of possible states at a site, i.e. the number of species plus one.

The Markov matrix $M^{(3)}$ defines an integrable stochastic process. As usual, the main objects needed to deal with integrability are the R-matrix encoding the bulk dynamics and the K-matrices encoding the boundaries rates.

For the 2-species TASEP, we recall that the braided R-matrix reads

$$\check{R}^{(3)}(z) = 1 + (1 - z)m^{(3)}, \quad (\text{III.B.81})$$

with the property $-\check{R}^{(3)'}(1) = m^{(3)}$. The reader may refer to example (II.B.18) for the detailed properties of this R-matrix. The K-matrix for the left boundary is

$$K^{(3)}(z) = \begin{pmatrix} z^2 & 0 & 0 \\ -\frac{az(z^2-1)}{za+1} & \frac{z(a+z)}{za+1} & 0 \\ -\frac{z^2-1}{za+1} & -\frac{z^2-1}{za+1} & 1 \end{pmatrix} \quad (\text{III.B.82})$$

and the ones for the two choices of right boundary are

$$\hat{K}^{(3)}(z) = \begin{pmatrix} 1 & \frac{z^2-1}{(b+z)z} & \frac{z^2-1}{(b+z)z} \\ 0 & \frac{bz+1}{(b+z)z} & \frac{b(z^2-1)}{(b+z)z^2} \\ 0 & 0 & z^{-2} \end{pmatrix} \quad \text{and} \quad \check{K}^{(3)}(z) = \begin{pmatrix} 1 & \frac{z^2-1}{(b+z)z} & \frac{z^2-1}{(b+z)z} \\ 0 & \frac{bz+1}{(b+z)z} & 0 \\ 0 & 0 & \frac{bz+1}{(b+z)z} \end{pmatrix}. \quad (\text{III.B.83})$$

One obtains

$$-\frac{1}{2}K^{(3)'}(1) = B, \quad \frac{1}{2}\widehat{K}^{(3)'}(1) = \widehat{B} \quad \text{and} \quad \frac{1}{2}\check{K}^{(3)'}(1) = \check{B}^{(3)}. \quad (\text{III.B.84})$$

The reader may refer to example (II.C.24) for the detailed properties of these K matrices.

As explained in chapter II, we can construct a transfer matrix from these building blocks

$$t(z) = \text{tr}_0 \left(\widetilde{K}_0(z) R_{0,L}(z) \dots R_{0,1}(z) K_0(z) R_{1,0}(z) \dots R_{L,0}(z) \right), \quad (\text{III.B.85})$$

where $\widetilde{K}_0(z)$ satisfies⁸ (II.C.28).

It generates a family of commuting operators and is linked to the Markov matrix through

$$-\frac{1}{2}t'(1) = M^{(3)}. \quad (\text{III.B.86})$$

b) Matrix ansatz

We are now interested in the stationary state of the model. Finding the steady state of the Markov matrix (III.B.180) amounts to solving a linear system that grows exponentially with the size of the lattice. Following the general method developed in this chapter for integrable models, we will construct the stationary weights in a matrix product from *i.e.*, the weight of the configuration $\mathcal{C} = (\tau_1, \dots, \tau_L)$ in the stationary state will be written as

$$\mathcal{S}(\tau_1, \dots, \tau_L) = \frac{1}{Z_L} \langle\langle W | X_{\tau_1} X_{\tau_2} \dots X_{\tau_L} | V \rangle\rangle, \quad (\text{III.B.87})$$

where $Z_L = \langle\langle W | (X_0 + X_1 + X_2)^L | V \rangle\rangle$ is the normalization factor. This will basically allow us to reduce the *a priori* exponential complexity of the steady state (see the general construction with rooted trees in chapter I) to a polynomial computation. Following the general procedure exposed in section A, we know that the operators X_0, X_1 and X_2 can be constructed from

$$\mathbf{A}(1) = \mathbf{X} = \begin{pmatrix} X_0 \\ X_1 \\ X_2 \end{pmatrix}, \quad (\text{III.B.88})$$

where the vector $\mathbf{A}(z)$ satisfies the ZF and GZ relations (III.A.119) and (III.A.131) that we recall here

$$\check{R}^{(3)}(z_1/z_2) \mathbf{A}(z_1) \otimes \mathbf{A}(z_2) = \mathbf{A}(z_2) \otimes \mathbf{A}(z_1), \quad (\text{III.B.89})$$

$$\langle\langle W | K^{(3)}(z) \mathbf{A}(1/z) \rangle\rangle = \langle\langle W | \mathbf{A}(z) \text{ and } \overline{K}^{(3)}(z) \mathbf{A}(1/z) | V \rangle\rangle = \mathbf{A}(z) | V \rangle, \quad (\text{III.B.90})$$

where $\overline{K}^{(3)}(z)$ is $\widehat{K}^{(3)}(z)$ or $\check{K}^{(3)}(z)$ depending on the right boundary considered. For more details about the use of these relations in the context of Markov chains see [V3] or section A. We recall that, taking the derivative of these relations w.r.t. z_1 and setting $z_1 = z_2$, we recover the telescopic relations (III.B.173) and (III.B.179) used to prove the matrix ansatz:

$$m^{(3)} \mathbf{X} \otimes \mathbf{X} = \mathbf{X} \otimes \overline{\mathbf{X}} - \overline{\mathbf{X}} \otimes \mathbf{X} \quad (\text{III.B.91})$$

for the bulk and

$$\langle\langle W | B^{(3)} \mathbf{X} \rangle\rangle = \langle\langle W | \overline{\mathbf{X}}, \quad \text{and} \quad \overline{B}^{(3)} \mathbf{X} | V \rangle\rangle = -\overline{\mathbf{X}} | V \rangle \quad (\text{III.B.92})$$

for the boundaries, where

$$\begin{pmatrix} \overline{X}_0 \\ \overline{X}_1 \\ \overline{X}_2 \end{pmatrix} = \overline{\mathbf{X}} = -\mathbf{A}'(1). \quad (\text{III.B.93})$$

⁸Note that $\widetilde{K}_0(z)$ cannot be obtained directly from (II.C.27) here because $R_{0,1}(z)^{\dagger 1}$ is not invertible.

Remark B.11. *The exchange relations among the X_i 's are obtained from these telescopic relations (III.B.91). However, as already pointed out in section A, the generators \bar{X}_i 's are not necessarily scalars (they will not be scalars in the present case, see below). Therefore, more relations are required to close the algebra generated by the X_i 's (the telescopic relation (III.B.91) does not tell us how to exchange X_i with \bar{X}_j for instance). A systematic way to deal with this question [V3] is to use the relations (III.B.89) and (III.B.90).*

We thus need to build explicitly the vector $\mathbf{A}(z)$ and the boundary vectors $\langle\langle W|$ and $|V\rangle\rangle$ satisfying (III.B.89) and (III.B.90). For such a purpose, we assume the following expansion for the vector $\mathbf{A}(z)$:

$$\mathbf{A}(z) = \begin{pmatrix} z^2 + G_9 z + G_8 + G_7/z \\ G_6 z + G_5 + G_4/z \\ G_3 z + G_2 + G_1/z + 1/z^2 \end{pmatrix}, \quad (\text{III.B.94})$$

where the G_i 's belong to a non-commuting algebra.

Remark B.12. *This expansion appears as arbitrary at first sight but it is empirically chosen as follows. For a given expansion, the ZF relation (III.B.89) provides the commutation relations among the G_i 's, see for instance the algebraic relations (III.B.95) corresponding to the specific expansion above (III.B.94). The relations on the boundary vectors $\langle\langle W|$ and $|V\rangle\rangle$ are obtained through the GZ relations (III.B.90), see for instance (III.B.98) and (III.B.99). All these relations are in principle sufficient to fix the value of any word $\langle\langle W|G_{i_1}G_{i_2}\dots G_{i_k}|V\rangle\rangle$ up to a global normalization (in the same way as we were able to compute the stationary weights of the single species open TASEP using only the algebraic relations). If the algebra generated by the G_i 's is not rich enough (i.e if there is not enough generators in the expansion of $\mathbf{A}(z)$), we noticed that all the words of length 3 built from the G_i 's vanish⁹. We have observed that 9 generators (III.B.94) is the minimal choice that ensures that not all words of length 3 identically vanish.*

Now that the expansion of the vector $\mathbf{A}(z)$ is guessed and fixed, the algebra satisfied by the nine generators G_i is found by writing each component of the ZF relation and identifying the coefficients of the polynomials in z_1 and z_2 . The generators G_i satisfy a quadratic algebra, given by the following *exchange* relations:

$$\begin{aligned} [G_1, G_2] &= 0, \\ [G_1, G_3] &= 0, & [G_2, G_3] &= 0, \\ G_1 G_4 &= G_5, & G_2 G_4 &= G_6, & G_3 G_4 &= 0, \\ [G_1, G_5] &= G_6 - G_4 G_2, & G_2 G_5 &= G_1 G_6, & G_3 G_5 &= 0, & [G_4, G_5] &= 0, \\ [G_1, G_6] &= -G_4 G_3, & [G_2, G_6] &= -G_5 G_3, & G_3 G_6 &= 0, & [G_4, G_6] &= 0, \\ G_1 G_7 &= G_8, & G_2 G_7 &= G_9, & G_3 G_7 &= 1, & G_4 G_7 &= 0, \\ [G_1, G_8] &= G_9 - G_7 G_2, & G_2 G_8 &= G_1 G_9, & G_3 G_8 &= G_1, & [G_4, G_8] &= -G_7 G_5, \\ [G_1, G_9] &= 1 - G_7 G_3, & [G_2, G_9] &= G_1 - G_8 G_3, & G_3 G_9 &= G_2, & [G_4, G_9] &= -G_7 G_6, \\ [G_5, G_6] &= 0, & & & & & & (\text{III.B.95}) \\ G_5 G_7 &= 0, & G_6 G_7 &= 0, \\ G_5 G_8 &= G_4 G_9, & G_6 G_8 &= G_4, & [G_7, G_8] &= 0, \\ [G_5, G_9] &= G_4 - G_8 G_6, & G_6 G_9 &= G_5, & [G_7, G_9] &= 0, & [G_8, G_9] &= 0. \end{aligned}$$

Remark B.13. *From the knowledge of the exchange relations for the G_i 's, the algebra gener-*

⁹The ZF and GZ relations implies the telescopic relations and thus the relation $M^{[3]}\langle\langle W|\mathbf{X}\otimes\mathbf{X}|V\rangle\rangle = 0$. We are hence left with two possibilities: either the matrix product state gives the correct stationary state of the model or it is identically vanishing.

ated by the X_i 's can be obtained using (III.B.88), i.e

$$\begin{aligned} X_0 &= 1 + G_9 + G_8 + G_7 \\ X_1 &= G_6 + G_5 + G_4 \\ X_2 &= 1 + G_3 + G_2 + G_1 \end{aligned} \quad (\text{III.B.96})$$

and (III.B.95). As already mentioned, to write the relations defining this algebra we need to introduce six more generators \bar{X}_i and $\bar{\bar{X}}_i$ corresponding to

$$\begin{pmatrix} \bar{X}_1 \\ \bar{X}_2 \\ \bar{X}_3 \end{pmatrix} = -\mathbf{A}'(1) = \begin{pmatrix} -2 - G_9 + G_7 \\ -G_6 + G_4 \\ -G_3 + G_1 + 2 \end{pmatrix}, \quad \begin{pmatrix} \bar{\bar{X}}_1 \\ \bar{\bar{X}}_2 \\ \bar{\bar{X}}_3 \end{pmatrix} = \mathbf{A}''(1) = \begin{pmatrix} 2 + 2G_7 \\ 2G_4 \\ 2G_1 + 6 \end{pmatrix} \quad (\text{III.B.97})$$

Note that these generators \bar{X}_i are not scalar. As an example, we give some of the relations satisfied by these generators

$$\begin{aligned} X_2 X_1 &= X_1 \bar{X}_2 - \bar{X}_1 X_2 = \bar{X}_2 X_1 - X_2 \bar{X}_1 \\ X_3 X_1 &= X_1 \bar{X}_3 - \bar{X}_1 X_3 = \bar{X}_3 X_1 - X_3 \bar{X}_1 \\ &\dots \\ 2\bar{X}_2 X_1 &= X_1 \bar{\bar{X}}_2 - \bar{\bar{X}}_1 X_2 = \bar{\bar{X}}_2 X_1 - X_2 \bar{\bar{X}}_1 \\ 2\bar{X}_3 X_1 &= X_1 \bar{\bar{X}}_3 - \bar{\bar{X}}_1 X_3 = \bar{\bar{X}}_3 X_1 - X_3 \bar{\bar{X}}_1 \\ &\dots \end{aligned}$$

The algebra generated by X_i , \bar{X}_i and $\bar{\bar{X}}_i$ is the same as the one generated by the G_i 's, written in a different basis. We chose to present the commutation relations in the G_i basis because they are simpler.

The action of the G_i 's on the boundary vectors is derived from the GZ relations (III.A.131). For the left vector we have

$$\begin{aligned} \langle\langle W | (G_4 - a) &= 0, \\ \langle\langle W | G_7 &= 0, \\ \langle\langle W | (G_8 - 1) &= 0, \\ \langle\langle W | (a(G_1 - G_3) - G_5) &= 0, \\ \langle\langle W | (G_3 + G_6 + G_9 - G_1 - a) &= 0. \end{aligned} \quad (\text{III.B.98})$$

For the right vector, depending on the model under consideration we have

<p>For (M_1) :</p> $\begin{aligned} G_3 V\rangle\rangle &= 0, \\ (G_2 - 1) V\rangle\rangle &= 0, \\ (G_6 - b) V\rangle\rangle &= 0, \\ (b(G_7 - G_9) + G_5) V\rangle\rangle &= 0, \\ (G_1 + G_4 + G_7 - G_9 - b) V\rangle\rangle &= 0, \end{aligned}$	<p>For (M_2) :</p> $\begin{aligned} (G_3 - b) V\rangle\rangle &= 0, \\ (G_5 - bG_4) V\rangle\rangle &= 0, \\ G_6 V\rangle\rangle &= 0, \\ (b(b - G_1) + G_2 - 1) V\rangle\rangle &= 0, \\ (G_1 + G_4 + G_7 - G_9 - b) V\rangle\rangle &= 0. \end{aligned}$
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Note that the relations and generators G_i are not all independent. For instance, $G_3 G_5 = 0$ and $(G_2 - 1) |V\rangle\rangle = 0$ can be deduced from the other exchange and boundary relations.

We present below an explicit representation of the generators G_i 's and of the boundary vectors $\langle\langle W |$ and $|V\rangle\rangle$, that was found in [V7]. This representation is build as tensor product of several copies of the DEHP algebra. It proves rigorously the existence of the algebraic structure (III.B.95)-(III.B.99) and hence of the matrix product expression of the stationary state. This representation can also be useful to perform explicit computation of physical quantities. This fact will be illustrated with the computation of the normalization (III.B.191).

We now stress that using only the algebraic relations (III.B.95)-(III.B.99) (and not the explicit representation of the G_i 's and boundary vectors), any expression containing X_0 , X_1

and X_2 and placed between $\langle\langle W|$ and $|V\rangle\rangle$ can be reduced to a multiple of $\langle\langle W|V\rangle\rangle$. Therefore, the weights of any configuration and the partition function of the model can be in principle calculated from these relations. A computer program allowed us to obtain this way all the weights for systems of small sizes. We present below example of weights of configurations of arbitrary length that can be exactly computed using only these algebraic relations. These examples are given for the particular case $\alpha = 1/2$ and $\beta = 1$ (*i.e* for $a = 1$ and $b = 0$) for which the models (M_1) and (M_2) coincide. Indeed the computations simplify in this case

- A word containing only the letters X_1 and X_2 is evaluated as

$$\langle\langle W|Y^{(k)}(X_1, X_2)X_2^p|V\rangle\rangle = \frac{k+2}{p+k+2} \binom{2p+k+1}{p} \langle\langle W|V\rangle\rangle, \quad \text{for } p, k = 0, 1, 2, \dots, \quad (\text{III.B.100})$$

where $Y^{(k)}(X_1, X_2)$ is the empty word for $k = 0$ and is a word of length k containing only the letters X_1 and X_2 and ending with X_1 .

- A word starting with a power of X_0 on the left and followed by a combination of X_1 and X_2 is calculated as

$$\langle\langle W|X_0^p Y^{(k)}(X_1, X_2)|V\rangle\rangle = \frac{2p+1}{p+1} \binom{2p}{p} \langle\langle W|V\rangle\rangle, \quad \text{for } p, k = 0, 1, 2, \dots, \quad (\text{III.B.101})$$

where $Y^{(k)}(X_1, X_2)$ is as above.

- The partition function is given by

$$Z_L = \langle\langle W|C^L|V\rangle\rangle = (2L+1)A_L A_{L+1} \langle\langle W|V\rangle\rangle, \quad (\text{III.B.102})$$

where $C = X_1 + X_2 + X_3$ and $A_L = \frac{1}{L+1} \binom{2L}{L}$ is the Catalan number.

Note that in principle it should be possible to obtain similar formulas for general values of the parameters α and β . Nevertheless the computations and recursive relations given by the algebraic relations (III.B.95)-(III.B.99) appear as much more involved and their study lies beyond the scope of this manuscript.

c) Identification

Interesting physical quantities, such as the mean particles currents and densities of each species, can be exactly computed using an identification, or coloring argument, formalized in [176]. The idea is to identify two species of particles, or a species of particles with holes, to simplify the model. The model obtained comprises a single species of particle and can thus be identified as a single species open TASEP. All possible identifications are not consistent with the dynamics of the 2-TASEP. For instance it is not possible to identify particles of species 2 (the fastest particles) with holes, because the particles of species 1 behave differently with respect to holes (that they overtake) and to particles of species 2 (that overtake them).

The 2-TASEP models (M_1) and (M_2) can both be mapped to the one-species TASEP model using two possible identifications:

1. One can identify holes and species 1 to get a one-species TASEP model for which the phase diagram is given in table (V.A.28). The boundary conditions read

$$\begin{array}{ll} \text{left boundary} & \text{right boundary} \\ (M_1) : & (0, 1) \xrightarrow{\alpha} 2 \qquad 2 \xrightarrow{1} (0, 1) \\ (M_2) : & (0, 1) \xrightarrow{\alpha} 2 \qquad 2 \xrightarrow{\beta} (0, 1) \end{array} \quad (\text{III.B.103})$$

2. One can identify species 1 and 2 to get another version of the one-species TASEP model. In that case the two models (M_1) and (M_2) produce the same boundary conditions:

$$\begin{array}{ll} \text{left boundary} & \text{right boundary} \\ (M_1) \& (M_2) : & 0 \xrightarrow{1} (1, 2) \qquad (1, 2) \xrightarrow{\beta} 0 \end{array} \quad (\text{III.B.104})$$

For the two-species TASEP, we denote by $\langle j_1 \rangle$, $\langle j_2 \rangle$ the mean particle currents in the stationary state for the particles of species 1 and 2 respectively ($\langle j_0 \rangle$ denotes the mean current of holes). The currents are counted positively when particles flow from the left to the right. In the same way, $\langle \rho_1^{(i)} \rangle$ and $\langle \rho_2^{(i)} \rangle$ denote the mean densities of particles of species 1 and 2 respectively on site i ($\langle \rho_0^{(i)} \rangle$ denotes the density of holes).

The exclusion property ensures that

$$\langle j_0 \rangle + \langle j_1 \rangle + \langle j_2 \rangle = 0, \quad \text{and} \quad \langle \rho_0^{(i)} \rangle + \langle \rho_1^{(i)} \rangle + \langle \rho_2^{(i)} \rangle = 1. \quad (\text{III.B.105})$$

Identification 1. allows us to compute the current $\langle j_2 \rangle$ and the density $\langle \rho_2^{(i)} \rangle$, while identification 2. yields the current $\langle j_1 \rangle + \langle j_2 \rangle = -\langle j_0 \rangle$ and the density $\langle \rho_1^{(i)} \rangle + \langle \rho_2^{(i)} \rangle$.

The identification procedure can be understood at the level of Markov matrices in the following way. We present here the case of the identification of species 1 and species 2 (but the case of identification of holes with species 1 can be treated similarly). When doing the aforementioned identification, we end up with the single species open TASEP defined in III.B.104 for both the models (M_1) and (M_2) . The stochastic evolution rules of this single species model can be, as usual, encoded in a Markov matrix written as the sum of local operators

$$M^{(2)} = B_1^{(2)} + \sum_{\ell=1}^{L-1} m_{\ell, \ell+1}^{(2)} + \overline{B}_L^{(2)}, \quad (\text{III.B.106})$$

where the local bulk Markov matrix between site ℓ and $\ell + 1$ and the boundary matrices are given by

$$m^{(2)} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}; \quad B^{(2)} = \begin{pmatrix} -1 & 0 \\ 1 & 0 \end{pmatrix}; \quad \overline{B}^{(2)} = \begin{pmatrix} 0 & \beta \\ 0 & -\beta \end{pmatrix}. \quad (\text{III.B.107})$$

We now define the rectangular matrix

$$u = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \end{pmatrix}. \quad (\text{III.B.108})$$

The role of this matrix can be intuitively understood as summing the two last entries of a vector of size 3. We have indeed

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x \\ y + z \end{pmatrix}. \quad (\text{III.B.109})$$

The validity of the identification 2 lies in the following intertwining relations for the local jump operators

$$u B^{(3)} = B^{(2)} u, \quad u \otimes u m^{(3)} = m^{(2)} u \otimes u, \quad u \overline{B}^{(3)} = \overline{B}^{(2)}. \quad (\text{III.B.110})$$

This is a rigorous way of saying that the process by the identification of species 1 and species 2 (which corresponds to summing the two last entries) is given by III.B.104. This can be immediately upgraded to an intertwining relation on the Markov matrices. If we define $U = u \otimes \cdots \otimes u$ then we have

$$U M^{(3)} = M^{(2)} U. \quad (\text{III.B.111})$$

Such intertwining relation have already been used for the multi-species ASEP on the ring [49, 170, 171].

Remark B.14. Note that the relations (III.B.110) on the local jump operators can be upgraded at the level of R and K matrices

$$u K^{(3)}(z) = K^{(2)}(z)u, \quad u \otimes u R^{(3)}(z) = R^{(2)}(z)u \otimes u, \quad u \bar{K}^{(3)}(z) = \bar{K}^{(2)}(z). \quad (\text{III.B.112})$$

where we have introduced the K -matrices for the single-species open TASEP

$$K^{(2)}(z) = \begin{pmatrix} z^2 & 0 \\ 1 - z^2 & 1 \end{pmatrix} \quad \text{and} \quad \bar{K}^{(2)}(z) = \begin{pmatrix} 1 & \frac{z^2-1}{(b+z)z} \\ 0 & \frac{bz+1}{(b+z)z} \end{pmatrix}. \quad (\text{III.B.113})$$

These reflection matrices are related to the boundary matrices through

$$-\frac{1}{2} \frac{d}{dz} K^{(2)}(z) \Big|_{z=1} = B^{(2)}, \quad \frac{1}{2} \frac{d}{dz} \bar{K}^{(2)}(z) \Big|_{z=1} = \bar{B}^{(2)}. \quad (\text{III.B.114})$$

These intertwining relations have strong implications on connection between steady states of the two species and single species models. Define the vector $\mathbf{X}^{(2)} = u \mathbf{X}$, where \mathbf{X} introduced in (III.B.88) satisfies the telescopic relations in the bulk (III.B.91) and on the boundaries (III.B.92). Then a direct computation, using the intertwining property (III.B.110), yields

$$m^{(2)} \mathbf{X}^{(2)} \otimes \mathbf{X}^{(2)} = \mathbf{X}^{(2)} \otimes \bar{\mathbf{X}}^{(2)} - \bar{\mathbf{X}}^{(2)} \otimes \mathbf{X}^{(2)} \quad (\text{III.B.115})$$

and

$$\langle\langle W | B^{(2)} \mathbf{X}^{(2)} = \langle\langle W | \bar{\mathbf{X}}^{(2)}, \quad \bar{B}^{(2)} \mathbf{X}^{(2)} | V \rangle\rangle = -\bar{\mathbf{X}}^{(2)} | V \rangle\rangle, \quad (\text{III.B.116})$$

where $\bar{\mathbf{X}}^{(2)} = u \bar{\mathbf{X}}$ with $\bar{\mathbf{X}}$ defined in (III.B.93).

Remark B.15. Once again this can be promoted to spectral parameter dependent relations. If we define $\mathbf{A}^{(2)}(z) = u \mathbf{A}(z)$ where the size three vector $\mathbf{A}(z)$ satisfies the ZF and GZ relation associated to the two species model, then the size two vector $\mathbf{A}^{(2)}(z)$ satisfies the ZF and GZ relation associated to the single species model. Note that going the other direction is much harder: finding a size three vector, that fulfill ZF and GZ relations, from a size two vector, that satisfies these relations for the single species model, requires a more involved construction which will be exposed when dealing with the explicit representation.

This immediately implies that the matrix product state

$$\langle\langle W | \mathbf{X}^{(2)} \otimes \dots \otimes \mathbf{X}^{(2)} | V \rangle\rangle = \langle\langle W | \begin{pmatrix} X_0 \\ X_1 + X_2 \end{pmatrix} \otimes \dots \otimes \begin{pmatrix} X_0 \\ X_1 + X_2 \end{pmatrix} | V \rangle\rangle \quad (\text{III.B.117})$$

is the (unnormalized) steady state of $M^{(2)}$. The Perron-Frobenius theorem tells us that the steady state of $M^{(2)}$ is unique: the previous matrix product state (III.B.117) is thus equal to the usual matrix product steady state of the single species open TASEP (constructed from the matrices E and D , see [46]) up to a global normalization (that is easily evaluated on a particular configuration)

$$\langle\langle W | \mathbf{X}^{(2)} \otimes \dots \otimes \mathbf{X}^{(2)} | V \rangle\rangle = \frac{\langle\langle W | X_0^L | V \rangle\rangle}{\langle\langle W | E^L | V \rangle\rangle} \langle\langle W | \begin{pmatrix} E \\ D \end{pmatrix} \otimes \dots \otimes \begin{pmatrix} E \\ D \end{pmatrix} | V \rangle\rangle, \quad (\text{III.B.118})$$

where we recall that the matrices E and D satisfy

$$DE = D + E, \quad \langle\langle W | E = \langle\langle W |, \quad D | V \rangle\rangle = \frac{1}{\beta} | V \rangle\rangle, \quad (\text{III.B.119})$$

because we are in the particular case $\alpha = 1$. Note that we made a slight abuse of notation, writing always $\langle\langle W |$ and $| V \rangle\rangle$ for both the boundary vectors for the well-known single species solution [46] and also for the two species model, but the reader has to be careful that they are not equal. Nevertheless there should be hopefully no ambiguity in the relation (III.B.118), the boundary vectors can indeed be distinguished by the matrices they are acting on.

From (III.B.118) we deduce immediately that

$$\begin{aligned}
\langle j_1 \rangle + \langle j_2 \rangle &= \frac{\langle\langle W|(X_0 + X_1 + X_2)^{i-1}(X_1 + X_2)X_0(X_0 + X_1 + X_2)^{L-i-1}|V\rangle\rangle}{\langle\langle W|(X_0 + X_1 + X_2)^L|V\rangle\rangle} \\
&= \frac{\langle\langle W|(E + D)^{i-1}DE(E + D)^{L-i-1}|V\rangle\rangle}{\langle\langle W|(E + D)^L|V\rangle\rangle} \\
&= \frac{\mathcal{Z}_{L-1}(1, \beta)}{\mathcal{Z}_L(1, \beta)},
\end{aligned}$$

where

$$\mathcal{Z}_L(\alpha, \beta) = \frac{\alpha\beta}{\alpha + \beta - 1} \sum_{p=1}^L B_{L,k} \frac{\left(\frac{1}{\alpha}\right)^{p+1} - \left(\frac{1}{\beta}\right)^{p+1}}{\frac{1}{\alpha} - \frac{1}{\beta}} \quad (\text{III.B.120})$$

is the normalization of the single species open TASEP computed in (III.A.20). The combinatorial coefficients

$$B_{n,k} = \frac{k(2n - 1 - k)!}{n!(n - k)!} \quad (\text{III.B.121})$$

were defined in (III.A.22). Note that the formula of the normalization have a slight difference with the one given in (III.A.20) because we evaluate explicitly here the scalar product $\langle\langle W|V\rangle\rangle = \alpha\beta/(\alpha + \beta - 1)$ using the representation (III.A.14). There is also a slight change of notation with the calligraphic \mathcal{Z}_L to distinguish it from Z_L the normalization of the two species model. We precise also in the notation the injection rate α and the extraction rate β because these parameters may vary when doing the different identification.

Thanks to (III.B.118) we can also compute

$$\langle\rho_1^{(i)} + \rho_2^{(i)}\rangle = \frac{\langle\langle W|(X_0 + X_1 + X_2)^{i-1}(X_1 + X_2)(X_0 + X_1 + X_2)^{L-i}|V\rangle\rangle}{\langle\langle W|(X_0 + X_1 + X_2)^L|V\rangle\rangle} \quad (\text{III.B.122})$$

$$= \frac{\langle\langle W|(E + D)^{i-1}D(E + D)^{L-i}|V\rangle\rangle}{\langle\langle W|(E + D)^L|V\rangle\rangle} \quad (\text{III.B.123})$$

$$= \sum_{k=1}^{L-i} B_{k,1} \frac{\mathcal{Z}_{L-k}(1, \beta)}{\mathcal{Z}_L(1, \beta)} + \frac{\mathcal{Z}_{i-1}(1, \beta)}{\mathcal{Z}_L(1, \beta)} \sum_{k=1}^{L-i} B_{L-i,k} \frac{1}{\beta^{k+1}}. \quad (\text{III.B.124})$$

The last equality is obtained using the result (III.A.36).

We can repeat exactly the same procedure with the identification 1 (defined in III.B.104), that we recall give access to the mean particle current $\langle j_2 \rangle$ and the mean particle density $\langle\rho_2^{(i)}\rangle$. The mean particle current of species 2 is thus given by

$$\langle j_2 \rangle = \frac{\mathcal{Z}_{L-1}(\alpha, 1)}{\mathcal{Z}_L(\alpha, 1)}, \quad \text{for } (M_1) \quad \text{and} \quad \langle j_2 \rangle = \frac{\mathcal{Z}_{L-1}(\alpha, \beta)}{\mathcal{Z}_L(\alpha, \beta)}, \quad \text{for } (M_2). \quad (\text{III.B.125})$$

The mean particle density of species 2 at site i is equal to

$$\langle\rho_2^{(i)}\rangle = \sum_{k=1}^{L-i+1} B_{k,1} \frac{\mathcal{Z}_{L-k}(\alpha, 1)}{\mathcal{Z}_L(\alpha, 1)} \quad (\text{III.B.126})$$

for model (M_1) and

$$\langle\rho_2^{(i)}\rangle = \sum_{k=1}^{L-i} B_{k,1} \frac{\mathcal{Z}_{L-k}(\alpha, \beta)}{\mathcal{Z}_L(\alpha, \beta)} + \frac{\mathcal{Z}_{i-1}(\alpha, \beta)}{\mathcal{Z}_L(\alpha, \beta)} \sum_{k=1}^{L-i} B_{L-i,k} \frac{1}{\beta^{k+1}} \quad (\text{III.B.127})$$

for model (M_2) .

To summarize, gathering the results obtained through both identifications, we obtain that

- The mean particle currents are given by

$$\langle j_0 \rangle = -\frac{\mathcal{Z}_{L-1}(1, \beta)}{\mathcal{Z}_L(1, \beta)}, \quad \langle j_1 \rangle = \frac{\mathcal{Z}_{L-1}(1, \beta)}{\mathcal{Z}_L(1, \beta)} - \frac{\mathcal{Z}_{L-1}(\alpha, 1)}{\mathcal{Z}_L(\alpha, 1)} \quad \text{and} \quad \langle j_2 \rangle = \frac{\mathcal{Z}_{L-1}(\alpha, 1)}{\mathcal{Z}_L(\alpha, 1)}. \quad (\text{III.B.128})$$

for the model (M_1) and

$$\langle j_0 \rangle = -\frac{\mathcal{Z}_{L-1}(1, \beta)}{\mathcal{Z}_L(1, \beta)}, \quad \langle j_1 \rangle = \frac{\mathcal{Z}_{L-1}(1, \beta)}{\mathcal{Z}_L(1, \beta)} - \frac{\mathcal{Z}_{L-1}(\alpha, \beta)}{\mathcal{Z}_L(\alpha, \beta)} \quad \text{and} \quad \langle j_2 \rangle = \frac{\mathcal{Z}_{L-1}(\alpha, \beta)}{\mathcal{Z}_L(\alpha, \beta)}. \quad (\text{III.B.129})$$

for the model (M_2).

- The average densities of particles at site i are given by

$$\langle \rho_0^{(i)} \rangle = 1 - \sum_{k=1}^{L-i} B_{k,1} \frac{\mathcal{Z}_{L-k}(1, \beta)}{\mathcal{Z}_L(1, \beta)} - \frac{\mathcal{Z}_{i-1}(1, \beta)}{\mathcal{Z}_L(1, \beta)} \sum_{k=1}^{L-i} B_{L-i,k} \frac{1}{\beta^{k+1}}, \quad (\text{III.B.130})$$

$$\langle \rho_1^{(i)} \rangle = \sum_{k=1}^{L-i} B_{k,1} \frac{\mathcal{Z}_{L-k}(1, \beta)}{\mathcal{Z}_L(1, \beta)} + \frac{\mathcal{Z}_{i-1}(1, \beta)}{\mathcal{Z}_L(1, \beta)} \sum_{k=1}^{L-i} B_{L-i,k} \frac{1}{\beta^{k+1}} \quad (\text{III.B.131})$$

$$- \sum_{k=1}^{L-i+1} B_{k,1} \frac{\mathcal{Z}_{L-k}(\alpha, 1)}{\mathcal{Z}_L(\alpha, 1)}, \quad (\text{III.B.132})$$

$$\langle \rho_2^{(i)} \rangle = \sum_{k=1}^{L-i+1} B_{k,1} \frac{\mathcal{Z}_{L-k}(\alpha, 1)}{\mathcal{Z}_L(\alpha, 1)}. \quad (\text{III.B.133})$$

for the model (M_1) and

$$\langle \rho_0^{(i)} \rangle = 1 - \sum_{k=1}^{L-i} B_{k,1} \frac{\mathcal{Z}_{L-k}(1, \beta)}{\mathcal{Z}_L(1, \beta)} - \frac{\mathcal{Z}_{i-1}(1, \beta)}{\mathcal{Z}_L(1, \beta)} \sum_{k=1}^{L-i} B_{L-i,k} \frac{1}{\beta^{k+1}}, \quad (\text{III.B.134})$$

$$\langle \rho_1^{(i)} \rangle = \sum_{k=1}^{L-i} B_{k,1} \frac{\mathcal{Z}_{L-k}(1, \beta)}{\mathcal{Z}_L(1, \beta)} + \frac{\mathcal{Z}_{i-1}(1, \beta)}{\mathcal{Z}_L(1, \beta)} \sum_{k=1}^{L-i} B_{L-i,k} \frac{1}{\beta^{k+1}} \quad (\text{III.B.135})$$

$$- \sum_{k=1}^{L-i} B_{k,1} \frac{\mathcal{Z}_{L-k}(\alpha, \beta)}{\mathcal{Z}_L(\alpha, \beta)} - \frac{\mathcal{Z}_{i-1}(\alpha, \beta)}{\mathcal{Z}_L(\alpha, \beta)} \sum_{k=1}^{L-i} B_{L-i,k} \frac{1}{\beta^{k+1}}, \quad (\text{III.B.136})$$

$$\langle \rho_2^{(i)} \rangle = \sum_{k=1}^{L-i} B_{k,1} \frac{\mathcal{Z}_{L-k}(\alpha, \beta)}{\mathcal{Z}_L(\alpha, \beta)} + \frac{\mathcal{Z}_{i-1}(\alpha, \beta)}{\mathcal{Z}_L(\alpha, \beta)} \sum_{k=1}^{L-i} B_{L-i,k} \frac{1}{\beta^{k+1}}. \quad (\text{III.B.137})$$

for the model (M_2). In chapter V we will study the large size limit of these results which will allow us to compute the phase diagrams of both models.

In the particular case $\alpha = 1/2$ and $\beta = 1$ that we studied previously, the results are much simpler (we recall that for these specific values of α and β the models (M_1) and (M_2) coincide)

- The mean particle currents are given by

$$\langle j_0 \rangle = -\frac{L+2}{2(2L+1)}, \quad \langle j_1 \rangle = \frac{1}{2(2L+1)} \quad \text{and} \quad \langle j_2 \rangle = \frac{L+1}{2(2L+1)}. \quad (\text{III.B.138})$$

- The average densities of particles at site i are given by

$$\langle \rho_0^{(i)} \rangle = \frac{1}{A_{L+1}} \sum_{k=0}^{i-1} A_k A_{L-k}, \quad (\text{III.B.139})$$

$$\langle \rho_1^{(i)} \rangle = \frac{1}{A_{L+1}} \sum_{k=i}^L \frac{L-k+1}{L+2} A_k A_{L-k}, \quad (\text{III.B.140})$$

$$\langle \rho_2^{(i)} \rangle = \frac{1}{A_{L+1}} \sum_{k=i}^L \frac{k+1}{L+2} A_k A_{L-k}. \quad (\text{III.B.141})$$

We just saw that densities and particle currents can be computed using the identification method. However, we stress that the algebraic relations (III.B.95)-(III.B.99) are necessary to compute all the individual weights and correlations between different type of particles: this cannot be obtained from the identification procedure.

We mention finally that similar algebras, with at most nine generators, can be defined to compute the weights of the stationary state of the other integrable 2-TASEP models found in this manuscript (see discussion in [V5]).

We now address the problem of finding an explicit representation of the nine generators and boundary vectors.

d) Explicit representation of the matrix ansatz algebra

This section is devoted to the construction of an explicit representation for the boundary vectors $\langle\langle W|$ and $|V\rangle\rangle$ and for the generators G_i 's (which will thus give a representation for the matrices X_0 , X_1 and X_2).

This representation for the 2-TASEP will be constructed in terms of tensor products of the fundamental operators A , d and e that appear in the solution of the one-species exclusion process [46]. These operators A , d and e define a quadratic algebra and satisfy

$$de = 1, \quad A = 1 - ed, \quad dA = 0, \quad Ae = 0. \quad (\text{III.B.142})$$

The relation with the operators D and E of [46] is $d = D - 1$, $e = E - 1$ and $A = DE - ED$.

We also define the following parameters

$$a = \frac{1 - \alpha}{\alpha} \quad \text{and} \quad b = \frac{1 - \beta}{\beta}. \quad (\text{III.B.143})$$

Finally, we shall need four commuting copies of the algebra (III.B.142), (e_n, d_n, A_n) , $n = 1, 2, 3, 4$. A simple way to achieve this is to make four-fold tensor products:

$$\begin{aligned} e_1 &= e \otimes 1 \otimes 1 \otimes 1, \\ e_2 &= 1 \otimes e \otimes 1 \otimes 1, \\ e_3 &= 1 \otimes 1 \otimes e \otimes 1, \\ e_4 &= 1 \otimes 1 \otimes 1 \otimes e, \end{aligned} \quad (\text{III.B.144})$$

and similarly for d_n and A_n .

We are now in a position to present explicit matrices for the 2-TASEP with open boundaries

Proposition B.16.

$$X_0 = \left(1 + aA_1A_2 + e_2d_3\right)(1 + e_4) + \left(e_2 + e_3 + aA_1A_2e_3 + e_1A_3\right)(1 + d_4), \quad (\text{III.B.145})$$

$$X_1 = ad_1A_2(1 + e_4) + \left(ad_1A_2e_3 + aA_2A_3\right)(1 + d_4), \quad (\text{III.B.146})$$

$$X_2 = \left(d_2 + d_3\right)(1 + e_4) + \left(1 + d_2e_3 + e_1d_2A_3\right)(1 + d_4). \quad (\text{III.B.147})$$

We get the following realization for the 9 generators G

$$\begin{aligned} G_1 &= d_3e_4 + e_1d_2A_3 + d_2e_3 + d_4; & G_2 &= d_3 + d_2e_4 + d_2e_3d_4 + e_1d_2A_3d_4; & G_3 &= d_2 \\ G_4 &= \lambda(d_1A_2e_3 + A_2A_3); & G_5 &= \lambda(d_1A_2e_4 + d_1A_2e_3d_4 + A_2A_3d_4); & G_6 &= \lambda d_1A_2 \\ G_7 &= \lambda A_1A_2e_3 + e_2; & G_8 &= \lambda A_1A_2e_4 + e_2d_3e_4 + \lambda A_1A_2e_3d_4 + e_2d_4 + e_1A_3 + e_3 \\ G_9 &= \lambda A_1A_2 + e_2d_3 + e_4 + e_1A_3d_4 + e_3d_4 \end{aligned} \quad (\text{III.B.148})$$

Proof. It can be easily checked using a symbolic calculation program [213] that the representation presented here indeed obeys the commutation relations (III.B.95). However, we give below a more elegant proof of this fact, taking advantage of a factorization property of the vector $\mathbf{A}(z)$, that is obtained using the identification procedure. ■

Remark B.17. *It is important to realize that the integer suffices on the left and right hand sides of (III.B.145)–(III.B.147) are unrelated: on the left $\tau = 0, 1, 2$ corresponds to particle species whereas on the right $n = 1, 2, 3, 4$ labels the tensor product as in the example (III.B.144).*

To construct the vectors $\langle\langle W|$ and $|V\rangle\rangle$, we first define the elementary vectors $\langle\langle x|$ and $|x\rangle\rangle$ that obey

$$\langle\langle x|e = x \langle\langle x| \text{ and } d|x\rangle\rangle = x|x\rangle\rangle. \quad (\text{III.B.149})$$

It is known [46] that explicit representations of such elementary vectors exist. Here we use the representation exposed previously in this chapter (III.A.14) where

$$\langle\langle x|y\rangle\rangle = \frac{1}{1 - xy}. \quad (\text{III.B.150})$$

Proposition B.18. *The left boundary vector reads:*

$$\langle\langle W|_{1234} = \langle\langle 1|_1 \langle\langle 0|_2 \langle\langle 0|_3 \langle\langle 0|_4, \quad (\text{III.B.151})$$

where the indices indicate again which copy of the (A, d, e) algebra acts on the vector. To make the notation less cluttered, we shall simply write $\langle\langle W|$ instead of $\langle\langle W|_{1234}$. Note that the left vector is the same for the models (M_1) and (M_2) .

The right boundary vector depends on the choice of the dynamics at the right boundary (i.e. on the choice of the model (M_1) or (M_2)). We have

$$|V(M_1)\rangle\rangle_{1234} = \left| \frac{b}{a} \right\rangle\rangle_1 |0\rangle\rangle_2 |1\rangle\rangle_3 |b\rangle\rangle_4 \text{ for } (M_1) \quad (\text{III.B.152})$$

$$\text{and } |V(M_2)\rangle\rangle_{1234} = |0\rangle\rangle_1 |b\rangle\rangle_2 |1\rangle\rangle_3 |b\rangle\rangle_4 \text{ for } (M_2). \quad (\text{III.B.153})$$

We shall simply write $|V\rangle\rangle$ for the right vector, without specifying the indices and which model we consider. This should be unambiguous from the context.

Proof. It can be checked by direct computation that the relations (III.B.98) and (III.B.99) are indeed satisfied. However, we provide below a simpler proof of this fact using a factorization of the vector $\mathbf{A}(z)$. \blacksquare

e) Factorized form for the representation

The expressions (III.B.145)–(III.B.147) for the X_τ 's can be written in a factorized form which will be useful to compute the normalization but also to prove the validity of the representation.

Definition B.19. *We define the Lax operators by $\mathbb{L}^{(3)}(z) = L^{(3)}(z)\tilde{L}^{(3)}(z)$ where*

$$L^{(3)}(z) = \begin{pmatrix} z + \lambda A_1 A_2 & ze_1 & ze_2 \\ \lambda d_1 A_2 & \lambda A_2 & 0 \\ d_2 & e_1 d_2 & 1 \end{pmatrix} \text{ and } \tilde{L}^{(3)}(z) = \begin{pmatrix} 1 & e_3 \\ 0 & A_3 \\ d_3/z & 1/z \end{pmatrix}, \quad (\text{III.B.154})$$

and $\mathbb{L}^{(2)}(z) = L^{(2)}(z)\tilde{L}^{(2)}(z)$ where

$$L^{(2)}(z) = \begin{pmatrix} z & ze_4 \\ d_4 & 1 \end{pmatrix} \text{ and } \tilde{L}^{(2)}(z) = \begin{pmatrix} 1 \\ 1/z \end{pmatrix}. \quad (\text{III.B.155})$$

Proposition B.20. *The vector $\mathbf{A}(z)$ can be factorized as*

$$\mathbf{A}(z) = \mathbb{L}^{(3)}(z)\mathbb{L}^{(2)}(z) = L^{(3)}(z)\tilde{L}^{(3)}(z)L^{(2)}(z)\tilde{L}^{(2)}(z). \quad (\text{III.B.156})$$

Proof. This property can be directly check using the explicit expression of the vector $\mathbf{A}(z)$ given by the expansion (III.B.94) and the explicit representation of the G_i 's (III.B.148). \blacksquare

As mentioned previously, we can prove the ZF and GZ relations (III.B.89) and (III.B.90) by direct computations. However, using the factorization (III.B.156), we can split the proof of these relations into simpler ones, involving only one or two copies of the DEHP algebra each, instead of dealing simultaneously with the four copies.

