

Fluctuations in Stochastic Interacting Particle Systems

Gunter M. Schütz^{1,2}

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¹Institute of Complex Systems II, Forschungszentrum Jülich, 52425 Jülich, Germany
Email: g.schuetz@fz-juelich.de

²Interdisziplinäres Zentrum für komplexe Systeme, Universität Bonn, Brühler Str. 7, 53119 Bonn, Germany
URL: <http://www.izks.uni-bonn.de>

Abstract

We consider from a microscopic perspective fluctuations in stochastic lattice gas models. We make use of multilinear algebra and the representation theory of Lie algebras and universal enveloping algebras to derive rigorously duality functions for the simple exclusion process. This provides detailed information about fluctuations of the density in the symmetric simple exclusion process (SSEP) on any graph and about the microscopic structure and dynamics of shocks in the asymmetric simple exclusion process (ASEP) on the integer lattice \mathbb{Z} . We go on to prove a generic fluctuation theorem for integrated currents from well-known fluctuation relations such as the Jarzynski relation and the Gallavotti-Cohen symmetry for stochastic processes with finite state space arise as simple corollaries. As a third result we describe briefly how nonlinear fluctuating hydrodynamics yields an intriguing infinite discrete family of dynamical universality classes. The dynamical exponents characterizing these universality classes are Kepler ratios of neighbouring Fibonacci numbers or their limiting case which is the golden mean. The scaling form of the corresponding dynamical structure functions for the Fibonacci models is an asymmetric Lévy distribution.

Contents

1	Introduction	4
1.1	Exclusion processes	4
1.1.1	The Asymmetric Simple Exclusion Process	4
1.1.2	Multispecies and multilane exclusion processes	8
1.2	Some linear algebra	10
1.2.1	Matrices and vectors	11
1.2.2	Addition and multiplication of matrices	12
1.2.3	The Kronecker product	13
1.3	Generator of Markov processes in matrix form	16
1.3.1	Matrix formulation of the generator	17
1.3.2	Expectations in matrix formulation	19
1.3.3	Stationarity and reversibility	20
2	Duality	24
2.1	Duality and Symmetry	25
2.2	The symmetric simple exclusion process	26
2.2.1	Generator of the SSEP in matrix form	26
2.2.2	Equilibrium measures	28
2.2.3	Duality functions for the SSEP	31
2.2.4	Density profile and dynamical structure function	33
2.3	Selfduality of the 1-d ASEP	34
2.3.1	Periodic boundary conditions with constant rates	35
2.3.2	Generator of the ASEP with reflecting boundaries	35
2.3.3	Grandcanonical equilibrium measure	36
2.3.4	Duality functions for the 1-d ASEP	37
2.3.5	Microscopic structure of shocks in the ASEP	38
2.4	Recipe for the quantum Hamiltonian of exclusion processes	41
3	Fluctuations of current and density	42
3.1	Tools	42
3.1.1	Counting processes	42
3.1.2	Time-dependent transition rates	45
3.2	The fundamental fluctuation relation	46
3.3	Some specific fluctuation theorems	49
3.3.1	Integral fluctuation relations	49
3.3.2	Detailed fluctuation relations	51
3.3.3	Gallavotti-Cohen-Theorem for stochastic interacting particle systems	53
4	Dynamical universality classes	54
4.1	Multi-lane exclusion processes	55
4.2	Brief outline of nonlinear fluctuating hydrodynamics	56
4.3	Fibonacci universality classes	58

4.4	Ballistic universality class in conditioned dynamics	60
5	Conclusions	60

1 Introduction

Stochastic interacting particle systems with short-range interaction exhibit a remarkably rich variety of critical phenomena even in one dimension when they are in a steady state far from equilibrium. This is in contrast to thermal equilibrium for which there is a famous quite general rule that says, simply put, no phase transition in one dimension at positive temperature for equilibrium systems with short-range interactions [99, 57, 80, 18]. One observes in non-equilibrium steady states anomalous (non-diffusive) transport and universal non-diffusive dynamical scaling, boundary-induced phase transition, spontaneous symmetry breaking, long-range order and phase coexistence and more. Since one is away from equilibrium, these phenomena cannot be explained from the properties of a free energy. The fundamental question of interest is therefore how such critical phenomena that appear on macroscopic scale arise from the microscopic dynamics of such systems, in particular, from conservation laws and other kinetic constraints on the microscopic dynamics.

A major contribution to this program has come from exact results on microscopic stochastic lattice gas models for driven diffusive systems [61, 21, 62, 54, 87, 88, 10]. These are systems of classical interacting particles that move under the action of a random force preferentially in one direction and/or where at the system boundaries particles can exchange with external reservoirs at different densities, thus maintaining a non-equilibrium steady state that supports macroscopic currents. Some of these exact results have been obtained by exploiting a very simple mathematical relation between the Markov generator of such processes and the Hamiltonian operator of certain quantum systems [63, 87]. This link suggests to use mathematical tools from algebra to treat probabilistic problems. In these lectures we introduce some of these methods which require no knowledge of quantum physics at all.

1.1 Exclusion processes

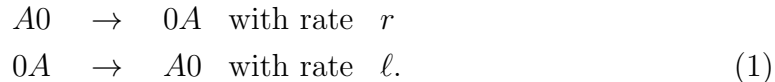
In order to make these general ideas more concrete we introduce some basic lattice gas models called exclusion processes. These are Markov processes also called stochastic interacting particle systems. We start with the simplest model of driven diffusive systems of identical conserved particles with hard-core interaction, which is the asymmetric simple exclusion process (ASEP, see below) in one space dimension [96].

1.1.1 The Asymmetric Simple Exclusion Process

The asymmetric simple exclusion process (ASEP) has become a paradigmatic example for a driven diffusive system and has attained a status in the study of nonequilibrium systems somewhat similar to the role that the Ising model plays in equilibrium statistical mechanics. The ASEP is a Markov process in continuous time which can be described informally as follows.

Each site k of the integer lattice Λ is occupied by at most one particle which is specified by the random variable $\eta_k \in \{0, 1\}$ indicating whether site k is vacant

or occupied. The set of configurations $\boldsymbol{\eta} := \{\eta_k : k \in \Lambda\}$ is therefore $\Omega = \{0, 1\}^\Lambda$. Particles hop randomly in continuous time to the right neighboring site with rate r and to the left with rate ℓ respectively, provided the target site is empty. Otherwise the attempted move is rejected. Hopping attempts take place independently with an exponential waiting time distribution with mean $\tau_w = 1/(r + \ell)$ (Fig. 1). We present this hopping rule as follows:



Here the symbol A represents occupation by a single particle and 0 represents an empty site. For definiteness we shall assume $r \geq \ell$ corresponding to an average drift on positive lattice direction, or clockwise in case of a finite periodic lattice. For $\ell = 0$ the process is called totally asymmetric simple exclusion process (TASEP).

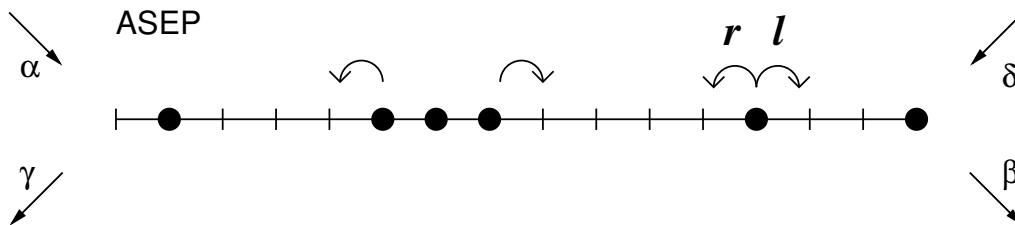


Figure 1: Pictorial representation of the ASEP with open boundaries and bulk hopping rates r to the right and $l \equiv \ell$ to the left. Some but not all possible jumps are indicated.

The ASEP was first invented in an early biophysics context already in 1968 as a model to describe the kinetics of protein synthesis through ribosomes moving along m-RNA templates [64, 85], and later became the “mother” of lattice gas models for automobile traffic [67], see [82] for a thorough discussion of these developments and applications to real biological systems and traffic flow. Despite being one-dimensional in its simplest formulation it also serves as a model to capture features of driven noisy dynamics in zeolites, carbon nanotubes, artificial narrow channels for colloidal particles, or, via various mappings, for interface dynamics in two dimensions and polymer dynamics and flux lines in three dimensions.

For a finite lattice with L sites one has to specify boundary conditions. Most commonly studied are periodic boundary conditions, reflecting boundaries (hopping confined to a box) [81], and open boundary conditions [56, 19, 83] where particles may enter and exit the lattice at the boundary sites 1 and L under the exclusion constraint with rates $\alpha, \beta, \gamma, \delta$ as indicated in Fig. 1. The parametrization $\alpha = r\lambda_-\rho_-$, $\gamma = \ell\lambda_-(1 - \rho_-)$ as left boundary rates and $\beta = r\lambda_+(1 - \rho_+)$, $\delta = \ell\lambda_+\rho_+$ as right boundary rates may be interpreted as a connection to particle reservoirs with constant density ρ_- at the left boundary and density ρ_+ at the right boundary, respectively. The parameters λ_\pm describe a hopping mechanism between the reservoirs and the chain which may differ from the hopping inside the chain.

For periodic boundary conditions the total particle number $N = \sum_{k \in \Lambda} \eta_k$ is conserved and the invariant measure for the process with a fixed number of particles is easily seen to be uniform. This fact allows for the construction of a family of invariant measures which are Bernoulli product measures with parameter ρ . This measure is also a (translation invariant) invariant measure of the ASEP defined on the infinite lattice \mathbb{Z} . Here $\rho = \mathbf{E}_\rho \eta_k$ is the particle density. The *instantaneous current*

$$j_k := r\eta_k(1 - \eta_{k+1}) - \ell(1 - \eta_k)\eta_{k+1} \quad (2)$$

has expectation

$$j^* := \mathbf{E}_\rho j_k = (r - \ell)\rho(1 - \rho). \quad (3)$$

The *stationary current* j^* tells us the net number of particle that flow in positive direction per infinitesimal time unit across a lattice bond $\langle k, k + 1 \rangle$.

The open ASEP is ergodic. The exactly known unique invariant measure is non-trivial and has an intriguing phase diagram. The bulk density ρ , which is determined by the two boundary densities ρ_\pm , undergoes a nonequilibrium discontinuous transition along the line $0 < \rho_- = 1 - \rho_+ < 1/2$ between a low-density phase with bulk density $\rho = \rho_-$ to a high-density phase with bulk density $\rho = \rho_+$. There are nonequilibrium continuous transitions from both phases to a maximal current phase with $\rho = 1/2$, which one has inside the region $1/2 < \rho_- \leq 1, 0 \leq \rho_+ < 1/2$ [60]. The microscopic density profiles are non-trivial in all phases [83, 20]. At the first-order transition line one has phase coexistence with a left domain of density ρ_- and a right domain of density ρ_+ , separated by a domain wall. On macroscopic scale this domain wall corresponds to a shock, i.e., a density discontinuity. Inside the maximal current phase the local density decays algebraically from the boundaries to its asymptotic bulk value $1/2$. The theory of boundary-induced phase transitions [55, 69] demonstrates that these phase transitions arise on microscopic level from the interplay of the shock motion and the flow of local perturbations as described by the so-called dynamical structure function. In this way one understands and extends the hydrodynamic derivation of the phase diagram, first proposed by Krug [56] and only quite recently proved rigorously by Bahadoran [2].

Also the dynamical properties of the ASEP are quite well understood. On microscopic scale the local density $\rho_k(t)$ defined by the expectation of the local occupation number at time t , starting from some initial measure μ_0 satisfies, due to particle number conservation, away from the boundaries the lattice continuity equation

$$\frac{d}{dt}\rho_k(t) = j_{k-1}(t) - j_k(t) \quad (4)$$

where $j_k(t)$ is the expectation of the instantaneous current (2). This equation does not allow for an explicit solution. However, it can be proved that on macroscopic Eulerian scale the density profile of the ASEP evolves according to the inviscid Burgers equation [79]

$$\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x}j(\rho) = \frac{\partial}{\partial t}\rho + (r - \ell)(1 - 2\rho)\frac{\partial}{\partial x}\rho = 0 \quad (5)$$

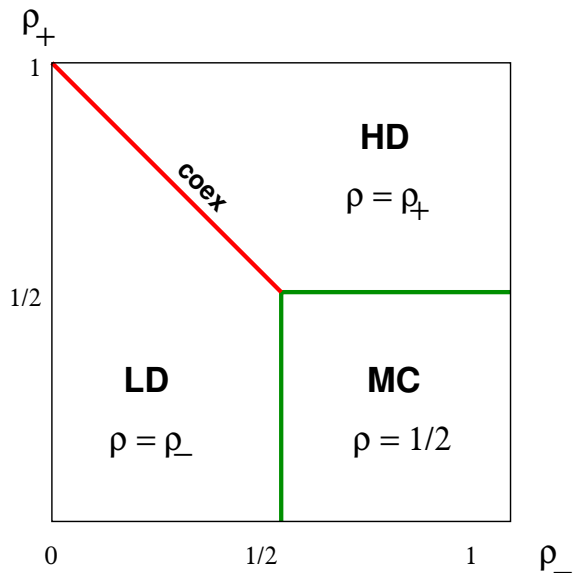


Figure 2: Phase diagram of the ASEP with open boundaries. LD (HD) denotes the low (high) density phase, and MC the maximal current phase. The red coexistence line marks a discontinuous phase transition between bulk densities ρ_- and ρ_+ . The green phase transition lines correspond to a continuous phase transition between bulk densities ρ_{\pm} and $1/2$.

where $\rho = \rho(x, t)$ is the coarse-grained local density.

The density develops a travelling shock discontinuity unless the initial density profile is monotonously decreasing. The shock velocity of shock with left density ρ_- and right density ρ_+ is given by the Rankine-Hugoniot condition [58]

$$v_s(\rho_+, \rho_-) = \frac{j_+ - j_-}{\rho_+ - \rho_-} \quad (6)$$

with the stationary currents j_{\pm} in the two branches of the shock, which in the present case are given by $j_{\pm}^{\alpha} = w(q - q^{-1})\rho_{\pm}(1 - \rho_{\pm})$. Looking at diffusive scale into the vicinity of the shock one finds that it performs a diffusive motion around its mean position [29] with diffusion coefficient

$$D_s(\rho_+, \rho_-) = \frac{1}{2} \frac{j_+ + j_-}{\rho_+ - \rho_-} \quad (7)$$

The shock has been shown to be sharp even on microscopic lattice scale [28, 20, 5].

The dynamical structure function

$$S_k(t) := \mathbf{E}_{\rho} (\eta_k(t)\eta_0(0)) - \rho^2 \quad (8)$$

describes the flow and spreading of local fluctuations (Fig. 3). On large scales it is expected to acquire a universal scaling form

$$S_k(t) \sim t^{-z} F((k - v_c t)^z/t). \quad (9)$$

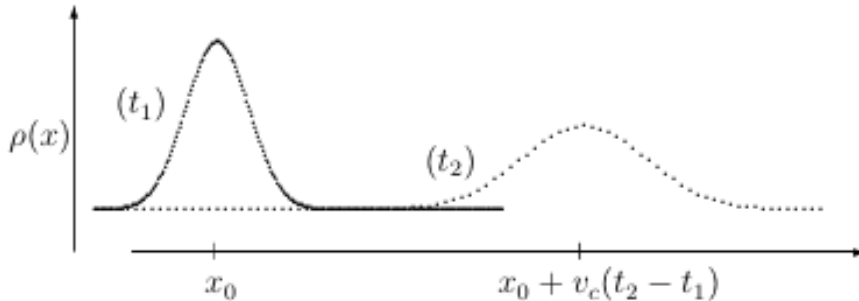


Figure 3: Schematic plot of the dynamical structure at two times $t_2 > t_1$ with center of mass at lattice x_0 at $t = t_1$.

This means that the center of mass of a fluctuations travels with collective velocity

$$v_c := \frac{d}{d\rho} j^*(\rho) = (r - \ell)(1 - 2\rho). \quad (10)$$

The dynamical exponent z which describes the spreading of a fluctuation around its peak characterizes the universality class. The symmetric version (SSEP) with $r = \ell$ is in the diffusive universality class with dynamical exponent $z = 2$ and Gaussian scaling function. On the other hand, the ASEP is in the celebrated universality class of the Kardar-Parisi-Zhang equation [50, 36] with dynamical exponent $z = 3/2$ and Prähofer-Spohn scaling function $F_{PS}(\cdot)$ [75, 76].

We point out that for the periodic or infinite lattice the compressibility

$$K := \sum_{k \in \Lambda} S_k(t) = \sum_{k \in \Lambda} \mathbf{E}_\rho(\eta_k(\eta_0 - \rho)) = \rho(1 - \rho) \quad (11)$$

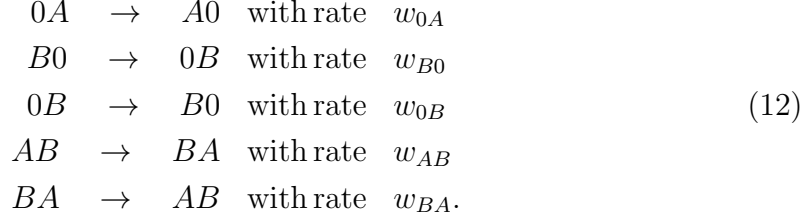
is time-independent due to particle number conservation for any conservative lattice gas with sufficiently rapidly decaying stationary correlations $C_k := S_k(0) = \mathbf{E}_\rho(\eta_k(\eta_0 - \rho))$.

1.1.2 Multispecies and multilane exclusion processes

Models with more than one conservation law are much less understood. There are few exact results on invariant measures, but numerical simulations and analytical approximations indicate a wealth of intriguing behaviour. For an older review we refer to [88]. Some recent numerical results will be discussed below and therefore we briefly describe some simple models.

The perhaps simplest particle system with more than one conserved species of particles is a multi-species exclusion process where each lattice site can be found in at least three different states: empty, or occupied by either an A -particle or a B -particle. Such an exclusion process is described by the six hopping rates

$$A0 \rightarrow 0A \quad \text{with rate } w_{A0}$$



Since there are two conservation laws one has two evolution equations for the two local densities

$$\frac{d}{dt}\rho_k^A(t) = j_{k-1}^A(t) - j_k^A(t) \tag{13}$$

$$\frac{d}{dt}\rho_k^B(t) = j_{k-1}^B(t) - j_k^B(t) \tag{14}$$

where $j_k^{A,B}$ are the expectations of the respective instantaneous currents which in general lead to two coupled lattice continuity equations. The stationary distribution of this process and hence the current-density relations $j_A^*(\rho^A, \rho^B)$ and $j_B^*(\rho^A, \rho^B)$ are known only on certain parameter manifolds [88, 10]. For

$$w_{AB} + w_{0A} + w_{0B} = w_{A0} + w_{BA} + w_{B0} \tag{15}$$

the canonical measure with fixed particle numbers N_A and N_B is uniform which allows for the construction of a product measure parametrized by densities ρ_A and ρ_B [42]. The stationary currents are then given by

$$j_A^*(\rho_A, \rho_B) = (w_{A0} - w_{0A})\rho_A(1 - \rho_A) - (w_{B0} - w_{0B})\rho_A\rho_B \tag{16}$$

$$j_B^*(\rho_A, \rho_B) = (w_{B0} - w_{0B})\rho_B(1 - \rho_B) - (w_{A0} - w_{0A})\rho_A\rho_B. \tag{17}$$

The hopping asymmetry generates a coupling between the two densities, leading to a non-trivial coupled system

$$\frac{\partial}{\partial t}\rho_A + \frac{\partial}{\partial x}j_A^*(\rho_A, \rho_B) = 0 \tag{18}$$

$$\frac{\partial}{\partial t}\rho_B + \frac{\partial}{\partial x}j_B^*(\rho_A, \rho_B) = 0 \tag{19}$$

of hyperbolic conservation laws for the coarse-grained local densities $\rho_{A,B}(x, t)$. If, however, e.g. $w_{B0} = w_{0B}$ the macroscopic evolution is known: The density of the A -particles evolves autonomously as the in the single-species ASEP and the B -particle density can be integrated straightforwardly [77].

A different way of constructing models with more than one conservation law are coupled multi-lane models where hopping rates on one lane depend on the particle configuration also of other lanes, but no particle exchange between lanes take place. An interesting class are models where the invariant measure is not changed by the coupling to the other lanes. This can be realized e.g. in a two-lane TASEP by making the rate of jump from site k to site $k + 1$ proportional to a linear function

of the the number of particles on site k and $k + 1$ in the adjacent lane, i.e., for $n_k^\alpha := \eta_k^\alpha + \eta_{k+1}^\alpha$ one chooses rates $r_1(n_k^2)$ for lane 1 and $r_2(n_k^1)$ for lane 2 given by [71]

$$r_1(n_k^2) = 1 + \gamma n_k^2/2, \quad r_2(n_k^1) = b + \gamma n_k^1/2, \quad (20)$$

see Fig. 4 for illustration. It is easy to see that a product of two Bernoulli product measures is invariant under the stochastic dynamics of this process. One finds the two stationary currents

$$j_1^*(\rho_1, \rho_2) = \rho_1(1 - \rho_1)(1 + \gamma\rho_2), \quad j_2^*(\rho_1, \rho_2) = \rho_2(1 - \rho_2)(b + \gamma\rho_1). \quad (21)$$

Notice that like (generically) in the single-lane multi-species process described above the currents depend on both densities unless the interaction constant γ vanishes.

