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Phase transitions in nonequilibrium stochastic particle systems with local conservation laws

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Abstract

Stochastic particle systems far from equilibrium show a great variety of critical phenomena already in one dimension. Their understanding is a current topic of major research, especially for systems with several particle species which exhibit a particularly rich critical behavior. In lack of a general theory, the basic mechanisms are studied by analyzing the stationary measures of minimal models. In this thesis we concentrate on systems where the number of particles is locally conserved, of which there are two basic types:
Exclusion processes and in particular the asymmetric simple exclusion processes (ASEP) and its variants have been studied extensively as minimal models showing boundary induced phase transitions, which can be effectively described on a macroscopic level.
The zero range process (ZRP) without exclusion interaction is a minimal model for a condensation transition. This has become of recent interest providing a general criterion for phase separation in exclusion models with periodic boundary conditions.

The first part of this thesis is devoted to boundary induced phase transitions. One open question in this context concerns an effective description of complex boundary conditions. We derive exact expressions for the stationary measures of the ASEP on a semi-infinite lattice coupled to a particle reservoir. For more general boundary mechanisms we establish existence and uniqueness of an effective reservoir density, by characterizing stationary product measures with localized inhomogeneities. Another problem is the derivation of rigorous results on stationary measures with open boundaries in the presence of several particle species. To this aim we introduce a multi-component version of the ZRP, establish the hydrodynamic limit and solve the macroscopic system of hyperbolic conservation laws with open boundaries under very general conditions.

In the second part we present a rigorous analysis of the condensation transition in the ZRP with periodic boundaries. If the particle density exceeds a critical value, the system phase separates into a homogeneous background and a condensed phase. We prove this by showing the equivalence of the canonical and the grand-canonical stationary measures in the thermodynamic limit. We also show that for large systems the condensed phase typically concentrates only on a single, randomly located site. The first result is generalized to a ZRP with two species of particles, showing a far more complex critical behavior. Using random walk arguments supported by Monte Carlo simulations, we also derive a coarsening scaling law for the dynamics of the condensation. We discuss a generalization to two-component processes, and the dependence on the symmetry of the jump probabilities and on the space dimension.

Zusammenfassung

Stochastische Teilchensysteme fernab vom Gleichgewicht zeigen bereits in einer Raumdimension eine große Vielfalt an kritischen Phänomenen. Deren Verständnis ist Gegenstand aktueller Forschung, vor allem für Systeme mit mehreren Teilchensorten, die ein besonders reichhaltiges kritisches Verhalten aufweisen. Da eine allgemeine Theorie nicht vorliegt, werden die grundlegenden Mechanismen anhand des stationären Verhaltens von Minimalmodellen untersucht. In dieser Arbeit beschränken wir uns dabei auf Systeme, in denen die Teilchenzahl lokal erhalten ist. Man unterscheidet zwei grundlegende Arten:
Exklusionsprozesse und insbesondere der asymmetrische einfache Exklusionsprozess (ASEP) wurden ausführlich untersucht als Minimalmodelle für randinduzierte Phasenübergänge, die auf makroskopischer Ebene effektiv beschrieben werden können.
Der "Zero-Range" Prozess (ZRP) ohne Ausschlusswechselwirkung ist ein Minimalmodell für Kondensationsübergänge. Dies wurde kürzlich benutzt, um ein allgemeines Kriterium für Phasenseparation in Exklusionsprozessen mit periodischen Randbedingungen aufzustellen.

Der erste Teil der Arbeit widmet sich offenen Fragen zu randinduzierten Phasenübergängen, wie zum Beispiel einer effektiven Beschreibung komplexer Randbedingungen. In diesem Zusammenhang leiten wir exakte Ausdrücke für stationäre Maße des ASEP auf einem halbunendlichen Gitter mit Teilchenreservoir her. Für verallgemeinerte Randmechanismen zeigen wir Existenz und Eindeutigkeit einer effektiven Reservoirdichte, indem wir stationäre Produktmaße mit lokalisierten Inhomogenitäten charakterisieren. Eine weitere Frage betrifft rigorose Ergebnisse für stationäre Maße bei offenen Randbedingungen mit mehreren Teilchensorten. Dazu führen wir den ZRP mit mehreren Komponenten ein, zeigen den Hydrodynamischen Limes und geben eine weitgehend allgemeine Lösung des makroskopischen Systems hyperbolischer Erhaltungsgleichungen mit offenen Randbedingungen.

Im zweiten Teil präsentieren wir eine rigorose Untersuchung des Kondensationsüberganges im ZRP mit periodischen Randbedingungen. Übersteigt die Teilchendichte einen kritischen Wert, separiert das System in einen homogene Hintergrund und eine kondensierte Phase. Im Beweis zeigen wir die Äquivalenz von kanonischen und großkanonischen stationären Maßen im hydrodynamischen Limes. Darüber hinaus zeigen wir, dass die kondensierte Phase in großen Systemen typischerweise auf nur einen zufälligen Gitterplatz konzentriert ist. Das erste Resultat wird auf einen ZRP mit zwei Teilchensorten verallgemeinert, der ein wesentlich komplexeres kritisches Verhalten zeigt. Unter Benutzung von heuristischen Argumenten und Monte Carlo Simulationen leiten wir ein "Coarsening" Skalengesetz für die Zeitentwicklung der Kondensation her. Wir diskutieren eine Verallgemeinerung zu Prozessen mit zwei Teilchensorten und die Abhängigkeit von der Symmetrie der Sprungwahrscheinlichkeiten und von der Raumdimension.

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Contents

Notation

$\mathbb{Z}$	integer numbers
$\mathbb{Z}^+ = \{1, 2, \ldots\}$	positive integer numbers
$\mathbb{N} = \{0, 1, 2, \ldots\}$	nonnegative integer numbers
$\mathbb{R}$	real numbers
$[a]$	largest integer smaller or equal to $a \in \mathbb{R}$
$\delta_{.,.}$ or $\delta(.,.)$	Kronecker delta function on $\mathbb{Z}^2$
$\chi_A(.)$	indicator function of the set A
$\Theta(.)$	Heaviside step function with $\Theta(0) = 0$ and $\Theta(k) = 1$, $k > 0$
${}_2F_1$	hypergeometric function (p. 83)
$a \wedge b$	minimum of a and $b \in \mathbb{R}$
$(a)_k$	Pochhammer symbol (p. 83)
$\partial_x = \frac{\partial}{\partial x}$	partial derivative with respect to x
$\lvert . \rvert$	cardinality of a set, absolute value, Euclidean norm
$\propto$	proportional
$\simeq$, $\sim$	asymptotically equal, asymptotically proportional (pp. 39, 100)
$\langle w \lvert A \rvert v \rangle$	scalar product in bra-ket notation with operator A (p. 22)
τ_x	translation with $x \in \Lambda$ (p. 8)
$(\mathbf{k}^i, k_i \pm 1)$	vector with modified component i (p. 59)