Proposition B.21. *One can show that the following relations hold*

$$\check{R}^{(3)}(z_1/z_2)L^{(3)}(z_1) \otimes L^{(3)}(z_2) = L^{(3)}(z_2) \otimes L^{(3)}(z_1)\check{R}^{(3)}(z_1/z_2), \quad (\text{III.B.157})$$

$$\check{R}^{(2)}(z_1/z_2)L^{(2)}(z_1) \otimes L^{(2)}(z_2) = L^{(2)}(z_2) \otimes L^{(2)}(z_1)\check{R}^{(2)}(z_1/z_2), \quad (\text{III.B.158})$$

$$\check{R}^{(3)}(z_1/z_2)\tilde{L}^{(3)}(z_1) \otimes \tilde{L}^{(3)}(z_2) = \tilde{L}^{(3)}(z_2) \otimes \tilde{L}^{(3)}(z_1)\check{R}^{(2)}(z_1/z_2), \quad (\text{III.B.159})$$

$$\check{R}^{(2)}(z_1/z_2)\tilde{L}^{(2)}(z_1) \otimes \tilde{L}^{(2)}(z_2) = \tilde{L}^{(2)}(z_2) \otimes \tilde{L}^{(2)}(z_1), \quad (\text{III.B.160})$$

where we used the braided R -matrix for the single-species TASEP, built on the local operator $m^{(2)}$ (see (III.B.107)):

$$\check{R}^{(2)}(x) = 1 + (1-x)m^{(2)}. \quad (\text{III.B.161})$$

Proof. This is directly checked by a straightforward computation. \blacksquare

Note that these “generalized” RLL relations not only allow us to factorize the difficulty to deal with the four-fold tensor space but also permit to reduce step by step the size of the L matrices through intertwining relations involving the R matrix of the 2 species model and of the single species model. These kind of relations are deeply inspired by the identification procedure exposed previously.

Corollary B.22. *These identities imply*

$$\check{R}^{(3)}(z_1/z_2)\mathbb{L}^{(3)}(z_1) \otimes \mathbb{L}^{(3)}(z_2) = \mathbb{L}^{(3)}(z_2) \otimes \mathbb{L}^{(3)}(z_1)\check{R}^{(2)}(z_1/z_2), \quad (\text{III.B.162})$$

$$\check{R}^{(2)}(z_1/z_2)\mathbb{L}^{(2)}(z_1) \otimes \mathbb{L}^{(2)}(z_2) = \mathbb{L}^{(2)}(z_2) \otimes \mathbb{L}^{(2)}(z_1). \quad (\text{III.B.163})$$

Corollary B.23. *The vector $\mathbf{A}(z)$ satisfies the ZF relation.*

Proof. Using the factorization (III.B.156) and applying the relations (III.B.162) and (III.B.163) successively, we prove the ZF relation (III.B.89). \blacksquare

Proposition B.24. *The following relations hold*

$$\begin{aligned} \langle\langle W|_{123} K(z)\mathbb{L}^{(3)}(1/z) = \langle\langle W|_{123} \mathbb{L}^{(3)}(z)K^{(2)}(z) ; \langle\langle W|_4 K^{(2)}(z)\mathbb{L}^{(2)}(1/z) = \langle\langle W|_4 \mathbb{L}^{(2)}(z) \\ \overline{K}(z)\mathbb{L}^{(3)}(1/z) |V\rangle\rangle_{123} = \mathbb{L}^{(3)}(z)\overline{K}^{(2)}(z) |V\rangle\rangle_{123} ; \overline{K}^{(2)}(z)\mathbb{L}^{(2)}(1/z) |V\rangle\rangle_4 = \mathbb{L}^{(2)}(z) |V\rangle\rangle_4 , \end{aligned} \quad (\text{III.B.164})$$

Finally, relations (III.B.164) imply equations (III.B.90).

Remark B.25. *Note that $\tilde{L}(z)$ can be obtained from $L(z)$. We define the transposition in the space of generators as follows*

$$e^t = d , d^t = e , A^t = A \text{ and } \langle\langle x|^t = |x\rangle\rangle \quad (\text{III.B.165})$$

Let us remark that starting from an $L^{(3)}(z)$ solution to the relation (III.B.157), the matrix

$$\overline{L}^{(3)}(z) = UL^{(3)}(1/z)^tU \text{ where } U = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad (\text{III.B.166})$$

is also a solution of (III.B.157). We have used the following property of the matrix $R^{(3)}(z)$

$$U_1U_2R_{21}^{(3)}(z)U_1U_2 = R^{(3)}(z) . \quad (\text{III.B.167})$$

This symmetry was already pointed out in (II.C.111). Starting from the realization (III.B.154) for $L^{(3)}(z)$, one gets

$$\overline{L}^{(3)}(z) = \begin{pmatrix} 1 & d_1e_2 & e_2 \\ 0 & \lambda A_2 & \lambda e_1 A_2 \\ d_2/z & d_1/z & 1/z + \lambda A_1 A_2 \end{pmatrix} . \quad (\text{III.B.168})$$

The trivial representation for the e, d, A algebra is defined as $e = d = 1$ and $A = 0$. These values are consistent with the relation (III.B.142) and the definition of A . In the $\overline{L}^{(3)}(z)$ matrix,

we may choose the trivial representation for the generators in the space 1 (i.e. $e_1 = d_1 = 1$ and $A_1 = 0$). Changing the name of space 2 to space 3 and putting $\lambda = 1$, one establishes a link with the matrix $\tilde{L}^{(3)}(z)$:

$$\bar{L}^{(3)}(z) \Big|_{e_1=d_1=1, A_1=0, \lambda=1} = \begin{pmatrix} 1 & e_3 & e_3 \\ 0 & A_3 & A_3 \\ d_3/z & 1/z & 1/z \end{pmatrix} = \tilde{L}^{(3)}(z) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \end{pmatrix}. \quad (\text{III.B.169})$$

The procedure to choose the trivial representation to get a simpler matrix has been used previously for the periodic case in [49].

Let us remark that taking the derivative of the RLL relations w.r.t. z_1 and setting $z_1 = z_2 = 1$, we obtain generalized telescopic relations. For instance, (III.B.162) implies that

$$m^{(3)}\mathbb{L}^{(3)} \otimes \mathbb{L}^{(3)} - \mathbb{L}^{(3)} \otimes \mathbb{L}^{(3)}m^{(2)} = \mathbb{L}^{(3)'} \otimes \mathbb{L}^{(3)} - \mathbb{L}^{(3)} \otimes \mathbb{L}^{(3)'}. \quad (\text{III.B.170})$$

and (III.B.163) implies

$$m^{(2)}\mathbb{L}^{(2)} \otimes \mathbb{L}^{(2)} = \mathbb{L}^{(2)'} \otimes \mathbb{L}^{(2)} - \mathbb{L}^{(2)} \otimes \mathbb{L}^{(2)'}, \quad (\text{III.B.171})$$

where

$$\mathbb{L}^{(3)} := \mathbb{L}^{(3)}(1), \quad \mathbb{L}^{(3)'} := \mathbb{L}^{(3)'}(1), \quad \mathbb{L}^{(2)} := \mathbb{L}^{(2)}(1), \quad \text{and} \quad \mathbb{L}^{(2)'} := \mathbb{L}^{(2)'}(1). \quad (\text{III.B.172})$$

Remark that this generalized “hat relation” already appeared in the solution of the periodic multi-species ASEP [171]. The present matrix $\mathbb{L}^{(3)}$ provides a new solution to this relation, adapted for the open boundaries case (see below).

Combining equations (III.B.170) and (III.B.171) yields the usual bulk relation

$$m^{(3)}\mathbf{X} \otimes \mathbf{X} = \mathbf{X} \otimes \bar{\mathbf{X}} - \bar{\mathbf{X}} \otimes \mathbf{X}, \quad (\text{III.B.173})$$

where

$$\mathbf{X} = \mathbb{L}^{(3)}\mathbb{L}^{(2)}, \quad \text{and} \quad \bar{\mathbf{X}} = -\mathbb{L}^{(3)}\mathbb{L}^{(2)'} - \mathbb{L}^{(3)'}\mathbb{L}^{(2)} \quad (\text{III.B.174})$$

which consistent with $\mathbf{X} = \mathbf{A}(1)$ and $\bar{\mathbf{X}} = -\mathbf{A}'(1)$.

In the same way taking the derivative of generalized GZ relations (III.B.164) w.r.t. z and setting $z = 1$, we obtain generalized telescopic relations on the boundaries. The following identities hold for $\mathbb{L}^{(3)}$

$$\langle\langle W|_{123} \left(B\mathbb{L}^{(3)} - \mathbb{L}^{(3)}B^{(2)} \right) = -\langle\langle W|_{123}\mathbb{L}^{(3)'} \quad (\text{III.B.175})$$

$$\left(\bar{B}\mathbb{L}^{(3)} - \mathbb{L}^{(3)}\bar{B}^{(2)} \right) |V\rangle\rangle_{123} = \mathbb{L}^{(3)'} |V\rangle\rangle_{123}. \quad (\text{III.B.176})$$

Similar relations also exist for $\mathbb{L}^{(2)}$

$$\langle\langle 0|_4 B^{(2)}\mathbb{L}^{(2)} = -\langle\langle 0|_4 \mathbb{L}^{(2)'} \quad (\text{III.B.177})$$

$$\bar{B}^{(2)}\mathbb{L}^{(2)}|b\rangle\rangle_4 = \mathbb{L}^{(2)'}|b\rangle\rangle_4. \quad (\text{III.B.178})$$

Combining equations (III.B.175)-(III.B.178) leads us to the boundary relations

$$\langle\langle W|B\mathbf{X} = \langle\langle W|\bar{\mathbf{X}} \quad \text{and} \quad \bar{B}\mathbf{X}|V\rangle\rangle = -\bar{\mathbf{X}}|V\rangle\rangle. \quad (\text{III.B.179})$$

In [174] a multi-species ASEP with reflective open boundaries has been studied, and another solution (with vanishing hat operators) of the generalized “hat relation” (III.B.170) was provided to construct the steady state in a matrix product form. In this model the boundary counterparts of the “hat relation” (III.B.175)-(III.B.176) were automatically satisfied because the boundary matrices B and \bar{B} vanish.

We recall that matrix product expression for the stationary probability vector reads

$$|\mathcal{S}\rangle = \frac{1}{Z_L} \langle\langle W | \mathbf{X} \otimes \mathbf{X} \otimes \cdots \otimes \mathbf{X} | V \rangle\rangle. \quad (\text{III.B.180})$$

The factorization $\mathbf{X} = \mathbb{L}^{(3)}\mathbb{L}^{(2)}$ leads to

$$|\mathcal{S}\rangle = \frac{1}{Z_L} \mathbb{P}^{(3)} \mathbb{P}^{(2)}, \quad (\text{III.B.181})$$

where

$$\mathbb{P}^{(3)} = \langle\langle W |_{123} \mathbb{L}^{(3)} \otimes \cdots \otimes \mathbb{L}^{(3)} | V \rangle\rangle_{123} \text{ and } \mathbb{P}^{(2)} = \langle\langle W |_4 \mathbb{L}^{(2)} \otimes \cdots \otimes \mathbb{L}^{(2)} | V \rangle\rangle_4. \quad (\text{III.B.182})$$

Here, $\mathbb{P}^{(3)}$ is a $3^L \times 2^L$ matrix and $\mathbb{P}^{(2)}$ is a 2^L -component vector so that \mathcal{S} is a 3^L -component vector as expected. We also remark that $\mathbb{P}^{(2)}$ (up to a normalisation) is identical to the steady-state vector of the one species TASEP with open boundaries. Therefore, we have

$$M^{(2)}\mathbb{P}^{(2)} = 0, \quad (\text{III.B.183})$$

where $M^{(2)}$ is the Markov matrix of the one-species TASEP. We also have the intertwining relation

$$M^{(3)}\mathbb{P}^{(3)} = \mathbb{P}^{(3)}M^{(2)}. \quad (\text{III.B.184})$$

Finally, thanks to the factorization property (III.B.156) of $\mathbf{A}(z)$ we know that

$$\mathbf{X} = \mathbf{A}(1) = L^{(3)}\tilde{L}^{(3)}L^{(2)}\tilde{L}^{(2)}, \quad (\text{III.B.185})$$

with $L^{(3)} := L^{(3)}(1)$, $\tilde{L}^{(3)} := \tilde{L}^{(3)}(1)$, $L^{(2)} := L^{(2)}(1)$ and $\tilde{L}^{(2)} := \tilde{L}^{(2)}(1)$. The stationary state can thus be further decomposed as

$$|\mathcal{S}\rangle = \frac{1}{Z_L} \mathbb{P}^{(3)} \mathbb{P}^{(2)} = \frac{1}{Z_L} P^{(3)} \tilde{P}^{(3)} P^{(2)} \tilde{P}^{(2)}, \quad (\text{III.B.186})$$

with

$$P^{(3)} = \langle\langle W |_{12} L^{(3)} \otimes L^{(3)} \otimes \cdots \otimes L^{(3)} | V \rangle\rangle_{12} \quad (\text{III.B.187})$$

$$\tilde{P}^{(3)} = \langle\langle W |_3 \tilde{L}^{(3)} \otimes \tilde{L}^{(3)} \otimes \cdots \otimes \tilde{L}^{(3)} | V \rangle\rangle_3 \quad (\text{III.B.188})$$

$$P^{(2)} = \langle\langle W |_4 L^{(2)} \otimes L^{(2)} \otimes \cdots \otimes L^{(2)} | V \rangle\rangle_4 \quad (\text{III.B.189})$$

$$\tilde{P}^{(2)} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 1 \end{pmatrix} \otimes \cdots \otimes \begin{pmatrix} 1 \\ 1 \end{pmatrix}. \quad (\text{III.B.190})$$

Let us note that $P^{(3)}$ is a $3^L \times 3^L$ matrix, $\tilde{P}^{(3)}$ is a $3^L \times 2^L$ matrix, $P^{(2)}$ is a $2^L \times 2^L$ matrix and $\tilde{P}^{(2)}$ is a 2^L -component vector with constant components.

f) Computation of the normalization from the explicit representation

We may now use the factorisation properties of the previous subsection to calculate the normalisation Z_L of the stationary probabilities. The results we obtain are

$$Z_L = \frac{a}{a-b} \mathcal{Z}_L(\alpha, 1) \mathcal{Z}_L(1, \beta) \quad \text{for } (M_1) \quad (\text{III.B.191})$$

$$Z_L = (1-ab) \mathcal{Z}_L(\alpha, \beta) \mathcal{Z}_L(1, \beta) \quad \text{for } (M_2)$$

where $\mathcal{Z}_L(\alpha, \beta)$ is the partition function of the open one-species TASEP with injection rate α and extraction rate β . Its exact expression [46] is given by

$$\mathcal{Z}_L(\alpha, \beta) = \langle\langle a | (2+e+d)^L | b \rangle\rangle = \langle\langle a | (D+E)^L | b \rangle\rangle = \sum_{p=0}^L \frac{p(2L-p-1)!}{L!(L-p)!} \frac{\left(\frac{1}{\alpha}\right)^{p+1} - \left(\frac{1}{\beta}\right)^{p+1}}{\frac{1}{\alpha} - \frac{1}{\beta}} \langle\langle a | b \rangle\rangle. \quad (\text{III.B.192})$$

From the matrix ansatz, we know that

$$Z_L = \langle\langle W | (X_0 + X_1 + X_2)^L | V \rangle\rangle. \quad (\text{III.B.193})$$

Using the factorization (III.B.185), we obtain

$$X_0 + X_1 + X_2 = (1, 1, 1) \cdot \begin{pmatrix} X_0 \\ X_1 \\ X_2 \end{pmatrix} = (1, 1, 1) L^{(3)} \tilde{L}^{(3)} \mathbb{L}^{(2)}. \quad (\text{III.B.194})$$

We first compute

$$(1, 1, 1) \cdot L^{(3)} = \left(1 + a(A_1 + d_1)A_2 + d_2, e_1(1 + d_2) + aA_2, 1 + e_2 \right). \quad (\text{III.B.195})$$

Then, from the relations $\langle\langle 1 | (A + d) = \langle\langle 1 |$ and $\langle\langle 1 | e = \langle\langle 1 |$, we deduce

$$\langle\langle 1 | (1, 1, 1) \cdot L^{(3)} = \left(1 + aA_2 + d_2, 1 + aA_2 + d_2, 1 + e_2 \right) \langle\langle 1 | \quad (\text{III.B.196})$$

This implies that the space 1 drops out (because neither $\tilde{L}^{(3)}$ nor $\mathbb{L}^{(2)}$ act on it). Remarking that

$$\begin{aligned} \left(1 + aA_2 + d_2, 1 + aA_2 + d_2, 1 + e_2 \right) \tilde{L}^{(3)} &= \left(1 + aA_2 + d_2, 1 + e_2 \right) \begin{pmatrix} 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tilde{L}^{(3)} \\ &= \left(1 + aA_2 + d_2, 1 + e_2 \right) \begin{pmatrix} 1 & A_3 + e_3 \\ d_3 & 1 \end{pmatrix} \end{aligned}$$

and using $(A + e)|1\rangle\rangle = |1\rangle\rangle$ and $d|1\rangle\rangle = |1\rangle\rangle$, we have

$$\begin{pmatrix} 1 & A_3 + e_3 \\ d_3 & 1 \end{pmatrix} |1\rangle\rangle_3 = |1\rangle\rangle_3 \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = |1\rangle\rangle_3 \begin{pmatrix} 1 \\ 1 \end{pmatrix} (1, 1) \quad (\text{III.B.197})$$

so that space 3 also drops out. Gathering the different results, we obtain

$$\begin{cases} Z_L = \langle\langle 1 | b/a \rangle\rangle_1 \langle\langle 0 | (2 + aA_2 + d_2 + e_2)^L | 0 \rangle\rangle_2 \langle\langle 0 | 1 \rangle\rangle_3 \langle\langle 0 | (2 + e_4 + d_4)^L | b \rangle\rangle_4 & \text{for } (M_1) \\ Z_L = \langle\langle 1 | 0 \rangle\rangle_1 \langle\langle 0 | (2 + aA_2 + d_2 + e_2)^L | b \rangle\rangle_2 \langle\langle 0 | 1 \rangle\rangle_3 \langle\langle 0 | (2 + e_4 + d_4)^L | b \rangle\rangle_4 & \text{for } (M_2). \end{cases} \quad (\text{III.B.198})$$

We conclude the derivation of (III.B.191) by using (III.B.192) and by observing that

$$\langle\langle 0 | (2 + aA + d + e)^L | b \rangle\rangle = \frac{\langle\langle 0 | b \rangle\rangle}{\langle\langle a | b \rangle\rangle} \mathcal{Z}_L(\alpha, \beta) \quad (\text{III.B.199})$$

because the operators $\tilde{e} = aA + e$ and d obeys the same algebraic rules as e and d , but now $\langle\langle 0 |$ is a left eigenvector of \tilde{e} with eigenvalue a .

To summarize, the 2-TASEP models studied here provide the first example of integrable multi-species open TASEP in which none the particles currents of the species vanishes in the stationary state. The stationary state is analytically expressed in a matrix product form, which is written using an algebra involving 9 generators. This translates into the presence of non-scalar 'hat operators'. The telescopic relations are not sufficient to encode all the algebraic relations satisfied by these 9 generators. These algebraic relations are provided by the ZF and GZ relations together with a convenient change of generators basis. It allows us to compute some physical quantities or some particular stationary weights using only these algebraic relations. The integrable structure of the model gives a guideline to construct an explicit representation of the matrix product algebra. A lot remains to be understood to construct such explicit representations for general integrable multi-species open (T)ASEP. We will come back to these 2-TASEP models in chapter V to study their properties in the thermodynamic limit. We will be in particular interested in their phase diagrams.

3 An open multi-species SSEP

This section is devoted to the study of diffusive multi-species open model that was introduced recently in [V8]. The interest of this model lies in the fact that it describes a system driven out-of-equilibrium by two reservoirs, and also in the fact that there is an arbitrary fixed number of species. We will see that the algebraic structure of the non-equilibrium steady state provides very convenient tools for physical quantities computations. The discussion and results exposed here are deeply based on the content of [V8], with minor modifications. The reader is thus encouraged to refer to this paper for details.

a) Presentation of the model

We consider a system involving N species of particles which diffuse on a one dimensional lattice comprising L sites. Each site i can be in $N + 1$ different states $\tau_i = 0, \dots, N$ depending on its occupancy. More precisely, we set $\tau_i = s$ if the site at position i carries a particle of species s , with $1 \leq s \leq N$, and we set $\tau_i = 0$ if the site is empty. Hence a configuration of the lattice will be denoted by a L -uplet $\boldsymbol{\tau} = (\tau_1, \dots, \tau_L) \in \{0, \dots, N\}^L$.

The dynamics is stochastic. During an infinitesimal time dt , in the bulk, there is a probability dt that a particle of a given species jumps to its left or right neighbor site, providing that it is empty. There is also a probability dt that two particles of different species, located on two adjacent sites, exchange their positions. At the left boundary, a particle of species s' (or a hole) located on the first site can be replaced by a particle of species s with probability $dt \times \alpha_s/a$. A particle of species s' can also be absorbed in the left reservoir (*i.e* replaced by a hole) with probability $dt \times \alpha_0/a$. In the same way, at the right boundary, a particle of species s' (or a hole) located on the last site can be replaced by a particle of species s with probability $dt \times \beta_s/b$. A particle of species s' can also be absorbed in the right reservoir (*i.e* replaced by a hole) with probability $dt \times \beta_0/b$. See figure III.7 for a graphical illustration.

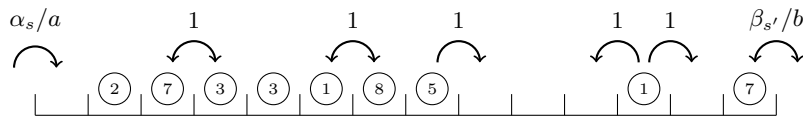


Figure III.7: Dynamical rules of the open multi-species SSEP.

Later on, the parameters $\alpha_1, \dots, \alpha_N$ (respectively β_1, \dots, β_N) will be interpreted as the particles densities at the left (respectively right) reservoir. The parameter α_0 (respectively β_0) is interpreted as the density of holes at the left (respectively right) reservoir. We have thus the constraints

$$\sum_{\tau=0}^N \alpha_{\tau} = 1, \quad \text{and} \quad \sum_{\tau=0}^N \beta_{\tau} = 1. \quad (\text{III.B.200})$$

The number a (respectively b) will be seen as the distance between the left reservoir and the first site (respectively the distance between the right reservoir and the last site), the lattice spacing being one in the bulk.

The update rules of the stochastic process described above are summarized in the following table where the rates of the allowed transitions are depicted above the arrows:

Left	Bulk	Right	
$\tau' \xrightarrow{\alpha_{\tau}/a} \tau$	$\tau' \tau \xrightarrow{1} \tau \tau'$	$\tau' \xrightarrow{\beta_{\tau}/b} \tau$	(III.B.201)
$0 \leq \tau, \tau' \leq N$	$0 \leq \tau, \tau' \leq N$	$0 \leq \tau, \tau' \leq N$	

Let us remark that the dynamics in the bulk is symmetric between the different species of particle and the holes: we cannot distinguish the different species of particles or even particles and holes from the bulk dynamics. It is thus possible to relabel the species or even to interpret

species s as holes and holes as species s (modifying accordingly the label of injection/extraction rates). This observation led us to present the expression of physical quantities (computed below) in the most symmetric way. Note that we already stick with this symmetry willing in the presentation of the injection/extraction rates on the boundaries (we did note single out the notation of "injection/extraction" rates for the holes: we introduced the reservoirs densities of holes α_0 and β_0).

Let us stress that the injection and extraction rate of each species at the boundaries are not the most general. The particular model presented here is motivated by the fact that it is integrable (see discussion below). It turns out that it has a nice physical interpretation. Taking into account the constraints (III.B.200), we are left with $2 \times N$ free parameters. For a generic choice of these parameters, the system will be driven out of equilibrium by the two reservoirs.

Remark B.26. *The system will reach, in the long time limit, a thermodynamic equilibrium if and only if the reservoir densities of each species of particle are the same on the left and on the right, namely: $\alpha_s = \beta_s$, for all $1 \leq s \leq N$ (that implies also, because of (III.B.200), that $\alpha_0 = \beta_0$). The detailed balance condition is indeed satisfied only in this case.*

b) Markov matrix and integrability.

In this subsection we recall briefly the mathematical formalism (exposed precisely in chapter II) needed to write the probability density function of the model and its time evolution (master equation) in a concise vector form. This will be also of great help to compute and express in a simple form the stationary probability density function.

Following the discussion of chapter II, we first attach to each site of the lattice a vector space \mathbb{C}^{N+1} with basis $|0\rangle, |1\rangle, \dots, |N\rangle$, where $|\tau\rangle = (\underbrace{0, \dots, 0}_\tau, 1, \underbrace{0, \dots, 0}_{N-\tau})^t$. The set of all configurations of the lattice is thus embedded in $\underbrace{\mathbb{C}^{N+1} \otimes \dots \otimes \mathbb{C}^{N+1}}_L$ with natural basis $|\tau_1\rangle \otimes \dots \otimes |\tau_L\rangle$,

where $\tau_i = 0, 1, \dots, N$. We denote by $P_t(\tau_1, \dots, \tau_L)$ the probability for the system to be in configuration (τ_1, \dots, τ_L) at time t . These probabilities can be encompassed in a single vector

$$|P_t\rangle = \begin{pmatrix} P_t(0, \dots, 0, 0) \\ P_t(0, \dots, 0, 1) \\ \vdots \\ P_t(N, \dots, N, N) \end{pmatrix} = \sum_{0 \leq \tau_1, \dots, \tau_L \leq N} P_t(\tau_1, \dots, \tau_L) |\tau_1\rangle \otimes \dots \otimes |\tau_L\rangle. \quad (\text{III.B.202})$$

This allows us to write in a compact form the master equation, governing the time evolution of the probability density

$$\frac{d|P_t\rangle}{dt} = M|P_t\rangle, \quad (\text{III.B.203})$$

where the Markov matrix M is given by

$$M = B_1 + \sum_{i=1}^{L-1} m_{i,i+1} + \bar{B}_L. \quad (\text{III.B.204})$$

The matrices B , \bar{B} and m are the local jump operators. The indices denote the sites, or equivalently the copies of \mathbb{C}^{N+1} , on which the operators act non trivially (they act as the identity in the other copies). The matrix B encodes the dynamics at the left boundary and acts on the first site as

$$B|\tau'\rangle = -\frac{1}{a}|\tau'\rangle + \sum_{0 \leq \tau \leq N} \frac{\alpha_s}{a}|\tau\rangle, \quad 0 \leq \tau' \leq N, \quad (\text{III.B.205})$$

which leads to the explicit expression

$$B = \frac{1}{a} \begin{pmatrix} \alpha_0 - 1 & \alpha_0 & \alpha_0 & \dots & \dots & \alpha_0 \\ \alpha_1 & \alpha_1 - 1 & \alpha_1 & \dots & \dots & \alpha_1 \\ \alpha_2 & \alpha_2 & \alpha_2 - 1 & \dots & \dots & \alpha_2 \\ \vdots & \vdots & & \ddots & & \vdots \\ \alpha_{N-1} & \alpha_{N-1} & \dots & \dots & \alpha_{N-1} - 1 & \alpha_{N-1} \\ \alpha_N & \alpha_N & \dots & \dots & \alpha_N & \alpha_N - 1 \end{pmatrix}. \quad (\text{III.B.206})$$

In the same way, the matrix \bar{B} encodes the dynamics at the right boundary and acts on the last site as

$$\bar{B}|\tau'\rangle = -\frac{1}{b}|\tau'\rangle + \sum_{0 \leq \tau \leq N} \frac{\beta_s}{b}|\tau\rangle, \quad 0 \leq \tau' \leq N, \quad (\text{III.B.207})$$

which leads to the explicit expression

$$\bar{B} = \frac{1}{b} \begin{pmatrix} \beta_0 - 1 & \beta_0 & \beta_0 & \dots & \dots & \beta_0 \\ \beta_1 & \beta_1 - 1 & \beta_1 & \dots & \dots & \beta_1 \\ \beta_2 & \beta_2 & \beta_2 - 1 & \dots & \dots & \beta_2 \\ \vdots & \vdots & & \ddots & & \vdots \\ \beta_{N-1} & \beta_{N-1} & \dots & \dots & \beta_{N-1} - 1 & \beta_{N-1} \\ \beta_N & \beta_N & \dots & \dots & \beta_N & \beta_N - 1 \end{pmatrix}. \quad (\text{III.B.208})$$

Finally the matrix m acts on two adjacent sites and encodes the dynamics in the bulk as

$$m|\tau'\rangle \otimes |\tau\rangle = |\tau\rangle \otimes |\tau'\rangle - |\tau'\rangle \otimes |\tau\rangle. \quad (\text{III.B.209})$$

It can be expressed as $m = P - 1$, where P is the permutation operator, namely $P|v\rangle \otimes |w\rangle = |w\rangle \otimes |v\rangle$ if $|v\rangle, |w\rangle \in \mathbb{C}^{N+1}$.

Remark B.27. *The well-known SSEP model with one species of particles plus holes is recovered from this framework for $N = 1$ (one has then to identify species 1 with holes). The present parameters are in this case related to the usual one α, β, γ and δ by $\alpha_0 = \gamma/(\alpha + \gamma)$, $\alpha_1 = \alpha/(\alpha + \gamma)$, $\beta_0 = \beta/(\beta + \delta)$, $\beta_1 = \delta/(\beta + \delta)$, $a = 1/(\alpha + \gamma)$ and $b = 1/(\beta + \delta)$. Note that this corresponds to the change of variable already used to study the one species SSEP, see for instance [16].*

This model is integrable. We can indeed construct an R -matrix satisfying the Yang-Baxter equation (with additive spectral parameter) (II.B.12)

$$R(z) = \frac{z + P}{z + 1}. \quad (\text{III.B.210})$$

It relates to the bulk local jump operator through $P.R'(0) = m$. It fulfills also the regularity, unitarity and Markov conditions. We can also define two reflection matrices K and \bar{K} (that we already encountered in (II.C.59)) satisfying the reflection equations (II.C.7) and (II.C.8) (with additive spectral parameters) respectively

$$K(z) = 1 + \frac{2za}{z+a}B \quad \text{and} \quad \bar{K}(z) = 1 + \frac{2zb}{z-b}\bar{B}. \quad (\text{III.B.211})$$

They satisfy also the regularity, unitarity and Markov conditions. The boundary local jump operators can be recovered by taking the derivative $K'(0)/2 = B$ and $-\bar{K}'(0)/2 = \bar{B}$.

As presented in chapter II, these objects are the building blocks of the transfer matrix $t(z)$ (see (II.C.34)), which generates a family of commuting operators (including the Markov matrix).

c) **Matrix ansatz**

This section is devoted to the construction of the stationary state of the model. More precisely we want to compute the vector $|\mathcal{S}\rangle$ which satisfies the stationary version of the master equation (III.B.203), that is $M|\mathcal{S}\rangle = 0$.

Following the Leitmotiv of this chapter, the integrability of the model can be exploited to express this vector in a matrix product form, *i.e* the probability to observe a configuration (τ_1, \dots, τ_L) in the steady state can be written as

$$\mathcal{S}(\tau_1, \dots, \tau_L) = \frac{1}{Z_L} \langle\langle W | X_{\tau_1} X_{\tau_2} \dots X_{\tau_L} | V \rangle\rangle, \quad (\text{III.B.212})$$

where we recall that $Z_L = \langle\langle W | C^L | V \rangle\rangle$ is a normalization, so that the entries of $|\mathcal{S}\rangle$ sum to 1. We recall also the notation

$$C = X_1 + \dots + X_N. \quad (\text{III.B.213})$$

For the matrix product state (III.B.212) to compute the stationary distribution correctly, the operators X_0, \dots, X_N and the boundary vectors $\langle\langle W |$ and $|V\rangle\rangle$ have to satisfy precise algebraic relations. As presented in this chapter, these relations take their root in the ZF and GZ relations. More precisely the matrices X_0, \dots, X_N are obtained through the relation

$$\mathbf{X} = \begin{pmatrix} X_0 \\ X_1 \\ \vdots \\ X_N \end{pmatrix} = \mathbf{A}(0) \quad (\text{III.B.214})$$

where $\mathbf{A}(z)$ satisfies the ZF relation $\check{R}(z_1 - z_2) \mathbf{A}(z_1) \otimes \mathbf{A}(z_2) = \mathbf{A}(z_2) \otimes \mathbf{A}(z_1)$. The boundary vectors $\langle\langle W |$ and $|V\rangle\rangle$ are chosen to satisfy the GZ relations $\langle\langle W | K(z) \mathbf{A}(-z) = \langle\langle W | \mathbf{A}(z)$ and $\overline{K}(z) \mathbf{A}(-z) |V\rangle\rangle = \mathbf{A}(z) |V\rangle\rangle$. The ZF relation implies the bulk telescopic relation

$$m \mathbf{X} \otimes \mathbf{X} = \mathbf{X} \otimes \overline{\mathbf{X}} - \overline{\mathbf{X}} \otimes \mathbf{X}, \quad (\text{III.B.215})$$

with $\overline{\mathbf{X}} = \mathbf{A}'(0)$. The GZ relations provide the boundary telescopic relations

$$\langle\langle W | B \mathbf{X} = \langle\langle W | \overline{\mathbf{X}}, \quad (\text{III.B.216})$$

and

$$\overline{B} \mathbf{X} |V\rangle\rangle = -\overline{\mathbf{X}} |V\rangle\rangle. \quad (\text{III.B.217})$$

Altogether this ensures that the vector

$$|\mathcal{S}\rangle = \frac{1}{Z_L} \langle\langle W | \mathbf{X} \otimes \mathbf{X} \otimes \dots \otimes \mathbf{X} |V\rangle\rangle \quad (\text{III.B.218})$$

is the steady state of the model.

The first step is to guess an "optimal" (in the sense of the smallest number of generators) expansion for the vector $\mathbf{A}(z)$.

Definition B.28. *We define the vector*

$$\mathbf{A}(z) = \begin{pmatrix} z\lambda_0 + X_0 \\ z\lambda_1 + X_1 \\ \vdots \\ z\lambda_N + X_N \end{pmatrix} = z\overline{\mathbf{X}} + \mathbf{X}, \quad (\text{III.B.219})$$

with

$$\overline{\mathbf{X}} = \begin{pmatrix} \lambda_0 \\ \lambda_1 \\ \vdots \\ \lambda_N \end{pmatrix} = \mathbf{A}'(0). \quad (\text{III.B.220})$$

Now we are equipped to write explicitly the ZF relation and identify the coefficients of the different powers of z in each components. We obtain that the following property.

Proposition B.29. *The ZF relation is equivalent to the fact that the operators X_1, \dots, X_N belong to a Lie algebra¹⁰. They satisfy the commutation relations*

$$[X_\tau, X_{\tau'}] = \lambda_\tau X_{\tau'} - \lambda_{\tau'} X_\tau, \quad 0 \leq \tau, \tau' \leq N, \quad (\text{III.B.221})$$

The last step is to write explicitly the GZ relations to derive the algebraic relations between the matrices X_0, \dots, X_N and the boundary vectors $\langle\langle W|$ and $|V\rangle\rangle$. By again collecting the coefficients of the powers of z in each components of the GZ relations we obtain the following properties.

Proposition B.30. *The action of the operators X_τ on the left boundary vector $\langle\langle W|$ is given by*

$$\langle\langle W|(\alpha_\tau C - X_\tau) = a\lambda_\tau \langle\langle W|, \quad 0 \leq \tau \leq N, \quad (\text{III.B.222})$$

where C is defined in (III.B.213). Note that these N relations are not all independent (the sum of these equations is trivial), only $N - 1$ are necessary. In the same way the action of the operators X_s on the right boundary vector $|V\rangle\rangle$ read

$$(\beta_\tau C - X_\tau)|V\rangle\rangle = -b\lambda_\tau |V\rangle\rangle, \quad 0 \leq \tau \leq N. \quad (\text{III.B.223})$$

Again, only $N - 1$ of these equations are independent.

The computation of length-1 words $\langle\langle W|X_\tau|V\rangle\rangle$, for $0 \leq \tau \leq N$, from the relations (III.B.222) and (III.B.223) yields the equations

$$(\alpha_\tau - \beta_\tau)\langle\langle W|C|V\rangle\rangle = (a + b)\lambda_\tau \langle\langle W|V\rangle\rangle, \quad 0 \leq \tau \leq N. \quad (\text{III.B.224})$$

These equations fix the values of the numbers λ_τ (up to a common factor) as

$$\lambda_\tau = \alpha_\tau - \beta_\tau, \quad 0 \leq \tau \leq N. \quad (\text{III.B.225})$$

These particular values of the λ_τ 's solve the previous set of equations and ensure that the length-1, 2, 3 words $\langle\langle W|X_\tau|V\rangle\rangle$, $\langle\langle W|X_\tau X_{\tau'}|V\rangle\rangle$, $\langle\langle W|X_\tau X_{\tau'} X_{\tau''}|V\rangle\rangle$ are completely fixed by the algebraic relations (III.B.221), (III.B.222) and (III.B.223) (up to a global factor $\langle\langle W|V\rangle\rangle$), are non vanishing and provide the correct stationary weights (this was check using formal computation software).

Unfortunately, we were not able to find an explicit representation for the operators X_τ and the boundary vectors $\langle\langle W|$ and $|V\rangle\rangle$. However, we will show that the commutation relations (III.B.221) and the relations on the boundary vectors (III.B.222) and (III.B.223) allow us to compute the currents and correlation functions, see subsection d), and to prove an additivity principle, see chapter V.

Remark B.31. *Once again the matrix ansatz solution of the usual SSEP with one species of particles and holes can be obtained for $N = 1$, by doing the same change of parameters as mentioned in the remark B.27, and setting $D = X_1/\lambda_1$ and $E = -X_0/\lambda_0 = X_0/\lambda_1$. They satisfy $DE - ED = D + E$ and $\langle\langle W|(\alpha E - \gamma D) = \langle\langle W|$, $(\delta E - \beta D)|V\rangle\rangle = -|V\rangle\rangle$.*

Remark B.32. *We already mentioned that the system reaches a thermodynamic equilibrium if and only if $\alpha_\tau = \beta_\tau$ for all $0 \leq \tau \leq N$. In this case we have $\lambda_\tau = 0$ for all $0 \leq \tau \leq N$, which implies that the operators X_τ commute one with each other and can be chosen proportional to the identity operator. We hence set $X_\tau := r_\tau$, with r_0, \dots, r_N real numbers. It is straightforward to check that $r_\tau = \alpha_\tau = \beta_\tau$ satisfy the boundary relations (III.B.222) and (III.B.223).*

¹⁰The Lie algebra (III.B.221) is not semi-simple since there is an abelian ideal of rank N generated by the elements $\lambda_0 X_\tau - \lambda_\tau X_0$ for $1 \leq \tau \leq N$. Hence it does not belongs to the well known classification of semi-simple Lie algebras. It could be interesting to study the decomposition into solvable and semi-simple parts of this algebra but this is beyond the scope of this manuscript.

The steady state is given by

$$|\mathcal{S}\rangle = \begin{pmatrix} r_0 \\ \vdots \\ r_N \end{pmatrix} \otimes \begin{pmatrix} r_0 \\ \vdots \\ r_N \end{pmatrix} \otimes \cdots \otimes \begin{pmatrix} r_0 \\ \vdots \\ r_N \end{pmatrix}. \quad (\text{III.B.226})$$

This shows that in the thermodynamic equilibrium, the occupation numbers τ_1, \dots, τ_L are independent and identically distributed random variables.

d) Computation of physical quantities

The algebraic structure of the stationary state described in (III.B.221), (III.B.222) and (III.B.223) proves very powerful in the computation of physical quantities such as the correlation functions and the particle currents. The first step is to evaluate the normalization Z_L .

Proposition B.33. *Assuming that the scalar product of the boundary vectors $\langle\langle W|V \rangle\rangle = 1$, the normalization of the steady state defined by $Z_L = \langle\langle W|C^L|V \rangle\rangle$ is equal to*

$$Z_L = \frac{\Gamma(a + b + L)}{\Gamma(a + b)}, \quad (\text{III.B.227})$$

where the gamma function satisfies the functional relation $\Gamma(x + 1) = x\Gamma(x)$.

Proof. We first remark that because of constraints (III.B.200), we have

$$\sum_{\tau=0}^N \lambda_\tau = \sum_{\tau=0}^N \alpha_\tau - \sum_{\tau=0}^N \beta_\tau = 1 - 1 = 0. \quad (\text{III.B.228})$$

It allows us to compute

$$[X_\tau, C] = \sum_{\tau'=0}^N [X_\tau, X_{\tau'}] = \lambda_\tau \sum_{\tau'=0}^N X_{\tau'} - X_\tau \sum_{\tau'=0}^N \lambda_{\tau'}, \quad (\text{III.B.229})$$

and leads to the very useful relation

$$[X_\tau, C] = \lambda_\tau C, \quad \text{or equivalently} \quad X_\tau C = C(X_\tau + \lambda_\tau). \quad (\text{III.B.230})$$

Using this equality n times we obtain

$$X_\tau C^n = C^n(X_\tau + n\lambda_\tau). \quad (\text{III.B.231})$$

We are now equipped to compute the normalization

$$\begin{aligned} Z_L &= \langle\langle W|C^L|V \rangle\rangle = \frac{a\lambda_0}{\alpha_0} Z_{L-1} + \frac{1}{\alpha_0} \langle\langle W|X_0 C^{L-1}|V \rangle\rangle \\ &= \frac{\lambda_0}{\alpha_0} (a + L - 1) Z_{L-1} + \frac{1}{\alpha_0} \langle\langle W|C^{L-1} X_0|V \rangle\rangle \\ &= \frac{\lambda_0}{\alpha_0} (a + b + L - 1) Z_{L-1} + \frac{\beta_0}{\alpha_0} Z_L. \end{aligned} \quad (\text{III.B.232})$$

The first line is obtained thanks to relation (III.B.222) for $\tau = 0$. We get the second line through relation (III.B.231) for $\tau = 0$ and $n = L - 1$. The last equality is established using (III.B.223) for $\tau = 0$. Finally (III.B.232) can be rearranged and leads to the recursive relation

$$Z_L = (a + b + L - 1) Z_{L-1}. \quad (\text{III.B.233})$$

Keeping in mind that $Z_0 = \langle\langle W|V \rangle\rangle = 1$, we can solve the previous relation and we obtain (III.B.227). \blacksquare

We now turn to the study of the mean stationary current of the particles of species s between site i and $i + 1$. It is defined by the average algebraic number of particles of species s crossing the bound between sites i and $i + 1$ per unit of time:

$$\langle j_s \rangle = \frac{\langle\langle W | C^{i-1} X_s (C - X_s) C^{L-i-1} | V \rangle\rangle}{Z_L} - \frac{\langle\langle W | C^{i-1} (C - X_s) X_s C^{L-i-1} | V \rangle\rangle}{Z_L}. \quad (\text{III.B.234})$$

Once again the algebraic structure of the steady state allows us to derive an exact expression for this quantity.