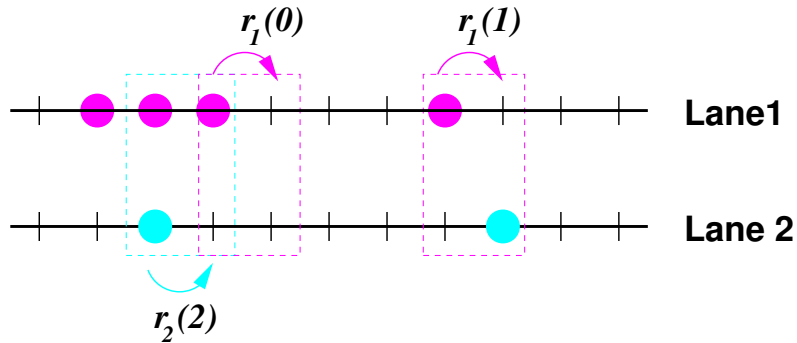


Figure 4: Twolane TASEP without hopping between lanes. Some possible jumps and their rates according to (20) are shown. The boxes drawn with broken lines indicate on which sites in the neighbouring lane the jump rate depends.

1.2 Some linear algebra

In order to obtain more information about stochastic lattice gas models we introduce below methods which are known under the flag *quantum Hamiltonian formalism*. The term quantum Hamiltonian formalism may sound scary to a non-physicist. In actual fact, however, this formalism is based on elementary notions from linear algebra of finite-dimensional vector spaces. Hence one can work within this framework without any reference to quantum mechanics and this is how we shall approach this way of looking at stochastic interacting particle systems.

The fundamental ingredients are standard matrix multiplication and the perhaps some less familiar Kronecker product of matrices, sometimes also called outer product. We recall both types of matrix products. In the following and throughout this work we use the Kronecker-symbol defined by

$$\delta_{\alpha,\beta} = \begin{cases} 1 & \text{if } \alpha = \beta \\ 0 & \text{else} \end{cases} \quad (22)$$

for α, β from any set. Complex conjugation is denoted by a bar as e.g. in \bar{z} .

1.2.1 Matrices and vectors

A $m \times n$ matrix A is a number array

$$A = \begin{pmatrix} A_{11} & A_{12} & A_{13} & \dots \\ A_{21} & A_{22} & A_{23} & \dots \\ A_{31} & A_{32} & A_{33} & \dots \\ A_{41} & A_{42} & A_{43} & \dots \\ A_{51} & A_{52} & A_{53} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

with $m \geq 1$ rows and $n \geq 1$ columns and matrix elements A_{kl} in row k and column l . The matrix elements A_{kl} will be mostly real numbers, but they can also be complex in certain applications. Hence we shall generally assume $A_{kl} \in \mathbb{C}$. We discuss some special cases.

(a) If $m = n = 1$ the matrix reduces a single number and we shall not differentiate between numbers and 1×1 -matrices.

(b) If $n = 1$ and $m > 1$ a matrix Φ is a column array of m numbers. We call such a matrix a *ket-vector* that we denote by the so-called ket-symbol $|\Phi\rangle$. The matrix elements Φ_{1l} with $1 \leq l \leq m$ will be denoted in simplified form by Φ_l and called components of the ket-vector. Thus

$$|\Phi\rangle = \begin{pmatrix} \Phi_1 \\ \Phi_2 \\ \vdots \\ \Phi_m \end{pmatrix}.$$

The vector with $\Phi_i = \delta_{ik}$ is a canonical basis vector of the vector space \mathbb{C}^m denoted by $|e_k\rangle$. The set $\mathbb{B}_m := \{|e_k\rangle : k \in \{1, \dots, m\}\}$ spans \mathbb{C}^m and is called the canonical basis.

(c) If $m = 1$ and $n > 1$ a matrix Ψ is a row array of n numbers. We call such a matrix a *bra-vector* that we denote by the so-called bra-symbol $\langle\Psi|$. The matrix elements Ψ_{k1} with $1 \leq k \leq n$ will be denoted in simplified form as Ψ_k and called components of the bra-vector. Thus

$$\langle\Psi| = (\Psi_1, \Psi_2, \dots, \Psi_n).$$

Defining $\langle e_k| = |e_k\rangle^T$ one realizes that the set $\mathbb{B}^* := \{\langle e_k| : k \in \{1, \dots, n\}\}$ spans \mathbb{C}^n . Since any finite-dimensional vector space is isomorphic to its dual, we can think of the bra-vectors \mathbb{B}_n^* as representing the canonical basis of the dual space $\mathbb{C}^{n*} \cong \mathbb{C}^n$.

The letter or number inside the ket-symbol $|\cdot\rangle$ or the bra-symbol $\langle\cdot|$ is not to be understood as the argument of some function, but just as a symbol that collectively represents the components of the vector. When we use the term matrix we shall tacitly assume that $m, n \geq 2$. The distinction between “proper” matrices on the

one hand and the two types of vectors or simple numbers on the other hand is useful because many fundamental linear algebra operations can be represented as products involving numbers, bra- and ket-vectors and proper matrices with more than one column or row.

We usually denote proper matrices by capital letters or small letters with circumflex accent as e.g. in \hat{a} . The unit matrix of dimension $n > 2$ with components $A_{kl} = \delta_{k,l}$ is denoted by $\mathbf{1}$ and for $n = 2$ we use the notation $\mathbb{1}$. Since multiplication of a vector with the unit matrix is the same as multiplication with the scalar unity 1 of the field F we do not usually differentiate between the two operations, i.e., in equations for matrices we often write a multiple $x\mathbf{1}$ of the unity matrix simply as x .

1.2.2 Addition and multiplication of matrices

Any two matrices A and B which have the same number of rows and columns can be multiplied by a number and added to form a matrix $C = xA + yB$ with the rule that $C_{kl} = xA_{kl} + yB_{kl}$ where $x, y \in \mathbb{C}$. Square matrices with $m = n$ form a ring with a multiplication rule that can be generalized to non-square matrices as follows.

Definition 1.1 (*Matrix product*) For $m, n, p \geq 1$ let A be a $m \times p$ -matrix and B be a $p \times n$ -matrix, both with matrix elements in some field F . The matrix product AB is an $m \times n$ matrix C with matrix elements $C_{kl} \equiv (AB)_{kl} \in F$ given by

$$C_{kl} = \sum_{j=1}^p A_{kj} B_{jl}, \quad 1 \leq k \leq m, \quad 1 \leq l \leq n. \quad (23)$$

Square matrices A, B of the same dimension $m = n = p$ satisfying

$$[A, B] := AB - BA = 0 \quad (24)$$

are said to commute.

Notice that unless $m = n$ the reverse product BA is not defined since the number of columns in the first factor must be equal to the number of rows in the second factor of any matrix product. For a square matrix A the p^{th} power of A is denoted A^p and is defined for strictly positive integers $p \in \mathbb{N}$ by iteration of (23). By convention $A^0 = \mathbf{1}$.

We discuss separately the special cases where at least one of the three number m, n, p is equal to one.

(a) If $n = 1$ and $p, m > 1$ then we can write the matrix B as a ket-vector $|\Phi\rangle$ with components $\Phi_k := B_{k1}$, $k \in \{1, \dots, p\}$. Then also the matrix product C is a ket-vector (with m components given by (23)) and the matrix product can be interpreted as a linear mapping $|\Phi\rangle \mapsto |\tilde{\Phi}\rangle$ given by $|\tilde{\Phi}\rangle = A|\Phi\rangle$, corresponding to the standard right multiplication of a matrix A with the column vector $|\Phi\rangle$.

(b) Likewise, for $m = 1$ and $p, n > 1$ we can write $A = \langle \Psi |$ as a bra-vector with p components with components $\Psi_l := A_{1l}$ and find that the matrix product is a linear mapping $\langle \Psi | \mapsto \langle \tilde{\Psi} |$ that yields the bra-vector $\langle \tilde{\Phi} | = \langle \Psi | B$ with n components given by (23), corresponding to the left multiplication of a matrix B with the row vector $\langle \Psi |$.

(c) If $p = 1$ and $m, n > 1$ then the matrix product actually turns into a product of two vectors. It maps a m -component ket-vector $|\Phi\rangle$ ($= m \times 1$ -matrix A) with components $\Phi_k := A_{k1}$ and an n -component bra-vector $\langle \Psi |$ ($= 1 \times n$ -matrix B) with components $\Psi_l := B_{1l}$ into a proper $m \times n$ matrix

$$C = |\Phi\rangle\langle \Psi| \quad (25)$$

with matrix elements $C_{kl} = \Phi_k \Psi_l$ as given by (23). This mapping, called dyadic product, is a special form of the Kronecker product discussed below.

(d) For $m = n = 1$ the matrix product reduces to a single number $C = \langle \Psi || \Phi \rangle = C_{11} \in F$ with

$$\langle \Psi || \Phi \rangle = \sum_{i=1}^p \Psi_i \Phi_i \equiv \langle \Psi | \Phi \rangle. \quad (26)$$

It defines a bilinear mapping $(\langle \Psi |, |\Phi\rangle) \mapsto C_{11}$ which can be interpreted as a dual pairing $d : \mathfrak{V}^* \times \mathfrak{V} \rightarrow F$, $(\langle \Psi |, |\Phi\rangle) \mapsto \langle \Psi | \Phi \rangle$ since it is natural to regard the bra-vector to be an element of the vector space dual to the vector space to which the ket-vector belongs. This motivates the simplified notation $\langle \Psi | \Phi \rangle$ of this matrix product with only one vertical bar.

Specifically, for the basis vectors we obtain from (26) the biorthogonality relation

$$\langle e_i | e_j \rangle = \delta_{ij}. \quad (27)$$

Notice the difference between the dual pairing (26) and the scalar product $s : \mathfrak{V} \times \mathfrak{V} \rightarrow F$ defined by the sesquilinear form $(|\Phi'\rangle, |\Phi\rangle) \mapsto \langle \Phi', \Phi \rangle := \sum_{i=1}^p \overline{\Phi'_i} \Phi_i$ which is linear in the second argument, but antilinear in the first. When $\langle \Phi' |$ has only real components (as is the case in most of our applications) this distinction is irrelevant, but should nevertheless be kept in mind.

1.2.3 The Kronecker product

The Kronecker product $A \otimes B$ is defined for arbitrary rectangular matrices (including vectors and numbers) as follows.

Definition 1.2 (*Kronecker product*) *Let A and B be two finite-dimensional matrices with $m_A \geq 1$ ($m_B \geq 1$) rows and $n_A \geq 1$ ($n_B \geq 1$) columns with matrix elements A_{ij} and B_{kl} respectively. The Kronecker product $A \otimes B$ is a $m_A m_B \times n_A n_B$ -matrix C with matrix elements*

$$C_{(i-1)m_B+k, (j-1)n_B+l} = A_{ij} B_{kl} \quad (28)$$

with $i \in \{1, \dots, m_A\}$, $j \in \{1, \dots, n_A\}$, $k \in \{1, \dots, m_B\}$, $l \in \{1, \dots, n_B\}$.

Alternatively we can write

$$A \otimes B = \begin{pmatrix} A_{11}B & A_{12}B & A_{13}B & \dots \\ A_{21}B & A_{22}B & A_{23}B & \dots \\ A_{31}B & A_{32}B & A_{33}B & \dots \\ A_{41}B & A_{42}B & A_{43}B & \dots \\ A_{51}B & A_{52}B & A_{53}B & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

Here each matrix “element” is itself a matrix, viz. the matrix B multiplied by the number A_{ij} . In general $A \otimes B \neq B \otimes A$. For $p \in \mathbb{N}_0$ the p -fold Kronecker product of a matrix A with itself is denoted by $A^{\otimes p}$ with the convention that $A^{\otimes 1} := A$ and $A^{\otimes 0} := 1$ where 1 is the unit element of F and not the unit matrix. We discuss special cases.

(a) Consider $n_A = n_B = 1$, i.e., the Kronecker product of ket-vectors $|\Phi^1\rangle, |\Phi^2\rangle$ with components Φ_i^1 where $i \in \{1, \dots, m_A\}$ and Φ_k^2 where $k \in \{1, \dots, m_B\}$. The tensor product $|\Phi^1\rangle \otimes |\Phi^2\rangle$ is a column vector of dimension $m_A m_B$ denoted by $|\Phi^1, \Phi^2\rangle$ and has factorized components $(|\Phi^1, \Phi^2\rangle)_{(i-1)m_B+k} = \Phi_i^1 \Phi_k^2$. Specifically, for the canonical basis vectors one gets $|e_i\rangle \otimes |e_k\rangle \equiv |e_i, e_k\rangle = |e_{(i-1)m_B+k}\rangle$. Thus the Kronecker product of two canonical basis vectors yields a canonical basis vector. The set $\mathbb{B}_{m_A m_B} := \{|e_{(i-1)m_B+k}\rangle : (i, k) \in \{1, \dots, m_A\} \times \{1, \dots, m_B\}\}$ forms the canonical basis of the tensor space $\mathbb{C}^{m_A} \otimes \mathbb{C}^{m_B} \cong \mathbb{C}^{m_A m_B}$.

(b) Similarly, for $m_A = m_B = 1$, i.e., for bra-vectors $\langle \Psi^1|, \langle \Psi^2|$ with components Ψ_j^1 where $j \in \{1, \dots, n_A\}$ and Ψ_l^2 where $l \in \{1, \dots, n_B\}$ the tensor product $\langle \Psi^1| \otimes \langle \Psi^2|$ is a row vector of dimension $n_A n_B$ denoted by $\langle \Psi^1, \Psi^2|$. It has factorized components $(\langle \Psi^1, \Psi^2|)_{(j-1)n_B+l} = \Psi_j^1 \Psi_l^2$ and for the canonical basis vectors one gets $\langle e_j, e_l| = \langle e_{(j-1)n_B+l}|$.

(c) For the Kronecker product of a bra-vector $\langle \Psi|$ and a ket-vector $|\Phi\rangle$ the definition (1.2) yields

$$\langle \Psi| \otimes |\Phi\rangle = |\Phi\rangle \otimes \langle \Psi| = |\Phi\rangle \langle \Psi| \quad (29)$$

with the dyadic product (25).

The Kronecker product is associative. Multiple Kronecker products of matrices define multilinear maps of the multiple tensor product of vector spaces defined by iterating the Kronecker product (1.2). They satisfy the multiplication rule

$$(A \otimes B)(C \otimes D) = (AC) \otimes (BD) \quad (30)$$

where we assume that the matrix products AC and BD are defined by (23).

We note an important factorization property of the dual pairing of Kronecker products of vectors which is an immediate consequence of the multilinearity of the Kronecker product encoded in (28).

Proposition 1.3 Let $\langle \Psi^k | (|\Phi^k\rangle)$ be a bra-vector (ket-vector) of dimension d_k with components $\Psi_i^k \in \mathbb{C}$ ($\Phi_i^k \in \mathbb{C}$) and $\langle \Psi^1, \Psi^2, \dots, \Psi^L | = \langle \Psi^1 | \otimes \langle \Psi^2 | \otimes \dots \otimes \langle \Psi^L |$ ($|\Phi^1, \Phi^2, \dots, \Phi^L\rangle = |\Phi^1\rangle \otimes |\Phi^2\rangle \otimes \dots \otimes |\Phi^L\rangle$) be the L -fold Kronecker product of these vectors. Then the dual pairing factorizes as

$$\langle \Psi^1, \Psi^2, \dots, \Psi^L | \Phi^1, \Phi^2, \dots, \Phi^L \rangle = \prod_{k=1}^L \langle \Psi^k | \Phi^k \rangle \quad (31)$$

with $\langle \Psi^k | \Phi^k \rangle$ given by (26).

When $\langle \Psi^k | = \langle \Psi |$ for all $k \in \{1, \dots, L\}$ then we write $\langle \Psi^1, \Psi^2, \dots, \Psi^L | = \langle \Psi |^{\otimes L}$ and analogously for ket-vectors and proper matrices A .

Finally we introduce *local operators* which act non-trivially only on component k in an L -fold tensor space. For simplicity we assume equal dimensions $d := d_1 = d_2 = \dots = d_L$.

Definition 1.4 (*Local operator*) Let $\mathbf{1}$ be the d -dimensional unit matrix and A be an arbitrary square matrix of dimension $d \geq 1$. The local operator A_k is the Kronecker product

$$A_k := \mathbf{1}^{\otimes(k-1)} \otimes A \otimes \mathbf{1}^{\otimes(L-k)}. \quad (32)$$

Notice the difference between the number $1 \in \mathbb{C}$ and the unit matrix $\mathbf{1}$ in this definition. The expression ‘‘local operator’’ come from the fact that when acting on a tensor vector $|\Phi^1, \dots, \Phi^L\rangle$ only the k^{th} factor is changed by the action of A_k . More precisely,

$$A_k (|\Phi^1\rangle \otimes \dots \otimes |\Phi^k\rangle \otimes \dots \otimes |\Phi^L\rangle) = |\Phi^1\rangle \otimes \dots \otimes |\tilde{\Phi}^k\rangle \otimes \dots \otimes |\Phi^L\rangle. \quad (33)$$

where $|\tilde{\Phi}^k\rangle = A|\Phi^k\rangle$.

From (30) one finds

$$A_k B_k = (AB)_k \quad (34)$$

which is equal to $B_k A_k$ if and only if $AB = BA$. On the other hand, by construction one has for two square matrices A, B of dimension k the commutation relation

$$A_k B_l = B_l A_k \text{ for } k \neq l \quad (35)$$

even when $AB \neq BA$. In order to avoid confusion concerning the role of the indices we point out that for $L = 2$ and $[A, B] \neq 0$ we have

$$A \otimes B = A_1 B_2 = B_2 A_1 \neq B \otimes A = B_1 A_2 = A_2 B_1. \quad (36)$$

We also note that for matrices $A^{(k)}$ one has

$$A_1^{(1)} A_2^{(2)} \dots A_L^{(L)} = A^{(1)} \otimes A^{(2)} \otimes \dots \otimes A^{(L)}. \quad (37)$$

The upper index defines the matrix while the lower index defines its position in the L -fold Kronecker product. We stress that $A^{(k)}$ is a matrix of dimension d while $A_k^{(k)}$ is a matrix of dimension d^L .

From Proposition (1.3) one finds for d -dimensional square matrices $A^{(k)}$ the factorization property

$$\langle \Psi^1, \Psi^2, \dots, \Psi^L | A_1^{(1)} A_2^{(2)} \dots A_L^{(L)} | \Phi^1, \Phi^2, \dots, \Phi^L \rangle = \prod_{k=1}^L \langle \Psi^k | A^{(k)} | \Phi^k \rangle. \quad (38)$$

We write explicitly two special cases of particular importance:

$$\frac{\langle \Psi^1, \Psi^2, \dots, \Psi^L | A_k | \Phi^1, \Phi^2, \dots, \Phi^L \rangle}{\langle \Psi^1, \Psi^2, \dots, \Psi^L | \Phi^1, \Phi^2, \dots, \Phi^L \rangle} = \frac{\langle \Psi^k | A | \Phi^k \rangle}{\langle \Psi^k | \Phi^k \rangle} \quad (39)$$

$$(\langle \Psi |)^{\otimes L} (|\Phi \rangle)^{\otimes L} = \langle \Psi | \Phi \rangle^L. \quad (40)$$

These computational properties of the matrix product (23) and of the Kronecker product defined in Def. (1.2) will be exploited throughout these notes.

1.3 Generator of Markov processes in matrix form

Markov processes provide very often a good description of classical physical processes and have gained particular attention in the context of interacting particle systems, both in mathematical probability theory [61, 62, 54] and in statistical physics [92, 21, 87, 27, 10, 9]. The link to quantum mechanical condensed matter systems that we mentioned above allows one to use ideas and techniques borrowed from many-body quantum mechanics even though stochastic interacting particle systems are completely classical. The fundamental idea very simple:

One writes the generator of a Markov process in terms of the intensity matrix of transition rates, expresses expectations as bilinear forms, and uses tools from algebra.

The point here is that in many cases of interest the intensity matrix is the same object as the quantum Hamiltonian operator of some many-body quantum system. Then one employs mathematical techniques from algebra that have proved useful in the treatment of quantum Hamiltonian operators. Quantum mechanics as such plays no part in extracting information about properties of the intensity matrix, only the purely mathematical machinery developed for many-body quantum systems comes into play.

To make clear some of the essential ideas we shall consider mostly irreducible systems with finite state space Ω . This allows us to straightforwardly adopt the strategy of describing the time evolution of the process by a *master equation* for the probability measure which is the differential form of the Chapman-Kolmogorov

equation. Solving the master equation, which is a first-order linear differential equation in the time variable, yields the probability of finding any given state the system may take given that it started from some initial state.

