

# Interacting particle systems

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These notes and other information about the course are available on  
<http://www.warwick.ac.uk/~masgav/teaching/ma4h3.html>

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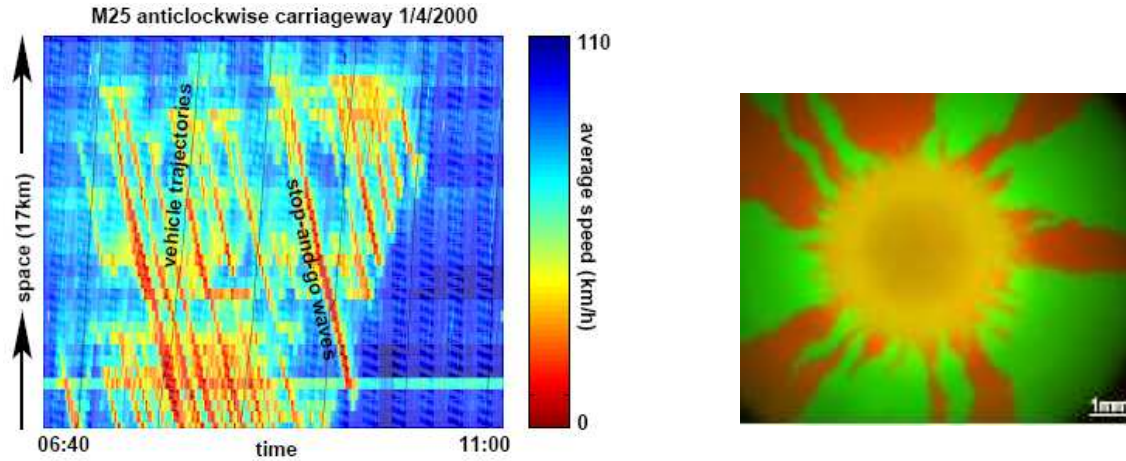
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## Introduction

Interacting particle systems (IPS) are mathematical models of complex phenomena involving a large number of interrelated components. There are numerous examples within all areas of natural and social sciences, such as traffic flow on motorways or communication networks, opinion dynamics, spread of epidemics or fires, genetic evolution, reaction diffusion systems, crystal surface growth, financial markets, etc. The central question is to understand and predict emergent behaviour on macroscopic scales, as a result of the microscoping dynamics and interactions of individual components. Qualitative changes in this behaviour depending on the system parameters are known as collective phenomena or phase transitions and are of particular interest.

In IPS the components are modeled as particles confined to a lattice or some discrete geometry. But applications are not limited to systems endowed with such a geometry, since continuous degrees of freedom can often be discretized without changing the main features. So depending on the specific case, the particles can represent cars on a motorway, molecules in ionic channels, or prices of asset orders in financial markets, to name just a few examples. In principle such systems often evolve according to well-known laws, but in many cases microscopic details of motion are not fully accessible. Due to the large system size these influences on the dynamics can be approximated as effective random noise with a certain postulated distribution. The actual origin of the noise, which may be related to chaotic motion or thermal interactions, is usually ignored. On this level the statistical description in terms of a random process where particles move and interact according to local stochastic rules is an appropriate mathematical model. It is neither possible nor required to keep track of every single particle. One is rather interested in predicting measurable quantities which correspond to expected values of certain observables, such as the growth rate of the crystalline surface or the flux of cars on the motorway. Although describing the system only on a mesoscopic level as explained above, stochastic particle systems are usually referred to as microscopic models and we stick to this convention. On a macroscopic scale, a continuum description of systems with a large number of particles is given by coarse-grained density fields, evolving in time according to a partial differential equation. The form of this equation depends on the particular application, and its mathematical connection to microscopic particle models is one of the fundamental questions in complexity science.

The focus of these notes is not on detailed models of real world phenomena, but on simple paradigmatic IPS that capture the main features of real complex systems. Several such models have been introduced in the seminal paper [Spi70]. They allow for a detailed mathematical analysis leading to a deeper understanding of the fundamental principles of emergence and collective phenomena. The notes provide an introduction into the well developed mathematical theory for the description of the dynamics of IPS, involving graphical representations and an analytic description using semigroups and generators. Since the external conditions for real systems are often constant or slowly varying with respect to the system dynamics, observations are typically available in a time stationary situation. This is described by the invariant measures of the stochastic particle systems which are thus of major interest in their analysis, and are introduced at the end of Section 1 which covers the basic theory. Later sections provide a more detailed discussion of several examples of basic IPS, probabilistic techniques used for their analysis such as coupling, duality and relative entropy methods are introduced along. The second main aspect of the notes, also covered in Sections 2 to 4, is to get acquainted with different types of collective phenomena in complex systems. We will discuss their intimate relationship with symmetries and conservation laws of the dynamics, and make connections to the classical theory of phase transitions in statistical mechanics.



**Figure 1:** Left: Traffic data gathered from inductance loops showing car speeds on the M25 London orbital motorway averaged over 1 minute intervals (taken from [R.E.Wilson: Mechanisms for spatio-temporal pattern formation in highway traffic models. *Philos Transact A Math Phys Eng Sci.* 366(1872), 2017-2032 (2008)]). Right: segregation pattern of a neutral genetic marker in *E. coli* growth from a mixed population of circular shape (taken from [O. Hallatschek et. al.: Genetic drift at expanding frontiers promotes gene segregation. *PNAS* 104(50), 19926-19930 (2007)]).

Necessary prerequisites for the reader are basic knowledge in undergraduate mathematics, in particular probability theory and stochastic processes. For the latter, discrete time Markov chains are sufficient since the concept of continuous time processes will be introduced in Section 1. Acquaintance with measure theoretic concepts is helpful but not necessary.

Before we get immersed into mathematics let us quickly discuss two real world examples of recent studies, to illustrate the motivation and the origin of the processes which we will work with. The left of Figure 1 shows colour-coded data for the car speed on the M25 London orbital motorway as a function of space and time. The striped patterns of low speed correspond to stop-and-go waves in during rush hour. Often there is no obvious external cause such as an accident or road closure, so this pattern has to be interpreted as an intrinsic collective phenomenon emerging from the interactions of cars on a busy road. A minimal mathematical description of this situation in terms of IPS would be to take a one-dimensional lattice  $\Lambda = \mathbb{Z}$  (or a subset thereof), and at each site  $x \in \Lambda$  denote the presence or absence of a car with an occupation number  $\eta_x = 1$  or 0, respectively. So the state space of our mathematical model is given by the set  $\{0, 1\}^\Lambda$  denoting all possible configurations  $\eta = (\eta_x)_{x \in \Lambda}$ . In terms of dynamics, we only want to model normal traffic on a single lane road without car crashes or overtaking. So cars are allowed to proceed one lattice site to the right, say, with a given rate<sup>1</sup>, provided that the site in front is not occupied by another car. The rate may depend on the surrounding configuration of cars (e.g. number of empty sites ahead), and relatively simple choices depending only on three or four neighbouring sites can already lead to interesting patterns and the emergence of stop-and-go waves. There are numerous such approaches in the literature known as cellular automata models for traffic flow, see e.g. [D. Helbing: Traffic and related self-driven many-particle systems. *Rev. Mod. Phys* **73**, 10671141 (2001)] and references therein. The defining features of this process in terms of IPS are that no particles are created or destroyed (conservation of the number of particles) and that there is at

<sup>1</sup>The concept of 'rate' and exact mathematical formulations of the dynamics will be introduced in Section 1.

most one particle per site (exclusion rule). Processes with both or only the first property will be discussed in detail in Sections 2 and 3, respectively.

The right of Figure 1 shows segregation patterns of a microbial species (*E. coli*) when grown in rich growth medium from a mixed initial population of circular shape. Each individual appears either red or green as a result of a neutral genetic marker that only affects the colour. A possible IPS model of this system has a state space  $\{0, R, G\}^\Lambda$ , where the lattice is now two dimensional, say  $\Lambda = \mathbb{Z}^2$  for simplicity, and 0 represents an empty site,  $R$  the presence of a red and  $G$  of a green individual. The dynamics can be modeled by letting each individual split into two ( $R \rightarrow 2R$  or  $G \rightarrow 2G$ ) with a given rate, and then place the offspring on an empty neighbouring site. If there is no empty neighbouring site the reproduction rate is zero (or equivalently the offspring is immediately killed). Therefore we have two equivalent species competing for the same resource (empty sites), and spatial segregation is a result of the fact that once the red particles died out in a certain region due to fluctuations, all the offspring is descending from green ancestors. Note that in contrast to the first example, the number of particles in this model is not conserved. The simplest such process to model extinction or survival of a single species is called contact process, and is discussed in detail in Section 4.

# 1 Basic theory

In general, let  $X$  be a compact metric space with measurable structure given by the Borel  $\sigma$ -algebra. A *continuous time stochastic process*  $\boldsymbol{\eta} = (\eta_t : t \geq 0)$  is a family of random variables  $\eta_t$  taking values in  $X$ , which is called the *state space* of the process. Let

$$D[0, \infty) = \{\eta. : [0, \infty) \rightarrow X \text{ càdlàg}\} \quad (1.1)$$

be the set of right continuous functions with left limits (càdlàg), which is the *canonical path space* for a stochastic process on  $X$ . To define a reasonable measurable structure on  $D[0, \infty)$ , let  $\mathcal{F}$  be the smallest  $\sigma$ -algebra on  $D[0, \infty)$  such that all the mappings  $\eta. \mapsto \eta_s$  for  $s \geq 0$  are measurable w.r.t.  $\mathcal{F}$ . That means that every path can be evaluated or observed at arbitrary times  $s$ , i.e.

$$\{\eta_s \in A\} = \{\eta. | \eta_s \in A\} \in \mathcal{F} \quad (1.2)$$

for all measurable subsets  $A \in X$ . If  $\mathcal{F}_t$  is the smallest  $\sigma$ -algebra on  $D[0, \infty)$  relative to which all the mappings  $\eta. \mapsto \eta_s$  for  $s \leq t$  are measurable, then  $(\mathcal{F}_t : t \geq 0)$  provides a filtration for the process. The filtered space  $(D[0, \infty), \mathcal{F}, (\mathcal{F}_t : t \geq 0))$  provides a generic choice for the probability space of a stochastic process which can be defined as a probability measure  $\mathbb{P}$  on  $D[0, \infty)$ .

**Definition 1.1** A (*homogeneous*) *Markov process* on  $X$  is a collection  $(\mathbb{P}^\zeta : \zeta \in X)$  of probability measures on  $D[0, \infty)$  with the following properties:

- (a)  $\mathbb{P}^\zeta(\eta. \in D[0, \infty) : \eta_0 = \zeta) = 1$  for all  $\zeta \in X$ , i.e.  $\mathbb{P}^\zeta$  is normalized on all paths with initial condition  $\eta_0 = \zeta$ .
- (b) The mapping  $\zeta \mapsto \mathbb{P}^\zeta(A)$  is measurable for every  $A \in \mathcal{F}$ .
- (c)  $\mathbb{P}^\zeta(\eta_{t+}. \in A | \mathcal{F}_t) = \mathbb{P}^{\eta_t}(A)$  for all  $\zeta \in X$ ,  $A \in \mathcal{F}$  and  $t > 0$ . (Markov property)

Note that the Markov property as formulated in (c) implies that the process is (time-)homogeneous, since the law  $\mathbb{P}^{\eta_t}$  does not have an explicit time dependence. Markov processes can be generalized to be inhomogeneous, but the whole content of these lectures will concentrate only on homogeneous processes.

## 1.1 Continuous time Markov chains and graphical representations

Let  $X$  now be a countable set. Then a Markov process  $\boldsymbol{\eta} = (\eta_t : t \geq 0)$  is called a *Markov chain* and it can be characterized by *transition rates*  $c(\zeta, \zeta') \geq 0$ , which have to be specified for all  $\zeta, \zeta' \in X$ . For a given process  $(\mathbb{P}^\zeta : \zeta \in X)$  the rates are defined via

$$\mathbb{P}^\zeta(\eta_t = \zeta') = c(\zeta, \zeta')t + o(t) \quad \text{as } t \searrow 0, \quad (1.3)$$

and represent probabilities per unit time. We will see in the next subsection how a given set of rates determines the path measures of a process. Now we would like to get an intuitive understanding of the time evolution and the role of the transition rates. We denote by

$$W_\zeta := \inf\{t \geq 0 : \eta_t \neq \zeta\} \quad (1.4)$$

the *holding time* in state  $\zeta$ . The value of this time is related to the total exit rate out of state  $\zeta$ ,

$$c_\zeta := \sum_{\zeta' \in X} c(\zeta, \zeta'). \quad (1.5)$$

If  $c_\zeta = 0$ ,  $\zeta$  is an *absorbing state* and  $W_\zeta = \infty$  a.s. .

**Proposition 1.1** *If  $c_\zeta > 0$ ,  $W_\zeta \sim \text{Exp}(c_\zeta)$  and  $\mathbb{P}^\zeta(\eta_{W_\zeta} = \zeta') = c(\zeta, \zeta')/c_\zeta$ .*

**Proof.**  $W_\zeta$  has the '*loss of memory*' property

$$\mathbb{P}^\zeta(W_\zeta > s + t | W_\zeta > s) = \mathbb{P}^\zeta(W_\zeta > s + t | \eta_s = \zeta) = \mathbb{P}^\zeta(W_\zeta > t), \quad (1.6)$$

the distribution of the holding time  $W_\zeta$  does not depend on how much time the process has already spent in state  $\zeta$ . Thus  $\mathbb{P}^\zeta(W_\zeta > s + t) = \mathbb{P}^\zeta(W_\zeta > s) \mathbb{P}^\zeta(W_\zeta > t)$ . This is the functional equation for an exponential and implies that

$$\mathbb{P}^\zeta(W_\zeta > t) = e^{\lambda t} \quad (\text{with initial condition } \mathbb{P}^\zeta(W_\zeta > 0) = 1). \quad (1.7)$$

The exponent is given by

$$\lambda = \frac{d}{dt} \mathbb{P}^\zeta(W_\zeta > t) \Big|_{t=0} = \lim_{t \searrow 0} \frac{\mathbb{P}^\zeta(W_\zeta > t) - 1}{t} = -c_\zeta, \quad (1.8)$$

since with (1.3)

$$\mathbb{P}^\zeta(W_\zeta > 0) = 1 - \mathbb{P}^\zeta(\eta_t \neq \zeta) + o(t) = 1 - c_\zeta t + o(t). \quad (1.9)$$

Now, conditioned on a jump occurring we have

$$\mathbb{P}^\zeta(\eta_t = \zeta' | W_\zeta < t) = \frac{\mathbb{P}^\zeta(\eta_t = \zeta')}{\mathbb{P}^\zeta(W_\zeta < t)} \rightarrow \frac{c(\zeta, \zeta')}{c_\zeta} \quad \text{as } t \searrow 0 \quad (1.10)$$

by L'Hopital's rule. With right-continuity of paths, this implies the second statement.  $\square$

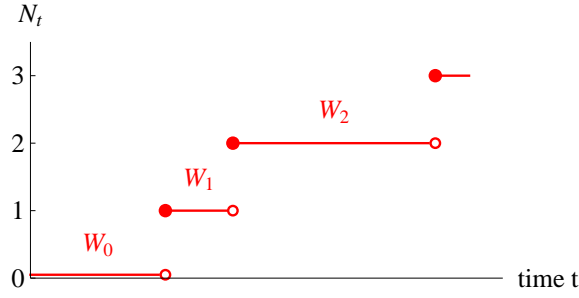
Let  $W_1, W_2, \dots$  be a sequence of independent exponentials  $W_i \sim \text{Exp}(\lambda_i)$ . Remember that  $\mathbb{E}(W_i) = 1/\lambda_i$  and

$$\min\{W_1, \dots, W_n\} \sim \text{Exp}\left(\sum_{i=1}^n \lambda_i\right). \quad (1.11)$$

The sum of iid exponentials with  $\lambda_i = \lambda$  is  $\Gamma$ -distributed,

$$\sum_{i=1}^n W_i \sim \Gamma(n, \lambda) \quad \text{with PDF} \quad \frac{\lambda^n w^{n-1}}{(n-1)!} e^{-\lambda w}. \quad (1.12)$$

**Example.** A *Poisson process*  $\mathbf{N} = (N_t : t \geq 0)$  with rate  $\lambda$  (short  $PP(\lambda)$ ) is a Markov process with  $X = \mathbb{N} = \{0, 1, \dots\}$  and  $c(n, m) = \lambda \delta_{n+1, m}$ .



**Figure 2:** Sample path (càdlàg) of a Poisson process with holding times  $W_0, W_1, \dots$

With iidrv's  $W_i \sim Exp(\lambda)$  we can write  $N_t = \max\{n : \sum_{i=1}^n W_i \leq t\}$ . This implies

$$\begin{aligned} \mathbb{P}(N_t = n) &= \mathbb{P}\left(\sum_{i=1}^n W_i \leq t < \sum_{i=1}^{n+1} W_i\right) = \int_0^t \mathbb{P}\left(\sum_{i=1}^n W_i = s\right) \mathbb{P}(W_{n+1} > t - s) ds = \\ &= \int_0^t \frac{\lambda^n s^{n-1}}{(n-1)!} e^{-\lambda s} e^{-\lambda(t-s)} ds = \frac{(\lambda t)^n}{n!} e^{-\lambda t}, \end{aligned} \quad (1.13)$$

so  $N_t \sim Poi(\lambda t)$  has a Poisson distribution. Alternatively a Poisson process can be characterized by the following.

**Proposition 1.2**  $(N_t : t \geq 0) \sim PP(\lambda)$  if and only if it has stationary, independent increments, i.e.

$$N_{t+s} - N_s \sim N_t - N_0 \quad \text{and} \quad N_{t+s} - N_s \quad \text{independent of} \quad (N_u : u \leq s), \quad (1.14)$$

and for each  $t$ ,  $N_t \sim Poi(\lambda t)$ .

**Proof.** By the loss of memory property and (1.13) increments have the distribution

$$N_{t+s} - N_s \sim Poi(\lambda t) \quad \text{for all} \quad s \geq 0, \quad (1.15)$$

and are independent of  $N_s$  which is enough together with the Markov property.

The other direction follows by deriving the jump rates from the properties in (1.14) using (1.3).  $\square$

Remember that for independent Poisson variables  $Y_1, Y_2, \dots$  with  $Y_i \sim Poi(\lambda_i)$  we have  $\mathbb{E}(Y_i) = Var(Y_i) = \lambda_i$  and

$$\sum_{i=1}^n Y_i \sim Poi\left(\sum_{i=1}^n \lambda_i\right). \quad (1.16)$$

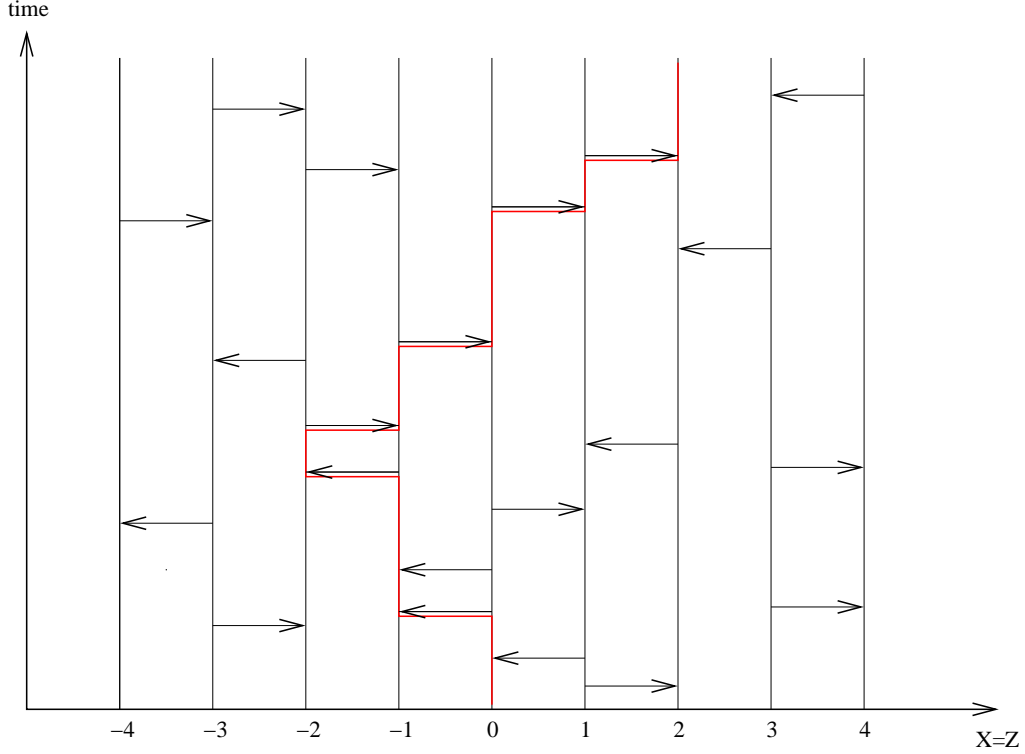
With Prop. 1.2 this immediately implies that adding independent Poisson processes  $(N_t^i : t \geq 0) \sim PP(\lambda_i)$ ,  $i = 1, 2, \dots$  results in a Poisson process, i.e.

$$M_t = \sum_{i=1}^n N_t^i \quad \Rightarrow \quad (M_t : t \geq 0) \sim PP\left(\sum_{i=1}^n \lambda_i\right). \quad (1.17)$$

**Example.** A continuous-time simple random walk  $(\eta_t : t \geq 0)$  on  $X = \mathbb{Z}$  with jump rates  $p$  to the right and  $q$  to the left is given by

$$\eta_t = R_t - L_t \quad \text{where} \quad (R_t : t \geq 0) \sim PP(p), \quad (L_t : t \geq 0) \sim PP(q). \quad (1.18)$$

The process can be constructed by the following graphical representation:



In each column the arrows  $\rightarrow \sim PP(p)$  and  $\leftarrow \sim PP(q)$  are independent Poisson processes. Together with the initial condition, the trajectory of the process shown in red is then uniquely determined. An analogous construction is possible for a general Markov chain, which is a continuous time random walk on  $X$  with jump rates  $c(\zeta, \zeta')$ . In this way we can also construct interacting random walks.

## 1.2 Two basic IPS

Let  $\Lambda$  be any countable set, the *lattice* for example think of regular lattices  $\Lambda = \mathbb{Z}^d$ , connected subsets of these or  $\Lambda = \Lambda_L := (\mathbb{Z}/L\mathbb{Z})^d$  a finite  $d$ -dimensional torus with  $L^d$  sites. We will consider two basic processes on the state space<sup>1</sup>  $X = \{0, 1\}^\Lambda$  of *particle configurations*  $\eta = (\eta(x) : x \in \Lambda)$ .  $\eta(x) = 1$  means that there is a particle at site  $x$  and if  $\eta(x) = 0$  site  $x$  is empty. Alternatively,  $\eta : \Lambda \rightarrow \{0, 1\}$  can be viewed as a function from  $\Lambda$  to  $\{0, 1\}$ .

<sup>1</sup>Why is  $X$  is a compact metric space?

The discrete topology  $\sigma_x$  on the local state space  $S = \{0, 1\}$  is simply given by the power set, i.e. all subsets are 'open'. The *product topology*  $\sigma$  on  $X$  is then given by the smallest topology such that all the canonical projections  $\eta(x) : X \rightarrow \{0, 1\}$  (particle number at a site  $x$  for a given configuration  $\eta$ ) are continuous (pre-images of open sets are open). That means that  $\sigma$  is generated by sets

$$\eta(x)^{-1}(U) = \{\eta : \eta(x) \in U\}, \quad U \subseteq \{0, 1\}, \quad (1.19)$$

which are called *open cylinders*. Finite intersections of these sets

$$\{\eta : \eta(x_1) \in U_1, \dots, \eta(x_n) \in U_n\}, \quad n \in \mathbb{N}, U_i \subseteq \{0, 1\} \quad (1.20)$$

are called *cylinder sets* and any open set on  $X$  is a (finite or infinite) union of cylinder sets. Clearly  $\{0, 1\}$  is compact  $\sigma_x$  is finite, and by *Tychonoff's theorem* any product of compact topological spaces is compact (w.r.t. the product topology). This holds for any general finite local state space  $S$  and  $X = S^\Lambda$ .