Proposition B.34. *The analytical expression of the mean current of particle of species s between site i and $i + 1$ is given by*

$$\langle j_s \rangle = \frac{\lambda_s}{L - 1 + a + b}, \quad (\text{III.B.235})$$

which is independent of the site i , as expected from the conservation of the particles number in the bulk. Note that this expression remains also valid for the mean current of holes in the system

$$\langle j_0 \rangle = \frac{\lambda_0}{L - 1 + a + b}. \quad (\text{III.B.236})$$

We recover immediately by summing these exact expression the property given by the exclusion constraint

$$\langle j_0 \rangle + \langle j_1 \rangle + \dots + \langle j_N \rangle = 0. \quad (\text{III.B.237})$$

Proof. We present the proof for $0 \leq \tau \leq N$, which includes the current of all the particle species and of the holes. We have

$$\langle j_\tau \rangle = \frac{\langle\langle W | C^{i-1} [X_\tau, C - X_\tau] C^{L-i-1} | V \rangle\rangle}{Z_L} = \frac{\langle\langle W | C^{i-1} [X_\tau, C] C^{L-i-1} | V \rangle\rangle}{Z_L} = \lambda_\tau \frac{Z_{L-1}}{Z_L},$$

where the last equality is obtained thanks to (III.B.230). Hence using (III.B.227) we get the desired expression (III.B.235). ■

Remark B.35. *In the thermodynamic equilibrium case, that is when $\lambda_\tau = 0$ for all τ , all the particles (and holes) currents vanish, as expected.*

Other physical quantities of prime interest are the equal time correlation functions in the stationary state. We recall that for a given configuration, we set $\rho_\tau^{(i)} = 1$ if the site i is in local configuration τ and $\rho_\tau^{(i)} = 0$ else. The algebraic structure of the steady state, revealed by the matrix product formulation, offers a very efficient framework to compute the equal time multi-points correlation functions in the stationary state $\langle \rho_{s_1}^{(i_1)} \rho_{s_2}^{(i_2)} \dots \rho_{s_k}^{(i_k)} \rangle$, where $\langle \cdot \rangle$ stands for the expectation with respect to the stationary measure. We will compute below only the one and two points correlation functions, which are of particular interest for a physical point of view. In principle closed expressions for the higher order correlation functions can also be derived using the computational techniques presented below.

The one point function $\langle \rho_s^{(i)} \rangle$ (respectively $\langle \rho_0^{(i)} \rangle$) represents the mean density of particles of a given species s (respectively of holes) at a given site i . It can be expressed through the matrix product formalism as

$$\langle \rho_\tau^{(i)} \rangle = \frac{\langle\langle W | C^{i-1} X_\tau C^{L-i} | V \rangle\rangle}{Z_L}, \quad 0 \leq \tau \leq N. \quad (\text{III.B.238})$$

Proposition B.36. *Using the algebraic structure (see the proof below), it can be reduced to the closed expression*

$$\langle \rho_\tau^{(i)} \rangle = \frac{(b + L - i)\alpha_\tau + (a + i - 1)\beta_\tau}{a + b + L - 1}. \quad (\text{III.B.239})$$

Note that the density profile is the linear interpolation between the left reservoir with density α_τ located at distance a from the first site and the right reservoir with density β_τ located at distance b from the last site. We recover the Fourier law.

Proof. The mean particle density of species s (or holes) at site i can be computed using the algebraic structure given by the matrix product form

$$\langle \rho_\tau^{(i)} \rangle = \frac{\langle\langle W|C^{i-1}X_\tau C^{L-i}|V \rangle\rangle}{Z_L} = (L-i)\lambda_\tau \frac{Z_{L-1}}{Z_L} + \frac{\langle\langle W|C^{L-1}X_\tau|V \rangle\rangle}{Z_L} \quad (\text{III.B.240})$$

$$= (b+L-i)\lambda_\tau \frac{Z_{L-1}}{Z_L} + \beta_\tau = \frac{(b+L-i)\alpha_\tau + (a+i-1)\beta_\tau}{a+b+L-1}. \quad (\text{III.B.241})$$

The second equality is obtained using relation (III.B.231). We use then (III.B.223) to get the second line of the equation and the last equality is established thanks to expression (III.B.227). ■

The two-point correlation function can also be written in a matrix product form

$$\langle \rho_\tau^{(i)} \rho_{\tau'}^{(j)} \rangle = \frac{\langle\langle W|C^{i-1}X_\tau C^{j-i-1}X_{\tau'} C^{L-j}|V \rangle\rangle}{Z_L}. \quad (\text{III.B.242})$$

It leads to the following proposition.

Proposition B.37. *We have a factorized expression for the connected two-point function*

$$\begin{aligned} \langle \rho_\tau^{(i)} \rho_{\tau'}^{(j)} \rangle_c &:= \langle \rho_\tau^{(i)} \rho_{\tau'}^{(j)} \rangle - \langle \rho_\tau^{(i)} \rangle \langle \rho_{\tau'}^{(j)} \rangle \\ &= -\lambda_\tau \lambda_{\tau'} \frac{(a+i-1)(b+L-j)}{(a+b+L-1)^2(a+b+L-2)}. \end{aligned} \quad (\text{III.B.243})$$

The formulas (III.B.239) and (III.B.243) are very similar to the ones derived for the usual one-species SSEP [16, 209] and appear as direct generalisation for the multi-species case.

Proof. For the two-point function, using again (III.B.231) and (III.B.223), we have

$$\langle \rho_\tau^{(i)} \rho_{\tau'}^{(j)} \rangle = \frac{\langle\langle W|C^{i-1}X_\tau C^{j-i-1}X_{\tau'} C^{L-j}|V \rangle\rangle}{Z_L} \quad (\text{III.B.244})$$

$$= \lambda_{\tau'}(L-j+b) \frac{\langle\langle W|C^{i-1}X_\tau C^{L-i-1}|V \rangle\rangle}{Z_L} + \beta_{\tau'} \langle \rho_\tau^{(i)} \rangle \quad (\text{III.B.245})$$

Replacing L by $L-1$ in the expression (III.B.239) we obtain

$$\begin{aligned} \frac{\langle\langle W|C^{i-1}X_\tau C^{L-i-1}|V \rangle\rangle}{Z_L} &= \frac{Z_{L-1}}{Z_L} \frac{(b+L-1-i)\alpha_\tau + (a+i-1)\beta_\tau}{a+b+L-2} \\ &= \frac{Z_{L-1}}{Z_L} \left(\langle \rho_\tau^{(i)} \rangle - \lambda_\tau \frac{i-1+a}{(L-1+a+b)(L-2+a+b)} \right) \end{aligned}$$

Substituting back in (III.B.245) leads to

$$\langle \rho_\tau^{(i)} \rho_{\tau'}^{(j)} \rangle = \langle \rho_\tau^{(i)} \rangle \langle \rho_{\tau'}^{(j)} \rangle - \lambda_\tau \lambda_{\tau'} \frac{(a+i-1)(b+L-j)}{(a+b+L-1)^2(a+b+L-2)}, \quad (\text{III.B.246})$$

which concludes the proof. ■

To summarize, we introduced here an integrable multi-species open SSEP. The dynamics on the boundaries has a simple physical interpretation: it models the interaction with a particles reservoirs with fixed densities of each species. The stationary state of the model is given analytically in terms of a simple matrix product expression. The generators indeed belong to a Lie algebra, which allows us to compute exactly physical quantities using only these algebraic relations (and without any explicit representation). We will encounter again this model in chapter V while studying its properties in the hydrodynamic limit.

In the whole present chapter, we dealt with matrix product expressions of the steady states of one dimensional exclusion processes. We encountered several matrix ansatz algebras and we explained their connections to the integrable structure of the models. The matrix product expressions allowed us to compute exactly physical quantities in the stationary state. But

these quantities were only related to 'static' observables (such as particles densities) or to the average value of 'dynamic' observables (such as particles currents). To get access to the full statistics of these 'dynamic' observables, we need (as explained in chapter I) to study a current counting deformation of the Markov matrices. We are going to see in the next chapter, how the matrix product states can be used to obtain the ground state of such deformed Markov matrices. It will be achieved through the study of the specific example of the single species open ASEP. As a byproduct, we will derive a matrix product expression of some symmetric polynomials: the Koornwinder polynomials (in a particular case). This stresses, once more, the wide range of applications of the matrix product states.

Chapter IV

q-KZ equation and fluctuations of the current

We saw in the previous chapter the efficiency of the matrix product states to encode exactly the stationary state of a wide range of stochastic processes. But we already stressed that the potential applications of such matrix product states goes far beyond the computation of steady states associated to Markov matrices. We now present another application of the matrix product formalism in out-of-equilibrium statistical physics. The goal is to extend the previous matrix ansatz construction of steady states to the computation of the fluctuations of the particles current. It was argued in chapter I that the generating function of the cumulants of the current can be computed through the ground state of a current counting deformation of the Markov matrix. We construct in the present chapter a further deformation of this ground state in a matrix product form that is conjectured to converge to the ground state in some limit. The interest of such construction lies both on the physical and mathematical side.

The physical motivation arises from the possible interpretation of the large deviation function of the current (that is obtained from the generating function through a Legendre transformation, see chapter I) as a dynamical generalization of the thermodynamic potential [27] (this large deviation function is expected to exhibit singularities at the dynamical phase transitions). It is thus important to derive the simplest expression as possible of the current generating function.

The mathematical motivation arises from the use of matrix product states to construct solutions to quantum deformation of the Knizhnik-Zamolodchikov equations (q KZ equations) that were introduced in the context of representation theory of quantum affine algebra [214]. These are a set of difference equations depending on the parameters t and s for periodic systems and also on the parameters a, b, c and d for open boundaries systems. These equations involve a vector, whose components depends on several variables, and relate precisely the permutation of variables in the vector with the mixing of components of the same vector. Once again the integrability plays a central role in the setting of the q KZ equations and ensures their consistency. It has been established that when the parameters satisfy the constraint

$$t^{k+1}s^{r-1}abcd = 1 \tag{IV..1}$$

for some integers k and r , there exist solutions to the q KZ equations that are polynomial in the variables [215–218]. The parameter k is called the rank and the parameter r is called the level of the equation. These polynomial solutions are often related [219] to representations of the double quantum affine algebra [220–222] and expressed in terms of Macdonald or Koornwinder polynomials [49, 141, 216]. The latter polynomials play a central role in combinatorics and representation theory [223].

It is now well established that, in the context of stochastic processes, these q KZ equations for special case $s = 1$ play a central role in the computation of the stationary states [49, 75, 141, 224]. This fact is deeply related (at least for stochastic interacting particles systems) to the construction exposed in chapter III with the ZF and GZ relations [V3, 105]. The main novelties

presented in this chapter are on one hand an interplay between the parameter s involved in the q KZ equations and a current counting deformation parameter ξ of the Markov matrix and on the other hand the matrix product construction of the associated polynomial solutions to the q KZ equations. On the mathematical side it leads to a matrix product construction of some Koornwinder polynomials. On the physical side it allows to construct the ground state of the deformed Markov matrix and gives access to the generating function of the cumulants of the current. The q KZ equations point out once again a bridge between the theory of symmetric polynomials and physical observables in integrable stochastic processes [225, 226]. The results presented here are mainly extracted from the work [V6].

A Current counting deformation and q -KZ equation

We focus our study on the ASEP [39, 40] for two reasons. On the physical side, it has become over the last decades a paradigmatic model in non-equilibrium statistical mechanics [36, 41]. It is an example of a physical system exhibiting a macroscopic current in a stationary regime. Such systems, which cannot be described by the usual thermal equilibrium formalism, can be seen as the simplest out-of-equilibrium situation one can imagine [35, 38, 90]. On the mathematical side, as seen in chapter II, the ASEP enjoys the property of being integrable.

Several exact results have been obtained for the current large deviation function of the ASEP using a deformed current-counting transition matrix [18, 120, 227–230]. The works [18, 120, 227, 229, 230] build upon the matrix product method [46], used to compute the stationary state of the undeformed ASEP. In this chapter we continue in this vein, relying particularly on the integrability of the ASEP [29, 126] and the connection between integrability and the matrix product method [V3, 105]. We note also the approach of [228], in which the Bethe ansatz was used to obtain the cumulant generating function in the thermodynamic limit.

More precisely, the integrable structure of the ASEP gives rise to a connection with Hecke algebras, that are at the heart of the definition of Macdonald and Koornwinder polynomials [49, 141, 224]. The Macdonald polynomials are associated with the periodic system, and in [49] this connection is exploited to derive a matrix product formula for the symmetric Macdonald polynomials. The connection between the open system and Koornwinder polynomials was first identified in [141], then fully established in [224]. However a matrix product formula, and the link to the general form of the Koornwinder polynomials is still lacking.

Our aim is to exploit the integrable structure of the ASEP with deformed current-counting matrix, to make a connection to the general form of the Koornwinder polynomials. This in turns leads to a connection between the symmetric Koornwinder polynomials and the generating function of the cumulants of the current. We do this by introducing scattering relations and q KZ equations with a further deformation, through which we define a twice deformed ground state vector. We give a matrix product construction of this ground state vector and of the symmetric Koornwinder polynomial associated with it. This leads us to conjecture a beautiful relation between the generating function of the cumulants of the current, and a certain limit of symmetric Koornwinder polynomials.

We consider here the ASEP with only *partial* asymmetry, but it would be interesting also to consider the *totally* asymmetric simple exclusion process (TASEP)¹. The TASEP exhibits broadly similar behaviour to the general ASEP physically, but often the involved mathematical expressions are much simpler. The stationary state of the TASEP can be expressed in matrix product form [46], but was also given by directly solving certain recursion relations [47]. The results related to current fluctuations in the TASEP [229] are also much simpler than those for the general ASEP. In our notation, the TASEP relates to the $t \rightarrow \infty$ limit of the Koornwinder polynomials, which has been previously studied [231]. Thus it would be interesting to study this limit in the TASEP context, and to see if any simplifications occur.

In the following subsections we recall briefly the main tools that are needed in this work: (i) the ASEP, the current-counting deformation of the associated Markov matrix, and the link with

¹That is with $q = 0$ in the model, as defined below.

the generating function of cumulants of the current, (ii) the Hecke algebra and Koornwinder polynomials, (iii) the integrable structure of the ASEP.

1 Deformed Markov matrix

a) Definition of the model and Gallavotti-Cohen symmetry

The open boundary ASEP is a stochastic model that we introduced previously through the local jump operators (II.A.23) and (II.A.31). We recall that, in the bulk of the lattice particles hop right one site with rate p , and left with rate q , so long as the target site is empty (the exclusion rule). With open boundaries, particles may enter and exit at the first and last sites. If site 1 is empty (occupied), a particle is injected (extracted) with rate α (γ). At site L , particles are extracted with rate β and injected with rate δ . These rules are summarised in figure IV.1.

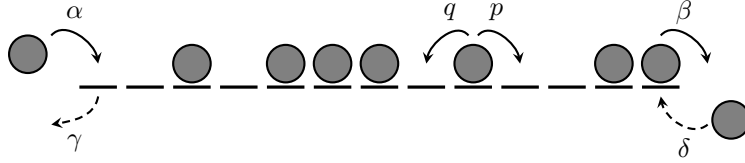


Figure IV.1: Transition rates for the ASEP with open boundaries.

We recall that we attach to each site i a boolean variable $\tau_i \in \{0, 1\}$ indicating if the site is empty ($\tau_i = 0$) or occupied ($\tau_i = 1$). The state of a single site is represented by a vector $|\tau_i\rangle \in \mathbb{C}^2$, where

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

The state of the lattice is given by a vector $|\tau\rangle = |\tau_1, \dots, \tau_L\rangle \in (\mathbb{C}^2)^{\otimes L}$ with

$$|\tau_1, \dots, \tau_L\rangle = |\tau_1\rangle \otimes \dots \otimes |\tau_L\rangle.$$

The ASEP transition rates are then encoded in the transition matrix $M(\xi = 1)$, where²

$$M(\xi) = \sqrt{\alpha\gamma}B_1(\xi) + \sum_{i=1}^{L-1} \sqrt{pq}w_{i,i+1} + \sqrt{\beta\delta}\bar{B}_L, \quad (\text{IV.A.1})$$

and

$$\sqrt{\alpha\gamma}B(\xi) = \begin{pmatrix} -\alpha & \xi^{-1}\gamma \\ \xi\alpha & -\gamma \end{pmatrix}, \quad \sqrt{\beta\delta}\bar{B} = \begin{pmatrix} -\delta & \beta \\ \delta & -\beta \end{pmatrix}, \quad \sqrt{pq}w = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -q & p & 0 \\ 0 & q & -p & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (\text{IV.A.2})$$

The indices on the matrices indicate the sites on which they act non trivially. The matrix $M(\xi)$ is stochastic only for $\xi = 1$, but the introduction of this fugacity allows the study of the current generating function, as will be discussed below. The stochastic matrix $M(\xi = 1)$ has a unique eigenvector with eigenvalue 0, that is

$$M(1)|\Psi\rangle = 0, \quad |\Psi\rangle = \sum_{\tau} \psi_{\tau}|\tau\rangle.$$

Normalizing this vector gives the stationary distribution of the system: letting

$$\mathcal{Z} = \langle 1|\Psi\rangle, \quad \langle 1| = (1, 1)^{\otimes L},$$

²The unusual normalisation is to ease the notation in later sections.

the stationary probability of a configuration τ is

$$\mathcal{S}(\tau) = \frac{1}{\mathcal{Z}} \psi_\tau.$$

If we now consider the deformed transition matrix $M(\xi)$, then the deformed ground state vector satisfies

$$M(\xi)|\Psi(\xi)\rangle = \Lambda_0(\xi)|\Psi(\xi)\rangle,$$

with $\Lambda_0(\xi) \rightarrow 0$ as $\xi \rightarrow 1$. As already stressed in chapter I, the eigenvalue $\Lambda_0(\xi)$ for general ξ is an object of prime interest in the context of out-of-equilibrium statistical physics, because of its connection to the generating function of the cumulants of the current, $E(\mu) = \Lambda_0(e^\mu)$. It has been shown recently [18, 120, 229, 230] that the cumulants of the current for finite systems can be extracted analytically at any order at the price of solving non-linear implicit equations. We recall that the Legendre transformation of $E(\mu)$ provides the large deviation function of the particle current in the stationary state,

$$G(j) = \min_{\mu} (\mu j - E(\mu)),$$

which is expected to be a possible generalisation of thermodynamic potential to non-equilibrium systems [27]. In words, $G(j)$ describes the non-typical fluctuations of the mean particle flux³. The reader can refer to chapter I or to [18] for more details.

The eigenvalue $\Lambda_0(\xi)$ is invariant under the Gallavotti–Cohen symmetry [21, 22]

$$\xi \rightarrow \xi' = \frac{\gamma\delta}{\alpha\beta} \left(\frac{q}{p}\right)^{L-1} \xi^{-1}. \quad (\text{IV.A.3})$$

This translates immediately into a symmetry on the large deviation function of the particle current.

$$G(j) - G(-j) = j \ln \left(\frac{\gamma\delta}{\alpha\beta} \left(\frac{q}{p}\right)^{L-1} \right). \quad (\text{IV.A.4})$$

This symmetry arises from the relation between the transition matrix and its transpose:

$$M(\xi') = U_{\text{GC}} M(\xi)^T U_{\text{GC}}^{-1}, \quad (\text{IV.A.5})$$

where ξ' is as defined in (IV.A.3) and

$$U_{\text{GC}} = \begin{pmatrix} 1 & 0 \\ 0 & \frac{\delta}{\beta} \left(\frac{q}{p}\right)^{L-1} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & \frac{\delta}{\beta} \left(\frac{q}{p}\right)^{L-2} \end{pmatrix} \otimes \cdots \otimes \begin{pmatrix} 1 & 0 \\ 0 & \frac{\delta}{\beta} \end{pmatrix}. \quad (\text{IV.A.6})$$

The relation (IV.A.5) implies that $M(\xi)$ and $M(\xi')$ have the same spectrum and thus the largest eigenvalue is the same:

$$\Lambda_0(\xi') = \Lambda_0(\xi).$$

As a further consequence of this symmetry, given a solution of the left eigenvalue problem

$$\langle \Phi(\xi) | M(\xi) = \Lambda(\xi) \langle \Phi(\xi) |.$$

there is a corresponding solution of the right eigenvalue problem

$$M(\xi') |\Psi(\xi')\rangle = \Lambda(\xi) |\Psi(\xi')\rangle,$$

with

$$|\Psi(\xi')\rangle = U_{\text{GC}} |\Phi(\xi)\rangle,$$

and ξ' as defined in (IV.A.3). Note that here and in the following we use the convention $\langle \cdot |^T = | \cdot \rangle$, where T denotes the usual transposition. We will explain in the following sections the connection that can be made between the ground state $|\Psi(\xi)\rangle$ and the theory of Koornwinder polynomials that we present now.

³More precisely, we recall that, if we denote by Q_T the algebraic number of particles exchanged between the system and the left reservoir during the time interval $[0, T]$, then $G(j)$ is characterised by $P(Q_T/T = j) \sim \exp(-TG(j))$ for large T .

b) Integrability of the deformed Markov matrix

We recall that the ASEP is an integrable model – the deformed transition matrix $M(\xi)$ belongs to an infinite family of commuting matrices [126] (see also [V3, 224]). The generating function of these commuting matrices is called the transfer matrix. The key ingredients to construct this transfer matrix are matrices $\check{R}(z)$, $K(z)$, and $\overline{K}(z)$ satisfying the braided Yang–Baxter relation (II.B.4), the reflection equation (II.C.1) and the reversed reflection equation (II.C.8) respectively. They also satisfy the unitarity and regularity properties.

For the open boundary ASEP the matrices are given by

$$\check{R}(z) = 1 + r(z)m, \quad (\text{IV.A.7})$$

$$K(x; \xi) = 1 + k(z; t_0^{1/2}, u_0^{1/2})B(\xi), \quad (\text{IV.A.8})$$

$$\overline{K}(z) = 1 + k(z^{-1}; t_L^{1/2}, u_L^{1/2})\overline{B}, \quad (\text{IV.A.9})$$

where

$$r(z) = \frac{z-1}{t^{-1/2}z - t^{1/2}}, \quad k(z; t_i^{1/2}, u_i^{1/2}) = \frac{z^2 - 1}{t_i^{-1/2}z^2 - (u_i^{1/2} - u_i^{-1/2})z - t_i^{1/2}}, \quad (\text{IV.A.10})$$

and w , $B(\xi)$, \overline{B} are written in terms of the Hecke parameters as

$$B(\xi) = \begin{pmatrix} -t_0^{-1/2} & \xi^{-1}t_0^{-1/2} \\ \xi t_0^{1/2} & -t_0^{-1/2} \end{pmatrix}, \quad \overline{B} = \begin{pmatrix} -t_L^{-1/2} & t_L^{1/2} \\ t_L^{-1/2} & -t_L^{1/2} \end{pmatrix}, \quad m = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -t^{-1/2} & t^{1/2} & 0 \\ 0 & t^{-1/2} & -t^{1/2} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (\text{IV.A.11})$$

We will write $K(z)$ for $K(z; \xi)$, except when it is necessary to distinguish between values of ξ . Note that the local (physical) transition matrices are obtained from (IV.A.7) – (IV.A.9) through

$$\sqrt{pq}w = (q-p)\check{R}'(1), \quad \sqrt{\alpha\gamma}B(\xi) = \frac{1}{2}(q-p)K'(1; \xi), \quad \sqrt{\beta\delta}\overline{B} = -\frac{1}{2}(q-p)\overline{K}'(1),$$

and the Gallavotti–Cohen symmetry on the transition matrices now reads

$$\begin{aligned} \check{R}_i(z) &= U_{\text{GC}}\check{R}_i(z)^T U_{\text{GC}}^{-1}, \\ K_1(z; \xi') &= U_{\text{GC}}K_1(z; \xi)^T U_{\text{GC}}^{-1}, \\ \overline{K}_L(z) &= U_{\text{GC}}\overline{K}_L(z)^T U_{\text{GC}}^{-1}, \end{aligned}$$

with ξ' and U_{GC} defined in (IV.A.3) and (IV.A.6) respectively.

2 Second deformation

a) Scattering matrices

Instead of the transfer matrix approach, one can define scattering matrices [141, 232], although the two methods are closely related. We first define a modified left boundary matrix

$$\tilde{K}(z) = K(s^{-1/2}z), \quad (\text{IV.A.12})$$

in order to introduce the Hecke parameter s . The matrix $\tilde{K}(z)$ satisfies deformed unitary and reflection relations

$$\begin{aligned} \tilde{K}(sz)\tilde{K}(z^{-1}) &= 1, \\ \check{R}_1(z_2/z_1)\tilde{K}_1(z_2)\check{R}_1(s^{-1}z_1z_2)\tilde{K}_1(z_1) &= \tilde{K}_1(z_1)\check{R}_1(s^{-1}z_1z_2)\tilde{K}_1(z_2)\check{R}_1(z_2/z_1), \end{aligned}$$

and has the Gallavotti–Cohen symmetry

$$\tilde{K}_1(z; \xi') = U_{\text{GC}} \tilde{K}_1(z; \xi)^T U_{\text{GC}}^{-1}.$$

For $1 \leq i \leq L$, define the scattering matrices

$$\begin{aligned} \mathcal{S}_i(\mathbf{z}) = & \check{R}_{i-1} \left(\frac{z_{i-1}}{sz_i} \right) \dots \check{R}_1 \left(\frac{z_1}{sz_i} \right) \\ & \cdot \tilde{K}_1 \left(\frac{1}{z_i} \right) \\ & \cdot \check{R}_1 \left(\frac{1}{z_i z_1} \right) \dots \check{R}_{i-1} \left(\frac{1}{z_i z_{i-1}} \right) \cdot \check{R}_i \left(\frac{1}{z_i z_{i+1}} \right) \dots \check{R}_{L-1} \left(\frac{1}{z_i z_L} \right) \\ & \cdot \bar{K}_L(z_i) \\ & \cdot \check{R}_{L-1} \left(\frac{z_L}{z_i} \right) \dots \check{R}_i \left(\frac{z_{i+1}}{z_i} \right). \end{aligned} \quad (\text{IV.A.13})$$

Using the Yang–Baxter, reflection relations, and unitarity, we see that the scattering matrices satisfy a deformed commutation relation

$$\mathcal{S}_i(\dots, sz_j, \dots) \mathcal{S}_j(z_1, \dots, z_L) = \mathcal{S}_j(\dots, sz_i, \dots) \mathcal{S}_i(z_1, \dots, z_L).$$

When $s = 1$, $[\mathcal{S}_i(\mathbf{z}), \mathcal{S}_j(\mathbf{z})] = 0$ for all i, j , and in fact in that case there is a direct relation to the transfer matrix approach [V3, 126, 224]⁴:

$$\mathcal{S}_i(\mathbf{z}) = t(z_i | \mathbf{z}), \quad (\text{IV.A.14})$$

where $t(z | \mathbf{z})$ is the usual transfer matrix with spectral parameter z and inhomogeneity parameters $\mathbf{z} = z_1, \dots, z_L$ (the reader may refer to chapter II for a precise definition).

At $s = 1$, we also have the important relations

$$\mathcal{S}_i(\mathbf{z})|_{s=z_1=\dots=z_L=1} = 1, \quad \frac{\partial}{\partial z_i} \mathcal{S}_i(\mathbf{z})|_{s=z_1=\dots=z_L=1} = \frac{2}{p-q} M(\xi). \quad (\text{IV.A.15})$$

Considering s general again, we would like to find solutions of the scattering relation

$$\mathcal{S}_i(\mathbf{z}) |\Psi(\dots, z_i, \dots)\rangle = |\Psi(\dots, sz_i, \dots)\rangle, \quad (\text{IV.A.16})$$

where

$$|\Psi(\mathbf{z})\rangle = \sum_{\boldsymbol{\tau}} \psi_{\boldsymbol{\tau}}(\mathbf{z}) |\boldsymbol{\tau}\rangle. \quad (\text{IV.A.17})$$

Taking the derivative of (IV.A.16) with respect to z_i and specialising with $z_1 = \dots = z_L = s = 1$, this would imply

$$M(\xi) |\Psi(\mathbf{1})\rangle = 0. \quad (\text{IV.A.18})$$

For $\xi = 1$ this is the unnormalized stationary vector of the ASEP with eigenvalue 0. For $\xi \neq 1$, the ground state eigenvalue is non-zero, and so (IV.A.18) should not have a solution at this point (that is $s = 1$, $\xi \neq 1$). However, in section D, we will discuss how there could be a solution of (IV.A.16) for $s \rightarrow 1$, $\xi \neq 1$, and how it relates to the current-counting eigenvalue.

⁴Note that for $s \neq 1$ there is no obvious link between the scattering matrices and the usual transfer matrix, as far as we know.

b) q-KZ equation

It can be checked directly that sufficient conditions for a solution of the scattering relation (IV.A.16) are

$$\check{R}_i(z_{i+1}/z_i)|\Psi(\dots, z_i, z_{i+1}, \dots)\rangle = |\Psi(\dots, z_{i+1}, z_i, \dots)\rangle, \quad 1 \leq i \leq L-1, \quad (\text{IV.A.19})$$

$$\tilde{K}_1(z_1^{-1})|\Psi(z_1^{-1}, z_2, \dots)\rangle = |\Psi(sz_1, z_2, \dots)\rangle, \quad (\text{IV.A.20})$$

$$\bar{K}_L(z_L)|\Psi(\dots, z_{L-1}, z_L)\rangle = |\Psi(\dots, z_{L-1}, 1/z_L)\rangle. \quad (\text{IV.A.21})$$

Note that the Yang–Baxter, reflection, and unitary conditions ensure the consistency of this definition. We will refer to (IV.A.19) – (IV.A.21) as the q KZ equations, although in our notation the q has been replaced by the parameter s . These q -difference equations were first introduced in [214] and appear as q -deformation of the KZ equations [233].

Motivated by the connection to the ASEP stationary state, we make the following definition:

Definition A.1. *We call a solution*

$$|\Psi(\mathbf{z}; s, \xi)\rangle = \sum_{\tau} \psi_{\tau}(\mathbf{z}; s, \xi)|\tau\rangle$$

of equations (IV.A.19) – (IV.A.21) a twice deformed inhomogeneous ground state vector, with deformation parameters s and ξ .

As indicated at the end of the previous section, such a vector with $s = \xi = 1$ is the inhomogeneous ground state vector of the open boundary ASEP, and can be constructed in matrix product form [**V3**, **V9**] or from specialised non-symmetric Koornwinder polynomials [224]. We will show that more general solutions exist when s and ξ obey some relations.

We define left q KZ equations

$$\langle\Phi(\dots, z_i, z_{i+1}, \dots)|\check{R}_i(z_{i+1}/z_i) = \langle\Phi(\dots, z_{i+1}, z_i, \dots)|, \quad 1 \leq i \leq L-1, \quad (\text{IV.A.22})$$

$$\langle\Phi(z_1^{-1}, z_2, \dots)|\tilde{K}_1(z_1^{-1}) = \langle\Phi(sz_1, z_2, \dots)|, \quad (\text{IV.A.23})$$

$$\langle\Phi(\dots, z_{L-1}, z_L)|\bar{K}_L(z_L) = \langle\Phi(\dots, z_{L-1}, 1/z_L)|, \quad (\text{IV.A.24})$$

with

$$\langle\Phi(\mathbf{z})| = \sum_{\tau} \phi_{\tau}(\mathbf{x})\langle\tau|. \quad (\text{IV.A.25})$$

These would imply a solution of a left scattering equation (analogous to (IV.A.16)) with a scattering matrix, defined by reversing the order of matrices in the definition (IV.A.13).

The Gallavotti–Cohen symmetry allows us to relate solutions of the left and right q KZ equations.

Lemma A.2. *For any vector $\langle\Phi(\mathbf{z}; s, \xi)|$ satisfying the left q KZ equations (IV.A.22) – (IV.A.24), the vector*

$$|\Psi(\mathbf{z}; s, \xi')\rangle = U_{GC}|\Phi(\mathbf{z}; s, \xi)\rangle, \quad (\text{IV.A.26})$$

with

$$\xi' = t_0^{-1}t_L^{-1}t^{-(L-1)}\xi^{-1}, \quad (\text{IV.A.27})$$

is a solution to the right q KZ equations (IV.A.19) – (IV.A.21).

Proof. This is checked by transposing the left q KZ equations and using the Gallavotti–Cohen symmetry on the \check{R} , \tilde{K} and \bar{K} matrices. ■

B Koornwinder polynomials and link with q-KZ equation

We now introduce the symmetric and non-symmetric Koornwinder polynomials, which form the other main theme of this chapter. The symmetric Koornwinder polynomials [234, 235] are a family of multivariate orthogonal polynomials generalising the Askey–Wilson polynomials. The symmetric Koornwinder polynomials can be constructed from their non-symmetric counterparts, which arise from the polynomial representation of the affine Hecke algebra of type C_L [222, 236].

1 Non-symmetric Koornwinder polynomials

a) Hecke algebra and Noumi representation

The affine Hecke algebra of type C_L is generated by elements T_0, T_1, \dots, T_L , with parameters $t^{1/2}$, $t_0^{1/2}$ and $t_L^{1/2}$. The generators satisfy the quadratic relations,

$$\begin{aligned} (T_0 - t_0^{1/2})(T_0 + t_0^{-1/2}) &= 0, \\ (T_i - t^{1/2})(T_i + t^{-1/2}) &= 0, \quad 1 \leq i \leq L-1, \\ (T_L - t_L^{1/2})(T_L + t_L^{-1/2}) &= 0, \end{aligned}$$

the braid relations

$$\begin{aligned} T_1 T_0 T_1 T_0 &= T_0 T_1 T_0 T_1 \\ T_i T_{i+1} T_i &= T_{i+1} T_i T_{i+1}, \quad 1 \leq i \leq L-2, \\ T_L T_{L-1} T_L T_{L-1} &= T_{L-1} T_L T_{L-1} T_L, \end{aligned}$$

and otherwise commute. That is

$$T_i T_j = T_j T_i, \quad |i - j| \geq 2.$$

The algebra contains a family of mutually commuting elements [222, 237]

$$Y_i = T_i \dots T_{L-1} T_L \dots T_0 T_1^{-1} \dots T_{i-1}^{-1}, \quad 1 \leq i \leq L. \quad (\text{IV.B.1})$$

We are interested in the representation of this algebra due to Noumi [221] (see also [222]), acting on Laurent polynomials in z_1, \dots, z_L . The Noumi representation contains three additional parameters, $u_0^{1/2}$, $u_L^{1/2}$, and $s^{1/2}$, and is defined in terms of operators s_i acting on the x_i as

$$s_0 : z_1 \rightarrow s z_1^{-1}, \quad s_L : z_L \rightarrow z_L^{-1}, \quad s_i : z_i \leftrightarrow z_{i+1}, \quad 1 \leq i \leq L-1. \quad (\text{IV.B.2})$$

The elements s_0, s_1, \dots, s_L generate the affine Weyl W group of type C_L . The *finite* Weyl group W_0 is the subgroup generated by s_1, \dots, s_L .

Then in the Noumi representation, the generators of the affine Hecke algebra are given by

$$\begin{aligned} T_0^{\pm 1} &= t_0^{\pm 1/2} - t_0^{-1/2} \frac{(z_1 - a)(z_1 - b)}{z_1(z_1 - s z_1^{-1})} (1 - s_0), \\ T_i^{\pm 1} &= t^{\pm 1/2} - \frac{t^{1/2} z_i - t^{-1/2} z_{i+1}}{(z_i - z_{i+1})} (1 - s_i), \quad 1 \leq i \leq L-1, \\ T_L^{\pm 1} &= t_L^{\pm 1/2} + t_L^{-1/2} \frac{(c z_L - 1)(d z_L - 1)}{z_L(z_L - z_L^{-1})} (1 - s_L), \end{aligned} \quad (\text{IV.B.3})$$

with

$$a = s^{1/2} t_0^{1/2} u_0^{1/2}, \quad b = -s^{1/2} t_0^{1/2} u_0^{-1/2}, \quad c = t_L^{1/2} u_L^{1/2}, \quad d = -t_L^{1/2} u_L^{-1/2}.$$

One can check directly that the definitions (IV.B.3) satisfy the relations of the Hecke algebra. Formally, we define the field $\mathbb{F} = \mathbb{C}(s^{1/2}, t^{1/2}, t_0^{1/2}, u_0^{1/2}, t_L^{1/2}, u_L^{1/2})$, and let $\mathcal{R} = \mathbb{F}[z_1, \dots, z_L]$

be the ring of Laurent polynomials in L variables over \mathbb{F} . The map sending the generators of the Hecke algebra to the operators defined in (IV.B.3) gives a representation of the algebra on \mathcal{R} [222].

Later we will see that to relate the ASEP to the Noumi representation of the Hecke algebra we should take

$$t^{1/2} = \sqrt{\frac{p}{q}}, \quad t_0^{1/2} = \sqrt{\frac{\alpha}{\gamma}}, \quad t_L^{1/2} = \sqrt{\frac{\beta}{\delta}},$$

and

$$u_0^{1/2} - u_0^{-1/2} = \frac{p - q + \gamma - \alpha}{\sqrt{\alpha\gamma}}, \quad u_L^{1/2} - u_L^{-1/2} = \frac{p - q + \delta - \beta}{\sqrt{\beta\delta}}.$$

For the remainder of this paper we will use this parameterisation in preference to the physical parameters of the ASEP, or the combinations a, b, c, d appearing in (IV.B.3).

b) Non-symmetric Koornwinder polynomials

Before defining the non-symmetric Koornwinder polynomials, we will introduce some notation and definitions concerning integer vectors, $\lambda \in \mathbb{Z}^L$, with

$$\lambda = (\lambda_1, \dots, \lambda_L).$$

We call such a vector a *composition*. For a given composition, λ , we write monomials

$$\mathbf{z}^\lambda = z_1^{\lambda_1} \dots z_L^{\lambda_L}.$$

A *partition* is a composition satisfying

$$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_L \geq 0.$$

We denote by λ^+ the unique partition obtained from a composition λ by reordering and changing signs so that the entries are non-negative and in decreasing order.

There are two partial orderings on compositions that will be relevant [236]. First define the *dominance order*: for $\mu, \lambda \in \mathbb{Z}^L$

$$\mu \leq \lambda \iff \sum_{i=1}^j (\mu_i - \lambda_i) \leq 0, \quad \forall j, 1 \leq j \leq L.$$

Then $\mu < \lambda$ if $\mu \leq \lambda$ and $\mu \neq \lambda$. The second partial ordering ‘ \preceq ’ is defined as

$$\mu \preceq \lambda \iff \mu^+ < \lambda^+ \text{ or } (\mu^+ = \lambda^+ \text{ and } \mu \leq \lambda).$$

Then, $\mu \prec \lambda$ if $\mu \preceq \lambda$ and $\mu \neq \lambda$.

Definition B.1. *The non-symmetric Koornwinder polynomial $E_\lambda(\mathbf{z})$, indexed by composition λ , is the unique Laurent polynomial satisfying*

$$\begin{aligned} Y_i E_\lambda(\mathbf{z}) &= y(\lambda)_i E_\lambda(\mathbf{z}), \quad 1 \leq i \leq L, \\ E_\lambda(\mathbf{z}) &= \mathbf{z}^\lambda + \sum_{\lambda' \prec \lambda} c_{\lambda\lambda'} \mathbf{z}^{\lambda'}, \end{aligned}$$

where Y_i is defined in (IV.B.1) in the Noumi representation, $y(\lambda)_i$ is the eigenvalue, and $c_{\lambda\lambda'}$ are coefficients.

The composition λ determines the eigenvalue $y(\lambda)_i$ [222]. The two following cases will appear directly in this work:

- For $m > 0$, $\lambda = ((-m)^L) = (-m, \dots, -m)$,

$$y(\lambda)_i = t_0^{-1/2} t_L^{-1/2} s^{-m} t^{-(i-1)}. \quad (\text{IV.B.4})$$

- For $m \geq 0$, $\lambda = (m^L) = (m, \dots, m)$,

$$y(\lambda)_i = t_0^{1/2} t_L^{1/2} s^m t^{L-i}. \quad (\text{IV.B.5})$$

However, other non-symmetric Koornwinder polynomials will appear implicitly, and we define the following space:

Definition B.2. For a partition λ of length L , define \mathcal{R}^λ as the space spanned by $\{E_\mu | \mu \in \mathbb{Z}^L, \mu^+ = \lambda\}$.

2 Symmetric Koornwinder polynomials

a) Finite difference operator and symmetric Koornwinder polynomials

The symmetric Koornwinder polynomials were introduced in [234], as eigenfunctions of the s -difference operator

$$D = \sum_{i=1}^L g_i(\mathbf{z})(T_{s,i} - 1) + \sum_{i=1}^L g_i(\mathbf{z}^{-1})(T_{s,i}^{-1} - 1), \quad (\text{IV.B.6})$$

where $g_i(\mathbf{z})$ is defined by

$$g_i(\mathbf{z}) = \frac{(1 - az_i)(1 - bz_i)(1 - cz_i)(1 - dz_i)}{(1 - z_i^2)(1 - sz_i^2)} \prod_{\substack{j=1 \\ j \neq i}}^L \frac{(1 - tz_i z_j^{-1})(1 - tz_i z_j)}{(1 - z_i z_j^{-1})(1 - z_i z_j)}, \quad (\text{IV.B.7})$$

and $T_{s,i}$ is the i^{th} s -shift operator

$$T_{s,i} f(z_1, \dots, z_i, \dots, z_L) = f(z_1, \dots, sz_i, \dots, z_L). \quad (\text{IV.B.8})$$

Definition B.3. For a partition λ , the symmetric Koornwinder polynomial $P_\lambda(\mathbf{z})$ is characterised by the eigenvalue equation

$$DP_\lambda = d_\lambda P_\lambda, \quad (\text{IV.B.9})$$

with eigenvalue

$$d_\lambda = \sum_{i=1}^L \left[t_0 t_L t^{2L-i-1} (s^{\lambda_i} - 1) + t^{i-1} (s^{-\lambda_i} - 1) \right], \quad (\text{IV.B.10})$$

and where the coefficient of \mathbf{x}^λ in P_λ is equal to 1.

b) Link with the non-symmetric polynomials

The symmetric Koornwinder polynomials are W_0 -invariant (that is, invariant under the action of s_1, \dots, s_L , defined in (IV.B.2)), and their relation to the non-symmetric Koornwinder polynomials was given in [222].

Theorem B.4 (Corollary 6.5 of [222]). *The symmetric Koornwinder polynomial P_λ can be characterised as the unique W_0 -invariant polynomial in \mathcal{R}^λ which has the coefficient of \mathbf{z}^λ equal to 1.*

3 Link with the q -KZ equation

a) Reformulation of the q -KZ equation

We use the Noumi representation of the Hecke algebra to write the q KZ equations in component form. To specify a lattice configuration τ we use ‘ \circ ’ for an empty site ($\tau_i = 0$), ‘ \bullet ’ for a filled site ($\tau_i = 1$) and ‘ \dots ’ for unspecified values. Then, for example, we write $\psi_{\circ\dots}$ to indicate the weight for any configuration with the first site empty ($\tau_1 = 0$)

Lemma B.5. *The qKZ equations (IV.A.19) – (IV.A.21) for the deformed ground state vector are equivalent to the following exchange relations on the components:*

$$T_0\psi_{\circ\dots} = \xi^{-1}t_0^{-1/2}\psi_{\bullet\dots}, \quad (\text{IV.B.11})$$

$$T_L\psi_{\dots\bullet} = t_L^{-1/2}\psi_{\dots\circ}, \quad (\text{IV.B.12})$$

and for $1 \leq i \leq L - 1$,

$$T_i\psi_{\dots\circ\dots} = t^{1/2}\psi_{\dots\circ\dots}, \quad (\text{IV.B.13})$$

$$T_i\psi_{\dots\bullet\dots} = t^{1/2}\psi_{\dots\bullet\dots}, \quad (\text{IV.B.14})$$

$$T_i\psi_{\dots\circ\dots} = t^{-1/2}\psi_{\dots\circ\dots}, \quad (\text{IV.B.15})$$

where the marked sites are in positions $i, i + 1$.

Proof. This can be checked directly. ■

Note that the parameters s and ξ both enter through (IV.B.11), with s contained within the T_0 operator.

Lemma B.6. *The left qKZ equations (IV.A.22) – (IV.A.24) for a vector of form (IV.A.25) are equivalent to the following exchange relations on the components:*

$$T_0\phi_{\circ\dots} = \xi t_0^{1/2}\phi_{\bullet\dots}, \quad (\text{IV.B.16})$$

$$T_L\phi_{\dots\bullet} = t_L^{1/2}\phi_{\dots\circ}, \quad (\text{IV.B.17})$$

and for $1 \leq i \leq L - 1$,

$$T_i\phi_{\dots\circ\dots} = t^{1/2}\phi_{\dots\circ\dots}, \quad (\text{IV.B.18})$$

$$T_i\phi_{\dots\bullet\dots} = t^{1/2}\phi_{\dots\bullet\dots}, \quad (\text{IV.B.19})$$

$$T_i\phi_{\dots\circ\dots} = t^{1/2}\phi_{\dots\circ\dots}, \quad (\text{IV.B.20})$$

where the marked sites are in positions $i, i + 1$.

b) Reference state

Lemma B.7. *For any vector $|\Psi(\mathbf{z}; s, \xi)\rangle$ satisfying the qKZ equations (IV.A.19) – (IV.A.21), the empty lattice weight $\psi_{\circ\dots\circ}$ (where the ‘...’ here stands for empty sites) is an eigenfunction of the Y_i operators (IV.B.1), satisfying*

$$Y_i\psi_{\circ\dots\circ} = \xi^{-1}t_0^{-1/2}t_L^{-1/2}t^{-(i-1)}\psi_{\circ\dots\circ}. \quad (\text{IV.B.21})$$

Proof. This follows by direct computation with the exchange relations in Lemma B.5. ■

Lemma B.7 immediately suggests the following connection to the non-symmetric Koornwinder polynomials:

1. Taking $\xi = s^m$, $m > 0$, the eigenvalue in (IV.B.21) is given by (IV.B.4), corresponding to the non-symmetric Koornwinder polynomial labelled by the composition $((-m)^L)$.
2. Taking $\xi = t_0^{-1}t_L^{-1}t^{-(L-1)}s^{-m}$, $m \geq 0$, the eigenvalue instead corresponds to (IV.B.5), for the composition (m^L) .