The idea of formulating the master equation in terms of a many-body quantum Hamiltonian is not new. Systematic treatments of various aspects of the quantum Hamiltonian formalism go back to [49, 23, 33, 1]. A mathematically rigorous account is given in [97, 63] and a detailed (non-rigorous) review is [87]. The extension to infinite systems can usually be made without great difficulty if the state space is countably infinite or by taking appropriate limits of expectation values if the state space of the infinite system is not countable.

1.3.1 Matrix formulation of the generator

We recall the definition of a Markov process η_t with state space Ω and transition rates $w_{\eta',\eta}$ for a transition from a configuration $\eta \in \Omega$ to a configuration $\eta' \in \Omega$ in terms of a generator \mathcal{L} acting on suitably chosen functions $f(\eta)$ through the relation

$$\mathcal{L}f(\eta) = \sum_{\eta' \in \Omega \setminus \eta} w_{\eta',\eta} [f(\eta') - f(\eta)]. \quad (41)$$

Now we introduce the central object of interest.

Definition 1.5 *The intensity matrix H of the process η_t with state space Ω is the matrix with elements*

$$H_{\eta'\eta} = \begin{cases} -w_{\eta',\eta} & \eta \neq \eta' \\ \sum_{\eta' \in \Omega \setminus \eta} w_{\eta',\eta} & \eta = \eta'. \end{cases} \quad (42)$$

Remark 1.6 *The intensity matrix is often represented in transposed form and with opposite sign and also called transition rate matrix. By definition of a transition rate one has $-H_{\eta'\eta} \in \mathbb{R}_0^+$ (positivity of rates) and $\sum_{\eta \in \Omega} H_{\eta'\eta} = 0$ (probability conservation). We shall call any matrix with these properties an intensity matrix.*

The defining equation (41) then becomes

$$\mathcal{L}f(\eta) = - \sum_{\eta' \in \Omega} f(\eta') H_{\eta'\eta} \quad (43)$$

with summation over η on the r.h.s. included. This follows from splitting the sum on the r.h.s. into two terms $-(f(\eta)H_{\eta\eta} + \sum_{\eta' \in \Omega \setminus \eta} f(\eta')H_{\eta'\eta})$ from which one recovers (41) by using (42). According to (23) the r.h.s. of (43) represents the left multiplication of the matrix H with a row vector with components $f(\eta')$.

Taking the expectation \mathbf{E}^μ under a measure μ , one gets from (43) (after renaming dummy variables inside the sums)

$$\frac{d}{dt} \mathbf{E}_{\mu_t} f = \mathbf{E}_{\mu_t} [\mathcal{L}f] = - \sum_{\eta' \in \Omega} f(\eta') \sum_{\eta'' \in \Omega} H_{\eta'\eta''} \mu_t(\eta'') = \sum_{\eta \in \Omega} f(\eta) \mathcal{L}^T \mu_t(\eta). \quad (44)$$

Choosing as $f(\eta)$ the indicator function $1_\eta : \Omega \rightarrow \{0, 1\}$, $\xi \mapsto 1_\eta(\xi) = \delta_{\eta,\xi}$ the second equality yields

$$\mathcal{L}^T \mu(\eta) = - \sum_{\eta' \in \Omega} H_{\eta\eta'} \mu(\eta') \quad (45)$$

where the r.h.s. represents the right multiplication of the matrix H with a column vector with components $\mu(\xi)$. The semigroup property of Markov processes then implies for the time-evolving measure μ_t the *master equation*

$$\frac{d}{dt} \mu_t(\eta) = - \sum_{\eta' \in \Omega} H_{\eta\eta'} \mu_t(\eta') = \sum_{\eta' \in \Omega \setminus \eta} (w_{\eta\eta'} \mu_t(\eta') - w_{\eta'\eta} \mu_t(\eta)) \quad (46)$$

which is the adjoint version of (43) for functions $f(\eta)$. The quantity

$$j_t(\eta', \eta) := w_{\eta'\eta} \mu_t(\eta) - w_{\eta\eta'} \mu_t(\eta') \quad (47)$$

is called the (instantaneous) *probability current* from η to η' .

The matrix multiplications (43) and (45) lead us consider the actual matrix in a basis. We assume Ω to be countable so that to each configuration η one can associate bijectively an integer $\iota(\eta) \in \mathbb{N}$ that enumerates the configurations. We shall call $\iota(\eta)$ the enumeration function. It is natural to choose the canonical basis vectors denoted by $\langle e_i |$ (represented as row vectors with components $(e_i)_j = \delta_{i,j}$) through the bijective map $\eta \mapsto \langle e_{\iota(\eta)} | =: \langle \eta |$ and to define also the column vectors $|\eta\rangle := \langle \eta |^T$. A given enumeration function thus fixes uniquely the matrix H which without explicit enumeration function would be fixed only up to permutations of the canonical basis vectors.

With the canonical basis vectors and an enumeration function at hand we define the function vector

$$\langle f | := \sum_{\eta \in \Omega} f(\eta) \langle \eta | \quad (48)$$

and the *probability vector*

$$|\mu(t)\rangle := \sum_{\eta \in \Omega} \mu_t(\eta) |\eta\rangle \quad (49)$$

for a time-dependent measure $\mu(t)$.

Observing biorthogonality one realizes that a function f can be expressed as dual pairing $f(\eta) = \langle f | \eta \rangle$ and similarly $\mu_t(\eta) = \langle \eta | \mu(t) \rangle$. These observations allow us to rewrite (41) in the form

$$\mathcal{L} f(\eta) = - \langle f | H | \eta \rangle \quad (50)$$

and the master equation (46) can be written in vector form as

$$\frac{d}{dt} |\mu(t)\rangle = - H |\mu(t)\rangle. \quad (51)$$

with

$$H = - \sum_{\eta \in \Omega} \sum_{\eta' \in \Omega \setminus \eta} w_{\eta'\eta} (E^{\eta'\eta} - \hat{1}_\eta) \quad (52)$$

where

$$E^{\eta'\eta} := |\eta'\rangle\langle\eta|, \quad \hat{1}_\eta := |\eta\rangle\langle\eta|. \quad (53)$$

Integration then expresses the time-dependent measure

$$|\mu(t)\rangle = e^{-Ht}|\mu\rangle \quad (54)$$

in terms of an arbitrary initial measure $\mu = \mu(0)$. In slight abuse of language we shall call also the intensity matrix H the generator of the process. We shall call the exponential $\exp(-Ht)$ the transition matrix at time t .

Some comments on the spectrum of H for finite state space Ω are in place. Obviously, $\dim(H) = |\Omega|$. Since H is real all eigenvalues are either real or come in complex conjugate pairs. The negative sign for the off-diagonal elements is by convention. It ensures, by the theorem of Gershgorin [32], that all eigenvalues of H are either 0 or have strictly positive real part. Consequently, the eigenvalues of the transition matrix $\exp(-Ht)$ are either 1 or strictly inside the unit circle in the complex plane for all times $t \in \mathbb{R}_0^+$. This rules out periodicity of the process. If the process η_t is irreducible then the matrix H is also irreducible and has unique lowest eigenvalue 0. By Perron-Frobenius [66] the corresponding right and left eigenvector can be chosen to have strictly positive real components. More generally, the following two statements on reducible chains are equivalent: (i) Ω has exactly n mutually communicating subsets Ω_α . (ii) The eigenvalue 0 of H is n -fold degenerate. The process restricted to a single communicating subset is ergodic since it is both aperiodic and irreducible.

1.3.2 Expectations in matrix formulation

In order to work with this matrix reformulation of the generator we introduce some further key objects. All summations run over the full set Ω unless stated otherwise.

Definition 1.7 (a) *The summation vector is the constant bra-vector*

$$\langle s| := \sum_{\eta} \langle\eta|. \quad (55)$$

(b) *The function matrix \hat{f} for a function $f : \Omega \rightarrow \mathbb{C}$ and the measure matrix $\hat{\mu}$ for a probability measure μ are the diagonal matrices*

$$\hat{f} := \sum_{\eta} f(\eta)|\eta\rangle\langle\eta|, \quad \hat{\mu} := \sum_{\eta} \mu(\eta)|\eta\rangle\langle\eta|. \quad (56)$$

(c) *The time-dependent function matrix $\hat{f}(t)$ is defined by*

$$\hat{f}(t) := e^{Ht}\hat{f}e^{-Ht}. \quad (57)$$

If $\hat{f}(t) = \hat{f}(0)$ for all $t \in \mathbb{R}$ we say that f is conserved.

(d) Let $S : \Omega \times \Omega \rightarrow \mathbb{C}$ be a function and \hat{S} be a matrix with elements $S_{\eta,\xi} = S(\eta, \xi)$. If \hat{S} satisfies

$$[H, \hat{S}] = 0. \quad (58)$$

then S is called a symmetry of the process.

The function matrix for the indicator function 1_η is the projector $\hat{1}_\eta = |\eta\rangle\langle\eta|$, i.e. the dyadic product of the canonical basis vector $|\eta\rangle$ with its transpose. For a strictly positive measure any power $\hat{\mu}^\alpha$ exists. Therefore, in particular, the inverse $\hat{\mu}^{-1}$ exists. Conservation of f implies the commutation relation $[H, \hat{f}] = 0$. Therefore a conserved f is a symmetry of the process. Notice that conservation of f implies $\langle f | H = 0$, which means that f is a harmonic function. The converse, however, is not true: A function may be harmonic, but not conserved. Nevertheless, a non-constant harmonic function implies existence of a conserved function S with the property $\langle s | \hat{S} = \langle f |$.

Since by construction in each column of H all matrix elements sum up to zero the summation vector is a left eigenvector of H with eigenvalue 0, i.e.,

$$\langle s | H = 0. \quad (59)$$

This fact expresses conservation of probability since $\langle s | \mu(t) \rangle = \langle s | e^{-Ht} | \mu \rangle = \langle s | \mu \rangle = 1$ with $\mu = \mu_0$. For the function vector $\langle f |$ (48) we have trivially that

$$\langle s | \hat{f} = \langle f |. \quad (60)$$

This yields for the expectation of a function $f(\eta)$ the various equivalent matrix representations

$$\mathbf{E}_{\mu_t} f \equiv \langle f \rangle_{\mu_t} = \langle s | \hat{f} | \mu(t) \rangle = \langle s | \hat{f} e^{-Ht} | \mu \rangle = \langle s | \hat{f}(t) | \mu \rangle \equiv \langle f_t \rangle_\mu \quad (61)$$

where in the rightmost expression we use the notation $f_t(\eta) = f(\eta_t)$.

The expectation – which we shall denote by angular brackets – is an average both over histories of the process and over the initial distribution μ . Of course, if the initial distribution is concentrated on a particular configuration ξ , the brackets reduce to an average over histories. For a process starting at a configuration ξ the expectation of the indicator function 1_η yields the conditional probability (sometimes called *propagator*)

$$P(\eta, t | \xi, 0) = \langle s | \hat{1}_\eta e^{-Ht} | \xi \rangle = \langle \eta | e^{-Ht} | \xi \rangle = \langle \xi | e^{-H^T t} | \eta \rangle. \quad (62)$$

Multi-time expectations can be expressed analogously using the propagator and the Chapman-Kolmogorov equation arising from the Markov property of the process.

1.3.3 Stationarity and reversibility

One of the most basic questions to ask is the behaviour at late times of the stochastic evolution. If the process is ergodic then the measure in the limit $t \rightarrow \infty$ is

independent of the initial state and one would like to know for interacting particle systems quantities like the mean density, density fluctuations, or the spatial structure of the particle distribution and its correlations. For transition rates that are constant in time this asymptotic measure is invariant under time translations and hence called stationary. We shall denote any normalized stationary measure by μ^* , its associated probability vector by $|\mu^*\rangle$ and the diagonal measure matrix by $\hat{\mu}^*$. From the considerations of the previous subsections it is clear that $|\mu^*\rangle$ is a right eigenvector of H with eigenvalue zero,

$$H|\mu^*\rangle = 0. \quad (63)$$

Trivially, one has

$$|\mu^*\rangle = \hat{\mu}^*|s\rangle \quad (64)$$

where $|s\rangle := \langle s|^T$ has constant components $s_\eta = 1$. If the process is ergodic then $\mu^* = \mu_\infty$ is unique and the diagonal matrix power $(\hat{\mu}^*)^\alpha$ with diagonal elements $(\mu^*(\eta))^\alpha$ exists for every $\alpha \in \mathbb{C}$.

In the context of physical systems at thermal equilibrium the configurations η are the microstates and the stationary measure is the Gibbs measure

$$\mu^*(\eta) = \frac{1}{Z} \exp(-\beta U(\eta)) \quad (65)$$

which is proportional to the *Boltzmann weight* $\exp(-\beta U(\eta))$. Here $\beta = 1/(k_B T)$ is proportional to the inverse temperature T , k_B is the Boltzmann constant and $U(\eta)$ is called the energy of the microstate η (Fig. 5) and

$$Z = \sum_{\eta \in \Omega} \exp(-\beta U(\eta)) \quad (66)$$

is the partition function, related to the free energy F by

$$F = -k_B T \ln Z. \quad (67)$$

For many applications, however, one has to think the other way round and construct a process such that for a given energy function the Gibbs measure is stationary. This is the case e.g. in Monte Carlo simulations of equilibrium systems. One possibility of solving this problem is implementing *detailed balance* on the transition probabilities (or rates respectively).

Definition 1.8 (*Detailed balance*) *A Markov process η_t with state space Ω and transition rates $w(\eta', \eta)$ is said to satisfy detailed balance (or to be reversible) if there exists a strictly positive measure $\pi(\eta)$ such that*

$$\pi(\eta)w(\eta', \eta) = \pi(\eta')w(\eta, \eta') \quad \forall \eta, \eta' \in \Omega. \quad (68)$$

A measure π with this property is called reversible. If $Z := \sum_{\eta} \pi(\eta) < \infty$ then Z is called the partition function. The normalized measure $\pi^ := \pi/Z$ is called the equilibrium measure.*

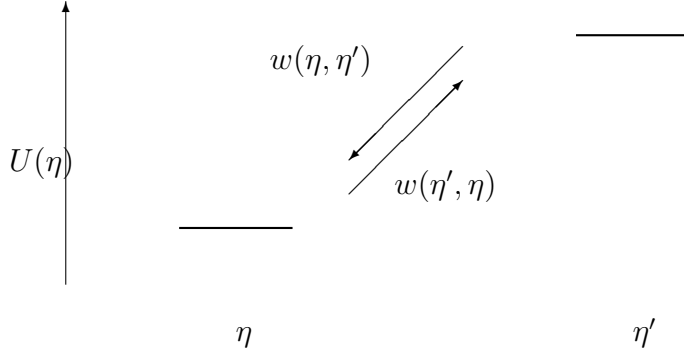


Figure 5: Stochastic transitions between two states of different equilibrium energies U, U' .

Remark 1.9 *The equilibrium measure entering the detailed balance definition is a stationary measure of the process. The invariance follows immediately from the master equation (46) since due to (68) each term in the sum over η' on the r.h.s. of (46) is equal to zero and therefore the time-derivative of π vanishes. Often any stationary measure is called an equilibrium measure which is confusing from a physics viewpoint. Therefore we reserve "equilibrium" to reversible processes and use "stationary" or "non-equilibrium" for non-reversible processes.*

Detailed balance means for a Gibbs measure that the ratio of transition rates between two microstates η, η' equals the exponential $\exp(-\beta\Delta U)$ of the energy gain $\Delta U = U(\eta') - U(\eta)$ incurred by the transition (Fig. 5). Thus the transition rate ratio is the equilibrium ratio of the probabilities of finding these states. Processes satisfying detailed balance are also called equilibrium processes.

For the generator H of a reversible process we note the following.

Proposition 1.10 *Let π be a strictly positive measure on the state space Ω . For an ergodic process η_t with generator H the following statements are equivalent:*

- (i) *The process satisfies detailed balance with reversible measure π .*
- (ii) *$H^T = \hat{\pi}^{-1}H\hat{\pi}$, where H^T is the transpose of H .*
- (iii) *H can be written in the form $H = F\hat{\pi}^{-1}$ for some symmetric intensity matrix F .*

Proof: (a) Assume (i) is true. By strict positivity π^{-1} exists and the detailed balance condition (68) can be recast as $\pi^{-1}(\eta')w(\eta', \eta)\pi(\eta) = w(\eta, \eta')$. This is assertion (ii) in terms of each matrix element.

(b) Assume (ii) is true. Writing out the matrix equation (ii) in terms of each matrix element one gets (i). Moreover, (ii) can be recast as $H\hat{\pi} = \hat{\pi}H^T = (H\hat{\pi})^T$ which implies that $H\hat{\pi}$ is symmetric. That $F := H\hat{\pi}$ is an intensity matrix follows from the fact that F has non-positive off-diagonal elements (meaning: non-negative

transition rates) and $0 = \langle s | H \hat{\pi} = \langle s | F$, which is conservation of probability. Thus (iii) follows from (ii).

(c) Assume (iii) is true. Since F is symmetric it follows that $H^T = \hat{\pi}^{-1} F = \hat{\pi}^{-1} H \hat{\pi}$. Thus (ii) follows from (iii). \square

Property (ii) can be seen as a special property of a diagonal similarity transformation of the generator H with the invariant measure π . Generalizing diagonal similarity transformations with the invariant measure π to processes not satisfying detailed balance leads us to introduce two more notions of interest.

Definition 1.11 (*Reversed process and ground state transformation*) *Let μ be a strictly positive stationary solution of the master equation (46) for a generator H . Then*

$$H^* := \hat{\mu} H^T \hat{\mu}^{-1} \quad (69)$$

is called generator of the time-reversed (or simply reversed) process. The transformation to the matrix \tilde{H} defined by

$$\tilde{H} := \hat{\mu}^{-1/2} H \hat{\mu}^{1/2} \quad (70)$$

is called the ground state transformation.

The reversed process has the same invariant measure, the same waiting time distribution for all states, and the same allowed transitions as the original process H , but different and often complicated non-local transition rates

$$w_{\eta', \eta}^{rev} = w_{\eta, \eta'} \frac{\mu(\eta')}{\mu(\eta)}. \quad (71)$$

With these notions Proposition (1.10) has a simple corollary that is worth noting.

Corollary 1.12 *Let the process η_t with generator H be ergodic and reversible. Then (i) $H^* = H$ and (ii) \tilde{H} is symmetric.*

Thus for a reversible ergodic process the spectrum of H is real and strictly positive except for its unique lowest eigenvalue which is 0.¹ The notion of reversibility has its origin in the following property of the two-time equilibrium correlation function

$$\lim_{\tau \rightarrow \infty} \langle f_1(\tau + t) f_2(\tau) \rangle = \langle f_1(t) f_2(0) \rangle_{\pi^*}. \quad (72)$$

What one calculates with this quantity are time-dependent fluctuations in a system which had sufficient time to reach equilibrium. Since the system is assumed to have a unique stationary distribution, this expression is independent of the initial state. Reversibility implies

¹On other words, detailed balance implies that the eigenvalues of the generator are all real and that the related symmetrized generator obtained from the ground state transformation can be interpreted as Hamiltonian of some quantum system. One sees that the use of the term quantum Hamiltonian formalism is justified by more than the formal analogy between Schrödinger equation and master equation.

Proposition 1.13 *Let η_t be reversible w.r.t. a measure π^* and f_1 and f_2 functions of the configurations η . Then*

$$\langle f_1(t)f_2(0) \rangle_{\pi^*} = \langle f_2(0)f_1(-t) \rangle_{\pi^*}. \quad (73)$$

Proof: By definition $\hat{f}_1, \hat{f}_2, \hat{\pi}^*$ are all diagonal and hence commute and are invariant under transposition. Therefore

$$\begin{aligned} \langle f_2(t)f_1(0) \rangle_{\pi^*} &= \langle s | \hat{f}_1 e^{-Ht} \hat{f}_2 | \pi^* \rangle \\ &= \langle s | \hat{\pi}^* \hat{f}_1 e^{-H^T t} \hat{f}_2 (\hat{\pi}^*)^{-1} | \pi^* \rangle \\ &= \langle \pi^* | \hat{f}_1 e^{-H^T t} \hat{f}_2 | s \rangle \\ &= \langle s | \hat{f}_2 e^{-Ht} \hat{f}_1 | \pi^* \rangle \\ &= \langle f_2(t)f_1(0) \rangle_{\pi^*} = \langle f_2(0)f_1(-t) \rangle_{\pi^*} \end{aligned} \quad (74)$$

where the last equality follows from time-translation invariance of the equilibrium distribution. \square

Time-reversal symmetry can be extended straightforwardly to multi-time correlators.