Note that if  $\Lambda$  is infinite,  $X$  is uncountable. But for the processes we consider the particles move/interact only locally, so a description with jump rates still makes sense. More specifically, for a given  $\eta \in X$  there are only countably many  $\eta'$  for which  $c(\eta, \eta') > 0$ . Define the configurations  $\eta^x$  and  $\eta^{xy} \in X$  for  $x \neq y \in \Lambda$  by

$$\eta^x(z) = \begin{cases} \eta(z) & , z \neq x \\ 1 - \eta(x) & , z = x \end{cases} \quad \text{and} \quad \eta^{xy}(z) = \begin{cases} \eta(z) & , z \neq x, y \\ \eta(y) & , z = x \\ \eta(x) & , z = y \end{cases}, \quad (1.21)$$

so that  $\eta^x$  corresponds to creation/annihilation of a particle at site  $x$  and  $\eta^{xy}$  to motion of a particle between  $x$  and  $y$ . Then following standard notation we write for the corresponding jump rates

$$c(x, \eta) = c(\eta, \eta^x) \quad \text{and} \quad c(x, y, \eta) = c(\eta, \eta^{xy}). \quad (1.22)$$

**Definition 1.2** Let  $p(x, y) \geq 0$ ,  $x, y \in \Lambda$ , which can be regarded as rates of a cont.-time random walk on  $\Lambda$ . The *exclusion process (EP)* on  $X$  is characterized by the jump rates

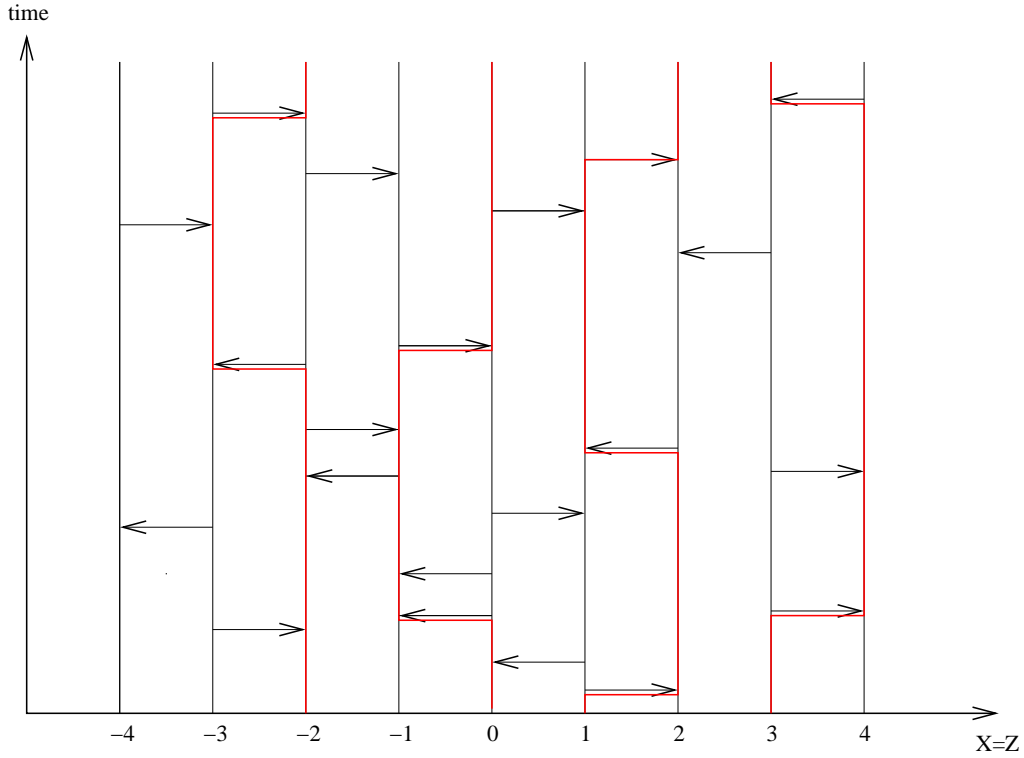
$$c(x, y, \eta) = p(x, y)\eta(x)(1 - \eta(y)), \quad x, y \in \Lambda \quad (1.23)$$

where particles only jump to empty sites (exclusion interaction). If  $\Lambda$  is a regular lattice and  $p(x, y) > 0$  only if  $x \sim y$  are nearest neighbours, the process is called *simple EP (SEP)*. If in addition  $p(x, y) = p(y, x)$  for all  $x, y \in \Lambda$  it is called *symmetric SEP (SSEP)* and otherwise *asymmetric SEP (ASEP)*.

Note that particles only move and are not created or annihilated, therefore the number of particles in the system is conserved in time. In general such IPS are called *lattice gases*. The ASEP in one dimension  $d = 1$  is one of the most basic and most studied models in IPS, a common quick way of defining it is

$$10 \xrightarrow{p} 01, \quad 01 \xrightarrow{q} 10 \quad (1.24)$$

where particles jump to the right (left) with rate  $p(q)$ .



The graphical construction is analogous to the single particle process given above, with the additional constraint of the exclusion interaction.

**Definition 1.3** The *contact process (CP)* on  $X$  is characterized by the jump rates

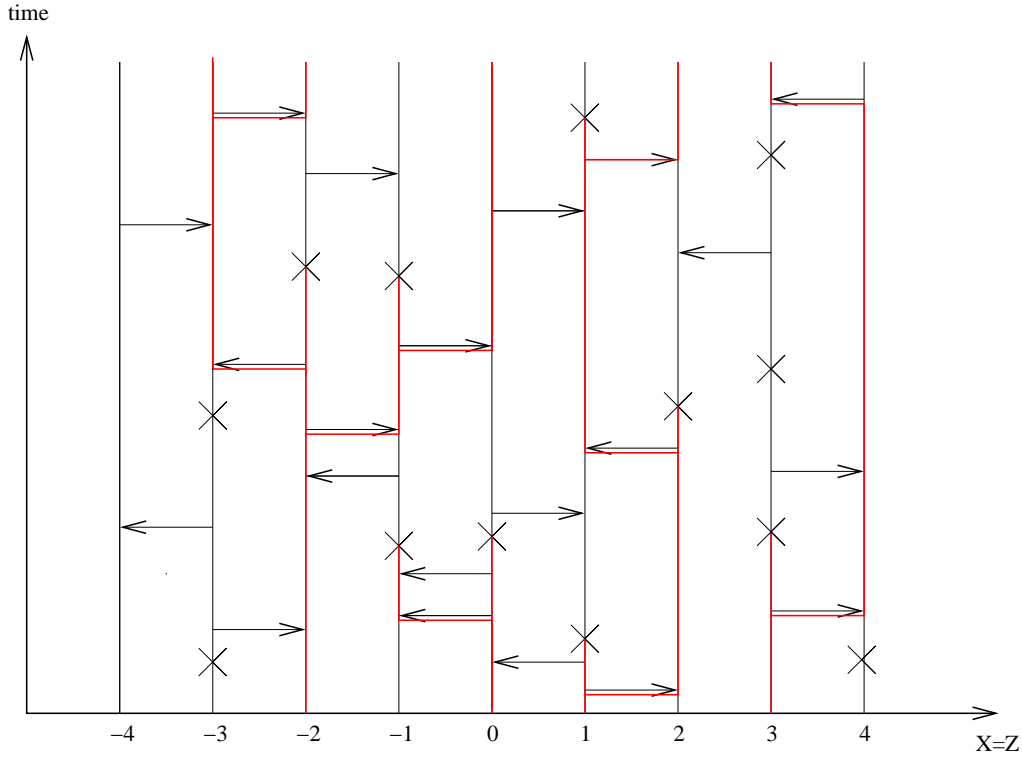
$$c(x, \eta) = \begin{cases} 1 & , \eta(x) = 1 \\ \lambda \sum_{y \sim x} \eta(y) & , \eta(x) = 0 \end{cases} , \quad x \in \Lambda . \quad (1.25)$$

Particles are interpreted as infected sites which recover with rate 1 and are infected independently with rate  $\lambda > 0$  by neighbouring particles  $y \sim x$ , to be understood w.r.t. some graph structure on  $\Lambda$  (e.g. a regular lattice).

In contrast to the SEP the CP does not have a conserved quantity like the number of particles, but it does have an absorbing state  $\eta = 0$ , since there is no spontaneous infection. A compact notation for the CP on any lattice  $\Lambda$  is

$$1 \xrightarrow{1} 0 , \quad 0 \rightarrow 1 \text{ with rate } \lambda \sum_{y \sim x} \eta(y) . \quad (1.26)$$

The graphical construction below contains now a third independent Poisson process  $\times \sim PP(1)$  on each line marking the recovery events. The infection events are marked by the independent  $PP(\lambda)$  Poisson processes  $\rightarrow$  and  $\leftarrow$ .



### 1.3 Semigroups and generators

Let  $X$  be a compact metric space and denote by

$$C(X) = \{f : X \rightarrow \mathbb{R} \text{ continuous}\} \quad (1.27)$$

the set of real-valued continuous functions, which is a Banach space with sup-norm  $\|f\|_\infty = \sup_{\eta \in X} |f(\eta)|$ . Functions  $f$  can be regarded as observables, and we are interested in their time evolution.

**Definition 1.4** For a given process  $\eta = (\eta_t : t \geq 0)$  on  $X$ , for each  $t \geq 0$  we define the operator

$$S(t) : C(X) \rightarrow C(X) \quad \text{by} \quad S(t)f(\eta) := \mathbb{E}^\eta f(\eta_t). \quad (1.28)$$

In general  $f \in C(X)$  does not imply  $S(t)f \in C(X)$ , but all the processes we consider have this property and are called *Feller processes*.

**Proposition 1.3** Let  $\eta$  be a Feller process on  $X$ . Then the family  $(S(t) : t \geq 0)$  is a **Markov semigroup**, i.e.

- (a)  $S(0) = Id$ , (identity at  $t = 0$ )
- (b)  $t \mapsto S(t)f$  is right-continuous for all  $f \in C(X)$ , (right-continuity)
- (c)  $S(t+s)f = S(t)S(s)f$  for all  $f \in C(X)$ ,  $s, t \geq 0$ , (Markov property)
- (d)  $S(t)1 = 1$  for all  $t \geq 0$ , (conservation of probability)
- (e)  $S(t)f \geq 0$  for all non-negative  $f \in C(X)$ . (positivity)

**Proof.** (a)  $S(0)f(\eta) = E^\eta(f(\eta_0)) = f(\eta)$  since  $\eta_0 = \eta$  which is equivalent to (a) of Def. 1.1.  
(b) follows from right-continuity of  $\eta_t$  and continuity of  $f$ .  
(c) follows from the Markov property of  $\eta_t$  (Def. 1.1(c))

$$\begin{aligned} S(t+s)f(\eta) &= \mathbb{E}^\eta f(\eta_{t+s}) = \mathbb{E}^\eta \left( \mathbb{E}(f(\eta_{t+s}) | \mathcal{F}_t) \right) = \mathbb{E}^\eta \left( \mathbb{E}^{\eta_t}(f(\eta_{t+s})) \right) = \\ &= \mathbb{E}^\eta ((S(s)f)(\eta_t)) = S(t)S(s)f . \end{aligned} \quad (1.29)$$

(d)  $S(t)1 = \mathbb{E}^\eta(\mathbb{1}_{\eta_t}(X)) = 1$  since  $\eta_t \in X$  for all  $t \geq 0$  (conservation of probability).  
(e) is immediate by definition.  $\square$

**Theorem 1.4** Suppose  $(S(t) : t \geq 0)$  is a Markov semigroup on  $C(X)$ . Then there exists a unique (Feller) Markov process  $(\eta_t : t \geq 0)$  on  $X$  such that

$$\mathbb{E}^\zeta f(\eta_t) = S(t)f(\zeta) \quad \text{for all } f \in C(X), \zeta \in X \text{ and } t \geq 0 . \quad (1.30)$$

**Proof.** for a reference see [L85] Theorem I.1.5

**Interpretation.** The operator  $S(t)$  determines the expected value of observables  $f$  on  $X$  at time  $t$  for a given Markov process  $\eta$ . Specification of all these expected values provides a full representation of  $\eta$  which is dual to the path measures  $(\mathbb{P}^\zeta : \zeta \in X)$ , since  $C(X)$  is dual to the set  $\mathcal{P}(X)$  of all probability measures on  $X$ .

For an initial distribution  $\mu \in \mathcal{P}(X)$  we write

$$\mathbb{P}^\mu := \int_X \mathbb{P}^\zeta \mu(d\zeta) \in \mathcal{P}(D[0, \infty)) \quad (1.31)$$

for the path measure  $\mathbb{P}^\mu$  with  $\mathbb{P}^\mu(\eta_0 \in \cdot) = \mu$ . Thus

$$\mathbb{E}^\mu f(\eta_t) = \int_X S(t)f d\mu \quad \text{for all } f \in C(X) . \quad (1.32)$$

**Definition 1.5** For a process  $(S(t) : t \geq 0)$  with initial distribution  $\mu$  we denote by  $\mu S(t) \in \mathcal{P}(X)$  the *distribution at time  $t$* , which is uniquely determined by

$$\int_X f d[\mu S(t)] := \int_X S(t)f d\mu \quad \text{for all } f \in C(X) . \quad (1.33)$$

**Remark.** The fact that probability measures on  $X$  can be characterised by all expected values of functions in  $C(X)$  is a direct consequence of the Riesz representation theorem.

Since  $(S(t) : t \geq 0)$  has the semigroup structure given in Prop. 1.3(c), in analogy with the proof of Prop. 1.1 we expect that it has the form of an exponential generated by the linearization  $S'(0)$ , i.e.

$$S(t) = \text{"exp}(tS'(0))\text{"} = Id + S'(0)t + o(t) \quad \text{with } S(0) = Id , \quad (1.34)$$

which is made precise in the following.

**Definition 1.6** The generator  $\mathcal{L} : D_{\mathcal{L}} \rightarrow C(X)$  for the process  $(S(t) : t \geq 0)$  is given by

$$\mathcal{L}f := \lim_{t \searrow 0} \frac{S(t)f - f}{t} \quad \text{for } f \in D_{\mathcal{L}}, \quad (1.35)$$

where the domain  $D_{\mathcal{L}} \subseteq C(X)$  is the set of functions for which the limit exists.

In general  $D_{\mathcal{L}} \subsetneq C(X)$  is a proper subset for processes on infinite lattices, and we will see later that this is in fact the case even for the simplest examples SEP and CP.

**Proposition 1.5**  $\mathcal{L}$  as defined above is a **Markov generator**, i.e.

- (a)  $1 \in D_{\mathcal{L}}$  and  $\mathcal{L}1 = 0$ , (conservation of probability)
- (b) for  $f \in D_{\mathcal{L}}$ ,  $\lambda \geq 0$ :  $\min_{\zeta \in X} f(\zeta) \geq \min_{\zeta \in X} (f - \lambda \mathcal{L}f)(\zeta)$ , (positivity)
- (c)  $D_{\mathcal{L}}$  is dense in  $C(X)$  and the range  $\mathcal{R}(Id - \lambda \mathcal{L}) = C(X)$  for sufficiently small  $\lambda > 0$ .

**Proof.** (a) is immediate from the definition (1.35) and  $S(t)1 = 1$ , the rest is rather technical and can be found in [L85] Section I.2.

**Theorem 1.6 (Hille-Yosida)** There is a one-to-one correspondence between Markov generators and semigroups on  $C(X)$ , given by (1.35) and

$$S(t)f = e^{t\mathcal{L}}f := \lim_{n \rightarrow \infty} \left( Id - \frac{t}{n}\mathcal{L} \right)^{-n} f \quad \text{for } f \in C(X), t \geq 0. \quad (1.36)$$

Furthermore, for  $f \in D_{\mathcal{L}}$  also  $S(t)f \in D_{\mathcal{L}}$  for all  $t \geq 0$  and

$$\frac{d}{dt} S(t)f = S(t)\mathcal{L}f = \mathcal{L}S(t)f, \quad (1.37)$$

called the **forward** and **backward equation**, respectively.

**Proof.** For a reference see [L85], Theorem I.2.9.

**Remarks.** Properties (a) and (b) in Prop. 1.5 are related to conservation of probability  $S(t)1 = 1$  and positivity of the semigroup (see Prop. 1.3). By taking closures a linear operator is uniquely determined by its values on a dense set. So property (c) in Prop. 1.5 ensures that the semigroup  $S(t)$  is defined for all  $f \in C(X)$ , and that  $Id - \frac{t}{n}\mathcal{L}$  is actually invertible for  $n$  large enough, as is required in (1.36).

$S(t) = e^{t\mathcal{L}}$  is nothing more than a notation analogous to scalar exponentials, given that  $S(t)f$  is the unique solution to the backward equation

$$\frac{d}{dt} u(t) = \mathcal{L}u(t), \quad u(0) = f. \quad (1.38)$$

In general, for Markov chains with countable  $X$  and jump rates  $c(\eta, \eta')$  the generator is given by

$$\mathcal{L}f(\eta) = \sum_{\eta' \in X} c(\eta, \eta')(f(\eta') - f(\eta)). \quad (1.39)$$

Using (1.3) this follows for small  $t \searrow 0$  from

$$\begin{aligned} S(t)f(\eta) &= \mathbb{E}^\eta(f(\eta_t)) = \sum_{\eta' \in X} \mathbb{P}^\eta(\eta_t = \eta') f(\eta') = \\ &= \sum_{\eta' \neq \eta} c(\eta, \eta') f(\eta') t + f(\eta) \left(1 - \sum_{\eta' \neq \eta} c(\eta, \eta') t\right) + o(t) \end{aligned} \quad (1.40)$$

and the definition (1.35) of  $\mathcal{L}$ .

**Example.** For the simple random walk with state space  $X = \mathbb{Z}$  we have

$$c(\eta, \eta + 1) = p \quad \text{and} \quad c(\eta, \eta - 1) = q, \quad (1.41)$$

while all other transition rates vanish. The generator is given by

$$\mathcal{L}f(\eta) = p(f(\eta + 1) - f(\eta)) + q(f(\eta - 1) - f(\eta)), \quad (1.42)$$

and in the symmetric case  $p = q$  it is proportional to the discrete Laplacian.

For the indicator function  $f = \mathbb{1}_\eta : X \rightarrow \{0, 1\}$  we have

$$\int_X S(t)f d\mu = [\mu S(t)](\eta) =: p_t(\eta) \quad (1.43)$$

for the distribution at time  $t$  with  $p_0(\eta) = \mu(\eta)$ . Using this and (1.39) we get for the right-hand side of (1.38) for all  $\eta \in X$

$$\begin{aligned} \int_X \mathcal{L}S(t)\mathbb{1}_\eta d\mu &= \sum_{\zeta \in X} \mu(\zeta) \sum_{\zeta' \in X} c(\zeta, \zeta') (S(t)\mathbb{1}_\eta(\zeta') - S(t)\mathbb{1}_\eta(\zeta)) = \\ &= \sum_{\zeta \in X} [\mu S(t)](\zeta) \left( c(\zeta, \eta) - \mathbb{1}_\eta(\zeta) \sum_{\zeta' \in X} c(\zeta, \zeta') \right) = \\ &= \sum_{\zeta \in X} p_t(\zeta) c(\zeta, \eta) - p_t(\eta) \sum_{\zeta' \in X} c(\eta, \zeta'). \end{aligned} \quad (1.44)$$

In summary we get

$$\frac{d}{dt} p_t(\eta) = \sum_{\eta' \in X} \left( p_t(\eta') c(\eta', \eta) - p_t(\eta) c(\eta, \eta') \right), \quad p_0(\eta) = \mu(\eta). \quad (1.45)$$

This is called the *master equation*, with intuitive gain and loss terms into state  $\eta$  on the right-hand side. It makes sense only for countable  $X$ , and in that case it is actually equivalent to (1.38), since the indicator functions form a basis of  $C(X)$ .

For IPS (with possibly uncountable  $X$ ) we can formally write down similar expressions. For a general lattice gas (e.g. SEP) we have

$$\mathcal{L}f(\eta) = \sum_{x, y \in \Lambda} c(x, y, \eta) (f(\eta^{xy}) - f(\eta)) \quad (1.46)$$

and for pure reaction systems like the CP

$$\mathcal{L}f(\eta) = \sum_{x \in \Lambda} c(x, \eta) (f(\eta^x) - f(\eta)). \quad (1.47)$$

For infinite lattices  $\Lambda$  convergence of the sums is an issue and we have to find a proper domain  $D_{\mathcal{L}}$  of functions  $f$  for which they are finite.

**Definition 1.7** For  $X = \{0, 1\}^\Lambda$ ,  $f \in C(X)$  is a *cylinder function* if there exists a finite subset  $\Delta \subseteq \Lambda$  such that  $f(\eta^x) = f(\eta)$  for all  $x \notin \Delta$ ,  $\eta \in X$ , i.e.  $f$  depends only on a finite set of coordinates of a configuration. We write  $C_0(X) \subseteq C(X)$  for the set of all cylinder functions.

**Examples.** The indicator function  $\mathbb{1}_\eta$  is in general not a cylinder function (only on finite lattices), whereas the local particle number  $\eta(x)$  or the product  $\eta(x)\eta(x+y)$  are. These functions are important observables, and their expectations correspond to *particle densities*

$$\rho(t, x) = \mathbb{E}^\mu(\eta_t(x)) \quad (1.48)$$

and *two-point correlation functions*

$$\rho(t, x, x+y) = \mathbb{E}^\mu(\eta_t(x)\eta_t(x+y)) . \quad (1.49)$$

For  $f \in C_0(X)$  the sum (1.47) contains only finitely many non-zero terms, but (1.46) might still diverge, corresponding to infinitely many particle exchanges attempted in a finite set of sites. This is not the case for the SEP since particles only jump to neighbouring sites, but for more general processes we have to restrict the jump rates to be sufficiently local.

**Proposition 1.7** *Suppose that*

$$\sup_{y \in \Lambda} \sum_{x \in \Lambda} \sup_{\eta \in X} c(x, y, \eta) < \infty . \quad (1.50)$$

*Then the closure of the operator  $\mathcal{L}$  defined in (1.46), as well as (1.47), is uniquely defined by its values on  $C_0(X)$  and is a Markov generator.*

**Proof.** see [L85], Theorem I.3.9

Generators are linear operators and modulo technicalities regarding domains (which can be substantial in more general situations than ours) Prop. 1.5 then implies that the sum of two or more generators is again a Markov generator. In that way we can define more general processes, e.g. the sum of (1.46) and (1.47) would define a contact process with nearest-neighbour particle motion.

## 1.4 Stationary measures and reversibility

**Definition 1.8** A measure  $\mu \in \mathcal{P}(X)$  is *stationary* or *invariant* if  $\mu S(t) = \mu$  or, equivalently,

$$\int_X S(t)f d\mu = \int_X f d\mu \quad \text{or shorter} \quad \mu(S(t)f) = \mu(f) \quad \text{for all } f \in C(X) . \quad (1.51)$$

To simplify notation here and in the following we will often use the standard notation  $\mu(f) = \int_X f d\mu$  for integration. The set of all invariant measures of a process is denoted by  $\mathcal{I}$ . A measure  $\mu$  is called *reversible* if

$$\mu(fS(t)g) = \mu(gS(t)f) \quad \text{for all } f, g \in C(X) . \quad (1.52)$$

Taking  $g = 1$  in (1.52) we see that every reversible measure is also stationary. Stationarity of  $\mu$  implies that

$$\mathbb{P}^\mu(\eta_t \in A) = \mathbb{P}^\mu(\eta_{t+} \in A) \quad \text{for all } t \geq 0, A \in \mathcal{F}, \quad (1.53)$$

using the Markov property (Def. 1.1(c)) with notation (1.31) and (1.51). Using  $\eta_t \sim \mu$  as initial distribution, the definition of a stationary process can be extended to negative times on the path space  $D(-\infty, \infty)$ . If  $\mu$  is also reversible, this implies

$$\mathbb{P}^\mu(\eta_{t+} \in A) = \mathbb{P}^\mu(\eta_{t-} \in A) \quad \text{for all } t \geq 0, A \in \mathcal{F}, \quad (1.54)$$

i.e. the process is time-reversible. More details on this are given at the end of this section.

**Proposition 1.8** *Consider a Feller process on a compact state space  $X$  with generator  $\mathcal{L}$ . Then*

$$\mu \in \mathcal{I} \quad \Leftrightarrow \quad \mu(\mathcal{L}f) = 0 \quad \text{for all } f \in C_0(X), \quad (1.55)$$

and similarly

$$\mu \text{ is reversible} \quad \Leftrightarrow \quad \mu(f\mathcal{L}g) = \mu(g\mathcal{L}f) \quad \text{for all } f, g \in C_0(X). \quad (1.56)$$

**Proof.** Follows from the definitions of semigroup/generator and  $\mu(f_n) \rightarrow \mu(f)$  if  $\|f_n - f\|_\infty \rightarrow 0$  by continuity of  $f_n, f$  and compactness of  $X$ .  $\square$

Analogous to the master equation (and using the same notation), we can get a meaningful relation for Markov chains by inserting indicator functions  $f = \mathbb{1}_\eta$  and  $g = \mathbb{1}_{\eta'}$  for  $\eta' \neq \eta$  in the stationarity condition (1.55). This yields with (1.39)

$$\mu(\mathcal{L}\mathbb{1}_\eta) = \sum_{\eta' \in X} (\mu(\eta') c(\eta', \eta) - \mu(\eta) c(\eta, \eta')) = 0 \quad \text{for all } \eta \in X, \quad (1.57)$$

so that  $\mu$  is a stationary solution of the master equation (1.45). A short computation yields

$$\mu(\mathbb{1}_\eta \mathcal{L} \mathbb{1}_{\eta'}) = \sum_{\zeta \in X} \mu(\zeta) \mathbb{1}_\eta(\zeta) \sum_{\xi \in X} c(\zeta, \xi) (\mathbb{1}_{\eta'}(\xi) - \mathbb{1}_{\eta'}(\zeta)) = \mu(\eta) c(\eta, \eta'). \quad (1.58)$$

Inserting this into the reversibility condition (1.56) on both sides we get

$$\mu(\eta') c(\eta', \eta) = \mu(\eta) c(\eta, \eta') \quad \text{for all } \eta, \eta' \in X, \eta \neq \eta', \quad (1.59)$$

which are called *detailed balance relations*. So if  $\mu$  is reversible, every individual term in the sum (1.57) vanishes. On the other hand, not every solution of (1.57) has to fulfill (1.59), i.e. there are stationary measures which are not reversible. The detailed balance equations are typically easy to solve for  $\mu$ , so if reversible measures exist they can be found as solutions of (1.59).