Note that case 2 is obtained from case 1 by sending

$$\xi \rightarrow t_0^{-1}t_L^{-1}t^{-(L-1)}\xi^{-1},$$

which is exactly the Gallavotti–Cohen symmetry (IV.A.3). In section C we will give a direct matrix product construction of the inhomogeneous ground state vector for case 1, that is $\xi = s^m$. To solve case 2, we will use the Gallavotti–Cohen symmetry on solutions of *left* q KZ equations, which we will present next. We note that an alternative approach, as followed in [224, 238], would be to take $\psi_{\circ\dots\circ}$ as the non-symmetric Koornwinder polynomial given in case 1 or case 2, then show that a solution of the exchange relations (IV.B.11) – (IV.B.15) can be constructed from this reference state.

Lemma B.8. *For any vector $\langle\Phi(\mathbf{z}; s, \xi)|$ satisfying the left q KZ equations (IV.A.22) – (IV.A.24), the empty lattice weight $\phi_{\circ\dots\circ}$ is an eigenfunction of the Y_i operators (IV.B.1), satisfying*

$$Y_i \phi_{\circ\dots\circ} = \xi t_0^{1/2} t_L^{1/2} t^{L-i} \phi_{\circ\dots\circ}. \quad (\text{IV.B.22})$$

Again, the same two constraints on ξ and s appear, but with the correspondence to the non-symmetric Koornwinder polynomials reversed: taking $\xi = s^m$, $m \geq 0$, would correspond to the composition (m^L) ; taking $\xi = t_0^{-1} t_L^{-1} t^{-(L-1)} s^{-m}$, $m > 0$, would correspond to the composition $((-m)^L)$.

C Matrix product solution to the q -KZ equation

1 Construction of the solution

a) General construction

The matrix product ansatz for the twice deformed inhomogeneous ground state vectors is written

$$|\Psi(\mathbf{z}; s, \xi)\rangle = \langle\langle W | \mathbb{S} \mathbb{A}(z_1) \otimes \dots \otimes \mathbb{A}(z_L) | V \rangle\rangle, \quad (\text{IV.C.1})$$

with

$$\mathbb{A}(z) = \begin{pmatrix} A_0(z) \\ A_1(z) \end{pmatrix}.$$

The entries $A_0(z)$, $A_1(z)$ as well as \mathbb{S} are operators in some auxiliary algebraic space, and the left and right vectors $\langle\langle W |$ and $|V\rangle\rangle$ contract this space to give a scalar value.

Writing out (IV.C.1) gives the 2^L component vector

$$|\Psi(\mathbf{z}; s, \xi)\rangle = \begin{pmatrix} \langle\langle W | \mathbb{S} A_0(z_1) \dots A_0(z_{L-1}) A_0(z_L) | V \rangle\rangle \\ \langle\langle W | \mathbb{S} A_0(z_1) \dots A_0(z_{L-1}) A_1(z_L) | V \rangle\rangle \\ \langle\langle W | \mathbb{S} A_0(z_1) \dots A_1(z_{L-1}) A_0(z_L) | V \rangle\rangle \\ \vdots \\ \langle\langle W | \mathbb{S} A_1(z_1) \dots A_1(z_{L-1}) A_1(z_L) | V \rangle\rangle \end{pmatrix},$$

with entries

$$\psi_{\tau}(\mathbf{z}; s, \xi) = \langle\langle W | \mathbb{S} A_{\tau_1}(z_1) \dots A_{\tau_{L-1}}(z_{L-1}) A_{\tau_L}(z_L) | V \rangle\rangle.$$

Lemma C.1. *Sufficient conditions for a vector of form (IV.C.1) to satisfy the q KZ equations (IV.A.19) – (IV.A.21) are the following:*

$$\check{R} \begin{pmatrix} z_{i+1} \\ z_i \end{pmatrix} \mathbb{A}(z_i) \otimes \mathbb{A}(z_{i+1}) = \mathbb{A}(z_{i+1}) \otimes \mathbb{A}(z_i), \quad (\text{IV.C.2})$$

$$\tilde{K}(z_1^{-1}) \langle\langle W | \mathbb{S} \mathbb{A}(z_1^{-1}) = \langle\langle W | \mathbb{S} \mathbb{A}(s z_1), \quad (\text{IV.C.3})$$

$$\bar{K}(z_L) \mathbb{A}(z_L) | V \rangle\rangle = \mathbb{A}(z_L^{-1}) | V \rangle\rangle. \quad (\text{IV.C.4})$$

Equation (IV.C.2) is the Zamolodchikov–Faddeev (ZF) algebra [193, 239]. Equations (IV.C.3), (IV.C.4) are a deformation of the Ghoshal–Zamolodchikov (GZ) relations [194]. The undeformed GZ relations are obtained by setting \mathbb{S} to the identity and $s = 1$. The matrix product ansatz for the open boundary ASEP can be expressed as a solution of the undeformed relations, and solutions for related models have also been found and studied [V3, V10].

b) Definition of the algebra

We now give an explicit construction of the q KZ solution when $\xi = s^m$, $m \geq 1$. We first define certain algebraic objects through the relations they satisfy.

Definition C.2. We define algebraic objects⁵ satisfying the following relations: operators a , a^\dagger and S :

$$\begin{aligned} aa^\dagger - ta^\dagger a &= 1 - t, \\ aS &= \sqrt{s}Sa, \\ Sa^\dagger &= \sqrt{s}a^\dagger S. \end{aligned} \tag{IV.C.5}$$

And paired boundary vectors $\langle\langle w|$ and $|v\rangle\rangle$:

$$\begin{aligned} \langle\langle w| \left(t_0^{1/2} a - t_0^{-1/2} a^\dagger \right) &= \langle\langle w| \left(u_0^{1/2} - u_0^{-1/2} \right), \\ \left(t_L^{1/2} a^\dagger - t_L^{-1/2} a \right) |v\rangle\rangle &= \left(u_L^{1/2} - u_L^{-1/2} \right) |v\rangle\rangle, \end{aligned} \tag{IV.C.6}$$

and $\langle\langle \tilde{w}|$ and $|\tilde{v}\rangle\rangle$:

$$\begin{aligned} \langle\langle \tilde{w}| \left(t_0^{1/2} a - t_0^{-1/2} a^\dagger \right) &= \langle\langle \tilde{w}| \left(t_0^{1/2} - t_0^{-1/2} \right), \\ \left(t_L^{1/2} a^\dagger - t_L^{-1/2} a \right) |\tilde{v}\rangle\rangle &= \left(t_L^{1/2} - t_L^{-1/2} \right) |\tilde{v}\rangle\rangle. \end{aligned} \tag{IV.C.7}$$

Elements of this algebra have appeared in many places in the context of the ASEP. The first algebraic relation of (IV.C.5) and the relations (IV.C.6) were first stated in [240] to study the stationary state of the open ASEP. This work shed new light on the DEHP algebra introduced in [46] by showing that it can be recast in a form of a q -deformed oscillator algebra by an appropriate shift and normalisation of the generators. The representation of the algebraic elements involved in the first relation of (IV.C.5) and in the relations (IV.C.6) were found in [240], and permitted explicit computations. In particular the author of that work pointed out the relevance of the parametrisation used here. More precisely the parameters $\kappa_+(\alpha, \gamma)$ and $\kappa_+(\beta, \delta)$ defined in [240] by $\kappa_+(x, y) = \frac{1}{2x} \left(y - x + p - q + \sqrt{(y - x + p - q)^2 + 4xy} \right)$ play a central role in the representation of the algebra, and are relevant in describing the phase transitions of the system. The precise relations with the parameters used here are $\kappa_+(\alpha, \gamma) = u_0^{1/2} t_0^{-1/2}$ and $\kappa_+(\beta, \delta) = u_L^{1/2} t_L^{-1/2}$.

The other relations (IV.C.5), (IV.C.6) and (IV.C.7) appear previously in [18, 120, 230, 241] to compute the fluctuations of the current. We recall an infinite dimensional representation of this algebra: $|v\rangle\rangle, |\tilde{v}\rangle\rangle, \dots$ are vectors of a Fock space endowed with the usual scalar product. In this manuscript the scalar product of two vectors $|x\rangle\rangle$ and $|y\rangle\rangle$ of this Fock space is denoted by $\langle\langle x| \cdot |y\rangle\rangle$. The operators a and a^\dagger are linear operators on this Fock space. Let us stress here that the creation operator a^\dagger is not the Hermitian conjugate of the annihilation operator a (it is a standard notation which appears often in the literature, see for instance [240]).

The representation of the algebra is defined on the Fock space $\text{Span}\{|k\rangle\rangle\}_{k=0}^\infty$. The bulk matrices are given by

$$\begin{aligned} a &= \sum_{k=1}^{\infty} (1 - t^k) |k-1\rangle\rangle \langle\langle k|, & a^\dagger &= \sum_{k=0}^{\infty} |k+1\rangle\rangle \langle\langle k|, \\ S &= \sum_{k=0}^{\infty} s^{k/2} |k\rangle\rangle \langle\langle k|. \end{aligned}$$

The boundary vectors are written

$$\langle\langle w| = \sum_{k=0}^{\infty} w_k \langle\langle k|, \quad |v\rangle\rangle = \sum_{k=0}^{\infty} v_k |k\rangle\rangle,$$

⁵These are s -deformations of the usual q -bosons that we recover for $q = t$ and $s = t^2$.

and

$$\langle\langle \tilde{w} | = \sum_{k=0}^{\infty} \tilde{w}_k \langle\langle k |, \quad | \tilde{v} \rangle\rangle = \sum_{k=0}^{\infty} \tilde{v}_k |k \rangle\rangle.$$

As a consequence of the boundary relations, the coefficients appearing in $\langle\langle w |, |v \rangle\rangle$ satisfy the recursion relations

$$\begin{aligned} w_{k+1} + t_0^{1/2}(u_0^{1/2} - u_0^{-1/2})w_k - t_0(1 - t^k)w_{k-1} &= 0, \\ (t; t)_{k+1}v_{k+1} + t_L^{1/2}(u_L^{1/2} - u_L^{-1/2})(t; t)_k v_k - t_L(1 - t^k)(t; t)_{k-1}v_{k-1} &= 0, \end{aligned}$$

with $w_{-1} = v_{-1} = 0$. We have used the t -Pochhammer symbol

$$(x; t)_n = \prod_{k=0}^{n-1} (1 - t^k x).$$

The t -Pochhammer symbol can be defined for $n = \infty$ if $t < 1$:

$$(x; t)_{\infty} = \prod_{k=0}^{\infty} (1 - t^k x),$$

and we use the notation

$$(x, y, z, \dots; t)_{\infty} = (x; t)_{\infty} (y; t)_{\infty} (z; t)_{\infty} \dots$$

The t -Hermite polynomials are given by

$$H_n(x, y) = \sum_{k=0}^n \frac{(t; t)_n}{(t; t)_k (t; t)_{n-k}} x^k y^{n-k},$$

and satisfy the recursion relation

$$H_{n+1}(x, y) - (x + y)H_n(x, y) + xy(1 - t^n)H_{n-1}(x, y) = 0.$$

Thus we find

$$\begin{aligned} w_n &= H_n(t_0^{1/2} u_0^{-1/2}, -t_0^{1/2} u_0^{1/2}), \\ v_n &= \frac{H_n(t_L^{1/2} u_L^{-1/2}, -t_L^{1/2} u_L^{1/2})}{(t; t)_n}. \end{aligned} \tag{IV.C.8}$$

The coefficients \tilde{w}_n, \tilde{v}_n are obtained by setting $u_i = t_i$ in the equation above.

To compute the normalisation factors in the q KZ solution, we will make use of the t -Mehler formula

$$\sum_{n=0}^{\infty} H_n(x, y) H_n(w, z) \frac{\lambda^n}{(t; t)_n} = \frac{(xywz\lambda^2; t)_{\infty}}{(xw\lambda, xz\lambda, yw\lambda, yz\lambda; t)_{\infty}}.$$

For the normalisation, we need to compute

$$\langle\langle w | S^a | v \rangle\rangle = \sum_{n=0}^{\infty} w_n \left(s^{n/2} \right)^a v_n.$$

Using the coefficients (IV.C.8) and the t -Mehler formula gives

$$\begin{aligned} \langle\langle w | S^a | v \rangle\rangle &= \\ &= \frac{\left(t_0^{1/2} t_L^{1/2} s^a; t \right)_{\infty}}{\left(t_0^{1/2} u_0^{-1/2} t_L^{1/2} u_L^{-1/2} s^{a/2}, -t_0^{1/2} u_0^{-1/2} t_L^{1/2} u_L^{1/2} s^{a/2}, -t_0^{1/2} u_0^{1/2} t_L^{1/2} u_L^{-1/2} s^{a/2}, t_0^{1/2} u_0^{1/2} t_L^{1/2} u_L^{1/2} s^{a/2}; t \right)_{\infty}}. \end{aligned} \tag{IV.C.9}$$

We also need to compute $\langle\langle \tilde{w} | S^a | \tilde{v} \rangle\rangle$, but this is obtained from (IV.C.9) by setting $u_i = t_i$, $i = 0, L$.

c) Construction of the solutions

In the matrix product construction we will need several commuting copies (a_n, a_n^\dagger, S_n) of the algebra (a, a^\dagger, S) defined in (IV.C.5). Similarly to the construction (III.B.144), a simple way to build these commuting copies is to define

$$\begin{aligned} a_n &= \underbrace{1 \otimes \cdots \otimes 1}_{n-1} \otimes a \otimes 1 \otimes 1 \otimes \cdots, \\ a_n^\dagger &= \underbrace{1 \otimes \cdots \otimes 1}_{n-1} \otimes a^\dagger \otimes 1 \otimes 1 \otimes \cdots, \\ S_n &= \underbrace{1 \otimes \cdots \otimes 1}_{n-1} \otimes S \otimes 1 \otimes 1 \otimes \cdots, \end{aligned} \quad (\text{IV.C.10})$$

We introduce also the corresponding boundary vectors

$$\begin{aligned} \langle\langle w|_n &= \underbrace{1 \otimes \cdots \otimes 1}_{n-1} \otimes \langle\langle w| \otimes 1 \otimes 1 \otimes \cdots, \\ \langle\langle \tilde{w}|_n &= \underbrace{1 \otimes \cdots \otimes 1}_{n-1} \otimes \langle\langle \tilde{w}| \otimes 1 \otimes 1 \otimes \cdots, \\ |v\rangle_n &= \underbrace{1 \otimes \cdots \otimes 1}_{n-1} \otimes |v\rangle \otimes 1 \otimes 1 \otimes \cdots, \\ |\tilde{v}\rangle_n &= \underbrace{1 \otimes \cdots \otimes 1}_{n-1} \otimes |\tilde{v}\rangle \otimes 1 \otimes 1 \otimes \cdots, \end{aligned} \quad (\text{IV.C.11})$$

The subscript indices on a, a^\dagger, S and $\langle\langle w|, \langle\langle \tilde{w}|, |v\rangle, |\tilde{v}\rangle$ in (IV.C.10) and (IV.C.11) thus denote the position of the operator or vector in the tensor product.

In the following, as a matter of convention, we will reserve the symbol ‘ \otimes ’ for objects belonging to the space of lattice configurations (see (IV.C.1) for example), and use the index notation to denote the tensor product in the auxiliary algebraic space (see (IV.C.12), (IV.C.13) for example). The aim is to provide a notational distinction between these two spaces and two tensor products.

Building on these commuting copies of the algebra, we define

$$\mathbb{S}^{(m)} = (S_{2m-1})^{2m-1} \times (S_{2m-2})^{2m-2} \times \cdots \times (S_3)^3 \times (S_2)^2 \times S_1, \quad (\text{IV.C.12})$$

$$\mathbb{A}^{(m)}(z) = L_{2m-1, 2m-2}(z) \cdot \cdots \cdot L_{5,4}(z) \cdot L_{3,2}(z) \cdot b(z), \quad (\text{IV.C.13})$$

with

$$L_{k+1,k}(z) = \begin{pmatrix} 1 & a_{k+1} \\ z a_{k+1}^\dagger & z \end{pmatrix} \cdot \begin{pmatrix} 1/z & a_k/z \\ a_k^\dagger & 1 \end{pmatrix}, \quad b(z) = \begin{pmatrix} 1/z + a_1 \\ z + a_1^\dagger \end{pmatrix}. \quad (\text{IV.C.14})$$

The symbol \cdot indicates the usual matrix product in the physical space. For example, expanding the definition of $L_{k+1,k}(z)$ gives

$$L_{j,k}(z) = \begin{pmatrix} 1/z + a_j a_k^\dagger & a_k/z + a_j \\ a_j^\dagger + z a_k^\dagger & a_j^\dagger a_k + z \end{pmatrix}.$$

To lighten the notation, we will sometimes write $L(z)$ instead of $L_{k+1,k}(z)$ when there is no ambiguity.

We also define boundary vectors

$$\langle\langle W^{(m)}| = \langle\langle w|_{2m-1} \langle\langle \tilde{w}|_{2m-2} \cdots \langle\langle w|_3 \langle\langle \tilde{w}|_2 \langle\langle w|_1 \quad (\text{IV.C.15})$$

$$|V^{(m)}\rangle\rangle = |v\rangle_{2m-1} |\tilde{v}\rangle_{2m-2} \cdots |v\rangle_3 |\tilde{v}\rangle_2 |v\rangle_1. \quad (\text{IV.C.16})$$

Proposition C.3. For integer $m > 0$ and $\xi = s^m$,

$$|\Psi^{(m)}(\mathbf{z}; s)\rangle = \frac{1}{\Omega^{(m)}} \langle\langle W^{(m)} | \mathbb{S}^{(m)} \mathbb{A}^{(m)}(z_1) \otimes \dots \otimes \mathbb{A}_L^{(m)}(z_L) | V^{(m)} \rangle\rangle, \quad (\text{IV.C.17})$$

with normalization factor

$$\Omega^{(m)} = \langle\langle W^{(m)} | \mathbb{S}^{(m)} | V^{(m)} \rangle\rangle, \quad (\text{IV.C.18})$$

is a solution of the q KZ equations (IV.A.19) – (IV.A.21).

Note that the dependence on ξ has disappeared in the vector $|\Psi^{(m)}(\mathbf{z}; s)\rangle$ because of the constraint $\xi = s^m$.

Proof. The normalization factor $\Omega^{(m)}$ can be chosen freely, but we must show that the choice (IV.C.18) is non-zero. To do so, we compute $\Omega^{(m)}$ using the infinite dimensional representation of the algebra defined in (IV.C.5) – (IV.C.7), see subsection b). Then to prove that $|\Psi^{(m)}(\mathbf{z}; s)\rangle$ is a q KZ solution, it is sufficient to show that (IV.C.2), (IV.C.3), (IV.C.4) are satisfied.

By a direct computation, using the algebraic relations (IV.C.5), it can be checked that the vector $b(z)$ and the matrix $L_{k+1,k}(z)$ satisfy the relations

$$\begin{aligned} \check{R}(z_{i+1}/z_i) b(z_i) \otimes b(z_{i+1}) &= b(z_{i+1}) \otimes b(z_i), \\ \check{R}(z_{i+1}/z_i) L(z_i) \otimes L(z_{i+1}) &= L(z_{i+1}) \otimes L(z_i) \check{R}(z_{i+1}/z_i). \end{aligned}$$

These elementary exchange relations can be used successively several times to give (IV.C.2). On the right boundary, using relations (IV.C.6), (IV.C.7) gives

$$\begin{aligned} \overline{K}(z_L) b(z_L) |v\rangle_1 &= b(1/z_L) |v\rangle_1, \\ \overline{K}(z_L) L_{k+1,k}(z_L) |v\rangle_{k+1} |\tilde{v}\rangle_k &= L_{k+1,k}(1/z_L) \overline{K}(z_L) |v\rangle_{k+1} |\tilde{v}\rangle_k. \end{aligned}$$

Using these properties several times, it is straightforward to prove (IV.C.4). Finally, on the left boundary, the vector $b(z)$ satisfies

$$\langle\langle w |_1 S_1 \check{K}(z_1^{-1}) \Big|_{\xi=s} b(z_1^{-1}) = \langle\langle w |_1 S_1 b(sz_1),$$

and the matrix $L_{k+1,k}(z)$ satisfies

$$\begin{aligned} \langle\langle w |_{k+1} \langle\langle \tilde{w} |_k (S_{k+1})^{2a+1} (S_k)^{2a} \check{K}(z_1^{-1}) \Big|_{\xi=s^{a+1}} L_{k+1,k}(z_1^{-1}) \\ = \langle\langle w |_{k+1} \langle\langle \tilde{w} |_k (S_{k+1})^{2a+1} (S_k)^{2a} L_{k+1,k}(sz_1) \check{K}(z_1^{-1}) \Big|_{\xi=s^a}. \end{aligned}$$

In words, the last equation means that the parameter ξ is multiplied by a factor s when the matrix L passes through the matrix \check{K} . Thus by imposing the constraint $\xi = s^m$ and applying these relations successively, relation (IV.C.3) follows. \blacksquare

d) Construction of the solutions to the left q KZ equation

We now present briefly the construction of row vector solutions of the *left* q KZ equations (IV.A.22) – (IV.A.24) in the matrix product form

$$\langle\langle \Phi(\mathbf{z}; s, \xi) | = \langle\langle W | \mathbb{S} \mathbb{A}(z_1) \otimes \dots \otimes \mathbb{A}(z_L) | V \rangle\rangle, \quad (\text{IV.C.19})$$

with

$$\mathbb{A}(z) = \left(A_0(z), A_1(z) \right). \quad (\text{IV.C.20})$$

Lemma C.4. *Sufficient conditions for a vector of form (IV.C.19) to satisfy the left qKZ equations (IV.A.22) – (IV.A.24) are the following:*

$$\mathbb{A}(z_i) \otimes \mathbb{A}(z_{i+1}) \check{R} \left(\frac{z_{i+1}}{z_i} \right) = \mathbb{A}(z_{i+1}) \otimes \mathbb{A}(z_i), \quad (\text{IV.C.21})$$

$$\langle\langle W | \mathbb{S} \mathbb{A}(z_1^{-1}) \tilde{K}(z_1^{-1}) \rangle\rangle = \langle\langle W | \mathbb{S} \mathbb{A}(sz_1) \rangle\rangle, \quad (\text{IV.C.22})$$

$$\mathbb{A}(z_L) |V\rangle\rangle \bar{K}(z_L) = \mathbb{A}(z_L^{-1}) |V\rangle\rangle. \quad (\text{IV.C.23})$$

We will construct a solution at $\xi = s^m$, with $m \geq 0$ an integer. We define the following objects:

$$\begin{aligned} b_{\text{left}}(z) &= (1, 1), \\ \mathbb{A}_{\text{left}}^{(m)}(z) &= b_{\text{left}}(z) \cdot L_{1,2}(1/z) \cdot \dots \cdot L_{2m-1,2m}(1/z), \\ \mathbb{S}_{\text{left}}^{(m)} &= S_1 \times (S_2)^2 \times \dots \times (S_{2m-1})^{2m-1} \times (S_{2m})^{2m}, \\ \langle\langle W_{\text{left}}^{(m)} | &= \langle\langle w |_1 \langle\langle \tilde{w} |_2 \langle\langle w |_3 \dots \langle\langle w |_{2m-1} \langle\langle \tilde{w} |_{2m}, \\ |V_{\text{left}}^{(m)} \rangle\rangle &= |v\rangle\rangle_1 | \tilde{v} \rangle\rangle_2 |v\rangle\rangle_3 \dots |v\rangle\rangle_{2m-1} | \tilde{v} \rangle\rangle_{2m}. \end{aligned} \quad (\text{IV.C.24})$$

The algebraic objects are as given in Definition C.2, and $L(z)$ is defined in (IV.C.14).

Proposition C.5. *For integer $m \geq 0$ and $\xi = s^m$,*

$$\langle\Phi^{(m)}(\mathbf{z}; s) | = \frac{1}{\Omega_{\text{left}}^{(m)}} \langle\langle W_{\text{left}}^{(m)} | \mathbb{S}_{\text{left}}^{(m)} \mathbb{A}_{\text{left}}^{(m)}(z_1) \otimes \dots \otimes \mathbb{A}_{\text{left}}^{(m)}(z_L) |V_{\text{left}}^{(m)} \rangle\rangle, \quad (\text{IV.C.25})$$

with normalization factor

$$\Omega_{\text{left}}^{(m)} = \langle\langle W_{\text{left}}^{(m)} | \mathbb{S}_{\text{left}}^{(m)} |V_{\text{left}}^{(m)} \rangle\rangle, \quad (\text{IV.C.26})$$

is a solution of the left qKZ equations (IV.A.22) – (IV.A.24).

Proof. We give the elementary exchange relations, which imply (IV.C.21) – (IV.C.23), and thus a solution of the left qKZ equations.

In the bulk,

$$\begin{aligned} b_{\text{left}}(z_i) \otimes b_{\text{left}}(z_{i+1}) \check{R}(z_{i+1}/z_i) &= b_{\text{left}}(z_{i+1}) \otimes b_{\text{left}}(z_i), \\ L(1/z_i) \otimes L(1/z_{i+1}) \check{R}(z_{i+1}/z_i) &= \check{R}(z_{i+1}/z_i) L(1/z_{i+1}) \otimes L(1/z_i), \end{aligned}$$

from which (IV.C.21) follows. On the right boundary

$$\begin{aligned} b_{\text{left}}(z_L) \bar{K}(z_L) &= b_{\text{left}}(1/z_L), \\ L_{k,k+1}(1/z_L) \bar{K}(z_L) |v\rangle\rangle_k | \tilde{v} \rangle\rangle_{k+1} &= \bar{K}(z_L) L_{k,k+1}(z_L) |v\rangle\rangle_k | \tilde{v} \rangle\rangle_{k+1}, \end{aligned}$$

from which (IV.C.23) follows. On the left boundary

$$b_{\text{left}}(1/z_1) \tilde{K}(z_1^{-1}) \Big|_{\xi=1} = b_{\text{left}}(sz_1),$$

and

$$\begin{aligned} \langle\langle w |_k \langle\langle \tilde{w} |_{k+1} (S_k)^{2a-1} (S_{k+1})^{2a} L_{k,k+1}(z_1) \tilde{K}(z_1^{-1}) \Big|_{\xi=s^a} \\ = \langle\langle w |_k \langle\langle \tilde{w} |_{k+1} (S_k)^{2a-1} (S_{k+1})^{2a} \tilde{K}(z_1^{-1}) \Big|_{\xi=s^{a-1}} L(1/(sz_1)). \end{aligned}$$

With the constraint $\xi = s^m$, these imply (IV.C.22). ■

2 Computation of Koornwinder polynomials

We still need to show that the construction gives a non-zero vector. Before doing so, we introduce some notation, then look at some examples.

Definition C.6. For a lattice configuration $\tau = (\tau_1, \dots, \tau_L)$, define the composition $\lambda^{(m)}(\tau)$, with

$$\lambda^{(m)}(\tau)_i = \begin{cases} -m, & \tau_i = 0, \\ m, & \tau_i = 1. \end{cases}$$

The corresponding partition is $\lambda^{(m)+}(\tau) = (m^L)$.

Example C.7. With $m = 1$, $\mathbb{A}^{(1)}(z) = b(z)$. For $L = 1$,

$$\begin{aligned} \Omega^{(1)}|\Psi^{(1)}(z_1; s) \rangle &= \langle\langle w|_1 S_1 b(z_1) |v \rangle\rangle_1 \\ &= \left(\begin{array}{c} \langle\langle w|_1 S_1 \left(\frac{1}{z_1} + a_1 \right) |v \rangle\rangle_1 \\ \langle\langle w|_1 S_1 \left(z_1 + a_1^\dagger \right) |v \rangle\rangle_1 \end{array} \right), \end{aligned}$$

which is a real valued vector of size 2. For $L = 2$,

$$\begin{aligned} \Omega^{(1)}|\Psi^{(1)}(z_1, z_2; s) \rangle &= \langle\langle w|_1 S_1 b(z_1) \otimes b(z_2) |v \rangle\rangle_1 \\ &= \left(\begin{array}{c} \langle\langle w|_1 S_1 \left(\frac{1}{z_1} + a_1 \right) \left(\frac{1}{z_2} + a_1 \right) |v \rangle\rangle_1 \\ \langle\langle w|_1 S_1 \left(\frac{1}{z_1} + a_1 \right) \left(z_2 + a_1^\dagger \right) |v \rangle\rangle_1 \\ \langle\langle w|_1 S_1 \left(z_1 + a_1^\dagger \right) \left(\frac{1}{z_2} + a_1 \right) |v \rangle\rangle_1 \\ \langle\langle w|_1 S_1 \left(z_1 + a_1^\dagger \right) \left(z_2 + a_1^\dagger \right) |v \rangle\rangle_1 \end{array} \right), \end{aligned}$$

which is a real valued vector of size 4. In general,

$$\Omega^{(1)}|\Psi^{(1)}(\mathbf{z}; s) \rangle = \langle\langle w|_1 S_1 b(z_1) \otimes \dots \otimes b(z_L) |v \rangle\rangle_1.$$

Note that the normalization $\Omega^{(1)} = \langle\langle w|_1 S_1 |v \rangle\rangle_1$ ensures that each component $\psi_\tau^{(1)}$ has leading term $\mathbf{z}^{\lambda^{(1)}(\tau)}$ with coefficient 1, and all other terms correspond to compositions μ with

$$\mu^+ < \lambda^{(1)+}(\tau) = (1^L).$$

Example C.8. With $m = 2$,

$$\mathbb{A}^{(2)}(z) = L_{3,2}(z) \cdot b(z).$$

Then for $L = 1$,

$$\begin{aligned} \Omega^{(2)}|\Psi^{(2)}(z_1; s) \rangle &= \langle\langle w|_3 \langle\langle \tilde{w}|_2 \langle\langle w|_1 (S_3)^3 (S_2)^2 S_1 \left(L_{3,2}(z_1) \cdot b(z_1) \right) |v \rangle\rangle_3 | \tilde{v} \rangle\rangle_2 |v \rangle\rangle_1 \\ &= \langle\langle w|_3 \langle\langle \tilde{w}|_2 (S_3)^3 (S_2)^2 L_{3,2}(z_1) |v \rangle\rangle_3 | \tilde{v} \rangle\rangle_2 \cdot \langle\langle w|_1 S_1 b(z_1) |v \rangle\rangle_1 \\ &= \langle\langle w|_3 \langle\langle \tilde{w}|_2 (S_3)^3 (S_2)^2 L_{3,2}(z_1) |v \rangle\rangle_3 | \tilde{v} \rangle\rangle_2 \cdot \Omega^{(1)}|\Psi^{(1)}(z_1; s) \rangle, \end{aligned}$$

with

$$\begin{aligned} &\langle\langle w|_3 \langle\langle \tilde{w}|_2 (S_3)^3 (S_2)^2 L_{3,2}(z_1) |v \rangle\rangle_3 | \tilde{v} \rangle\rangle_2 \\ &= \langle\langle w|_3 \langle\langle \tilde{w}|_2 (S_3)^3 (S_2)^2 \begin{pmatrix} z_1^{-1} + a_3 a_2^\dagger & z_1^{-1} a_2 + a_3 \\ a_3^\dagger + z_1 a_2^\dagger & a_3^\dagger a_2 + z_1 \end{pmatrix} |v \rangle\rangle_3 | \tilde{v} \rangle\rangle_2. \end{aligned}$$

For $L = 2$,

$$\begin{aligned} \Omega^{(2)}|\Psi^{(2)}(z_1, z_2; s)\rangle &= \langle\langle w|_3 \langle\langle \tilde{w}|_2 \langle\langle w|_1 (S_3)^3 (S_2)^2 S_1 \left(L_{3,2}(z_1) \cdot b(z_1) \right) \\ &\quad \otimes \left(L_{3,2}(z_2) \cdot b(z_2) \right) |v\rangle\rangle_3 |\tilde{v}\rangle\rangle_2 |v\rangle\rangle_1. \end{aligned}$$

The matrix $L_{3,2}(z_2)$ can be brought past $b(z_1)$ as they are in different physical spaces, and their entries are in different auxiliary algebraic spaces. Thus we obtain

$$\Omega^{(2)}|\Psi^{(2)}(z_1, z_2; s)\rangle = \langle\langle w|_3 \langle\langle \tilde{w}|_2 (S_3)^3 (S_2)^2 L_{3,2}(z_1) \otimes L_{3,2}(z_2) |v\rangle\rangle_3 |\tilde{v}\rangle\rangle_2 \cdot \left(\Omega^{(1)}|\Psi^{(1)}(z_1, z_2; s)\rangle \right),$$

where

$$\begin{aligned} &\langle\langle w|_3 \langle\langle \tilde{w}|_2 (S_3)^3 (S_2)^2 L_{3,2}(z_1) \otimes L_{3,2}(z_2) |v\rangle\rangle_3 |\tilde{v}\rangle\rangle_2 \\ &= \langle\langle w|_3 \langle\langle \tilde{w}|_2 (S_3)^3 (S_2)^2 \begin{pmatrix} z_1^{-1} + a_3 a_2^\dagger & z_1^{-1} a_2 + a_3 \\ a_3^\dagger + z_1 a_2 & a_3 a_2 + z_1 \end{pmatrix} \otimes \begin{pmatrix} z_2^{-1} + a_3 a_2^\dagger & z_2^{-1} a_2 + a_3 \\ a_3^\dagger + z_2 a_2 & a_3 a_2 + z_2 \end{pmatrix} |v\rangle\rangle_3 |\tilde{v}\rangle\rangle_2, \end{aligned}$$

is a real valued 4×4 matrix The normalization factor is

$$\Omega^{(2)} = \langle\langle w|_3 \langle\langle \tilde{w}|_2 \langle\langle w|_1 (S_3)^3 (S_2)^2 S_1 |v\rangle\rangle_3 |\tilde{v}\rangle\rangle_2 |v\rangle\rangle_1,$$

and it can be checked directly for $L = 1, 2$ that each component $\psi_\tau^{(2)}$ has leading term $\mathbf{z}^{\lambda^{(2)}(\tau)}$ with coefficient 1, and all other terms correspond to compositions μ with

$$\mu^+ < \lambda^{(2)+}(\tau) = (2^L).$$

We now give the general form.

Theorem C.9. *The qKZ equations have a solution when $\xi = s^m$, written recursively on m : For $m > 1$*

$$\begin{aligned} |\Psi^{(m)}(\mathbf{z}; s)\rangle &= \frac{1}{\langle\langle w|S^{2m-1}|v\rangle\rangle \langle\langle \tilde{w}|S^{2m-2}|\tilde{v}\rangle\rangle} \langle\langle w|_{2m-1} \langle\langle \tilde{w}|_{2m-2} (S_{2m-1})^{2m-1} (S_{2m-2})^{2m-2} \quad \text{(IV.C.27)} \\ &\quad L_{2m-1,2m-2}(z_1) \otimes \dots \otimes L_{2m-1,2m-2}(z_L) |v\rangle\rangle_{2m-1} |\tilde{v}\rangle\rangle_{2m-2} \cdot |\Psi^{(m-1)}(\mathbf{z}; s)\rangle, \end{aligned}$$

with

$$|\Psi^{(1)}(\mathbf{z}; s)\rangle = \frac{1}{\langle\langle w|S|v\rangle\rangle} \langle\langle w|_1 S_1 b(z_1) \otimes \dots \otimes b(z_L) |v\rangle\rangle_1. \quad \text{(IV.C.28)}$$

The components of the solution, $\psi_\tau^{(m)}(\mathbf{x}; s)$, have leading term $\mathbf{z}^{\lambda^{(m)}(\tau)}$, and all other terms correspond to compositions μ with

$$\mu^+ < \lambda^{(m)+}(\tau) = (m^L).$$

Proof. The recursive form (IV.C.27), (IV.C.28) is obtained by a reordering of the matrix product form (IV.C.17), as in Example C.8.

The second part of the claim, on the degree and normalization of components of the solution, can be proven inductively. We assume the property holds at $m-1$ and use (IV.C.27) to obtain the solution at m . That is, we multiply by the ‘increment’ matrix

$$\begin{aligned} &\frac{1}{\langle\langle w|S^{2m-1}|v\rangle\rangle \langle\langle \tilde{w}|S^{2m-2}|\tilde{v}\rangle\rangle} \langle\langle w|_{2m-1} \langle\langle \tilde{w}|_{2m-2} (S_{2m-1})^{2m-1} (S_{2m-2})^{2m-2} \\ &\quad L_{2m-1,2m-2}(z_1) \otimes \dots \otimes L_{2m-1,2m-2}(z_L) |v\rangle\rangle_{2m-1} |\tilde{v}\rangle\rangle_{2m-2}, \end{aligned}$$

which is a real valued $2^L \times 2^L$ matrix. The following points can be deduced by writing (IV.C.27) and the increment matrix in component form:

- A term \mathbf{z}^μ with $\mu^+ = (m^L)$ can only be produced from the leading order terms of the $m - 1$ solution, which correspond to the partition $((m - 1)^L)$, and thus we can ignore sub-leading terms.
- The diagonal entries of the increment matrix produce the term $\mathbf{z}^{\lambda^{(m)}(\boldsymbol{\tau})}$ with coefficient 1 (plus lower order terms) in $\psi_{\boldsymbol{\tau}}^{(m)}$, from the corresponding component of the $m - 1$ solution.
- The off-diagonal entries of the increment matrix, acting on the leading order term of a component of the $m - 1$ solution, either reduces the degree or leaves it unchanged.

These points are sufficient to show that the degree and normalization properties hold at m , assuming they hold at $m - 1$. As the $m = 1$ case was checked in Example C.7, the properties hold for all m . \blacksquare

Similar results hold for the solution of the left qKZ equations at $s = \xi^m$ as stated in the following theorem.

Theorem C.10. *For integer $m \geq 0$ and $\xi = s^m$, solutions of the left qKZ equations can be constructed in matrix product form, and can be defined recursively. For $m > 0$*

$$\langle \Phi^{(m)}(\mathbf{z}; s) | = \frac{1}{\langle\langle w | S^{2m-1} | v \rangle\rangle \langle\langle \tilde{w} | S^{2m} | \tilde{v} \rangle\rangle} \langle \Phi^{(m-1)}(\mathbf{z}; s) | \cdot \langle\langle w |_{2m-1} \langle\langle \tilde{w} |_{2m} (S_{2m-1})^{2m-1} (S_{2m})^{2m} L_{2m-1,2m} \left(\frac{1}{z_1} \right) \otimes \dots \otimes L_{2m-1,2m} \left(\frac{1}{z_L} \right) | v \rangle\rangle_{2m-1} | \tilde{v} \rangle\rangle_{2m} \quad (\text{IV.C.29})$$

with

$$\langle \Phi^{(0)}(\mathbf{z}; s) | = \langle 1 | = (1, 1)^{\otimes L} \quad (\text{IV.C.30})$$

The solution is non-zero: the component of the solution, $\phi_{\boldsymbol{\tau}}^{(m)}(\mathbf{z}; s)$, contains the term $\mathbf{z}^{-\lambda^{(m)}(\boldsymbol{\tau})}$ with coefficient 1, and all terms correspond to compositions μ with

$$\mu^+ \leq \lambda^{(m)+}(\boldsymbol{\tau}) = (m^L).$$

Proof. The proof of this theorem is very similar to that for Theorem C.9. We will, however, comment briefly on the terms appearing in each component $\phi_{\boldsymbol{\tau}}^{(m)}(\mathbf{x})$, and the normalization. To do so, we look at the normalized ‘increment matrix’ taking the $m - 1$ solution to the m solution:

$$\frac{1}{\langle\langle w | S^{2m-1} | v \rangle\rangle \langle\langle \tilde{w} | S^{2m} | \tilde{v} \rangle\rangle} \langle\langle w |_{2m-1} \langle\langle \tilde{w} |_{2m} (S_{2m-1})^{2m-1} (S_{2m})^{2m} L_{2m-1,2m} \left(\frac{1}{z_1} \right) \otimes \dots \otimes L_{2m-1,2m} \left(\frac{1}{z_L} \right) | v \rangle\rangle_{2m-1} | \tilde{v} \rangle\rangle_{2m}$$

The diagonal entries of this matrix contain the term $\mathbf{z}^{-\lambda^{(1)}(\boldsymbol{\tau})}$ with coefficient 1, which produce the term $\mathbf{z}^{-\lambda^{(m)}(\boldsymbol{\tau})}$ in $\phi_{\boldsymbol{\tau}}^{(m)}$. In the top row of the increment matrix, the entry in column $\boldsymbol{\tau}'$ has leading term

$$\frac{\langle\langle \tilde{w} | S^{2m} a^{\sum_i \tau'_i} | \tilde{v} \rangle\rangle}{\langle\langle \tilde{w} | S^{2m} | \tilde{v} \rangle\rangle} z_1 \dots z_N, \quad (\text{IV.C.31})$$

and as a consequence, each component $\phi_{\boldsymbol{\tau}}^{(m)}$ contains the term $\mathbf{z}^{(m^N)}$ with the same coefficient as in (IV.C.31). \blacksquare

Corollary C.11. *For $m > 0$ and $\xi = t_0^{-1} t_L^{-1} t^{-(L-1)} s^{-m}$, the right qKZ equations (IV.A.19) – (IV.A.21) have solution*

$$|\Psi(\mathbf{z}; s, \xi = t_0^{-1} t_L^{-1} t^{-(L-1)} s^{-m})\rangle = U_{GC} |\Phi^{(m)}(\mathbf{z}; s)\rangle. \quad (\text{IV.C.32})$$

Proof. This follows from Lemma A.2. ■

The $m = 0$ case is a bit special: $|\Psi(\mathbf{z}; s, \xi = t_0^{-1}t_L^{-1}t^{-(L-1)})\rangle = U_{\text{GC}}|1\rangle$. The solution does not depend on \mathbf{z} and s . Imposing in addition that $\xi = 1$, i.e. $t_0t_Lt^{L-1} = 1$, gives a very simple ASEP stationary state. Indeed the system is at thermal equilibrium in this case: written in the usual ASEP parameters the constraint is $\frac{\alpha\beta}{\gamma\delta} \left(\frac{p}{q}\right)^{L-1} = 1$.

a) Normalization and symmetric Koornwinder polynomials

We can now make the connection between solutions of the $q\text{KZ}$ equations, and the symmetric and non-symmetric Koornwinder polynomials.

Lemma C.12. *The component $\psi_{\circ\dots\circ}^{(m)}$ of the vector $|\Psi^{(m)}(\mathbf{z}, s)\rangle$ is the non-symmetric Koornwinder polynomial $E_{((-m)L)}$. All other components can be constructed through the relations*

$$\begin{aligned}\psi_{\circ\dots\circ\bullet}^{(m)} &= t_L^{-1/2}T_L^{-1}\psi_{\circ\dots\circ\circ}^{(m)}, \\ \psi_{\dots\bullet\circ\dots}^{(m)} &= t^{-1/2}T_i^{-1}\psi_{\dots\circ\bullet\dots}^{(m)}, \quad 1 \leq i \leq L-1.\end{aligned}\tag{IV.C.33}$$

The set of all components $\{\psi_{\tau}^{(m)}\}$ forms a basis for $\mathcal{R}^{(mL)}$, the space spanned by non-symmetric Koornwinder polynomials $\{E_{\mu} | \mu \in \mathbb{Z}^L, \mu^+ = (m^L)\}$.

Proof. By Theorem C.9, and Lemma B.7 with $\xi = s^m$, $\psi_{\circ\dots\circ}^{(m)}$ is an eigenfunction of the Y_i operators, and is a Laurent polynomial with the required degree and normalisation. Thus by uniqueness, we can identify $\psi_{\circ\dots\circ}^{(m)} = E_{((-m)L)}$. The relations (IV.C.33) come from the exchange relations (IV.B.15) and (IV.B.12).