Remark 1.14 *Detailed balance means that all stationary probability currents (47) vanish, thus exposing a direct link between probability currents and reversibility. Notice, however, that a system that does not satisfy detailed balance for the microscopic transition rates may nevertheless be reversible on macroscopic scales. A simple example is a translation-invariant random walk whose increments have zero mean and finite variance. Then by the central limit theorem the large scale behaviour is that of a diffusive particle whose probability distribution satisfies the reversible free diffusion equation, irrespective of whether or not the microscopic increments satisfy detailed balance w.r.t. the stationary uniform measure.*

2 Duality

Duality is a powerful tool in the study of some interacting particles as in some cases it allows for expressing one problem in terms of a much simpler problem. We discuss this property for the SSEP where it was first pointed out by Spitzer in 1970 [96]. Later, by importing known results about quantum spin systems, it was realized that this duality arises from a non-abelian symmetry of the generator [84] known as $SU(2)$ symmetry and eventually extended to the ASEP [86] which has a related symmetry that we shall not discuss in detail. The relationship between symmetries and duality was brought into a neat and systematic form by Giardinà et al. [31] which triggered renewed interest in duality, see also [43] for a survey. We begin by defining duality and presenting it in matrix form [97].

2.1 Duality and Symmetry

Definition 2.1 Let x_t be a Markov process with countable state space Ξ and intensity matrix G and η_t be a Markov process with countable state space Ω and intensity matrix H . Furthermore, let $D : \Xi \times \Omega \rightarrow \mathbb{R}$ be a bounded measurable function. The processes x_t and η_t are said to be dual w.r.t. the duality function D if

$$\mathbf{E}_x D(x_t, \eta) = \mathbf{E}_\eta D(x, \eta_t). \quad (75)$$

The $|\Omega| \times |\Xi|$ matrix

$$\hat{D} := \sum_{x \in \Xi} \sum_{\eta \in \Omega} D(x, \eta) |x\rangle\langle \eta| \quad (76)$$

with matrix elements $D_{x,\eta} = D(x, \eta)$ is called the duality matrix. For $|\Omega| = |\Xi|$ a duality function of the form $D(x, \eta) = \sum_x d(x) \delta_{x,\eta}$ is called diagonal. If $H = G$ then the process is said to be self-dual w.r.t. D .

Remark 2.2 In terms of transition probabilities P for x_t and Q for η_t the defining relation (75) reads

$$\sum_{x' \in \Xi} D(x', \eta) P(x', t | x, 0) = \sum_{\eta' \in \Omega} D(x, \eta') Q(\eta', t | \eta, 0). \quad (77)$$

This yields an equivalent formulation of duality in matrix form by taking the time derivative at $t = 0$. With (62) one obtains [97]

$$\hat{D}H = G^T \hat{D}. \quad (78)$$

Remark 2.3 A process with strictly positive invariant measure and its reversed are dual w.r.t. the diagonal duality function $D^*(\eta, \eta') = \sum_x \mu^{-1}(\eta) \delta_{\eta,\eta'}$ where $\mu > 0$ is the common invariant measure. This follows directly from the definition (69) of the reversed process and the matrix representation $\hat{D} = \hat{\mu}^*$ of the diagonal duality function.

Following [31, 6] we show now that symmetries of a generator may lead to non-trivial dualities.

Theorem 2.4 Let H be the matrix representation of the generator of an ergodic Markov process η_t with countable state space and H^{rev} be the matrix form of the generator of the reversed process x_t . Assume that there exists an intertwiner \hat{S} such that

$$\hat{S}H = H^{rev}\hat{S}. \quad (79)$$

Then H is self-dual with duality function $D(x, \eta) = D_{x,\eta}$ given by the matrix elements of the duality matrix

$$\hat{D} = \hat{\mu}^{-1}\hat{S}. \quad (80)$$

with the diagonal stationary distribution matrix of definition (1.7).

Proof: Given the hypothesis (79), self-duality with duality matrix (80) follows from the chain of equalities

$$DH = \hat{\mu}^{-1} \hat{S}H = \hat{\mu}^{-1} H^{rev} \hat{S} = \hat{\mu}^{-1} H^{rev} \hat{\mu} D = H^T D. \quad (81)$$

The first and the third equality are the definition (80), the second equality is the hypothesis (79) of the theorem, and the fourth equality is the definition (69) of the reversed process. \square

Remark 2.5 *It follows that if H is reversible then the hypothesis (79) reads $\hat{S}H = H\hat{S}$, i.e. according to (58) \hat{S} is a symmetry of H .*

Corollary 2.6 *Let H be the matrix representation of the generator of an ergodic Markov process η_t with countable state space and strictly positive invariant measure μ and S be a symmetry of H . Then H and H^{rev} are dual w.r.t. the duality function $D(\eta, \eta') = \mu^{-1}(\eta)S(\eta, \eta')$.*

2.2 The symmetric simple exclusion process

Above we have introduced in informal fashion the ASEP on the one-dimensional integer lattice. For symmetric hopping rates $r = \ell =: w$ the process is called symmetric simple exclusion process (SSEP). Basically, what this process does is to randomly interchange the occupation variables of a pair of sites. It has a natural generalization to arbitrary graphs and link-dependent hopping rates and can then informally be described as follows. Let $\Gamma = (\Lambda, \Upsilon)$ be a finite graph with nodes $k \in \Lambda$ and undirected links $\langle k, l \rangle \in \Upsilon$. A configuration of the SSEP is denoted by $\boldsymbol{\eta} := \{\eta_k : k \in \Lambda\}$ with the $L = |\Lambda|$ occupation numbers $\eta_k \in \{0, 1\}$. Each link $\langle k, l \rangle$ carries a ‘‘clock’’ that rings after an exponentially distributed random time with parameter $w_{kl} \equiv w_{lk}$. When the clock rings the occupation numbers η_k and η_l are interchanged, corresponding to a particle jump across bond $\langle k, l \rangle$ if one of the two sites is occupied and the other is empty.

This process has a non-Abelian symmetry under the Lie-group $SU(2)$ which implies that its generator H written as a matrix commutes with the representation matrices of the Lie algebra $\mathfrak{sl}(2)$. In order to exploit this fact for deriving duality relations we first write the generator in matrix form.

2.2.1 Generator of the SSEP in matrix form

Definition 2.7 *Let Λ be a finite set of cardinality L , $\eta_j \in \{0, 1\}$ for $j \in \Lambda$ the occupation number of an exclusion process, $\Omega_L = \{0, 1\}^L$, the state space and $\boldsymbol{\eta} = \{\eta_j : j \in \Lambda\}$ be a configuration of an exclusion process. For a pair $\langle k, l \rangle \in \Lambda \times \Lambda$ the $\langle k, l \rangle$ -permutation of a configuration $\boldsymbol{\eta} \in \Omega_L$ is the mapping $\pi^{kl} : \Omega_L \rightarrow \Omega_L$ such that $\pi^{kl}(\boldsymbol{\eta}) \mapsto \boldsymbol{\eta}^{kl}$ with interchanged occupation numbers*

$$\eta_j^{kl} = \eta_j + (\eta_k - \eta_l) (\delta_{j,l} - \delta_{k,l}). \quad (82)$$

The informal description of the SSEP on the Graph Γ means that the transition rates are given by

$$w_{\boldsymbol{\eta}', \boldsymbol{\eta}} = \sum_{\langle k, l \rangle \in \Upsilon} w_{kl} (\eta_k(1 - \eta_l) + (1 - \eta_k)\eta_l) \delta_{\boldsymbol{\eta}', \boldsymbol{\eta}^{kl}} = w_{kl} \quad (83)$$

for all links $\langle k, l \rangle$. Thus the generator reads

$$\mathcal{L}f(\boldsymbol{\eta}) = \sum_{\langle k, l \rangle \in \Upsilon} w_{kl} [f(\boldsymbol{\eta}^{kl}) - f(\boldsymbol{\eta})] = \sum_{\boldsymbol{\eta}' \in \Omega_L} \sum_{\langle k, l \rangle \in \Upsilon} w_{kl} (\delta_{\boldsymbol{\eta}', \boldsymbol{\eta}^{kl}} - \delta_{\boldsymbol{\eta}', \boldsymbol{\eta}}) f(\boldsymbol{\eta}') \quad (84)$$

from which one reads off the matrix elements

$$H_{\boldsymbol{\eta}', \boldsymbol{\eta}} = - \sum_{\langle k, l \rangle \in \Upsilon} w_{kl} (\delta_{\boldsymbol{\eta}', \boldsymbol{\eta}^{kl}} - \delta_{\boldsymbol{\eta}', \boldsymbol{\eta}}) \quad (85)$$

of the generator H of the SSEP.

In order to fix the canonical basis vectors $\langle \boldsymbol{\eta} | = \langle e_{\iota(\boldsymbol{\eta})} |$ and $| \boldsymbol{\eta} \rangle = \langle \boldsymbol{\eta} |^T$ for the intensity matrix, i.e., the matrix form of the generator, we choose the enumeration function

$$\iota(\boldsymbol{\eta}) = 1 + \sum_{k=1}^L \eta_k 2^{L-k}. \quad (86)$$

Thus $\iota(\boldsymbol{\eta})$ is the decimal value plus 1 of the binary number $\eta_1 \eta_2 \dots \eta_L$. By the definition of the Kronecker product (1.2) this choice of enumeration function corresponds to the tensor basis

$$\langle \boldsymbol{\eta} | = \langle \eta_1, \dots, \eta_L | \equiv \langle \eta_1 | \otimes \dots \otimes \langle \eta_L | \quad (87)$$

with the one-site basis vectors

$$\langle \eta_k | = (1 - \eta_k, \eta_k). \quad (88)$$

This yields the constant summation vector in the tensor form

$$\langle s | = (1, 1)^{\otimes L}. \quad (89)$$

In order to write the generator as a matrix it is useful to introduce the unit matrix $\mathbf{1}$ and three Pauli matrices

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (90)$$

where i is the imaginary unit. From these we construct the so-called spin-lowering and raising operator

$$\sigma^+ = \frac{1}{2}(\sigma^x + i\sigma^y) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \sigma^- = \frac{1}{2}(\sigma^x - i\sigma^y) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad (91)$$

which are nilpotent of degree 2 and the projectors

$$\hat{n} = \frac{1}{2}(\mathbf{1} + \sigma^z) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad \hat{v} = \frac{1}{2}(\mathbf{1} - \sigma^z) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad (92)$$

on a particle and vacancy vector respectively.

From the action of these matrices on the single-site basis vectors one reads off

$$(\mathbf{1} + \sigma_k^+ \sigma_l^- + \sigma_k^- \sigma_l^+ - \hat{n}_k \hat{v}_l - \hat{v}_k \hat{n}_l) |\boldsymbol{\eta}\rangle = |\boldsymbol{\eta}^{kl}\rangle. \quad (93)$$

The orthogonality relations $\langle \boldsymbol{\eta}' | \boldsymbol{\eta}^{kl} \rangle = \delta_{\boldsymbol{\eta}', \boldsymbol{\eta}^{kl}}$ and $\langle \boldsymbol{\eta}' | \boldsymbol{\eta} \rangle = \delta_{\boldsymbol{\eta}', \boldsymbol{\eta}}$ then yields from the matrix elements (85) the matrix representation

$$H_{\boldsymbol{\eta}', \boldsymbol{\eta}} = - \sum_{\langle k, l \rangle} w_{kl} \langle \boldsymbol{\eta}' | (\sigma_k^+ \sigma_l^- + \sigma_k^- \sigma_l^+ - \hat{n}_k \hat{v}_l - \hat{v}_k \hat{n}_l) | \boldsymbol{\eta} \rangle. \quad (94)$$

of the generator of the SSEP in terms of spin operators. In quantum mechanics this matrix is known as the Hamiltonian of the spin-1/2 Heisenberg ferromagnet. We can write

$$H = \sum_{\langle k, l \rangle} w_{kl} h_{kl} \quad (95)$$

with the hopping matrices

$$h_{kl} = - (\sigma_k^+ \sigma_l^- + \sigma_k^- \sigma_l^+ - \hat{n}_k \hat{v}_l - \hat{v}_k \hat{n}_l) \quad (96)$$

$$= -\frac{1}{2} (\sigma_k^x \sigma_l^x + \sigma_k^y \sigma_l^y + \sigma_k^z \sigma_l^z - \mathbf{1}). \quad (97)$$

2.2.2 Equilibrium measures

Since H is symmetric it follows that $|u\rangle = \langle s|^T$ is a stationary measure. Moreover, the SSEP obviously satisfies detailed balance (68) w.r.t. this measure. Thus the uniform measure

$$|u^*\rangle := \frac{1}{|\Omega_L|} |s\rangle = 2^{-L} |s\rangle \quad (98)$$

is an equilibrium measure with an energy $E(\boldsymbol{\eta}) = \text{const}$ that does not depend on the configuration $\boldsymbol{\eta}$. Since particle number is conserved the SSEP defined on Ω is trivially non-ergodic. However, since the dynamics is a sequence of permutations, the SSEP restricted to the state space $\Omega_{L,N} := \{\boldsymbol{\eta} \in \Omega_L : \sum_{k \in \Lambda} \eta_k = N\}$ of fixed particle number $N \in \{0, \dots, L\}$ is ergodic. Since there are $|\Omega_{L,N}| = \binom{L}{N}$ ways of distributing N exclusion particles on L sites, the *canonical* uniform measure

$$|\pi_{L,N}\rangle = \sum_{\boldsymbol{\eta} \in \Omega_{L,N}} |\boldsymbol{\eta}\rangle, \quad |\pi_{L,N}^*\rangle = \frac{1}{Z} \sum_{\boldsymbol{\eta} \in \Omega_{L,N}} |\boldsymbol{\eta}\rangle \quad (99)$$

with canonical partition function

$$Z_{L,N} = \binom{L}{N} \quad (100)$$

is the unique equilibrium measure $\pi_{L,N}^*$ on $\Omega_{L,N}$. One has for $\boldsymbol{\eta} \in \Omega_L$

$$\pi_{L,N}^*(\boldsymbol{\eta}) = \binom{L}{N}^{-1} \delta_{N,N(\boldsymbol{\eta})} \quad (101)$$

where

$$N(\boldsymbol{\eta}) = \sum_{k \in \Lambda} \eta_k \quad (102)$$

is the number of particles in the configuration $\boldsymbol{\eta}$. The canonical partition function (100) yields the canonical free energy

$$F_{L,N} = -\ln Z_{L,N}. \quad (103)$$

Clearly, any normalized convex combination of the unnormalized canonical invariant measure $u_{L,N}(\boldsymbol{\eta}) := \delta_{N,N(\boldsymbol{\eta})}$ defines an equilibrium measure. Of particular importance is the *grandcanonical measure*

$$\pi_{L,\phi}^*(\boldsymbol{\eta}) := \frac{1}{Z_L(\phi)} \sum_{N=0}^L e^{\phi N} u_{L,N}(\boldsymbol{\eta}) \quad (104)$$

with so-called chemical potential ϕ and *grandcanonical partition function*

$$Z_L(\phi) := \sum_{\boldsymbol{\eta} \in \Omega_L} \sum_{N=0}^L e^{\phi N} u_{L,N}(\boldsymbol{\eta}) = \sum_{N=0}^L e^{\phi N} Z_{L,N} = (1 + e^\phi)^L. \quad (105)$$

The simple form of this partition function comes from the fact that the grandcanonical measure can be written in product form as

$$\pi_{L,\phi}^*(\boldsymbol{\eta}) := \frac{1}{Z_L(\phi)} \prod_{k \in \Lambda} (1 - \eta_k + e^\phi \eta_k) \quad (106)$$

which is a Bernoulli product measure.

By construction the particle number $N(\boldsymbol{\eta})$ in this *grandcanonical ensemble* of configuration is not a fixed number even though for any given realization of the process it is. Instead one has

$$\rho(\phi) := \frac{\langle N \rangle_\phi}{L} = \frac{1}{L} \sum_{\boldsymbol{\eta} \in \Omega_L} N(\boldsymbol{\eta}) \pi_{L,\phi}(\boldsymbol{\eta}) = \frac{1}{L} \frac{d}{d\phi} \ln Z_L(\phi) = \frac{e^\phi}{1 + e^\phi} \quad (107)$$

Defining the inverse function

$$\phi(\rho) = \ln \rho - \ln(1 - \rho) \quad (108)$$

one finds for the composite function $\tilde{Z}_L(\rho) = (Z_L \circ \phi)(\rho)$ the density dependence

$$\tilde{Z}_L(\rho) = Z_L(\phi(\rho)) = (1 - \rho)^{-L}. \quad (109)$$

of the grandcanonical partition function and the corresponding ρ -parametrization

$$\tilde{\pi}_{L,\rho}^*(\boldsymbol{\eta}) := \pi_{L,\phi(\rho)}^*(\boldsymbol{\eta}) = \sum_{N=0}^L (1-\rho)^{L-N} \rho^N u_{L,N}(\boldsymbol{\eta}) \quad (110)$$

of the grandcanonical measure (104).

One realizes that – as expected – the grandcanonical free energy

$$G(L, \phi) := -\ln Z_{L,\phi} = -L \ln(1 + e^\phi) \quad (111)$$

is extensive in L . In the associated canonical free energy defined by the Legendre transform

$$F(L, \rho) = G(L, \phi(\rho)) + L\rho\phi(\rho) = L[(1-\rho)\ln(1-\rho) + \rho\ln\rho] \quad (112)$$

one recognizes the thermodynamic limit (103)

$$\lim_{L \rightarrow \infty} F_{L,\rho L} = F(L, \rho) \quad (113)$$

of the canonical free energy. This indicates equivalence of the canonical ensemble with $N = \rho L$ particles and the grandcanonical ensemble at density ρ in the thermodynamic limit.

The grandcanonical probability vector $|\pi_{L,\phi}^*\rangle$ is obtained from (99). Defining the unnormalized canonical stationary probability vector

$$|\pi_{L,N}\rangle = \sum_{\boldsymbol{\eta} \in \Omega_{L,N}} |\boldsymbol{\eta}\rangle \quad (114)$$

and the particle number operator

$$\hat{N} = \sum_{\boldsymbol{\eta} \in \Omega_L} N(\boldsymbol{\eta}) |\boldsymbol{\eta}\rangle \langle \boldsymbol{\eta}| \quad (115)$$

one gets $f(N)|\pi_{L,N}\rangle = f(\hat{N})|\pi_{L,N}\rangle$ since each component in $|\pi_{L,N}\rangle$ with non-zero weight has exactly N particles which means that $N|\pi_{L,N}\rangle = \hat{N}|\pi_{L,N}\rangle$. Thus

$$\begin{aligned} |\pi_{L,\phi}^*\rangle &= Z_L^{-1}(\phi) \sum_{N=0}^L e^{\phi N} |\pi_{L,N}\rangle \\ &= Z_L^{-1}(\phi) \sum_{N=0}^L e^{\phi \hat{N}} |\pi_{L,N}\rangle \\ &= Z_L^{-1}(\phi) e^{\phi \hat{N}} \sum_{N=0}^L \sum_{\boldsymbol{\eta} \in \Omega_{L,N}} |\boldsymbol{\eta}\rangle \\ &= Z_L^{-1}(\phi) e^{\phi \sum_{k=1}^L \hat{n}_k} |u\rangle \end{aligned}$$

$$\begin{aligned}
&= Z_L^{-1}(\phi) \prod_{k=1}^L (\hat{v}_k + e^\phi \hat{n}_k) |u\rangle \\
&= (1 + e^\phi)^{-L} ((1, e^\phi)^T)^{\otimes L} \\
&= \frac{1}{(1 + e^\phi)^L} \begin{pmatrix} 1 \\ e^\phi \end{pmatrix}^{\otimes L} = \begin{pmatrix} 1 - \rho(\phi) \\ \rho(\phi) \end{pmatrix}^{\otimes L} \tag{116}
\end{aligned}$$

which is an L -fold tensor product.

This tensor structure of the grandcanonical probability vector makes the computation of correlations trivial. From (38) one has

$$\langle \eta_{k_1} \dots \eta_{k_m} \rangle_\phi = \rho^m(\phi) \tag{117}$$

when all k_i are mutually different. Therefore one finds the static structure function

$$C_{k,l} := \langle \eta_k \eta_l \rangle_\phi - \rho^2(\phi) = \rho(\phi)(1 - \rho(\phi))\delta_{k,l}. \tag{118}$$

This yields the compressibility

$$K(\rho) = \frac{1}{L} \sum_{k \in \Lambda} \sum_{l \in \Lambda} C_{k,l} = \frac{1}{L} \langle (N - \rho L)^2 \rangle = \rho(1 - \rho). \tag{119}$$

Of course, this result could directly have been obtained from the usual thermodynamic relation

$$\tilde{K}(\phi) = \frac{d}{d\phi} \rho(\phi) = \frac{e^\phi}{(1 + e^\phi)^2} \tag{120}$$

and using (108).

2.2.3 Duality functions for the SSEP

From the structure of the hopping matrices in (97) it is clear that the generator is symmetric under the action of the Lie-algebra $\mathfrak{su}(2)$ [4], i.e., H satisfies the commutation relations

$$[H, S^p m] = [H, S^z] = 0 \tag{121}$$

with the representation matrices

$$S^\pm = \sum_{k \in \Lambda} \sigma_k^\pm, \quad S^z = \frac{1}{2} \sum_{k \in \Lambda} \sigma_k^z \tag{122}$$

which satisfy the $\mathfrak{su}(2)$ commutation relations

$$[S^+, S^-] = 2S^z, \quad [S^z, S^\pm] = \pm S^\pm. \tag{123}$$

Using the symmetry approach to duality discussed above, the well-known self-duality of the SSEP [96, 61] stated in a generalized form in the following theorem becomes a trivial corollary of the $\mathfrak{su}(2)$ symmetry.