d	space dimension
n	number of particle species
Λ	lattice, connected subset of $\mathbb{Z}^d$
Λ_L	finite lattice of size L^d
L	length of a lattice in one space direction
x, y	lattice sites
E	local state space, subset of $\mathbb{N}$
η_{max}	maximum number of particles per site
$\eta(x)$	local configuration (number of particles) at a given site
$\boldsymbol{\eta} = \big(\eta(x)\big)_{x\in\Lambda}$	configuration of the process
$\boldsymbol{\eta}^{x\to y}$	configuration after a particle jumped from x to y (p. 6)
$\boldsymbol{\eta}^{x\leftrightarrow y}$	configuration after exchange of $\eta(x)$ and $\eta(y)$ (p. 20)
$X = E^\Lambda$	state space of the process on Λ
$X_L = E^{\Lambda_L}$	state space of the process on Λ_L
$\Sigma_L(\boldsymbol{\eta})$	number of particles in configuration $\boldsymbol{\eta} \in X_L$ (p. 9)
N	fixed number of particles
$X_{L,N}$	canonical state space with fixed number of particles (p. 9)
$\mu_{L,N}$	canonical stationary measure on $X_{L,N}$ (p. 9)
$Z(L, N)$	canonical partition function (p. 31)

$D[0,\infty)$	set of right continuous paths with left limits
$(\boldsymbol{\eta}_t)_{t\in[0,\infty)}$	path (realization) of the process
$\mathbb{P}^{\boldsymbol{\eta}}$	probability measure on path space with initial condition $\boldsymbol{\eta}_0 = \boldsymbol{\eta}$
$\mathbb{E}^{\boldsymbol{\eta}}$	expectation value with respect to $\mathbb{P}^{\boldsymbol{\eta}}$
$c(x, y, \boldsymbol{\eta})$	jump rate of a particle from site x to y given a configuration $\boldsymbol{\eta}$ (p. 7)
$\mathcal{L}$	Markov generator of the process (pp. 7, 116)
$\mathcal{L}_b$, $\mathcal{L}_v$	boundary and volume part of the generator $\mathcal{L} = \mathcal{L}_b + \mathcal{L}_v$ (p. 8)
$S(t)$	Markov semigroup of the process (pp. 6, 115)
$C_{(b)}(X, \mathbb{R})$	set of (bounded) continuous functions $f : X \to \mathbb{R}$
$C_0(X, \mathbb{R})$	set of cylinder functions $f : X \to \mathbb{R}$ (p. 7)
$C^k(X, \mathbb{R})$	set of k times continuously differentiable functions $f : X \to \mathbb{R}$
$L(X, \mathbb{R})$	set of Lipschitz continuous functions $f : X \to \mathbb{R}$ (p. 30)
$P(X)$	set of probability measures on X
$\langle . \rangle_\mu$	expectation value with respect to a measure $\mu \in P(X)$
μ^k	k-point marginal of a measure $\mu \in P(X)$ (pp. 21, 78)
$H(\mu\|\nu)$	relative entropy of $\mu \in P(X)$ with respect to $\nu \in P(X)$ (p. 118)
$\mathcal{I}$	set of stationary measures (p. 8)
$\mathcal{I}_e$	set of extremal stationary measures (p. 9)

ρ, $\boldsymbol{\rho} = (\rho_i)_{i=1\ldots n}$	particle density, vector for n-species systems
ν_ρ, $\nu_{\boldsymbol{\rho}}$	product measure of density ρ, $\boldsymbol{\rho}$ (p. 21)
μ, $\boldsymbol{\mu} = (\mu_i)_{i=1\ldots n}$	chemical potential, vector for n-species systems
$\bar{\nu}_\mu$, $\bar{\nu}_{\boldsymbol{\mu}}$	product measure with chemical potential μ, $\boldsymbol{\mu}$ (p. 59)
ϕ, $\boldsymbol{\phi} = (\phi_i)_{i=1\ldots n}$	fugacity $\phi = \exp[\mu] \in [0,\infty)$, vector for n-species systems
$\bar{\nu}_\phi$, $\bar{\nu}_{\boldsymbol{\phi}}$	product measure with fugacity ϕ, $\boldsymbol{\phi}$ (p. 31)
R, $\mathbf{R}$, R_i	particle density as a function of fugacity or chem. potential (pp. 31, 60)
M, $\mathbf{M}$, M_i	chemical potential as a function of particle density (p. 61)
Φ, $\boldsymbol{\Phi}$, Φ_i	fugacity as a function of particle density (pp. 31, 88)
D_μ	domain of R, $\mathbf{R}$ as a function of chemical potential (p. 60)
D_ϕ	domain of R, $\mathbf{R}$ as a function of fugacity (p. 31)
D_ρ	range of the function R, $\mathbf{R}$ (pp. 31, 60)
$Z(\phi)$, $Z(\boldsymbol{\phi})$	grand canonical partition function (p. 31)
$Z(\mu)$, $Z(\boldsymbol{\mu})$	grand canonical partition function (p. 60)
ϕ_c	radius of convergence of $Z(\phi)$ (p. 31)
ρ_c, $\boldsymbol{\rho}_c$, $\rho_{c,i}$	critical density (p. 31), of species i (p. 90)
j, $\mathbf{J}$, J_i	stationary current as a function of density (pp. 12, 33, 61)
g, g_i	jump rates of the zero range process (pp. 29, 58)
p, p_i	jump probabilities of the zero range process (pp. 29, 58)
m, m^k	typical condensate size, size of the k-th largest condensate (p. 104, 107)
$\mathcal{C}_L(t)$	set of cluster sites as a function of time (p. 101)
$M_L(t)$	total number of particles in condensates (p. 101)

We use some shorthands to simplify notation concerning events and measures. Let μ be a measure on some countable set Ω. Then we write $\mu(A) := \sum_{\omega\in A} \mu(\omega)$ for all $A \subset \Omega$, and $\{f \in D\} := \{\omega | f(\omega) \in D\}$ for measurable $D \subset \mathbb{R}$ and random variables $f : \Omega \to \mathbb{R}$.

Chapter 1

Introduction

The stochastic particle systems we consider in this thesis consist of randomly moving particles on a lattice, whose motion is influenced by interactions between each other. They are frequently applied in physics, biology or the social sciences as mathematical models for various phenomena which involve a large number of identical components. A direct example from epitaxial growth is given by diffusive motion of atoms on the surface of a crystal, corresponding to a lattice of about 10^{20} sites per square meter. But applications are not limited to systems endowed with such a lattice geometry, since continuous degrees of freedom can often be discretized without changing the main features. So depending on the specific case, the 'particles' can also be cars on a freeway, 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 then 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 stochastic particle system 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 freeway. Although describing the system only on the mesoscopic level 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 hydrodynamic partial differential equation. The form of this equation depends on the particular application, and its derivation from a microscopic particle model is one of the fundamental tasks of statistical mechanics [129].

The external conditions for real systems are usually constant or slowly varying with respect to the system dynamics, so 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. In case of equilibrium or reversible systems, the dynamics is governed by an energy function which also determines the stationary behavior.