The preceding parts of this lemma give the preconditions for Proposition 1 and Corollary 1 of [224], from which it follows that $\{\psi_{\tau}^{(m)}\}$ forms a basis for $\mathcal{R}^{(mL)}$. ■

Lemma C.13. *The component $\phi_{\circ\dots\circ}^{(m)}$ of the vector $\langle\Phi^{(m)}(\mathbf{z}, s)|$ is the non-symmetric Koornwinder polynomial $E_{(mL)}$. All other components can be constructed through the relations*

$$\begin{aligned}\phi_{\circ\dots\circ\bullet}^{(m)} &= t_L^{1/2}T_L^{-1}\phi_{\circ\dots\circ\circ}^{(m)}, \\ \phi_{\dots\bullet\circ\dots}^{(m)} &= t^{1/2}T_i^{-1}\phi_{\dots\circ\bullet\dots}^{(m)}, \quad 1 \leq i \leq L-1.\end{aligned}$$

The set of all components $\{\phi_{\tau}^{(m)}\}$ forms a basis for $\mathcal{R}^{(mL)}$.

Proof. This follows in the same way, with reference to Theorem C.10, and Lemmas B.8 and B.6. ■

Lemma C.14. *Given a solution $|\Psi(\mathbf{z}; s, \xi)\rangle$ of the $q\text{KZ}$ equations (IV.A.19) – (IV.A.21), the sum of components*

$$\mathcal{Z}(\mathbf{z}; s, \xi) = \langle 1 | \Psi(\mathbf{z}; s, \xi) \rangle \tag{IV.C.34}$$

is W_0 invariant.

Proof. We first note that $\langle 1 |$ is a left eigenvector of \check{R}_i, \bar{K}_L with eigenvalue 1 (see (IV.A.7), (IV.A.9)). Then applying $\langle 1 |$ to the bulk and right boundary $q\text{KZ}$ equations (IV.A.19), (IV.A.21) we see that $\mathcal{Z}(\mathbf{z}; s, \xi)$ is invariant under s_i , $1 \leq i \leq L$, and hence is W_0 invariant. ■

Theorem C.15. *The sum of components of $|\Psi^{(m)}(\mathbf{z}; s)\rangle$ is the symmetric Koornwinder polynomial $P_{(mL)}$. That is*

$$P_{(mL)}(\mathbf{z}) = \mathcal{Z}^{(m)}(\mathbf{z}; s), \tag{IV.C.35}$$

where

$$\mathcal{Z}^{(m)}(\mathbf{z}; s) = \langle 1 | \Psi^{(m)}(\mathbf{z}; s) \rangle, \tag{IV.C.36}$$

and $|\Psi^{(m)}(\mathbf{z}; s)\rangle$ is the $q\text{KZ}$ solution with $\xi = s^m$, constructed as in Theorem C.9.

Proof. By Lemmas C.12 and C.14, $\mathcal{Z}^{(m)}(\mathbf{z}; s)$ is W_0 invariant, and belongs to the space $\mathcal{R}^{(m^L)}$, and from Theorem C.9, we see that it contains $\mathbf{z}^{(m^L)}$ with coefficient 1. The result then follows from the characterisation of symmetric Koornwinder polynomials in [222], quoted in Theorem B.4. ■

We note that Theorem C.15 implies a matrix product construction for the symmetric Koornwinder polynomial $P_{(m^L)}$. Direct computations from this form would be difficult, but the structure leads to certain conjectures that we discuss in Section D. We also note that an integral form for the polynomial $P_{(m^L)}$ is already known [242]. The solution of the left q KZ equation is also related to the same symmetric Koornwinder polynomial.

Theorem C.16. *The sum of components of $U_{GC}|\Phi^{(m)}(\mathbf{z}; s)\rangle$ is proportional to the symmetric Koornwinder polynomial $P_{(m^L)}$. That is*

$$P_{(m^L)}(\mathbf{z}) \propto \mathcal{Z}^{(m)}(\mathbf{z}; s, \xi'), \quad (\text{IV.C.37})$$

where

$$\mathcal{Z}^{(m)}(\mathbf{z}; s, \xi') = \langle 1 | U_{GC} | \Phi^{(m)}(\mathbf{z}; s) \rangle, \quad (\text{IV.C.38})$$

with $\xi' = t_0^{-1} t_L^{-1} t^{-(L-1)} s^{-m}$.

Proof. Note that $U_{GC}|\Phi^{(m)}(\mathbf{z}; s)\rangle$ is the solution of the right q KZ equations at ξ' , and the proof follows as in Theorem C.15. However, because of the structure of the components $\phi_{\mathbf{r}}^{(m)}$ (see Theorem C.10 and (IV.C.25)), and the multiplication by matrix U_{GC} , the coefficient of $\mathbf{z}^{(m^L)}$ in $\mathcal{Z}^{(m)}(\mathbf{z}; s, \xi')$ is not 1. Thus the identification with $P_{(m^L)}$ can only be made up to normalization. ■

D Current fluctuations conjecture

1 Quasi-classical limit

The aim of this section is to make contact between the machinery developed previously, and the generating function of the cumulants of the current. The idea is quite simple and arises from the following observation: the constraint $\xi = s^m$ that was imposed in order to solve the q KZ equations, can be satisfied by setting $s = \xi^{1/m}$, leaving ξ free instead of s , which then implies $s \rightarrow 1$ as $m \rightarrow \infty$. It appears then natural to think that the scattering relation (IV.A.16) may degenerate, in this $s \rightarrow 1$ limit, to an eigenvector equation. Then as $m \rightarrow \infty$, the vector $|\Psi^{(m)}(\mathbf{z}; s = \xi^{1/m})\rangle$ should thus converge in some sense to an eigenvector of the scattering matrix. To move towards this direction, we make the following conjectures.

Conjecture D.1. *It is conjectured that*

$$\lim_{m \rightarrow \infty} \frac{|\Psi^{(m)}(\mathbf{z}; s = \xi^{1/m})\rangle}{\mathcal{Z}^{(m)}(\mathbf{z}; s = \xi^{1/m})} = |\Psi_0(\mathbf{z}; \xi)\rangle, \quad (\text{IV.D.1})$$

$$\lim_{m \rightarrow \infty} \frac{\ln(\xi)}{m} \ln \left(\mathcal{Z}^{(m)}(\mathbf{z}; s = \xi^{1/m}) \right) = F_0(\mathbf{z}; \xi), \quad (\text{IV.D.2})$$

with $|\Psi_0\rangle$ and F_0 regular functions of \mathbf{z} .

These conjectures are supported by strong numerical evidences (up to 3 sites) and by the fact that the matrix product construction of $|\Psi^{(m)}(\mathbf{z}; s)\rangle$ is similar to the one presented in [18, 230]. In those works, the authors developed a method called the ‘‘perturbative matrix ansatz’’, which allowed them to approximate the ground state of $M(\xi)$, at any order in the current counting parameter ξ . Let us also mention that these kind of results have already been observed in the context of q KZ equations of different models, and are known as the ‘‘quasi-classical’’ limit [243, 244].

Note that the second part of the conjecture can be immediately rewritten in terms of symmetric Koornwinder polynomials as

$$\lim_{m \rightarrow \infty} \frac{\ln(\xi)}{m} \ln \left(P_{(mL)}(\mathbf{z}; s = \xi^{1/m}) \right) = F_0(\mathbf{z}; \xi). \quad (\text{IV.D.3})$$

In the following these conjectures will be considered as facts and properties will be deduced from them. But one has to keep in mind that the validity of the deduced results relies obviously on the validity of these conjectures.

2 Generating function of the cumulants of the current

Proposition D.2. *The function $F_0(\mathbf{z}; \xi)$ is W_0 invariant and its derivative, with respect to any of the x_i , is invariant under the Gallavotti-Cohen symmetry $\xi \rightarrow \xi' = t_0^{-1} t_L^{-1} t^{-(L-1)} \xi^{-1}$.*

Proof. The W_0 invariance directly follows from the W_0 invariance of the symmetric Koornwinder polynomials. The Gallavotti-Cohen symmetry follows from theorems C.15 and C.16 which give that

$$\begin{aligned} P_{(mL)}(\mathbf{z}; s = \zeta^{1/m}) &= \mathcal{Z}^{(m)}(\mathbf{z}; s = \zeta^{1/m}, \xi = \zeta) \\ &\propto \mathcal{Z}^{(m)}(\mathbf{z}; s = \zeta^{1/m}, \xi = t_0^{-1} t_L^{-1} t^{-(L-1)} \zeta^{-1}) \end{aligned}$$

with a proportionality coefficient independent of \mathbf{z} . Taking the large m limit it translates into the fact that $F_0(\mathbf{z}; \xi') = F_0(\mathbf{z}; \xi) + c$ with c a constant term independent of \mathbf{z} , which concludes the proof. \blacksquare

In the following we will specify when needed the dependence on s and ξ of the scattering matrix $\mathcal{S}_i(\mathbf{z}; s, \xi)$ defined in (IV.A.13).

Proposition D.3. *The vector $|\Psi_0(\mathbf{z}; \xi)\rangle$ is an eigenvector of the scattering matrices evaluated at $s = 1$, with*

$$\mathcal{S}_i(\mathbf{z}; 1, \xi) |\Psi_0(\mathbf{z}; \xi)\rangle = \exp \left(z_i \frac{\partial F_0}{\partial z_i}(\mathbf{z}; \xi) \right) |\Psi_0(\mathbf{z}; \xi)\rangle. \quad (\text{IV.D.4})$$

Proof. Our starting point is the scattering relation (IV.A.16) applied with $s = \xi^{1/m}$. We divide by $\mathcal{Z}^{(m)}(\mathbf{z}; s = \xi^{1/m})$ to obtain

$$\begin{aligned} \mathcal{S}_i(\mathbf{z}; s = \xi^{1/m}, \xi) &\frac{|\Psi^{(m)}(\dots, z_i, \dots; s = \xi^{1/m})\rangle}{\mathcal{Z}^{(m)}(\dots, z_i, \dots; s = \xi^{1/m})} \\ &= \frac{\mathcal{Z}^{(m)}(\dots, \xi^{1/m} z_i, \dots; s = \xi^{1/m})}{\mathcal{Z}^{(m)}(\dots, z_i, \dots; s = \xi^{1/m})} \frac{|\Psi^{(m)}(\dots, \xi^{1/m} z_i, \dots; s = \xi^{1/m})\rangle}{\mathcal{Z}^{(m)}(\dots, \xi^{1/m} z_i, \dots; s = \xi^{1/m})}. \end{aligned}$$

We then have the limits

$$\begin{aligned} \lim_{m \rightarrow \infty} \mathcal{S}_i(\mathbf{z}; s = \xi^{1/m}, \xi) &= \mathcal{S}_i(\mathbf{z}; 1, \xi), \\ \lim_{m \rightarrow \infty} \frac{|\Psi^{(m)}(\dots, z_i, \dots; s = \xi^{1/m})\rangle}{\mathcal{Z}^{(m)}(\dots, z_i, \dots; s = \xi^{1/m})} &= |\Psi_0(\dots, z_i, \dots; \xi)\rangle, \\ \lim_{m \rightarrow \infty} \frac{|\Psi^{(m)}(\dots, \xi^{1/m} z_i, \dots; s = \xi^{1/m})\rangle}{\mathcal{Z}^{(m)}(\dots, \xi^{1/m} z_i, \dots; s = \xi^{1/m})} &= |\Psi_0(\dots, z_i, \dots; \xi)\rangle, \\ \lim_{m \rightarrow \infty} \frac{\mathcal{Z}^{(m)}(\dots, \xi^{1/m} z_i, \dots; s = \xi^{1/m})}{\mathcal{Z}^{(m)}(\dots, z_i, \dots; s = \xi^{1/m})} &= \exp \left(z_i \frac{\partial F_0}{\partial z_i}(\mathbf{z}; \xi) \right), \end{aligned}$$

which yield the desired result. \blacksquare

Proposition D.4. *The vector $|\Psi_0(\mathbf{1}; \xi)\rangle$ is an eigenvector of the deformed Markov matrix, with*

$$M(\xi)|\Psi_0(\mathbf{1}; \xi)\rangle = \frac{p-q}{2} \frac{\partial^2 F_0}{\partial z_i^2}(\mathbf{1}; \xi)|\Psi_0(\mathbf{1}; \xi)\rangle. \quad (\text{IV.D.5})$$

This implies immediately the following expression for the generating function of the cumulants of the current:

$$E(\mu) = \Lambda_0(e^\mu) = \frac{p-q}{2} \frac{\partial^2 F_0}{\partial z_i^2}(\mathbf{1}; e^\mu). \quad (\text{IV.D.6})$$

Proof. This is proven by taking the derivative of (IV.D.4) with respect to z_i and then setting $z_1 = \dots = z_L = 1$. One has to make basic use of the properties given in (IV.A.15), and notice the fact that $\frac{\partial F_0}{\partial z_i}(\mathbf{1}; \xi) = 0$ because F_0 is W_0 invariant. ■

Note that despite revealing a beautiful connection between the symmetric functions and the fluctuations of the current, in practice, the last expression does not help to compute the cumulants of the current because a closed expression for F_0 is missing.

However a step can be made toward an exact expression of F_0 , using the characterization of the symmetric Koornwinder polynomials as eigenfunctions of the finite difference operator D defined in (IV.B.6). The eigenvalue $d_{(mL)}$ of this operator associated to the symmetric Koornwinder polynomial $P_{(mL)}$ is given for $s = \xi^{1/m}$ by

$$d_0(\xi) = \frac{1-t^L}{1-t}(\xi-1)(t_0 t_L t^{L-1} - 1/\xi). \quad (\text{IV.D.7})$$

It is straightforward to check that $d_0(\xi)$ is invariant under the Gallavotti-Cohen symmetry, that is $d_0(\xi) = d_0(\xi')$.

In the following we will explicitly write the dependence on s of the functions $g_i(\mathbf{z}; s)$ defined in (IV.B.7).

Proposition D.5. *We have the following characterization of the function F_0 :*

$$\begin{aligned} & \sum_{i=1}^L g_i(\mathbf{z}; 1) \left[\exp\left(z_i \frac{\partial F_0}{\partial z_i}(\mathbf{z}; \xi)\right) - 1 \right] + \sum_{i=1}^L g_i(\mathbf{z}^{-1}; 1) \left[\exp\left(-z_i \frac{\partial F_0}{\partial z_i}(\mathbf{z}; \xi)\right) - 1 \right] \\ & = d_0(\xi) \end{aligned}$$

Proof. This follows directly from the relation (IV.B.9) applied for the symmetric Koornwinder polynomial $P_{(mL)}$ and $s = \xi^{1/m}$. Dividing the latter relation by $P_{(mL)}(\mathbf{z}; s = \xi^{1/m})$ and taking the large m limit yield the desired result. ■

It would be interesting to understand if this characterization of the function F_0 can be related to a Baxter $t-Q$ relation [29]. It has been shown in [V9] that the normalisation of the stationary state (corresponding to the case $s = \xi = 1$) satisfies a $t-Q$ difference equation. We can mention also in this context the work [120] where the authors constructed a Baxter Q operator for the open ASEP (with current-counting deformation) and derived the corresponding $t-Q$ relations.

Chapter V

Hydrodynamic limit

In the previous chapters we focused essentially on the study of systems defined on a finite size lattice. We computed exactly physical observables in these models. A lot of efforts were put on the comprehension of the mathematical structures related to the stochastic processes, in particular the algebraic and combinatorial aspects of the Markov matrices and of the stationary states. The emphasis was mainly put on the mathematical methods involved in the exact computations rather than on the physical interpretation of the results.

This chapter focuses mainly on the physical description of the models and tries to follow the usual purpose of statistical physics. The goal is to try to bridge the gap between the microscopic scale and the macroscopic scale. At the microscopic scale, we know precisely the interactions between each elementary components of the system (typically the Coulomb interactions between atoms forming a plasma). At the macroscopic scale, we would like to identify, for a system composed of a huge number of components, a few number of relevant physical macroscopic observables (typically the temperature or the pressure). We would like to infer physical laws or principles satisfied by these observables, in order to describe efficiently the behavior of the system at this scale (typically an equation of state such as the law of ideal gas).

In our precise case the system is composed by a big number of particles evolving on a lattice and the microscopic dynamics is defined by the Markov matrix associated to the model. From this stochastic dynamics defined at the particle scale, we would like to infer the macroscopic behavior of the system. In other words, we would like to construct a simple formalism to answer easily questions like: what is the mean particles flow (and also its fluctuations) through the system? or is it likely to observe a high concentration of particles at some place? We can easily see the potential wide range of applications (in population dynamics, traffic flow, biology...) of such theory. The essential feature of such description lies in the fact the system comprises a huge number of individual components, so that the details of the microscopic dynamics can be averaged out at the macroscopic scale to give rise to a universal macroscopic description of the system.

The first step, that we need to focus on, is thus to take what is commonly called the thermodynamic limit, or the hydrodynamic limit. It consists in letting the size L of the lattice go to infinity. We will in particular determine the behavior of the physical observables, computed exactly for a finite size lattice in chapter III, in this limit. We will see that they give precious hints concerning the macroscopic behavior of the system, such as transitions between different regimes, called phase transitions (for instance a transition from fluid traffic flow to jammed traffic flow) or such as the relaxation time toward the stationary state.

We will see in a second time that, while taking this large size $L \rightarrow \infty$ limit, we can define macroscopic variables (that can be heuristically interpreted as local particle density or local particle current) whose stochastic evolution follows simple laws as $L \rightarrow \infty$. We will typically observe large deviation principles for these macroscopic variables that are expected to be an efficient generalization of thermodynamic potentials to non-equilibrium systems. This could be though as a prelude toward a general theory to describe out-of-equilibrium systems.

A Hydrodynamic limit and density profile

1 Hydrodynamic limit

a) Continuous limit of the lattice

We want to let the lattice size L go to infinity, *i.e.* to have an infinite number of sites in the system. We precise here the mathematical meaning of this limit. The lattice is seen as embedded in the segment $[0, 1]$ of the real line. The site i is located at coordinate

$$x = \frac{i}{L}. \quad (\text{V.A.1})$$

When the number of sites L increases and tends to infinity, the distance between two adjacent sites, which is equal to $1/L$, decreases and converges toward 0. For a given $x \in [0, 1]$, it is straightforward to check that the coordinate of the site $\lfloor Lx \rfloor$ (where $\lfloor \cdot \rfloor$ denotes the floor function), which is equal to $\lfloor Lx \rfloor / L$, converges toward x when L goes to infinity. In this thermodynamic limit we can thus define physical quantities depending on a continuous variable $x \in [0, 1]$.

For instance we can define a function

$$\bar{\rho}_\tau(x) = \lim_{L \rightarrow \infty} \langle \rho_\tau^{\lfloor Lx \rfloor} \rangle, \quad (\text{V.A.2})$$

which stands for the mean particle density of species τ at position $x \in [0, 1]$ in the thermodynamic limit.

We define also the limit of the two-point function

$$\bar{\rho}_{\tau, \tau'}(x, y) = \lim_{L \rightarrow \infty} \langle \rho_\tau^{\lfloor Lx \rfloor} \rho_{\tau'}^{\lfloor Ly \rfloor} \rangle, \quad (\text{V.A.3})$$

and more generally the multi-point correlation function

$$\bar{\rho}_{\tau(1), \dots, \tau(k)}(x_1, \dots, x_k) = \lim_{L \rightarrow \infty} \langle \rho_{\tau(1)}^{\lfloor Lx_1 \rfloor} \dots \rho_{\tau(k)}^{\lfloor Lx_k \rfloor} \rangle. \quad (\text{V.A.4})$$

The limits of the connected correlation functions are more subtle because we might need to rescale the function with a L -dependent factor to obtain a non-vanishing (and non-diverging) real value when performing the large L limit. For instance for the connected two-point function we may have

$$\bar{\rho}_{\tau, \tau'}^c(x, y) = \lim_{L \rightarrow \infty} f(L) \langle \rho_\tau^{\lfloor Lx \rfloor} \rho_{\tau'}^{\lfloor Ly \rfloor} \rangle_c, \quad (\text{V.A.5})$$

where the function f depends on the model under consideration (see examples below).

Similar issues appear when defining the thermodynamic limit of the particle current on the lattice, where the rescaling of the current may also depend on the model under consideration. We will encounter two different classes of model in the examples below: models in which the lattice current does not need to be rescaled and that are called ballistic, and models in which the lattice current has to be multiplied by a factor L and that are called diffusive.

Note that in the case of a single species model, *i.e.* for $N = 1$, we will lighten the notation by writing $\bar{\rho}(x)$, $\bar{\rho}(x, y)$, $\bar{\rho}^c(x, y), \dots$ instead of $\bar{\rho}_1(x)$, $\bar{\rho}_{1,1}(x, y)$, $\bar{\rho}_{1,1}^c(x, y), \dots$

In what follows, we provide a detailed study of the thermodynamic limit of the models that we encountered in chapter III: the DiSSEP, the 2-TASEP and the multi-species SSEP.

b) Limit of observables in the DiSSEP

In this subsection, we study the thermodynamic limit of the DiSSEP. Once again this work was realized in details in [V10] and we expose hereafter the results obtained there. The computations will be based on the exact expressions derived for a finite size lattice in chapter III. We are interested in the case where there exists a competition between the diffusion of particles and the evaporation/condensation of pairs. It is indeed possible that, when performing

the thermodynamic limit in a naive way, the effect of one process completely overcomes the other process.

In order to maintain the competition in the continuous limit, we have to scale properly the parameters of the model. In other words, the mean time for a particle to go through the lattice by diffusion must be comparable to the time for it to be evaporated.

In order to evaluate quantitatively this competition, let us write the time evolution of the one-point correlation function for $1 < i < L$

$$\frac{d\langle\tau_i\rangle_t}{dt} = \langle\tau_{i-1}(1-\tau_i)\rangle_t + \langle(1-\tau_i)\tau_{i+1}\rangle_t - \langle(1-\tau_{i-1})\tau_i\rangle_t - \langle\tau_i(1-\tau_{i+1})\rangle_t \quad (\text{V.A.6})$$

$$+ \lambda^2 \left(\langle(1-\tau_{i-1})(1-\tau_i)\rangle_t + \langle(1-\tau_i)(1-\tau_{i+1})\rangle_t - \langle\tau_{i-1}\tau_i\rangle_t - \langle\tau_i\tau_{i+1}\rangle_t \right) \\ = \langle\tau_{i-1}\rangle_t + \langle\tau_{i+1}\rangle_t - 2\langle\tau_i\rangle_t + \lambda^2 \left(2 - \langle\tau_{i-1}\rangle_t - \langle\tau_{i+1}\rangle_t - 2\langle\tau_i\rangle_t \right), \quad (\text{V.A.7})$$

where $\langle\cdot\rangle_t$ stands for the expectation with respect to the probability density $P_t(\mathcal{C})$ whose time evolution obeys the master equation. Note that although the two-point correlation functions cancel when going from (V.A.6) to (V.A.7), the mean field approximation is not exact in the sense that the connected two-point function does not vanish, see (III.B.45).

We want to take the large L limit in equation (V.A.7). For $x \in [0, 1]$, we define

$$\bar{\rho}_t(x) = \lim_{L \rightarrow \infty} \langle\tau_{\lfloor Lx \rfloor}\rangle_{L^2t}. \quad (\text{V.A.8})$$

Note that the time has been speeded up by a factor L^2 which is necessary in diffusive systems to observe non-trivial behavior. We obtain

$$\frac{\partial \bar{\rho}_t}{\partial t}(x) = \frac{\partial^2 \bar{\rho}_t}{\partial x^2}(x) + 2 \left(\lim_{L \rightarrow \infty} L^2 \lambda^2 \right) (1 - 2\bar{\rho}_t(x)) \quad (\text{V.A.9})$$

We see on the previous equation that we have to take $\lambda = \lambda_0/L$ in order to have a balance between diffusion and creation-annihilation. In this case we obtain

$$\frac{\partial \bar{\rho}_t}{\partial t} = \frac{\partial^2 \bar{\rho}_t}{\partial x^2} + 2\lambda_0^2(1 - 2\bar{\rho}_t) \quad (\text{V.A.10})$$

with the boundary conditions $\bar{\rho}_t(0) = \rho_l$ and $\bar{\rho}_t(1) = \rho_r$. This equation shows that the correlation length for this scaling is finite. Indeed, the stationary density shown in equation V.A.13 decays as $\bar{\rho}(x) - 1/2 \sim \exp(-2\lambda_0 x)$ for x far from the boundaries. The correlation length can thus be defined as $1/(2\lambda_0)$.

Without rescaling λ w.r.t L and without speeding up the time in (V.A.8) (or for $\lambda = \lambda_0/L^\mu$ with $\mu < 1$ and speeding up the time with a factor $L^{2\mu}$ in (V.A.8)), the diffusive term drops out and the density satisfies

$$\frac{\partial \bar{\rho}_t}{\partial t} = 2\lambda^2(1 - 2\bar{\rho}_t). \quad (\text{V.A.11})$$

In the case where $\lambda = \lambda_0/L^\mu$ for $\mu > 1$ (and keeping the definition (V.A.8) as it is), the system becomes a pure diffusive model for large L and one gets for the density

$$\frac{\partial \bar{\rho}_t}{\partial t} = \frac{\partial^2 \bar{\rho}_t}{\partial x^2}. \quad (\text{V.A.12})$$

Thermodynamic limit of the observables We are now interested in evaluating the thermodynamic limit of the physical quantities computed for a finite size lattice in chapter III. We will perform this limit in the case where there is a competition between diffusion and evaporation/condensation, *i.e* when we take $\lambda = \lambda_0/L$.

We are first interested in the one point correlation function in the continuous limit.

Proposition A.1. *The mean particle density in the thermodynamic limit is given for $x \in [0, 1]$ by the exact expression*

$$\bar{\rho}(x) = \lim_{L \rightarrow \infty} \langle \tau_{[Lx]} \rangle = \frac{1}{2} + \frac{1}{2 \sinh 2\lambda_0} \left(q_1 e^{-2\lambda_0(x-1/2)} + q_2 e^{2\lambda_0(x-1/2)} \right), \quad (\text{V.A.13})$$

where

$$q_1 = (\rho_l + \rho_r - 1) \sinh(\lambda_0) - (\rho_r - \rho_l) \cosh(\lambda_0), \quad (\text{V.A.14})$$

and

$$q_2 = (\rho_l + \rho_r - 1) \sinh(\lambda_0) + (\rho_r - \rho_l) \cosh(\lambda_0). \quad (\text{V.A.15})$$

It is easy to check that it satisfies the stationary version of (V.A.10).

Proof. It can be directly computed from the expression (III.B.42) for a finite size lattice. ■

We can also compute the connected two-point correlation function in this limit. We can see that it scales as $\frac{1}{L}$, *i.e.* it has weak correlations.

Proposition A.2. *For $x, y \in [0, 1]$, $x < y$, we have the following analytical expression of the connected two-point correlation function in the thermodynamic limit*

$$\bar{\rho}^c(x, y) = \lim_{L \rightarrow \infty} L \times \langle \tau_{[Lx]} \tau_{[Ly]} \rangle_c = \frac{2\lambda_0 q_1 q_2}{(\sinh 2\lambda_0)^3} \sinh 2\lambda_0 (1 - y) \sinh 2\lambda_0 x. \quad (\text{V.A.16})$$

For $\lambda_0 \ll 1$, this connected two-point correlation function behaves algebraically w.r.t. x and y whereas it behaves exponentially and is short range for $\lambda_0 \gg 1$.

Proof. Once again this is directly evaluated from the finite size lattice expression (III.B.44). ■

We can also study the particle lattice current and condensation current.

Proposition A.3. *The thermodynamic limit of the mean particle currents are given for $x \in [0, 1]$ by*

$$\bar{j}_{lat}(x) := \lim_{L \rightarrow \infty} L \times \langle j_{lat}^{[Lx] \rightarrow [Lx]+1} \rangle = \frac{\lambda_0}{\sinh 2\lambda_0} \left(q_1 e^{-2\lambda_0(x-1/2)} - q_2 e^{2\lambda_0(x-1/2)} \right), \quad (\text{V.A.17})$$

and

$$\bar{j}_{cond}(x) := \lim_{L \rightarrow \infty} L^2 \times \langle j_{cond}^{[Lx], [Lx]+1} \rangle = \frac{-2\lambda_0^2}{\sinh 2\lambda_0} \left(q_1 e^{-2\lambda_0(x-1/2)} + q_2 e^{2\lambda_0(x-1/2)} \right). \quad (\text{V.A.18})$$

Proof. These formulas are derived from the explicit expression of the currents for a finite size lattice (III.B.51) and (III.B.53) ■

Note that these expressions are consistent with the fact that when the system reaches a thermodynamic equilibrium, that is for $\rho_l = \rho_r = 1/2$ (or equivalently $q_1 = q_2 = 0$), both currents vanish.

The particle conservation law (III.B.54) becomes in the thermodynamic limit

$$-\frac{d\bar{j}_{lat}}{dx}(x) + \bar{j}_{cond}(x) = 0,$$

which is satisfied by the expressions above. In the same way, relations (III.B.55) and (III.B.56) become in the thermodynamic limit:

$$\frac{d\bar{\rho}}{dx}(x) + \bar{j}_{lat}(x) = 0, \quad \bar{j}_{cond}(x) = 2\lambda_0^2 \left(1 - 2\bar{\rho}(x) \right). \quad (\text{V.A.19})$$

Behavior of the density and the currents Depending on the values of q_1 and q_2 defined in (V.A.14) and (V.A.15), the behavior of the density may change:

- the density is not monotonic when $e^{-2\lambda_0} < \frac{q_1}{q_2} < e^{2\lambda_0}$, which implies that q_1 and q_2 have the same sign. In that case, it possesses an extremum at \bar{x} satisfying $e^{4\lambda_0(\bar{x}-1/2)} = \frac{q_1}{q_2}$. The lattice current vanishes at this point.
 - the density presents a maximum

$$\bar{\rho}(\bar{x}) = \frac{1}{2} - \frac{\sqrt{q_1 q_2}}{\sinh(2\lambda_0)} \quad (\text{V.A.20})$$

when $q_1, q_2 < 0$. Let us remark that in this case, the density is everywhere smaller than $1/2$. Example of such behavior can be seen on figure V.1.

The lattice current changes direction at the point \bar{x} , as expected since the lattice current goes from high density to low density. At this point, the condensation current is minimal but positive, since the density is smaller than $1/2$, so that condensation is promoted.

- It presents a minimum

$$\bar{\rho}(\bar{x}) = \frac{1}{2} + \frac{\sqrt{q_1 q_2}}{\sinh(2\lambda_0)} \quad (\text{V.A.21})$$

when $q_1, q_2 > 0$. In this case, the density is everywhere greater than $1/2$.

The condensation current is negative but maximal, so that the evaporation is minimal. As previously, the lattice current changes sign at \bar{x} , still going from high density to low density. Example of such behavior can be seen on figure V.2.

- The density is monotonic from ρ_l to ρ_r when $\frac{q_1}{q_2} < e^{-2\lambda_0}$ or $\frac{q_1}{q_2} > e^{2\lambda_0}$. In this case, the lattice current never vanishes. Example of such behavior can be seen on figure V.3.

The condensation current follows the same pattern, due to the relation (V.A.19). The lattice current behaves as follows:

- it is not monotonic when $e^{-2\lambda_0} < -\frac{q_1}{q_2} < e^{2\lambda_0}$, which implies that q_1 and q_2 have opposite sign. There is an extremum at \bar{x} satisfying $e^{4\lambda_0(\bar{x}-1/2)} = -\frac{q_1}{q_2}$. The condensation current vanishes at this point.

- When $q_1 < 0$, the lattice current presents a maximum

$$\bar{j}_{lat}(\bar{x}) = -\frac{2\lambda_0}{\sinh(2\lambda_0)} \sqrt{-q_1 q_2}. \quad (\text{V.A.22})$$

- When $q_1 > 0$, it presents a minimum (see figure V.3)

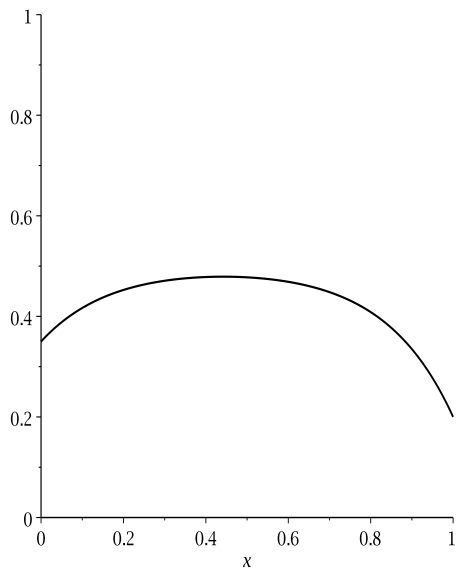
$$\bar{j}_{lat}(\bar{x}) = \frac{2\lambda_0}{\sinh(2\lambda_0)} \sqrt{-q_1 q_2}. \quad (\text{V.A.23})$$

- The lattice current is monotonic when $-\frac{q_1}{q_2} < e^{-2\lambda_0}$ or $-\frac{q_1}{q_2} > e^{2\lambda_0}$, see figures V.1 and V.2.

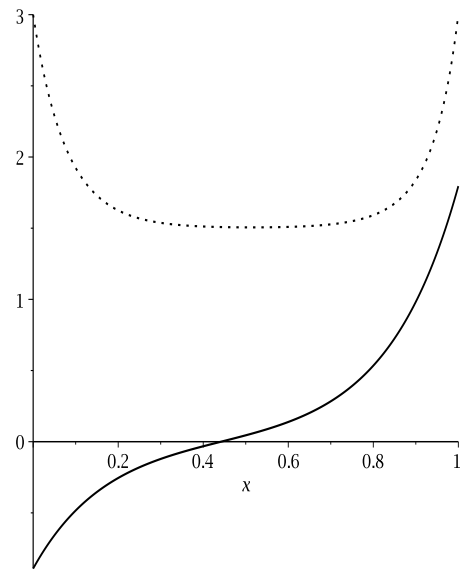
We now turn to the study of the behavior of the lattice current in the large system size limit.

Proposition A.4. *The thermodynamic limit of the variance of the lattice current, computed exactly in (III.B.73) for any size, takes the form:*

$$\begin{aligned} E^{(2)}(x) &= 2q_1 q_2 \lambda_0^2 \left\{ (2x-1) \frac{\sinh(2\lambda_0(2x-1))}{(\sinh(2\lambda_0))^3} - \frac{\cosh(2\lambda_0) \cosh(2\lambda_0(2x-1)) + 1}{(\sinh(2\lambda_0))^4} \right\} \\ &- q_2^2 \lambda_0 \frac{e^{4\lambda_0 x} + e^{-4\lambda_0(1-x)} - e^{4\lambda_0(2x-1)} + 3}{4(\sinh(2\lambda_0))^3} - q_1^2 \lambda_0 \frac{e^{4\lambda_0(1-x)} + e^{-4\lambda_0 x} - e^{4\lambda_0(1-2x)} + 3}{4(\sinh(2\lambda_0))^3} \\ &+ \frac{\lambda_0 \cosh(2\lambda_0 x) \cosh(2\lambda_0(1-x))}{\sinh(2\lambda_0)}. \end{aligned} \quad (\text{V.A.24})$$

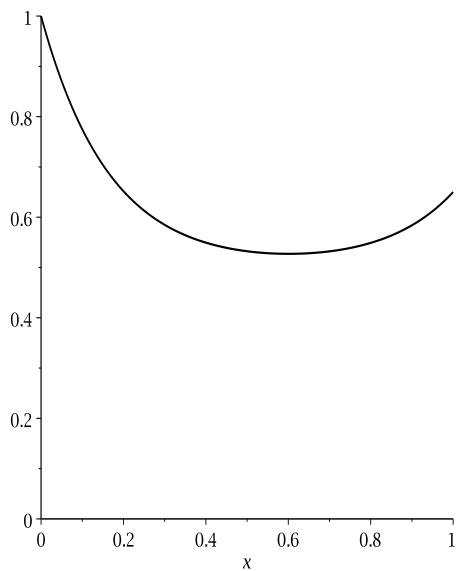


(a) Density

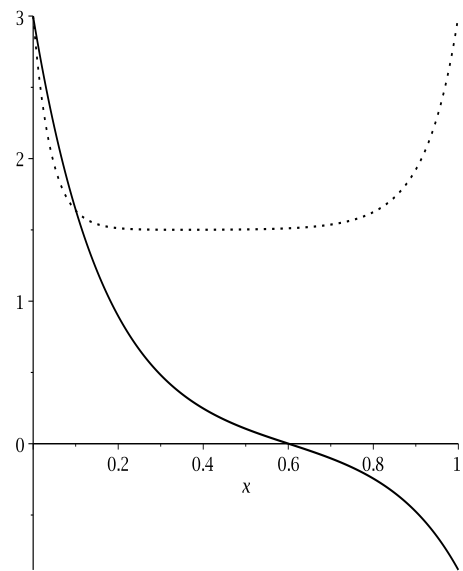


(b) Mean value (—) and variance (···) of the lattice current

Figure V.1: Plot of the density and of the lattice current for $\rho_l = 0.35$, $\rho_r = 0.2$ and $\lambda_0 = 3$.



(a) Density



(b) Mean value (—) and variance (···) of the lattice current

Figure V.2: Plot of the density and of the lattice current for $\rho_l = 1$, $\rho_r = 0.65$ and $\lambda_0 = 3$.

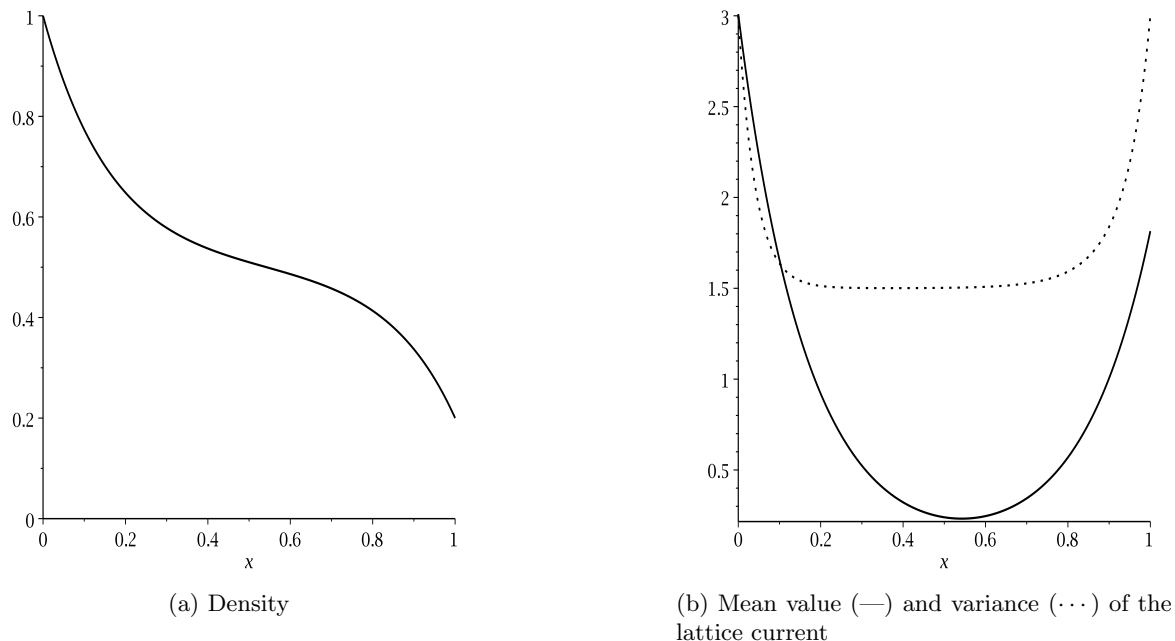


Figure V.3: Plot of the density and of the lattice current for $\rho_l = 1$, $\rho_r = 0.2$ and $\lambda_0 = 3$.

As all physical quantities of the model, the variance is invariant under the transformation $q_1 \leftrightarrow q_2$ and $x \rightarrow 1-x$, which is the left-right symmetry. The particle-hole symmetry amounts to change $q_1 \rightarrow -q_1$ and $q_2 \rightarrow -q_2$: it leaves $E^{(2)}$ invariant, transforms $\bar{\rho}(x)$ into $1 - \bar{\rho}(x)$ and changes the sign of the currents. The symmetry $\lambda \rightarrow -\lambda$ reads $\lambda_0 \rightarrow -\lambda_0$ and $q_1 \leftrightarrow (-q_2)$ and leaves all quantities invariant.

Remark A.5. By taking the limit $\lambda_0 \rightarrow 0$ in the previous quantities, i.e in the limit where the evaporation/condensation is negligible, we recover the well-known SSEP expressions [209]:

$$\begin{aligned} \lim_{\lambda_0 \rightarrow 0} \bar{\rho}(x) &= \rho_l(1-x) + \rho_r x, & \lim_{\lambda_0 \rightarrow 0} \bar{\rho}^c(x, y) &= -x(1-y)(\rho_l - \rho_r)^2, \\ \lim_{\lambda_0 \rightarrow 0} \bar{j}_{lat}(x) &= \rho_l - \rho_r, & \lim_{\lambda_0 \rightarrow 0} E^{(2)}(x) &= \rho_l + \rho_r - \frac{2}{3}(\rho_l^2 + \rho_l \rho_r + \rho_r^2). \end{aligned}$$

We are finally interested in the study of the dynamical properties of the model: using the Bethe equations (II.C.139) and (II.C.141), we study the approach to the stationary state at large times for a large system. We must compute the eigenvalue, denoted by G , for the first excited state (*i.e.* the one with the greatest non-vanishing eigenvalue).

We start by presenting the main results for the gap then we give the sketch of the numerical evidences for them.

- In the case when evaporation rate λ is independent of the size of the system L , there is a non-vanishing gap. The values of this gap depends on the boundaries parameters and on λ . We present these different values of the gaps on Figure V.4. They are consistent with the analytical result obtained for $\lambda = 1$, see (III.B.28).
- If the rate λ behaves as $\frac{1}{L^\mu}$ for large system, the model is gapless and we get

$$G \sim \frac{1}{L^{2\mu}} \text{ for } 0 < \mu < 1 \text{ and } G \sim \frac{1}{L^2} \text{ for } \mu \geq 1. \quad (\text{V.A.25})$$

We show in figure V.5 numerical evidence for such a behavior. We plot

$$z(L) = \frac{\ln(G_L) - \ln(G_{L-1})}{\ln(L-1) - \ln(L)} \quad (\text{V.A.26})$$

as a function of $\frac{1}{L}$: as $\frac{1}{L}$ tends to 0, it tends to 2μ (resp. 2) for $\mu < 1$ (resp. $\mu \geq 1$). The $\frac{1}{L^2}$ behavior of the gap for $\mu > 1$ is expected since the system becomes in this case a diffusive model in the thermodynamic limit as discussed around equation (V.A.12).

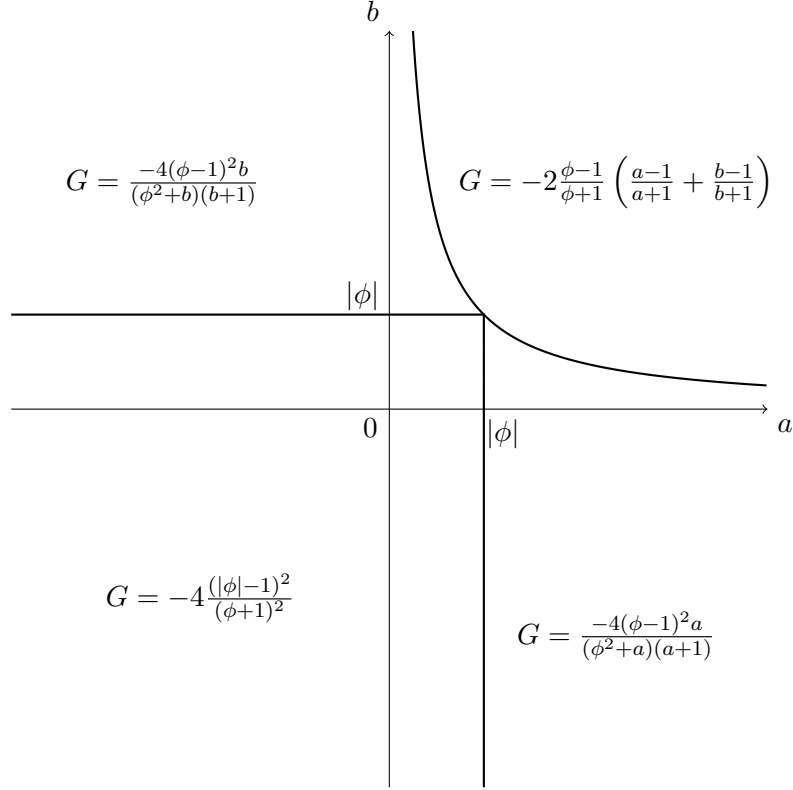


Figure V.4: Value of the gap G depending on the parameters a , b and ϕ . The equation of the curve is $b = \phi^2/a$. (This particular figure is drawn for $\phi = 1/4$ ($\lambda = 0.6$) even though similar behavior is valid for any ϕ).