Theorem 2.8 *The SSEP on a lattice Λ with state space $\Omega = \{0, 1\}^\Lambda$ is selfdual w.r.t. the duality function*

$$D(\zeta, \eta) = \prod_{k \in \Lambda} (\alpha + \beta \eta_k)^{\gamma + \delta \zeta_k} \quad (124)$$

for all $\eta, \zeta \in \{0, 1\}^\Lambda$ and $\alpha, \beta, \gamma, \delta \in \mathbb{R}$.

Remark 2.9 *For $\gamma = 0$ the duality function (124) can be written in alternative form as follows. Let $\mathbf{x}(\zeta) := \{k : \zeta_k = 1\}$ be the set of occupied sites $x_i \in \Lambda$ of the configuration ζ and $N(\mathbf{x}) = |\mathbf{x}|$ be the number of particles in the configuration \mathbf{x} . This mapping induces an obvious bijection between the state space $\Omega = \{0, 1\}^\Lambda$ and the coordinate set Ξ of possible distinct occupied sites and thus allows for describing the ASEP in terms of the evolution \mathbf{x}_t of particle coordinates. With $a = \alpha^\delta$, $b = (\alpha + \beta)^\delta - \alpha^\delta$ the duality function (124) then becomes*

$$\tilde{D}(\mathbf{x}, \eta) = \prod_{i=1}^{N(\mathbf{x})} (a + b \eta_{x_i}) \quad (125)$$

for all $\mathbf{x} \in \Xi$ and $\eta \in \Omega$. For $\alpha = 0$, $\beta = \delta = 1$ corresponding to $a = 0$ and $b = 1$ one recovers the well-known duality function formulated and proved in a different way in [61] and which goes back to [96].

Proof: The $SU(2)$ -symmetry implies that the L -fold Kronecker product $\hat{D} = A^{\otimes L}$ is a symmetry operator for any $\times 2$ matrix A . Since the SSEP is reversible with uniform invariant measure (98) this yields the duality function $D(\zeta, \eta) = \langle \zeta | \hat{D} | \eta \rangle$. The factorization of the symmetry operator and also of the dual pairing (see (38)) yields

$$D(\zeta, \eta) = \prod_{k \in \Lambda} \langle \zeta_k | A | \eta_k \rangle \quad (126)$$

Explicit computation of the two-dimensional bilinear form

$$\langle \zeta_k | A | \eta_k \rangle = (1 - \zeta_k, \zeta_k) \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} 1 - \eta_k \\ \eta_k \end{pmatrix} \quad (127)$$

yields $(\alpha + \beta \eta_k)^{\gamma + \delta \zeta_k}$ with $A_{11} = \alpha^\gamma$, $A_{12} = (\alpha + \beta)^\gamma$, $A_{21} = \alpha^{\gamma + \delta}$, $A_{22} = (\alpha + \beta)^{\gamma + \delta}$.
□

Remark 2.10 *The duality function (124) is not unique. Any measurable function of the symmetry operators $S^{\pm, z}$ (122) yields a duality function.*

One realizes that the mapping to the quantum Hamiltonian immediately reveals the well-known $\mathfrak{sl}(2)$ symmetry of the generator of the SSEP and therefore provides instantly self-duality functions. Moreover, the matrix formulation reduces to proof of selfduality to elementary multilinear algebra. The $\mathfrak{sl}(2)$ symmetry allows for the derivation of similarly strong results for multi-time correlation functions $\langle n_{i_1}(t_1) \dots n_{i_k}(t_k) \rangle$.

Remark 2.11 Any Markov process whose generator is a function of the hopping matrices $e_{k,l} = \sigma_k^x \sigma_l^x + \sigma_k^y \sigma_l^y + \sigma_k^z \sigma_l^z - \mathbf{1}$ is $\mathfrak{sl}(2)$ symmetric and therefore self-dual w.r.t. the same duality functions as the SSEP. The approach can be straightforwardly generalized to the partial symmetric exclusion process [84, 53]. The partial exclusion process is the spin- s version of this model where each lattice site i can be occupied by at most $2s_i$ particles and where single-particle hopping from site i to site j occurs with rate $n_i(2s_j - n_j)$.

2.2.4 Density profile and dynamical structure function

We focus now on the case $\alpha = \gamma = 0$ and $\beta = \delta = 1$ in the duality function (124). The self-duality has the remarkable consequence that for any initial measure with support on configurations with any number of particles the joint expectations of n occupation numbers can be expressed in terms of transition probabilities for initial states with only n particles. In particular, for the density profile $\rho_k(t) = \mathbf{E}_{\mu_t} \eta_k$ one finds by inserting the duality function in the form (125) for $N = 1$ into the definition (77) of duality. Inserting $D(x, \boldsymbol{\eta}) = \eta_x$ into the r.h.s. of (77) and using the propagator representation (62) of the transition probability yields for an initial configuration $\boldsymbol{\eta}$

$$\sum_{\boldsymbol{\eta}'} \eta_x \langle \boldsymbol{\eta}' | e^{-Ht} | \boldsymbol{\eta} \rangle = \sum_{\boldsymbol{\eta}'} \langle \boldsymbol{\eta}' | \hat{n}_x e^{-Ht} | \boldsymbol{\eta} \rangle = \langle s | \hat{n}_x e^{-Ht} | \boldsymbol{\eta} \rangle \quad (128)$$

since $\langle \boldsymbol{\eta}' | \hat{n}_x = \eta_x \langle \boldsymbol{\eta}' |$. On the other hand, the l.h.s. of (77) becomes

$$\sum_{x' \in \Lambda} \eta_{x'} P(x', t | x, 0) = \sum_{x' \in \Lambda} \langle s | \hat{n}_{x'} | \boldsymbol{\eta} \rangle P(x, t | x', 0) \quad (129)$$

since for a single particle one has $\Xi = \Lambda$ and since the generator for the SSEP is symmetric.

This yields for an arbitrary initial measure μ the density profile

$$\rho_x(t) = \langle s | \eta_x e^{-Ht} | \mu \rangle = \sum_{x' \in \Lambda} \rho_{x'}(0) P(x, t | x', 0). \quad (130)$$

This means that irrespective of the lattice and of the jump rates between lattice points the time evolution of the local density in a system of any number of interacting particles is completely determined by the (non-interacting) time evolution of a single particle. Specifically, on the d -dimensional hypercubic lattice \mathbb{Z}^d with translation-invariant nearest-neighbour hopping the single-particle propagator satisfies a discrete diffusion equation which can be solved in explicit form in terms of modified Bessel functions

$$I_n(t) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dp e^{ipn - t \cos p}. \quad (131)$$

On \mathbb{Z}^d with hopping rates w_i in each direction one then has for point $\vec{x} = (x_1, \dots, x_d)$

$$\rho_{\vec{x}}(t) = \prod_{j=1}^d \sum_{x'_j \in \mathbb{Z}} \rho_{x'_j}(0) e^{-w_j t} I_{x_j - x'_j}(w_j t). \quad (132)$$

As a corollary of (130) we note

$$\langle s | \eta_x e^{-Ht} = \sum_{x' \in \Lambda} P(x, t | x', 0) \langle s | \hat{n}_{x'}. \quad (133)$$

For the dynamical structure function defined by

$$S_{x,y}(t) := \mathbf{E}_\rho (\eta_x(t) \eta_y(0)) - \rho^2 \quad (134)$$

this yields

$$\begin{aligned} S_{x,y}(t) &= \langle s | \eta_x e^{-Ht} \eta_y | \rho \rangle - \rho^2 \\ &= \sum_{x' \in \Lambda} P(x, t | x', 0) \langle s | \hat{n}_{x'} \hat{n}_y | \rho \rangle - \rho^2 \\ &= \sum_{x' \in \Lambda} P(x, t | x', 0) (\rho^2 + \rho(1 - \rho) \delta_{x',y}) - \rho^2 \\ &= \rho(1 - \rho) P(x, t | y, 0) \end{aligned} \quad (135)$$

where we have used reversibility of the SSEP and conservation of probability which gives $\sum_{x' \in \Lambda} P(x, t | x', 0) = \sum_{x' \in \Lambda} P(x', t | x, 0) = 1$ for the single-particle process.

On the translation-invariant hypercubic lattice with nearest-neighbour jumps with rates w_i in direction i the dynamical structure function $S_{\vec{x}}(t) := S_{\vec{x}, \vec{0}}(t)$ becomes

$$S_{\vec{x}}(t) = \prod_{j=1}^d e^{-2w_j t} I_{x_j - x'_j}(2w_j t). \quad (136)$$

In the scaling limit $x_i(t) = r_i \sqrt{4w_i t}$ and $t \rightarrow \infty$ the modified Bessel function becomes a Gaussian. Thus

$$\prod_{j=1}^d \sqrt{4\pi w_j} \lim_{t \rightarrow \infty} t^{d/2} S_{\vec{x}(t)}(t) = e^{-\sum_{j=1}^d r_j^2}. \quad (137)$$

We read off the dynamical exponent $z = 2$ and the universal Gaussian scaling function with diagonal diffusion matrix $D_{ij} = 2w_i \delta_{ij}$.

Higher order correlation functions can be studied using the Bethe ansatz [35, 52, 87]. One finds that *all n -point correlation functions of the symmetric exclusion process are, to leading order in time, identical to the same n -point correlators of non-interacting particles.* Corrections are of order $1/\sqrt{t}$, see [14] for a related rigorous result. Hence diffusive scaling with dynamical exponent $z = 2$ leaves finite-order correlation functions invariant up to an overall amplitude.

2.3 Selfduality of the 1-d ASEP

The ASEP on the graph Γ is the asymmetric generalization of the SSEP with directed hopping rates w_{kl} for jumps from site k to site l and w_{lk} for the reversed jump. Little is known about this process on general graphs where it does not have

a symmetry analogous to the $\mathfrak{sl}(2)$ -symmetry of the SSEP and where not even the invariant measure is known. We restrict our attention to the most-studied one-dimensional finite integer lattice $\Lambda = [L^-, L^+] \setminus \mathbb{Z}$ with nearest-neighbour jumps with rates $r_k \equiv w_{kk+1} > 0, \ell_{k+1} \equiv w_{k+1k} > 0$ for constant hopping bias .

2.3.1 Periodic boundary conditions with constant rates

For constant bond hopping rates $r_k = r, \ell_k = \ell$ it is straightforward to prove that for periodic boundary conditions the product measure (106) is a family of stationary distribution of the ASEP [96]. Therefore the stationary distribution is the same as the equilibrium distribution of the SSEP, even though the ASEP does not satisfy detailed balance and hence is not an equilibrium process. The lack of reversibility is reflected in the fact that the stationary current

$$j = r\langle \eta_k (1 - \eta_{k+1}) \rangle - \ell\langle \eta_{k+1} (1 - \eta_k) \rangle = (r - \ell)\rho(1 - \rho) \quad (138)$$

is non-zero.

2.3.2 Generator of the ASEP with reflecting boundaries

For reflecting boundaries where hopping between the boundary sites L^- and L^+ is not allowed it is convenient to define the parameters

$$q \equiv e^f = \sqrt{\frac{r_k}{\ell_{k+1}}}, \quad w_k = \sqrt{r_k \ell_{k+1}} \quad (139)$$

and define the system size

$$L = L^+ + 1 - L^-. \quad (140)$$

With the local hopping rates

$$w_{kk+1}(\boldsymbol{\eta}) = w_k (q\eta_k(1 - \eta_{k+1}) + q^{-1}(1 - \eta_k)\eta_{k+1}), \quad k \in \{L^-, \dots, L^+ - 1\} \quad (141)$$

the transition rate from a configuration $\boldsymbol{\eta}$ to a configuration $\boldsymbol{\eta}'$ is given by

$$w_{\boldsymbol{\eta}', \boldsymbol{\eta}} = \sum_{k=L^-}^{L^+-1} w_{kk+1}(\boldsymbol{\eta}) \delta_{\boldsymbol{\eta}', \boldsymbol{\eta}^{kk+1}}. \quad (142)$$

and the generator reads

$$\mathcal{L}f(\boldsymbol{\eta}) = \sum_{k=L^-}^{L^+-1} w_{kk+1}(\boldsymbol{\eta}) [f(\boldsymbol{\eta}^{kk+1}) - f(\boldsymbol{\eta})]. \quad (143)$$

Using the Pauli matrices (90) one finds

$$H = \sum_{k=L^-}^{L^+-1} w_k h_k \quad (144)$$

with non-symmetric hopping matrices

$$h_k = -q (\sigma_k^+ \sigma_{k+1}^- - \hat{n}_k \hat{v}_{k+1}) - q^{-1} (\sigma_k^- \sigma_{k+1}^+ - \hat{v}_k \hat{n}_{k+1}). \quad (145)$$

2.3.3 Grandcanonical equilibrium measure

The hopping matrices can be symmetrized by the ground state transformation

$$V := q^{\sum_{k=L^-}^{L^+} k \hat{n}_k}. \quad (146)$$

One has

$$h_k^T = V^{-2} h_k V^2 \quad (147)$$

$$\tilde{h}_k := V^{-1} h_k V = \tilde{h}_k^T. \quad (148)$$

This implies that this ASEP is reversible and together with particle number conservation one concludes that

$$\pi_{L,\phi}^*(\boldsymbol{\eta}) = \frac{1}{Z_{L,\phi}} \langle \boldsymbol{\eta} | V^2 | \boldsymbol{\eta} \rangle = \frac{1}{Z_{L,\phi}} q^{2 \sum_{k=L^-}^{L^+} (k - \kappa(\phi)) \eta_k}, \quad \kappa(\phi) = -\phi/(2f) \quad (149)$$

is an equilibrium measure² for any chemical potential $\phi \in \mathbb{R}$, corresponding to a linear potential

$$U(\mathbf{x}) = -\epsilon \sum_{i=1}^{N(\mathbf{x})} x_i \quad (150)$$

with $\epsilon = 2k_B T f$ for a configuration \mathbf{x} with particles at sites x_i . This is a product measure with grandcanonical partition function

$$Z_{L,\phi} = \prod_{k=L^-}^{L^+} (1 + q^{2k-2\kappa(\phi)}). \quad (151)$$

Correspondingly the associated probability vector is a tensor product

$$|\pi_{L,\phi}^*\rangle = \frac{1}{Z_{L,\phi}} e^{\phi \hat{N}} V^2 |s\rangle = |\rho_1\rangle \otimes \cdots \otimes |\rho_L\rangle \quad (152)$$

with marginals

$$|\rho_k\rangle = (1 + q^{2k-2\kappa(\phi)})^{-1} \begin{pmatrix} 1 \\ q^{2k-2\kappa(\phi)} \end{pmatrix}. \quad (153)$$

This is the blocking measure [61] restricted to Λ .

The stationary particle density is not uniform, but given by

$$\rho_k = \frac{q^{2k-2\kappa(\phi)}}{1 + q^{2k-2\kappa(\phi)}} = \frac{1}{2} (1 + \tanh(f(k - \kappa(\phi)))) , \quad (154)$$

see Fig. (??). This means that the stationary local density is approximately equal to 1/2 near the lattice point $k^* = [\kappa(\phi)]$ provided that $k^* \in \Lambda$. The density approaches 1(0) to the right(left) on a length scale of order $1/f^2$. Thus on macroscopic scale the density has a shock discontinuity at $x^* = \kappa(\phi)/L \in [b^-, b^+]$ where $b^\pm = \lim_{L \rightarrow \infty} L^\pm/L$.

²The measure (149) as well as all related measures and functions introduced below depend both on L^- and L^+ . In order to avoid heavy notation we indicate this dependence only by the volume L .

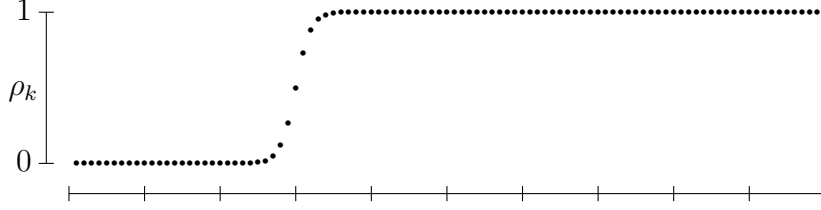


Figure 6: Stationary density profile of the ASEP with reflecting boundaries with 100 sites. The position of the step is determined by the particle number, its width depends on the driving field. Here we have chosen $\beta f = 1/2$, corresponding to $q = \sqrt{e}$.

2.3.4 Duality functions for the 1-d ASEP

The process is symmetric under the quantum algebra $U_q[\mathfrak{gl}(2)]$ [68] which is the q -deformed universal enveloping algebra of $\mathfrak{gl}(2)$ [47, 48]. This implies that the generator H given by (144) commutes with the symmetry operators $S^\pm(q)$ and S^z where [86]

$$S^+(q) = \sum_{k=L^-}^{L^+} q^{\hat{N}_k} \sigma_k^+, \quad S^-(q) = \sum_{k=L^-}^{L^+} q^{-\hat{V}_k} \sigma_k^- \quad (155)$$

with the non-local particle balance operators

$$\hat{N}_k = \sum_{j=k+1}^{L^+} \hat{n}_j - \sum_{j=L^-}^{k-1} \hat{n}_j, \quad \hat{V}_k = \sum_{j=k+1}^{L^+} \hat{v}_j - \sum_{j=L^-}^{k-1} \hat{v}_j, \quad (156)$$

The particle balance function

$$N_k(\boldsymbol{\eta}) := \sum_{j=k+1}^{L^+} \eta_j - \sum_{j=L^-}^{k-1} \eta_j \quad (157)$$

gives the difference between the number of particles to right and left of site k . Hence $N_k(\boldsymbol{\eta}_t) - N_k(\boldsymbol{\eta}_0)$ is the integrated particle current across site k up to time t .

By the duality theorem (2.4) the ASEP with reflecting boundary conditions defined by (144) is self-dual w.r.t.

$$D^{gen}(\boldsymbol{\zeta}, \boldsymbol{\eta}) = \pi_{L,0}^{-1}(\boldsymbol{\zeta}) \langle \boldsymbol{\zeta} | F(S^+(q), S^-(q), S^z) | \boldsymbol{\eta} \rangle \quad (158)$$

where $F(S^+(q), S^-(q), S^z)$ is some bounded function of the symmetry operators and $\pi_{L,0}^{-1}(\boldsymbol{\zeta}) = q^{-2 \sum_{k \in \Lambda} \zeta_k}$ is the unnormalized equilibrium measure of the ASEP.

The computation of the matrix elements of $F(S^+(q), S^-(q), S^z)$ is less forward than in the $\mathfrak{sl}(2)$ case. We note [6]

Proposition 2.12 *For all $q \in \mathbb{C} \setminus 0$ the symmetry operator*

$$Y^+(q) = \sum_{r=0}^L \frac{(S^+(q))^r}{[r]_q!} \quad (159)$$

with the q -numbers

$$[x]_q = \frac{q^x - q^{-x}}{q - q^{-1}}, \quad x \in \mathbb{C}, \quad [n]_q! = \prod_{k=1}^n [k]_q, \quad k \in \mathbb{N} \quad (160)$$

has matrix elements

$$\langle \zeta | Y^+(q) | \boldsymbol{\eta} \rangle = \prod_{k=L^-}^{L^+} (Q_k(\boldsymbol{\eta}))^{\zeta_k} \quad (161)$$

with $Q_k(\boldsymbol{\eta}) = \eta_k q^{-N_k(\boldsymbol{\eta})}$.

This result yields from (158) the duality function of [86] in the coordinate representation \mathbf{x} of the configuration ζ :

Corollary 2.13 *The ASEP defined by (144) is selfdual w.r.t. the duality function*

$$D_\omega(\mathbf{x}, \boldsymbol{\eta}) = \prod_{i=1}^{N(\mathbf{x})} \eta_{x_i} q^{-2 \sum_{k=L^-}^{x_i-1} (1-\eta_k) + \omega N(\boldsymbol{\eta})}. \quad (162)$$

To see this notice first that Proposition (2.12) together with (158) implies that

$$\tilde{D}(\mathbf{x}, \boldsymbol{\eta}) = \prod_{i=1}^{N(\mathbf{x})} q^{-2x_i} \eta_{x_i} q^{-N_{x_i}(\boldsymbol{\eta})} \quad (163)$$

is a duality function. Because of particle conservation this duality function can be multiplied with any function of the particle numbers $N(\mathbf{x})$ and $N(\boldsymbol{\eta})$ to obtain a new duality function. So in particular we have that

$$\tilde{D}(\mathbf{x}, \boldsymbol{\eta}) q^{N(\mathbf{x})((1+\omega)N(\boldsymbol{\eta})+2L^- - 1)} = \prod_{i=1}^{N(\mathbf{x})} q^{(1+\omega)N(\boldsymbol{\eta})+2L^- - 1 - 2x_i} \eta_{x_i} q^{-N_{x_i}(\boldsymbol{\eta})} = D_\omega(\mathbf{x}, \boldsymbol{\eta}) \quad (164)$$

is also a duality function.