**Examples.** Consider the simple random walk on the torus  $X = \mathbb{Z}/L\mathbb{Z}$ , moving with rate  $p$  to the right and  $q$  to the left. The uniform measure  $\mu(\eta) = 1/L$  is an obvious solution to the stationary master equation (1.57). However, the detailed balance relations are only fulfilled in the symmetric case  $p = q$ . For the simple random walk on the infinite state space  $X = \mathbb{Z}$  the constant solution cannot be normalized, and in fact (1.57) does not have a normalized solution.

Another important example is a *birth-death chain* with state space  $X = \mathbb{N}$  and jump rates

$$c(\eta, \eta + 1) = \alpha, \quad c(\eta + 1, \eta) = \beta \quad \text{for all } \eta \geq 1. \quad (1.60)$$



In this case the detailed balance relations have the solution

$$\mu(\eta) = (\alpha/\beta)^\eta . \quad (1.61)$$

For  $\alpha < \beta$  this can be normalized, yielding a stationary, reversible measure for the process.

In particular not every Markov chain has a stationary distribution. If  $X$  is finite there exists at least one stationary distribution, as a direct result of linear algebra (Perron-Frobenius theorem). For IPS we have compact state spaces  $X$ , for which a similar result holds.

**Theorem 1.9** *For every Feller process with compact state space  $X$  we have:*

(a)  $\mathcal{I}$  is non-empty, compact and convex.

(b) Suppose the weak limit  $\mu = \lim_{t \rightarrow \infty} \pi S(t)$  exists for some initial distribution  $\pi \in \mathcal{P}(X)$ , i.e.

$$\pi S(t)(f) = \int_X S(t)f d\pi \rightarrow \mu(f) \quad \text{for all } f \in C(X) , \quad (1.62)$$

then  $\mu \in \mathcal{I}$ .

**Proof.** (a) Convexity of  $\mathcal{I}$  follows directly from the fact that a convex combination of two probability measures  $\mu_1, \mu_2 \in \mathcal{P}(X)$  is again a probability measure,

$$\lambda\mu_1 + (1 - \lambda)\mu_2 \in \mathcal{P}(X) \quad \text{for all } \lambda \in [0, 1] , \quad (1.63)$$

and that the stationarity condition (1.55) is linear in  $\mu$ .

$\mathcal{I}$  is a closed subset of  $\mathcal{P}(X)$ , i.e.

$$\mu_1, \mu_2, \dots \in \mathcal{I}, \mu_n \rightarrow \mu \text{ weakly, implies } \mu \in \mathcal{I} , \quad (1.64)$$

again since (1.55) is linear (and in particular continuous) in  $\mu$ . Under the topology of weak convergence  $\mathcal{P}(X)$  is compact since  $X$  is compact, and therefore also  $\mathcal{I} \subseteq \mathcal{P}(X)$  is compact.

Non-emptiness: By compactness of  $\mathcal{P}(X)$  there exists a convergent subsequence of  $\mu S(t)$  for every  $\mu \in \mathcal{P}(X)$ . With (b) the limit is in  $\mathcal{I}$ .

(b)  $\mu = \lim_{t \rightarrow \infty} \pi S(t) \in \mathcal{I}$  since for all  $f \in C(X)$ ,

$$\begin{aligned} \mu(S(s)f) &= \lim_{t \rightarrow \infty} \int_X S(s)f d[\pi S(t)] = \lim_{t \rightarrow \infty} \int_X S(t)S(s)f d\pi = \\ &= \lim_{t \rightarrow \infty} \int_X S(t+s)f d\pi = \lim_{t \rightarrow \infty} \int_X S(t)f d\pi = \\ &= \lim_{t \rightarrow \infty} \int_X f d[\pi S(t)] = \mu(f) . \end{aligned} \quad (1.65)$$

□

By the Krein Milman theorem, statement (a) implies that  $\mathcal{I}$  is the closed convex hull of its extreme points  $\mathcal{I}_e$ . Elements of  $\mathcal{I}_e$  are called *extremal invariant measures*.

What about uniqueness of stationary distributions?

**Definition 1.9** A Markov process  $(\mathbb{P}^\eta : \eta \in X)$  is called *irreducible*, if for all  $\eta, \eta' \in X$

$$\mathbb{P}^\eta(\eta_t = \eta') > 0 \quad \text{for some } t \geq 0. \quad (1.66)$$

So an irreducible MP can sample the whole state space, and if  $X$  is countable this implies that it has at most one stationary distribution. For IPS with uncountable state space this does in general not hold, and non-uniqueness can be the result of absorbing states (e.g. CP), or the presence of conservation laws on infinite lattices (e.g. SEP) as is discussed later.

**Definition 1.10** A Markov process with semigroup  $(S(t) : t \geq 0)$  is *ergodic* if

- (a)  $\mathcal{I} = \{\mu\}$  is a singleton, and (unique stationary measure)
- (b)  $\lim_{t \rightarrow \infty} \pi S(t) = \mu$  for all  $\pi \in \mathcal{P}(X)$ . (convergence to equilibrium)

Phase transition are related to the breakdown of ergodicity in irreducible systems, in particular non-uniqueness of stationary measures.

**Proposition 1.10** *An irreducible Markov chain with finite state space  $X$  is ergodic.*

**Proof.** A result of linear algebra, in particular the Perron-Frobenius theorem: The finite matrix  $c(\eta, \eta')$  has eigenvalue 0 with unique eigenvector  $\mu$ .

Therefore, mathematically phase transitions occur only in infinite systems. Infinite systems are often interpreted/studied as limits of finite systems, which show traces of a phase transition by divergence or non-analytic behaviour of certain observables. In terms of applications, infinite systems are approximations or idealizations of real systems which may large but are always finite, so results have to interpreted with care.

There is a well developed mathematical theory of phase transitions for reversible systems provided by the framework of Gibbs measures (see e.g. [G88]). But for IPS which are in general non-reversible, the notion of phase transitions is not well defined and we will try to get an understanding by looking at several examples.

#### **Further remarks on reversibility.**

We have seen before that a stationary process can be extended to negative times on the path space  $D(-\infty, \infty)$ . A time reversed stationary process is again a stationary Markov process and the time evolution is given by adjoint operators as explained in the following.

Let  $\mu \in \mathcal{P}(X)$  be the stationary measure of the process  $(S(t) : t \geq 0)$  and consider

$$L^2(X, \mu) = (f \in C(X) : \mu(f^2) < \infty) \quad (1.67)$$

the set of square integrable test functions. With the inner product  $\langle f, g \rangle = \mu(fg)$  the closure of this (w.r.t. the metric given by the inner product) is a Hilbert space, and the generator  $\mathcal{L}$  and the  $S(t)$  are bounded linear operators on  $L^2(X, \mu)$ . They are uniquely defined by their values on  $C(X)$ , which is a dense subset of the closure of  $L^2(X, \mu)$ . Therefore they have an *adjoint* operator  $\mathcal{L}^*$  and  $S(t)^*$ , respectively, uniquely defined by

$$\langle S(t)^* f, g \rangle = \mu(g S(t)^* f) = \mu(f S(t) g) = \langle f, S(t) g \rangle \quad \text{for all } f, g \in L^2(X, \mu), \quad (1.68)$$

and analogously for  $\mathcal{L}^*$ . To compute the action of the adjoint operator note that for all  $g \in L^2(X, \mu)$

$$\begin{aligned} \mu(gS(t)^*f) &= \int_X fS(t)g \, d\mu = \mathbb{E}^\mu(f(\eta_0)g(\eta_t)) = \mathbb{E}^\mu\left(\mathbb{E}(f(\eta_0)|\eta_t)g(\eta_t)\right) = \\ &= \int_X \mathbb{E}(f(\eta_0)|\eta_t = \zeta)g(\zeta) \, \mu(d\zeta) = \mu\left(g \mathbb{E}(f(\eta_0)|\eta_t = \cdot)\right), \end{aligned} \quad (1.69)$$

where the identity between the first and second line is due to  $\mu$  being the stationary measure. Since this holds for all  $g$  it implies that

$$S(t)^*f(\eta) = \mathbb{E}(f(\eta_0)|\eta_t = \eta), \quad (1.70)$$

so the adjoint operator describes the evolution of the time-reversed process. Similarly, it can be shown that the adjoint generator  $\mathcal{L}^*$  is actually the generator of the adjoint semigroup  $S(t)^* : t \geq 0$  (modulo some technicalities with domains of definition). The process is time-reversible if  $\mathcal{L} = \mathcal{L}^*$  and therefore reversibility is equivalent to  $\mathcal{L}$  and  $S(t)$  being *self-adjoint* as in (1.52) and (1.56).

## 2 The asymmetric simple exclusion process

As given in Def. 1.2 an *exclusion process (EP)* has state space  $X = \{0, 1\}^\Lambda$  on a lattice  $\Lambda$ . The process is characterized by the generator

$$\mathcal{L}f(\eta) = \sum_{x,y \in \Lambda} c(x,y,\eta) (f(\eta^{xy}) - f(\eta)) \quad (2.1)$$

with jump rates

$$c(x,y,\eta) = p(x,y) \eta(x)(1 - \eta(y)) . \quad (2.2)$$

### 2.1 Stationary measures and conserved quantities

**Definition 2.1** For a function  $\rho : \Lambda \rightarrow [0, 1]$  the *product measure*  $\nu_\rho$  on  $X$  is defined by the marginals

$$\nu_\rho(\eta(x_1) = n_1, \dots, \eta(x_k) = n_k) = \prod_{i=1}^k \nu_{\rho(x_i)}^1(\eta(x_i) = n_i) \quad (2.3)$$

for all  $k, x_i \neq x_j$  and  $n_i \in \{0, 1\}$ , where the *single-site marginals* are given by

$$\nu_{\rho(x_i)}^1(\eta(x_i) = 1) = \rho(x_i) \quad \text{and} \quad \nu_{\rho(x_i)}^1(\eta(x_i) = 0) = 1 - \rho(x_i) . \quad (2.4)$$

In other words the  $\eta(x)$  are independent Bernoulli rvs with *local density*  $\rho(x) = \nu(\eta(x))$ .

**Theorem 2.1** (a) Suppose  $p(\cdot, \cdot)/C$  is doubly stochastic for some  $C > 0$ , i.e.

$$\sum_{y' \in \Lambda} p(x, y') = \sum_{x' \in \Lambda} p(x', y) = C \quad \text{for all } x, y \in \Lambda , \quad (2.5)$$

then  $\nu_\rho \in \mathcal{I}$  for all constants  $\rho \in [0, 1]$  (*uniform density*).

(b) If  $\lambda : \Lambda \rightarrow [0, \infty)$  fulfills  $\lambda(x) p(x, y) = \lambda(y) p(y, x)$ ,  
then  $\nu_\rho \in \mathcal{I}$  with density  $\rho(x) = \frac{\lambda(x)}{1 + \lambda(x)}$ ,  $x \in \Lambda$ .

**Proof.** For stationarity we have to show that  $\nu_\rho(\mathcal{L}f) = 0$  for all  $f \in C_0(X)$ . By linearity, it is enough to check this for simple cylinder functions

$$f_A(\eta) = \begin{cases} 1 & , \eta(x) = 1 \text{ for each } x \in A \\ 0 & , \text{otherwise} \end{cases} \quad (2.6)$$

for all finite  $A \subseteq \Lambda$ . Then

$$\nu_\rho(\mathcal{L}f_A) = \sum_{x,y \in \Lambda} p(x,y) \int_X \eta(x)(1 - \eta(y)) (f(\eta^{xy}) - f(\eta)) d\nu_\rho , \quad (2.7)$$

and for  $x \neq y$  the integral terms in the sum look like

$$\int_X f(\eta) \eta(x)(1 - \eta(y)) d\nu_\rho = \begin{cases} 0 & , y \in A \\ (1 - \rho(y)) \prod_{u \in A \cup \{x\}} \rho(u) & , y \notin A \end{cases}$$

$$\int_X f(\eta^{xy}) \eta(x)(1 - \eta(y)) d\nu_\rho = \begin{cases} 0 & , x \in A \\ (1 - \rho(y)) \prod_{u \in A \cup \{x\} \setminus \{y\}} \rho(u) & , x \notin A \end{cases} . \quad (2.8)$$

This follows from the fact that the integrands take values only in  $\{0, 1\}$  and the rhs is basically the probability of the integrand being 1. Then re-arranging the sum we get

$$\nu_\rho(\mathcal{L}f_A) = \sum_{\substack{x \in A \\ y \notin A}} \left[ \rho(y)(1 - \rho(x))p(y, x) - \rho(x)(1 - \rho(y))p(x, y) \right] \prod_{u \in A \setminus \{x\}} \rho(u). \quad (2.9)$$

Under the assumption of (b) the square bracket vanishes for all  $x, y$  in the sum, since

$$\frac{\rho(x)}{1 - \rho(x)} p(x, y) = \frac{\rho(y)}{1 - \rho(y)} p(y, x). \quad (2.10)$$

For  $\rho(x) \equiv \rho$  in (a) we get

$$\nu_\rho(\mathcal{L}f_A) = \rho^{|A|} (1 - \rho) \sum_{\substack{x \in A \\ y \notin A}} [p(y, x) - p(x, y)] = 0 \quad (2.11)$$

due to  $p(\cdot, \cdot)$  being proportional to a doubly-stochastic.  $\square$

For the ASEP (1.24) in one dimension with  $\Lambda = \mathbb{Z}$  we have:

- Theorem 2.1(a) holds with  $C = p + q$  and therefore  $\nu_\rho \in \mathcal{I}$  for all  $\rho \in [0, 1]$ . These measures have homogeneous density; they are reversible iff  $p = q$ , which is immediate from time-reversibility.
- Also Theorem 2.1(b) is fulfilled with  $\lambda(x) = c(p/q)^x$  for all  $c > 0$ , since  $c(p/q)^x p = c(p/q)^{x+1} q$ . Therefore

$$\nu_\rho \in \mathcal{I} \quad \text{with} \quad \rho(x) = \frac{c(p/q)^x}{1 + c(p/q)^x} \quad \text{for all } c \in \Lambda. \quad (2.12)$$

For  $p \neq q$  these are not homogeneous and since e.g. for  $p > q$  the density of particles (holes) is exponentially decaying as  $x \rightarrow \pm\infty$  they concentrate on configurations such that

$$\sum_{x < 0} \eta(x) < \infty \quad \text{and} \quad \sum_{x \geq 0} (1 - \eta(x)) < \infty. \quad (2.13)$$

These are called *blocking measures* and turn out to be reversible also for  $p \neq q$ .

- There are only countably many configurations with property (2.13), forming the disjoint union of

$$X_n = \left\{ \eta : \sum_{x < n} \eta(x) = \sum_{x \geq n} (1 - \eta(x)) < \infty \right\}, \quad n \in \Lambda. \quad (2.14)$$

Conditioned on  $X_n$ , the ASEP is an irreducible MC with unique stationary distribution  $\nu_n := \nu_\rho(\cdot | X_n)$ . Liggett ('76) showed that all extremal measures of the ASEP are

$$\mathcal{I}_e = \{ \nu_\rho : \rho \in [0, 1] \} \cup \{ \nu_n : n \in \mathbb{Z} \}. \quad (2.15)$$

To stress the role of the boundary conditions let us consider another example. For the ASEP on a one-dimensional torus  $\Lambda_L = \mathbb{Z}/L\mathbb{Z}$  we have:

- Theorem 2.1(a) still applies so  $\nu_\rho \in \mathcal{I}$  for all  $\rho \in [0, 1]$ . But part (b) does no longer hold due to periodic boundary conditions, so there are no blocking measures.  
Under  $\nu_\rho$  the total number of particles in the system is a binomial rv

$$\Sigma_L(\eta) := \sum_{x \in \Lambda} \eta(x) \sim Bi(L, \rho) \quad \text{where} \quad \nu_\rho(\Sigma_L = N) = \binom{L}{N} \rho^N (1 - \rho)^{L-N} \quad (2.16)$$

The  $\{\nu_\rho : \rho \in [0, 1]\}$  are called *grand-canonical measures/ensemble*.

- If we fix the number of particles at time 0, i.e.  $\Sigma_L(\eta_0) = N$ , we condition the ASEP on

$$X_{L,N} = \{\eta : \Sigma_L(\eta) = N\} \subsetneq X_L. \quad (2.17)$$

For each  $N \in \mathbb{N}$ , the process is irreducible on  $X_{L,N}$  and  $|X_{L,N}| = \binom{L}{N}$  is finite. Therefore it has a unique stationary measure  $\pi_{L,N}$  on  $X_{L,N}$  and the  $\{\pi_{L,N} : N = 0, \dots, L\}$  are called *canonical measures/ensemble*.

**Definition 2.2**  $h \in C(X)$  is a *conserved quantity* for a process  $\eta = (\eta_t : t \geq 0)$  if

$$h(\eta_t) = h(\eta_0) \quad \text{for all } t \geq 0. \quad (2.18)$$

**Remarks.** For Feller processes (2.18) implies

$$S(t)h(\eta) = S(t)^*h(\eta) = h(\eta) \quad \text{for all } \eta \in X. \quad (2.19)$$

If  $h \in C_0(X)$  (e.g. on finite lattices) then this is equivalent to

$$\mathcal{L}h(\eta) = \mathcal{L}^*h(\eta) = 0 \quad \text{for all } \eta \in X, \quad (2.20)$$

where  $S(t)$  and  $\mathcal{L}$  are semigroup and generator of  $\eta$ . If  $h$  is conserved then so is  $g \circ h$  for all  $g : \mathbb{R} \rightarrow \mathbb{R}$ .

**Proposition 2.2** Suppose that for a Feller process  $\mu \in \mathcal{I}$ ,  $h \in C(X)$  is conserved and  $g : \mathbb{R} \rightarrow [0, \infty)$  is such that  $g \circ h \in C(X)$  and  $\mu(g \circ h) = 1$ . Then  $(g \circ h)\mu \in \mathcal{I}$ .

**Proof.** For all  $t \geq 0$  and  $f \in C(X)$  we have

$$(g \circ h)\mu(S(t)f) = \int_X (S(t)f)(\eta) g(h(\eta)) \mu(d\eta) = \int_X f S(t)^*g(h) d\mu = (g \circ h)\mu(f),$$

and therefore  $(g \circ h)\mu \in \mathcal{I}$ . □

We can apply this result to characterize the stationary measures  $\pi_{L,N}$  for the ASEP on  $X_{L,N}$  given above. For all  $\rho \in (0, 1)$  we can condition the product measures  $\nu_\rho$  on  $X_{L,N}$ , i.e. define

$$\tilde{\pi}_{L,N} := \nu_\rho(\cdot | \Sigma_L = N) = \frac{\mathbb{1}_{\Sigma_L = N} \nu_\rho}{\binom{L}{N} \rho^N (1 - \rho)^{L-N}}. \quad (2.21)$$

Since with  $\Sigma_L \in C(X)$  also  $\mathbb{1}_{\Sigma_L = N} : X \rightarrow \{0, 1\}$  is conserved,  $\tilde{\pi}_{L,N}$  as defined above is stationary for all  $N \in \mathbb{N}$ . In fact,

$$\tilde{\pi}_{L,N}(\eta) = \begin{cases} 0 & , \eta \notin X_{L,N} \\ \frac{\rho^N (1 - \rho)^{L-N}}{\binom{L}{N} \rho^N (1 - \rho)^{L-N}} = 1 / \binom{L}{N} & , \eta \in X_{L,N} \end{cases}, \quad (2.22)$$

so it concentrates on  $X_{L,N}$  and it is uniform, in particular independent of  $\rho$ . Since the stationary measure on  $X_{L,N}$  is unique, we have  $\tilde{\pi}_{L,N} = \pi_{L,N}$ .

We can write the grand-canonical product measures  $\nu_\rho$  as convex combinations

$$\nu_\rho = \sum_{N=0}^L \binom{L}{N} \rho^N (1-\rho)^{L-N} \pi_{L,N}, \quad (2.23)$$

but this is not possible for the  $\pi_{L,N}$  since they concentrate on particular subsets  $X_{L,N} \subsetneq X_L$ . Thus for the ASEP on  $\Lambda_L = \mathbb{Z}/L\mathbb{Z}$  we have

$$\mathcal{I}_e = \{\pi_{L,N} : N = 0, \dots, L\} \quad (2.24)$$

given by the canonical measures. So for each value of the conserved quantity  $\Sigma_L$  we have an extremal stationary measure and these are the only elements of  $\mathcal{I}_e$ . This is the appropriate notion of *uniqueness of stationary measures* for systems with a conserved quantity on finite lattices.

For the ASEP on the infinite lattice  $\Lambda = \mathbb{Z}$  uniqueness would correspond to  $\mathcal{I}_e = \{\nu_\rho : \rho \in [0, 1]\}$ , since for every translation invariant distribution the actual number of particles will be infinity. But we have seen in (2.15) that this is not the case, since we also have extremal blocking measures. Therefore we have non-uniqueness of stationary measures which is called a *phase transition*. Since the blocking measures are also not translation invariant but the dynamics of the system is, the nature or type of this phase transition is called (spontaneous) symmetry breaking.

Later we will see other types of phase transitions, and examples which are a bit more exciting than this one.

### General remarks on symmetries.

**Definition 2.3** A bijection  $\tau : X \rightarrow X$  is a *symmetry* for a Feller process  $(S(t) : t \geq 0)$  if

$$(S(t)f) \circ \tau = S(t)(f \circ \tau) \quad \text{for all } f \in C(X) \text{ and } t \geq 0. \quad (2.25)$$

Note that this is equivalent to

$$(\mathcal{L}f) \circ \tau = \mathcal{L}(f \circ \tau) \quad \text{for all } f \in C_0(X) \quad (2.26)$$

or  $\mathbb{P}^{\tau\eta}(\eta \in A) = \mathbb{P}^\eta(\tau\eta \in A)$  for all space-time events  $A \in \mathcal{F}$  on path space  $D[0, \infty)$ . An example we have seen above is *translation invariance*, i.e. shifting the initial condition by a lattice spacing and then running the process is the same as running the process and then shifting the path.

**Proposition 2.3** *Symmetries are groups, i.e. if  $\tau, \tau'$  are symmetries for  $(S(t) : t \geq 0)$  so is  $\tau \circ \tau'$  and the inverse  $\tau^{-1}$ .*

**Proof.** Let  $\tau, \tau'$  be symmetries for  $(S(t) : t \geq 0)$ . Then for all  $f \in C(X)$ ,

$$(S(t)f) \circ (\tau \circ \tau') = ((S(t)f) \circ \tau) \circ \tau' = (S(t)(f \circ \tau)) \circ \tau' = S(t)(f \circ \tau \circ \tau'). \quad (2.27)$$

Further,

$$(S(t)(f \circ \tau^{-1})) \circ \tau = S(t)(f \circ \tau^{-1} \circ \tau) = S(t)f \quad (2.28)$$

and therefore

$$S(t)(f \circ \tau^{-1}) = (S(t)(f \circ \tau^{-1})) \circ \tau \circ \tau^{-1} = (S(t)f) \circ \tau^{-1}. \quad (2.29)$$

□

For example the group corresponding to *translation invariance* of the one-dimensional ASEP is the set of lattice shifts  $(\tau_x : x \in \mathbb{Z})$  where  $(\tau_x\eta)(y) = \eta(y - x)$ .

**Proposition 2.4** Let  $\tau$  be a symmetry for  $(S(t) : t \geq 0)$  and  $\mu \in \mathcal{I}$ . Then  $\mu \circ \tau \in \mathcal{I}$ .

**Proof.** Since with  $\tau$  also  $\tau^{-1}$  is a symmetry, we have for all  $f \in C(X)$  and  $t \geq 0$

$$\begin{aligned} (\mu \circ \tau)(S(t)f) &= \int_X (S(t)f)(\eta) (\mu \circ \tau)(d\eta) = \int_X (S(t)f)(\tau^{-1}\zeta) \mu(d\zeta) = \\ &= \int_X (S(t)(f \circ \tau^{-1}))(\zeta) \mu(d\zeta) = \int_X f \circ \tau^{-1} d\mu = (\mu \circ \tau)(f), \end{aligned} \quad (2.30)$$

where we have used a change of variable  $\zeta = \tau\eta$ . Therefore  $\mu \circ \tau \in \mathcal{I}$ .  $\square$

For example for product measures  $\nu_\rho$  with constant density  $\rho \in [0, 1]$  we have  $\nu_\rho \circ \tau_x = \nu_\rho$  for all lattice shifts  $\tau_x$  so these measures are translation invariant. On the other hand the blocking measures have  $x$ -dependent densities and are not translation invariant, but of course  $\mathcal{I}$  contains all translates of these measures.