The stationary process shows a time reversal symmetry and additional tools for the analysis become available. This is only the case if the stochastic dynamics have certain symmetry properties, but on the other hand many systems show an inherent bias in the stochastic dynamics. Examples are freeway traffic, where cars go only in one direction, or charged particles in an electric field. For such nonequilibrium systems the stationary distribution has to be derived from the dynamics in lack of an energy function, and they are of primary interest in this thesis.

Of particular importance in the analysis are phase transitions, resulting from collective behavior of particles over large distances which leads to qualitative differences in the stationary properties on changing the system parameters. A fundamental task of statistical mechanics is to understand the emergence of such macroscopic phenomena from the microscopic interactions. For equilibrium systems this has been studied extensively in the physics literature [72], and there is a well established mathematical theory of phase transitions in terms of Gibbs measures [56]. For non-reversible systems this is still a topic of major interest, and although there has been a lot of progress in the past years, there is no systematic, general approach comparable to equilibrium statistical mechanics. So far the notion of a phase transition has been used in a rather phenomenological sense, by studying generic model systems and categorizing the observed critical phenomena [107, 124]. On the other hand, non-reversible systems have a much richer structure than their equilibrium counterparts, and a great variety of critical phenomena can be observed already in one spatial dimension.

A decisive influence on the dynamical and stationary behavior of a stochastic particle system is given by the presence of conservation laws. In many systems there exist quantities which are locally conserved during time evolution and may only enter or exit the system through boundaries, such as on and off ramps for cars on a freeway (as long as one excludes events like car accidents from the consideration). Examples with non-conserving dynamics such as spread of infection or reaction diffusion systems [124] show a different critical behavior and often exhibit phase transitions into absorbing states [68]. In this thesis we concentrate on lattice gases, where the particles are locally conserved and the hydrodynamic equation is given by a hyperbolic conservation law [26]. For such systems there are basically two types of critical phenomena which are explained below. To understand their basic principles, these phenomena have been studied for minimal models with limited direct applications, but which capture the essential mechanisms of real systems.

A variety of minimal lattice gas models has been introduced in [128], for which one can distinguish between two basic types. In exclusion processes, the maximum number of particles on a lattice site is restricted to one, corresponding to a hard core or exclusion interaction. A paradigmatic model of this class is the asymmetric simple exclusion process (ASEP), where particles jump to (empty) nearest neighbor sites with biased rates on a one-dimensional lattice. It was originally introduced as a model for the kinetics of protein synthesis [102] and has been studied extensively in the physics literature, since it can be applied to various phenomena such as interface growth, directed polymers [92], as well as freeway traffic [23]. Furthermore it can be mapped on vertex models and quantum spin chains [124]. There are detailed results on the stationary properties of the ASEP which are summarized in Part III of [100]. It is a topic of current research to extend these results to exclusion models with more complex interactions.

The most basic model without restrictions on the number of particles per site is the zero range process (ZRP), where the jump rate of a particle only depends on the occupation number at its departure site, resembling an interaction of range zero. The process is defined in arbitrary space dimension and its stationary measures have product form under very general conditions [3]. This simple structure could be used for deducing several results for exclusion models, in particular for disordered systems, since they can often be mapped on the ZRP. It has also been applied to sandpile dynamics, to 1+1 dimensional interface growth by the step flow mechanism or to structural glasses under the name backgammon model. In addition, the process provides a minimal model for condensation transitions which can be analyzed in detail due to the simple form of the stationary measure. For a review including applications and results on the ZRP see [40] and references therein.

On the basis of these simplified models, there has been a lot of recent research concerning the stationary behavior of driven lattice gases. In the following, we shortly describe part of the results and some remaining open questions which are addressed in this thesis.

Unlike in equilibrium, for non-reversible systems which are in contact with particle reservoirs at their boundary, the stationary behavior is the result of an interplay between boundary and bulk effects. This leads to boundary induced critical phenomena [89] which can be captured in terms of an extremal principle for the current [124], as the result of a macroscopic analysis of the motion and stability of domain walls, separating regions of different densities. A key ingredient in this analysis is the characterization of the boundary in terms of a single density variable. If the system is not simply coupled to a boundary reservoir but shows a more complex mechanism of particle injection and ejection, one expects that the latter can be replaced by an effective density, but there are practically no rigorous results. We address this question in Chapter 3, where the ASEP is studied on a semi-infinite lattice giving an exact expression for the stationary measure in case of reservoir coupling. For any generalized boundary mechanism we establish existence and uniqueness of an effective density, by characterizing stationary product measures for which boundary inhomogeneities remain localized within a finite region. Our method allows an explicit calculation of the effective density, but the approach is restricted to models with ASEP bulk dynamics. We also propose a less explicit definition of the effective boundary density for general systems and discuss the limitations of this concept.

Recently processes with two or more particle species have been of particular interest, showing a much richer critical behavior than one-component systems, including for example spontaneous symmetry breaking even in one dimension [125]. A major topic is the identification of a principle governing the selection of stationary measures for open boundary conditions, analogous to the single species case. The first step in this direction is the derivation of the hydrodynamic behavior which has only recently been understood in some specific cases. In this context we introduce the n-component ZRP in Chapter 4 and characterize stationary product measures for periodic boundary conditions. Following the derivation for one-component systems [84], we establish the hydrodynamic limit given by a system of hyperbolic conservation laws. Stationary solutions of these equations take a particularly simple form in a transformed variable and are stated explicitly. With these results, the ZRP is one of the few examples of multi-species systems, where the selection of stationary measures on a macroscopic level is well understood under very general conditions.

In addition to boundary induced phenomena, multi-species systems exhibit phase separation also on periodic lattices [125]. In this context the (one-component) ZRP recently received attention as an effective model of domain wall dynamics for such phenomena. The correspondence to a condensation transition in the ZRP has provided a general criterion to determine the existence of phase separation in driven systems with conserved density [76]. Apart from this relation, the condensation in the ZRP is of interest in its own right as an example of a phase transition in an exactly solvable model. So far this phenomenon has been studied only non-rigorously [40]. In Chapter 5 we give exact results on the condensation transition in the context of the equivalence of ensembles. We prove that a typical stationary configuration in large systems consists of a background phase at some critical density, and that essentially all excess particles condense on a single, randomly located site. The first result is generalized to a ZRP with two species of particles, showing a far more complex critical behavior, involving simultaneous condensation.

In Chapter 6 we investigate the relaxation dynamics of the condensation with uniform initial distribution, using non-rigorous random walk arguments corroborated by Monte Carlo simulations. The time evolution of the condensed phase shows an interesting coarsening behavior which is a well known phenomenon in the context of phase separation. For the ZRP we derive a scaling law, governing the cluster growth in the condensed phase, for which there have been only numerical results in special cases so far. We discuss the dependence on the symmetry of the jump rates, on the space dimension and a generalization to two-component processes. For the late stage of the dynamics we derive an effective master equation which governs the saturation of the system towards a typical stationary configuration. Given the correspondence to exclusion models, the results of Chapters 5 and 6 also provide new information on the stability and the dynamics of domain walls in two-component systems. This already proved to be a key ingredient in the theory of boundary induced phase transitions in systems with one conservation law and thus may shed light on similar phenomena in two-component systems.