2.3.5 Microscopic structure of shocks in the ASEP

This duality function is not local and therefore it cannot be used to compute the dynamical structure of the ASEP. However, it carries non-trivial information about the distribution of the time-integrated current [41] and for constant bond hopping rates $w_k = w$ also about the microscopic structure and dynamics of shocks [5, 7]. It turns out that just as in the SSEP the time evolution of an n -point density correlation is given by the transition probabilities of only n particles in the SSEP, the time evolution of a shock measure for the ASEP defined on the infinite integer lattice \mathbb{Z} with n microscopic shocks is given by the transition probabilities of a modified ASEP with only n particles. To be precise, we state the result of [5] for a single microscopic shock where the modified ASEP reduces to a biased random walk.

Definition 2.14 (*Shock measure*) A shock measure ν_x on $\{0, 1\}^{\mathbb{Z}}$ indexed by the microscopic shock position $x \in \mathbb{Z}$ is the product measure given by the marginals

$$\nu_x(\eta_k) = \begin{cases} 1 & k = x \\ \rho_0 \delta_{\eta_k, 1} + (1 - \rho_-) \delta_{\eta_k, 0} & k < x \\ \rho_1 \delta_{\eta_k, 0} + (1 - \rho_+) \delta_{\eta_k, 1} & k > x \end{cases} \quad (165)$$

The restriction to Λ for $x \in \Lambda$

$$\mu_x^L(\boldsymbol{\eta}) := \prod_{k=L^-}^{L^+} \nu_x^k(\eta_k) \quad (166)$$

is also called shock measure with microscopic shock position x .

Then one has [5, 3, 7]:

Theorem 2.15 Let $\nu_x(t)$ denote the measure at time t of the ASEP on \mathbb{Z} with constant rates $r = wq > 0$, $\ell = wq^{-1} > 0$, starting from a shock measure ν_x defined in (2.14) with

$$\frac{\rho_+(1 - \rho_-)}{\rho_-(1 - \rho_+)} = q^2. \quad (167)$$

Then, for any $x \in \mathbb{Z}$

$$\nu_x(t) = \sum_{y \in \mathbb{Z}} P(y, t | x, 0) \nu_y \quad (168)$$

where $P(y, t | x, 0)$ is the transition probability of a biased random walk with jump rates

$$p_{\pm} = (r - \ell) \frac{\rho_{\pm}(1 - \rho_{\pm})}{\rho_+ - \rho_-} \quad (169)$$

to the right (+) and left (-) respectively.

Corollary 2.16 The shock is microscopically sharp at all times and performs on macroscopic scale a diffusive motion with drift velocity

$$v_s = p_+ - p_- = (r - \ell)(1 - \rho_+ - \rho_-) \quad (170)$$

and diffusion coefficient

$$D_s = \frac{1}{2}(p_+ + p_-) = (r - \ell) \frac{\rho_-(1 - \rho_-) + \rho_+(1 - \rho_+)}{\rho_+ - \rho_-}. \quad (171)$$

Remark 2.17 The microscopic sharpness follows from the product structure of the shock measure (166). One recognizes in the microscopic shock velocity (170) the Rankine-Hugoniot velocities (6) since $j_{\pm} := w(q - q^{-1})\rho_{\pm}(1 - \rho_{\pm})$ is the expectation of the particle current to the right and to the left of shock. The shock diffusion coefficients (171) are consistent with the general result (7) of [29] on shock motion in the ASEP on diffusive scale.

We outline the proof and refer for the technical details to [5, 7]. An alternative probabilistic proof is given in [3].

Consider first the finite lattice Λ . We recall (77) which reads for the duality function (162) with a single-particle configuration ζ

$$\begin{aligned}
\sum_{y \in \Lambda} D_\omega(y, \boldsymbol{\eta}) P(y, t|x, 0) &= \sum_{\boldsymbol{\eta}' \in \Omega} \eta'_x q^{-2 \sum_{k=L^-}^{x-1} (1-\eta'_k) + \omega N(\boldsymbol{\eta}')} \langle \boldsymbol{\eta}' | e^{-Ht} | \boldsymbol{\eta} \rangle \\
&= \sum_{\boldsymbol{\eta}' \in \Omega} \langle \boldsymbol{\eta}' | \hat{n}_x q^{-2 \sum_{k=L^-}^{x-1} (1-\hat{n}_k) + \omega \hat{N}} e^{-Ht} | \boldsymbol{\eta} \rangle \\
&= \langle s | \hat{n}_x q^{-2 \sum_{k=L^-}^{x-1} (1-\hat{n}_k) + \omega \hat{N}} e^{-Ht} | \boldsymbol{\eta} \rangle \\
&= \langle \boldsymbol{\eta} | e^{-H^T t} \hat{n}_x q^{-2 \sum_{k=L^-}^{x-1} (1-\hat{n}_k) + \omega \hat{N}} | s \rangle
\end{aligned} \tag{172}$$

On the other hand, for the l.h.s. we have

$$D_\omega(y, \boldsymbol{\eta}) = \eta_y q^{-2 \sum_{k=L^-}^{y-1} (1-\eta_k) + \omega N(\boldsymbol{\eta})} = \langle \boldsymbol{\eta} | \hat{n}_y q^{-2 \sum_{k=L^-}^{y-1} (1-\hat{n}_k) + \omega \hat{N}(\boldsymbol{\eta})} | s \rangle \tag{173}$$

Next we observe that

$$\hat{n}_x q^{-2 \sum_{k=L^-}^{x-1} (1-\hat{n}_k) + \omega \hat{N}(\boldsymbol{\eta})} | s \rangle = Z_x^{-1} | \nu_x \rangle \tag{174}$$

with densities

$$\rho_- = \frac{q^\omega}{q^{-2} + q^\omega}, \quad \rho_+ = \frac{q^\omega}{1 + q^\omega} \tag{175}$$

and normalization constant

$$Z_x = (q^{-2} + q^\omega)^{x-L^-} (1 + q^\omega)^{L^+ - x} = \frac{(1 + q^\omega)^{L^+}}{(q^{-2} + q^\omega)^{L^-}} \left(\frac{\rho_+}{\rho_-} \right)^x \tag{176}$$

Thus selfduality yields

$$\sum_{y \in \Lambda} Z_y^{-1} | \nu_y \rangle P(y, t|x, 0) = e^{-H^T t} Z_x^{-1} | \nu_x \rangle. \tag{177}$$

or equivalently

$$\sum_{y \in \Lambda} | \nu_y \rangle \left(\frac{\rho_+}{\rho_-} \right)^{x-y} P(y, t|x, 0) = e^{-H^T t} | \nu_x \rangle. \tag{178}$$

Notice now the trivial random walk property that up to a boundary term

$$\left(\frac{\rho_+}{\rho_-} \right)^{x-y} P(y, t|x, 0) = e^{-\lambda t} \tilde{P}(y, t|x, 0) \tag{179}$$

where $\tilde{P}(y, t|x, 0)$ is the transition probability of a random walk with rates $\tilde{p}_\pm = (q\rho_-/\rho_+)^{\pm 1}$ and $\lambda = p_+ + p_- - q - q^{-1}$. Thus

$$\sum_{y \in \Lambda} \tilde{P}(y, t|x, 0) | \nu_y \rangle = e^{-(H^T - \lambda)t} | \nu_x \rangle. \tag{180}$$

On the other hand, $\tilde{H} = H^T - \lambda$ is, up to another boundary term, the generator of the ASEP with inverse hopping asymmetry q^{-1} . Using coupling arguments it can be shown that in the thermodynamic limit these boundary terms are irrelevant [5]. Thus we arrive at

$$\sum_{y \in \mathbb{Z}} \tilde{P}(y, t | x, 0) | \nu_y \rangle = | \nu_x(t) \rangle^{\triangleleft} \quad (181)$$

where the upper left-pointing triangle indicates the evolution under the ASEP on \mathbb{Z} with reversed bias.

The densities satisfy

$$\frac{\rho_+(1 - \rho_-)}{\rho_-(1 - \rho_+)} = q^{-2}. \quad (182)$$

Therefore

$$q - q^{-1} = q(1 - q^{-2}) = \frac{p_+}{w} \frac{\rho_- - \rho_+}{\rho_+(1 - \rho_+)} \quad (183)$$

$$= q^{-1}(q^2 - 1) = \frac{p_-}{w} \frac{\rho_- - \rho_+}{\rho_-(1 - \rho_-)} \quad (184)$$

which yields the transition rates

$$p_{\pm} = (r - \ell) \frac{\rho_- - \rho_+}{\rho_{\pm}(1 - \rho_{\pm})} \quad (185)$$

for the random walk. Substituting $q \rightarrow q^{-1}$ then proves the theorem.

2.4 Recipe for the quantum Hamiltonian of exclusion processes

To construct H for a given process without going through the explicit matrix multiplications we note that any changes of the state of the system are represented by offdiagonal matrices. To be precise, they represent attempts rather than actual changes: Acting on a state with an already occupied site with σ^- yields zero, i.e. no change in the probability vector. This reflects the rejection of any attempt at creating a second particle on a given site. Thus the exclusion of double occupancy is encoded in the properties of the Pauli matrices.

Simultaneous events are represented by products of Pauli matrices acting on different sites. E.g. hopping of a particle from site i to site j is equivalent to annihilating a particle at site i and at the same time creating one at site j . Thus it is given by the matrix $\sigma_i^+ \sigma_j^-$. The hopping attempt is successful only if site i is occupied and site j is empty. Otherwise acting with $\sigma_i^+ \sigma_j^-$ on the state gives zero and hence no change. The rate of hopping (or of any other possible stochastic event) is the numerical prefactor of each hopping matrix (or other attempt matrix). Of course, in principle the rate may depend on the configuration of the complete system. Suppose the hopping rate is given by a function $w(\boldsymbol{\eta})$ where $\boldsymbol{\eta}$ is the configuration prior to hopping. In this case the hopping matrix is given by $\sigma_i^+ \sigma_j^- \hat{w}$

where the diagonal operator \hat{w} is obtained from the rate $w(\boldsymbol{\eta})$ by replacing any η_i by the projector $\text{hat}n_i$. If e.g. for some reason hopping from site i to site j should occur only if a third site k is empty, then the hopping matrix would be given by $\sigma_i^+ \sigma_j^- (1 - n_k)$. For a hopping rate which is proportional to the number of particles on neighboring sites one finds the matrix $\sigma_i^+ \sigma_j^- (1 + w \sum_k \hat{n}_k)$. The construction of the attempt matrices for other processes or for n -states model is analogous.

For two-states models one notes the useful identities

$$\langle s | \sigma_i^+ = \langle s | \hat{n}_i, \quad \langle s | \sigma_i^- = \langle s | (\hat{v}_i \quad (186)$$

which follow immediately from the tensor structure of the summation vector and the definition of the local Pauli matrices. With these relations it is easy to construct the diagonal part of the quantum Hamiltonian in order to ensure conservation of probability. To each off-diagonal attempt matrix one constructs a diagonal matrix by replacing all σ_i^+ by \hat{n}_i and by replacing all σ_i^- by \hat{v}_i . E.g. to hopping from i to j with rate w represented by $-w\sigma_i^+ \sigma_j^-$ one adds $w\hat{n}_i \hat{v}_j$. The (negative) sum of all attempt matrices minus their diagonal counterparts is then the full generator. In the same way one constructs the diagonal parts of n -states models by using the analogues of Eqs. (186). Conservation of probability (59) is then automatically satisfied.

3 Fluctuations of current and density

Fluctuation theorems relate the probability of a positive value of some observable to the probability of the negative of that quantity [26, 38, 91, 40]. Prominent examples for such relations include the Jarzynski relation for the distribution of non-equilibrium work [44] and the Gallavotti-Cohen theorem [30] for the distribution of the entropy production in deterministic dynamics and a related result by Lebowitz and Spohn for the particle current in stochastic interacting particle systems [59]. The latter two have been established in a mathematically rigorous fashion.

It has become clear that currents play an important role in understanding the non-equilibrium properties of a particle system. Therefore we consider here fluctuation theorems that concern currents such as the current of particles in a particle system such as the ASEP (cf. (2)). To this end we keep track of the trajectory of a process, i.e., the whole sequence of transitions from an initial configuration η_0 at time 0 to a final state η_t at time $t > 0$. In order to do so we first need to introduce some more tools.

3.1 Tools

3.1.1 Counting processes

The time-integrated particle current provides an example of what we shall call a *counting process* C_t with state space \mathbb{R} , defined informally by the following properties [38].

Property 1: The value of C_t changes only at a transition of the underlying process with an increment $r_{\eta',\eta} \in \mathbb{R}$ for a transition $\eta \rightarrow \eta'$.

Property 2: The transition rates $w_{\eta',\eta}$ of the process η_t do not depend on C_t .

We also introduce the extended counting process by adding “boundary values” that do not depend on C_t :

Property 3: For given functions $r^i : \Omega \rightarrow \mathbb{R}$, $r^f : \Omega \rightarrow \mathbb{R}$ the extended counting process is the random number $R_t = r_{\eta_0}^i + C_t + r_{\eta_t}^f$.

Notice that in general a counting process C_t is not Markovian. The joint process $\sigma_t = (\eta_t, C_t)$ with state space $\Xi = \Omega \times \mathbb{R}$, however, is Markov with generator

$$\mathcal{S}f(\eta, C) = \sum_{\eta' \in \Omega \setminus \eta} w_{\eta',\eta} [f(\eta', C + r_{\eta',\eta}) - f(\eta, C)]. \quad (187)$$

The values C_t, R_t of a counting process at time t can be regarded as a functional of the trajectories of the underlying process η_t as we note in the following proposition which is an immediate consequence of the definition of the counting process, see Fig. 7 illustration.

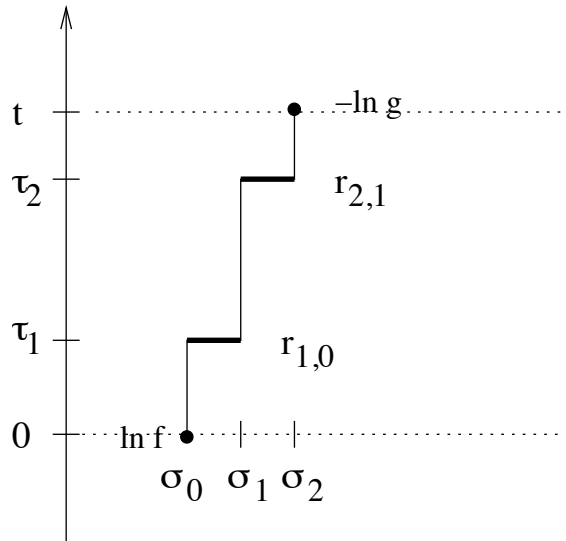


Figure 7: A stochastic trajectory with the sequence of configurations $\{\sigma_0, \sigma_1, \sigma_2\}$ such that $\sigma_t = \sigma_2$. Time points upwards, the horizontal direction is the abstract space of configurations. The increment $r_{\sigma_i, \sigma_j}(\tau)$ is abbreviated as $r_{i,j}$ and the boundary values are $r^i = \ln f(\sigma_0)$ and $r^f = -\ln g(\sigma_2)$. Therefore $C_t = r_{0,1} + r_{1,2}$ and $R_t = \ln f(\sigma_0) + r_{0,1} + r_{1,2} - \ln g(\sigma_2)$.

Proposition 3.1 *Let η_t be a Markov process with finite state space Ω and $C_0 = 0$. Then for a trajectory $\eta_{[0,t]}$ of the process with $n_t \geq 0$ transitions at random times $t_k \in (0, t)$, $1 \leq k \leq n_t$ and $\eta_\tau = \eta_{t_k}$ for $t_k \leq \tau < t_{k+1} \leq t$, $0 \leq k < n_t$ and $\eta_\tau = \eta_t$ for $t_{n_t} \leq \tau \leq t$ one has*

$$C_t = \sum_{k=1}^{n_t} r_{\eta_{t_k}, \eta_{t_{k-1}}} \quad (188)$$

and

$$R_t = r_{\eta_0}^i + \sum_{k=1}^{n_t} r_{\eta_{t_k}, \eta_{t_{k-1}}} + r_{\eta_t}^f. \quad (189)$$

The physical scenario described by a counting process is the following. One imagines that besides the physical random process described by η_t there is some physical property such as the energy of a heat reservoir that can be measured and whose value is C_t . This quantity does not directly depend on the state η_t but changes by an amount $r_{\eta', \eta}$ whenever the underlying transition $\eta \rightarrow \eta'$ occurs. Moreover, it is assumed that this physical property does not perturb the dynamics of the process. The extended counting process then yields a physical property that depends also on the boundary states of the physical random process. Here “boundary” refers to the temporal boundaries of the trajectory at times $\tau = 0$ and $\tau = t$ (Fig. 7). Concrete examples of physical importance will be discussed below.

As a direct consequence of (187) we note the factorization property

$$\mathcal{S}(f(\eta)e^{-\lambda C}) = e^{-\lambda C} \tilde{\mathcal{L}}_\lambda f(\eta) \quad (190)$$

with the *tilted generator*

$$\tilde{\mathcal{L}}_\lambda f(\eta) = \sum_{\eta' \in \Omega \setminus \eta} w_{\eta', \eta} [e^{-\lambda r_{\eta', \eta}} f(\eta') - f(\eta)]. \quad (191)$$

This factorization property of the generator has the important consequence that for a factorized initial measure $\mu(\eta, C) = \mu(\eta)\delta_{C,0}$ one has

$$\langle f_t e^{-\lambda C_t} \rangle_\mu = e^{-\lambda C_0} \sum_{\eta \in \Omega} f(\eta) \tilde{\mu}_{\lambda, t}(\eta) \quad (192)$$

where the tilted measure $\tilde{\mu}_{\lambda, t}$ with $\tilde{\mu}_{\lambda, 0} = \mu$ derives from the time evolution of the initial measure $\mu =$ under the semigroup generated by the tilted generator $\tilde{\mathcal{L}}_\lambda$ [16].

In matrix form one has

$$\tilde{H}_\lambda = - \sum_{\eta \in \Omega} \sum_{\eta' \in \Omega \setminus \eta} w_{\eta', \eta} \left(e^{-\lambda r_{\eta', \eta}} E^{\eta', \eta} - \hat{1}_\eta \right) \quad (193)$$

with the transition matrix $E^{\eta', \eta}$ defined in (53). Even though \tilde{H} is not a stochastic generator the evolution under \tilde{H} has a straightforward stochastic interpretation by appealing to the interpretation of C_t as a trajectory functional. Each stochastic

trajectory generated by the underlying process H gets weighted under the evolution of \tilde{H} by a factor $e^{-\lambda r_{\eta',\eta}}$ whenever a transition $\eta \rightarrow \eta'$ occurs. Hence the tilted transition probability, or equivalently the generating function (192) of the counter C_t for $f(\cdot) = 1_{\eta'}(\cdot)$ and initial measure concentrated on η ,

$$P_\lambda(\eta'; t|\eta; 0) = \langle \eta' | e^{-\tilde{H}_\lambda t} | \eta \rangle \quad (194)$$

can be interpreted as a measure for the weighted trajectories from a configuration η to a configuration η' for a time interval of length t .

Thus, taking $f_t(\eta) = 1$ and arbitrary initial measure $\mu(\eta)$ one obtains the generating function

$$G(\lambda, t) := \langle e^{-\lambda C_t} \rangle_\mu = \langle s | e^{-\tilde{H}_\lambda t} | \mu \rangle \quad (195)$$

of the counting function C_t . Likewise, the tilted correlation function

$$C_{12}(\lambda, t) := \langle s | \hat{f}_2 e^{-\tilde{H}_\lambda t} \hat{f}_1 | \mu \rangle \quad (196)$$

is the measure for the weighted trajectories drawn from an initial distribution μ with *boundary weights* $r_{\eta_0}^i = \ln(f_1(\eta_0))$ and $r_{\eta_t}^f = \ln(f_2(\eta_t))$. Therefore, choosing $f_1(\eta) = f^{-\lambda}(\eta)$, $f_2(\eta) = g^\lambda(\eta)$ and initial measure $\mu(\eta) = f(\eta)/Z$ with partition function $Z = \langle s | f \rangle$, one thus finds for the extended counting process

$$\langle e^{-\lambda R_t} \rangle_f = \langle s | \hat{g}^\lambda e^{-\tilde{H}_\lambda t} \hat{f}^{-\lambda} | f \rangle \quad (197)$$

which means that the generating function of the extended counting process is a tilted correlation function.

3.1.2 Time-dependent transition rates

Above we have tacitly assumed that the transition rates of the Markov process were independent of time. When we make them explicitly time-dependent the finite-time transition matrix is no longer $\exp(-Ht)$, but given by the time-ordered exponential $\mathcal{T} \left[\exp(-\int_0^t d\tau H(\tau)) \right]$ defined for general square matrices as follows.

Definition 3.2 *Let $H(t)$ be a finite-dimensional square matrix parametrized by time t . The time-ordered exponential of $\int_0^t d\tau H(\tau)$ is the infinite sum*

$$\mathcal{T} \left[e^{-\int_0^t d\tau H(\tau)} \right] = \sum_{n=0}^{\infty} (-1)^n G_n(t) \quad (198)$$

where the matrix $G_n(t)$ is defined recursively by

$$G_n(t) := \int_0^t d\tau H(\tau) G_{n-1}(\tau), \quad n \geq 1 \quad (199)$$

and $G_0(t) = \mathbf{1}$.