There are other symmetries of the ASEP on  $\mathbb{Z}$ , for example particle-hole and space inversion, also called *CP-invariance*, given by

$$\tau\eta(x) = 1 - \eta(-x). \quad (2.31)$$

Here  $\nu_\rho \circ \tau = \nu_{1-\rho}$  and  $\nu_n \circ \tau = \nu_{-n}$  for the blocking measures, so only two elements of  $\mathcal{I}$ ,  $\nu_{1/2}$  and the blocking measure  $\nu_0$  are invariant under  $\tau$ . This is, however, not very suprising, since CP-invariance is already broken by the conservation law on a finite lattice. On the state space  $X_{L,N}$  we have for the number of particles

$$(\Sigma_L \circ \tau)(\eta) = N - \Sigma_L(\eta) \quad (2.32)$$

which is in general different from  $\Sigma_L(\eta)$ . This is in contrast to translation invariance, for which  $\Sigma_L \circ \tau_x = \Sigma_L$  for finite systems. Therefore the breaking of translation invariance is really a result of the infinite lattice and therefore connected to a phase transition.

In general, if  $\tau$  is a symmetry for  $(S(t) : t \geq 0)$  which is not already broken by a conservation law, and  $\mathcal{I}$  contains measures  $\mu$  for which  $\mu \circ \tau \neq \mu$  the system is said to exhibit (*spontaneous*) *symmetry breaking*. Note that by Prop. 2.4 symmetry breaking always implies non-uniqueness of stationary measures and is therefore a phase transition.



## 2.2 Currents and conservation laws

Consider the one-dimensional ASEP on  $\Lambda = \mathbb{Z}$  or  $\Lambda_L = \mathbb{Z}/L\mathbb{Z}$ . Remember the forward equation from Theorem 1.6

$$\frac{d}{dt}S(t)f = S(t)\mathcal{L}f \quad \text{which holds for all } f \in C_0(X). \quad (2.33)$$

Integrating w.r.t. the initial distribution  $\mu$  the equation becomes

$$\frac{d}{dt}\mu(S(t)f) = \mu(S(t)\mathcal{L}f) = (\mu S(t))(\mathcal{L}f). \quad (2.34)$$

Using  $f(\eta) = \eta(x)$  and writing  $\mu_t := \mu S(t)$  for the distribution at time  $t$  we have

$$\mu_t(f) = \mathbb{E}^\mu(\eta_t(x)) =: \rho(x, t) \quad (2.35)$$

for the *particle density* at site  $x$  at time  $t$ . Note that  $\eta(x)$  is a cylinder function and we have

$$\begin{aligned} (\mathcal{L}f)(\eta) &= \sum_{y \in \Lambda} \left( p\eta(y)(1 - \eta(y+1)) + q\eta(y+1)(1 - \eta(y)) \right) (f(\eta^{y,y+1}) - f(\eta)) = \\ &= -p\eta(x)(1 - \eta(x+1)) + q\eta(x+1)(1 - \eta(x)) \\ &\quad - q\eta(x)(1 - \eta(x-1)) + p\eta(x-1)(1 - \eta(x)). \end{aligned} \quad (2.36)$$

Taking expectations w.r.t.  $\mu_t$  and writing

$$\mu_t(\eta(x)(1 - \eta(x+1))) = \mu_t(1_x 0_{x+1}) \quad (2.37)$$

we get with (2.33)

$$\frac{d}{dt}\rho(x, t) = \underbrace{p\mu_t(1_{x-1}0_x) + q\mu_t(0_x1_{x+1})}_{\text{gain}} - \underbrace{p\mu_t(1_x0_{x+1}) + q\mu_t(0_{x-1}1_x)}_{\text{loss}}. \quad (2.38)$$

**Definition 2.4** The *average current* of particles across the directed edge  $(x, x+1)$  is given by

$$j(x, x+1, t) := \mu_t(c(x, y, \eta) - c(y, x, \eta)). \quad (2.39)$$

For the ASEP this is non-zero only across nearest-neighbour bonds and given by

$$j(x, x+1, t) = p\mu_t(1_x0_{x+1}) - q\mu_t(0_x1_{x+1}). \quad (2.40)$$

Then we can write, using the lattice derivative  $\nabla_x j(x-1, x, t) = j(x, x+1, t) - j(x-1, x, t)$ ,

$$\frac{d}{dt}\rho(x, t) + \nabla_x j(x-1, x, t) = 0 \quad (2.41)$$

which is the (lattice) *continuity equation*. It describes the time evolution of the density  $\rho(x, t)$  in terms of higher order (two-point) correlation functions. The form of this equation implies that the particle density is conserved, i.e. on the finite lattice  $\Lambda_L = \mathbb{Z}/L\mathbb{Z}$  with periodic boundary conditions we have

$$\frac{d}{dt} \sum_{x \in \Lambda_L} \rho(x, t) = - \sum_{x \in \Lambda_L} \nabla_x j(x-1, x, t) = 0. \quad (2.42)$$

In general on any finite subset  $A \in \Lambda$

$$\frac{d}{dt} \sum_{x \in A} \rho(x, t) = - \sum_{x \in \partial A} \nabla_x j(x-1, x, t), \quad (2.43)$$

where  $\partial A$  is the boundary of  $A$ . The other terms in the telescoping sum on the right-hand side cancel, which is a primitive version of Gauss' integration theorem (we have not been very careful with the notation at the boundary here).

In the special case  $p = q$  (2.41) simplifies significantly. Let's take  $p = q = 1$ , then adding and subtracting an auxiliary term we see

$$\begin{aligned} j(x, x+1, t) &= \mu_t(1_x 0_{x+1}) + \mu_t(1_x 1_{x+1}) - \mu_t(1_x 1_{x+1}) - \mu_t(0_x 1_{x+1}) = \\ &= \mu_t(1_x) - \mu_t(1_{x+1}) = \rho(x, t) - \rho(x+1, t) = -\nabla_x \rho(x, t). \end{aligned} \quad (2.44)$$

So the current is given by the lattice derivative of the density, and (2.41) turns into a closed equation

$$\frac{d}{dt} \rho(x, t) = \Delta_x \rho(x, t) = \rho(x-1, t) - 2\rho(x, t) + \rho(x+1, t). \quad (2.45)$$

Thus the particle density of the SSEP behaves like the probability density of a single simple random walk with jump rates  $p = q = 1$ .

To describe this behaviour on large scales we scale the lattice constant by a factor of  $1/L$  and embed it in the continuum, i.e.  $\frac{1}{L}\Lambda \subseteq \mathbb{R}$  and  $\frac{1}{L}\Lambda_L \subseteq \mathbb{T} = \mathbb{R}/[0, 1)$  for the torus. Using the macroscopic space variable  $y = x/L \in \mathbb{R}, \mathbb{T}$  we define

$$\tilde{\rho}(y, t) := \rho([yL], t) \quad (2.46)$$

for the macroscopic *density field* and use a Taylor expansion

$$\rho(x \pm 1, t) = \tilde{\rho}(y \pm \frac{1}{L}, t) = \tilde{\rho}(y, t) \pm \frac{1}{L} \partial_y \tilde{\rho}(y, t) + \frac{1}{2L^2} \partial_y^2 \tilde{\rho}(y, t) + o(\frac{1}{L^2}) \quad (2.47)$$

to compute the lattice Laplacian in (2.45). This leads to

$$\Delta_x \rho(x, t) = \frac{1}{L^2} \partial_y^2 \tilde{\rho}(y, t), \quad (2.48)$$

since first order terms vanish due to symmetry. In order to get a non-degenerate equation in the limit  $L \rightarrow \infty$ , we have to scale time as  $s = t/L^2$ . This corresponds to speeding up the process by a factor of  $L^2$ , in order to see diffusive motion of the particles on the scaled lattice. Using both in (2.45) we obtain in the limit  $L \rightarrow \infty$

$$\partial_s \tilde{\rho}(y, s) = \partial_y^2 \tilde{\rho}(y, s), \quad (2.49)$$

the *heat equation*, describing the diffusion of particles on large scales.

If we use a stationary measure  $\mu_t = \mu$  in the continuity equation (2.41) we get

$$0 = \frac{d}{dt} \mu(1_x) = j(x-1, x) - j(x, x+1), \quad (2.50)$$

which implies that the *stationary current*  $j(x, x+1) := p\mu(1_x 0_{x+1}) - q\mu(0_x 1_{x+1})$  is site-independent. Since we know the stationary measures for the ASEP from the previous section we can compute it explicitly. For the homogeneous product measure  $\mu = \nu_\rho$  we get

$$j(x, x+1) := p\nu_\rho(1_x 0_{x+1}) - q\nu_\rho(0_x 1_{x+1}) = (p-q)\rho(1-\rho) = f(\rho), \quad (2.51)$$

which is actually just a function of the total particle density  $\rho \in [0, 1]$ . We can use this to arrive at a scaling limit of the continuity equation for the asymmetric case  $p \neq q$ . We use the same space scaling  $y = x/L$  as above and write

$$\nabla_x j(x-1, x, t) = \frac{1}{L} \partial_y \tilde{j}(y - \frac{1}{L}, y, t) + o(\frac{1}{L}), \quad (2.52)$$

with a similar notation  $\tilde{j}$  as for  $\tilde{\rho}$  above. In the asymmetric case the first order terms in the spatial derivative do not vanish and we have to scale time as  $s = t/L$ , speeding up the process only by a factor  $L$  to see ballistic motion. In the limit  $L \rightarrow \infty$  this leads to the *conservation law (PDE)*

$$\partial_s \tilde{\rho}(y, s) + \partial_y \tilde{j}(y, s) = 0, \quad (2.53)$$

where we have redefined  $\tilde{j}$  as

$$\tilde{j}(y, s) := \lim_{L \rightarrow \infty} j([yL] - 1, [yL], sL). \quad (2.54)$$

Since we effectively take microscopic time  $t = sL \rightarrow \infty$  in that definition, it is plausible to assume that

$$\tilde{j}(y, s) = f(\rho(y, s)) \quad (2.55)$$

is in fact the stationary current corresponding to the local density  $\rho(y, s)$ . This is equivalent to the process becoming locally stationary in the limit  $L \rightarrow \infty$ , the only (slowly) varying quantity remaining on a large scale is the macroscopic density field. Local stationarity (also called local equilibrium) implies for example

$$\mu S(sL)(1_{[yL]} 0_{[yL]+1}) \rightarrow \nu_{\rho(y,s)}(1_0 0_1) = \rho(y, s)(1 - \rho(y, s)) \quad \text{as } L \rightarrow \infty. \quad (2.56)$$

In the following we write again  $\tilde{\rho} = \rho$  to avoid notational overload, the notation was only introduced to make the scaling argument clear.

**Definition 2.5** The ASEP on  $\frac{1}{L}\mathbb{Z}$  or  $\frac{1}{L}\mathbb{Z}/L\mathbb{Z}$  with initial distribution  $\mu$ , such that

$$\rho(y, 0) = \lim_{L \rightarrow \infty} \mu(1_{[yL]}) \quad (2.57)$$

exists, is in *local equilibrium* if

$$\mu S(Ls)\tau_{-[yL]} \rightarrow \nu_{\rho(y,s)} \quad \text{weakly (locally), as } L \rightarrow \infty, \quad (2.58)$$

where  $\rho(y, s)$  is a solution of the *Burgers* equation

$$\partial_s \rho(y, s) + \partial_y f(\rho(y, s)) = 0 \quad \text{where } f(\rho) = (p - q)\rho(1 - \rho), \quad (2.59)$$

with initial condition  $\rho(y, 0)$ .

By local weak convergence we mean

$$\mu S(Ls)\tau_{-[yL]}(f) \rightarrow \nu_{\rho(y,s)}(f) \quad \text{for all } f \in C_0(X). \quad (2.60)$$

Local equilibrium has been established rigorously for the ASEP in a so-called *hydrodynamic limit*, the formulation of this result requires the following definition.

**Definition 2.6** For each  $t \geq 0$  we define the *empirical measure*

$$\pi_t^L := \frac{1}{L} \sum_{x \in \Lambda} \eta_t(x) \delta_{x/L} \in \mathcal{M}(\mathbb{R}) \text{ or } \mathcal{M}(\mathbb{T}), \quad (2.61)$$

and the measure-valued process  $(\pi_t^L : t \geq 0)$  is called the *empirical process*.

The  $\pi_t^L$  describe the discrete particle densities on  $\mathbb{R}, \mathbb{T}$ . They are (random) measures depending on the configurations  $\eta_t$  and for  $A \subseteq \mathbb{R}, \mathbb{T}$  we have

$$\pi_t^L(A) = \frac{1}{L} \left( \# \text{ of particles in } A \cap \frac{1}{L}\Lambda \text{ at time } t \right). \quad (2.62)$$

**Theorem 2.5** Consider the ASEP  $(\eta_t : t \geq 0)$  on the lattice  $\frac{1}{L}\mathbb{Z}$  or  $\frac{1}{L}\mathbb{Z}/L\mathbb{Z}$  with initial distribution  $\mu$  which has a limiting density  $\rho(y, 0)$  analogous to (2.57). Then as  $L \rightarrow \infty$

$$\pi_{sL}^L \rightarrow \rho(\cdot, s) dy \quad \text{weakly, in probability,} \quad (2.63)$$

where  $\rho(y, s)$  is a solution of (2.59) on  $\mathbb{R}$  or  $\mathbb{T}$  with initial condition  $\rho(y, 0)$ .

Here weak convergence means that for every  $g \in C_0(\mathbb{R})$  continuous with compact support

$$\pi_{sL}^L(g) = \frac{1}{L} \sum_{x \in \Lambda} g(x/L) \eta_t(x) \rightarrow \int_{\mathbb{R}, \mathbb{T}} g(y) \rho(y, s) dy. \quad (2.64)$$

The left-hand side is still random, and convergence holds in probability, i.e. for all  $\epsilon > 0$

$$\mathbb{P}^\mu \left( \left| \frac{1}{L} \sum_{x \in \Lambda} g(x/L) \eta_t(x) - \int_{\mathbb{R}, \mathbb{T}} g(y) \rho(y, s) dy \right| > \epsilon \right) \rightarrow 0 \quad \text{as } L \rightarrow \infty. \quad (2.65)$$

The fact that the limiting macroscopic density is non-random can be understood as a time-dependent version of the law of large numbers.

The proof is far beyond the scope of this course. Hydrodynamic limits are still an area of major research and technically quite involved. Relevant results can be found in [KL99] Chapter 8. The above result was first proved in '81 by Rost for the TASEP ( $q = 0$ ), and in '91 by Rezakhanlou for a more general class of models.

### 2.3 Hydrodynamics and the dynamic phase transition

In the previous section we were often talking about solutions to the Burgers equation (2.59), not mentioning that it is far from clear whether that equation actually has a unique solution. A useful method to solve a conservation law of the form

$$\partial_t \rho(x, t) + \partial_x f(\rho(x, t)) = 0, \quad \rho(x, 0) = \rho_0(x) \quad (2.66)$$

with general *flux function*  $f$  are characteristic equations.

**Definition 2.7** A function  $x : \mathbb{R} \rightarrow \mathbb{R}, \mathbb{T}$  is a *characteristic* for the PDE (2.66) if

$$\frac{d}{dt} \rho(x(t), t) = 0 \quad \text{for all } t \geq 0, \quad (2.67)$$

i.e. the solution is constant along  $x(t)$  and given by the initial conditions,  $\rho(x(t), t) = \rho_0(x(0))$ .

Using the PDE (2.66) to compute the total derivative we get

$$\begin{aligned}\frac{d}{dt}\rho(x(t), t) &= \partial_t \rho(x(t), t) + \partial_x \rho(x(t), t) \dot{x}(t) = \\ &= -f'(\rho(x(t), t)) \partial_x \rho(x(t), t) + \partial_x \rho(x(t), t) \dot{x}(t) = 0,\end{aligned}\quad (2.68)$$

which implies that

$$\dot{x}(t) = f'(\rho(x(t), t)) = f'(\rho_0(x(0))) \quad (2.69)$$

is a constant given by the derivative of the flux function. So the *characteristic velocity*  $u$  is given by the local density through the function

$$u(\rho) = f'(\rho) = (p - q)\rho(1 - \rho). \quad (2.70)$$

It turns out that a general theory can be based on understanding the solutions to the *Riemann problem*, which is given by step initial data

$$\rho_0(x) = \begin{cases} \rho_l & , x \leq 0 \\ \rho_r & , x > 0 \end{cases}. \quad (2.71)$$

Discontinuous solutions of a PDE have to be understood in a weak sense.

**Definition 2.8**  $\rho : \mathbb{R} \times [0, \infty) \rightarrow \mathbb{R}$  is a *weak solution* to the conservation law (2.66) if  $\rho \in L^1_{loc}(\mathbb{R} \times [0, \infty))$  and for all  $\phi \in C^1(\mathbb{R} \times [0, \infty))$  with compact support and  $\phi(x, 0) = 0$ ,

$$\int_{\mathbb{R}} \int_0^\infty \partial_t \phi(x, t) \rho(x, t) dx dt + \int_{\mathbb{R}} \int_0^\infty f(\rho(x, t)) \partial_x \phi(x, t) dx dt = 0. \quad (2.72)$$

$L^1_{loc}$  means that for all compact  $A \subseteq \mathbb{R} \times [0, \infty)$ ,  $\int_A |\rho(x, t)| dx dt < \infty$ .

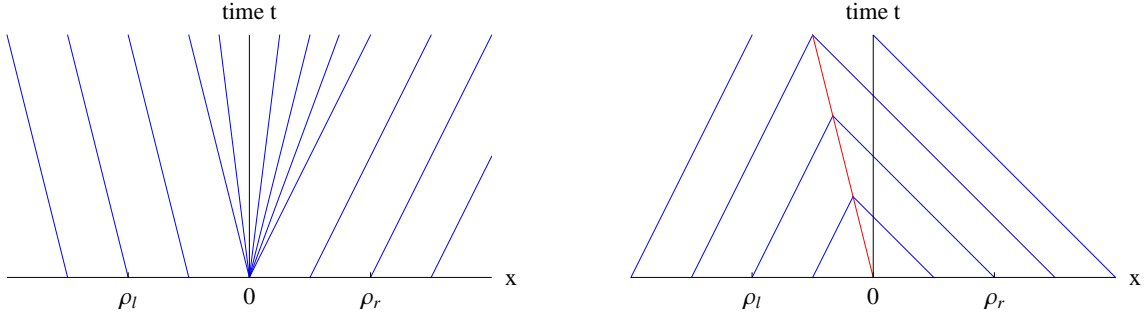
The characteristics do not determine a unique solution everywhere, so weak solutions are not unique. However, for given initial density profile, the IPS shows a unique time evolution on the macroscopic scale. This unique *admissible solution* can be recovered from the variety of weak solutions to (2.66) by several regularization methods. The *viscosity method* is directly related to the derivation of the continuum equation in a scaling limit. For every  $\epsilon > 0$  consider the equation

$$\partial_t \rho^\epsilon(x, t) + \partial_x f(\rho^\epsilon(x, t)) = \epsilon \partial_x^2 f(\rho^\epsilon(x, t)), \quad \rho^\epsilon(x, 0) = \rho_0(x). \quad (2.73)$$

This is a parabolic equation and has a unique smooth global solution for all  $t > 0$ , even when starting from non-smooth initial data  $\rho_0$ . This is due to the regularizing effect of the diffusive term (confer e.g. to the heat equation starting with initial condition  $\delta_0(x)$ ), which captures the fluctuations in large finite IPS. The term can be interpreted as a higher order term of order  $1/L^2$  which disappears in the scaling limit from a particle system. Then one can define the unique admissible weak solution to (2.66) as

$$\rho(\cdot, t) := \lim_{\epsilon \rightarrow 0} \rho^\epsilon(\cdot, t) \quad \text{in } L^1_{loc}\text{-sense as above for all } t > 0. \quad (2.74)$$

It can be shown that this limit exists, and further that for one-dimensional conservation laws the precise form of the viscosity is not essential, i.e. one could also add the simpler term  $\epsilon \partial_x^2 \rho^\epsilon(x, t)$  leading to the same weak limit solution.



**Figure 3:** Characteristics for the Riemann problem with  $\rho_l < \rho_r$  (left) showing a rarefaction fan, and  $\rho_l > \rho_r$  (right), showing a shock. The curve is shock location is shown in red and the speed is given by (2.77).

For the Riemann problem, there are two basic scenarios for the time evolution of step initial data shown in Fig. 3. For  $\rho_r < \rho_l$  we have for the characteristic speed  $u(\rho_r) > u(\rho_l)$  and the solution is given by the *rarefaction fan*

$$\rho(x, t) = \begin{cases} \rho_l & , x \leq u(\rho_l)t \\ \rho_r & , x > u(\rho_r)t \\ \rho_l + (x - tu(\rho_l)) \frac{\rho_l - \rho_r}{t(u(\rho_l) - u(\rho_r))} & , u(\rho_l)t < x \leq u(\rho_r)t \end{cases} . \quad (2.75)$$

So the step dissolves and the solution interpolates linearly between the points uniquely determined by the characteristics. For  $\rho_r > \rho_l$  we have  $u(\rho_r) < u(\rho_l)$  and the step is stable, called a *shock solution*,

$$\rho(x, t) = \begin{cases} \rho_l & , x \leq vt \\ \rho_r & , x > vt \end{cases} . \quad (2.76)$$

The *shock speed*  $v = v(\rho_l, \rho_r)$  can be derived by the conservation of mass,

$$v(\rho_l, \rho_r) = \frac{j(\rho_r) - j(\rho_l)}{\rho_r - \rho_l} . \quad (2.77)$$

Understanding the Riemann problem is sufficient to construct solutions to general initial data by approximation with piecewise constant functions.

In the following we will use our knowledge on solutions to the Riemann problem to understand the time evolution of the ASEP with step initial distribution

$$\mu = \nu_{\rho_l, \rho_r} \quad \text{product measure with} \quad \nu_{\rho_l, \rho_r}(1_x) = \begin{cases} \rho_l & , x \leq 0 \\ \rho_r & , x > 0 \end{cases} . \quad (2.78)$$

**Theorem 2.6** For the ASEP on  $\Lambda = \mathbb{Z}$  with  $p > q$  we have as  $t \rightarrow \infty$

$$\nu_{\rho_l, \rho_r} S(t) \rightarrow \begin{cases} \nu_{\rho_r} & , \rho_r \geq \frac{1}{2}, \rho_l > 1 - \rho_r & (I) \\ \nu_{\rho_l} & , \rho_l \leq \frac{1}{2}, \rho_r < 1 - \rho_r & (II) \\ \nu_{1/2} & , \rho_l \geq \frac{1}{2}, \rho_r \leq \frac{1}{2} & (III) \end{cases} \quad (2.79)$$

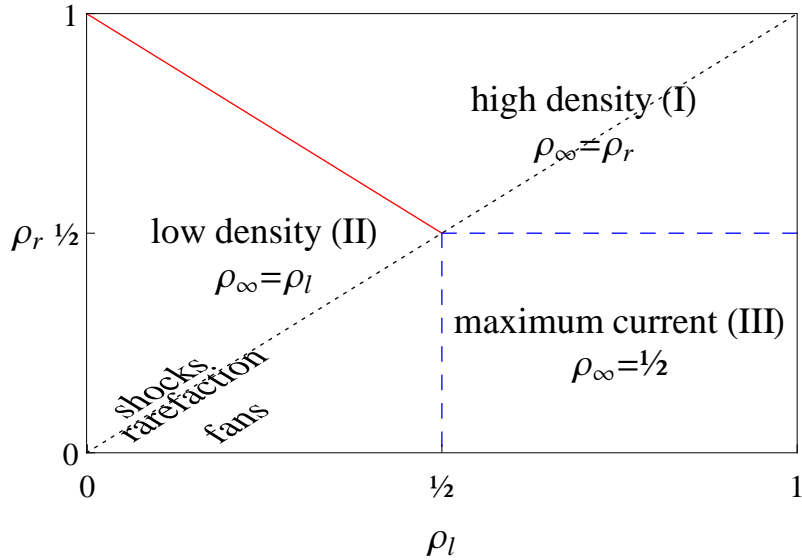
**Proof.** by studying shock and rarefaction fan solutions of the conservation law (2.66).

Note that all the limiting distributions are stationary product measures of the ASEP, as required

by Theorem 1.9. But depending on the initial distribution, the system selects different stationary measures in the limit  $t \rightarrow \infty$ , which do not depend smoothly on  $\rho_l$  and  $\rho_r$ . Therefore this phenomenon is called a *dynamic phase transition*. The set  $\mathcal{I}$  of stationary measures is not changed, but the long-time behaviour of the process depends on the initial conditions in a non-smooth way. This behaviour can be captured in a *phase diagram*, whose axes are given by the (fixed) parameters of our problem,  $\rho_l$  and  $\rho_r$ . We choose the limiting density

$$\rho_\infty := \lim_{t \rightarrow \infty} \nu_{\rho_l, \rho_r} S(t)(\eta(0)) \quad (2.80)$$

as the *order parameter*, which characterizes the phase transition. The *phase regions* correspond to areas of qualitatively distinct behaviour of  $\rho_\infty$  as a function of  $\rho_l$  and  $\rho_r$ .