The thesis is organized as follows: In the first section of Chapter 2 we give a precise mathematical definition of interacting particle systems, based on material from [99]. We introduce the notion of a phase transition in our context and explain the basic concepts of hydrodynamic limits. The rest of Chapter 2 contains a detailed summary of previous work on exclusion processes and the ZRP which is relevant for the subsequent presentation of our results. As indicated above, in Chapters 3 and 4 we address open questions concerning boundary induced critical phenomena and the hydrodynamic characterization of stationary measures for open systems. Chapters 5 and 6 are devoted to a static and dynamical analysis of the condensation transition of the ZRP on a periodic lattice. We comment on the relevance of individual contributions at the end of each chapter, where we also discuss possible extensions for future research. In the appendix we shortly summarize the construction of stochastic particle systems on the basis of the Markov semigroup, properties of the relative entropy, and coupling techniques used in Chapter 3.

Chapter 2

Interacting particle systems

2.1 Definition and general properties

In this section we give a precise mathematical description of stochastic particle systems following the presentation in [99], and introduce the basic tools to study their critical behavior.

2.1.1 Construction of the dynamics

The Markov process

Interacting particle systems are continuous time Markov processes with a discrete state space $X = E^\Lambda$. The lattice Λ can be any countable set, but throughout this thesis we concentrate on connected subsets of $\mathbb{Z}^d$. At each lattice site $x \in \Lambda$ the local state is denoted by $\eta(x) \in E$ such that $\boldsymbol{\eta} = \big(\eta(x)\big)_{x\in\Lambda} \in X$ gives the configuration of the system. In general the local state space E can be any countable set, but to fix ideas we take $E = \{0, 1, \dots, \eta_{max}\}$ with $\eta_{max} \in \mathbb{Z}^+$ and interpret $\eta(x)$ as the number of particles at site x. In particular, $\eta_{max} < \infty$ implies that E is compact and we can apply standard construction techniques. A generic example for this are exclusion processes with $E = \{0, 1\}$, discussed in Section 2.2. Modifications necessary for non-compact E can be found in Section 2.3.1, where we construct the zero range process with $E = \mathbb{N}$.

Endowed with the product topology, $X = E^\Lambda$ is a compact metric space with measurable structure given by the σ-algebra of Borel sets. The time evolution of the process is given by a path $\boldsymbol{\eta}_\cdot : [0, \infty) \to X$, where the generic path space $D[0, \infty)$ is restricted to right continuous paths with left limits.

Definition. A *Markov process* with state space X is defined as a family of probability measures $\big\{\mathbb{P}^{\boldsymbol{\eta}} \big| \boldsymbol{\eta} \in X\big\}$ on $D[0, \infty)$ with the following properties:

a) $\mathbb{P}^{\boldsymbol{\eta}}\big[\{\boldsymbol{\zeta}_\cdot \in D[0,\infty) \,\big|\, \boldsymbol{\zeta}_0 = \boldsymbol{\eta}\}\big] = 1$ for all $\boldsymbol{\eta} \in X$, i.e. $\mathbb{P}^{\boldsymbol{\eta}}$ is normalized on all paths with initial configuration $\boldsymbol{\eta}_0 = \boldsymbol{\eta}$.

b) The mapping $\boldsymbol{\eta} \mapsto \mathbb{P}^{\boldsymbol{\eta}}[A]$ is measurable for every $A \in \mathcal{F}$.

c) $\mathbb{P}^{\boldsymbol{\eta}}\big[\{\boldsymbol{\eta}_{t+\cdot} \in A\} \,\big|\, \mathcal{F}_t\big] = \mathbb{P}^{\boldsymbol{\eta}_t}[A]$ $a.s.$ for every $\boldsymbol{\eta} \in X$ and $A \in \mathcal{F}$.

The Markov property c) ensures that the probability of some future event $\{\boldsymbol{\eta}_{t+\cdot} \in A\}$ depends on the past $\mathcal{F}_t$ only through the present configuration $\boldsymbol{\eta}_t$. $(\mathcal{F}_t)_{t\geq 0}$ is the filtration on $D[0,\infty)$ induced by the process and $\mathcal{F} = \bigcup_{t\geq 0} \mathcal{F}_t$. More precisely, $\mathcal{F}_t$ is the smallest σ-algebra relative to which all mappings $\boldsymbol{\eta}_\cdot \mapsto \boldsymbol{\eta}_s$ for $s \leq t$ are measurable.

In [128] a variety of interacting Markov processes has been introduced. Throughout this thesis we focus on processes with local conservation of the number of particles, so-called *lattice gases*, where particles move on the lattice without being created or annihilated. The dynamics is specified by transition rates $c(x, y, \boldsymbol{\eta})$ at which a particle at site $x \in \Lambda$ jumps to site y, depending on the current configuration $\boldsymbol{\eta}$. The intuitive meaning of c is

$$\mathbb{P}^{\boldsymbol{\eta}}\big[\{\boldsymbol{\eta}_t = \boldsymbol{\eta}^{x\to y}\}\big] = c(x, y, \boldsymbol{\eta})t + o(t) \quad \text{as } t \searrow 0\,. \tag{2.1}$$

$\boldsymbol{\eta}^{x\to y}$ is the configuration resulting from $\boldsymbol{\eta}$ after a particle at site x jumped to site y, i.e. $\eta^{x\to y}(z) = \eta(z) - \delta_{x,z} + \delta_{y,z}$ for all $z \in \Lambda$. Strictly speaking (2.1) is only correct if Λ is finite, since otherwise the probabilities on the left are typically zero for $t > 0$. For infinite lattices it is often not clear if there exists a Markov process which corresponds to that description. This question was addressed in [67], giving a direct graphical construction of the process in space-time for $\Lambda = \mathbb{Z}^d$, limited to nearest neighbor interactions. For general interactions it is more convenient to characterize Markov processes via the corresponding Markov semigroup (see e.g. [79]). In the context of lattice gases this approach was first used in [71] for $\Lambda = \mathbb{Z}$ and later generalized in [95] to arbitrary countable lattices. Since this approach is standard by now, we only give a brief outline of the construction in the following and summarize a precise version of the statements and definitions in the Appendix A.1. A more detailed treatment can be found in [99], Chapter I.