To prove these result, we must study in detail the Bethe equations (II.C.139) and (II.C.141). The comparison of the eigenvalues obtained by the exact diagonalisation of M or by the numerical resolutions of the Bethe equations for small system (up to 10 sites), show that the gap is obtained for $N = 1$ in (II.C.140) and (II.C.141) or is equal to $G = -\alpha - \beta - \gamma - \delta = -2\frac{\phi-1}{\phi+1} \left(\frac{a-1}{a+1} + \frac{b-1}{b+1} \right)$ (which corresponds to $N = 0$ in (II.C.138) and (II.C.139)). We assume that this behavior holds for any L then we must solve only (II.C.139) for $N = 1$. This Bethe equation can be written as the vanishing of a polynomial of degree $2L + 2$ w.r.t. v_1 . This polynomial has two obvious roots ϕ and $-\phi$ which are not physical since they corresponds to a vanishing “eigenvector”. The remaining factor is a polynomial of degree $2L$ w.r.t. v_1 which can be transformed, thanks to (II.C.140) (and up to a normalization), to a polynomial of degree L w.r.t. E . Then, the Bethe equation (II.C.141) for $N = 1$ becomes

$$\sum_{p=0}^L \frac{(1+\phi)^{2p} E^p}{4^p} \sum_{q=0}^{L-p} \phi^{2q} \left[ab \binom{p+q}{q} \binom{L-q-2}{p-2} + (a+b) \binom{p+q-1}{q} \binom{L-q-1}{p-1} + \binom{p+q-2}{q} \binom{L-q}{p} \right] = 0 \quad (\text{V.A.27})$$

The L.H.S. of the previous equation is a factor of the characteristic polynomial of the Hamiltonian H (II.C.135) or of the Markov matrix M (III.B.2). It is possible now to find numerically the roots of the polynomial (V.A.27) for large system (up to 150 sites) and pick up the largest ones. Performing this computation for different values of λ and of the boundary parameters, we obtain the results for the gap summarized previously, see figure V.4.

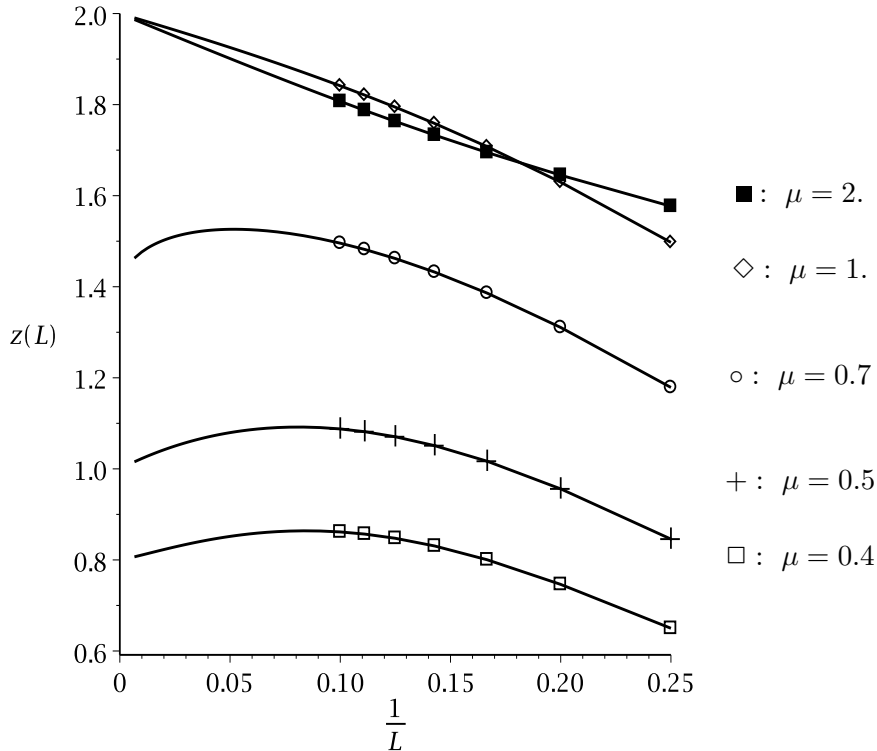


Figure V.5: Behavior of the gap in the thermodynamic limit when λ behaves as $\frac{1}{L^\mu}$: plot of $z(L) = \frac{\ln(G_L) - \ln(G_{L-1})}{\ln(L-1) - \ln(L)}$ as a function of $\frac{1}{L}$. The lines represent the values obtained from Bethe ansatz (for $4 \leq L \leq 150$), while the dots correspond to direct diagonalisation of H (for $4 \leq L \leq 10$).

c) Limit of observables in 2-TASEP

We are now interested in another example that we encountered in chapter III: the open two-species TASEP. We expressed the stationary state in a matrix product form and computed exactly the mean particle currents and the particle densities for a finite size lattice. The goal is now to study this model in the thermodynamic limit. The results presented here are mainly extracted from the work [V7].

The stationary state of the exclusion process can exhibit different qualitative features and different analytical expressions for macroscopic quantities in the infinite size limit, $L \rightarrow \infty$. The system is said to exhibit various phases, that depend on the values of the boundary exchange rates. These different phases can be discriminated by the values of the currents and by the shapes of the density profiles. More refined features, such as correlations length or even dynamical behavior, can even lead us to define subphases (see [42] for details and references). We stressed in chapter III that the value of the mean particle currents and the mean density profiles can be exactly obtained, from the the study of single species open TASEP, through the identification procedure. The first step to compute analytically the asymptotic behavior of the particle currents and densities in the two species TASEP is thus to determine the asymptotic behavior of these quantities in the single species TASEP.

The phase diagram of the one-species TASEP has been well-known for a long time; first determined using a mean-field approximation [45, 153], it was rigorously established and precisely investigated after the finding of the exact solution [42, 46, 47]. The phase diagram is determined by the behavior of the stationary current $\langle j \rangle$ and bulk density of particles in the limit $L \rightarrow \infty$ [42]. The different phases are summarized in table (V.A.28).

Region	Phase	Current \bar{j}	Bulk density
$\alpha < \beta, \alpha < \frac{1}{2}$	Low-density (LD)	$\alpha(1 - \alpha)$	α
$\beta < \alpha, \beta < \frac{1}{2}$	High-density (HD)	$\beta(1 - \beta)$	$1 - \beta$
$\alpha > \frac{1}{2}, \beta > \frac{1}{2}$	Maximal current (MC)	$\frac{1}{4}$	$\frac{1}{2}$

(V.A.28)

We recall briefly the main steps of the asymptotic study of the particle current and density. The goal is to take the large size limit $L \rightarrow \infty$ in the exact expression (III.A.30) and (III.A.36) derived for a finite size lattice. These quantities are expressed in terms of the normalization Z_n (III.A.20). The key point is thus to evaluate the asymptotic behavior of this normalization. Following the lines of [46] we first define

$$R_n(x) = \sum_{p=2}^{n+1} \frac{(p-1)(2n-p)!}{n!(n+1-p)!} x^p, \quad (\text{V.A.29})$$

which is of particular interest because

$$Z_n = \langle\langle W|C^n|V \rangle\rangle = \frac{R_n(1/\beta) - R_n(1/\alpha)}{1/\beta - 1/\alpha} \langle\langle W|V \rangle\rangle. \quad (\text{V.A.30})$$

An asymptotic expression of $R_n(1/\beta)$, respectively of $R_n(1/\alpha)$, can be obtained by determining the value of p which gives the dominant contribution to the sum (V.A.29):

$$R_n\left(\frac{1}{\beta}\right) \simeq \begin{cases} \frac{1}{\sqrt{\pi}(2\beta-1)^2} \frac{4^n}{n^{3/2}}, & \text{for } \beta > \frac{1}{2} \\ \frac{2}{\sqrt{\pi}} \frac{4^n}{n^{1/2}}, & \text{for } \beta = \frac{1}{2} \\ (1-2\beta) \frac{1}{\beta^{n+1}(1-\beta)^{n+1}}, & \text{for } \beta < \frac{1}{2}. \end{cases} \quad (\text{V.A.31})$$

This provides an asymptotic expression of the normalization Z_n depending on the value of α and β . We present here the case where $\alpha \leq \beta$. By symmetry, the case $\beta < \alpha$ can then be obtained by interchanging α and β in the expressions below. We have

$$Z_n \simeq \begin{cases} \frac{\alpha\beta}{\sqrt{\pi}(\beta-\alpha)} \left(\frac{1}{(2\alpha-1)^2} - \frac{1}{(2\beta-1)^2} \right) \frac{4^n}{n^{3/2}}, & \text{for } \frac{1}{2} < \alpha < \beta, \\ \frac{\alpha^2}{\sqrt{\pi}(2\alpha-1)^3} \frac{4^n}{n^{3/2}}, & \text{for } \frac{1}{2} < \alpha = \beta, \\ \frac{2\beta}{\sqrt{\pi}(2\beta-1)} \frac{4^n}{n^{1/2}}, & \text{for } \alpha = \frac{1}{2} < \beta, \\ 4^n, & \text{for } \alpha = \beta = \frac{1}{2}, \\ \frac{\beta(1-2\alpha)}{(\beta-\alpha)(1-\alpha)} \frac{1}{\alpha^n(1-\alpha^n)}, & \text{for } \alpha < \frac{1}{2} \text{ and } \alpha < \beta, \\ \frac{(1-2\alpha)^2}{(1-\alpha)^2} \frac{n}{\alpha^n(1-\alpha^n)}, & \text{for } \alpha = \beta < \frac{1}{2}. \end{cases} \quad (\text{V.A.32})$$

We are now in position to give the asymptotic behavior of the particle current.

Proposition A.6. *In the limit $L \rightarrow \infty$, the expression of the mean particle current (III.A.30) tends to*

$$\bar{j} := \lim_{L \rightarrow \infty} \langle j \rangle = \begin{cases} \frac{1}{4}, & \text{for } \alpha \geq \frac{1}{2}, \text{ and } \beta \geq \frac{1}{2}, \\ \alpha(1 - \alpha), & \text{for } \alpha < \frac{1}{2}, \text{ and } \beta > \alpha, \\ \beta(1 - \beta), & \text{for } \beta < \frac{1}{2}, \text{ and } \alpha > \beta. \end{cases} \quad (\text{V.A.33})$$

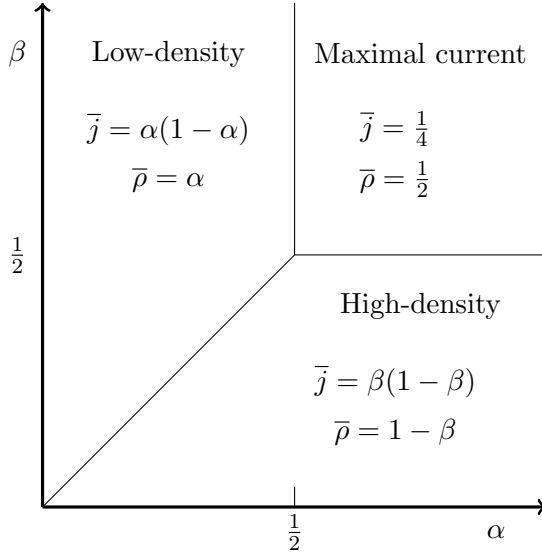


Figure V.6: Phase diagram of the single species open TASEP.

The previous proposition show that the system displays three different macroscopic behavior (called phases) depending on the value of the injection/extraction rates. These phases are represented in figure V.6.

The region where $\bar{j} = 1/4$ is called the maximal-current phase and the region where $\bar{j} = \alpha(1-\alpha)$, respectively $\bar{j} = \beta(1-\beta)$, is called the low-density phase, respectively high-density phase. This denomination will make sense below through the computation of the asymptotic behavior of the particle density. A careful study of the exact expression of the particle density for a finite size lattice (III.A.36) combined with the asymptotic behavior of the quantity $R_n(1/\beta)$ (V.A.31) yields [46] the shape of the particle density near the right boundary

$$\lim_{L \rightarrow \infty} \langle \tau_{L-j} \rangle = \begin{cases} \frac{1}{2} - \frac{1}{2\sqrt{\pi j}} + \mathcal{O}\left(\frac{1}{j^{3/2}}\right), & \text{for } \alpha, \beta > \frac{1}{2} \quad (\text{MC}) \\ \alpha + \mathcal{O}\left(\exp\left(-\frac{j}{\xi}\right)\right) & \text{for } \alpha < \beta < \frac{1}{2} \quad (\text{LD}) \\ \alpha + \mathcal{O}\left(\frac{1}{j^{3/2}} \exp\left(-\frac{j}{\xi}\right)\right) & \text{for } \alpha < \frac{1}{2} < \beta \quad (\text{LD}) \\ 1 - \beta & \text{for } \beta < \frac{1}{2}, \beta < \alpha \quad (\text{HD}) \end{cases} \quad (\text{V.A.34})$$

Note that the shape of the particle density near the left boundary can be obtained from the previous results using the symmetry $\langle \tau_j \rangle = 1 - \langle \tau_{L+1-j} \rangle|_{\alpha \leftrightarrow \beta}$.

We stress also that on the particular line defined by $\alpha = \beta$ and $\alpha, \beta < 1/2$, called the shock line, the shape of the particle density is different from the one of the low and high density phases, it is a linear interpolation between the reservoir densities α and $1 - \beta = 1 - \alpha$. More precisely we have

$$\lim_{L \rightarrow \infty} \langle \tau_{\lfloor Lx \rfloor} \rangle = \alpha + (1 - 2\alpha)x. \quad (\text{V.A.35})$$

The phase diagrams of the (M_1) and (M_2) models can be determined rigorously without having to compute exactly the steady-state probabilities. Indeed, the various phases of these two species models can be extracted from the knowledge of the one-species TASEP phase diagram, by using the two possible identifications described in (III.B.103) and (III.B.104) and called identification 1. and 2. respectively.

We recall that identification 1. allows us to compute the current $\langle j_2 \rangle$ and the density $\langle \rho_2^{(i)} \rangle$, whereas identification 2. yields the current $\langle j_1 \rangle + \langle j_2 \rangle = -\langle j_0 \rangle$ and the density $\langle \rho_1^{(i)} \rangle + \langle \rho_2^{(i)} \rangle$. Gathering these results, we obtain the phase diagrams depicted in figure V.7.

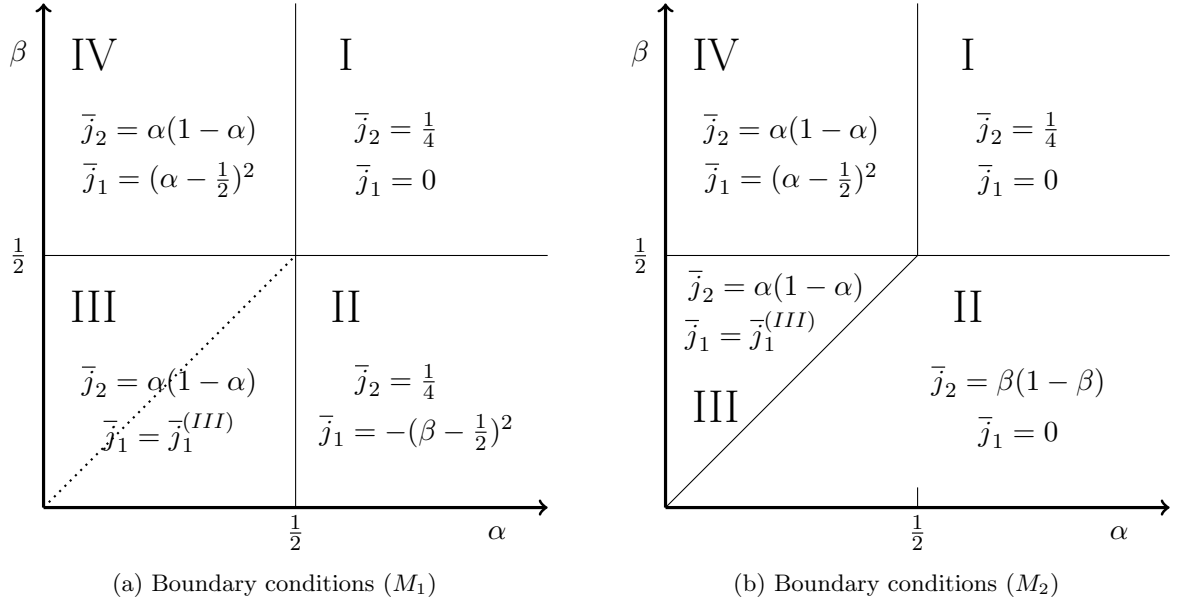


Figure V.7: Phase diagrams of the 2-TASEP with open boundaries for the boundary conditions (M_1) and (M_2) (we have used the notation $\bar{j}_1^{(III)} = (\beta - \alpha)(1 - \alpha - \beta)$).

Phase diagram of the (M_1) model The phase diagram of the (M_1) model is displayed in Figure V.7(a). It comprises four phases. Using the identification procedure, we observe that $\bar{\rho}_2$ behaves as the density for the one-species TASEP with boundary rates $(\alpha, 1)$, while $\bar{\rho}_1 + \bar{\rho}_2$ behaves as the density for the one-species TASEP with boundary rates $(1, \beta)$. The values of the currents and particle densities in each phase (see fig V.7(a)) are readily found by this identification.

Phase I: For $\alpha > \frac{1}{2}$ and $\beta > \frac{1}{2}$, particles of species 2 exhibit a maximal current, whereas the current of the particles of species 1 vanishes. The bulk density of particles of species 2 and of holes is equal to $1/2$, while the number of particles of species 2 in the bulk is vanishingly small. The density profiles of particles of species 1 and 2 are characterised by power law decays to the bulk values:

$$\lim_{L \rightarrow \infty} \langle \rho_2^{(L-j)} \rangle = \frac{1}{2} - \frac{1}{2\sqrt{\pi j}} + \mathcal{O}\left(\frac{1}{j^{3/2}}\right) \quad \text{and} \quad \lim_{L \rightarrow \infty} \langle \rho_1^{(L-j)} \rangle = \mathcal{O}\left(\frac{1}{j^{3/2}}\right).$$

The system is similar to the one-species TASEP in its maximal current phase.

Phase II: For $\alpha > \frac{1}{2}$ and $\beta < \frac{1}{2}$, none of the currents \bar{j}_1, \bar{j}_2 and \bar{j}_0 vanishes. This is a genuine 2-TASEP phase with boundaries permeable to all the species. The two species and the holes coexist in the bulk with non-zero bulk densities and density profiles characterised by power-law decays:

$$\lim_{L \rightarrow \infty} \langle \rho_2^{(L-j)} \rangle = \frac{1}{2} - \frac{1}{2\sqrt{\pi j}} + \mathcal{O}\left(\frac{1}{j^{3/2}}\right) \quad \text{and} \quad \lim_{L \rightarrow \infty} \langle \rho_1^{(L-j)} \rangle = \frac{1}{2} - \beta + \frac{1}{2\sqrt{\pi j}} + \mathcal{O}\left(\frac{1}{j^{3/2}}\right).$$

First-class particles are in their maximal current phase. Boundary effects are long-range for species 1 and 2.

Phase III: For $\alpha < \frac{1}{2}$ and $\beta < \frac{1}{2}$, we obtain a ‘massive’ phase in which boundary effects are localized: after a finite correlation length, the system reaches its bulk behaviour,

$$\lim_{L \rightarrow \infty} \langle \rho_2^{(L-j)} \rangle = \alpha + \mathcal{O}\left(\frac{1}{j^{3/2}} \exp\left(-\frac{j}{\xi}\right)\right) \quad \text{and} \quad \lim_{L \rightarrow \infty} \langle \rho_1^{(L-j)} \rangle = 1 - \alpha - \beta + \mathcal{O}\left(\frac{1}{j^{3/2}} \exp\left(-\frac{j}{\xi}\right)\right).$$

The current of second-class particles \bar{j}_2 vanishes along the line $\alpha = \beta < \frac{1}{2}$ and changes its sign across this line.

Phase IV: This phase, obtained for $\alpha < \frac{1}{2}$ and $\beta > \frac{1}{2}$, is massive for first-class particles but ‘massless’ (exhibiting long-range correlations characterised by power laws) for second-class particles and holes. Here again, the two species and the holes coexist in the bulk:

$$\lim_{L \rightarrow \infty} \langle \rho_2^{(L-j)} \rangle = \alpha + \mathcal{O}\left(\frac{1}{j^{3/2}} \exp\left(-\frac{j}{\xi}\right)\right) \quad \text{and} \quad \lim_{L \rightarrow \infty} \langle \rho_1^{(L-j)} \rangle = \frac{1}{2} - \alpha - \frac{1}{2\sqrt{\pi j}} + \mathcal{O}\left(\frac{1}{j^{3/2}}\right).$$

Holes are in their maximal current phase $\bar{j}_0 = -1/4$.

Phase diagram of the (M_2) model The phase diagram of the (M_2) model also comprises four phases, displayed in Figure V.7(b). The diagram is qualitatively different from that of the (M_1) model. Here, $\bar{\rho}_2$ behaves as the density for the one-species TASEP with boundary rates (α, β) , while $\bar{\rho}_1 + \bar{\rho}_2$ behaves as the density for the one-species TASEP with boundary rates $(1, \beta)$.

Phase I: For $\alpha > \frac{1}{2}$ and $\beta > \frac{1}{2}$, first-class particles exhibit a maximal current. This phase is similar to Phase I of model (M_1) .

Phase II: This phase is obtained for $\beta < \alpha < \frac{1}{2}$. Particles of species 2 are in their high density phase. The density of particles of species 1 in the bulk vanishes.

$$\lim_{L \rightarrow \infty} \langle \rho_2^{(L-j)} \rangle = 1 - \beta \quad \text{and} \quad \lim_{L \rightarrow \infty} \langle \rho_1^{(L-j)} \rangle = 0.$$

Phase III: For $\alpha < \beta < \frac{1}{2}$, the two species and the holes are simultaneously present with non-vanishing currents. The current of particles of species one \bar{j}_1 is strictly positive. This phase is massive for the two classes of particles and the holes:

$$\lim_{L \rightarrow \infty} \langle \rho_2^{(L-j)} \rangle = \alpha + \mathcal{O}\left(\exp\left(-\frac{j}{\xi}\right)\right) \quad \text{and} \quad \lim_{L \rightarrow \infty} \langle \rho_1^{(L-j)} \rangle = 1 - \alpha - \beta + \mathcal{O}\left(\exp\left(-\frac{j}{\xi}\right)\right).$$

Shock Line: This line corresponds to $\alpha = \beta < \frac{1}{2}$. The density profiles $\bar{\rho}_1$ and $\bar{\rho}_2$ display a linear behaviour that reflect a coexistence between a low density and a high density regions:

$$\lim_{L \rightarrow \infty} \langle \rho_2^{(\lfloor Lx \rfloor)} \rangle = \alpha + x(1 - 2\alpha) \quad \text{and} \quad \lim_{L \rightarrow \infty} \langle \rho_1^{(\lfloor Lx \rfloor)} \rangle = (1 - 2\alpha)(1 - x). \quad (\text{V.A.36})$$

The density profile of particles of species 2 takes the values α and $1 - \alpha$ with a discontinuous shock between the two regions. The particles of species 1 have a plateau density of $1 - 2\alpha$ to the left of the shock and zero density to the right shock. This means effectively that in the stationary state in the infinite system limit only the left reservoir is active as far as particles of species 1 are concerned.

Phase IV This phase, obtained for $\alpha < \frac{1}{2}$ and $\beta > \frac{1}{2}$, is similar to Phase IV of the (M_1) model.

d) Limit of observables in the multi-species SSEP

We now turn to the study of the multi-species SSEP in the thermodynamic limit. We compute in particular the large size limit $L \rightarrow \infty$ of the mean particle currents, of the mean particle densities and of the two-point functions.

Proposition A.7. *The thermodynamic limit of the mean particle current of species τ ($0 \leq \tau \leq N$) is given by the exact expression*

$$\bar{j}_\tau := \lim_{L \rightarrow \infty} L \times \langle j_\tau \rangle = \lambda_\tau. \quad (\text{V.A.37})$$

Proof. This formula is derived by a straightforward computation, starting from the expression of the particle current on the finite size lattice (III.B.235). ■

Note that the formula above is valid for $\tau = 0$ and gives the mean current of holes on the lattice. We observed in chapter III, with the exact computations on the finite size lattice, that the exclusion constraint implied $\langle j_0 \rangle + \dots + \langle j_N \rangle = 0$. This result is directly recovered, in the thermodynamic limit, from the formula above

$$\sum_{\tau=0}^N \bar{j}_\tau = \sum_{\tau=0}^N \lambda_\tau = 0, \quad (\text{V.A.38})$$

where the last equality is obtained using the definition (III.B.225) and the constraints (III.B.200).

Note also that we multiplied the mean particle current $\langle j_\tau \rangle$ with a factor L when performing the large size limit to obtain a finite and non vanishing value. This is characteristic of diffusive system in contrast with bulk driven systems (that are called ballistic) where the scaling is not needed, see for instance (V.A.33).

Proposition A.8. *The thermodynamic limit of the mean particle density of species τ ($0 \leq \tau \leq N$) at position $x \in [0, 1]$ on the lattice is given by the exact expression*

$$\bar{\rho}_\tau(x) := \lim_{L \rightarrow \infty} \langle \rho_\tau^{(\lfloor Lx \rfloor)} \rangle = \alpha_\tau(1-x) + \beta_\tau x. \quad (\text{V.A.39})$$

Proof. This is obtained through a direct computation, using the expression of the particle density for a finite size lattice (III.B.239). ■

Note that the proposition above provides for $\tau = 0$ the density of holes on the lattice. The exclusion constraint that we had on the finite size lattice $\langle \rho_0^{(i)} \rangle + \dots + \langle \rho_N^{(i)} \rangle = 1$ is easily observed in the thermodynamic limit

$$\sum_{\tau=0}^N \bar{\rho}_\tau(x) = (1-x) \sum_{\tau=0}^N \alpha_\tau + x \sum_{\tau=0}^N \beta_\tau = (1-x) + x = 1, \quad (\text{V.A.40})$$

where we made use of the constraints (III.B.200).

We observe that the mean particle density of species τ is the linear interpolation between the density of species τ in the left reservoir α_τ and the density of species τ in the right reservoir β_τ . We have indeed $\bar{\rho}_\tau(0) = \alpha_\tau$ and $\bar{\rho}_\tau(1) = \beta_\tau$.

Proposition A.9. *The large size limit of the connected two-point function between a particle of species τ and a particle of species τ' located respectively at x and y on the lattice (with $0 \leq x \leq y \leq 1$) is given by the exact expression*

$$\bar{\rho}_{\tau,\tau'}(x,y) := \lim_{L \rightarrow \infty} L \times \langle \rho_\tau^{(\lfloor Lx \rfloor)} \rho_{\tau'}^{(\lfloor Ly \rfloor)} \rangle_c = -\lambda_\tau \lambda_{\tau'} x(1-y). \quad (\text{V.A.41})$$

Proof. This is again obtained by direct computation starting from the formula (III.B.243) for the finite size lattice. ■

Note that we multiplied the connected two-point function with a factor L when performing the large size limit. It shows that the correlations in the system decrease algebraically as $1/L$.

2 Large deviation functional of the density profile

The previous subsection was devoted to the evaluation of the physical quantities (mean particle currents, mean particle densities, two-point function,...), that have been computed exactly for a finite size lattice, in the thermodynamical limit. That was performed on a series of examples studied in details on a finite size lattice in chapter III. We observed that in this large size limit, the expressions of the physical quantities became simpler. Now we would like to push further this study of the thermodynamic limit with a coarse-grained description of the physical models. The idea is to define local average of the occupation variables $\rho_0^{(i)}, \dots, \rho_N^{(i)}$ (we recall that these

variables define uniquely the configuration of the system). These averages will be computed over several sites i giving rise to a coarse-grained variable. In the spirit of the law of large number (where the average of independent identically distributed random variables converges to the expectation with probability 1), we expect these coarse-grained variables to behave nicely in the large size limit, typically to display a deterministic behavior. It means intuitively that, in the thermodynamic limit, we are almost sure to observe a density profile that is equal to a typical density profile. We will see that (on particular example) we can even get a refined result and evaluate the probability to deviate from this typical profile. This probability is, on the example treated below, exponentially small in the system size and will lead to a large deviation principle. As explained in chapter I, the large deviation functional could be a generic and powerful formalism to describe the macroscopic behavior of out-of-equilibrium statistical physics systems.

a) Definition

The first step toward a coarse-grained description of the stationary state of the model in the thermodynamic limit is to define precisely coarse-grained, or average, variables. In order to formalize the problem, we split the full system which contains $L = nl$ sites into n subsystems (called “boxes” below) containing l sites each, see figure V.8. This leads to the following definition.

Definition A.10. For all particle species (and holes) $\tau \in \{0, \dots, N\}$ and all box number $1 \leq k \leq n$, we define the average variable

$$\rho_{\tau}^{\{k\}} = \frac{1}{l} \sum_{i=kl+1}^{(k+1)l} \rho_{\tau}^{(i)}, \quad (\text{V.A.42})$$

which corresponds to the average number of particles of species τ in the box k for a given configuration.

We expect these variables to display some deterministic behavior in the limit $l \rightarrow \infty$ (that is when the number of sites involved in the average goes to infinity).

Definition A.11. It will be useful to introduce the row vector $\boldsymbol{\rho}^{\{k\}}$ encompassing the average variables of each species (and holes) in the box k :

$$\boldsymbol{\rho}^{\{k\}} = (\rho_0^{\{k\}}, \dots, \rho_N^{\{k\}}). \quad (\text{V.A.43})$$

Note that the average variables fulfill the exclusion constraint $\rho_0^{\{k\}} + \dots + \rho_N^{\{k\}} = 1$, for all $1 \leq k \leq n$ (this is directly derived from the exclusion constraint $\rho_0^{(i)} + \dots + \rho_N^{(i)} = 1$ which holds on every site i).

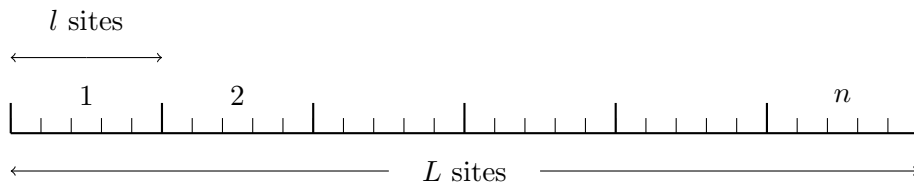


Figure V.8: The system of length L is divided into n boxes of length l .

The second step is to determine precisely which observable of these coarse-grained variables is both physically relevant and simple enough to be exactly computed in the thermodynamic limit. We are interested in evaluating the probability of observing in the stationary state a given density profile in the limit of large system size L . A density profile is defined by a fixed number of particles of each species (and holes) $\tau = 0, \dots, N$ in each boxes $k = 1, \dots, n$.

We thus want to study the joint probability law of the average variables. This motivates the following definition.

Definition A.12. *We denote by*

$$P_L(\{\boldsymbol{\rho}^{\{1\}}, \boldsymbol{\rho}^{\{2\}}, \dots, \boldsymbol{\rho}^{\{n\}}\} \mid \boldsymbol{\alpha}, \boldsymbol{\beta}) \quad (\text{V.A.44})$$

the probability to find simultaneously $\rho_\tau^{\{k\}} \times l$ particles of species τ in the box k for $\tau = 0, \dots, N$ and $k = 1, \dots, n$. We have introduced in this notation the two row vectors of size $N + 1$, encompassing the particle (and hole) densities at the two reservoirs

$$\boldsymbol{\alpha} = (\alpha_0, \dots, \alpha_N) \quad \text{and} \quad \boldsymbol{\beta} = (\beta_0, \dots, \beta_N). \quad (\text{V.A.45})$$

For l large (and thus L large), that is when the size of the boxes used to define the coarse-grained variables goes to infinity, we expect the joint probability $P_L(\{\boldsymbol{\rho}^{\{1\}}, \boldsymbol{\rho}^{\{2\}}, \dots, \boldsymbol{\rho}^{\{n\}}\} \mid \boldsymbol{\alpha}, \boldsymbol{\beta})$ to follow a large deviation principle

$$P_L(\{\boldsymbol{\rho}^{\{1\}}, \boldsymbol{\rho}^{\{2\}}, \dots, \boldsymbol{\rho}^{\{n\}}\} \mid \boldsymbol{\alpha}, \boldsymbol{\beta}) \sim \exp\left(-L\mathcal{F}_n(\{\boldsymbol{\rho}^{\{1\}}, \boldsymbol{\rho}^{\{2\}}, \dots, \boldsymbol{\rho}^{\{n\}}\} \mid \boldsymbol{\alpha}, \boldsymbol{\beta})\right). \quad (\text{V.A.46})$$

In the limit where we have in addition the number of boxes n going also to infinity, we can define a continuous coordinate x such that $k = xL$ and a vector $\boldsymbol{\rho}(x) = \boldsymbol{\rho}^{\{k\}}$. We obtain in this case a large deviation functional $\mathcal{F}(\{\boldsymbol{\rho}(x)\} \mid \boldsymbol{\alpha}, \boldsymbol{\beta})$

$$P_L(\{\boldsymbol{\rho}(x)\} \mid \boldsymbol{\alpha}, \boldsymbol{\beta}) \sim \exp(-L\mathcal{F}(\{\boldsymbol{\rho}(x)\} \mid \boldsymbol{\alpha}, \boldsymbol{\beta})). \quad (\text{V.A.47})$$

We will now study this joint probability law and show these large deviation principles on the particular example of the multi-species SSEP that we encountered many times in this manuscript. The results presented below are mainly taken out of the work [V8].

b) Multi-species SSEP case

We now turn to the computation of the joint probability law $P_L(\{\boldsymbol{\rho}^{\{1\}}, \boldsymbol{\rho}^{\{2\}}, \dots, \boldsymbol{\rho}^{\{n\}}\} \mid \boldsymbol{\alpha}, \boldsymbol{\beta})$ for the multi-species SSEP. This computation can be drastically simplified by using a powerful tool: the additivity principle. This was first introduced in [245] (see also [16] for the connection with matrix ansatz) to compute the large deviation functional of the single species open SSEP and has then been successfully applied to compute the one of the single species open ASEP [246, 247]. The general idea is to relate the probability of observing a given configuration of the lattice in the stationary state with the probabilities of the subsystems that are obtained by cutting the original system into two pieces. The difficult part lies in the correct tuning of the injection/extraction rates that have to be introduced at the level of the cutting. We stress that this approach is completely rigorous in the sense that the formula obtained to relate the full system to the two subsystems is exact. The interest of this additivity principle is to reduce, or factorize, the complexity of the computations on the full system into computations on the subsystems that we expect to be simpler. The result that we present below holds for a finite size lattice of any length. Note that similar ideas of additivity have also been used directly in the thermodynamic limit to compute large deviation functionals [248] (which by analogy with the free energy should behave as an extensive quantity). More details about that will be presented altogether with the macroscopic fluctuation theory.

Additivity principle from matrix ansatz. In order to write an additivity principle, we first need the following definition.

Definition A.13. *We introduce the vector*

$$\bar{\boldsymbol{\rho}}(u) = (1 - u)\boldsymbol{\alpha} + u\boldsymbol{\beta} \quad (\text{V.A.48})$$

which achieves the linear interpolation between the particle densities at the left (respectively right) reservoir $\boldsymbol{\alpha}$ (respectively $\boldsymbol{\beta}$).

This vector thus contains the mean particle densities at position $u \in [0, 1]$ on the lattice in the stationary state $\bar{\rho}_\tau(u)$, that have been computed in (V.A.39).

Definition A.14. We denote by $\mathcal{S}_L(\tau_1, \dots, \tau_L | \alpha, \beta, a, b)$ the probability of the configuration (τ_1, \dots, τ_L) in the stationary state for a system of size L with boundary parameters α , β , a and b .

We recall that the definition of the boundary parameters and of the dynamics of the model can be found in subsection a). Up to now the length of the lattice and the boundary parameters were omitted in the notation $\mathcal{S}(\tau_1, \dots, \tau_L)$ because there was no ambiguity, but this precision will make sense when formulating the additivity principle. As already mentioned, the idea of the additivity principle is to express the stationary weights of a system of size L in terms of the stationary weights of the two subsystems of size L' and L'' (with $L = L' + L''$) obtained by cutting the original system in two parts. The results presented in this subsection are heavily inspired by what was done in [16, 249] for the usual SSEP (with one species of particles plus holes).

Proposition A.15. For the present model, the additivity principle reads¹

$$\begin{aligned} \mathcal{S}_L(\tau_1, \dots, \tau_L | \alpha, \beta, a, b) &= -\frac{\Gamma(a+b+L')\Gamma(L''+1)}{\Gamma(a+b+L)} \oint_{u=1} \frac{du}{2i\pi} \frac{1}{u^{a+b+L'}(1-u)^{L''+1}} \text{(V.A.49)} \\ &\times \mathcal{S}_{L'}(\tau_1, \dots, \tau_{L'} | \alpha, \bar{\rho}(u), a, b) \mathcal{S}_{L''}(\tau_{L'+1}, \dots, \tau_L | \bar{\rho}(u), \beta, 1-b, b) \end{aligned}$$

This additivity property can be rewritten using the matrix product formalism. Since the algebraic relations (III.B.221), (III.B.222) and (III.B.223) involving the operators X_τ and the boundary vectors $\langle\langle W |$ and $|V\rangle\rangle$ depend explicitly on the boundary parameters, we need to introduce some more notations. We denote by $\tilde{X}_\tau(u)$, $\langle\langle \tilde{W}(u) |$ and $|\tilde{V}(u)\rangle\rangle$ the operators and boundary vectors associated to the system with parameters α and a for the left reservoir and $\bar{\rho}(u)$ and b for the right reservoir. Namely they satisfy (III.B.221), (III.B.222) and (III.B.223) where β_τ has been replaced by $(1-u)\alpha_\tau + u\beta_\tau$ for all τ :

$$[\tilde{X}_\tau(u), \tilde{X}_{\tau'}(u)] = \tilde{\lambda}_\tau(u)\tilde{X}_{\tau'}(u) - \tilde{\lambda}_{\tau'}(u)\tilde{X}_\tau(u) = u(\lambda_\tau\tilde{X}_{\tau'}(u) - \lambda_{\tau'}\tilde{X}_\tau(u)), \quad \text{(V.A.50)}$$

where

$$\tilde{\lambda}_\tau(u) = \alpha_s - [(1-u)\alpha_\tau + u\beta_\tau] = u\lambda_\tau, \quad \text{(V.A.51)}$$

and for the boundaries

$$\langle\langle \tilde{W}(u) | (\alpha_\tau \tilde{C}(u) - \tilde{X}_\tau(u)) = au\lambda_\tau \langle\langle \tilde{W}(u) |, \quad \text{(V.A.52)}$$

and

$$([(1-u)\alpha_\tau + u\beta_\tau]\tilde{C}(u) - \tilde{X}_\tau(u))|\tilde{V}(u)\rangle\rangle = -bu\lambda_\tau|\tilde{V}(u)\rangle\rangle, \quad \text{(V.A.53)}$$

where

$$\tilde{C}(u) = \tilde{X}_0(u) + \dots + \tilde{X}_N(u). \quad \text{(V.A.54)}$$

In the same way we denote by $\hat{X}_\tau(u)$, $\langle\langle \hat{W}(u) |$ and $|\hat{V}(u)\rangle\rangle$ the operators and boundary vectors associated to the system with parameters $\bar{\rho}(u)$ and $1-b$ for the left reservoir and β and b for the right reservoir. Namely they satisfy (III.B.221), (III.B.222) and (III.B.223) where α_τ has been replaced by $(1-u)\alpha_\tau + u\beta_\tau$ for all τ and a has been replaced by $1-b$:

$$[\hat{X}_\tau(u), \hat{X}_{\tau'}(u)] = \hat{\lambda}_\tau(u)\hat{X}_{\tau'}(u) - \hat{\lambda}_{\tau'}(u)\hat{X}_\tau(u) = (1-u)(\lambda_\tau\hat{X}_{\tau'}(u) - \lambda_{\tau'}\hat{X}_\tau(u)), \quad \text{(V.A.55)}$$

where

$$\hat{\lambda}_\tau(u) = [(1-u)\alpha_\tau + u\beta_\tau] - \beta_\tau = (1-u)\lambda_\tau, \quad \text{(V.A.56)}$$

and for the boundaries

$$\langle\langle \hat{W}(u) | ([(1-u)\alpha_\tau + u\beta_\tau]\hat{C}(u) - \hat{X}_\tau(u)) = (1-b)(1-u)\lambda_\tau \langle\langle \hat{W}(u) |, \quad \text{(V.A.57)}$$

¹The integration contour is chosen to contain the pole at $u = 1$ but not the pole at $u = 0$.

and

$$(\beta_\tau \widehat{C}(u) - \widehat{X}_\tau(u)) |\widehat{V}(u)\rangle = -b(1-u)\lambda_\tau |\widehat{V}(u)\rangle, \quad (\text{V.A.58})$$

where

$$\widehat{C}(u) = \widehat{X}_0(u) + \dots + \widehat{X}_N(u). \quad (\text{V.A.59})$$

Proposition A.16. *We have the formula:*

$$\begin{aligned} \langle\langle W | X_{\tau_1} \dots X_{\tau_L} | V \rangle\rangle &= - \oint_{u=1} \frac{du}{2i\pi} \frac{1}{u^{a+b+L'}(1-u)^{L''+1}} \quad (\text{V.A.60}) \\ &\times \langle\langle \widetilde{W}(u) | \widetilde{X}_{\tau_1}(u) \dots \widetilde{X}_{\tau_{L'}}(u) | \widetilde{V}(u) \rangle\rangle \langle\langle \widehat{W}(u) | \widehat{X}_{\tau_{L'+1}}(u) \dots \widehat{X}_{\tau_L}(u) | \widehat{V}(u) \rangle\rangle. \end{aligned}$$

Proof. For $i = 1, \dots, L'$ we perform the change of variables

$$X_{\tau_i} = \alpha_{\tau_i} C - L_{\tau_i} \quad \text{and} \quad \widetilde{X}_{\tau_i}(u) = \alpha_{\tau_i} \widetilde{C}(u) - \widetilde{L}_{\tau_i}(u). \quad (\text{V.A.61})$$

The new operators L_τ and $\widetilde{L}_\tau(u)$ behave conveniently on the left boundary

$$\langle\langle W | L_\tau = a\lambda_\tau \langle\langle W | \quad \text{and} \quad \langle\langle \widetilde{W}(u) | \widetilde{L}_\tau(u) = ua\lambda_\tau \langle\langle \widetilde{W}(u) |. \quad (\text{V.A.62})$$

When we expand the product $X_{\tau_1} \dots X_{\tau_{L'}}$ (respectively the product $\widetilde{X}_{\tau_1}(u) \dots \widetilde{X}_{\tau_{L'}}(u)$), we can push the L_τ (respectively the $\widetilde{L}_\tau(u)$) to the left through the C 's (respectively the $\widetilde{C}(u)$'s) using the relation $[L_\tau, C] = -\lambda_\tau C$ (respectively the relation $[\widetilde{L}_\tau(u), \widetilde{C}(u)] = -u\lambda_\tau \widetilde{C}(u)$). At the end the expansion of $X_{\tau_1} \dots X_{\tau_{L'}}$ involve monomials of the form $\lambda_{s_1} \dots \lambda_{s_k} L_{s_{k+1}} \dots L_{s_{n'}} C^{L'-n'}$. The expansion of the product $\widetilde{X}_{\tau_1}(u) \dots \widetilde{X}_{\tau_{L'}}(u)$ is exactly the same but with the previous monomial replaced by $u^k \lambda_{s_1} \dots \lambda_{s_k} \widetilde{L}_{s_{k+1}}(u) \dots \widetilde{L}_{s_{n'}}(u) \widetilde{C}(u)^{L'-n'}$.

In the same way for $i = L' + 1, \dots, L' + L''$ we perform the change of variables

$$X_{\tau_i} = \beta_{\tau_i} C - R_{\tau_i} \quad \text{and} \quad \widehat{X}_{\tau_i}(u) = \beta_{\tau_i} \widehat{C}(u) - \widehat{R}_{\tau_i}(u). \quad (\text{V.A.63})$$

The new operators R_τ and $\widehat{R}_\tau(u)$ behave conveniently on the right boundary

$$R_\tau |V\rangle = -b\lambda_\tau |V\rangle \quad \text{and} \quad \widehat{R}_\tau(u) |\widehat{V}(u)\rangle = -(1-u)b\lambda_\tau |\widehat{V}(u)\rangle. \quad (\text{V.A.64})$$

Following the same idea as previously, the expansion of $X_{\tau_{L'+1}} \dots X_{\tau_L}$ involve monomials of the form $\lambda_{s_1} \dots \lambda_{s_k} C^{L''-n''} R_{s_{k+1}} \dots R_{s_{n''}}$. The expansion of the product $\widetilde{X}_{\tau_{L'+1}}(u) \dots \widetilde{X}_{\tau_L}(u)$ is exactly the same but with the previous monomial replaced by $(1-u)^k \lambda_{s_1} \dots \lambda_{s_k} \widehat{C}(u)^{L''-n''} \widehat{R}_{s_{k+1}}(u) \dots \widehat{R}_{s_{n''}}(u)$.