- (I) *High density phase*: The limiting density  $\rho_\infty = \rho_r$ , since particles drifting to the right are jamming behind the region of high density.
- (II) *Low density phase*: The limiting density is  $\rho_\infty = \rho_l$ , since particles can drift to the right without jamming.
- (III) *Maximum current phase*: The solution to the PDE is a rarefaction fan with negative (positive) characteristic velocity  $u$  on the left (right). Thus the limiting density is given by the density  $1/2$  with vanishing  $u(1/2) = 0$ .

The dashed blue line is a continuous phase transition line, i.e. crossing this line the function  $\rho_\infty(\rho_l, \rho_r)$  is continuous. The full red line is a first order transition line, across which the density jumps from  $\rho_l < 1/2$  to  $\rho_r > 1/2$ . The exact behaviour of the system on that line is discussed in the next section.

Above the dashed diagonal the solutions of the conservation law (2.66) are given by shocks, and below by rarefaction fans.

## 2.4 Open boundaries and matrix product ansatz

In the following we consider the ASEP on the lattice  $\Lambda_L = \{1, \dots, L\}$  with *open boundary conditions*. So in addition to the bulk rates

$$10 \xrightarrow{p} 01 \quad \text{and} \quad 01 \xrightarrow{q} 10, \quad (2.81)$$

we have to specify boundary rates for creation and annihilation of particles at sites  $x = 1$  and  $L$ ,

$$|0 \xrightarrow{\alpha} |1, \quad |1 \xrightarrow{\gamma} |0, \quad |1 \xrightarrow{\beta} 0| \quad \text{and} \quad 0| \xrightarrow{\delta} 1|. \quad (2.82)$$

In principle we are free to choose  $\alpha, \beta, \gamma$  and  $\delta \geq 0$  independently. We would like to model the situation where the system is coupled to *particle reservoirs* at both ends with densities  $\rho_l$  and  $\rho_r \in [0, 1]$ , which implies

$$\alpha = \rho_l p, \quad \gamma = q(1 - \rho_l), \quad \beta = p(1 - \rho_r) \quad \text{and} \quad \delta = q\rho_r. \quad (2.83)$$

The generator of the process is then given by the sum

$$\begin{aligned} \mathcal{L}f(\eta) &= \mathcal{L}_{bulk}f(\eta) + \mathcal{L}_{bound}f(\eta) = \\ &= \sum_{x=1}^{L-1} \left( p\eta(x)(1 - \eta(x+1)) - q\eta(x+1)(1 - \eta(x)) \right) (f(\eta^{x,x+1}) - f(\eta)) + \\ &\quad + \left( p\rho_l(1 - \eta(1)) - q\eta(1)(1 - \rho_l) \right) (f(\eta^1) - f(\eta)) + \\ &\quad + \left( p\eta(L)(1 - \rho_r) - q\rho_r(1 - \eta(L)) \right) (f(\eta^L) - f(\eta)). \end{aligned} \quad (2.84)$$

Note that for  $\rho_l, \rho_r \in (0, 1)$  the conservation law is broken at the boundaries and the ASEP is a finite state irreducible Markov chain on  $X_L = \{0, 1\}^{\Lambda_L}$ . Therefore with Prop. 1.10 the process is ergodic and has a unique stationary measure  $\mu_L = \mu_L(\rho_l, \rho_r)$  depending on the boundary parameters.

Following the analysis of the previous section, the scaled stationary density profile

$$\rho(y) := \lim_{L \rightarrow \infty} \mu_L(1_{[yL]}) \quad \text{with } y \in [0, 1] \quad (2.85)$$

should be a stationary solution of the conservation law (2.66). This is given by the boundary value problem

$$0 = \partial_y f(\rho(y)) = (p - q)(1 - 2\rho(y))\partial_y \rho(y) \quad \text{with} \quad \rho(0) = \rho_l, \quad \rho(1) = \rho_r, \quad (2.86)$$

which has constant solutions. This is a first order equation which is not well posed having two boundary conditions  $\rho_l \neq \rho_r$ . So jumps at the boundary cannot be avoided and obviously the solution can be any arbitrary constant. Again one can apply the viscosity method as in the previous section to get a unique solution for all  $\epsilon > 0$  and retrieve a unique admissible stationary profile  $\rho(y)$  in the limit  $\epsilon \rightarrow 0$ .

Understanding the motion of shocks and rarefaction fans, we can derive the stationary profile  $\rho(y)$  also from the time dependent solution  $\rho(y, t)$  in the limit  $t \rightarrow \infty$ . As initial condition we can choose

$$\rho_0(y) = \begin{cases} \rho_l & , 0 \leq y \leq a \\ \rho_r & , a < y \leq 1 \end{cases} \quad \text{for some } a \in (0, 1). \quad (2.87)$$



Then the macroscopic stationary profile  $\rho(y) = \rho_{bulk}$  is given by a constant that corresponds exactly to the densities observed in Theorem 2.6 for the infinite system, i.e.

$$\rho_{bulk} = \begin{cases} \rho_r & , \rho_r \geq \frac{1}{2}, \rho_l > 1 - \rho_r & \text{(high density)} \\ \rho_l & , \rho_l \leq \frac{1}{2}, \rho_r < 1 - \rho_r & \text{(low density)} \\ 1/2 & , \rho_l \geq \frac{1}{2}, \rho_r \leq \frac{1}{2} & \text{(maximum current)} \end{cases} . \quad (2.88)$$

In contrast to the previous section this is only correct in the scaling limit. For finite  $L$  boundary effects produce visible deviations and in particular correlations. So the stationary measure is not of product form, except for the trivial case  $\rho_l = \rho_r$ .

A very powerful ansatz to represent the non-product stationary distribution in this case is given by using products of matrices.

**Theorem 2.7** Consider the ASEP on  $\Lambda_L = \{0, \dots, L\}$  with boundary densities  $\rho_l, \rho_r \in (0, 1)$  and bulk rates  $p, q$ . Suppose that the (possibly infinite) matrices  $D, E$  and vectors  $\mathbf{w}, \mathbf{v}$  satisfy

$$\begin{aligned} pDE - qED &= D + E \\ \mathbf{w}^T (\rho_l p E - (1 - \rho_l) q D) &= \mathbf{w} \\ ((1 - \rho_r) p D - \rho_r q E) \mathbf{v} &= \mathbf{v} . \end{aligned} \quad (2.89)$$

These relations are called a **quadratic algebra**. For  $\eta \in X_L$  put

$$g_L(\eta) = \mathbf{w}^T \prod_{x=1}^L (\eta(x) D + (1 - \eta(x)) E) \mathbf{v} . \quad (2.90)$$

If this is a well defined number in  $\mathbb{R}$  for all  $\eta \in X_L$  and the normalization

$$Z_L = \sum_{\eta \in X_L} g_L(\eta) \neq 0 , \quad (2.91)$$

then the stationary distribution of the ASEP is given by  $\mu_L(\eta) = g_L(\eta)/Z_L$ .

The matrices are purely auxiliary and have no interpretation in terms of the particle system.

**Proof.**  $(\eta_t : t \geq 0)$  is a finite state irreducible MC and has a unique stationary measure  $\mu_L$ , given by the stationary solution of the master equation

$$\frac{d}{dt} \mu_L(\eta) = 0 = \sum_{\eta' \in X_L} (\pi_L(\eta') c(\eta', \eta) - \pi_L(\eta) c(\eta, \eta')) \quad \text{for all } \eta \in X_L . \quad (2.92)$$

(This is the stationarity condition  $\mu_L(\mathcal{L}f) = 0$  for  $f = \mathbb{1}_\eta$ .)

Therefore it suffices to show that  $g_L$  given in (2.90) fulfills the master equation, then it can automatically be normalized. In our case the (unnormalized) individual terms in the sum are of the form

$$g_L(\eta^{x,x+1}) c(x, x+1, \eta^{x,x+1}) - g_L(\eta) c(x, x+1, \eta) \quad (2.93)$$

for the bulk and similar for the boundaries. They can be simplified using the quadratic algebra (2.89). Using the first rule we get for the bulk

$$\begin{aligned} g_L(\dots, 0, 1, \dots) q - g_L(\dots, 1, 0, \dots) p &= -g_{L-1}(\dots, 1, \dots) - g_{L-1}(\dots, 0, \dots) \quad \text{and} \\ g_L(\dots, 1, 0, \dots) p - g_L(\dots, 0, 1, \dots) q &= g_{L-1}(\dots, 1, \dots) + g_{L-1}(\dots, 0, \dots) . \end{aligned} \quad (2.94)$$

In general we can write for  $x \in \{1, \dots, L-1\}$

$$g_L(\eta^{x,x+1})c(\eta^{x,x+1}, \eta) - g_L(\eta)c(\eta, \eta^{x,x+1}) = (1 - 2\eta(x))g_{L-1}(\dots, \eta(x-1), \eta(x), \dots) - (1 - 2\eta(x+1))g_{L-1}(\dots, \eta(x), \eta(x+1), \dots). \quad (2.95)$$

For the boundaries we get analogously

$$g_L(\eta^1)c(1, \eta^1) - g_L(\eta)c(1, \eta) = -(1 - 2\eta(1))g_{L-1}(\eta(2), \dots) \quad \text{and} \\ g_L(\eta^L)c(L, \eta^L) - g_L(\eta)c(L, \eta) = (1 - 2\eta(L))g_{L-1}(\dots, \eta(L-1)). \quad (2.96)$$

The sum over all  $x \in \Lambda_L$  corresponds to the right-hand side of (2.92), and vanishes since it is a telescoping series.  $\square$

If the system is reversible then the terms (2.93) vanish individually. In the general non-reversible case they are therefore called **defects from reversibility**, and the quadratic algebra provides a simplification of those in terms of distributions for smaller system sizes.

The normalization is given by

$$Z_L = \mathbf{w}^T C^L \mathbf{v} \quad \text{with} \quad C = D + E \quad (2.97)$$

and correlation functions can be computed as

$$\rho(x) = \mu_L(1_x) = \frac{\mathbf{w}^T C^{x-1} D C^{L-x} \mathbf{v}}{\mathbf{w}^T C^L \mathbf{v}} \quad (2.98)$$

or for higher order with  $x > y$ ,

$$\mu_L(1_x 1_y) = \frac{\mathbf{w}^T C^{x-1} D C^{y-x-1} D C^{L-y} \mathbf{v}}{\mathbf{w}^T C^L \mathbf{v}}. \quad (2.99)$$

In particular for the stationary current we get

$$j(x) = \frac{\mathbf{w}^T C^{x-1} (pDE - qED) C^{L-x-1} \mathbf{v}}{\mathbf{w}^T C^L \mathbf{v}} = \frac{\mathbf{w}^T C^{L-1} \mathbf{v}}{\mathbf{w}^T C^L \mathbf{v}} = \frac{Z_{L-1}}{Z_L}, \quad (2.100)$$

which is independent of the lattice site as expected.

For  $\rho_l = \rho_r = \rho$  and  $p \neq q$  the algebra (2.89) is fulfilled by the one-dimensional matrices

$$E = \frac{1}{\rho(p-q)}, \quad D = \frac{1}{(1-\rho)(p-q)} \quad \text{and} \quad w = v = 1 \quad (2.101)$$

since

$$pDE - qED = \frac{(p-q)}{(p-q)^2 \rho(1-\rho)} = \frac{1}{(p-q)\rho(1-\rho)} = D + E = C \quad (2.102)$$

and  $\rho pE - (1-\rho)qD = (1-\rho)pD - \rho qE = 1$ .

$E, D \in \mathbb{R}$  implies that  $\mu_L$  is a product measure, and the density is not surprising,

$$\rho(x) = \rho(1) = \frac{DC^{L-1}}{C^L} = \rho \quad \text{so} \quad \mu_L = \nu_\rho. \quad (2.103)$$

In general  $\mu_L$  is a product measure if and only if there exist scalars  $E, D$  fulfilling the algebra (2.89), and it turns out that for  $\rho_l \neq \rho_r$  this is not the case.

In the following let's focus on the totally asymmetric case  $p = 1, q = 0$  (TASEP) with  $\rho_l, \rho_r \in (0, 1)$ . The algebra simplifies to

$$DE = D + E, \quad \mathbf{w}^T E = \frac{1}{\rho_l} \mathbf{w}^T, \quad D\mathbf{v} = \frac{1}{1-\rho_r} \mathbf{v}. \quad (2.104)$$

The question is what kind of matrices fulfill these relations.

**Proposition 2.8** For  $p = 1, q = 0$ , if  $E, D$  are finite dimensional, then they commute.

**Proof.** Suppose  $u$  satisfies  $Eu = u$ . Then by the first identity  $Du = Du + u$  and hence  $u = 0$ . Therefore  $E - I$  is invertible and we can solve the first identity

$$D = E(E - I)^{-1} \quad \text{which implies that } D \text{ and } E \text{ commute.} \quad \square \quad (2.105)$$

So  $D$  and  $E$  have to be infinite dimensional, and possible choices are

$$D = \begin{pmatrix} 1 & 1 & 0 & 0 & \dots \\ 0 & 1 & 1 & 0 & \dots \\ 0 & 0 & 1 & 1 & \dots \\ \vdots & \vdots & \ddots & \ddots & \ddots \end{pmatrix}, \quad E = \begin{pmatrix} 1 & 0 & 0 & 0 & \dots \\ 1 & 1 & 0 & 0 & \dots \\ 0 & 1 & 1 & 0 & \dots \\ \vdots & \vdots & \ddots & \ddots & \ddots \end{pmatrix} \quad (2.106)$$

with corresponding vectors

$$\mathbf{w}^T = \left( 1, \frac{1 - \rho_l}{\rho_l}, \left( \frac{1 - \rho_l}{\rho_l} \right)^2, \dots \right) \quad \text{and} \quad \mathbf{v}^T = \left( 1, \frac{\rho_r}{1 - \rho_r}, \left( \frac{\rho_r}{1 - \rho_r} \right)^2, \dots \right). \quad (2.107)$$

Correlation functions can be computed without using any representations by repeatedly applying the algebraic relations. Using the rules

$$DE = C, \quad DC = D^2 + C, \quad CE = C + E^2 \quad \text{and} \\ \mathbf{w}^T E^k = \frac{1}{\rho_l^k} \mathbf{w}^T, \quad D^k \mathbf{v} = \frac{1}{(1 - \rho_r)^k} \mathbf{v}, \quad (2.108)$$

the probability of every configuration can be written as a combination of terms of the form  $Z_k = \mathbf{w}^T C^k \mathbf{v}$ . Explicit formulas can be derived which look rather complicated, for the current we get the following limiting behaviour,

$$j = \frac{Z_{L-1}}{Z_L} \rightarrow \begin{cases} \rho_r(1 - \rho_r) & , \rho_r > 1/2, \rho_l > 1 - \rho_r \\ \rho_l(1 - \rho_l) & , \rho_l < 1/2, \rho_r < 1 - \rho_l \\ 1/4 & , \rho_r \leq 1/2, \rho_l \geq 1/2 \end{cases} \quad \text{as } L \rightarrow \infty. \quad (2.109)$$

This is consistent with the hydrodynamic result. Using the MPA one can show rigorously.

**Theorem 2.9** Suppose  $p = 1, q = 0$  and let  $x_L$  be a monotone sequence of integers such that  $x_L \rightarrow \infty$  and  $L - x_L \rightarrow \infty$  for  $L \rightarrow \infty$ . Then

$$\mu_L \tau_{x_L} \rightarrow \begin{cases} \nu_{\rho_r} & , \rho_r > 1/2, \rho_l > 1 - \rho_r \\ \nu_{\rho_l} & , \rho_l < 1/2, \rho_r < 1 - \rho_l \\ \nu_{1/2} & , \rho_r \leq 1/2, \rho_l \geq 1/2 \end{cases} \quad \text{weakly, locally.} \quad (2.110)$$

If  $\rho_l < 1/2 < \rho_r$  and  $\rho_l + \rho_r = 1$  (first order transition line), then

$$\mu_L \tau_{x_L} \rightarrow (1 - a)\nu_{\rho_l} + a\nu_{\rho_r} \quad \text{where} \quad a = \lim_{L \rightarrow \infty} \frac{x_L}{L}. \quad (2.111)$$

**Proof.** see [L99], Section III.3

Note that on the first order transition line we have a shock measure with diffusing shock location, where the left part of the system has distribution  $\nu_{\rho_l}$  and the right part  $\nu_{\rho_r}$ . This phenomenon is called *phase coexistence*, and is described by a mixture of the form (2.111).

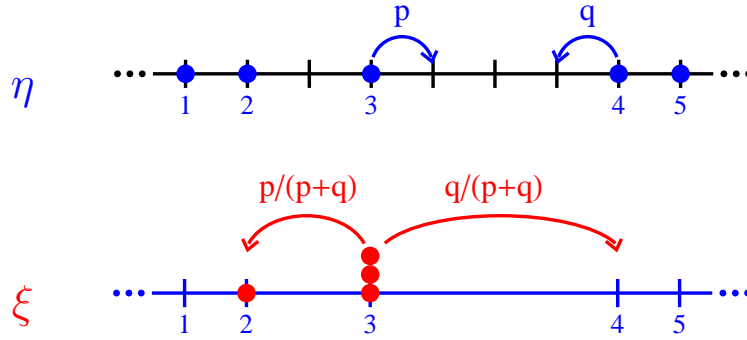
### 3 Zero-range processes

#### 3.1 From ASEP to ZRPs

Consider the ASEP on the lattice  $\Lambda_L = \mathbb{Z}/L\mathbb{Z}$ . For each configuration  $\eta \in X_L = \{0, 1\}^{\Lambda_L}$  label the particles  $j = 1, \dots, N$  with  $N = \sum_{x \in \Lambda_L} \eta_x$  and let  $x_j \in \Lambda_L$  be the position of the  $j$ th particle. We attach the labels such that the positions are ordered  $x_1 < \dots < x_N$ . We map the configuration  $\eta$  to a configuration  $\xi \in \mathbb{N}^{\Lambda_N}$  on the lattice  $\Lambda_N = \{1, \dots, N\}$  by

$$\xi(j) = x_{j+1} - x_j - 1. \quad (3.1)$$

Here the lattice site  $j \in \Lambda_N$  corresponds to particle  $j$  in the ASEP and  $\xi_j \in \mathbb{N}$  to the distance to the next particle  $j + 1$ . Note that  $\eta$  and  $\xi$  are equivalent descriptions of an ASEP configuration up to the position  $x_1$  of the first particle.



As can be seen from the construction, the dynamics of the ASEP ( $\eta_t : t \geq 0$ ) induce a process ( $\xi_t : t \geq 0$ ) on the state space  $\mathbb{N}^{\Lambda_N}$  with rates

$$c(\xi, \xi^{j \rightarrow j+1}) = q(1 - \delta_{0, \xi(j)}) \quad \text{and} \quad c(\xi, \xi^{j \rightarrow j-1}) = p(1 - \delta_{0, \xi(j)}), \quad (3.2)$$

where we write  $\xi^{x \rightarrow y} = \begin{cases} \xi(x) - 1, & z = x \\ \xi(y) + 1, & z = y \\ \xi(z), & z \neq x, y \end{cases}$ .

Since the order of particles in the ASEP is conserved, we have  $\xi_t(j) \geq 0$  and therefore  $\xi_t \in \mathbb{N}^{\Lambda_N}$  for all  $t \geq 0$ . Note also that the number of  $\xi$ -particles is

$$\sum_{j \in \Lambda_N} \xi(j) = L - N = \text{number of wholes in ASEP}, \quad (3.3)$$

which is conserved in time, and therefore ( $\xi_t : t \geq 0$ ) is a lattice gas. There is no exclusion interaction for this process, i.e. the number of particles per site is not restricted. With analogy to quantum mechanics this process is sometimes called a *bosonic* lattice gas, whereas the ASEP is a *fermionic* system.

The  $\xi$ -process defined above is an example of a more general class of bosonic lattice gases, zero-range processes, which we introduce in the following. From now on we will switch back to our usual notation denoting configurations by  $\eta$  and lattice sizes by  $L$ .

**Definition 3.1** Consider a lattice  $\Lambda$  (any discrete set) and the state space  $X = \mathbb{N}^\Lambda$ . Let  $p(x, y)$  be the transition probabilities of a single random walker on  $\Lambda$  with  $p(x, x) = 0$ , called the *jump probabilities*. For each  $x \in \Lambda$  define the *jump rates*  $g_x : \mathbb{N} \rightarrow [0, \infty)$  as a non-negative function of the number of particles  $\eta(x)$  at site  $x$ . Then the process  $(\eta_t : t \geq 0)$  on  $X$  defined by the generator

$$\mathcal{L}f(\eta) = \sum_{x, y \in \Lambda} g_x(\eta(x))p(x, y)(f(\eta^{x \rightarrow y}) - f(\eta)) \quad (3.4)$$

is called a *zero-range process (ZRP)*.

The interpretation of the generator is that each site  $x$  loses a particle with rate  $g(\eta(x))$ , which then jumps to a site  $y$  with probability  $p(x, y)$ . For this description to make sense we set  $g(0) = 0$ , to avoid occurrence of negative occupation numbers. In addition we also want to assure that the process is *non-degenerate*, so we also assume that  $p(x, y)$  is irreducible on  $\Lambda$  and

$$g_x(n) = 0 \quad \Leftrightarrow \quad n = 0 \quad \text{for all } x \in \Lambda . \quad (3.5)$$

**Remarks.**

- ZRPs are interacting random walks with *zero-range* interaction, since the jump rate of a particle at site  $x \in \Lambda$  depends only on the number of particles  $\eta(x)$  at that site.
- The above  $\xi$ -process is a simple example of a (non-degenerate) ZRP with  $\Lambda = \mathbb{Z}/N\mathbb{Z}$  and

$$g_x(n) \equiv p + q , \quad p(x, x + 1) = \frac{q}{p + q} \quad \text{and} \quad p(x, x - 1) = \frac{p}{p + q} . \quad (3.6)$$

- On finite lattices  $\Lambda_L$  of size  $L$ , non-degeneracy implies that ZRPs are irreducible finite state Markov chains on

$$X_{L, N} = \{ \eta \in \mathbb{N}^{\Lambda_L} \mid \Sigma_L(\eta) = N \} \quad (3.7)$$

for all fixed particle numbers  $N \in \mathbb{N}$  (remember the shorthand  $\Sigma_L(\eta) = \sum_{x \in \Lambda_L} \eta(x)$ ). Therefore they have a unique stationary distribution  $\pi_{L, N}$  on  $X_{L, N}$ .

On infinite lattices the number of particles is in general also infinite, but as opposed to exclusion processes the local state space of a ZRP is  $\mathbb{N}$ . This is not compact, and therefore in general also  $X$  is not compact and the construction of the process with semigroups and generators given in Chapter 1 does not apply directly and has to be modified.

In addition to non-degeneracy (3.5) we assume a sub-linear growth of the jump rates, i.e.

$$\bar{g} := \sup_{x \in \Lambda} \sup_{n \in \mathbb{N}} |g_x(n + 1) - g_x(n)| < \infty , \quad (3.8)$$

and restrict to the state space

$$X_\alpha = \{ \eta \in \mathbb{N}^\Lambda \mid \|\eta\|_\alpha < \infty \} \quad \text{with} \quad \|\eta\|_\alpha = \sum_{x \in \Lambda} |\eta(x)| \alpha^{|x|} \quad (3.9)$$

for some  $\alpha \in (0, 1)$ . Let  $L(X) \subseteq C(X)$  be the set of *Lipshitz-continuous* test functions  $f : X_\alpha \rightarrow \mathbb{R}$ , i.e.

$$|f(\eta) - f(\zeta)| \leq l(f) \|\eta - \zeta\|_\alpha \quad \text{for all } \eta, \zeta \in X_\alpha . \quad (3.10)$$

**Theorem 3.1** Under the above conditions (3.8) to (3.10) the generator  $\mathcal{L}$  given in (3.4) is well-defined for  $f \in L(X) \cap C_0(X)$  and generates a Markov semigroup  $(S(t) : t \geq 0)$  on  $L(X)$  which uniquely specifies a ZRP  $(\eta_t : t \geq 0)$ .

**Proof.** Andjel (1982). The proof includes in particular the statement that  $\eta_0 \in X_\alpha$  implies  $\eta_t \in X_\alpha$  for all  $t \geq 0$ , which follows from showing that the semigroup is contractive, i.e.

$$|S(t)f(\eta) - S(t)f(\zeta)| \leq l(f)e^{3\bar{g}t/(1-\alpha)}\|\eta - \zeta\|_\alpha .$$

**Remarks.**

- Let  $\mu$  be a measure on  $\mathbb{N}^\Lambda$  with density

$$\mu(\eta(x)) \leq C_1 C_2^{|x|} \quad \text{for some } C_1, C_2 > 0 \quad (3.11)$$

(this includes in particular uniformly bounded densities). Then for all  $\alpha < 1/C_1$  we have  $\mu(X_\alpha) = 1$ , so the restricted state space is very large and contains most cases of interest.

- The conditions (3.8) to (3.10) are sufficient but not necessary, in particular (3.8) can be relaxed when looking on regular lattices and imposing a finite range condition on  $p(x, y)$ .

### 3.2 Stationary measures

Let  $(\eta_t : t \geq 0)$  be a (non-degenerate, well defined) ZRP on a lattice  $\Lambda$  with jump probabilities  $p(x, y)$  and jump rates  $g_x$ .