For illustration we write out explicitly the first few terms:

$$\mathcal{T} \left[e^{-\int_0^t d\tau H(\tau)} \right] = \mathbf{1} - \int_0^t d\tau H(\tau) + \int_0^t d\tau_1 H(\tau_1) \int_0^{\tau_1} d\tau_2 H(\tau_2) - \dots \quad (200)$$

Evidently one has $\frac{d}{dt}G_n(t) = H(t)G_{n-1}(t)$ for $n \geq 1$ and $\frac{d}{dt}G_0(t) = 0$. Thus, with the short-hand notation

$$P(t) = \mathcal{T} \left[e^{-\int_0^t d\tau H(\tau)} \right], \quad (201)$$

one has

$$\frac{d}{dt}P(t) = -H(t)P(t). \quad (202)$$

Since also $\lim_{t \searrow 0} P(t) = \mathbf{1}$ we find that

$$|\mu(t)\rangle = P(t)|\mu\rangle \quad (203)$$

is the time-dependent measure satisfying the master equation

$$\frac{d}{dt}|\mu(t)\rangle = -H(t)|\mu(t)\rangle \quad (204)$$

of a time-inhomogeneous Markov process with time-dependent transition rates $w_{\eta',\eta}(t)$. Thus the time-ordered exponential yields the transition matrix of the time-inhomogeneous Markov process. We shall refer to the time-dependence of the rates as *protocol* of the process since we have in mind an experiment where one changes a process in time in some specific way (called protocol) by means of some technical device.

For a similarity transformation (not dependent on t) one has

$$AP(t)A^{-1} = \mathcal{T} \left[e^{-\int_0^t d\tau AH(\tau)A^{-1}} \right]. \quad (205)$$

Notice that transposition yields

$$P^T(t) = \mathcal{T} \left[e^{-\int_0^t d\tau H^T(t-\tau)} \right] \quad (206)$$

with transposition *and* time-reversal of the protocol inside the exponential.

Since in defining the time-ordered exponential we have nowhere used that H is the generator of a stochastic process the formulas (204) - (206) apply also to the tilted generator, including the case where the increments are explicitly time-dependent. We write $r_{\eta',\eta}(t)$ to make such a dependence clear.

3.2 The fundamental fluctuation relation

Loosely speaking, fluctuation relations arise from comparing the probability of a trajectory of a process to the probability of a “time-reversed” trajectory. Here we prove a single master fluctuation theorem from which many fundamental fluctuation relations that have appeared in the literature follow as simple corollaries. It turns out that with the machinery developed above the proof of this master fluctuation

theorem itself reduces to a mathematical triviality. The significance of this master fluctuation relation and its famous corollaries is not mathematical depth but lies in the rather general applicability in physics, the validity arbitrarily far from equilibrium, and a unifying description of the various fluctuation theorems available for stochastic dynamics.

We are mostly interested in currents and therefore focus on antisymmetric increments satisfying $r_{\eta',\eta}(t) = -r_{\eta,\eta'}(t)$. We denote the associated counting process by J_t . Since fluctuation theorems arise from time reversal we differentiate between a *forward* process η_t^F and a *backward* process η_t^B .

Definition 3.3 (*Forward and backward process*) Fix an observation time $t > 0$ and let η_τ^F be a Markov process with countable state space Ω and time-dependent transition rates $w_{\eta'\eta}^F(\tau)$ such that for all $\tau \in [0, t]$ and all $\eta, \eta' \in \Omega \times \Omega$ either $w_{\eta'\eta}^F(\tau)w_{\eta\eta'}^F(\tau) > 0$ or $w_{\eta'\eta}^F(\tau) = w_{\eta\eta'}^F(\tau) = 0$. We say that for $\tau \in [0, t]$ the process η_τ^B with transition rates $w_{\eta'\eta}^B(\tau) = w_{\eta'\eta}^F(t - \tau)$ is the backward process associated to the forward process η_t^F and the set of functions $w_{\eta'\eta}^B(\tau)$ is the backward protocol associated with the forward protocol $w_{\eta'\eta}^F(\tau)$.

Remark 3.4 The backward process should not be confused with the time-reversed process defined by the reversed and weighted transition rates (71).

Expectations for the forward and backward process w.r.t. some initial measure μ are denoted by \mathbf{E}_μ^X with $X \in \{F, B\}$ indicating the process (forward or backward). For expectations with initial measure $\mu(\eta) = \delta_{\eta, \eta_0}$ concentrated on a fixed initial configuration η_0 we use the notation $\mathbf{E}_{\eta_0}^X$. Sums over such expectations are denoted by

$$\langle \cdot \rangle_f^X := \sum_{\eta_0 \in \Omega} f(\eta_0) \mathbf{E}_{\eta_0}^X(\cdot). \quad (207)$$

The central result from which the various fluctuation theorems derive is the following [38].

Theorem 3.5 (*Fundamental fluctuation relation*) Fix $t > 0$ and let η_τ^X with $X \in \{F, B\}$ be forward and backward Markov processes according to Definition (3.3) with finite state space Ω and associated counting processes J_τ^X with antisymmetric increments

$$r_{\eta'\eta}^X(\tau) = \ln \left(\frac{w_{\eta'\eta}^X(t)}{w_{\eta\eta'}^X(\tau)} \right) \quad (208)$$

for transitions satisfying $w_{\eta'\eta}^X(\tau)w_{\eta\eta'}^X(\tau) > 0$ and $r_{\eta'\eta}^X(\tau) = 0$ otherwise. Furthermore, let

$$R_t^F := \ln f(\eta_0^F) + J_t^F - \ln g(\eta_t^F), \quad R_t^B := \ln g(\eta_0^B) + J_t^B - \ln f(\eta_t^B) \quad (209)$$

with $f(\eta), g(\eta) \neq 0$ for all $\eta \in \Omega$ be the associated extended counting processes at time t . Then the generating functions

$$\Phi^F(\lambda, t) := \langle e^{-\lambda R_t^F} \rangle_f^F, \quad \Phi^B(\lambda, t) := \langle e^{-\lambda R_t^B} \rangle_g^B \quad (210)$$

of the trajectory functionals $R_t^{F,B}$ obey the symmetry

$$\Phi^F(\lambda, t) = \Phi^B(1 - \lambda, t) \quad (211)$$

for all $\lambda \in \mathbb{R}$.

Proof: First we note

Lemma 3.6 *Let H^F be the generator of the forward process η_τ^F and H^B be the generator of the backward process η_τ^B according to Definition (3.3) and let $J_\tau^{F,B}$ be the associated counting processes with increments (208). Then tilted evolution operators satisfy*

$$\left(\tilde{P}_\lambda^F(\tau)\right)^T = \tilde{P}_{1-\lambda}^B(\tau). \quad (212)$$

for all $\tau \in [0, t]$ and $\lambda \in \mathbb{R}$.

Proof: We recall the matrix representation (193) from which we obtain for the time-dependent case

$$\begin{aligned} \left(\tilde{H}_\lambda^F(t - \tau)\right)^T &= - \sum_{\eta \in \Omega} \sum_{\eta' \in \Omega \setminus \eta} w_{\eta'\eta}^F(t - \tau) \left(e^{-\lambda r_{\eta',\eta}^F(t-\tau)} E^{\eta\eta'} - \hat{1}_\eta \right) \\ &= - \sum_{\eta \in \Omega} \sum_{\eta' \in \Omega \setminus \eta} w_{\eta'\eta}^F(t - \tau) \left(\left(\frac{w_{\eta\eta'}^F(t - \tau)}{w_{\eta'\eta}^F(t - \tau)} \right)^\lambda E^{\eta\eta'} - \hat{1}_\eta \right) \\ &= - \sum_{\eta \in \Omega} \sum_{\eta' \in \Omega \setminus \eta} \left(w_{\eta\eta'}^F(t - \tau) \left(\frac{w_{\eta\eta'}^F(t - \tau)}{w_{\eta'\eta}^F(t - \tau)} \right)^{\lambda-1} E^{\eta\eta'} - w_{\eta'\eta}^F(t - \tau) \hat{1}_\eta \right) \\ &= - \sum_{\eta \in \Omega} \sum_{\eta' \in \Omega \setminus \eta} \left(w_{\eta\eta'}^B(\tau) \left(\frac{w_{\eta\eta'}^B(\tau)}{w_{\eta'\eta}^B(\tau)} \right)^{\lambda-1} E^{\eta\eta'} - w_{\eta'\eta}^B(\tau) \hat{1}_\eta \right) \\ &= - \sum_{\eta \in \Omega} \sum_{\eta' \in \Omega \setminus \eta} \left(w_{\eta\eta'}^B(\tau) \left(\frac{w_{\eta'\eta}^B(\tau)}{w_{\eta\eta'}^B(\tau)} \right)^{1-\lambda} E^{\eta\eta'} - w_{\eta'\eta}^B(\tau) \hat{1}_\eta \right) \\ &= - \sum_{\eta \in \Omega} \sum_{\eta' \in \Omega \setminus \eta} w_{\eta'\eta}^B(\tau) \left(\left(\frac{w_{\eta\eta'}^B(\tau)}{w_{\eta'\eta}^B(\tau)} \right)^{1-\lambda} E^{\eta\eta'} - \hat{1}_\eta \right) \\ &= - \sum_{\eta \in \Omega} \sum_{\eta' \in \Omega \setminus \eta} w_{\eta\eta'}^B(\tau) \left(e^{-(1-\lambda)r_{\eta',\eta}^B(t-\tau)} E^{\eta\eta'} - \hat{1}_\eta \right). \end{aligned} \quad (213)$$

where we have used the antisymmetry of the increments. Thus

$$\left(\tilde{H}_\lambda^F(t - \tau)\right)^T = \tilde{H}_{1-\lambda}^B(\tau). \quad (214)$$

The transposition property (206) of the time-ordered exponential then proves the Lemma. \square

Continuing with the proof of Theorem (3.5) we include now the boundary terms. We have

$$\Phi^F(\lambda, t) = \langle s | \hat{g}^\lambda \tilde{P}_\lambda^F(t) \hat{f}^{-\lambda} | f \rangle, \quad \Phi^B(\lambda, t) = \langle s | \hat{f}^\lambda \tilde{P}_\lambda^B(t) \hat{g}^{-\lambda} | g \rangle \quad (215)$$

with $|f\rangle = \sum_{\eta \in \Omega} f(\eta) |\eta\rangle$ and $|g\rangle = \sum_{\eta \in \Omega} g(\eta) |\eta\rangle$. By transposition we obtain

$$\Phi^F(\lambda, t) = \langle f | \hat{f}^{-\lambda} \left(\tilde{P}_t^F(\lambda) \right)^T \hat{g}^\lambda | s \rangle = \langle s | \hat{f}^{1-\lambda} \left(\tilde{P}_t^F(\lambda) \right)^T \hat{g}^{-(1-\lambda)} | g \rangle. \quad (216)$$

Lemma (3.6) then concludes the proof. \square

Remark 3.7 *We required the functions f and g to be non-vanishing for all η . However, one can generalize Theorem (3.5) by introducing indicator functions $1_X, 1_Y$ on subsets $X, Y \in \Omega$. Going through the same steps as above one obtains for*

$$\Phi_{YX}^F(\lambda, t) := \langle I_Y(\eta_t) e^{-\lambda R_t^F} I_X(\eta_0) \rangle_f^F, \quad \Phi_{YX}^B(\lambda, t) := \langle I_X(\eta_t) e^{-\lambda R_t^B} I_Y(\eta_0) \rangle_g^B \quad (217)$$

the extended fluctuation theorem

$$\Phi_{YX}^F(\lambda, t) = \Phi_{XY}^B(1 - \lambda, t) \quad (218)$$

In particular, choosing $X = |\eta_a\rangle\langle\eta_a|$ and $Y = |\eta_b\rangle\langle\eta_b|$ one obtains a symmetry relation for trajectories between fixed configurations η_a, η_b . This yields the detailed fluctuation theorems introduced in [45].

3.3 Some specific fluctuation theorems

In applications one thinks of a stochastic transition as being triggered by thermal processes in the physical environment into which the system described by the process is embedded. The choice of increments (208) then means that J_t is the change of entropy ΔS_{env} of the physical environment along a trajectory of the process [90]. Since for thermal systems at temperature T , the dissipated heat is given by

$$Q = T \Delta S_{\text{env}} \quad (219)$$

we can also think of this current J_t as defining a non-equilibrium heat term. Different physical scenarios are then described an appropriate choice of the boundary terms $r^i(\eta)$ and $r^f(\eta)$ in the extended process R_t . We list some well-known cases.

3.3.1 Integral fluctuation relations

Setting $\lambda = 1$ in (211) gives the ‘‘integral fluctuation relation’’ [65]

$$\langle e^{-R_t^F} \rangle_f^F = 1 \quad (220)$$

with *any* normalized choice of $r^i = \ln f$ and $r^f = -\ln g$. The specific choice of f and g determines the physical interpretation of R_t^F .

1) Jarzynski equality

Consider a process in which the rates obey detailed balance (68) at all times w.r.t. a time-dependent distribution

$$\mu_\tau^*(\eta) = e^{-\beta U_\tau(\eta)} / Z_\tau \quad (221)$$

with temperature $T = 1/\beta$, internal energy $U_\tau(\eta)$ of the configuration η , partition function

$$Z_\tau = \sum_{\eta \in \Omega} e^{-\beta U_\tau(\eta)} \quad (222)$$

and free energy

$$F_\tau = -T \ln Z_\tau. \quad (223)$$

Now we imagine preparing an experiment in which we start with initial distribution $f(\eta) = \mu_0^*(\eta)$ and measure at some fixed time $t > 0$ the quantity

$$g(\eta) = \mu_t^*(\eta). \quad (224)$$

Then (220) reads

$$\langle e^{-R_t^F} \rangle_f^F = \frac{Z_0}{Z_t} \langle s | e^{-\beta \hat{U}} \tilde{P}_1(t) e^{\beta \hat{U}} | \mu_0^* \rangle \quad (225)$$

In this case R_t^F is proportional to the dissipated work, which can be seen as follows.

Using the Boltzmann form of the time-dependent pseudo-equilibrium distribution μ_τ^* the boundary part of the functional R_t^F becomes

$$\ln f(\eta_0) - \ln g(\eta_t) = \frac{\Delta U}{T} - \frac{\Delta F}{T} \quad (226)$$

with the changes of internal energy $\Delta U := U(\eta_t) - U(\eta_0)$ and free energy $\Delta F := F_t - F_0$ resp. during the experimental time span t . Since the current part J_t is proportional to dissipated heat (219) one finds

$$R_t^F = \frac{Q}{T} + \frac{\Delta U}{T} - \frac{\Delta F}{T} \quad (227)$$

According to the first law of thermodynamics the work is given by $W = (Q + \Delta U)/T$ and hence R_t^F is the dissipated work.

Thus (220) yields the Jarzynski relation [44]

$$\langle e^{-W/T} \rangle = e^{-\Delta F/T}. \quad (228)$$

Notice that it is *not* assumed that the system during its time evolution is in its time-dependent pseudo-equilibrium state μ_τ^* , not even at the final measurement

time $\tau = t$. This is important as it implies one can measure equilibrium free energies from an average of the non-equilibrium work performed. The Jarzynski equality can also be related to some earlier work theorems [11, 12, 13]. A discussion of the connections can be found in [46].

2) Integral fluctuation theorem for entropy

Now consider a different experimental scenario. Prepare experimentally an initial distribution $\mu = f$ and measure a quantity g chosen to correspond to the final probability distribution of the process, i.e.,

$$g(\eta) = \langle \eta | P_t | f \rangle. \quad (229)$$

Then the boundary term of R_t^F can be written as

$$f(\eta_0) - g(\eta_t) = \ln \mu(\eta_0, 0) - \ln \mu(\eta_t, t) \quad (230)$$

where $\mu(\eta_t, t)$ is the solution of the time-dependent master equation (204).

Using the general definition

$$S = \mathbf{E}_\mu \ln \mu(\eta) = \sum_{\eta \in \Omega} \mu(\eta) \ln \mu(\eta) \quad (231)$$

of entropy these boundary terms can be interpreted as the change in “system” entropy $\Delta S_{\text{sys}} := S_{\text{sys}}(t) - S_{\text{sys}}(0)$ along a trajectory [90]. Hence in this case we have

$$R_t^F = \Delta S_{\text{env}} + \Delta S_{\text{sys}} =: \Delta S_{\text{tot}}, \quad (232)$$

and (220) becomes an integral relation for the *total* entropy change [90]

$$\langle e^{-\Delta S_{\text{tot}}} \rangle = 1. \quad (233)$$

Jensen’s inequality then implies $\langle \Delta S_{\text{tot}} \rangle \geq 0$. In other words, the fluctuation theorem is entirely consistent with the Second Law of Thermodynamics which, properly interpreted, is a statement about averages, not individual trajectories.

3.3.2 Detailed fluctuation relations

For general λ the master theorem (3.5) leads to various “stronger” fluctuation relation. To fix the idea we write the generating-function relation (211) formally as

$$\sum_R \text{Prob}^F(R_t^F = R) e^{-\lambda R} = \sum_R \text{Prob}^B(R_t^B = R) e^{-(1-\lambda)R}. \quad (234)$$

where $\text{Prob}^F(R_t^F = R)$ denotes the probability $R_t^F = R$ in the forward process (with initial distribution μ^F) and analogously for the backward process. This is trivially equivalent to

$$\sum_R \text{Prob}^F(R_t^F = R) e^{-\lambda R} = \sum_R \text{Prob}^B(R_t^B = R) e^{(1-\lambda)R}. \quad (235)$$

Validity for all $\lambda \in \mathbb{R}$ implies

$$\frac{\text{Prob}^B(R_t^B = -R)}{\text{Prob}^F(R_t^F = R)} = e^{-R} \quad (236)$$

which is time-reversal symmetry of the extended forward and backward counting processes, or, equivalently, of the generating function of the forward and backward trajectory functionals.

We point that if r^i and r^f are related by reversal of protocol, then R_t^F and R_t^B measure the same physical quantity in forward and reverse processes (with initial distributions f and g respectively). We can then denote this quantity by R_t without subscript and write (236) in the simplified form

$$\frac{p_B(-R_t)}{p_F(R_t)} = e^{-R_t} \quad (237)$$

which is known as the transient fluctuation theorem, see [38] for a more detailed discussion. Here $p_F(R_t)$ denotes the probability distribution for the physical quantity \mathcal{R} in the forward process and $p_B(R_t)$ is the corresponding distribution for the backward process. We point out some examples.

1) Crooks' fluctuation theorem

Choose for rates obeying time-dependent detailed balance,

$$f(\eta_0) = \mu^*(\eta_0) \quad \text{and} \quad g(\eta_t) = \mu^*(\eta_t). \quad (238)$$

which allows the identification of R_t as proportional to the dissipated work $W_d = Q + \Delta U - \Delta F$. 237 then becomes the fluctuation theorem

$$\frac{p_B(-W_d)}{p_F(W_d)} = e^{-W_d/T}, \quad (239)$$

which is due to [17].

2) Evans-Searles fluctuation theorem

For constant rates the forward and reverse processes are obviously identical. If we also take $f = g$ then we can drop the subscripts on the probability distributions $p_F(R_t)$ and $p_B(R_t)$ and one obtains the Evans-Searles fluctuation theorem [25, 89, 26].

A special case corresponds to taking $f = g = \mu^*$. Experimentally, this simply means allowing a system (with time-independent rates) to relax to stationarity before starting the measurement. In this case we can identify R_t with the total entropy change. This yields a fluctuation theorem for entropy changes in the steady state [90]

$$\frac{p(-\Delta S_{\text{tot}})}{p(\Delta S_{\text{tot}})} = e^{-\Delta S_{\text{tot}}}, \quad (240)$$

which is essentially a stochastic form of the original fluctuation theorem proposed by [24].

3.3.3 Gallavotti-Cohen-Theorem for stochastic interacting particle systems

In this subsection we focus on *time-independent* rates (in which case backward and forward processes are identical) and discuss the limit $t \rightarrow \infty$ of the fundamental fluctuation relation (218). For finite state space the result is quite simple [59] and the analogue of the Gallavotti-Cohen theorem [30].