Markov semigroup and generator

Let $P(X)$ be the set of probability measures on X. $C(X, \mathbb{R})$ denotes the set of continuous functions $f : X \to \mathbb{R}$ and is regarded as a Banach space with $\|f\| = \sup_{\boldsymbol{\eta}\in X} |f(\boldsymbol{\eta})|$. The rate function c is assumed to be nonnegative, uniformly bounded and continuous as a function of $\boldsymbol{\eta}$ in the product topology on X. A one-parameter family $\{S(t), t \geq 0\}$ of bounded linear operators on $C(X, \mathbb{R})$ is called a semigroup, if $S(0) = I$ and $S(s + t) = S(s)S(t)$ for all $s, t \geq 0$. It can be shown (see Theorem A.1 in the appendix), that every semigroup which is strongly continuous, nonnegative and $S(t)1 = 1$ for all $t \geq 0$, called *Markov semigroup*, uniquely defines a Markov process on X via

$$\mathbb{E}^{\boldsymbol{\eta}}\big[f(\boldsymbol{\eta}_t)\big] := S(t)\, f(\boldsymbol{\eta}) \quad \text{for all } f \in C(X, \mathbb{R}),\ \boldsymbol{\eta} \in X \text{ and } t \geq 0\,. \tag{2.2}$$

Such a Markov process has the additional property $S(t)f \in C(X, \mathbb{R})$ for all $f \in C(X, \mathbb{R})$, $t \geq 0$, and is called a *Feller process*. The operators $S(t)$ determine the time evolution of functions $f \in C(X, \mathbb{R})$, which can be interpreted as observables. According to the Hille-Yosida theorem (Theorem A.2) every Markov semigroup is generated by an operator $\mathcal{L} : C_0(X, \mathbb{R}) \to C(X, \mathbb{R})$ and $u(t) = S(t)\, f \in C(X, \mathbb{R})$ is the unique solution to the backward equation

$$\tfrac{d}{dt}u(t) = \mathcal{L}u(t)\,, \quad u(0) = f\,. \tag{2.3}$$

Here $C_0(X,\mathbb{R}) \subset C(X,\mathbb{R})$ denotes the set of cylinder functions, which depend only on finitely many lattice sites. The *Markov generator* for lattice gases is given by

$$\mathcal{L}f(\boldsymbol{\eta}) = \sum_{x,y\in\Lambda} c(x,y,\boldsymbol{\eta})\big[f(\boldsymbol{\eta}^{x\to y}) - f(\boldsymbol{\eta})\big] \,. \tag{2.4}$$

The restriction of $\mathcal{L}$ to $C_0(X,\mathbb{R})$ is important for convergence of the sum under natural summability conditions on $c(x,y,\boldsymbol{\eta})$.

Theorem 2.1 (Liggett) *Suppose that*

$$\sup_{y\in\Lambda}\sum_{x\in\Lambda}\sup_{\boldsymbol{\eta}\in X} c(x,y,\boldsymbol{\eta}) < \infty \,. \tag{2.5}$$

Then $C_0(X,\mathbb{R})$ is a core (see Appendix A.1) for the operator $\mathcal{L}$ defined in (2.4) and the closure of $\mathcal{L}$ is the generator of a strongly continuous Markov semigroup on $C(X,\mathbb{R})$ and thus of a Feller Markov process on X.

Proof. See [99], Theorem I.3.9.

By (2.5) the total rate of particles jumping to a site y is uniformly bounded, which guarantees a well defined first arrival event for every configuration $\boldsymbol{\eta}$. The time dependent distribution of the process with initial distribution $\pi \in P(X)$ is denoted by $\pi S(t)$ and uniquely defined by

$$\big\langle f\big\rangle_{\pi S(t)} = \big\langle S(t)f\big\rangle_{\pi} \,, \quad f\in C(X,\mathbb{R}) \,, \tag{2.6}$$

as a consequence of the Riesz representation theorem. This is connected to the description on path space via $\mathbb{P}^{\boldsymbol{\eta}}\big[\{\boldsymbol{\eta}_t \in A\}\big] = \delta_{\boldsymbol{\eta}} S(t)(A)$ for all $A \subset X$ with Dirac measure $\delta_{\boldsymbol{\eta}} \in P(X)$, but for the remainder of this thesis we stick to the semigroup notation.

Jump rates and boundary conditions

Theorem 2.1 is the most general result on the existence of lattice gases with compact state space. In particular, it follows that the dynamics of processes with finite state space is well defined. On infinite lattices one has to give extra conditions on the jump rates to ensure (2.5). It is sufficient to assume that c is of finite range $R \in \mathbb{Z}^+$, i.e.

$$c(x,y,\boldsymbol{\eta}) = 0 \quad \text{for all } x,y\in\Lambda \,, \text{ with } |x-y| > R \,, \tag{2.7}$$

and translation invariant. So $c(x,y,\boldsymbol{\eta})$ depends only on the difference $x-y$, and it can be written as

$$c(x,y,\boldsymbol{\eta}) = \tilde{c}(y-x,\boldsymbol{\eta}) \qquad \text{for all } x,y\in\Lambda \,. \tag{2.8}$$

Although much more restrictive than necessary, these conditions have an intuitive interpretation and are fulfilled by the processes we consider in the following, so from now in we assume (2.7) and (2.8).

Note that (2.8) in general does not imply translation invariance in the sense

$$c(x, y, \boldsymbol{\eta}) = c(x + a, y + a, \tau_a \boldsymbol{\eta}) \qquad \text{for all } a, x, y \in \Lambda \,, \tag{2.9}$$

with $(\tau_a \boldsymbol{\eta})(x) = \eta(x - a)$. This is only true if the underlying lattice Λ also has this property, i.e. $\tau_a \Lambda = \Lambda$. Generic choices of such translation invariant lattices are $\Lambda = \mathbb{Z}^d$ or finite lattices with periodic boundary conditions such as $\Lambda = (\mathbb{Z}/L\mathbb{Z})^d$ that we consider in Chapters 4 to 6. Another typical choice are lattices with (non-periodic) boundaries which are not translation invariant, such as $\Lambda = \{1, \dots, L\}$ or $\Lambda = \mathbb{Z}^+$ as in Chapter 3. In this case, one would like to allow for particle creation and annihilation within a certain boundary region $\partial\Lambda \subset \Lambda$ to describe, for example, the coupling to external particle reservoirs. This can be included in the above description by adding a boundary part $\mathcal{L}_b$ to the generator (2.4),

$$\mathcal{L}_b f(\boldsymbol{\eta}) = \sum_{x \in \partial\Lambda} \Big(c(b, x, \boldsymbol{\eta}) \big[f(\boldsymbol{\eta}^{b \to x}) - f(\boldsymbol{\eta}) \big] + c(x, b, \boldsymbol{\eta}) \big[f(\boldsymbol{\eta}^{x \to b}) - f(\boldsymbol{\eta}) \big] \Big) \,. \tag{2.10}$$

This is understood in the same way as (2.4) where $b \notin \Lambda$ is interpreted as a dummy boundary site. The rates $c(b, ., \boldsymbol{\eta})$ and $c(., b, \boldsymbol{\eta})$ concentrate on the boundary region $\partial\Lambda$ and to get well defined dynamics they have to be uniformly bounded for all $\boldsymbol{\eta} \in X$. analogous to (2.5).