**Lemma 3.2** There exists a positive harmonic function  $\lambda = (\lambda_x : x \in \Lambda)$  such that

$$\sum_{y \in \Lambda} p(y, x) \lambda_y = \lambda_x , \quad (3.12)$$

which is unique up to multiples.

**Proof.** Existence of non-negative  $\lambda_x$  follows directly from  $p(x, y)$  being the transition probabilities of a random walk on  $\Lambda$ , irreducibility of  $p(x, y)$  implies uniqueness up to multiples and strict positivity.  $\square$

Note that we do not assume  $\lambda$  to be normalizable, which is only the case if the corresponding random walk is positive recurrent. Since (3.12) is homogeneous, every multiple of  $\lambda$  is again a solution. In the following we fix  $\lambda_0 = 1$  (for some lattice site  $0 \in \Lambda$ , say the origin) and denote the one-parameter family of solutions to (3.12) by

$$\{\phi\lambda : \phi \geq 0\} , \quad (3.13)$$

where the parameter  $\phi$  is called the *fugacity*.

**Theorem 3.3** For each  $\phi \geq 0$ , the product measure  $\nu_\phi$  with marginals

$$\nu_\phi^x(\eta(x) = n) = \frac{w_x(n)(\phi\lambda_x)^n}{z_x(\phi)} \quad \text{and} \quad w_x(n) = \prod_{k=1}^n \frac{1}{g_x(k)} \quad (3.14)$$

is stationary, provided that the local normalization (also called **partition function**)

$$z_x(\phi) = \sum_{n=0}^{\infty} w_x(n)(\phi\lambda_x)^n < \infty \quad \text{for all } x \in \Lambda. \quad (3.15)$$

**Proof.** To simplify notation in the proof we will write

$$\nu_\phi^x(n) := \nu_\phi^x(\eta(x) = n), \quad (3.16)$$

and we will assume that  $\Lambda$  is finite. Our argument can be immediately extended to infinite lattices. First note that using  $w_x(n) = 1 / \prod_{k=1}^n g_x(k)$  we have for all  $n \geq 0$

$$\nu_\phi^x(n+1) = \frac{1}{z_x(\phi)} w_x(n+1)(\phi\lambda_x)^{n+1} = \frac{\phi\lambda_x}{g_x(n+1)} \nu_\phi^x(n). \quad (3.17)$$

We have to show that for all cylinder test functions  $f$

$$\nu_\phi(\mathcal{L}f) = \sum_{\eta \in X} \sum_{x,y \in \Lambda} g_x(\eta(x)) p(x,y) (f(\eta^{x \rightarrow y}) - f(\eta)) \nu_\phi(\eta) = 0, \quad (3.18)$$

which will be done by two changes of variables.

1. For all  $x, y \in \Lambda$  we change variables in the sum over  $\eta$

$$\sum_{\eta \in X} g_x(\eta(x)) p(x,y) f(\eta^{x \rightarrow y}) \nu(\eta) = \sum_{\eta \in X} g_x(\eta(x) + 1) p(x,y) f(\eta) \nu(\eta^{y \rightarrow x}). \quad (3.19)$$

Using (3.17) we have

$$\begin{aligned} \nu(\eta^{y \rightarrow x}) &= \nu_\phi^x(\eta(x) + 1) \nu_\phi^y(\eta(y) - 1) \prod_{z \neq x,y} \nu_\phi^z(\eta(z)) = \\ &= \frac{\phi\lambda_x}{g_x(\eta(x) + 1)} \nu_\phi^x(\eta(x)) \frac{g_y(\eta(y))}{\phi\lambda_y} \nu_\phi^y(\eta(y)) \prod_{z \neq x,y} \nu_\phi^z(\eta(z)) = \\ &= \nu_\phi(\eta) \frac{\lambda_x g_y(\eta(y))}{\lambda_y g_x(\eta(x))}. \end{aligned} \quad (3.20)$$

Plugging this into (3.18) we get

$$\nu_\phi(\mathcal{L}f) = \sum_{\eta \in X} f(\eta) \nu_\phi(\eta) \sum_{x,y \in \Lambda} \left( g_y(\eta(y)) p(x,y) \frac{\lambda_x}{\lambda_y} - g_x(\eta(x)) p(x,y) \right). \quad (3.21)$$

2. Exchanging summation variables  $x \leftrightarrow y$  in the first part of the above sum we get

$$\nu_\phi(\mathcal{L}f) = \sum_{\eta \in X} f(\eta) \nu_\phi(\eta) \sum_{x \in \Lambda} \frac{g_x(\eta(x))}{\lambda_x} \sum_{y \in \Lambda} (p(y,x) \lambda_y - p(x,y) \lambda_x) = 0, \quad (3.22)$$

since

$$\sum_{y \in \Lambda} (p(y,x) \lambda_y - p(x,y) \lambda_x) = \sum_{y \in \Lambda} (p(y,x) \lambda_y) - \lambda_x = 0. \quad (3.23)$$

Note that terms of the form  $\nu_\phi^y(-1)$  do not appear in the above sums, since  $g_y(0) = 0$ .  $\square$

**Example.** Take  $\Lambda = \Lambda_L = \mathbb{Z}/L\mathbb{Z}$ ,  $p(x, y) = p\delta_{y, x+1} + q\delta_{y, x-1}$  and  $g_x(k) = 1 - \delta_{k, 0}$  corresponding to nearest-neighbour jumps on a one-dimensional lattice with periodic boundary conditions. Then we have  $\lambda_x = 1$  for all  $x \in \Lambda_L$  and the stationary weights are just  $w_x(n) = 1$  for all  $n \geq 0$ . So the stationary product measures  $\nu_\phi$  have geometric marginals

$$\nu_\phi^x(\eta(x) = n) = (1 - \phi)\phi^n \quad \text{since} \quad z_x(\phi) = \sum_{k=0}^{\infty} \phi^k = \frac{1}{1 - \phi}, \quad (3.24)$$

which are well defined for all  $\phi \in [0, 1)$ .

**Remarks.**

- The partition function  $z_x(\phi) = \sum_{n=0}^{\infty} w_x(n)(\phi\lambda_x)^n$  is a power series with radius of convergence

$$r_x = \left( \limsup_{n \rightarrow \infty} w_x(n)^{1/n} \right)^{-1} \quad \text{and so} \quad z_x(\phi) < \infty \quad \text{if} \quad \phi < r_x/\lambda_x. \quad (3.25)$$

If  $g_x^\infty = \lim_{k \rightarrow \infty} g_x(k)$  exists, we have

$$w_x(n)^{1/n} = \left( \prod_{k=1}^n g_x(k)^{-1} \right)^{1/n} = \exp\left(-\frac{1}{n} \sum_{k=1}^n \log g_x(k)\right) \rightarrow 1/g_x^\infty \quad (3.26)$$

as  $n \rightarrow \infty$ , so that  $r_x = g_x^\infty$ .

- The density at site  $x \in \Lambda$  is given by

$$\rho_x(\phi) = \nu_\phi^x(\eta(x)) = \frac{1}{z_x(\phi)} \sum_{k=1}^{\infty} k w_x(k) (\phi\lambda_x)^k. \quad (3.27)$$

Multiplying the coefficients  $w_x(k)$  by  $k$  (or any other polynomial) does not change the radius of convergence of the power series and therefore  $\rho_x(\phi) < \infty$  for all  $\phi < r_x/\lambda_x$ .

Furthermore  $\rho_x(0) = 0$  and it can be shown that  $\rho_x(\phi)$  is a monotone increasing function of  $\phi$  (see problem sheet). Note that for  $\phi > r_x/\lambda_x$  the partition function and  $\rho_x(\phi)$  diverge, but for  $\phi = r_x/\lambda_x$  convergence or divergence are possible.

- With Def. 2.4 the expected stationary current across a bond  $(x, y)$  is given by

$$j(x, y) = \nu_\phi^x(g_x) p(x, y) - \nu_\phi^y(g_y) p(y, x), \quad (3.28)$$

and using the form  $w_x(n) = 1/\prod_{k=1}^n g_x(k)$  of the stationary weight we have

$$\nu_\phi^x(g_x) = \frac{1}{z_x(\phi)} \sum_{n=1}^{\infty} g_x(n) w_x(n) (\phi\lambda_x)^n = \frac{\phi\lambda_x}{z_x(\phi)} \sum_{n=1}^{\infty} w_x(n-1) (\phi\lambda_x)^{n-1} = \phi\chi_x^{\lambda_x} \quad (3.29)$$

So the current is given by

$$j(x, y) = \phi(\lambda_x p(x, y) - \lambda_y p(y, x)), \quad (3.30)$$

which is proportional to the fugacity  $\phi$  and the stationary probability current of a single random walker.



**Example.** For the above example with  $\Lambda_L = \mathbb{Z}/L\mathbb{Z}$ ,  $p(x, y) = p\delta_{y, x+1} + q\delta_{y, x-1}$  and  $g_x(k) = 1 - \delta_{k, 0}$  the density is

$$\rho_x(\phi) = (1 - \phi) \sum_{k=1}^{\infty} k\phi^k = \frac{\phi}{1 - \phi} \quad (3.31)$$

and the current  $j(x, x+1) = \phi(p - q)$  for all  $x \in \Lambda_L$ . As we have seen before in one-dimensional systems the stationary current is bond-independent.

### 3.3 Equivalence of ensembles and relative entropy

In this section let  $(\eta_t : t \geq 0)$  be a homogeneous ZRP on the lattice  $\Lambda_L = \mathbb{Z}/L\mathbb{Z}$  with state space  $X_L = \mathbb{N}^{\Lambda_L}$ , jump rates  $g_x(n) \equiv g(n)$  and translation invariant jump probabilities  $p(x, y) = q(y - x)$ . This implies that the stationary product measures  $\nu_\phi$  given in Theorem 3.3 are translation with marginals

$$\nu_\phi^x(\eta(x) = n) = \frac{w(n)\phi^n}{z(\phi)}. \quad (3.32)$$

Analogous to Section 2.1 for exclusion processes, the family of measures

$$\{\nu_\phi : \phi \in [0, \phi_c)\} \quad \text{is called } \mathbf{grand-canonical ensemble}, \quad (3.33)$$

where  $\phi_c$  is the radius of convergence of the partition function  $z(\phi)$  (called  $r_x$  in the previous section for more general processes). We further assume that the jump rates are bounded away from 0, i.e.  $g(k) \geq C$  for  $k > 0$ , which implies that  $\phi_c > 0$  using (3.26). The particle density  $\rho(\phi)$  is characterized uniquely by the fugacity  $\phi$  as given in (3.27)

As noted before the ZRP is irreducible on

$$X_{L, N} = \{\eta \in \mathbb{N}^{\Lambda_L} \mid \Sigma_L(\eta) = N\} \quad (3.34)$$

for all fixed particle numbers  $N \in \mathbb{N}$ . It has a unique stationary measure  $\pi_{L, N}$  on  $X_{L, N}$  given by

$$\pi_{L, N}(\eta) = \frac{1}{Z_{L, N}} \prod_{x \in \Lambda_L} w(\eta(x)) \delta(\Sigma_L(\eta), N), \quad (3.35)$$

with *canonical partition function*  $Z_{L, N} = \sum_{\eta \in X_{L, N}} \prod_x w(\eta(x))$ .

The family of measures

$$\{\pi_{L, N} : N \in \mathbb{N}\} \quad \text{is called } \mathbf{canonical ensemble}. \quad (3.36)$$

In general these two ensembles are expected to be 'equivalent' as  $L \rightarrow \infty$ , in vague analogy to the law of large numbers for iid random variables. We will make this precise in the following. To do this we need to quantify the 'distance' of two probability measures.

**Definition 3.2** Let  $\mu_1, \mu_2 \in \mathcal{P}(\Omega)$  be two probability measures on a countable space  $\Omega$ . Then the *relative entropy* of  $\mu_1$  w.r.t.  $\mu_2$  is defined as

$$H(\mu_1; \mu_2) = \begin{cases} \mu_1 \left( \log \frac{\mu_1}{\mu_2} \right) = \sum_{\omega \in \Omega} \mu_1(\omega) \log \frac{\mu_1(\omega)}{\mu_2(\omega)} & , \text{ if } \mu_1 \ll \mu_2 \\ \infty & , \text{ if } \mu_1 \not\ll \mu_2 \end{cases}, \quad (3.37)$$

where  $\mu_1 \ll \mu_2$  is a shorthand for  $\mu_2(\omega) = 0 \Rightarrow \mu_1(\omega) = 0$  (called *absolute continuity*).

**Lemma 3.4 Properties of relative entropy**

Let  $\mu_1, \mu_2 \in \mathcal{P}(\Omega)$  be two probability measures on a countable space  $\Omega$ .

(i) **Non-negativity:**

$$H(\mu_1; \mu_2) \geq 0 \quad \text{and} \quad H(\mu_1; \mu_2) = 0 \Leftrightarrow \mu_1(\omega) = \mu_2(\omega) \text{ for all } \omega \in \Omega.$$

(ii) **Sub-additivity:**

Suppose  $\Omega = S^\Lambda$  with some local state space  $S \subseteq \mathbb{N}$  and a lattice  $\Lambda$ . Then for  $\Delta \subseteq \Lambda$  and marginals  $\mu_i^\Delta$ ,  $H(\mu_1^\Delta; \mu_2^\Delta)$  is increasing in  $\Delta$  and

$$H(\mu_1; \mu_2) \geq H(\mu_1^\Delta; \mu_2^\Delta) + H(\mu_1^{\Lambda \setminus \Delta}; \mu_2^{\Lambda \setminus \Delta}). \quad (3.38)$$

If  $\mu_1$  and  $\mu_2$  are product measures, then equality holds.

(iii) **Entropy inequality:**

For all bounded  $f \in C_b(\Omega)$  and all  $\epsilon > 0$  we have

$$\mu_1(f) \leq \frac{1}{\epsilon} \left( \log \mu_2(e^{\epsilon f}) + H(\mu_1; \mu_2) \right). \quad (3.39)$$

**Proof.** In the following let  $\mu_1 \ll \mu_2$  and  $h(\omega) = \mu_1(\omega)/\mu_2(\omega) \geq 0$ .

(i) Then

$$H(\mu_1; \mu_2) = \mu_2(h \log h) = \mu_2(\phi(h)) \quad \text{with} \quad \phi(u) := u \log u + 1 - u, \quad (3.40)$$

since  $\mu_2(1 - h) = 1 - \mu_1(1) = 1 - 1 = 0$ . Elementary properties of  $\phi$  are

$$\phi(u) \geq 0 \text{ for } u \geq 0 \quad \text{and} \quad \phi(u) = 0 \Leftrightarrow u = 1, \quad (3.41)$$

which implies that  $H(\mu_1; \mu_2) \geq 0$ . If  $\mu_1 = \mu_2$  the relative entropy obviously vanishes.

On the other hand, if  $H(\mu_1; \mu_2) = 0$  then  $\phi(h(\omega)) = 0$  whenever  $\mu_2(\omega) > 0$ , which implies  $h(\omega) = 1$  and thus  $\mu_1(\omega) = \mu_2(\omega)$ . Since  $\mu_1 \ll \mu_2$  equality also holds when  $\mu_2(\omega) = 0$ .

(ii) For  $\Omega = S^\Lambda$  we fix some  $\Delta \subsetneq \Lambda$  and write  $h(\eta) = \mu_1(\eta)/\mu_2(\eta)$  and  $h^\Delta(\eta(\Delta)) = \mu_1^\Delta(\eta(\Delta))/\mu_2^\Delta(\eta(\Delta))$  for marginal distributions with  $\Delta \subseteq \Lambda_L$ . Then  $h^\Delta$  is given by an expectation conditioned on the sub-configuration  $\eta(\Delta)$  on  $\Delta$ ,

$$h^\Delta(\eta(\Delta)) = \frac{\mu_1^\Delta}{\mu_2^\Delta}(\eta(\Delta)) = \mu_2 \left( \frac{\mu_1}{\mu_2} \middle| \eta(\Delta) \right) = \mu_2(h | \eta(\Delta)). \quad (3.42)$$

Since  $\phi$  is convex we can apply Jensen's inequality to get

$$\phi(h^\Delta(\eta(\Delta))) = \phi \left( \mu_2(h | \eta(\Delta)) \right) \leq \mu_2(\phi(h) | \eta(\Delta)). \quad (3.43)$$

Therefore with  $\mu_2 \left( \mu_2(\phi(h) | \eta(\Delta)) \right) = \mu_2(\phi(h))$  we have

$$H(\mu_1^\Delta; \mu_2^\Delta) = \mu_2(\phi(h^\Delta)) \leq \mu_2(\phi(h)) = H(\mu_1; \mu_2), \quad (3.44)$$

which implies that in general  $H(\mu_1^\Delta; \mu_2^\Delta)$  is increasing in  $\Delta$ .

Using the auxiliary measure  $\nu = \frac{\mu_1^\Delta}{\mu_2^\Delta} \mu_2$  monotonicity in  $\Delta$  implies

$$\begin{aligned} H(\mu_1; \mu_2) - H(\mu_1^\Delta; \mu_2^\Delta) &= \mu_1 \left( \log \frac{\mu_1 \mu_2^\Delta}{\mu_2 \mu_1^\Delta} \right) = \mu_1 \left( \log \frac{\mu_1}{\nu} \right) = H(\mu; \nu) \geq \\ &\geq H(\mu_1^{\Lambda \setminus \Delta}; \nu^{\Lambda \setminus \Delta}) = H(\mu_1^{\Lambda \setminus \Delta}; \mu_2^{\Lambda \setminus \Delta}), \end{aligned} \quad (3.45)$$

since  $\nu^{\Lambda \setminus \Delta} = \mu_2^{\Lambda \setminus \Delta}$  by definition ( $\mu_1^\Delta / \mu_2^\Delta$  does not change  $\mu_2$  on  $\Lambda \setminus \Delta$ ).  
 If  $\mu_1$  and  $\mu_2$  are product measures  $h = \mu_1 / \mu_2$  factorizes, leading to equality.  
 (iii) harder, see e.g. [KL99], Appendix 1. □

**Remarks.**

- $H(\mu_1; \mu_2)$  is not symmetric and therefore not a metric on  $\mathcal{P}(X)$ .
- (i) only holds if  $\mu_1, \mu_2$  are normalized probability measures, for general distributions the relative entropy can also be negative.
- $H(\mu_1; \mu_2)$  is a well studied concept from information theory, often also called *Kullback-Leibler divergence* or *information gain*.

**Theorem 3.5** *Consider the canonical and grand-canonical ensembles for a homogeneous ZRP as defined above. Then the **specific relative entropy***

$$h_L(\phi) := \frac{1}{L} H(\pi_{L,N}; \nu_\phi) \rightarrow 0 \tag{3.46}$$

in the **thermodynamic limit**  $L \rightarrow \infty$  and  $N/L \rightarrow \bar{\rho} \geq 0$ , provided that  $\phi \in [0, \phi_c)$  solves  $\rho(\phi) = \bar{\rho}$ .

**Proof.** First we fix some  $L \geq 0$ . Note that for all  $\eta \in X_L$  and  $\phi > 0$ ,  $\nu_\phi(\eta) > 0$ , so in particular  $\pi_{L,N} \ll \nu_\phi$  and we have

$$h_L(\phi) = \sum_{\eta \in X_{L,N}} \pi_{L,N}(\eta) \log \frac{\pi_{L,N}(\eta)}{\nu_\phi(\eta)}. \tag{3.47}$$

Using the form (3.32) and (3.35) of the two measures we get for  $\eta \in X_{L,N}$

$$\frac{\pi_{L,N}(\eta)}{\nu_\phi(\eta)} = \frac{\prod_x w(\eta(x))}{Z_{L,N}} \frac{z(\phi)^L}{\prod_x w(\eta(x)) \phi^{\eta(x)}} = \frac{z(\phi)^L}{Z_{L,N} \phi^N}. \tag{3.48}$$

So due to the special form of the ensembles we get the simple expression

$$h_L(\phi) = \frac{1}{L} \sum_{\eta \in X_{L,N}} \pi_{L,N}(\eta) \log \frac{z(\phi)^L}{Z_{L,N} \phi^N} = -\frac{1}{L} \log \frac{Z_{L,N} \phi^N}{z(\phi)^L}. \tag{3.49}$$

Further note that

$$Z_{L,N} = \sum_{\eta \in X_{L,N}} \prod_{x \in \Lambda_L} w(\eta(x)) = \nu_\phi(\Sigma_L(\eta) = N) \phi^{-N} z(\phi)^L, \tag{3.50}$$

and thus

$$h_L(\phi) = -\frac{1}{L} \log \nu_\phi(\Sigma_L(\eta) = N). \tag{3.51}$$

Since  $\phi < \phi_c$  we have  $\sum_n n^2 w(n) \phi^n < \infty$ . So under  $\nu_\phi$  the  $\eta(x)$  are iidrvs with finite variance and mean  $\nu_\phi^x(\eta(x)) = \rho(\phi) = \bar{\rho}$ . Now taking  $L \rightarrow \infty$  with  $N/L \rightarrow \bar{\rho}$  by the local central limit theorem

$$\nu_\phi(\Sigma_L(\eta) = N) = \nu_\phi\left(\sum_{x \in \Lambda_L} \eta(x) = N\right) = O(L^{-1/2}), \tag{3.52}$$

which corresponds to the width  $\sqrt{L}$  of the distribution of a sum of iidrv's. This implies that

$$h_L(\phi) = O\left(\frac{1}{L} \log L\right) \rightarrow 0 \quad \text{as } L \rightarrow \infty. \quad (3.53)$$

□

Note that this convergence result only holds if  $\bar{\rho}$  is in the range of the function  $\rho(\phi)$  for  $\phi \in [0, \phi_c)$ . Whenever this is not the case the system exhibits an interesting phase transition which is discussed in detail in the next section.

**Corollary 3.6** *Let  $f \in C_0(X)$  be a cylinder test function with  $\nu_\phi(e^{\epsilon f}) < \infty$  for some  $\epsilon > 0$ . Then*

$$\mu_{L,N}(f) \rightarrow \nu_\phi(f) \quad \text{as } L \rightarrow \infty, \quad (3.54)$$

*provided that  $\phi \in [0, \phi_c)$  solves  $\rho(\phi) = \bar{\rho} = \lim_{L \rightarrow \infty} N/L$ .*

**Proof.** Let  $\Delta \subseteq \Lambda_L$  be the finite range of dependence of the cylinder function  $f \in C_0(X)$ . Then we can plug  $f - \nu_\phi^\Delta(f)$  and  $\nu_\phi^\Delta(f) - f$  in the entropy inequality (3.39) to show that

$$|\pi_{L,N}(f) - \nu_\phi(f)| \leq H(\pi_{L,N}^\Delta; \nu_\phi^\Delta). \quad (3.55)$$

This involves extending the inequality to unbounded functions  $f$  with finite exponential moments and a standard  $\epsilon - \delta$  argument. It is rather lengthy and we do not present this here, for a reference see e.g. [Csiszár, Ann. Prob. 3, 146 (1975), Lemma 3.1].

Then sub-additivity (Lemma 3.4(ii)) gives

$$H(\pi_{L,N}^\Delta; \nu_\phi^\Delta) \leq \frac{|\Delta|}{L} H(\pi_{L,N}; \nu_\phi) = |\Delta| h_L(\phi) \rightarrow 0 \quad (3.56)$$

as  $L \rightarrow \infty$  which implies the statement. □

### Remarks.

- The above corollary implies e.g. convergence of the test function  $f(\eta) = \eta(x)$ , since for all  $\phi < \phi_c$

$$\sum_{n=0}^{\infty} e^{\epsilon n} w(n) \phi^n < \infty \quad \text{for } e^\epsilon \phi < \phi_c, \text{ i.e. } \epsilon < \log \frac{\phi_c}{\phi}. \quad (3.57)$$

So  $\pi_{L,N}(\eta(x)) = N/L \rightarrow \nu_\phi(\eta(x)) = \rho(\phi)$ , which is not very surprising since  $\phi$  is chosen to match the density  $\rho$ .

- The function  $f(\eta) = \eta(x)^2$  corresponding to the second moment is not covered by the above result, since  $e^{\epsilon n^2}$  grows too fast with  $n$  for all  $\epsilon > 0$ . However, convergence can be extended to functions  $f \in L^2(\nu_\phi)$  (with considerable technical effort, see e.g. appendix of [KL99]). Since  $\phi < \phi_c$  leads to an exponential decay of  $w(n)\phi^n$ , this extension includes all polynomial correlation functions.

### 3.4 Phase separation and condensation

Since ZRPs are bosonic lattice gases, they exhibit a condensation transition under certain conditions which is similar to Bose-Einstein condensation for bosons. As in the previous section we consider a homogeneous ZRP on the lattice  $\Lambda_L = \mathbb{Z}/L\mathbb{Z}$  with jump rates  $g(n)$  bounded away from 0 for  $n > 0$  and translation invariant jump probabilities  $p(x, y) = q(y - x)$ .