Theorem 3.8 (*Gallavotti-Cohen symmetry*) *Let η_t be an ergodic Markov process with finite state space Ω and transition rates $w_{\eta'\eta}$ satisfying either $w_{\eta'\eta}w_{\eta\eta'} > 0$ or $w_{\eta'\eta} = w_{\eta\eta'} = 0$. Furthermore, let J_t be the associated counting processes with antisymmetric increments*

$$r_{\eta'\eta} = \ln \left(\frac{w_{\eta'\eta}}{w_{\eta\eta'}} \right) \quad (241)$$

for transitions where $w_{\eta'\eta}w_{\eta\eta'} > 0$ and $r_{\eta'\eta} = 0$ otherwise and let

$$R_t := \ln f(\eta_0^F) + J_t - \ln g(\eta_t^F) \quad (242)$$

with $f(\eta), g(\eta) \neq 0$ for all $\eta \in \Omega$ be the associated extended counting process at time t . Then for the generating function

$$\Phi_\mu(\lambda, t) := \langle e^{-\lambda R_t} \rangle_\mu \quad (243)$$

with any initial measure μ one has the asymptotic behaviour

$$\lim_{t \rightarrow \infty} \frac{1}{t} \ln \Phi_\mu(\lambda, t) = -E_0(\lambda) \quad \forall \lambda \in \mathbb{R} \quad (244)$$

and the Gallavotti-Cohen symmetry

$$E_0(\lambda) = E_0(1 - \lambda) \quad \forall \lambda \in \mathbb{R} \quad (245)$$

where $E_0(\lambda) \in \mathbb{R}$ is the lowest eigenvalue of the tilted generator \tilde{H}_λ .

Proof: By definition

$$\Phi_\mu(\lambda, t) = \langle s | \hat{g}^\lambda e^{-\tilde{H}_\lambda t} \hat{f}^{-\lambda} | \mu \rangle. \quad (246)$$

The spectral decomposition

$$e^{-\tilde{H}_\lambda t} = \sum_k e^{-E_k(\lambda)t} | \Phi_k(\lambda) \rangle \langle \Psi_k(\lambda) | \quad (247)$$

into the dyadic product of biorthogonal left and right eigenvectors of \tilde{H}_λ yields

$$\Phi_\mu(\lambda, t) = e^{-E_0(\lambda)t} \sum_k e^{-(E_k(\lambda) - E_0(\lambda))t} a_k(\lambda) b_k(\lambda) \quad (248)$$

where $E_0(\lambda)$ denotes the lowest eigenvalue of \tilde{H}_λ and

$$a_k(\lambda) := \langle s | \hat{g}^\lambda | \Phi_k(\lambda) \rangle, \quad b_k(\lambda) := \langle \Psi_k(\lambda) | \hat{f}^{-\lambda} | \mu \rangle. \quad (249)$$

By Perron-Frobenius the lowest eigenvalue corresponding to index $k = 0$ in the decomposition is unique. Thus $\Re(E_k(\lambda) - E_0(\lambda)) > 0$ for all $k \neq 0$. Since in finite state space $a_k(\lambda)$ and $b_k(\lambda)$ are bounded (244) is proved. The Gallavotti-Cohen symmetry (244) then follows from (214) which here reduces to $\tilde{H}_\lambda^T = \tilde{H}_{1-\lambda}$. \square

Remark 3.9 *The assumption of finite state space is not a minor technicality, but essential for the validity of the theorem. For infinite state space the coefficients $a_0(\lambda)$ and/or $b_0(\lambda)$ may diverge so that (244) is not valid. A simple lattice gas model where this happens is the zero-range process where each lattice site can be occupied by an arbitrary number of particles, see [37, 78, 39].*

Remark 3.10 *If (244) holds then the symmetry relation (245) for the lowest eigenvalue implies the more popular (but not precise) version of the Gallavotti-Cohen symmetry*

$$\frac{p(J, t)}{p(-J, t)} = e^{-Jt} \quad (250)$$

for the probability density $p(J, t) = \text{Prob}[J_t = J]$ of the entropy production J_t .

Notice the independence of (244) and (245) of boundary terms. Heuristically this corresponds to the intuition that $J_t \propto t^\alpha$ for large t with some positive power α , while the boundary terms (which depend only on one point in time) are bounded as $t \rightarrow \infty$.

As pointed out in [59] the existence of the limit (244) implies a large deviation property for the probability distribution $p(j, t) := \text{Prob}[j_t = j]$ of the observed “average” current $j_t = J_t/t$. Specifically, the long-time limiting behaviour is given by

$$p(j, t) \sim e^{-t\hat{E}(j)} \quad (251)$$

where the large deviation function $\hat{E}(j)$ is the Legendre transformation, i.e.,

$$\hat{E}(j) = \max_\lambda \{E_0(\lambda) - \lambda j\}. \quad (252)$$

of $E_0(\lambda)$.

4 Dynamical universality classes

In the SSEP we have seen that local perturbations spread diffusively with dynamical exponent $z = 2$ while in the ASEP the spreading is superdiffusive and the KPZ-universality class with dynamical exponent $z = 3/2$. For a long time these were the only universality classes known to appear in driven diffusive systems. However, based

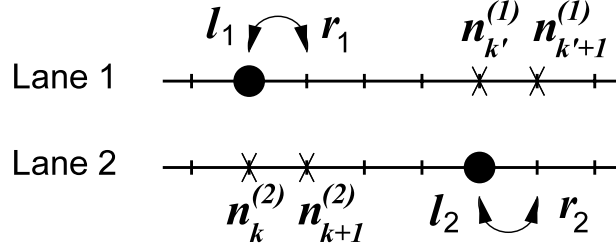


Figure 8: Schematic representation of the two-lane partially asymmetric simple exclusion process. A particle on lane 1 (2) hops to the neighbouring site (provided this target site is empty) with to the right or left with rates (253) that depend on the particle configuration on the adjacent sites of the other lane that are marked by a cross.

on numerical evidence and analytical results for other types of models also a dynamical exponent $z = 5/3$ has been reported [15, 100]. Thus the question arises which dynamical exponent can generally arise and what universal scaling functions describe the dynamical structure function. Of course, this question is posed rather imprecisely and very generally. We shall narrow down the quest for an answer to systems with n locally conserved species of particles and dynamics whose large scale behaviour is determined by the slow relaxation of these densities and not by other local kinetic constraints on the transition rates for the particles.

4.1 Multi-lane exclusion processes

We consider a two-lane asymmetric simple exclusion process on two parallel chains with L sites each and periodic boundary conditions. Particles do not change lanes. We denote the particle occupation number on site k in the first (upper) lane by $\eta_k^{(1)} \in \{0, 1\}$, and on the second (lower) lane by $\eta_k^{(2)} \in \{0, 1\}$. The total particle number is conserved in each lane and denoted N_λ .

The jump rates for particle on lane λ depend on the particle configuration on the adjacent lane. Particles on lane λ jump from site k to site $k+1$ with rate $r_\lambda(k, k+1)$ and from site $k+1$ to site k with rate $\ell_\lambda(k+1, k)$ (Fig. 8) as given by [72]

$$\begin{aligned}
 r_1(k, k+1) &= p_1 + b_1 n_k^{(2)} + c_1 n_{k+1}^{(2)} + d_1 n_k^{(2)} n_{k+1}^{(2)} \\
 \ell_1(k+1, k) &= q_1 + e_1 n_k^{(2)} + f_1 n_{k+1}^{(2)} + g_1 n_k^{(2)} n_{k+1}^{(2)} \\
 r_2(k, k+1) &= p_2 + b_2 n_k^{(1)} + c_2 n_{k+1}^{(1)} + d_2 n_k^{(1)} n_{k+1}^{(1)} \\
 \ell_2(k+1, k) &= q_2 + e_2 n_k^{(1)} + f_2 n_{k+1}^{(1)} + g_2 n_k^{(1)} n_{k+1}^{(1)}.
 \end{aligned} \tag{253}$$

The stationary distribution for this model is uniform distribution if $b_1 - e_1 = c_2 - f_2$, $b_2 - e_2 = c_1 - f_1$, $d_1 = g_1$ and $d_2 = g_2$. Correspondingly one has stationary grandcanonical product measures where each site of lane λ is occupied independently of the other sites with probability $\rho_\lambda \in [0, 1]$. Hence the ρ_λ are the conserved densities. From the hopping rates (253) and the product form of the grandcanonical

distribution one thus obtain the stationary current vector \vec{j} with components

$$\begin{aligned} j_1(\rho_1, \rho_2) &= \rho_1(1 - \rho_1)(a + \gamma\rho_2), \\ j_2(\rho_1, \rho_2) &= \rho_2(1 - \rho_2)(b + \gamma\rho_1). \end{aligned} \quad (254)$$

where

$$a = p_1 - q_1, \quad b = p_2 - q_2, \quad \gamma = b_1 + c_1 - e_1 - f_1. \quad (255)$$

For $b = 1$ we recover the totally asymmetric two-lane model of [70] which is a special case of the multi-lane model of [71]. We consider $a = 1, \gamma \neq 0$.

The fluctuation of the total particle number in the grandcanonical ensemble are described by the compressibility matrix K with matrix elements

$$K_{\lambda\mu} := \frac{1}{L} \langle (N_\lambda - \rho_\lambda L)(N_\mu - \rho_\mu L) \rangle = \rho_\lambda(1 - \rho_\lambda)\delta_{\lambda,\mu}. \quad (256)$$

where $\lambda, \mu \in \{1, 2\}$. This corresponds to

$$\kappa_\lambda := K_{\lambda\lambda} = \rho_\lambda(1 - \rho_\lambda), \quad \bar{\kappa} := K_{12} = 0. \quad (257)$$

4.2 Brief outline of nonlinear fluctuating hydrodynamics

In order to study fluctuations in this process we follow [94] and take the non-linear fluctuating hydrodynamics approach together with a mode-coupling analysis of the non-linear equation. We summarize here the main ingredients of this well-established description.

Let us denote microscopic time by the symbol τ rather than t as done in the previous section. We begin by describing the large-scale dynamics of the process under Eulerian scaling where the lattice spacing a is taken to zero such that the macroscopic coordinate $x = ka$ remains finite and where the microscopic time τ is taken to infinity such that the macroscopic time $t = \tau a$ is finite. One then assumes the validity of a law of large numbers such that the local distribution of particles can be described by a coarse-grained local density $\rho_\lambda(x, t)$ of the particle component λ . This leads the system of conservation laws [92, 54]

$$\frac{\partial}{\partial t} \vec{\rho}(x, t) + \frac{\partial}{\partial x} \vec{j}(x, t) = 0 \quad (258)$$

which follow rigorously or heuristically from the microscopic local conservation of the particle number. Here $\rho_\lambda(x, t)$ is a component of the density vector $\vec{\rho}(x, t)$, and $j_\lambda(x, t)$ is a component of the current vector $\vec{j}(x, t)$ which we regard as column vectors.

According to the assumption of local stationarity the current is a function of x and t only through its dependence on the local conserved densities. Therefore

$$\frac{\partial}{\partial t} \vec{\rho}(x, t) + J \frac{\partial}{\partial x} \vec{\rho}(x, t) = 0 \quad (259)$$

where J is the current Jacobian with matrix elements $J_{\lambda\mu} = \partial j_\lambda / \partial \rho_\mu$. The product JK of the Jacobian with the compressibility matrix (256) is symmetric [34] which guarantees hyperbolicity of the system (259) [98]. The eigenvalues v_α of J are the characteristic velocities of the system. If $v_1 \neq v_2$ the system is called strictly hyperbolic.

In order to extract information from this non-linear system of PDE's one expands the local densities $\rho_\lambda(x, t) = \rho_\lambda + u_\lambda(x, t)$ around their long-time stationary values ρ_λ . To linear order one gets

$$\partial_t \vec{u} = -J \partial_x \vec{u}. \quad (260)$$

where J is now fixed at the values stationary values ρ_λ . We transform to normal modes $\vec{\phi} = R \vec{u}$ where $RJR^{-1} = \text{diag}(v_\alpha)$ and the transformation matrix R is normalized such that $RKR^T = 1$. Thus we get, since we have a linear system,

$$\phi_\alpha(x, t) = \phi_0(x + v_\alpha t) \quad (261)$$

with initial data $\phi_\alpha(x, 0) = \phi_0(x)$. This result demonstrates the significance of the eigenvalues of the current Jacobian which are called characteristic velocities v_α . They are the velocities at which perturbations of the flat stationary density profile move.

In order to study the effect of the non-linearity we now expand to second order. This yields

$$\partial_t \vec{u} = -\partial_x \left(J \vec{u} + \frac{1}{2} \vec{u}^T \vec{H} \vec{u} \right) \quad (262)$$

where \vec{H} is a column vector whose entries $(\vec{H})_\lambda = H^\lambda$ are the Hessians with matrix elements $H_{\mu\nu}^\lambda = \partial^2 j_\lambda / (\partial \rho_\mu \partial \rho_\nu)$. The term $\vec{u}^T H^\lambda \vec{u}$ denotes the inner product in component space. One recognizes in (262) a system of coupled Burgers equations.

Finally, the effect of fluctuations, which occur on finer space-time scales where $t = \tau a^z$ with dynamical exponent $z > 1$, can be captured by adding phenomenological diffusion matrix D and white noise terms $\xi_i(x, t)$. For quadratic nonlinearities (259) then yields

$$\partial_t \vec{u} = -\partial_x \left(J \vec{u} + \frac{1}{2} \vec{u}^T \vec{H} \vec{u} - D \partial_x \vec{u} + B \vec{\xi} \right). \quad (263)$$

If the quadratic non-linearity is absent one has diffusive behaviour, up to possible logarithmic corrections that may arise from cubic non-linearities [22]. In normal modes one has

$$\partial_t \phi_\alpha = -\partial_x \left(v_\alpha \phi_\alpha + \vec{\phi}^T G^\alpha \vec{\phi} - \partial_x (\tilde{D} \vec{\phi})_\alpha + (\tilde{B} \vec{\xi})_\alpha \right) \quad (264)$$

with $\tilde{D} = RDR^{-1}$, $\tilde{B} = RB$ and

$$G^\alpha = \frac{1}{2} \sum_\lambda R_{\alpha\lambda} (R^{-1})^T H^\lambda R^{-1} \quad (265)$$

are the called the mode coupling matrices.

Consider now the dynamical structure matrix $\bar{S}_k(t)$ of the microscopic model defined on the lattice. Its matrix elements are the dynamical structure functions

$$\bar{S}_k^{\lambda\mu}(t) := \langle (n_k^{(\lambda)}(t) - \rho_\lambda)(n_0^{(\mu)}(t) - \rho_\mu) \rangle \quad (266)$$

which measure density fluctuations in the stationary state. In normal modes one then has

$$S_k^{\alpha\beta}(t) = [R\bar{S}_k(t)R^T]_{\alpha\beta} = \langle \phi_k^\alpha(t)\phi_0^\beta(0) \rangle \quad (267)$$

where the transformation R acts on the lattice density vector.

We focus from now on on strictly hyperbolic systems where all characteristic velocities are different. Then one expects that the off-diagonal elements of S decay quickly and for long times and large distances the diagonal elements which we denote by

$$S_\alpha(x, t) := S^{\alpha\alpha}(x, t) \quad (268)$$

with initial value $S_\alpha(x, 0) = \delta(x)$ remain significant. One expects the the scaling form

$$S_\alpha(x, t) \sim t^{-1/z_\alpha} f_\alpha((x - v_\alpha t)^{z_\alpha}/t) \quad (269)$$

with a dynamical exponent z_α that may be different for the different modes. The exponent in the power law prefactor is determined by mass conservation.

The dynamical structure function can interpreted as describing the stationary two-time correlations of the local density fluctuations. Alternatively, it can regarded as the expectation of the local density evolving from an initial initial distribution that is microscopically peaked around the origin $k = 0$ [72], corresponding to a δ -peak on macroscopic scale. Thus the characteristic velocity describes the velocity at which the center of mass of these peaks move [70] and the dynamical exponent describes the spreading around the center of mass.

4.3 Fibonacci universality classes

In order to analyze the system of nonlinear stochastic PDE's in more detail we employ mode coupling theory [94, 74]. The starting point for computing the $S_\alpha(x, t)$ are the one-loop mode coupling equations

$$\partial_t S_\alpha(x, t) = (-v_\alpha \partial_x + D_\alpha \partial_x^2) S_\alpha(x, t) + \int_0^t ds \int_{-\infty}^{\infty} dy S_\alpha(x - y, t - s) \partial_y^2 M_{\alpha\alpha}(y, s) \quad (270)$$

with the diagonal element $D_\alpha := \tilde{D}_{\alpha\alpha}$ of the phenomenological diffusion matrix and the memory kernel

$$M_{\alpha\alpha}(y, s) = 2 \sum_{\beta, \gamma} (G_{\beta\gamma}^\alpha)^2 S_\beta(y, s) S_\gamma(y, s). \quad (271)$$

The strategy is to rewrite this equation in terms of the Fourier transform

$$\hat{S}_\alpha(p, t) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-ipx} S_\alpha(x, t). \quad (272)$$

and then to plug into this equation the scaling ansatz

$$\hat{S}_\alpha(p, t) \sim e^{-iv_\alpha p t} \hat{f}_\alpha(p^{z_\alpha} t). \quad (273)$$

Remarkably, the coupled system of equation then becomes exactly solvable [73, 74]. One obtains equations for the dynamical exponents arising from requiring non-trivial scaling solutions and using the known results $z = 3/2$ for KPZ and $z = 2$ for diffusion. In a next step one can then solve for the actual scaling functions.

The scaling behaviour of the solutions of (270) is turns out to be determined by the diagonal terms $G_{\beta\beta}^\alpha$ of the mode coupling matrices G^α . We define the set

$$\mathbb{I}_\alpha := \{\beta : G_{\beta\beta}^\alpha \neq 0\} \quad (274)$$

of non-zero diagonal mode coupling coefficients. This means that \mathbb{I}_α is the set of modes β that give rise to a non-linear term in the time evolution of the mode α whose dynamical exponent and scaling function one wishes to compute.

The equations that determine the dynamical exponents for a system with n modes are then:

$$z_\alpha = \begin{cases} 2 & \text{if } \mathbb{I}_\alpha = \emptyset \\ 3/2 & \text{if } \alpha \in \mathbb{I}_\alpha \\ \min_{\beta \in \mathbb{I}_\alpha} \left[\left(1 + \frac{1}{z_\beta} \right) \right] & \text{else} \end{cases} \quad (275)$$

and

$$1 < z_\alpha \leq 2 \quad \forall \alpha \quad (276)$$

Remarkably the solution to this non-linear recursion yields as possible dynamical exponents the Kepler ratios of neighbouring Fibonacci numbers $z_\alpha = 2, 3/2, 5/3, 8/5, \dots$ or its limiting value which is the golden mean $z_\alpha = (1 + \sqrt{5})/2$.

Specifically, if all self-coupling term $G_{\alpha\alpha}^\alpha$ vanish then mode α is diffusive with $z_\alpha = 2$ and Gaussian scaling function (except for possible logarithmic corrections). If $G_{\alpha\alpha}^\alpha \neq 0$ and there is no diffusive mode β such that $G_{\beta\beta}^\alpha \neq 0$ then the mode is KPZ with $z_\alpha = 3/2$ and Prähofer-Spohn scaling function [75, 76]. If $G_{\alpha\alpha}^\alpha \neq 0$, but there is a diffusive mode β such that $G_{\beta\beta}^\alpha \neq 0$ then again $z_\alpha = 3/2$, but the scaling function is unknown [95]. If the self-coupling $G_{\alpha\alpha}^\alpha = 0$ but some $G_{\beta\beta}^\alpha \neq 0$ then the mode is a Fibonacci mode where the scaling function is an asymmetric Lévy distribution [73, 74]. The lowest Fibonacci mode has $z = 3/2$ like KPZ, but is not KPZ. The scaling function for this mode satisfies a fractional diffusion equation which has been proved rigorously in a system of harmonic oscillators that are perturbed by a conservative noise [8].

Thus non-linear hydrodynamics yields an infinite discrete family of dynamical universality classes. The ubiquitous diffusive universality class and the celebrated KPZ universality class are the lowest members of this family. We stress that this result is not confined to lattice gases but generally to any system with slow relaxation of the conserved modes.

4.4 Ballistic universality class in conditioned dynamics

Finally we consider the question whether one can have a “ballistic” universality class with $z = 1$. Such a universality class indeed exists as shown by Spohn for an exclusion process with long-range interactions [93]. No models with short-range interactions and $z = 1$ are known. However, the model of Spohn arises as “conditioned” dynamics of the usual ASEP, viz. the ASEP conditioned on carrying a large current. This observation then points to the existence of a much larger family of models with $z = 1$ with the conjecture that *all* stationary space-time correlation functions can be predicted from conformal invariance [51]. This conjecture arises from the mapping to quantum spin systems and then using well-established properties of the quantum ground state which is known to be described by conformal field theory.

5 Conclusions

It has been realized in recent years that the stochastic time evolution of many stochastic interacting particle systems can be mapped to quantum spin systems, and in special one-dimensional cases to integrable quantum chains. This insight has made available the tool box of quantum mechanics for these interacting particle systems far from equilibrium. With these methods many new exact results for their dynamical and stationary properties have been derived. It is also amusing to note that the Hamiltonians for such systems are mostly not hermitian and therefore from a quantum mechanical point of view not interesting. Stochastic interacting particle systems which can be described in this way comprise a large variety of phenomena in physics and beyond. In this way one obtains detailed information about the microscopic properties and large-scale fluctuations of lattice gas models with conserved particle species.

Going beyond these exact results we have shown that non-linear fluctuating hydrodynamics predicts an infinite discrete family of dynamical universality classes whose dynamical exponents are the Kepler ratios of neighbouring Fibonacci numbers. This fact encourages the search for other discrete families of nonequilibrium universality classes.

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