In the following, (2.4) is called bulk or volume part of the generator, denoted by $\mathcal{L}_v$. In case of translation invariant Λ or vanishing boundary rates, so-called closed boundary conditions, no particles can enter or leave the system and it is called *closed*. Whereas for open boundary conditions, i.e. non-vanishing boundary rates, particles can be exchanged with the outside and the system is called *open*. To avoid complicated degeneracies we also assume that

the jump rate c is irreducible on finite lattices, (2.11)

so that every configuration can be reached within a finite time. On closed lattices this is understood on a state space restricted to a fixed number of particles, so that the latter is the only conserved quantity. We come back to this point when discussing the stationary measures in the next subsection.

2.1.2 Stationary measures

Definition. A probability measure $\mu \in P(X)$ is said to be *stationary* or *invariant* if it satisfies $\mu S(t) = \mu$ for all $t > 0$. The set of all invariant measures for a given process is denoted by $\mathcal{I}$. The measure is called *reversible* if $\langle f\, S(t)\, g \rangle_\mu = \langle g\, S(t)\, f \rangle_\mu$ for all $f, g \in C(X, \mathbb{R})$.

It is clear that every reversible measure is invariant, taking $g \equiv 1$ in the above definition. The probabilistic meaning is that if μ is stationary, the process $\boldsymbol{\eta}_t$ with initial distribution μ has the same joint distributions as $\boldsymbol{\eta}_{t+s}$ for every $s \in [0, \infty)$. Therefore it can be extended to negative times, and if μ is also reversible, the processes $\boldsymbol{\eta}_t$ and $\boldsymbol{\eta}_{-t}$ have the same joint distributions. So reversible measures can only exist if the dynamics of the process fulfills certain symmetry relations. Analytically this corresponds to self-adjointness of the operators $S(t)$, which greatly simplifies further analysis. A discussion of this can be found in [99] Chapter II, or [129] Chapter II.1, whereas the processes we consider are in general non-reversible.

One central topic in the study of interacting particle systems is the characterization of the set $\mathcal{I}$ of invariant measures. Some general properties are summarized in the following.

Theorem 2.2 (Liggett) *Consider a Feller process on a compact state space X with generator $\mathcal{L}$. Then the following statements hold.*

a) $\mu \in \mathcal{I}$ if and only if $\langle \mathcal{L} f \rangle_\mu = 0$ for all $f \in C_0(X, \mathbb{R})$.
b) $\mathcal{I}$ is non-empty, compact and the closed convex hull of its extreme points $\mathcal{I}_e$.
c) If the weak limit $\mu = \lim_{t\to\infty} \pi S(t)$ exists for some $\pi \in P(X)$, then $\mu \in \mathcal{I}$.
d) Let $\mu_n \in \mathcal{I}(\mathcal{L}_n)$ be the stationary measures for processes with generators $\mathcal{L}_n : C_0(X, \mathbb{R}) \to C(X, \mathbb{R})$ and $\mu_n \to \mu$ weakly. Then $\mu \in \mathcal{I}(\mathcal{L})$ if there is a core $D \subset C_0(X, \mathbb{R})$ of $\mathcal{L}$ such that $\mathcal{L}f = \lim_{n\to\infty} \mathcal{L}_n f$ for all $f \in D$.

Proof. See [99], Propositions I.1.8. and I.2.14.

Remarks.

i) $\mathcal{I}$ is convex since $P(X)$ is closed under convex combinations and the stationarity condition of *a)* is linear in μ.
ii) Due to *c)* the invariant measures determine the long-time behavior of the process. If the latter is positive recurrent, the limit exists for all $\pi \in P(X)$. If it is also irreducible, the limit is independent of π and the invariant measure is unique. Such a process is called ergodic.
iii) *d)* is a consequence of the Trotter-Kurtz theorem (see Theorem A.3) that ensures the existence of the limiting process. It can be used to find elements of $\mathcal{I}$ for processes on infinite lattices as limiting stationary measures of processes with finite Λ. By varying the boundary conditions, different extremal invariant measures $\mu \in \mathcal{I}_e$ can be found in that way, but in general not all of them (see e.g. [99], Prop. I.2.14).

Canonical and grand canonical measures

On a finite lattice Λ_L with corresponding state space X_L we define the number of particles

$$\Sigma_L(\boldsymbol{\eta}) = \sum_{x\in\Lambda_L} \eta(x) \in \mathbb{N} \qquad \text{for all } \boldsymbol{\eta} \in X_L \,. \tag{2.12}$$

If the system is closed it is conserved in time, i.e. $\Sigma_L(\boldsymbol{\eta}_0) = \Sigma_L(\boldsymbol{\eta}_t)$ for all $t > 0$, which can formally be seen by inserting the indicator function $f = \chi_{\{\Sigma_L = N\}}$ in (2.3). So in this case the locally conserving dynamics leads to a (global) conservation of $\Sigma_L(\boldsymbol{\eta})$ and non-uniqueness of the stationary measure, since the state space X_L decomposes into non-communicating subsets $X_{L,N} = \{\boldsymbol{\eta} \in X_L | \Sigma_L(\boldsymbol{\eta}) = N\}$, $N \in \{0, 1, \ldots, L\,\eta_{max}\}$. By assumption (2.11) the process is irreducible on $X_{L,N}$ and thus has a unique stationary measure $\mu_{L,N}$ for each $N \in \mathbb{N}$. These so-called *canonical measures* are the extremal stationary measures for closed systems,

$$\mathcal{I}_e = \left\{ \mu_{L,N} \,\middle|\, N \in \{0, 1, \ldots, L\,\eta_{max}\} \right\} . \tag{2.13}$$

This is in contrast with open systems, where the number of particles is not conserved as they can enter and leave the system through the boundary. Therefore such systems are irreducible on X_L and have a unique stationary measure, i.e. $|\mathcal{I}_e| = 1$.

Another standard concept for closed systems are the *grand canonical measures*, given by convex combinations

$$\mu_{L,\phi} = Z(L,\phi)^{-1} \sum_{N=0}^{L\,\eta_{max}} \phi^N \, Z(L,N) \, \mu_{L,N} \; . \tag{2.14}$$

They are normalized by $Z(L,\phi) = \sum_{N=0}^{L\,\eta_{max}} \phi^N Z(L,N)$, and since $\eta_{max} < \infty$ they are well defined for every $\phi \in [0,\infty)$. For $\eta_{max} = \infty$ the situation is different and is discussed in Section 2.3.2 and Chapter 5. In principle, the factors $Z(L,N) > 0$ are arbitrary, but in many cases a generic choice is the normalization of the $\mu_{L,N}$ with respect to a 'natural' stationary weight (cf. Section 2.3.2). The variable ϕ is called *fugacity* and is often also written in terms of the *chemical potential* $\mu = \log \phi \in \mathbb{R}$. In contrast to the canonical measures, $\mu_{L,\phi}$ does not concentrate on one of the canonical state spaces $X_{L,N}$, and Σ_L is a random variable on $\{0,\dots,L\,\eta_{max}\}$ with exponential distribution $\frac{Z(L,N)}{Z(L,\phi)}\phi^N$ and expected value

$$\langle \Sigma_L \rangle_{\mu_{L,\phi}} = Z(L,\phi)^{-1} \sum_{N=0}^{L\,\eta_{max}} N \, \phi^N Z(L,N) = \phi \, \partial_\phi \log Z(L,\phi) \; . \tag{2.15}$$