**Definition 3.3** Let  $\rho(\phi) = \nu_\phi(\eta(x))$  be the density of the grand-canonical product measure  $\nu_\phi$  and  $\phi_c \in [0, \infty]$  be the radius of convergence of the partition function  $z(\phi)$ . Then we define the *critical density*

$$\rho_c = \lim_{\phi \nearrow \phi_c} \rho(\phi) \in [0, \infty]. \quad (3.58)$$

$\rho_c$  can take the value  $\infty$ , as we have seen above for the example

$$g(k) = 1 - \delta_{k,0} \quad \Rightarrow \quad \rho(\phi) = \frac{\phi}{1 - \phi} \nearrow \infty \quad \text{as } \phi \nearrow \phi_c = 1. \quad (3.59)$$

In fact, this is the 'usual' situation since it implies that there exists a grand-canonical stationary measure for all densities  $\rho \geq 0$ .

Are there examples with  $\rho_c < \infty$ ? To realize this we need

$$\sum_{n=0}^{\infty} n w(n) \phi_c^n < \infty, \quad (3.60)$$

i.e. the power series has to converge **at** the radius of convergence  $\phi_c$ . Therefore  $w(n)\phi_c^n$  has to decay sub-exponentially (by definition of  $\phi_c$ ), but fast enough for the sum to converge. A generic example is a power law decay

$$w(n) \phi_c^n \simeq n^{-b} \quad \text{as } n \rightarrow \infty \quad \text{with } b > 2. \quad (3.61)$$

Since we have the explicit formula  $w(n) = \prod_{k=1}^n g(k)^{-1}$  this implies for the jump rates

$$g(n) = \frac{w(n-1)}{w(n)} \simeq \frac{(n-1)^{-b} \phi_c^{-(n-1)}}{n^{-b} \phi_c^{-n}} = \phi_c (1 - 1/n)^{-b} \simeq \phi_c (1 + b/n). \quad (3.62)$$

Such a generic example

$$g(n) = 1 + b/n \quad \text{with } \phi_c = 1 \quad \text{and } w(n) \simeq \Gamma(1 + b) n^{-b} \quad (3.63)$$

was introduced by Evans ('00). For this model  $\rho_c$  can be computed explicitly,

$$\rho_c = \frac{1}{b-2} < \infty \quad \text{for } b > 2. \quad (3.64)$$

The interesting question is now, what happens to the equivalence of ensembles in the limit  $L \rightarrow \infty$  with  $N/L \rightarrow \bar{\rho} > \rho_c$ ?

**Theorem 3.7** Consider the canonical  $\pi_{L,N}$  and the grand-canonical measures  $\nu_\phi$  of a homogeneous ZRP, for which we assume that

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{k=1}^n \log g(k) \in \mathbb{R} \quad \text{exists}. \quad (3.65)$$

Then

$$h_L(\phi) := \frac{1}{L} H(\pi_{L,N}; \nu_\phi) \rightarrow 0 \quad \text{as } L \rightarrow \infty \quad \text{and } N/L \rightarrow \bar{\rho} \geq 0, \quad (3.66)$$

provided that for  $\bar{\rho} \leq \rho_c$ ,  $\phi \in [0, \phi_c]$  solves  $\rho(\phi) = \rho$  (**sub-critical case**) and for  $\bar{\rho} > \rho_c$ ,  $\phi = \phi_c$  (**super-critical case**).

**Proof.** Analogous to the proof of Theorem 3.5 we have

$$h_L(\phi) = -\frac{1}{L} \log \nu_\phi(\Sigma_L(\eta) = N), \quad (3.67)$$

and for  $\bar{\rho} \leq \rho_c$  or  $\rho_c = \infty$  this implies the result as before.

For  $\bar{\rho} > \rho_c$ ,  $\sum_{x \in \Lambda_L} \eta(x) = N$  is a large deviation event, and to get an upper bound on (3.67) we need a lower bound on its probability under the critical measure  $\nu_{\phi_c}$ .

$$\begin{aligned} \nu_{\phi_c} \left( \sum_{x \in \Lambda_L} \eta(x) = N \right) &\geq \\ &\geq \nu_{\phi_c}^1(\eta(1) = N - [\rho_c(L-1)]) \nu_{\phi_c}^{\Lambda_L \setminus \{1\}} \left( \sum_{x \in \Lambda_L \setminus \{1\}} \eta(x) = [\rho_c(L-1)] \right), \end{aligned} \quad (3.68)$$

which corresponds to putting an extensive amount of particles on lattice site 1 and distributing an amount which is typical under  $\nu_{\phi_c}$  on the remaining sites.

The second term can be treated by local limit theorems analogous to the previous result\* (see remark below). Since  $\phi_c$  is the radius of convergence of the partition function  $\nu_{\phi_c}^1$  has a subexponential tail, i.e.

$$\frac{1}{L} \log \nu_{\phi_c}^1(\eta(1) = N - [\rho_c(L-1)]) \rightarrow 0 \quad \text{as } L \rightarrow \infty, \quad (3.69)$$

since  $N - [\rho_c(L-1)] \simeq (\bar{\rho} - \rho_c)L \rightarrow \infty$  for  $\bar{\rho} > \rho_c$ . Existence of the limit is guaranteed by assumption (3.65) using

$$\log \nu_{\phi_c}^1(\eta(1) = n) = n \log(\phi_c w(n)^{1/n}) - \log z(\phi_c) \quad (3.70)$$

and (3.26). Plugging these results for (3.68) into (3.67) we get  $h_L(\phi_c) \rightarrow 0$  for  $\bar{\rho} > \rho_c$ .  $\square$

### Remarks.

- Existence of the *Cesàro* limit in (3.65) is a very weak assumption, it is certainly fulfilled if  $g(k)$  has a limit as  $k \rightarrow \infty$  as in our example above. It only excludes pathological cases where  $g(k)$  has an exponentially diverging subsequence.
- \*For  $b > 3$  the  $\eta(x)$  are iidrvs with finite variance and the second term in (3.68) is of order  $1/\sqrt{L}$ . For  $2 < b \leq 3$  the variance is infinite and the sum of  $\eta(x)$  has a non-normal limit distribution. Using adapted local limit theorems, the second term can be still be bounded below by terms of order  $1/L$  for all  $b > 2$ .
- Corollary 3.6 still applies, but note that in the super-critical case  $\nu_{\phi_c}(e^{\epsilon \eta(x)}) = \infty$  for all  $\epsilon > 0$  due to sub-exponential tails. So the test function  $f(\eta) = \eta(x)$  is not included in the result, which is to be expected, since for  $\rho > \rho_c$

$$\pi_{L,N}(\eta(x)) = N/L \rightarrow \rho > \rho_c = \nu_{\phi_c}(\eta(x)). \quad (3.71)$$

**Interpretation.**

- Elements  $\nu_\phi$  of the grand-canonical ensemble are also called *fluid phases*. For  $\rho > \rho_c$  the ensemble

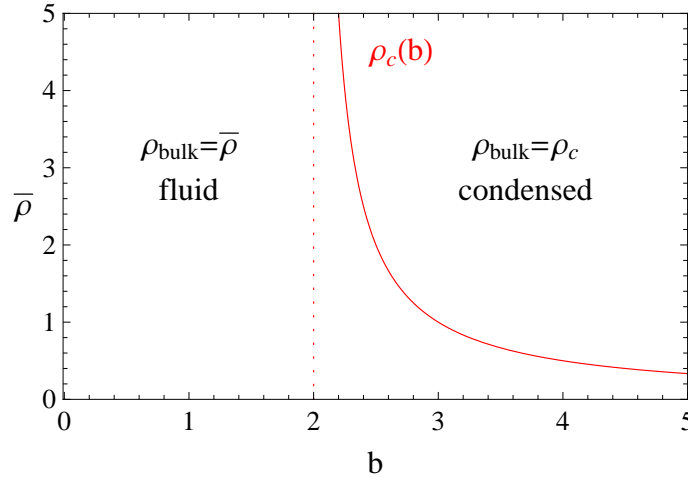
$$\{\nu_\phi : \phi \in [0, \phi_c]\} \quad \text{has density range} \quad [0, \rho_c], \quad (3.72)$$

and there are no fluid phases with density  $\rho > \rho_c$ .

- The limiting distribution in any finite fixed volume  $\Delta$  is given by the fluid phase  $\nu_{\phi_c}^\Delta$  with density is  $\rho_c$ . Therefore for large systems the *excess mass*  $(\rho - \rho_c)L$  concentrates in a region with vanishing volume fraction (volume  $o(L)$ ), the so-called *condensed phase*. This phenomenon is called *phase separation* in general, and since one of the phases covers only a vanishing fraction of the system this particular form of phase separation is called *condensation*.
- It can be shown that in fact the condensed phase concentrates on a *single* lattice site, i.e. for  $\rho > \rho_c$  we have a law of large numbers for the maximal occupation number in the canonical ensemble,

$$\pi_{L,N} \left( \left| \frac{1}{L} \max_{x \in \Lambda_L} \eta(x) - (\rho - \rho_c) \right| > \epsilon \right) \rightarrow 0 \quad \text{as } L \rightarrow \infty \quad \text{for all } \epsilon > 0. \quad (3.73)$$

For the above example with  $g(k) = 1 + b/k$ ,  $k > 0$  and  $\rho_c(b) = 1/(b - 2)$  these results can be summarized in the following phase diagram.



The axes are given by the system parameters  $b$  and the density  $\bar{\rho} = \lim_{L \rightarrow \infty} N/L$ . As order parameter we took the limiting *bulk density*  $\rho_{bulk} := \nu_\phi(\eta(x))$ , where  $\nu_\phi$  is the limit measure of Theorem 3.7. This leads to

$$\rho_{bulk} = \begin{cases} \bar{\rho} & , \bar{\rho} \leq \rho_c \\ \rho_c & , \bar{\rho} > \rho_c \end{cases}, \quad (3.74)$$

and the two phase regions we call *fluid* and *condensed*.  $\rho_{bulk}$  is continuous across the phase transition line (red), and therefore condensation is a continuous phase transition w.r.t. the order parameter  $\rho_{bulk}$ .

## 4 The contact process

The lattice  $\Lambda$ , an arbitrary countable set, is endowed with a graph structure by a directed edge set  $E \subseteq \Lambda \otimes \Lambda$ . We assume that  $(\Lambda, E)$  is connected, i.e. for all  $x, y \in \Lambda$  there exists a directed path of edges connecting  $x$  to  $y$ . The state space of the contact process (CP) is  $X = \{0, 1\}^\Lambda$  and the generator is

$$\mathcal{L}f(\eta) = \sum_{x \in \Lambda} \left( \eta(x) + \lambda(1 - \eta(x)) \sum_{y \sim x} \eta(y) \right) (f(\eta^x) - f(\eta)), \quad (4.1)$$

where  $y \sim x$  if  $(y, x) \in E$ . Infected sites ( $\eta(x) = 1$ ) recover independently with rate 1, and infect neighbouring sites independently with rate  $\lambda > 0$ .

### 4.1 Mean-field rate equations

Choosing  $f(\eta) = \eta(x)$ , denoting by  $\mu_t = \mu_0 S(t)$  the distribution at time  $t$  and writing  $\rho_t(x) = \mu_t(\eta(x)) \in [0, 1]$  for the density, we get from the backward equation (1.38)

$$\frac{d}{dt} \rho_t(x) = \mu_t(\mathcal{L}f) = -\rho_t(x) + \lambda \sum_{y \sim x} \mu_t(\eta(y)(1 - \eta(x))). \quad (4.2)$$

So the time evolution of the first moment  $\rho(t)$  involves second moments and is not a closed equation, similar to what we have seen for the ASEP in Section 2. The simplest way to close these equations is called the *mean-field assumption*:

$$\mu_t(\eta(y)(1 - \eta(x))) = \mu_t(\eta(y))\mu_t(1 - \eta(x)) = \rho_t(y)(1 - \rho_t(x)), \quad (4.3)$$

i.e.  $\mu_t$  is assumed to be a product measure and the  $\eta(x)$  to be independent. If the graph  $(\Lambda, E)$  is translation invariant, e.g. a regular lattice such as  $\mathbb{Z}^d$  or  $(\mathbb{Z}/L\mathbb{Z})^d$  or homogeneous trees, and the initial distribution  $\mu_0$  is as well, the system is homogeneous and we have the additional identity  $\rho_t(x) \equiv \rho_t$  for all  $x \in \Lambda$ . Using this and the mean-field assumption in (4.2) we get the *mean-field rate equation* for the CP

$$\frac{d}{dt} \rho_t = -\rho_t + m\lambda\rho_t(1 - \rho_t), \quad (4.4)$$

where  $m$  is the coordination number or vertex degree of the lattice  $\Lambda$ , i.e. the number of neighbours of a lattice site, such as  $m = 2d$  for  $d$ -dimensional cubic lattices.

#### Remarks.

- Of course there is no reason why the mean-field assumption should be correct. However, it turns out that for high coordination number the replacement

$$\mu_t \left( \sum_{y \sim x} \eta(y)(1 - \eta(x)) \right) \approx \sum_{y \sim x} \rho_t(y)(1 - \rho_t(x)) \quad (4.5)$$

leads to quantitatively good predictions. Due to a 'law of large numbers'-effect  $\sum_{y \sim x} \eta(y)$  can be replaced by its expected value when the number  $m$  of terms is large. For example this is the case for  $d$ -dimensional cubic lattices ( $m = 2d$ ) with  $d > 4$ . The highest dimension for which the mean-field assumption is not exact is often referred to as the *upper critical dimension* in the physics literature.



- For low dimensions/coordination numbers the mean-field assumption still is useful to get a first idea of the critical behaviour of the system, since it typically easy to derive and analyze. In most cases quantitative predictions are wrong (such as location of phase boundaries and critical exponents), but qualitative features are often predicted correctly (such as the number of phase regions or existence of critical points).

### Analysis of the rate equation.

The long-time behaviour of solutions to an equation of the form  $\frac{d}{dt}\rho_t = f(\rho_t)$  is given by stationary points of the right-hand side  $f(\rho) = 0$ . In our case for (4.4) these are given by

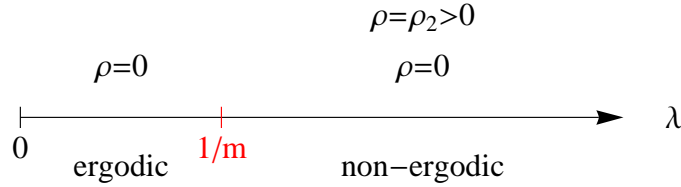
$$0 = -\rho + m\lambda\rho(1 - \rho) = -m\lambda\rho^2 + (m\lambda - 1)\rho, \quad (4.6)$$

which are the roots of a downward parabola, given by  $\rho_1 = 0$  and  $\rho_2 = 1 - 1/(m\lambda)$ .

$\rho \equiv \rho_1 = 0$  is always a stationary solution to the equation, corresponding to the absorbing state  $\eta = 0$  of the CP, called the *inactive phase*. For  $m\lambda > 1$  there is a second stationary density  $\rho_2 = 1 - 1/(m\lambda) \in (0, 1)$  called the *active phase*. The domains of attraction of these stationary points are determined by the sign of  $f(\rho)$ , and  $\rho_i$  is locally stable if  $f'(\rho_i) < 0$ . In summary we have

$$\begin{aligned} f'(0) = m\lambda - 1 &\Rightarrow \rho = 0 && \begin{array}{l} \text{stable for } m\lambda \leq 1 \\ \text{unstable for } m\lambda > 1 \end{array} \\ f'(\rho_2) = 1 - m\lambda &\Rightarrow \rho = \rho_2 && \begin{array}{l} \notin (0, 1] \text{ for } m\lambda \leq 1 \\ \text{stable for } m\lambda > 1 \end{array} \end{aligned}, \quad (4.7)$$

which leads to the following mean-field prediction of the phase diagram of the CP with the *critical value*  $\lambda_c = 1/m$ .



As opposed to previous sections the diagram is one-dimensional, since the number of particles in the CP is not conserved and  $\lambda$  is the only system parameter. The phase regions can be characterized by ergodicity of the infinite system, as is explained below.

### Remarks.

- The mean-field rate equation does not take into account fluctuations. Since the CP is irreducible on  $X \setminus \{0\}$ , on a finite lattice the states in the active phase are transient and the CP is ergodic with unique stationary measure  $\mu = \delta_0$ . However, if the infection rate  $\lambda$  is large enough and we start the system in the active phase (e.g.  $\eta_0(x) = 1$  for all  $x$ ), it remains active for a (random) time with mean of the order  $\exp(CL)$  where  $L$  is the size of the lattice. If  $L$  is large it takes the system very long to reach its stationary distribution and the active phase is said to be *metastable*.
- The lifetime of the active phase diverges for infinite lattice size. Therefore infinite systems exhibit a truly stationary active phase if  $\lambda$  is large enough. The system is no longer ergodic since it has two stationary distributions,  $\delta_0$  corresponding to the absorbing state (inactive phase) and  $\mu$  corresponding to the active phase.

- On  $\mathbb{Z}$  ( $d = 1$ ) precise numerical estimates (and rigorous bounds) show that  $\lambda_c = 1.64893$ , which is quite far from the mean-field value  $1/m = 1/2$  we predicted. Nevertheless, the qualitative prediction of a phase transitions turns out to be true. Comparing to the first remark it is actually not surprising that mean-field underestimates the critical value, since even for  $\lambda > 1/2$  the system can still die out due to fluctuations. Clearly  $\lambda_c$  should decrease with  $m$ , and in fact the numerical estimate for  $\mathbb{Z}^2$  is 0.4119 (MF prediction  $1/m = 0.25$ ).

## 4.2 Stochastic monotonicity and coupling

In this section we introduce a powerful technique which can be used to get rigorous results on the contact process. Let  $X = S^\Lambda$  be the state space of a particle system with  $S \subseteq \mathbb{N}$  and  $\Lambda$  some arbitrary discrete lattice.  $X$  is a partially ordered set, given by

$$\eta \leq \zeta \quad \text{if} \quad \eta(x) \leq \zeta(x) \quad \text{for all } x \in \Lambda. \quad (4.8)$$

**Definition 4.1** A function  $f \in C(X)$  is *increasing* if

$$\eta \leq \zeta \quad \text{implies} \quad f(\eta) \leq f(\zeta). \quad (4.9)$$

This leads to the concept of *stochastic monotonicity* for probability measures  $\mu_1, \mu_2$  on  $X$ :

$$\mu_1 \leq \mu_2 \quad \text{provided that} \quad \mu_1(f) \leq \mu_2(f) \quad \text{for all increasing } f \in C(X). \quad (4.10)$$

This definition is quite hard to work with, and the best way to understand and use stochastic monotonicity is in terms of *couplings*.

**Definition 4.2** A coupling of two measures  $\mu_1, \mu_2 \in \mathcal{P}(X)$  is a measure  $\mu$  on the product state space  $X \otimes X$  of pair configurations  $\eta = (\eta^1, \eta^2)$ , such that the marginals for  $i = 1, 2$  are

$$\mu^i = \mu_i \quad \text{i.e.} \quad \mu(\{\eta : \eta^i \in A\}) = \mu_i(A) \quad \text{for all measurable } A \subseteq X. \quad (4.11)$$

**Remark.** In other words, a coupling means constructing the random variables  $\eta^1(\omega)$  and  $\eta^2(\omega)$  on the same probability space  $(\Omega, \mathcal{A}, \mathbb{P})$ , such that

$$\mathbb{P}(\{\omega : \eta^i(\omega) \in A\}) = \mu_i(A) \quad \text{for all measurable } A \subseteq X. \quad (4.12)$$

**Theorem 4.1 (Strassen)** Suppose  $\mu_1, \mu_2 \in \mathcal{P}(X)$ . Then  $\mu_1 \leq \mu_2$  if and only if there exists a coupling  $\mu \in \mathcal{P}(X \otimes X)$  such that

$$\mu(\{\eta : \eta^1 \leq \eta^2\}) = 1 \quad (\eta^1 \leq \eta^2 \mu - a.s.). \quad (4.13)$$

**Proof.**  $\Leftarrow$ : Suppose such a coupling  $\mu$  exists. If  $f \in C(X)$  is increasing then  $f(\eta^1) \leq f(\eta^2)$   $\mu - a.s.$  and writing  $\pi^i : X \otimes X \rightarrow X$  for the projection on the  $i$ -th coordinate  $\pi^i(\eta) = \eta^i$ , we have

$$\mu_1(f) = \mu(f \circ \pi^1) \leq \mu(f \circ \pi^2) = \mu_2(f), \quad (4.14)$$

so that  $\mu_1 \leq \mu_2$ .

$\Rightarrow$ : involves a construction of the coupling on a probability space, see e.g. Theorem 2.4, p. 72 [L99]  $\square$

**Example.**

Let  $\nu_{\rho_1}, \nu_{\rho_2}$  be product measures on  $X = \{0, 1\}^\Lambda$  with  $\rho_1 \leq \rho_2$ . Then for each  $i = 1, 2$  the  $\eta^i(x)$  are iid  $Be(\rho_i)$  random variables. To construct a coupling  $\mu$  on  $X \otimes X$  let  $\Omega_x = (0, 1)$  and  $\mathbb{P}_x = U(0, 1)$  be the uniform measure independently for each  $x \in \Lambda$ . Then define

$$\eta^i(x)(\omega) := \begin{cases} 1 & , \omega_x \leq \rho_i \\ 0 & , \omega_x > \rho_i \end{cases} , \quad (4.15)$$

which implies that  $\eta^1(x)(\omega) \leq \eta^2(x)(\omega)$  for all  $\omega \in \Omega$  and  $x \in \Lambda$ . Taking the product over all lattice sites with  $\mathbb{P} = \prod_x \mathbb{P}_x$ , we can define a coupling measure on  $X \otimes X$  by

$$\mu := \mathbb{P} \eta^{-1} \quad \text{i.e.} \quad \mu(A) = \mathbb{P}\{\omega : \eta(\omega) \in A\} \quad \text{for all } A \in X \otimes X , \quad (4.16)$$

and we have  $\eta^1 \leq \eta^2 \mu - a.s.$ . Therefore the theorem implies  $\nu_{\rho_1} \leq \nu_{\rho_2}$ .

The idea of monotonicity and coupling can be extended to processes.

**Definition 4.3** Consider an IPS on  $X$  with generator  $(S(t) : t \geq 0)$ . The process is *attractive* or *monotone* if

$$f \text{ increasing} \quad \Rightarrow \quad S(t)f \text{ increasing for all } t \geq 0 , \quad (4.17)$$

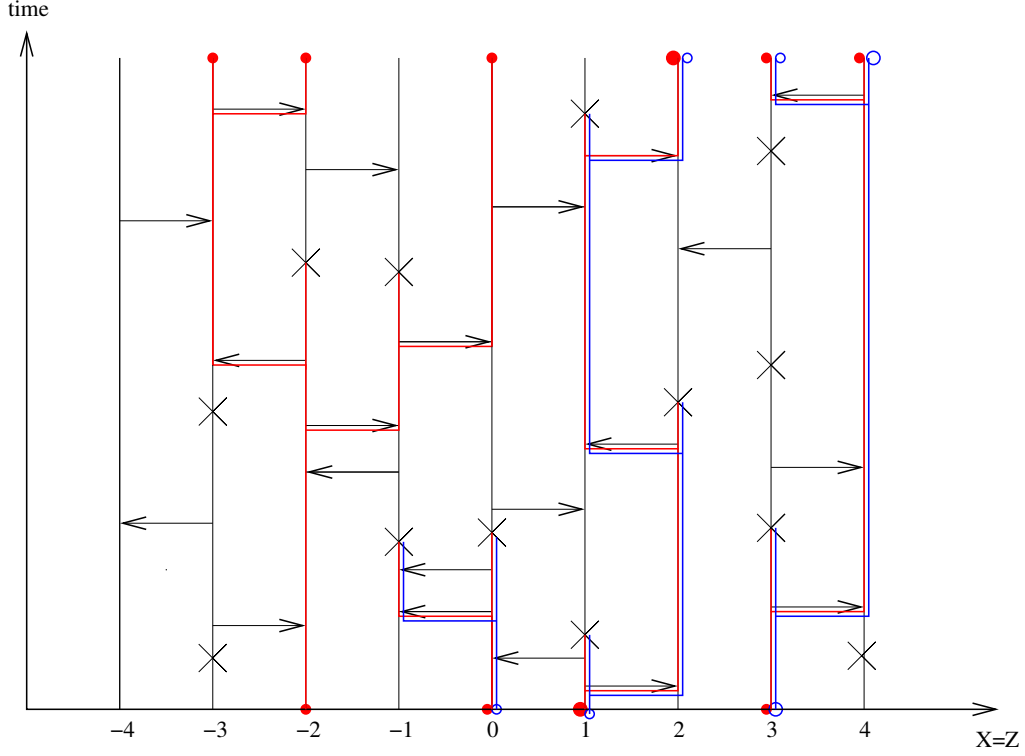
or equivalently

$$\mu_1 \leq \mu_2 \quad \Rightarrow \quad \mu_1 S(t) \leq \mu_2 S(t) \quad \text{for all } t \geq 0 . \quad (4.18)$$

Let  $\mathbb{P}_1, \mathbb{P}_2 \in \mathcal{P}(D[0, \infty))$  be the path space measures of two IPS  $(\eta_t^1 : t \geq 0)$  and  $(\eta_t^2; t \geq 0)$ . Then a *coupling* of the processes is given by a Markov process  $((\eta_t^1, \eta_t^2) : t \geq 0)$  on  $X \otimes X$  with measure  $\mathbb{P} \sim \mathcal{P}(D[0, \infty) \otimes D[0, \infty))$ , having marginal processes  $(\eta_t^i : t \geq 0) \sim \mathbb{P}_i$ , i.e.  $\mathbb{P}^i = \mathbb{P}_i$ .