Putting all these expansions together, we see that finally it remains to prove

$$\begin{aligned} \langle\langle W | C^{L'+L''-n'-n''} | V \rangle\rangle &= - \oint_{u=1} \frac{du}{2i\pi} \frac{1}{u^{a+b+L'-n'}(1-u)^{1+L''-n''}} \quad (\text{V.A.65}) \\ &\times \langle\langle \widetilde{W}(u) | \widetilde{C}(u)^{L'-n'} | \widetilde{V}(u) \rangle\rangle \langle\langle \widehat{W}(u) | \widehat{C}(u)^{L''-n''} | \widehat{V}(u) \rangle\rangle. \end{aligned}$$

This is established using result (III.B.227) and the fact that

$$\oint_{u=1} \frac{du}{2i\pi} \frac{1}{u^{a+b+L'-n'}(1-u)^{1+L''-n''}} = - \frac{(-1)^{L''-n''}}{(L''-n'')!} \left. \frac{d^{L''-n''}}{du^{L''-n''}} \frac{1}{u^{a+b+L'-n'}} \right|_{u=1} \quad (\text{V.A.66})$$

$$= - \frac{\Gamma(a+b+L'+L''-n'-n'')}{\Gamma(a+b+L'-n')\Gamma(1+L''-n'')} \quad (\text{V.A.67})$$

■

Large deviation functional of the density profile. We are now equipped to study the large deviation functional of the density profile. As a warm-up, we start with the particular case of the thermodynamic equilibrium, i.e. when $\alpha = \beta := \mathbf{r} = (r_0, \dots, r_N)$, see (III.B.226), which is much easier than the non-equilibrium case.

Proposition A.17. *In the thermodynamic equilibrium case, the large deviation functional is given by*

$$\mathcal{F}(\{\rho(x)\} | \mathbf{r}, \mathbf{r}) = \int_0^1 dx B(\rho(x), \mathbf{r}), \quad (\text{V.A.68})$$

where

$$B(\rho, \mathbf{r}) = \sum_{\tau=0}^N \rho_\tau \ln \left(\frac{\rho_\tau}{r_\tau} \right) \quad (\text{V.A.69})$$

We recall that $r_0 + \dots + r_N = 1$ and $\rho_0(x) + \dots + \rho_N(x) = 1$ for all x . Note that $B(\rho(x), \mathbf{r})$ is nothing else but the Kullback-Leibler divergence between the two discrete measure $\rho(x)$ and \mathbf{r} .

Proof. In the thermodynamic equilibrium case the stationary distribution is given by (III.B.226). Hence we can easily evaluate

$$P_L(\{\rho^{\{1\}}, \rho^{\{2\}}, \dots, \rho^{\{n\}}\} | \mathbf{r}, \mathbf{r}) = \prod_{k=1}^n \frac{l!}{(l\rho_0^{\{k\}})! \dots (l\rho_N^{\{k\}})!} r_0^{l\rho_0^{\{k\}}} \dots r_N^{l\rho_N^{\{k\}}}. \quad (\text{V.A.70})$$

Then using the Stirling formula we obtain

$$\lim_{l \rightarrow \infty} -\frac{1}{L} \ln P_L(\{\rho^{\{1\}}, \rho^{\{2\}}, \dots, \rho^{\{n\}}\} | \mathbf{r}, \mathbf{r}) = \frac{1}{n} \sum_{k=1}^n \sum_{\tau=0}^N \rho_\tau^{\{k\}} \ln \left(\frac{\rho_\tau^{\{k\}}}{r_\tau} \right). \quad (\text{V.A.71})$$

The limit of large n thus gives

$$\lim_{n \rightarrow \infty} \lim_{l \rightarrow \infty} -\frac{1}{L} \ln P_L(\{\rho^{\{1\}}, \rho^{\{2\}}, \dots, \rho^{\{n\}}\} | \mathbf{r}, \mathbf{r}) = \int_0^1 dx \sum_{\tau=0}^N \rho_\tau(x) \ln \left(\frac{\rho_\tau(x)}{r_\tau} \right), \quad (\text{V.A.72})$$

which yields the desired result. ■

The non-equilibrium case $\alpha \neq \beta$ is more involved.

Proposition A.18. *The large deviation functional of the density profile is given by*

$$\mathcal{F}(\{\rho(x)\} | \alpha, \beta) = \int_0^1 dx \left[B(\rho(x), \bar{\rho}(u(x))) + \ln u'(x) \right], \quad (\text{V.A.73})$$

where u is the monotonic solution of the differential equation

$$\frac{u''(x)}{(u'(x))^2} + \sum_{\tau=0}^N \lambda_\tau \frac{\rho_\tau(x)}{\bar{\rho}_\tau(u(x))} = 0 \quad (\text{V.A.74})$$

satisfying boundary conditions $u(0) = 0$ and $u(1) = 1$.

Before proving this expression, we formulate two remarks.

Remark A.19. *We can deduce from this expression that the most probable density profile is given by $\rho(x) = \bar{\rho}(x)$. The differential equation is indeed solved by the function $u(x) = x$ in this case because $\lambda_0 + \dots + \lambda_N = 0$. Injecting in (V.A.73) makes the large deviation function vanish.*

Remark A.20. *The thermodynamic equilibrium case can be of course recovered from the general case. Indeed we have $\bar{\rho}(u) = \alpha = \beta = \mathbf{r}$ for all u . Moreover the differential equation (V.A.74) reduces to $u''(x) = 0$ because $\lambda_s = 0$ for all s in this case. It is solved by the function $u(x) = x$. Injecting in (V.A.73) leads to (V.A.68) as expected.*

We now present the proof of (V.A.73)

Proof. The proof presented here follows heavily the lines of the proof written in [16, 249] for the one species SSEP. For the sake of simplicity, we will present the proof for the case where $a + b = 1$, but the generalization to the other cases is straightforward.

We want to evaluate the probability $P_L(\{\rho^{\{1\}}, \rho^{\{2\}}, \dots, \rho^{\{n\}}\} | \alpha, \beta)$ to find $\rho_\tau^{\{k\}} \times l$ particles (or holes) of species τ in the box k for $\tau = 0, \dots, N$ and $k = 1, \dots, n$. This is done by summing the probabilities of all the configurations satisfying these constraints. For each of these configurations, we use the additivity principle (V.A.49) to divide the system into two part of size $L' = kl$ (containing k boxes) and $L'' = (n - k)l$ (containing $n - k$ boxes), for a fixed $1 \leq k \leq n$. We thus obtain

$$P_{nl}(\{\rho^{\{1\}}, \dots, \rho^{\{n\}}\} | \alpha, \beta) = -\frac{(kl)!((n-k)l)!}{(nl)!} \oint \frac{du}{2i\pi} \frac{1}{u^{kl+1}(1-u)^{(n-k)l+1}} \\ \times P_{kl}(\{\rho^{\{1\}}, \dots, \rho^{\{k\}}\} | \alpha, \bar{\rho}(u)) P_{(n-k)l}(\{\rho^{\{k+1\}}, \dots, \rho^{\{n\}}\} | \bar{\rho}(u), \beta) \quad (\text{V.A.75})$$

In the large l limit, evaluating the previous expression at the saddle point, we obtain the following equation for the large deviation function

$$\mathcal{F}_n(\{\rho^{\{1\}}, \dots, \rho^{\{n\}}\} | \alpha, \beta) = \max_{0 < u < 1} \frac{k}{n} \ln\left(\frac{nu}{k}\right) + \frac{n-k}{n} \ln\left(\frac{n(1-u)}{n-k}\right) \\ + \frac{k}{n} \mathcal{F}_k(\{\rho^{\{1\}}, \dots, \rho^{\{k\}}\} | \alpha, \bar{\rho}(u)) + \frac{n-k}{n} \mathcal{F}_{n-k}(\{\rho^{\{k+1\}}, \dots, \rho^{\{n\}}\} | \bar{\rho}(u), \beta) \quad (\text{V.A.76})$$

We repeat n times the same procedure to obtain

$$\mathcal{F}_n(\{\rho^{\{1\}}, \dots, \rho^{\{n\}}\} | \alpha, \beta) = \max_{0=u_0 < u_1 < \dots < u_n=1} \frac{1}{n} \sum_{k=1}^n \mathcal{F}_1(\rho^{\{k\}} | \bar{\rho}(u_{k-1}), \bar{\rho}(u_k)) \\ + \ln((u_k - u_{k-1})n) \quad (\text{V.A.77})$$

In the large n limit, we can define the continuous variable $x = k/n$ and a function u such that $u(x) = u_k$. The sequence u_k being monotone, the difference $u_k - u_{k-1}$ is small in this limit. Hence we have that $\bar{\rho}(u_{k-1}) \simeq \bar{\rho}(u_k)$ and we can replace $\mathcal{F}_1(\rho^{\{k\}} | \bar{\rho}(u_{k-1}), \bar{\rho}(u_k))$ by the equilibrium value $\mathcal{F}_1(\rho^{\{k\}} | \bar{\rho}(u_k), \bar{\rho}(u_k)) = B(\rho^{\{k\}} | \bar{\rho}(u_k))$. We thus obtain

$$\mathcal{F}(\{\rho(x)\} | \alpha, \beta) = \max_{u(x)} \int_0^1 dx \left[B(\rho(x), \bar{\rho}(u(x))) + \ln u'(x) \right], \quad (\text{V.A.78})$$

where the maximum is evaluated over the increasing functions u satisfying $u(0) = 0$ and $u(1) = 1$. The Euler-Lagrange equation associated with the maximization over u of this functional gives the differential equation (V.A.74). ■

Let us stress that exact computation, from finite size lattice, of the large deviation functional of the density profile has only be achieved on a few out-of-equilibrium models, including the SSEP [245, 250] and the ASEP [246, 247].

B Macroscopic fluctuation theory

The computations done in the previous subsection were all about the stationary state of the models in the large size limit. We are now interested in the study of the full dynamics of the models in the thermodynamic limit. The idea is quite the same as for the study of the density profile in the stationary state. We would like to introduce coarse-grained variables (such as macroscopic particle density or current) that will depend on space and time. We expect that all the details of the microscopic dynamics of the model will be averaged out and that these coarse grained variables will satisfy deterministic equations depending only on a small number of physically relevant parameters in the large size limit.

For instance it has been proved rigorously for the ASEP with weak asymmetry, *i.e* $p - q = \nu/L$, that the macroscopic density $\rho(x, t)$ satisfies the Burger equation with viscosity²

$$\frac{\partial \rho}{\partial t} = \frac{\partial^2 \rho}{\partial x^2} - 2\nu \frac{\partial \rho(1 - \rho)}{\partial x}. \quad (\text{V.B.1})$$

In the particular case of the SSEP, *i.e* when $\nu = 0$, the macroscopic density satisfies the heat equation

$$\frac{\partial \rho}{\partial t} = \frac{\partial^2 \rho}{\partial x^2}. \quad (\text{V.B.2})$$

These results on deterministic equations tell that the probability to observe a given time evolution, path history, of the coarse-grained variables tends to 1 in the thermodynamic limit if this time evolution satisfies the deterministic equation and tends to 0 otherwise. We are now interested in a refined result. We would like to evaluate the probability of rare events, when the temporal evolution of the macroscopic variables deviates from the typical evolution governed by the deterministic equation. These rare events show up with an exponentially weak probability in the system size L , giving rise to a large deviation principle. This approach is called the macroscopic fluctuation theory (MFT) and is the whole topic of the remaining part of this chapter. We will see that this framework gives in principle access to the fluctuations of the particle current and density profile at the price of minimizing an action or equivalently at the price of solving a system of non linear coupled partial differential equations (the associated Euler-Lagrange equations). The MFT has been in particular successfully applied to characterize dynamical phase transitions, see for instance [19, 20]. For the sake of simplicity, we start by presenting this theory on the case of single species diffusive models (the theory was first introduced to describe this class of systems) and we show its efficiency to derive the fluctuations of the current and density in the stationary state. The goal is to present the main tools and techniques that are provided by this theory. We then present extensions of this theory (to dissipative systems or to multi-species systems) that are suitable to describe the models studied all along this manuscript: the DiSSEP and the multi-species SSEP. We will in particular derive results about current and density fluctuations in the stationary state through the MFT framework and check the consistency with exact computations that were done for a finite size lattice in chapter III.

1 Single species diffusive systems

a) General idea

The macroscopic fluctuation theory (MFT) is a general approach that aims to describe out of equilibrium diffusive particle gases in the thermodynamic limit. It was developed a few years ago by Bertini, De Sole, Gabrielli, Jona-Lasinio and Landim [251, 252], and has proven to be an efficient way to compute fluctuations of the current and of the density profile. One strength of this theory is to describe the diffusive systems through only two key parameters, the diffusion constant $D(\rho)$ and the conductivity $\sigma(\rho)$ which depend on the local particle density ρ . These parameters can be determined case by case from the microscopic dynamics of the model. See [253] for a detailed review. Some validations from a microscopic point of view were realised for exactly solvable models including the SSEP [16, 245, 249, 250].

The first step toward this macroscopic, or hydrodynamic, description is to define coarse-grained variables. We recall that we study here the case of systems with a single species of particle. The framework of the MFT presented here allows to describe models with possibly several particles on the same site (this number can have an upper bound to describe exclusion or not) and encompasses in particular the example of the single species SSEP. We recall that the occupation number $\rho_1^{(i)}$ is equal to the number of particles lying on site i . We introduce

²This equation can be heuristically derived by writing the time evolution of the mean particle density and performing a mean-field approximation, *i.e* simplifying the two-point correlation functions that appear into the product of two one-point functions.

the random variables $\rho^{(t,i)} := \rho_1^{(i)}(C_t)$. We recall also that the random variable C_t denote the configuration of the system at time t . Its probability law satisfies the master equation of the model. In other words $\rho^{(t,i)}$ is equal to the number of particle on the site i and at time t .

Definition B.1. We define, for L large, the macroscopic density of particles $\rho(x, t)$ at time³ t and at position $x \in [0, 1]$ on the lattice by

$$\rho(x, t) = \frac{1}{2\sqrt{L}} \sum_{|i-Lx| \leq \sqrt{L}} \rho^{(L^2t, i)}. \quad (\text{V.B.3})$$

Note that the macroscopic density $\rho(x, t)$ is a random variable which is intuitively understood as the average number of particles per site in a box of size $2\sqrt{L}$ (which explains the denominator in the definition) around site Lx at time L^2t .

We also need to define the macroscopic current of particles. We denote by $Q^{(t, i \rightarrow i+1)}$ the algebraic number of particles that have crossed the bound between sites i and $i+1$ (from left to right) during the time interval $[0, t]$. It allows us to give the following definition.

Definition B.2. We introduce, for L large,

$$Q(x, t) = \frac{1}{2L\sqrt{L}} \sum_{|i-Lx| \leq \sqrt{L}} Q^{(L^2t, i \rightarrow i+1)}. \quad (\text{V.B.4})$$

Definition B.3. The macroscopic particle current $j(x, t)$ at time t and at position x is then defined as

$$j(x, t) = \frac{\partial}{\partial t} Q(x, t). \quad (\text{V.B.5})$$

We mentioned that the hydrodynamic description of the model relies on two key parameters. This motivates the following definition.

Definition B.4. We introduce the diffusion constant $D(\rho)$ that satisfies for ρ_l and ρ_r both close to the value ρ

$$\lim_{t \rightarrow \infty} \frac{\langle Q^{(t, i \rightarrow i+1)} \rangle}{t} = \frac{D(\rho)(\rho_l - \rho_r)}{L} \quad (\text{V.B.6})$$

and the conductivity $\sigma(\rho)$ that satisfies for $\rho_l = \rho_r = \rho$

$$\lim_{t \rightarrow \infty} \frac{\langle (Q^{(t, i \rightarrow i+1)})^2 \rangle}{t} = \frac{\sigma(\rho)}{L} \quad (\text{V.B.7})$$

These two parameters are model dependent and has to be computed case by case from the microscopic dynamics of the model. They have been computed exactly in particular for the SSEP and for free random walkers (also called Brownian particles). We recall that the model of free random walkers is defined as a particular case of the zero range process with $p = q = 1$ and $w_n = n$ (see remark A.1).

Proposition B.5. For the single species SSEP we have

$$D(\rho) = 1, \quad \sigma(\rho) = 2\rho(1 - \rho), \quad (\text{V.B.8})$$

and for free random walkers we have

$$D(\rho) = 1, \quad \sigma(\rho) = 2\rho. \quad (\text{V.B.9})$$

We are now equipped to present the main result associated with MFT.

³Note that in order to do this hydrodynamic limit, we will rescale in all this section the time with a factor L^2 , as usual in this context of diffusive systems.

Proposition B.6. *The probability to observe a given path history of the macroscopic density and current profiles $\{\rho(x, t), j(x, t)\}$ during a time interval $[t_1, t_2]$ satisfies the large deviation principle*

$$P(\{\rho(x, t), j(x, t)\}) \sim \exp \left[-L \int_{t_1}^{t_2} dt \int_0^1 dx \frac{(j(x, t) + D(\rho(x, t))\partial_x \rho(x, t))^2}{2\sigma(\rho(x, t))} \right], \quad (\text{V.B.10})$$

where the fields satisfy the usual conservation law

$$\frac{\partial}{\partial t} \rho(x, t) = -\frac{\partial}{\partial x} j(x, t), \quad (\text{V.B.11})$$

and the boundary conditions

$$\rho(0, t) = \rho_l, \quad \rho(1, t) = \rho_r. \quad (\text{V.B.12})$$

Remark B.7. *The large deviation functional in (V.B.10) vanishes when the path history of the current and density profiles follows the typical time evolution (which can be seen as the Fick's law)*

$$j(x, t) = -D(\rho(x, t))\partial_x \rho(x, t). \quad (\text{V.B.13})$$

Remark B.8. *The large deviation functional can be heuristically interpreted as the description of current and density profiles satisfying a Langevin-like equation*

$$\begin{cases} \partial_t \rho(x, t) = \partial_x j(x, t) \\ j(x, t) = -D(\rho(x, t))\partial_x \rho(x, t) + \sqrt{\sigma(\rho(x, t))}\xi(x, t), \end{cases} \quad (\text{V.B.14})$$

where $\xi(x, t)$ is a Gaussian white noise with $\langle \xi(x, t) \rangle = 0$ and $\langle \xi(x, t)\xi(x', t') \rangle = \delta(x - x')\delta(t - t')/L$.

Remark B.9. *In the weakly asymmetric simple exclusion process (i.e the ASEP with the weak asymmetry scaling $p - q = \nu/L$), the large deviation functional is modified to*

$$\int_{t_1}^{t_2} dt \int_0^1 dx \frac{(j(x, t) + D(\rho(x, t))\partial_x \rho(x, t) - \nu\sigma(\rho(x, t)))^2}{2\sigma(\rho(x, t))}. \quad (\text{V.B.15})$$

For the ASEP without the weak asymmetry scaling, the situation is more complicated. The coarse grained variable $\rho(x, t)$ converges in the large size L limit (with a ballistic scaling, i.e time is accelerated with a factor L instead of a factor L^2 in the diffusive scaling case) to the inviscid Burger equation

$$\partial_t \rho(x, t) = -(p - q)\partial_x (\rho(x, t)(1 - \rho(x, t))) \quad (\text{V.B.16})$$

which is a well-known example of shock wave formation in partial differential equations theory. To the best of our knowledge, a macroscopic fluctuation theory description of such model has not yet been provided.

Note that from a physical point of view, the large deviation functional can be intuitively understood as an action (associated to a path history of the density and current profiles, that are the reduced phase space variables of the system in this coarse-grained description). The probability of the path history then reads as exponential of minus an action (which makes the physicists think to the path integral formalism in quantum mechanics). More precisely we have the following statement.

Proposition B.10. *The probability to observe at time t_2 a density profile $\rho_f(x)$ and a current profile $j_f(x)$, knowing that the density and current profiles were equal to $\rho_i(x)$ and $j_i(x)$, can be written as the path integral*

$$P(\rho_f(x), j_f(x) \mid \rho_i(x), j_i(x)) = \int \mathcal{D}\rho \mathcal{D}j \exp \left(-L \int_{t_1}^{t_2} dt \int_0^1 dx \frac{(j + D(\rho)\partial_x \rho)^2}{2\sigma(\rho)} \right) \quad (\text{V.B.17})$$

where the functional integral is performed over fields $\rho(x, t)$ and $j(x, t)$ that satisfy the particles conservation law

$$\partial_t \rho = -\partial_x j, \quad (\text{V.B.18})$$

the boundary conditions

$$\rho(0, t) = \rho_l, \quad \rho(1, t) = \rho_r, \quad (\text{V.B.19})$$

and the initial and final conditions

$$\rho(x, t_1) = \rho_i(x), \quad j(x, t_1) = j_i(x) \quad \text{and} \quad \rho(x, t_2) = \rho_f(x), \quad j(x, t_2) = j_f(x). \quad (\text{V.B.20})$$

In the large system size $L \rightarrow \infty$, the path integral (V.B.17) can be evaluated through a saddle point (for density and current profiles that minimize the action). This yields the following result.

Proposition B.11. *We have the large deviation principle*

$$P(\rho_f(x), j_f(x) \mid \rho_i(x), j_i(x)) \sim \exp\left(-L \min_{\rho, j} \int_{t_1}^{t_2} dt \int_0^1 dx \frac{(j + D(\rho)\partial_x \rho)^2}{2\sigma(\rho)}\right), \quad (\text{V.B.21})$$

where the minimum is taken over fields $\rho(x, t)$ and $j(x, t)$ satisfying the constraints (V.B.18), (V.B.19) and (V.B.20).

We thus have to minimize an action over two fields that are coupled through the equation (V.B.18). This problem of minimization under constraints can be tackled using the Lagrange multipliers. We introduce a third field $\pi(x, t)$ that will play the role of the Lagrange multipliers. The problem is reduced to the minimization of

$$\int_{t_1}^{t_2} dt \int_0^1 dx \left[\frac{(j + D(\rho)\partial_x \rho)^2}{2\sigma(\rho)} + (\partial_t \rho + \partial_x j)\pi \right] := \int_{t_1}^{t_2} dt \int_0^1 dx \mathcal{L}(\rho, \partial_x \rho, \partial_t \rho, j, \partial_x j), \quad (\text{V.B.22})$$

over the fields ρ and j that are now considered as independent. It is now possible to write down the Euler-Lagrange equations associated to this modified action. This yields the two following equations.

Proposition B.12. *The Euler-Lagrange equations satisfied by the optimal profiles $\hat{\rho}(x, t)$ and $\hat{j}(x, t)$ that minimize the action (V.B.22) are*

$$\hat{j} = \sigma(\hat{\rho})\partial_x \pi - D(\hat{\rho})\partial_x \hat{\rho} \quad (\text{V.B.23})$$

and

$$\partial_t \pi = -D(\hat{\rho})\partial_{xx} \pi - \frac{1}{2}\sigma'(\hat{\rho})(\partial_x \pi)^2. \quad (\text{V.B.24})$$

Proof. We have indeed

$$\frac{d}{dx} \partial_{\partial_x j} \mathcal{L} = \partial_j \mathcal{L}, \quad (\text{V.B.25})$$

which can be simplified to

$$\partial_x \pi = \frac{\hat{j} + D(\hat{\rho})\partial_x \hat{\rho}}{\sigma(\hat{\rho})}. \quad (\text{V.B.26})$$

This yields the first equation of the proposition. The second Euler-Lagrange equation is given by

$$\frac{d}{dt} \partial_{\partial_t \rho} \mathcal{L} + \frac{d}{dx} \partial_{\partial_x \rho} \mathcal{L} = \partial_\rho \mathcal{L}, \quad (\text{V.B.27})$$

which leads, through an explicit computation of the partial derivatives, to

$$\partial_t \pi + \frac{d}{dx} \left[D(\hat{\rho}) \frac{\hat{j} + D(\hat{\rho})\partial_x \hat{\rho}}{\sigma(\hat{\rho})} \right] = D'(\hat{\rho})\partial_x \pi - \frac{1}{2}\sigma'(\hat{\rho})(\partial_x \pi)^2. \quad (\text{V.B.28})$$

This can be simplified using the first Euler-Lagrange equation and yields the second equation of the proposition. \blacksquare

Proposition B.13. *The optimal density and current profiles $\hat{\rho}$ and \hat{j} that minimize the action (V.B.21) are obtained by solving the following system of coupled non-linear partial differential equations*

$$\partial_t \hat{\rho} = \partial_x (D(\hat{\rho}) \partial_x \hat{\rho}) - \partial_x (\sigma(\hat{\rho}) \partial_x \pi) \quad (\text{V.B.29})$$

and

$$\partial_t \pi = -D(\hat{\rho}) \partial_{xx} \pi - \frac{1}{2} \sigma'(\hat{\rho}) (\partial_x \pi)^2, \quad (\text{V.B.30})$$

where π is an auxiliary field and \hat{j} is obtained through

$$\hat{j} = \sigma(\hat{\rho}) \partial_x \pi - D(\hat{\rho}) \partial_x \hat{\rho}. \quad (\text{V.B.31})$$

Proof. We just need to prove the first equation. It is obtained starting from

$$\hat{j} = \sigma(\hat{\rho}) \partial_x \pi - D(\hat{\rho}) \partial_x \hat{\rho}, \quad (\text{V.B.32})$$

taking the derivative with respect to x and using the fact that $\partial_t \hat{\rho} = -\partial_x \hat{j}$. \blacksquare

These equations allow us in principle to compute large deviation functionals of the current and density profiles directly at the macroscopic scale without having to study in details the microscopic dynamics of the model and to deal often with intractable combinatorial problems. The microscopic dynamics of the system is completely encapsulated in the diffusion D and the conductivity σ . The formalism presented here can in principle apply to a wide range of diffusive systems. But in practice these coupled non-linear partial differential equations are very hard to solve. Even for the SSEP, for which the value of $D(\rho)$ and $\sigma(\rho)$ have been computed exactly and take a rather simple expression, the exact solutions to these coupled differential equations are not known to the best of our knowledge. Nevertheless, we will see below that several techniques have been developed within this MFT framework to compute explicitly current and density fluctuations in the particular case of the stationary state.

b) Stationary state

We are now interested in what can be deduced from the large deviation principle (V.B.10) about the properties of the stationary state of the model. It appears indeed plausible that knowing information about the full dynamics (through this estimation of a path history probability) may give insight on the steady state. More precisely, two quantities are of prime interest in non-equilibrium stationary state, because they could be a generalization of the thermodynamic potentials far from equilibrium: the large deviation function of the particle current and the large deviation functional of the density profile. It turns out that these quantities can be in principle obtained, for a wide range of diffusive models, using the MFT formalism.

It was shown in [251] that the large deviation functional of the density profile in the stationary state is obtained by determining the optimal density and current profile $\rho(x, t)$ and $j(x, t)$ which produces an atypical density profile starting from the stationary typical profile $\bar{\rho}(x)$. More precisely we have the statement

Proposition B.14. *The large deviation functional of the density profile can be expressed in the MFT formalism by*

$$\mathcal{F}(\{\rho(x)\}) = \min_{\rho(x,t), j(x,t)} \int_{-\infty}^T dt \int_0^1 dx \frac{(j(x, t) + D(\rho(x, t)) \partial_x \rho(x, t))^2}{2\sigma(\rho(x, t))}, \quad (\text{V.B.33})$$

where the minimum is taken over the density and current profiles $\rho(x, t)$ and $j(x, t)$ that satisfy the particle conservation law

$$\partial_t \rho(x, t) = -\partial_x j(x, t), \quad (\text{V.B.34})$$

the boundary conditions

$$\rho(0, t) = \rho_l, \quad \rho(1, t) = \rho_r, \quad (\text{V.B.35})$$

and the limit conditions

$$\rho(x, -\infty) = \bar{\rho}(x), \quad \rho(x, T) = \rho(x). \quad (\text{V.B.36})$$

The profile $\bar{\rho}(x)$ denotes the mean density profile of the model.

Remark B.15. Note that this correspond to large deviation principle we saw previously (V.B.21) with $t_1 = -\infty$, $t_2 = T$, $\rho_i(x) = \bar{\rho}(x)$, $j_i(x) = \bar{j}$ and $\rho_f = \rho(x)$ (the value of $j_f(x)$ is not fixed, we have also to minimize over this quantity).

Definition B.16. We introduce the following function

$$U(x) = \frac{\delta \mathcal{F}(\{\rho(x)\})}{\delta \rho(x)}. \quad (\text{V.B.37})$$

Proposition B.17. The function U' has to satisfy the Hamilton-Jacobi equation

$$\int_0^1 dx \left[\left(\frac{D(\rho)\rho'}{\sigma(\rho)} - U' \right)^2 - \left(\frac{D(\rho)\rho'}{\sigma(\rho)} \right)^2 \right] \frac{\sigma(\rho)}{2} = 0 \quad (\text{V.B.38})$$

Proof. Following the lines of [16], we observe that the large deviation functional (V.B.33) should not depend on the time T . We thus have that

$$\mathcal{F}(\{\rho(x)\}) = \min_{\delta\rho(x), j(x)} \left[\mathcal{F}(\{\rho(x) - \delta\rho(x)\}) + \delta T \int_0^1 dx \frac{(j(x) + D(\rho(x))\rho'(x))^2}{2\sigma(\rho(x))} \right]. \quad (\text{V.B.39})$$

The particle conservation law imposes that $\delta\rho(x) = -\delta T \times j'(x)$. The equation right above can thus be rewritten

$$\mathcal{F}(\{\rho(x)\}) = \min_{j(x)} \left[\mathcal{F}(\{\rho(x)\}) + \delta T \int_0^1 dx U(x)j'(x) + \delta T \int_0^1 dx \frac{(j(x) + D(\rho(x))\rho'(x))^2}{2\sigma(\rho(x))} \right]. \quad (\text{V.B.40})$$

The optimal current profile $\hat{j}(x)$ is obtained through the Euler-Lagrange equation

$$\frac{\hat{j}(x) + D(\rho(x))\rho'(x)}{\sigma(\rho(x))} = U'(x). \quad (\text{V.B.41})$$

Plugging back in (V.B.40) yields

$$\int_0^1 dx \left[U(x)\hat{j}'(x) + \frac{\sigma(\rho(x))}{2} U'(x)^2 \right] = 0. \quad (\text{V.B.42})$$

We can integrate by part $U(x)\hat{j}'(x)$ using the fact that $U(0) = U(1) = 0$ because of the boundary conditions. \blacksquare

Solving this Hamilton-Jacobi equation gives in principle access to the large deviation functional of the density profile $\mathcal{F}(\{\rho(x)\})$ through the relation (V.B.37). In practice for general values of the diffusion $D(\rho)$ and of the conductivity $\sigma(\rho)$ we don't know how to solve this equation. It has only been solved for a very few models including the SSEP [16, 249], the weakly asymmetric simple exclusion process [254, 255] and the Kipnis-Marchioro-Presutti model [256, 257].

We now turn to the study of the fluctuations of the current in the stationary state. We are interested in the large deviation of the integrated current

$$\int_0^1 dx Q(x, T) = \int_0^T dt \int_0^1 dx j(x, t) \quad (\text{V.B.43})$$

when the time $T \rightarrow \infty$. One way to address the problem is to first study the generating function of the cumulants of the integrated current $G(\tau)$ (the large deviation function can be

obtained from the generating function through a Legendre transform, see chapter I). We recall that $G(\tau)$ is defined as

$$G(\tau) = \lim_{T \rightarrow \infty} \lim_{L \rightarrow \infty} \frac{1}{LT} \ln \mathbb{E}_{[0,T]} \left(\exp \left(\tau \int_0^T dt \int_0^1 dx j(x,t) \right) \right) \quad (\text{V.B.44})$$

where $\mathbb{E}_{[0,T]}$ denotes the expectation value with respect to the probability distribution on the path history of current and density profiles on the time interval $[0, T]$. The large deviation principle given by the MFT (V.B.10) allows us to reduce this computation to an optimization problem

$$G(\tau) = \lim_{T \rightarrow \infty} \frac{1}{T} \sup_{\rho(x,t), j(x,t)} \left[\tau \int_0^T dt \int_0^1 dx j(x,t) - \int_0^T dt \int_0^1 dx \frac{(j(x,t) + D(\rho(x,t)) \partial_x \rho(x,t))^2}{2\sigma(\rho(x,t))} \right]. \quad (\text{V.B.45})$$

If some constraints are assumed on the dynamics of the model (the reader is invited to refer to [253] for details), this is equivalent to a stationary optimization problem where the optimal profiles can be chosen independent of time. In this case, due to the particle conservation law, we have $\partial_x j = -\partial_t \rho = 0$. Hence the optimal current profile is constant in space and we have

$$G(\tau) = \sup_{\rho(x), j} \left(\tau j - \int_0^1 dx \frac{(j + D(\rho(x)) \rho'(x))^2}{2\sigma(\rho(x))} \right) \quad (\text{V.B.46})$$

$$= \sup_j \left(\tau j - \inf_{\rho(x)} \int_0^1 dx \frac{(j + D(\rho(x)) \rho'(x))^2}{2\sigma(\rho(x))} \right). \quad (\text{V.B.47})$$

We recognize exactly a Legendre transformation with respect to j (see chapter I), and hence we can identify the large deviation of the integrated current. This yields the following proposition.

Proposition B.18. *The large deviation of the integrated current can be expressed as*

$$\mathcal{F}(j) = \min_{\rho(x)} \int_0^1 dx \frac{(j + D(\rho(x)) \rho'(x))^2}{2\sigma(\rho(x))} \quad (\text{V.B.48})$$

Proposition B.19. *The large deviation function of the current is given by*

$$\mathcal{F}(j) = j \int_{\rho_r}^{\rho_l} d\rho \frac{D(\rho)}{\sigma(\rho)} \left[\frac{1 + K\sigma(\rho)}{\sqrt{1 + 2K\sigma(\rho)}} - 1 \right], \quad (\text{V.B.49})$$

where the constant K is fixed by the condition

$$\int_{\rho_r}^{\rho_l} d\rho \frac{D(\rho)}{\sqrt{1 + 2K\sigma(\rho)}} = j. \quad (\text{V.B.50})$$

The large deviation function of the particle current is thus obtained in parametric form.

Proof. We want to minimize the action

$$\min_{\rho(x)} \int_0^1 dx \frac{(j + D(\rho(x)) \rho'(x))^2}{2\sigma(\rho(x))} \quad (\text{V.B.51})$$

over the density profile $\rho(x)$ for a fixed current j (independent of the position x). Expanding the square gives

$$\min_{\rho(x)} \int_0^1 dx \left[\frac{j^2}{2\sigma(\rho(x))} + \frac{D(\rho(x))^2 \rho'(x)^2}{2\sigma(\rho(x))} + \frac{j D(\rho(x)) \rho'(x)}{\sigma(\rho(x))} \right] \quad (\text{V.B.52})$$

$$= \min_{\rho(x)} \int_0^1 dx \left[\frac{j^2}{2\sigma(\rho(x))} + \frac{D(\rho(x))^2 \rho'(x)^2}{2\sigma(\rho(x))} \right] - \int_{\rho_r}^{\rho_l} d\rho \frac{D(\rho)}{\sigma(\rho)} \quad (\text{V.B.53})$$

We are thus only left with the minimization of the first term in the previous sum (the second one is now independent of the profile $\rho(x)$). The associated Euler-Lagrange equation reads

$$j^2 \partial_\rho \left(\frac{1}{2\sigma(\hat{\rho})} \right) + (\hat{\rho}')^2 \partial_\rho \left(\frac{D(\hat{\rho})^2}{2\sigma(\hat{\rho})} \right) = \partial_x \left(\frac{D(\hat{\rho})^2 \hat{\rho}'}{\sigma(\hat{\rho})} \right), \quad (\text{V.B.54})$$

where $\hat{\rho}(x)$ is the optimal density profile. Multiplying by $\hat{\rho}'(x)$ leads to

$$\partial_x \left(\frac{j^2}{2\sigma(\hat{\rho}(x))} - \frac{D(\hat{\rho}(x))^2 \hat{\rho}'(x)^2}{2\sigma(\hat{\rho}(x))} \right) = 0 \quad (\text{V.B.55})$$

Hence there exists an integration constant K such that

$$\hat{\rho}'(x)^2 = \frac{j^2(1 + 2K\sigma(\hat{\rho}(x)))}{D(\hat{\rho}(x))^2} \quad (\text{V.B.56})$$

The constant K is fixed to satisfy the conditions $\hat{\rho}(0) = \rho_l$ and $\hat{\rho}(1) = \rho_r$ on the boundaries. If the value of the current j does not deviate too much from the typical value \bar{j} , we expect the optimal profile to be monotone (more precisely decreasing if we assume that $\rho_l > \rho_r$). We thus have

$$- \frac{\hat{\rho}'(x) D(\hat{\rho}(x))}{\sqrt{1 + 2K\sigma(\hat{\rho}(x))}} = j. \quad (\text{V.B.57})$$

Integrating this last equation for x ranging from 0 to 1 leads to (V.B.50). Moreover, plugging the value of $\rho'(x)$ obtained in (V.B.57) in the action yields (V.B.49). \blacksquare

Remark B.20. *This parametric form of the current large deviation function was obtained in [248] with a different method by assuming an additivity principle of the large deviation function with respect to the system size. This principle reads*

$$\mathcal{F}_{L'+L''}(j, \rho_l, \rho_r) = \min_{\rho} (\mathcal{F}_{L'}(j, \rho_l, \rho) + \mathcal{F}_{L''}(j, \rho, \rho_r)), \quad (\text{V.B.58})$$

where $\mathcal{F}_L(j, \rho_l, \rho_r)$ denotes the large deviation functional of the current in a system of size L with reservoir densities ρ_l and ρ_r . The equivalence between these two methods suggests that the additivity principle holds only when the optimal density profile that produces a given current deviation is independent of time.

2 Single species systems with dissipation

a) Large deviation functional

The macroscopic fluctuation theory can be extended to a larger class of system with bulk dissipation [258, 259]. More precisely we are interested in models describing lattice gas with diffusive dynamics and creation/annihilation of particles in the bulk, which are driven out of equilibrium by two reservoirs at different densities. An example of such model is the DiSSEP that was presented and studied in details in chapter III.

We will start by presenting how the large deviation functional of the path history should be modified to include the creation/annihilation dynamics in addition to the diffusive part that we already encountered in the previous subsection. This will be a short summary of the work [258], the reader is invited to study this reference for the details. We will focus on the particular case of the DiSSEP. The MFT framework will be used to compute the variance of the current on the lattice that will be checked against the exact value computed from the microscopic point of view in chapter III (and whose thermodynamic limit was obtained in subsection b)).

Let us start by briefly presenting the key ingredients of the MFT related to our model. A detailed presentation can be found in [258, 259]. It has been shown that the microscopic behavior of the system can be averaged in the thermodynamic limit and can be described at the macroscopic level by a small number of relevant parameters: $D(\rho)$, $\sigma(\rho)$, $A(\rho)$ and $C(\rho)$.

These parameters depend on the microscopic dynamics of the model and have to be computed for each different model.

The two first are related to the diffusive dynamics on the lattice: $D(\rho)$ is the diffusion coefficient and $\sigma(\rho)$ is the conductivity already introduced in the previous subsection for purely diffusive systems. For systems with creation and annihilation, these parameters are defined by considering the systems in which the creation/annihilation dynamics has been switched off (leaving only the diffusive dynamics on), and applying on those reduced purely diffusive model the same definition B.4.

Proposition B.21. *For the DiSSEP, the diffusive dynamics is the same as for the SSEP and hence the diffusion and conductivity take the values*

$$D(\rho) = 1 \quad \text{and} \quad \sigma(\rho) = 2\rho(1 - \rho). \quad (\text{V.B.59})$$

The two other parameters $A(\rho)$ and $C(\rho)$ are related to the creation-annihilation dynamics. $A(\rho)$ can be understood intuitively as the mean number of particles annihilated per site and per unit of time when the density profile is identically flat and equal to ρ in the system whereas $C(\rho)$ stands for the mean number of particles created. A rigorous definition of these parameters for general dissipative models can be found in [258]. We give the precise definition in the case of the DiSSEP dynamics.

Definition B.22.

$$\frac{A(\rho)}{L^2} = \langle \lambda^2 \tau_{i-1} \tau_i \rangle_\rho + \langle \lambda^2 \tau_i \tau_{i+1} \rangle_\rho \quad (\text{V.B.60})$$

and

$$\frac{C(\rho)}{L^2} = \langle \lambda^2 (1 - \tau_{i-1})(1 - \tau_i) \rangle_\rho + \langle \lambda^2 (1 - \tau_i)(1 - \tau_{i+1}) \rangle_\rho, \quad (\text{V.B.61})$$

where $\langle \cdot \rangle_\rho$ denotes the expectation value with respect to the Bernoulli probability density

$$\binom{1 - \rho}{\rho} \otimes \dots \otimes \binom{1 - \rho}{\rho}. \quad (\text{V.B.62})$$

Note that for general dissipative processes this definition should be adapted accordingly to the local creation/annihilation dynamics in the bulk.

Proposition B.23. *For the DiSSEP, annihilation rate $A(\rho)$ is given by*

$$A(\rho) = 2\lambda_0^2 \rho^2 \quad (\text{V.B.63})$$

and the creation rate $C(\rho)$ by

$$C(\rho) = 2\lambda_0^2 (1 - \rho)^2. \quad (\text{V.B.64})$$

Before stating the large deviation principle associated to dissipative models, we first need to define the coarse-grained variable corresponding to the creation annihilation current. We denote by $K^{(t,i)}$ the number of particles created minus the number of particles annihilated at site i during the time interval $[0, t]$. It allows us to give the following definition.

Definition B.24. *We introduce, for L large,*

$$K(x, t) = \frac{1}{2\sqrt{L}} \sum_{|i-Lx| \leq \sqrt{L}} K^{(L^2 t, i)}. \quad (\text{V.B.65})$$

Definition B.25. *The macroscopic particle creation/annihilation current $k(x, t)$ at time t and at position x is then defined as*

$$k(x, t) = \frac{\partial}{\partial t} K(x, t). \quad (\text{V.B.66})$$

When the number of sites L goes to infinity, the probability of observing a given history of the density profile ρ , of the lattice current j and of the creation-annihilation current k during the time interval $[0, T]$, can be written as⁴

Proposition B.26.

$$\mathbb{P}_{[0,T]}(\{\rho, j, k\}) \sim \exp[-L\mathcal{I}_{[0,T]}(\rho, j, k)], \quad (\text{V.B.67})$$

with the large deviation functional

$$\mathcal{I}_{[0,T]}(\rho, j, k) = \int_0^T dt \int_0^1 dx \left\{ \frac{(j(x, t) + D(\rho(x, t))\partial_x \rho(x, t))^2}{2\sigma(\rho(x, t))} + \Phi(\rho(x, t), k(x, t)) \right\}, \quad (\text{V.B.68})$$

where

$$\Phi(\rho, k) = \frac{1}{2} \left[A(\rho) + C(\rho) - \sqrt{k^2 + 4A(\rho)C(\rho)} + k \ln \left(\frac{\sqrt{k^2 + 4A(\rho)C(\rho)} + k}{2C(\rho)} \right) \right]. \quad (\text{V.B.69})$$

The quantities ρ , j and k are related through the conservation equation

$$\partial_t \rho(x, t) = -\partial_x j(x, t) + k(x, t), \quad (\text{V.B.70})$$

and the value of ρ is fixed on the boundaries $\rho(0, t) = \rho_l$, $\rho(1, t) = \rho_r$.

Note that the factor $1/2$ in the definition of Φ is a slight modification in comparison to [258] due to the fact that we consider here creation-annihilation of pairs of particles instead of creation-annihilation of single particles.

The minimum of the large deviation functional $\mathcal{I}_{[0,T]}$ is achieved when the particle currents take their typical values, that is $j(x, t) = -D(\rho(x, t))\partial_x \rho(x, t)$ and $k(x, t) = C(\rho(x, t)) - A(\rho(x, t))$. The typical evolution of the density profile is hence given by

$$\partial_t \rho(x, t) = \partial_x (D(\rho(x, t))\partial_x \rho(x, t)) + C(\rho(x, t)) - A(\rho(x, t)) \quad (\text{V.B.71})$$

which matches (V.A.10) for the DiSSEP.

b) Check with finite size lattice exact computations

Using the previous formalism and following [258], it is possible to compute the local variance of the lattice current j in the stationary regime. Due to the fact that the dynamics of the model does not conserve the number of particle, this current and its fluctuations depend on the position in the system. Hence, given a function $\tau(x)$, we want to compute the generating function of the cumulants of the integrated current $\int_0^T dt \int_0^1 dx \tau(x) j(x, t)$ for T going to infinity. This leads to the following definition.