This formula reflects the fact that $Z(L,\phi)$ is the moment generating function of $Z(L,N)$. (2.15) is a monotonic increasing function of ϕ onto $[0, L\,\eta_{max}]$. The canonical measures are usually more convenient to study because they are often of product form, whereas $\mu_{L,N}$ has extra correlations introduced by the constraint $\Sigma_L = N$. In fact it is

$$\mu_{L,N} = \mu_{L,\phi}(\,.\,|\Sigma_L = N) \qquad \text{for all } \phi > 0. \tag{2.16}$$

Usually there is a law of large numbers for the sum $\Sigma_L(\boldsymbol{\eta})$, so that both concepts are equivalent in the limit $L \to \infty$, which is discussed in detail in Chapter 5. For periodic boundary conditions the canonical and grand canonical measures are translation invariant due to translation invariance of the dynamics (2.8).

For infinite lattices the number of particles is in general infinite and thus not well defined and the decomposition of the state space into irreducible subsets is not so clear. The reason is that the local conservation law does not imply the existence of a globally conserved quantity, as it was the case for finite lattices. Loosely speaking, on an infinite lattice 'infinity' can be a source or a sink of particles (cf. Theorem 3.1 in Chapter 3). The particle density $\rho(x) = \langle \eta(x) \rangle_\mu$ is a locally conserved quantity and can be used to index translation invariant measures. One expects that for translation invariant lattices $\Lambda = \mathbb{Z}^d$, excluding for example $\Lambda = \mathbb{Z}^+$ in Section 3, $\mathcal{I}_e$ contains a family of translation invariant stationary measures $\{\mu_\rho | \rho \in [0,\eta_{max}]\}$. Regarding the full range of ρ, this intuition can be false in case of a phase transition, as we discuss in the next subsection and Chapter 5. In addition, there might also be non-translation invariant extremal measures, as we see in Section 2.2.1.

The stationary current

The local conservation of the number of particles can be written as

$$\boldsymbol{\eta}_t(x) - \boldsymbol{\eta}_s(x) + \sum_{|y|\le R} J_{(x,x+y)}\big([s,t]\big) = 0\,, \tag{2.17}$$

where the *integrated current* $J_{(x,x+y)}([s,t]) : D[0,\infty) \to \mathbb{Z}$ is a random variable on path space, counting the number of jumps from site x to $x+y$ minus the number of jumps from $x+y$ to x during the time interval $[s,t]$. Inserting $f(\boldsymbol{\eta}) = \eta(x)$ in the backward equation (2.3) and taking the expectation with respect to some initial distribution $\pi \in P(X)$ we get an averaged version of (2.17), the *lattice continuity equation*

$$\partial_t \left\langle \eta(x) \right\rangle_{\pi S(t)} = \sum_{|y|\le R} \left\langle c(x+y,x,.) - c(x,x+y,.) \right\rangle_{\pi S(t)}\,. \tag{2.18}$$

The average current in an infinitesimal time interval is thus given by

$$\mathbb{E}^\pi\big[J_{(x,x+y)}([t,t+dt])\big] = \Big\langle c(x,x+y,.) - c(x+y,x,.) \Big\rangle_{\pi S(t)} dt + O(dt^2)\,, \tag{2.19}$$

where we use the notation $\mathbb{E}^\pi[\,.\,] = \big\langle \mathbb{E}^{\boldsymbol{\eta}}[\,.\,] \big\rangle_\pi$. For $\pi = \mu \in \mathcal{I}$ the lefthand side of (2.18) vanishes, leading to a condition for stationarity on the righthand side. If μ is also reversible, the summands on the right hand side of (2.18) vanish pairwise according to the condition of *detailed balance*,

$$c(x,y,\boldsymbol{\eta})\,\mu(\boldsymbol{\eta}) = c\big(y,x,\boldsymbol{\eta}^{x\to y}\big)\,\mu\big(\boldsymbol{\eta}^{x\to y}\big) \quad \text{for all } x,y \in \Lambda \text{ and } \boldsymbol{\eta} \in X. \tag{2.20}$$

In virtue of the situation in continuous space, discussed in Section 2.1.4, one would like to write (2.18) in conservative form, identifying a vector valued, local current $j(.,\boldsymbol{\eta}) : \Lambda \subset \mathbb{Z}^d \to \mathbb{R}^d$, such that the righthand side is given by a lattice derivative of j. This is possible if the particles only jump along the standard basis vectors e_k, $k = 1,\dots,d$ of the lattice $\Lambda \subset \mathbb{Z}^d$. We can define the microscopic current in direction k for all $x \in \Lambda$ and $\boldsymbol{\eta} \in X$ as the sum of rates for jumps passing the bond $(x, x+e_k)$ in positive direction minus the sum passing in negative direction. In particular this is always possible in one space dimension, for which we give examples in Section 2.2. We do not give further details here, since in higher dimensions this approach only works for restricted jump rates.

In the general case, we define the *particle drift* by

$$d(x,\boldsymbol{\eta}) = \sum_{|y|\le R} y\, c(x,x+y,\boldsymbol{\eta}) \;\in \mathbb{R}^d \qquad \text{for all } x \in \Lambda \subset \mathbb{Z}^d, \boldsymbol{\eta} \in X\,. \tag{2.21}$$

Note that in general this is not a particle current, but rather the average velocity of a particle at site x at a given configuration $\boldsymbol{\eta}$. However, its expectation value with respect to a translation invariant measure $\pi \in P(X)$ can be interpreted as a current by looking at a space integrated version of (2.18). Summing over all x in some volume $V \subsetneq \Lambda$, all terms except for the boundary terms vanish on the righthand side, which can thus be written as

$$\sum_{\substack{x\in V,|y|\le R\\ x+y\notin V}} \left\langle c(x+y,x,.) - c(x,x+y,.) \right\rangle_\pi = \sum_{x\in\partial V} s(x)\cdot \left\langle d(x,.) \right\rangle_\pi\,. \tag{2.22}$$

We use the standard notation $\partial V = \left\{x \in V \,\middle|\, \exists_{y \notin V} |x-y| = 1\right\}$ for the boundary of V and $s(x) = \sum_{z \notin V, |z-x|=1}(z-x)$ is the inward pointing normal boundary vector. The above notation motivates the following definition, since it is very similar to the continuum case discussed in (2.31). Consider a system on a finite periodic lattice Λ_L, for which translation invariant canonical measures $\mu_{L,[\rho L]}$ exist for all denisities $\rho \in [0, \eta_{max}]$ (see discussion above). We define the *current-density relation*, also called *fundamental diagram* of the process as

$$j(\rho) = \lim_{L\to\infty} \left\langle d(x,.) \right\rangle_{\mu_{L,[\rho L]}} \in \mathbb{R}^d \qquad \text{for all } \rho \in [0, \eta_{max}] \,. \tag{2.23}$$

For calculations it is usually more convenient to use the expectation values with respect to the (equivalent) grand canonical measures $\mu_{L,\phi}$. By definition, (2.23) is a pure bulk property of the system. But it is of great importance for open systems, since it enters the hydrodynamic equation (see Section 2.1.4) and thus, together with the boundary conditions, determines the bulk properties of the stationary measure as discussed in Section 2.2.3.