**Lemma 4.2** *The contact process is attractive.*

**Proof.** We couple two contact processes  $(\eta_t^1 : t \geq 0)$  (shown red) and  $(\eta_t^2; t \geq 0)$  (shown blue) using a graphical construction.



Both processes use the same realization of infection and recovery processes  $\rightarrow$ ,  $\leftarrow$  and  $\times$ , and the initial conditions fulfill  $\eta_0^2 \leq \eta_0^1$ . Then by inspection of the coupling construction this immediately implies that  $\eta_t^2 \leq \eta_t^1$  for all  $t \geq 0$  (example shown above). Therefore we have for all  $f \in C(X)$ ,

$$S(t)f(\eta_0^2) = \mathbb{E}^{\eta_0^2}(f(\eta_t^2)) \leq \mathbb{E}^{\eta_0^1}(f(\eta_t^1)) = S(t)f(\eta_0^1), \quad (4.19)$$

and since this holds for all ordered initial conditions the CP is attractive as given in Def. 4.3.  $\square$

More generally it can be shown that:

**Proposition 4.3** *A general spin system on  $\{0, 1\}^\Lambda$  with generator*

$$\mathcal{L}f(\eta) = \sum_{x \in \Lambda} c(x, \eta)(f(\eta^x) - f(\eta)) \quad (4.20)$$

*is attractive if and only if the jump rates (spin flip rates) fulfill*

$$\eta \leq \zeta \quad \text{implies} \quad \begin{cases} c(x, \eta) \leq c(x, \zeta) & , \text{ if } \eta(x) = \zeta(x) = 0 \\ c(x, \eta) \geq c(x, \zeta) & , \text{ if } \eta(x) = \zeta(x) = 1 \end{cases} . \quad (4.21)$$

**Proof.** Suppose the spin system is attractive, i.e.  $f$  increasing implies  $S(t)f$  increasing for all  $t \geq 0$ . Since  $f(\eta) = \eta(x)$  is increasing and in  $C_0(X)$  we have

$$\mathcal{L}f(\eta) = \lim_{t \searrow 0} \frac{S(t)f(\eta) - f(\eta)}{t}, \quad (4.22)$$

and for all  $\eta \leq \zeta$  with  $\eta(x) = \zeta(x)$

$$\mathcal{L}f(\eta) - \mathcal{L}f(\zeta) = \lim_{t \searrow 0} \frac{S(t)f(\eta) - S(t)f(\zeta) + \eta(x) - \zeta(x)}{t} \leq 0. \quad (4.23)$$

Therefore  $\mathcal{L}f(\eta) \leq \mathcal{L}f(\zeta)$  and since

$$\mathcal{L}f(\eta) = c(x, \eta)(1 - 2\eta(x)) \quad (4.24)$$

this implies 4.21.

The other direction involves a more general version of the coupling given in the proof of Lemma 4.2 above, see e.g. Theorem 2.2, p. 134 [L99].  $\square$

**Remark.** Property (4.21) asserts that 0 is more likely to flip to 1 in a environment of more 1s ( $\zeta \geq \eta$ ), and vice versa. That means that local occupation numbers 'attract' one another, explaining the term 'attractive' for such particle systems.

#### Lemma 4.4 Monotonicity in $\lambda$

Let  $(\eta_t^\lambda : t \geq 0)$  and  $(\eta_t^{\lambda'} : t \geq 0)$  be two CPs with infection rates  $\lambda \leq \lambda'$ . Then

$$\mu^\lambda \leq \mu^{\lambda'} \quad \text{implies} \quad \mu^\lambda S(t) \leq \mu^{\lambda'} S(t) \quad \text{for all } t > 0, \quad (4.25)$$

i.e. there exists a coupling such that

$$\eta_0^\lambda \leq \eta_0^{\lambda'} \quad \text{and} \quad \eta_t^\lambda \leq \eta_t^{\lambda'} \quad \text{for all } t > 0. \quad (4.26)$$

**Proof.** By Strassen's Theorem,  $\mu^\lambda \leq \mu^{\lambda'}$  implies existence of a coupling such that  $\eta_0^\lambda \leq \eta_0^{\lambda'}$ . Suppose first that  $\eta_0^\lambda = \eta_0^{\lambda'}$  and couple the processes  $(\eta_t^\lambda : t \geq 0)$  and  $(\eta_t^{\lambda'} : t \geq 0)$  by using coupled infection processes  $PP(\lambda)$  and  $PP(\lambda) + PP(\lambda' - \lambda) \sim PP(\lambda')$  in the graphical construction. Then clearly  $\eta_t^\lambda \leq \eta_t^{\lambda'}$  for all  $t > 0$ . Now by attractivity of the process  $(\eta_t^\lambda : t \geq 0)$  this also holds for initial conditions  $\eta_0^\lambda \leq \eta_0^{\lambda'}$ .  $\square$

### 4.3 Invariant measures and critical values

Consider a CP with infection rate  $\lambda$  on some connected graph  $(\Lambda, E)$  and let  $\delta_0$  be the point mass on the empty configuration and  $\delta_1$  on the full configuration  $\eta(x) = 1, x \in \Lambda$ . Since  $\eta \equiv 0$  is absorbing,  $\delta_0$  is stationary.

**Proposition 4.5** For all  $0 \leq s \leq t$  we have

$$\delta_1 S(s) \geq \delta_1 S(t), \quad \bar{\nu}_\lambda = \lim_{t \rightarrow \infty} \delta_1 S(t) \quad \text{exists and} \quad \bar{\nu}_\lambda \in \mathcal{I}_e. \quad (4.27)$$

$\bar{\nu}_\lambda$  is called the **upper invariant measure**, and we have  $\delta_0 \leq \mu \leq \bar{\nu}_\lambda$  for all  $\mu \in \mathcal{I}$ . Furthermore,  $\lambda < \lambda'$  implies  $\bar{\nu}_\lambda \leq \bar{\nu}_{\lambda'}$ , and for each  $x \in \Lambda$

$$\rho_x(\lambda) := \bar{\nu}_\lambda(\eta(x)) \quad \text{is monotone increasing in } \lambda. \quad (4.28)$$

**Proof.** Since  $\delta_1$  is maximal on  $X$  we have

$$\delta_1 \geq \delta_1 S(t - s) \quad \text{for all } 0 \leq s \leq t. \quad (4.29)$$

By attractivity of the CP and the Markov property this implies

$$\delta_1 S(s) \geq \delta_1 S(t - s) S(s) = \delta_1 S(t). \quad (4.30)$$

Therefore  $\delta_1 S(t)$  is a monotone sequence, and by compactness of  $\mathcal{P}(X)$  (in the topology of weak convergence) the limit exists and is stationary by Theorem 1.9(b). Furthermore  $\delta_0 \leq \mu \leq \delta_1$  for

all  $\mu \in \mathcal{P}$ . Every stationary measure can be written as  $\lim_{t \rightarrow \infty} \mu S(t)$  for some  $\mu$ , so by attractivity it will also be bounded by  $\delta_0$  and  $\bar{\nu}_\lambda$ .

Suppose that  $\bar{\nu}_\lambda \in \mathcal{I}$  is not extremal, i.e.  $\bar{\nu}_\lambda = \alpha\mu_1 + (1 - \alpha)\mu_2$  for  $\mu_1, \mu_2 \in \mathcal{I}$  and  $\alpha \in (0, 1)$ . Then  $\mu_1, \mu_2 \leq \bar{\nu}_\lambda$ , so for all increasing  $f \in C(X)$  we have  $\mu_1(f), \mu_2(f) \leq \bar{\nu}_\lambda(f)$ . Suppose now that  $\mu_1(f) < \bar{\nu}_\lambda(f)$ , then

$$\alpha\mu_1(f) + (1 - \alpha)\mu_2(f) < \alpha\bar{\nu}_\lambda(f) + (1 - \alpha)\bar{\nu}_\lambda(f) = \bar{\nu}_\lambda(f) \quad (4.31)$$

in contradiction to the assumption. So  $\mu_1(f) = \mu_2(f) = \bar{\nu}_\lambda(f)$  for all increasing  $f \in C(X)$ , and thus  $\mu_1 = \mu_2 = \bar{\nu}_\lambda$  and  $\bar{\nu}_\lambda \in \mathcal{I}_e$ .

By monotonicity in  $\lambda$  we have for all  $t \geq 0$

$$\delta_1 S^\lambda(t) \leq \delta_1 S^{\lambda'}(t), \quad (4.32)$$

provided that  $\lambda \leq \lambda'$ , which implies  $\bar{\nu}_\lambda \leq \bar{\nu}_{\lambda'}$ . Since  $\eta(x)$  is increasing this also holds for the corresponding densities.  $\square$

On a finite lattice  $\eta \equiv 0$  can be reached in finite time from any other configuration, and since  $\eta \equiv 0$  is absorbing this implies

$$\mu S(t) \rightarrow \delta_0 \quad \text{as } t \rightarrow \infty \quad \text{for all } \mu \in \mathcal{P}(X). \quad (4.33)$$

This holds in particular for  $\mu = \delta_1$ , and thus the upper invariant measure is  $\bar{\nu}_\lambda = \delta_0$  and the CP is ergodic for all  $\lambda \geq 0$ . On the other hand, on an infinite lattice it might be possible that  $\bar{\nu}_\lambda \neq \delta_0$  and the mean-field prediction of an active phase is correct. It turns out that this is indeed the case for high enough infection rate  $\lambda$  as we will see below.

**Definition 4.4** Denote by

$$\alpha_\eta := \mathbb{P}^\eta(\eta_t \neq 0 \text{ for all } t \geq 0) \quad (4.34)$$

the *survival probability* with initial configuration  $\eta \in X$ . For each  $x \in \Lambda$  denote by  $\xi_x \in X$  the configuration with  $\xi_x(y) = \delta_{y,x}$  having a single infection at  $x$ . The CP  $(\eta_t : t \geq 0)$  is said to *die out* if  $\alpha_{\xi_x} = 0$  for some  $x \in \Lambda$ , otherwise it is said to *survive*.

Note that condition (4.4) actually does not depend on the lattice site  $x$ , since  $\Lambda$  is connected and therefore the CP is irreducible on  $X \setminus \{0\}$ .

**Proposition 4.6** *If the CP dies out for infection rate  $\lambda' > 0$ , then it dies out for all  $\lambda \in [0, \lambda']$ . The **critical value**  $\lambda_c \in [0, \infty]$  is then given by*

$$\lambda_c := \sup \{ \lambda \geq 0 : \text{CP with infection rate } \lambda \text{ dies out} \}. \quad (4.35)$$

**Proof.** Monotonicity in  $\lambda$  of the CP (Lemma 4.4) and  $\eta_0^\lambda = \eta_0^{\lambda'}$  imply that if  $(\eta_t^{\lambda'} : t \geq 0)$  dies out so does  $(\eta_t^\lambda : t \geq 0)$ .

Since the CP with  $\lambda = 0$  certainly dies out, the supremum  $\lambda_c$  is well defined in  $[0, \infty]$ .  $\square$

**Proposition 4.7** *Analogous to above for any  $A \subseteq \Lambda$  write  $\xi_A \in X$  for  $\xi_A(y) = \mathbb{1}_A(y)$ . Then the survival probability is*

$$\alpha_{\xi_A} = \mathbb{P}^{\xi_A}(\eta_t \neq 0 \text{ for all } t \geq 0) = \bar{\nu}_\lambda(\{\xi_B : B \cap A \neq \emptyset\}), \quad (4.36)$$

and for  $\lambda < \lambda_c$  we have  $\bar{\nu}_\lambda = \delta_0$  for  $\lambda > \lambda_c$ ,  $\bar{\nu}_\lambda \neq \delta_0$ .

**Proof.** The result is based on the following *duality property* of the CP. For all  $A, B \subseteq \Lambda$  we have

$$\mathbb{P}^{\xi^A}(\eta_t(x) = 1 \text{ for some } x \in B) = \mathbb{P}^{\xi^B}(\eta_t(x) = 1 \text{ for some } x \in A). \quad (4.37)$$

For a proof of this see e.g. [L85] Theorem VI.1.7. Now choosing  $B = \Lambda$  we have  $\xi_B(x) = 1$  for all  $x \in \Lambda$  and

$$\mathbb{P}^{\xi^A}(\eta_t \neq 0) = \mathbb{P}^{\delta_1}(\eta_t(x) = 1 \text{ for some } x \in A). \quad (4.38)$$

Taking the limit  $t \rightarrow \infty$  implies the first statement. For  $\lambda < \lambda_c$  the process dies out with probability 1 for all initial configurations  $\xi_x$  and thus with  $A = \{x\}$  in (4.36) we have

$$\bar{\nu}_\lambda(\eta(x) = 1) = \bar{\nu}_\lambda(\eta(x)) = \rho_x(\lambda) = 0 \quad \text{for all } x \in \Lambda, \quad (4.39)$$

which implies that  $\bar{\nu}_\lambda = \delta_0$ . For  $\lambda > \lambda_c$  the process survives, and thus (4.39) has non-zero value and  $\bar{\nu}_\lambda \neq \delta_0$ .  $\square$

**Remark.** Note that Prop. 4.7 implies in particular that the density

$$\rho_x(\lambda) = \bar{\nu}_\lambda(\eta(x)) = \mathbb{P}^{\xi_x}(\eta_t \neq 0 \text{ for all } t \geq 0) \quad (4.40)$$

is equal to the survival probability.

Our results so far imply that there is a well defined critical value  $\lambda_c \in [0, \infty]$  such that the CP dies out and  $\bar{\nu}_\lambda = \delta_0$  for  $\lambda < \lambda_c$ , and the CP survives and  $\bar{\nu}_\lambda \neq \delta_0$  for  $\lambda > \lambda_c$ . On a finite lattice we have discussed above that  $\lambda_c = \infty$ . The crucial question on infinite lattices is now whether  $\lambda_c$  is *non-trivial*, i.e.  $\lambda_c \in (0, \infty)$ . Certainly the value of  $\lambda_c$  will depend on the lattice  $\Lambda$  but at least one can derive a quite general lower bound.

Let  $(\eta_t : t \geq 0)$  be the CP with infection rate  $\lambda$  on a connected graph  $(\Lambda, E)$ . Consider the auxiliary process  $(\zeta_t : t \geq 0)$  on the same graph with state space  $X = \mathbb{N}^\Lambda$  and generator

$$\mathcal{L}f(\zeta) = \sum_{x \in \Lambda} \left( \eta(x) (f(\zeta^{-x}) - f(\zeta)) + \lambda \sum_{y \sim x} \zeta(y) (f(\zeta^{+x}) - f(\zeta)) \right), \quad (4.41)$$

where we write  $\zeta^{\pm x}(y) = \begin{cases} \zeta(y) \pm 1 & , y = x \\ \zeta(y) & , y \neq x \end{cases}$ . In this process particles independently create new particles at connected sites with rate  $\lambda$  and die independently with rate 1, so the number of particles per site can be larger than 1. We couple this process to a CP  $(\eta_t : t \geq 0)$  by using the same Poisson processes  $PP(\lambda)$  and  $PP(1)$  for infection/creation and death/recovery in the graphical construction. If for the auxiliary process  $\zeta_t > 1$ , we use independent creation and death processes for the extra particles. This construction implies that the CP is *dominated* by the  $\zeta$ -process, i.e.

$$\eta_0 \leq \zeta_0 \quad \Rightarrow \quad \eta_t \leq \zeta_t \quad \text{for all } t \geq 0. \quad (4.42)$$

Therefore if  $(\zeta_t : t \geq 0)$  dies out then the CP dies out as well. Now let  $m$  be the maximal vertex degree of the graph  $(\Lambda, E)$ . Then the number of particles in the  $\zeta$ -process is dominated by a Markov chain  $N(t)$  on the state space  $\mathbb{N}$  with transition rates

$$c(n, n+1) = nm\lambda \quad \text{for } n \geq 0, \quad c(n, n-1) = n \quad \text{for } n \geq 1. \quad (4.43)$$

All the particles independently create new particles at rate  $m\lambda$  and die at rate 1. Again there exists an obvious coupling such that

$$\sum_{x \in \Lambda} \zeta_t(x) \leq N(t) \quad \text{for all } t \geq 0. \quad (4.44)$$

$N(t)$  is a well-known birth-death chain with absorbing state  $n = 0$ , and dies out with probability 1 if and only if  $m\lambda \leq 1$ . For  $m\lambda > 1$  the average  $\mathbb{E}(N(t))$  is monotone increasing and the process can survive with positive probability.

**Proposition 4.8** *Consider a CP on a connected graph  $(\Lambda, E)$  with maximal vertex degree  $m$ . Then  $\lambda_c \geq 1/m$ .*

**Proof.** With initial condition  $\xi_x$  as in Definition 4.4 and using the above coupling the number of active sites in the CP is dominated by the birth-death chain

$$\sum_{x \in \Lambda} \eta_t(x) \leq N(t) \quad \text{with} \quad N(0) = 1. \quad (4.45)$$

Therefore  $\lambda \leq 1/m$  implies that the CP dies out and thus  $\lambda_c \geq 1/m$ .  $\square$

Note that the lower bound coincides with the mean-field prediction  $\lambda_c = 1/m = 1/(2d)$  of Section 4.1. To get an upper bound on  $\lambda_c$  is in general harder. In the following we will concentrate on  $\Lambda = \mathbb{Z}^d$  and only give a small part of the proof.

#### 4.4 Results for $\Lambda = \mathbb{Z}^d$

Consider the CP on the regular lattice  $\Lambda = \mathbb{Z}^d$ .

**Theorem 4.9** *For the critical value  $\lambda_c(d)$  of a CP on the lattice  $\Lambda = \mathbb{Z}^d$  we have*

$$\frac{1}{2d} \leq \lambda_c(d) \leq \frac{2}{d} \quad \text{for all } d \geq 1. \quad (4.46)$$

**Proof.** The lower bound is given by Prop. 4.8, for the proof of  $\lambda_c(1) \leq 2$  see Theorem VI.1.33 in [L85]. For higher dimensions the required inequality  $\lambda_c(d) \leq \lambda_c(1)/d$  follows from

$$\mathbb{P}^{\xi_x}(\eta_t^d \neq 0) \geq \mathbb{P}^{\xi_x}(\eta_t^1 \neq 0), \quad t \geq 0, \quad (4.47)$$

where  $(\eta_t^d : t \geq 0)$  is the  $d$ -dimensional CP with rate  $\lambda$ , and  $(\eta_t^1 : t \geq 0)$  is a 1-dimensional CP with rate  $d\lambda$ . We show this by coupling the two processes such that for each  $y \in \mathbb{Z}$

$$\eta_t^1(y) = 1 \quad \text{implies} \quad \eta_t^d(x) = 1 \quad \text{for some } x \text{ such that } \pi_d(x) = y, \quad (4.48)$$

where for all  $x \in \mathbb{Z}^d$  we denote

$$\pi_d(x) = \pi_d(x_1, \dots, x_d) = x_1 + \dots + x_d \in \mathbb{Z}. \quad (4.49)$$

Suppose that  $A \subseteq \mathbb{Z}^d$  and  $B \subseteq \mathbb{Z}$  are finite and such that

$$B \subseteq \pi_d(A) = \{\pi_d(x) : x \in A\}, \quad (4.50)$$

i.e. for each  $y \in B$  there is (at least) one  $x \in A$  such that  $y = \pi_d(x)$ . Choose one of these  $\bar{x}$ , and associate its  $PP(1)$  death process with site  $y$ . Also, for all of the  $2d$  neighbours of  $\bar{x}$  we have

$$x \sim \bar{x} \quad \text{implies} \quad \pi_d(x) = y \pm 1 \sim y. \quad (4.51)$$

Now associate the infection processes  $PP(\lambda)$  pointing towards  $\bar{x}$  from all its neighbours with infections at  $y$ , which leads to a net infection rate of  $d\lambda$  from each of the two neighbours  $y \pm 1$ . Note



that all other deaths and infections in the  $d$ -dimensional CP that would correspond to  $y$  are not used in the coupling. With this construction both marginal processes  $(\eta_t^1 : t \geq 0)$  and  $(\eta_t^d : t \geq 0)$  have the right law, and clearly (4.48) is fulfilled, which finishes the proof.  $\square$

Using more involved techniques than we do here, lower and upper bound can be improved significantly, depending on the dimension  $d$ . Further it can be shown that

$$d \lambda_c(d) \rightarrow \frac{1}{2} \quad \text{as } d \rightarrow \infty, \quad (4.52)$$

supporting the physics wisdom that 'mean-field theory is exact in high dimensions'.

**Theorem 4.10 Complete convergence**

Suppose that  $\lambda > \lambda_c$ , then for every  $\eta \in X$  as  $t \rightarrow \infty$

$$\delta_\eta S(t) \rightarrow \alpha_\eta \bar{\nu}_\lambda + (1 - \alpha_\eta) \delta_0 \quad \text{weakly (locally)}, \quad (4.53)$$

where  $\alpha_\eta = \mathbb{P}^\eta(\eta_t \neq 0 \text{ for all } t \geq 0)$  is the survival probability.

**Proof.** See e.g. [L99], Theorem I.2.27.

**Remark.**

Taking the expected value w.r.t. an initial distribution  $\mu$  in (4.53) we get weak convergence of

$$\mu S(t) \rightarrow \mu(\alpha_\eta) \bar{\nu}_\lambda + (1 - \mu(\alpha_\eta)) \delta_0. \quad (4.54)$$

This holds in particular for all stationary  $\mu \in \mathcal{P}(X)$ , and therefore every stationary distribution is a convex combination of  $\delta_0$  and  $\bar{\nu}_\lambda$  and we have

$$\mathcal{I}_e = \{\delta_0, \bar{\nu}_\lambda\}. \quad (4.55)$$

**Theorem 4.11 Extinction time**

Suppose  $\lambda > \lambda_c$  and for the CP  $(\eta_t : t \geq 0)$  let

$$\tau := \inf\{t \geq 0 : \eta_t = 0\} \quad (4.56)$$

be the **extinction time** of the process. Then there exists  $\epsilon > 0$  such that for every initial condition  $\eta_0 = \eta \in X$

$$\mathbb{P}^\eta(\tau < \infty) \leq e^{-\epsilon|\eta|} \quad \text{where } |\eta| = \sum_{x \in \Lambda} \eta(x). \quad (4.57)$$

**Proof.** see [L99], Theorem I.2.30

Note that this implies that the supercritical CP can only die out with positive probability if the initial condition is finite  $|\eta| < \infty$ . If, however,  $\mu \in \mathcal{P}(X)$  is translation invariant and  $\mu(\eta(x)) > 0$ , then we have  $\mu(|\eta| = \infty) = 1$ , and therefore

$$\mathbb{P}^\eta(\tau = \infty) = \alpha_\eta = 1 \quad (4.58)$$

and the process survives with probability 1. With Theorem 4.10 this implies

$$\mu S(t) \rightarrow \bar{\nu}_\lambda \quad \text{as } t \rightarrow \infty. \quad (4.59)$$

**Theorem 4.12** *The critical contact process dies out.*

**Proof.** see [L99], Theorem I.2.25

This implies that the density

$$\rho(\lambda) = \bar{\nu}_\lambda(\eta(x)) = \mathbb{P}^{\xi_x}(\eta_t \neq 0 \text{ for all } t \geq 0) \quad (4.60)$$

which is independent of  $x$  due to translation invariance, is a continuous function of  $\lambda$ . By Proposition 4.5 it is also monotone increasing, for  $\lambda > \lambda_c$  and vanishes for  $\lambda < \lambda_c$  by Proposition 4.7. In particular, to leading order the behaviour at the critical point is given by

$$\rho(\lambda) \sim C(\lambda - \lambda_c)^\beta \quad (4.61)$$

for some exponent  $\beta > 0$ . The only rigorous bound is  $\beta \leq 1$ , and our mean-field result from section 4.1 predicts  $\lambda_c = 1/(2d)$  and for  $\lambda \geq \lambda_c$  similar we have to leading order

$$\rho(\lambda) = 1 - \frac{1}{2d\lambda} = 1 - \frac{1}{2d\lambda_c} \left(1 + \frac{\lambda - \lambda_c}{\lambda_c}\right)^{-1} \simeq \frac{\lambda - \lambda_c}{\lambda_c}, \quad (4.62)$$

which implies  $\beta = 1$ . In fact numerical estimates give values  $\beta \approx 0.28$  ( $d = 1$ ),  $0.58$  ( $d = 2$ ),  $0.81$  ( $d = 3$ ), and for  $d \geq 4$  the mean-field value  $\beta = 1$  should be 'exact'.

The CP has also been analyzed on other regular lattices, in particular homogeneous trees  $T^d$  (see e.g. Chapter I.4 in [L99]). In this case the critical behaviour turns out to be more complicated, there exists a second critical value  $\lambda_2 > \lambda_c$  and complete convergence in the sense of Theorem 4.10 only holds outside the interval  $[\lambda_c, \lambda_2]$ . Inside this interval there exist infinitely many extremal invariant measures and the infection survives globally but dies out locally.

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