Definition B.27. We introduce the generating function

$$\mathcal{F}(\{\tau(x)\}) = \lim_{T \rightarrow \infty} \lim_{L \rightarrow \infty} \frac{1}{LT} \ln \mathbb{E}_{[0,T]} \left(\exp \left(\int_0^T dt \int_0^1 dx \tau(x) j(x, t) \right) \right). \quad (\text{V.B.72})$$

The previous expression can be simplified using (V.B.67) and a saddle point method. It reduces to maximize a functional over the time dependent fields ρ , j and k . Assuming that the extremum of this functional is achieved for time independent profiles, we end up with the following expression (the reader is invited to refer to [258] for the details)

⁴The link with the quantities previously computed is given by the fact that in the stationary state the mean value of $j(x)$ is $\bar{j}_{lat}(x)$ and the mean value of $k(x)$ is $\bar{j}_{cond}(x)$.

Proposition B.28.

$$\mathcal{F}(\{\tau(x)\}) = \sup_{\rho, j} \left(\int_0^1 dx \tau(x) j(x) - \hat{\mathcal{I}}(\rho, j) \right), \quad (\text{V.B.73})$$

with

$$\hat{\mathcal{I}}(\rho, j) = \int_0^1 dx \left(\frac{(j(x) + D(\rho(x))\partial_x \rho(x))^2}{2\sigma(\rho(x))} + \Phi(\rho(x), \partial_x j(x)) \right). \quad (\text{V.B.74})$$

To compute the local variance of the lattice current j at the point y , it is enough to take $\tau(x) = \delta(x - y)$ and expand $\mathcal{F}(\{\epsilon\tau\})$ up to order ϵ^2 . For a small perturbation ϵ , the fields are expected to be close to their typical value

$$\rho(x) = \bar{\rho}(x) + \epsilon \frac{f(x)}{D(\bar{\rho}(x))}, \quad j(x) = -D(\bar{\rho}(x))\partial_x \bar{\rho}(x) + \epsilon q(x) \quad (\text{V.B.75})$$

with the constraint $f(0) = f(1) = 0$ due to the boundaries. We then obtain

$$\mathcal{F}(\{\epsilon\tau\}) = -\epsilon D(\bar{\rho}(y))\partial_x \bar{\rho}(y) + \frac{\epsilon^2}{2} E^{(2)}(y) \quad (\text{V.B.76})$$

with the variance of the lattice current at the point y

$$E^{(2)}(y) = 2 \sup_{q, f} \left\{ q(y) - \int_0^1 dx \left(\frac{(q(x) + f'(x))^2}{2\sigma(\bar{\rho}(x))} + \frac{(q'(x) + U(x)f(x))^2}{4(A(\bar{\rho}(x)) + C(\bar{\rho}(x)))} \right) \right\} \quad (\text{V.B.77})$$

and $U(x) = \frac{A'(\bar{\rho}(x)) - C'(\bar{\rho}(x))}{D(\bar{\rho}(x))} = 4\lambda_0^2$. We make the following change of variables to solve this optimization problem

$$\varphi(x) = \frac{q(x) + f'(x)}{\sigma(\bar{\rho}(x))}, \quad \psi(x) = \frac{q'(x) + U(x)f(x)}{2(A(\bar{\rho}(x)) + C(\bar{\rho}(x)))}, \quad (\text{V.B.78})$$

so that the Euler-Lagrange equations become for the DiSSEP:

$$\begin{cases} \psi'(x) = \varphi(x) - \delta(x - y) \\ \varphi'(x) = 4\lambda_0^2 \psi(x). \end{cases} \quad (\text{V.B.79})$$

Note that there are slight modifications in expressions (V.B.76) and (V.B.78) with respect to [258], in accordance with the modification of Φ (see discussion after (V.B.69)).

These equations can be solved analytically and we get

$$\begin{cases} \psi(x) = \frac{\theta(x \leq y) \sinh(2\lambda_0 x) \cosh(2\lambda_0(1 - y)) + \theta(x > y) \sinh(2\lambda_0(x - 1)) \cosh(2\lambda_0 y)}{\sinh 2\lambda_0} \\ \varphi(x) = \frac{2\lambda_0 [\theta(x \leq y) \cosh(2\lambda_0 x) \cosh(2\lambda_0(1 - y)) + \theta(x > y) \cosh(2\lambda_0(x - 1)) \cosh(2\lambda_0 y)]}{\sinh 2\lambda_0}. \end{cases} \quad (\text{V.B.80})$$

The function $q(x)$ can be also computed analytically by solving

$$q''(x) - 4\lambda_0^2 q(x) = \partial_x (2(A(\bar{\rho}(x)) + C(\bar{\rho}(x)))\psi(x)) - 4\lambda_0^2 \sigma(\bar{\rho}(x))\varphi(x). \quad (\text{V.B.81})$$

Note that it depends on y , see for instance the expressions (V.B.80). It allows us to deduce the expression of $q(x)$ at the special point y (as needed in (V.B.76))

$$q(y) = \int_0^1 dx [\sigma(\bar{\rho}(x))\varphi(x)^2 + 2(A(\bar{\rho}(x)) + C(\bar{\rho}(x)))\psi(x)^2], \quad (\text{V.B.82})$$

with φ and ψ are given above. Hence for the DiSSEP, the variance of the current lattice computed from MFT is

$$\begin{aligned} E^{(2)}(y) &= \int_0^1 dx [\sigma(\bar{\rho}(x))\varphi(x)^2 + 2(A(\bar{\rho}(x)) + C(\bar{\rho}(x)))\psi(x)^2] \\ &= \frac{4\lambda_0^2}{\sinh^2 2\lambda_0} \left[\cosh^2 2\lambda_0(1-y) \int_0^1 dx (\sigma(\bar{\rho}(x)) + \sinh^2 2\lambda_0 x) \right. \\ &\quad \left. + \cosh^2 2\lambda_0 y \int_0^1 dx (\sigma(\bar{\rho}(x)) + \sinh^2 2\lambda_0(1-x)) \right]. \end{aligned}$$

Using the explicit form for σ , we show that this result obtained from MFT matches perfectly the previous result (V.A.24) computed exactly from a microscopic description of the model.

The result obtained here points out the consistency of the MFT developed in [258], for a system with diffusion and dissipation, with exact computations performed for a finite size lattice.

3 Multi-species diffusive systems: the multi-SSEP case

a) Large deviation functional

In this section we propose, based on the exact microscopic computations, a hydrodynamic description of the multi-species SSEP which extends the MFT to systems with several species of particles. We check the consistency with the exact results derived in the previous subsection (about the large deviation functional of the density profile), the rigorous proof of the approach remains to be done.

The first step toward the hydrodynamic description of the multi-species SSEP is to defined coarse-grained, or average variables. In the same way as for the single species models, we introduce the random variables $\rho_\tau^{(t,i)} := \rho_\tau^{(i)}(C_t)$. We recall that the occupation number $\rho_\tau^{(i)}$ is equal to 1 if the local configuration at site i is equal to τ and 0 otherwise. We recall also that the random variable C_t denote the configuration of the system at time t . Its probability law satisfies the master equation of the model. In other words $\rho_\tau^{(t,i)}$ is equal to 1 if there is a particle (or hole) of species τ at site i and at time t and 0 otherwise.

Definition B.29. We define, for L large, the macroscopic density $\rho_\tau(x, t)$ of the species τ at time⁵ t and at position $x \in [0, 1]$ on the lattice by

$$\rho_\tau(x, t) = \frac{1}{2\sqrt{L}} \sum_{|i-Lx| \leq \sqrt{L}} \rho_\tau^{(L^2 t, i)}. \quad (\text{V.B.83})$$

We will also need the row vector

$$\boldsymbol{\rho}(x, t) = (\rho_0(x, t), \dots, \rho_N(x, t)). \quad (\text{V.B.84})$$

Note that the macroscopic density $\rho_\tau(x, t)$ is a random variable which is intuitively understood as the average number of particles of species τ in a box of size $2\sqrt{L}$ (which explains the denominator in the definition) around site Lx at time $L^2 t$.

We also need to define the macroscopic current of particles. We denote by $Q_\tau^{(t, i \rightarrow i+1)}$ the algebraic number of particles of species τ that have crossed the bound between sites i and $i+1$ (from left to right) during the time interval $[0, t]$. It allows us to give the following definition.

Definition B.30. We introduce, for L large,

$$Q_\tau(x, t) = \frac{1}{2L\sqrt{L}} \sum_{|i-Lx| \leq \sqrt{L}} Q_\tau^{(L^2 t, i \rightarrow i+1)}. \quad (\text{V.B.85})$$

⁵Again, in order to do this hydrodynamic limit, we will rescale in all this section the time with a factor L^2 , as usual in this context of diffusive systems.

Definition B.31. The macroscopic particle current $j_\tau(x, t)$ of species τ at time t and at position x is then defined as

$$j_\tau(x, t) = \frac{\partial}{\partial t} Q_\tau(x, t). \quad (\text{V.B.86})$$

We will also need the row vector

$$\mathbf{j}(x, t) = (j_0(x, t), \dots, j_N(x, t)). \quad (\text{V.B.87})$$

Rate function for the multi-species SSEP. The idea of the MFT is to express the probability to observe certain density profiles $\rho(x, t)$ and current profiles $\mathbf{j}(x, t)$ during the time interval $[t_1, t_2]$ as a large deviation principle. We present now one of the main result of this paper, which gives a new perspective on the rate function of diffusive models with exclusion which can be seen as that of a model of free particles but with an additional exclusion constraint.

Proposition B.32. We have the large deviation principle

$$P(\{\rho(x, t), \mathbf{j}(x, t)\}) \sim \exp \left[-L \int_{t_1}^{t_2} dt \int_0^1 dx \sum_{\tau=0}^N \frac{(j_\tau(x, t) + \partial_x \rho_\tau(x, t))^2}{4\rho_\tau(x, t)} \right], \quad (\text{V.B.88})$$

where the fields satisfy the usual conservation law

$$\frac{\partial}{\partial t} \rho(x, t) = -\frac{\partial}{\partial x} \mathbf{j}(x, t), \quad (\text{V.B.89})$$

the boundary conditions

$$\rho(0, t) = \alpha, \quad \rho(1, t) = \beta \quad (\text{V.B.90})$$

and the additional exclusion constraints

$$\rho_0(x, t) + \dots + \rho_N(x, t) = 1, \quad j_0(x, t) + \dots + j_N(x, t) = 0. \quad (\text{V.B.91})$$

The rate function (V.B.88) can be heuristically interpreted having in mind that, for Brownian particles, the diffusion constant is $D(\rho) = 1$ and the conductivity is $\sigma(\rho) = 2\rho$. The functional (V.B.88) is exactly the one that describes a model of independent Brownian particles of N different species, but on top of that we impose the exclusion constraint (V.B.91) which translates the fact that there is at most one particle per site. We recall that in our notation the holes (empty sites) are interpreted as a species of particles. This formula is supported by: (i) the consistency check with the large deviation functional of the density profile in the stationary state done in the next subsection, (ii) the following remark.

Remark B.33. The well known case of the SSEP with a single species and holes can be recovered from (V.B.88) by setting $N = 1$. We recall that the holes are labelled by 0 and the particles 1. We have in this case $j_1(x, t) = -j_0(x, t) := j(x, t)$ and $\rho_1(x, t) = 1 - \rho_0(x, t) := \rho(x, t)$ due to the constraints (V.B.91). Then the rate function in (V.B.88) becomes

$$\int_{t_1}^{t_2} dt \int_0^1 dx \frac{(j(x, t) + \partial_x \rho(x, t))^2}{4\rho(x, t)(1 - \rho(x, t))}, \quad (\text{V.B.92})$$

which agrees with the known expression for the single species SSEP (recall that the diffusion constant is given by $D(\rho) = 1$ and the conductivity by $\sigma(\rho) = 2\rho(1 - \rho)$).

b) Check with finite size lattice exact computations

Following what was done in [16], this framework allows us to express the probability to observe at time T a density profile $\rho(x)$ in the stationary state. We have to identify how this deviation is produced, i.e. we have to find the optimal path $\rho(x, t)$ such that $\rho(x, -\infty) = \bar{\rho}(x)$ and $\rho(x, T) = \rho(x)$:

$$\mathcal{F}(\{\rho(x)\} | \alpha, \beta) = \min_{\rho(x,t), \mathbf{j}(x,t)} \int_{-\infty}^T dt \int_0^1 dx \sum_{\tau=0}^N \frac{(j_\tau(x, t) + \partial_x \rho_\tau(x, t))^2}{4\rho_\tau(x, t)}. \quad (\text{V.B.93})$$

Note that the probability to observe a deviation in the density profile $\rho(x)$ does not depend on the time at which this deviation occurs. It means that (V.B.93) does not depend on T .

Cutting the integration interval $(-\infty, T]$ in (V.B.93) into two pieces $(-\infty, T - \delta T]$ and $[T - \delta T, T]$ yields

$$\mathcal{F}(\{\rho(x)\} | \alpha, \beta) = \min_{\delta\rho(x), \mathbf{j}(x)} \left[\mathcal{F}(\{\rho(x) - \delta\rho(x)\} | \alpha, \beta) + \delta T \int_0^1 dx \sum_{\tau=0}^N \frac{(j_\tau(x) + \rho'_\tau(x))^2}{4\rho_\tau(x)} \right], \quad (\text{V.B.94})$$

where we have used the definitions $\rho(x) - \delta\rho(x) = \rho(x, T - \delta T)$ and $\mathbf{j}(x) = \mathbf{j}(x, T)$. The conservation law reads $\delta\rho(x) = -\mathbf{j}'(x) \times \delta T$. The equation on the large deviation functional (V.B.94) above suggests to introduce the following quantity.

Definition B.34. *We define*

$$U_\tau(x) = \frac{\delta\mathcal{F}(\{\rho(x)\} | \alpha, \beta)}{\delta\rho_\tau(x)}. \quad (\text{V.B.95})$$

We can write using (V.B.94) an equation satisfied by the $U_s(x)$'s. Indeed, maximising (V.B.94) over the current profile $\mathbf{j}(x)$ with the constraint (V.B.91) yields

$$j_\tau(x) = -\rho'_\tau(x) + 2\rho_\tau(x)U'_\tau(x) - 2\rho_\tau(x)\mu(x), \quad (\text{V.B.96})$$

with the Lagrange multiplier

$$\mu(x) = \sum_{\tau=0}^N \rho_\tau(x)U'_\tau(x). \quad (\text{V.B.97})$$

Using the fact that $\sum_{\tau=0}^N j_\tau(0)U_\tau(0) = \sum_{\tau=0}^N j_\tau(1)U_\tau(1) = 0$ (because of the boundary conditions (V.B.90)), we can perform an integration by part and derive an equation satisfied by the functions $U'_\tau(x)$.

Proposition B.35. *The functions $U'_\tau(x)$ should satisfy the Hamilton-Jacobi equation*

$$\int_0^1 dx \left[\sum_{\tau=0}^N (\rho'_\tau(x)U'_\tau(x) - \rho_\tau(x)U'_\tau(x)^2) + \left(\sum_{\tau=0}^N \rho_\tau(x)U'_\tau(x) \right)^2 \right] = 0. \quad (\text{V.B.98})$$

We can check that the large deviation functional exactly computed in (V.A.73) indeed fulfills this equation.

Proposition B.36. *The function $U_\tau(x)$ obtained from the exact expression of the large deviation of the density profile (V.A.73) (derived from finite size lattice computations) that is given through direct computation by*

$$U_\tau(x) = \ln \left(\frac{\rho_\tau(x)}{\bar{\rho}_\tau(u(x))} \right) + 1, \quad (\text{V.B.99})$$

where the function u satisfies (V.A.74), is a solution to the Hamilton equation (V.B.98).

Proof. Using the constraints (V.B.91) and the expression of $U_\tau(x)$, the differential equation (V.A.74) can be rewritten

$$\frac{u''(x)}{u'(x)} = - \sum_{\tau=0}^N \rho_\tau(x) U'_\tau(x). \quad (\text{V.B.100})$$

This permits to show that

$$\left(\frac{u''}{u'} \right)' (x) = \sum_{\tau=0}^N (\rho'_\tau(x) U'_\tau(x) - \rho_\tau(x) U'_\tau(x)^2) + \left(\sum_{\tau=0}^N \rho_\tau(x) U'_\tau(x) \right)^2. \quad (\text{V.B.101})$$

Then we deduce that the left hand side of (V.B.98) is equal to

$$\int_0^1 dx \left(\frac{u''}{u'} \right)' (x) = \frac{u''(1)}{u'(1)} - \frac{u''(0)}{u'(0)} = 0, \quad (\text{V.B.102})$$

because $u''(1) = u''(0) = 0$ thanks to (V.A.74). ■

Remark B.37. *The computation presented above points out the consistency of the hydrodynamic description (V.B.88) with the exact computations performed on the finite size lattice (through matrix ansatz). This is thus a strong hint on the validity of the large deviation principle (V.B.88) in the multi-species case.*

Appendix A

Résumé en français

Physique statistique des systèmes hors d'équilibre

Un système physique est dit à l'équilibre thermodynamique s'il est à l'équilibre par rapport à toutes les grandeurs physiques imaginables. Il doit par exemple être à l'équilibre mécanique, thermique, électrodynamique, chimique. En d'autres termes c'est un système pour lequel on n'observe aucun courant macroscopique d'aucune grandeur physique (comme un courant d'énergie, de charge, de particules).

L'état de tels systèmes est obtenu en maximisant l'entropie sous certaines contraintes, dictées par l'interaction du système avec son environnement (l'énergie moyenne peut être fixée par exemple). Ce principe fondamental permet d'obtenir la célèbre distribution de Boltzmann

$$\mathcal{S}(\mathcal{C}) = \frac{e^{-\beta E(\mathcal{C})}}{Z}, \quad (\text{R.1})$$

où $\mathcal{S}(\mathcal{C})$ désigne la probabilité que le système soit dans la configuration \mathcal{C} et Z est la normalisation, appelée fonction de partition. Cela permet de définir un potentiel thermodynamique (énergie libre) et de décrire efficacement les propriétés macroscopiques du système (transitions de phase par exemple).

A l'opposé, un système physique est dit hors d'équilibre si il affiche des courants macroscopiques d'une ou plusieurs grandeurs physiques. L'archétype de tel modèle est donné par deux réservoirs de particules de densités différentes reliés par un tuyau. Le réservoir de forte densité se déverse dans celui de faible densité et on observe un courant de particules. Un système peut être hors d'équilibre parce qu'il est en phase de relaxation vers l'équilibre ou alors parce qu'il est maintenu hors d'équilibre par son environnement. On dit dans ce dernier cas que le système est dans un état stationnaire hors d'équilibre. Ce sont ces états stationnaires qui nous intéressent dans ce manuscrit.

Il n'existe pas de cadre général pour décrire de tels systèmes: on ne sait pas comment généraliser le principe fondamental de maximisation de l'entropie et la distribution de Boltzmann. L'objectif est donc d'étudier des modèles simples et de calculer exactement dans ces cas particuliers la distribution de l'état stationnaire, afin d'apporter un éclairage nouveau sur la structure générale.

Le cadre utilisé pour décrire de tels systèmes est celui des chaînes de Markov. Le système peut occuper un nombre fini de configurations. Pendant un intervalle de temps infinitésimal dt , le système se trouvant dans la configuration \mathcal{C} a une probabilité $m(\mathcal{C} \rightarrow \mathcal{C}')dt$ de sauter dans la configuration \mathcal{C}' . L'évolution temporelle de la distribution de probabilité du système est dictée par l'équation maîtresse

$$\frac{d\mathcal{P}_t(\mathcal{C})}{dt} = \sum_{\mathcal{C}' \neq \mathcal{C}} \mathcal{P}_t(\mathcal{C}')m(\mathcal{C}' \rightarrow \mathcal{C}) - \sum_{\mathcal{C}' \neq \mathcal{C}} \mathcal{P}_t(\mathcal{C})m(\mathcal{C} \rightarrow \mathcal{C}'), \quad (\text{R.2})$$

où $\mathcal{P}_t(\mathcal{C})$ désigne la probabilité que le système se trouve dans la configuration \mathcal{C} à l'instant t . Cette équation linéaire peut simplement se réécrire sous une forme matricielle en introduisant

un vecteur $|\mathcal{C}\rangle$ associé à chaque configuration \mathcal{C} , un vecteur regroupant les probabilités de toutes les configurations

$$|\mathcal{P}_t\rangle = \sum_{\mathcal{C}} \mathcal{P}_t(\mathcal{C})|\mathcal{C}\rangle, \quad (\text{R.3})$$

une matrice de Markov

$$M = \sum_{\mathcal{C}', \mathcal{C}} m(\mathcal{C} \rightarrow \mathcal{C}')|\mathcal{C}'\rangle\langle\mathcal{C}|, \quad (\text{R.4})$$

où l'on définit $m(\mathcal{C} \rightarrow \mathcal{C}') = \sum_{\mathcal{C}'' \neq \mathcal{C}} m(\mathcal{C} \rightarrow \mathcal{C}'')$. L'équation maîtresse devient

$$\frac{d|\mathcal{P}_t\rangle}{dt} = M|\mathcal{P}_t\rangle. \quad (\text{R.5})$$

On s'intéresse particulièrement à l'état stationnaire associée à cette équation (son existence est assurée par le théorème de Perron-Frobenius), on le notera $|\mathcal{S}\rangle$: il vérifie $M|\mathcal{S}\rangle = 0$.

Les systèmes à l'équilibre thermodynamique sont caractérisés par la relation de bilan détaillé

$$\mathcal{S}(\mathcal{C})m(\mathcal{C} \rightarrow \mathcal{C}') = \mathcal{S}(\mathcal{C}')m(\mathcal{C}' \rightarrow \mathcal{C}), \quad (\text{R.6})$$

qui résout de manière évidente la version stationnaire de l'équation maîtresse. Elle permet notamment de retrouver la distribution de Boltzmann et elle assure la réversibilité temporelle du système dans l'état stationnaire.

Le cas des systèmes hors d'équilibre est beaucoup plus complexe. La relation de bilan détaillé peut être généralisée mais elle ne conduit pas de manière évidente à une expression simple de la distribution stationnaire. Elle donne cependant de fructueux résultats, avec le théorème de fluctuation (qui permet notamment de retrouver les relations de dissipation-fluctuation d'Einstein, les relations de réciprocity d'Onsager). Elle suggère notamment l'étude de la fonction génératrice du courant de particules dans l'état stationnaire qui semble être une généralisation naturelle des potentiels thermodynamiques au cas hors d'équilibre.

On s'intéresse plus particulièrement dans ce manuscrit à des modèles d'exclusion. Ces modèles sont définis sur des réseaux unidimensionnels avec un nombre fini de site L sur lequel se déplacent des particules. Chaque site du réseau est soit vide, soit occupé par au plus une particule (ce qui correspond à une règle d'exclusion de type Fermi). Il y a N espèces différentes de particules. Le contenu du site i est décrit par une variable d'occupation locale $\tau_i \in \{0 \dots N\}$. $\tau_i = 0$ si le site est vide, et s'il est occupé $\tau_i = 1, \dots, N$ suivant l'espèce de la particule qui l'occupe. Une configuration sur le réseau est donc caractérisée par le L -uplet $\boldsymbol{\tau} = (\tau_1, \dots, \tau_L)$. Le réseau peut être connecté à des réservoirs de particules au niveau du site 1 ainsi que du site L ou alors avoir des conditions aux bords périodiques (géométrie d'anneau). On associe un vecteur $|\boldsymbol{\tau}\rangle$ à chaque configuration locale $\boldsymbol{\tau} = 0, \dots, N$ et on note $V \simeq \mathbb{C}^{N+1}$ l'espace vectoriel engendré par ces vecteurs.

L'évolution temporelle du système est stochastique. Les particules peuvent sauter sur des sites voisins (s'ils sont libres), réagir localement avec d'autres espèces, ou alors être créées ou détruites, et tout cela avec des taux de probabilité donnés. La dynamique étant locale, la matrice de Markov M peut se décomposer comme une somme d'opérateurs agissant localement sur le réseau. Dans le cas périodique, cela donne

$$M = \sum_{k=1}^L m_{k,k+1}, \quad (\text{R.7})$$

où m est un opérateur de saut local dans le bulk. C'est une matrice agissant sur l'espace tensoriel $V \otimes V$ et qui encode la dynamique du modèle sur deux sites adjacents (une composante V de l'espace tensoriel représente en quelque sorte un site du réseau). La matrice de Markov agit elle sur l'espace tensoriel $V^{\otimes L}$ (qui représente les L sites du réseau). Les indices représentent les composantes du produit tensoriel $V^{\otimes L}$ (*i.e* les sites) sur lesquels la matrice m agit non trivialement. Plus précisément on a

$$m_{k,k+1} = \underbrace{1 \otimes \dots \otimes 1}_{k-1} \otimes m \otimes \underbrace{1 \otimes \dots \otimes 1}_{L-k-1}. \quad (\text{R.8})$$

Pour les systèmes à bords ouverts, la matrice de Markov s'exprime comme

$$M = B_1 + \sum_{k=1}^{L-1} m_{k,k+1} + \bar{B}_L, \quad (\text{R.9})$$

où B et \bar{B} sont des matrices agissant sur V et qui encodent respectivement la dynamique avec le réservoir de gauche et de droite. La matrice

$$B_1 = B \otimes \underbrace{1 \otimes \cdots \otimes 1}_{L-1} \quad (\text{R.10})$$

agit sur le premier site du réseau et de manière similaire \bar{B}_L agit sur le dernier site du réseau.

Nous nous focalisons dans ce manuscrit sur des modèles d'exclusion qui sont exactement solubles. Le but est de calculer exactement la distribution stationnaire de tels modèles. On s'intéressera aussi aux fluctuations du courant de particules dans l'état stationnaire.

Les systèmes intégrables donnent un cadre idéal pour construire de manière systématique de tels modèles d'exclusion. La procédure est détaillée dans la section suivante.

Intégrabilité

L'idée essentielle des modèles intégrables a pris naissance en mécanique classique avec l'observation que la présence de grandeurs physiques conservées (typiquement l'énergie) était très utile à la résolution exacte des équations de Newton. Cette observation a été formalisée précisément (dans le cadre de la mécanique analytique) avec le théorème de Liouville. Celui-ci affirme que si un système évoluant dans un espace de phase de dimension $2n$ possède n grandeurs physiques indépendantes conservées, alors ses équations du mouvement peuvent être résolues par quadrature.

Cette idée a été transposée aux systèmes quantiques et aux chaînes de Markov: dans ce cadre une grandeur conservée est un opérateur qui commute avec l'Hamiltonien ou la matrice de Markov. Il n'existe pas d'équivalent du théorème de Liouville dans ce cadre, assurant que l'équation maîtresse peut être exactement résolue s'il y a assez de grandeurs conservées. Néanmoins leur présence est un indice fort d'une possible résolution analytique.

Pour les modèles d'exclusion, il existe un moyen systématique de générer simultanément une matrice de Markov avec des opérateurs qui commutent avec elle (et qui commutent entre eux deux à deux). L'ensemble de ces opérateurs et la matrice de Markov sont engendrés par une matrice de transfert $t(z)$, dépendant d'un paramètre spectral z . La propriété essentielle de cette matrice de transfert est qu'elle commute pour des valeurs différentes du paramètre spectral $[t(z), t(z')] = 0$. Elle est reliée très simplement à la matrice de Markov M par une relation du type $t'(1) \sim M$. La matrice de transfert est construite à partir d'un objet clef: la matrice $\check{R}(z)$, qui apparaît dans ce cadre comme la pierre angulaire de l'intégrabilité. Elle agit dans l'espace tensoriel $V \otimes V$. Elle est solution de la célèbre équation de Yang-Baxter (braïdée)

$$\check{R}_{12}(z)\check{R}_{23}(zz')\check{R}_{12}(z') = \check{R}_{23}(z')\check{R}_{12}(zz')\check{R}_{23}(z). \quad (\text{R.11})$$

C'est une équation portant sur des matrices agissant dans l'espace tensoriel $V \otimes V \otimes V$. Les indices désignent les composantes de l'espace tensoriel dans lequel les matrices agissent non trivialement. Par exemple

$$\check{R}_{12}(z) = \check{R}(z) \otimes 1, \quad \check{R}_{23}(z) = 1 \otimes \check{R}(z). \quad (\text{R.12})$$

L'équation de Yang-Baxter est essentielle pour prouver la propriété de commutation de la matrice de transfert. Dans le contexte des processus d'exclusion, la matrice $\check{R}(z)$ est directement connectée à l'opérateur de saut local m par une relation du type $\check{R}'(1) \sim m$

Pour les systèmes aux conditions aux bords périodiques la matrice de transfert s'exprime comme

$$t(z) = \text{tr}_0(R_{0L}(z) \cdots R_{01}(z)), \quad (\text{R.13})$$

où $R(z) = P\check{R}(z)$, avec P l'opérateur de permutation sur $V \otimes V$.

Pour les systèmes à bords ouverts, il est nécessaire d'introduire des matrices $K(z)$ et $\bar{K}(z)$, agissant sur V , qui assurent en quelque sorte l'intégrabilité des conditions aux bords. Celles-ci doivent être solution de l'équation de réflexion

$$\check{R}_{12}(z_1/z_2)K_1(z_1)\check{R}_{12}(z_1z_2)K_1(z_2) = K_1(z_2)\check{R}_{12}(z_1z_2)K_1(z_1)\check{R}_{12}(z_1/z_2), \quad (\text{R.14})$$

et d'une équation similaire pour $\bar{K}(z)$. C'est une équation portant sur des matrices agissant sur $V \otimes V$. Les indices indiquent encore une fois sur quelle composante de l'espace tensoriel les matrices agissent non trivialement. Cette relation est essentielle pour prouver la propriété de commutation de la matrice de transfert dans le cas ouvert. Les matrices $K(z)$ et $\bar{K}(z)$ sont directement connectées aux opérateurs de saut locaux B et \bar{B} par des relations du type $K'(1) \sim B$ et $\bar{K}'(1) \sim \bar{B}$. Pour de tels systèmes ouverts la matrice de transfert s'exprime comme

$$t(z) = \text{tr}_0(\tilde{K}_0(z)R_{0L}(z) \dots R_{01}(z)K_0(z)R_{10}(z) \dots R_{L0}(z)), \quad (\text{R.15})$$

où $\tilde{K}(z)$ s'exprime simplement en fonction de la matrice $\bar{K}(z)$.

Il apparaît donc très important de déterminer des solutions à l'équation de Yang-Baxter et à l'équation de réflexion afin de découvrir de nouveaux modèles hors d'équilibre exactement solubles. Des progrès ont été réalisés dans ce sens avec l'introduction de nouvelles structures algébriques qui permettent de générer des solutions de ces deux équations par une procédure de Baxtérization. Cette procédure peut être résumée comme étant une méthode pour créer une matrice $R(z)$ ou une matrice $K(z)$ à partir d'un opérateur de saut local m ou B vérifiant des relations algébriques spécifiques, en ajoutant de manière judicieuse un paramètre spectral. Cela a permis par exemple de proposer une classe de conditions aux bords intégrables pour la généralisation multi-espèces de l'ASEP.

On s'intéresse dans la section suivante à une méthode permettant de calculer exactement la distribution stationnaire des modèles intégrables hors d'équilibre.

Ansatz matriciel pour les états stationnaires hors d'équilibre

Depuis quelques décennies une technique s'est développée pour calculer analytiquement la distribution stationnaire de systèmes hors d'équilibre, appelée ansatz matriciel. Cette méthode a été introduite pour résoudre exactement le processus d'exclusion simple totalement asymétrique (TASEP, de l'acronyme anglais). Elle a depuis ce temps été largement utilisée pour résoudre d'autres modèles d'exclusion.

L'idée de l'ansatz matriciel est d'exprimer la distribution stationnaire comme un produit de matrices

$$\mathcal{S}(\tau_1, \dots, \tau_L) = \frac{1}{Z} \langle\langle W | X_{\tau_1} \dots X_{\tau_L} | V \rangle\rangle, \quad (\text{R.16})$$

avec Z une normalisation assurant que les probabilités stationnaires se somment bien à 1. X_{τ_i} est une matrice dépendant du site i . $\langle\langle W |$ est un vecteur ligne et $|V \rangle\rangle$ est un vecteur colonne de sorte que la contraction de ce produit de matrices est un nombre réel. Cet ansatz peut se réécrire de manière compacte sous forme vectorielle (qui nous est très utile pour la suite), en introduisant le vecteur

$$\mathbf{X} = \begin{pmatrix} X_0 \\ X_1 \\ \vdots \\ X_N \end{pmatrix}, \quad (\text{R.17})$$

contenant toutes les matrices. L'ansatz matriciel se réécrit alors

$$|\mathcal{S}\rangle = \langle\langle W | \mathbf{X} \otimes \dots \otimes \mathbf{X} | V \rangle\rangle. \quad (\text{R.18})$$

Les matrices X_0, \dots, X_N et les vecteurs $\langle\langle W |$ et $|V \rangle\rangle$ doivent bien sûr satisfaire des relations algébriques très précises pour que ce produit de matrices calcule correctement les probabilités stationnaires.

Dans le cas des modèles intégrables, il existe une manière systématique de déterminer ces relations algébriques, grâce à deux relations clefs: la relation de Zamolodchikov-Faddeev

$$\check{R} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \mathbf{A}(z_1) \otimes \mathbf{A}(z_2) = \mathbf{A}(z_2) \otimes \mathbf{A}(z_1), \quad (\text{R.19})$$

et les relations de Ghoshal-Zamolodchikov

$$\langle\langle W|K(z)\mathbf{A} \begin{pmatrix} 1 \\ z \end{pmatrix} = \langle\langle W|\mathbf{A}(z), \quad \overline{K}(z)\mathbf{A} \begin{pmatrix} 1 \\ z \end{pmatrix} |V\rangle\rangle = \mathbf{A}(z)|V\rangle\rangle. \quad (\text{R.20})$$

$\mathbf{A}(z)$ est un vecteur dont les entrées sont des éléments d'une algèbre non commutative.

Ces relations sont à la racine des relations télescopiques dans le bulk

$$m\mathbf{X} \otimes \mathbf{X} = \mathbf{X} \otimes \overline{\mathbf{X}} - \overline{\mathbf{X}} \otimes \mathbf{X}, \quad (\text{R.21})$$

et sur les bords

$$\langle\langle W|B\mathbf{X} = \langle\langle W|\overline{\mathbf{X}}, \quad \overline{B}\mathbf{X}|V\rangle\rangle = -\overline{\mathbf{X}}, \quad (\text{R.22})$$

qui s'obtiennent respectivement en prenant la dérivée de la relation Zamolodchikov-Faddeev par rapport à z_1 et en imposant $z_1 = z_2 = 1$, et en prenant la dérivée des relations de Ghoshal-Zamolodchikov par rapport à z et en imposant $z = 1$. Le vecteur \mathbf{X} est donné par $\mathbf{X} = \mathbf{A}(1)$ et le vecteur $\overline{\mathbf{X}}$ est obtenu par une relation du type $\overline{\mathbf{X}} \sim \mathbf{A}'(1)$. Ces relations télescopiques permettent de prouver très facilement que l'ansatz matriciel donne bien l'état stationnaire du modèle (on obtient en effet une somme télescopique en agissant avec la matrice de Markov sur l'état en produit de matrices).

Cette procédure peut être appliquée pour calculer l'état stationnaire de plusieurs nouveaux modèles, qui ont été découvert en résolvant l'équation de Yang-Baxter et l'équation de réflexion. L'un des modèles est une généralisation du processus d'exclusion simple symétrique (SSEP, de l'acronyme anglais) où des paires de particules peuvent condenser ou s'évaporer. Un autre modèle est un TASEP à deux espèces de particules avec des bords ouverts. Enfin le dernier modèle est une généralisation multi-espèces (avec un nombre quelconque d'espèces) du SSEP avec bords ouverts.

En résumé, les relations de Zamolodchikov-Faddeev et de Ghoshal-Zamolodchikov ont permis d'introduire des ansatz matriciels avec une structure algébrique riche (avec par exemple des opérateurs "chapeaux" non scalaires). De plus des calculs exacts de grandeurs physiques (courants et densités de particules) ont pu être réalisés grâce à cet ansatz matriciel.

Equations qKZ et fluctuations du courant

Nous venons de voir que l'ansatz matriciel est particulièrement efficace pour calculer exactement l'état stationnaire de certains processus d'exclusion. Mais son champ d'application ne se limite pas à cela. Nous allons voir une autre de ses applications, toujours dans le contexte de la physique statistique hors d'équilibre. Nous considérons le cas particulier de l'ASEP avec bords ouverts et nous nous intéressons aux fluctuations du courant de particules dans l'état stationnaire. La fonction génératrice des cumulants de cette observable s'obtient en déformant, à l'aide d'un paramètre ξ , la matrice de Markov du modèle de façon à pouvoir "compter" les particules qui sont injectées par le réservoir de gauche dans le système. La fonction génératrice est la plus grande valeur propre de cette matrice déformée.

Nous tentons de déterminer cette plus grande valeur propre ainsi que le vecteur propre associé (qu'on appelle le *ground state*) à l'aide des équations de Knizhnik-Zamolodchikov q -déformées (équations q KZ). Ces équations peuvent être vues de manière simplifiée comme des déformations, par un paramètre s , des relations Zamolodchikov-Faddeev et Ghoshal-Zamolodchikov.

Le résultat essentiel est que ces équations admettent une solution polynomiale, qui s'exprime sous forme de produit de matrices, lorsque la contrainte suivante est vérifiée:

$$\xi = s^n, \quad \text{avec } n \in \mathbb{N}. \quad (\text{R.23})$$

La normalisation du vecteur solution des équations qKZ dans ce cas est identifiée comme étant un polynôme de Koornwinder associé à une partition particulière. Cela offre une expression en produit de matrices pour ce polynôme.

De plus, nous avons conjecturé que dans la limite $n \rightarrow \infty$, le vecteur solution des équations qKZ converge vers le ground state de la matrice de Markov déformée. Cela révèle une connexion inédite entre les fluctuations du courant dans l'ASEP et la théorie des polynômes symétriques.

Limite hydrodynamique

Un des objectifs premiers de la physique statistique est de décrire de manière efficace le comportement macroscopique de systèmes physiques dans la limite où le nombre de leurs constituants tend vers l'infini. Le but est de déterminer à partir des interactions entre les constituants élémentaires au niveau microscopique, des variables macroscopiques (telles que la température ou la pression) ainsi que des lois physiques décrivant l'état du système (comme une équation d'état par exemple).

Dans le cadre des processus d'exclusion, nous nous intéressons donc à la limite thermodynamique, *i.e* lorsque le nombre de sites sur le réseau tend vers l'infini. Nous calculons la limite thermodynamique des observables (courants et densités de particules notamment) pour les nouveaux modèles introduits et étudiés sur le réseau de taille finie. Nous calculons aussi de manière exacte la fonction de grande déviation des profils de densité pour le SSEP multi-espèces, en utilisant un principe d'additivité prouvé grâce à l'ansatz matriciel.

Nous nous intéressons ensuite à une théorie développée dans les dernières années, appelée théorie des fluctuations macroscopiques (MFT, de l'acronyme anglais), qui vise à donner un cadre général pour décrire les systèmes diffusifs hors d'équilibre dans la limite thermodynamique. L'idée est d'introduire des variables macroscopiques de courants et de densités de particules (qui décrivent la valeur moyenne du courant et de la densité autour d'un point du réseau). Par analogie avec la loi des grands nombres, ces variables sont supposées avoir un comportement déterministe dans la limite thermodynamique. Plus précisément, il a été montré que la probabilité d'observer une trajectoire, une évolution temporelle, de ces variables macroscopiques vérifie un principe de grande déviation. D'un point de vue physique, la fonction de grande déviation peut être interprétée comme une action. Cela permet, au prix de résoudre des équations différentielles non linéaires (qui sont des équations d'Euler-Lagrange obtenues par minimisation de l'action), de calculer les fluctuations du courant et du profil de densité dans l'état stationnaire.

Les résultats exacts obtenus pour le modèle avec évaporation et condensation de paires de particules sur le réseau à taille finie ont été confrontés avec succès, dans la limite thermodynamique, avec les prédictions de la MFT. Cela constitue la première vérification de ce type pour les systèmes avec création et annihilation de particules dans le bulk. Enfin les résultats obtenus pour la généralisation multi-espèces du SSEP à bords ouverts (notamment concernant la fonction de grande déviation des profils de densités) ont permis de proposer une extension de la MFT à ce système diffusif à plusieurs espèces de particules. Cela apporte un nouveau point de vue sur la transcription de la contrainte d'exclusion dans la fonctionnelle de grande déviation (action) de la MFT.

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Approche intégrabiliste des modèles de physique statistique hors d'équilibre.

Malgré son indéniable succès pour décrire les systèmes physiques à l'équilibre thermodynamique (grâce à la distribution de Boltzmann, reflétant la maximisation de l'entropie, et permettant la construction systématique de potentiels thermodynamiques), la physique statistique n'offre pas de cadre général pour étudier les phénomènes hors d'équilibre, i.e dans lesquels on observe un courant moyen non nul d'une grandeur physique (énergie, charge, particules...). L'objectif de la thèse est de décrire de tels systèmes à l'aide de modèles très simples mais qui retranscrivent néanmoins les principales caractéristiques physiques de ceux-ci. Ces modèles sont constitués de particules se déplaçant de manière aléatoire sur un réseau unidimensionnel connecté à des réservoirs et soumises à un principe d'exclusion. L'enjeu est de calculer exactement l'état stationnaire du modèle, notamment le courant de particules, ses fluctuations et plus particulièrement sa fonction de grande déviation (qui pourrait jouer le rôle d'un potentiel thermodynamique hors d'équilibre). Une première partie de la thèse vise à construire des modèles dits intégrables, dans lesquels il est possible de mener à bien des calculs exacts de quantités physiques. De nouveaux modèles hors d'équilibre sont proposés grâce à la résolution dans des cas particuliers de l'équation de Yang-Baxter et de l'équation de réflexion. De nouvelles structures algébriques permettant la construction de ces solutions par une procédure de Baxterisation sont introduites. Une deuxième partie de la thèse consiste à calculer exactement l'état stationnaire de tels modèles en utilisant l'ansatz matriciel. Les liens entre cette technique et l'intégrabilité du modèle ont été mis en lumière au travers de deux relations clef: la relation de Zamolodchikov-Faddeev et la relation de Ghoshal-Zamolodchikov. L'intégrabilité a aussi été exploitée au travers des équations de Knizhnik-Zamolodchikov quantiques, afin de calculer les fluctuations du courant, mettant en lumière des connexions avec la théorie des polynômes symétriques (polynômes de Koornwinder en particulier). Enfin une dernière partie de la thèse porte sur la limite hydrodynamique des modèles étudiés, i.e lorsque la maille du réseau tend vers zéro et que le nombre de constituants du système tend vers l'infini. Les résultats exacts obtenus sur les modèles à taille finie ont permis de vérifier les prédictions de la théorie des fluctuations macroscopiques (concernant les fluctuations du courant et du profil de densité dans l'état stationnaire) et de l'étendre à des modèles comprenant plusieurs espèces de particules.

Integrabilist approach of non-equilibrium statistical physics models

Although statistical physics has been very successful to describe physical systems at thermal equilibrium (thanks to the Boltzmann distribution, which reflects the maximization of the entropy, and allows one to construct in a systematic way thermodynamic potentials), it remains elusive to provide an efficient framework to study phenomena that are out-of-equilibrium, i.e displaying non vanishing current of physical quantities (energy, charge, particles...). The goal of the thesis is to describe such systems with very simple models which retain nevertheless their main physical features. The models consist in particles evolving randomly on a one dimensional lattice connected to reservoirs and subject to hard-core repulsion. The challenge lies in computing exactly the stationary state of the model, especially the particle current, its fluctuations and more precisely its large deviation function (which is expected to play the role of an out-of-equilibrium thermodynamic potential). In the first part of the thesis we construct models, called integrable, in which we can perform exact computations of physical quantities. We introduce several new out-of-equilibrium models that are obtained by solving, in specific cases, the Yang-Baxter equation and the reflection equation. We provide new algebraic structures which allow us to construct the solutions through a Baxterisation procedure. In the second part of the thesis we compute exactly the stationary state of these models using a matrix ansatz. We shed light on the connection between this technique and the integrability of the model by pointing out two key relations: the Zamolodchikov-Faddeev relation and the Ghoshal-Zamolodchikov relation. The integrability is also exploited, through the quantum Knizhnik-Zamolodchikov equations, to compute the fluctuations of the particles current, unrevealing connections with the theory of symmetric polynomials (the Koornwinder polynomials in particular). Finally the last part of the thesis deals with the hydrodynamic limit of the models, i.e when the lattice spacing tends to 0 and the number of particles tends to infinity. The exact results obtained for a finite size system allow us to check the validity of the predictions of the macroscopic fluctuations theory (concerning the fluctuations of the current and the density profile in the stationary state) and to extend the theory to systems with several species of particles.