2.1.3 Phase transitions

The aim of this section is to specify the notion of a phase transition in case of non-reversible, translation invariant lattice gases and to quickly review and put into context standard notions from the theory of phase transitions for reversible systems. In the literature for equilibrium statistical mechanics there are several general approaches, which are known to be equivalent to some extent. One is the characterization of phase boundaries as regions of non-analyticity of the large deviation functional, called *free energy*. This approach is found in many textbooks (see e.g. [72]) and is closely related to the theory of Yang and Lee [140, 94], defining critical points as real roots of the grand canonical partition function. For nonequilibrium systems a general quantity comparable to the free energy has not been identitied so far (for recent work on this question see e.g. [36, 37] or [20] and references therein). Below we give a probabilistic characterization of phase transitions connected to the structure of the set $\mathcal{I}$ of stationary measures.

It is well known that equilibrium systems do not exhibit phase transitions in one dimension at non-zero temperature, provided that the interactions are short range and the local state variable takes only a finite number of possible values. Nonequilibrium systems have a much richer structure and a great variety of critical phenomena can be observed even in one dimension. On the other hand, there is no general concept such as the Gibbs ensemble for equilibrium systems, which determines the stationary measures at least in principle. For each system they have to be derived from the dynamics, which is in general a very difficult task. Thus the notion of a phase transition so far has been used in a rather phenomenological sense, by studying generic model systems and trying to categorize the observed critical phenomena (for a recent review see [107]). In contrast with equilibrium systems, there is no canonical definition of phase transitions covering all these phenomena. The one we propose below turns out to be a reasonable choice for the systems we consider, but should not be taken as a general declaration. As we shortly discuss below, it also has weaknesses, and in particular when working in a different context, there might be good reasons to use a different definition.

Definition of a phase transition

We know from the previous subsection that the set of stationary measures $\mathcal{I}$ is non-empty and it is the convex hull of its extreme points $\mathcal{I}_e$, which are also called *pure phases*. Since we always assume irreducibility of the process on finite lattices Λ_L, the structure of $\mathcal{I}_e$ is clear in this case. It is either a singleton if Λ_L is open, or consists of the canonical measures $\mu_{L,N}$ if it is closed. So the possibility of a phase transition is only given on infinite lattices, where $\mathcal{I}_e$ may be more complicated due to the infinite state space. Consider a process with local conservation of particles on the infinite lattice $\Lambda = \mathbb{Z}^d$. Since both, the dynamics and the lattice, are translation invariant we expect that there exists a translation invariant, extremal stationary measure μ_ρ for every density $\rho \in [0, \eta_{max}]$ and that these are the only extremal measures, i.e.

$$\mathcal{I}_e = \left\{ \mu_\rho \,\middle|\, \rho \in [0, \eta_{max}] \right\} . \tag{2.24}$$

Definition. If (2.24) is not fulfilled, the above process is said to exhibit a *phase transition*.

There are different critical phenomena that can be observed in case of a phase transition, which are introduced below in the context of the above definition. However, these notions originate from the physics literature, where they are used to describe properties of typical stationary configurations of large, finite systems. Although our definition is largely compatible to the physics convention, there might be discrepancies especially for systems with open boundaries, as is discussed towards the end of this section.

Spontaneous breaking of translation invariance: There are extremal measures $\mu \in \mathcal{I}_e$ which are not translation invariant.

Phase separation: There is some density $\rho \in [0, \eta_{max}]$ for which there is no extremal invariant measure, but only a mixture.

Condensation: This occurs only for systems with unbounded local state space E, if there are no extremal invariant measures beyond a critical density $\rho_c < \infty$.

Remarks.

i) A very basic example of spontaneously broken translation invariance is given by the so-called blocking measures (2.43) of the asymmetric simple exclusion process in Section 2.2.1. They are reversible and can be characterized as limit measures of systems with closed boundary conditions. The existence of such measures is quite common for non-reversible systems. Therefore one could argue that it might be reasonable to exclude them from the definition, but we rather prefer to have a concise statement.
This example demonstrates that for non-reversible systems the boundary conditions have a global effect on the stationary measures already in one dimension, because the non-zero current can transport boundary properties into the bulk. For equilibrium systems this applies only in higher dimensions, which we briefly discuss below for the most classical equilibrium example, the stochastic Ising model.

In general, there can be other symmetries in addition to translation invariance, and the system is said to exhibit spontaneaous symmetry breaking whenever there are extremal measures $\mu \in \mathcal{I}_e$ which do not reflect these symmetries. However, the presence of the conservation law for the number of particles alone naturally breaks internal symmetries, such as the spin-flip symmetry for the Ising model discussed below. Thus for the general formulation we stick to translation invariance which is not affected by the conservation law, and below we discuss other symmetries in the context of boundary induced critical phenomena.

ii) Consider a system on a finite, periodic lattice Λ_L with $N = [\rho L]$ particles. If there is no pure phase with density ρ the limit $L \to \infty$ of the canonical measures $\mu_{L,N}$ is usually a mixture of two pure phases. In a typical configuration for large lattices both phases are spatially separated in so-called *domains*. This does not have to imply symmetry breaking, since the domain boundaries are fluctuating and the measure itself can still be translation invariant. Phase separation in one dimensional systems with finite local state space E can occur in the presence of two or more particle species with different jump rates, as is discussed in Section 2.2.4.

iii) For unbounded local state space E it is possible that the grand canonical measures (2.14) are only defined up to a critical density ρ_c, as discussed in Section 2.3.2 for the zero range process. In the setting of the previous remark with $\rho > \rho_c$, the system separates into a homogeneous background phase with distribution μ_{ρ_c} and a condensate, which contains a non-zero fraction of the particles but concentrates only on a vanishing fraction of the system volume. In the limit $L \to \infty$, the canonical measures converge to the critical background distribution μ_{ρ_c} in a certain sense, which is shown in detail for the zero range process in Chapter 5.

There is an alternative dynamical interpretation of phase separation and condensation in terms of the ergodic behavior of the process on the infinite lattice $\mathbb{Z}^d$. Starting with a uniform initial distribution with density ρ for which there is no pure phase, the spatial separation into domains evolves dynamically. In case of phase separation these domains tend to grow in space and show an interesting coarsening phenomenon. The best known example are presumably the domains of different magnetization in the Ising model, which we shortly discuss below. In case of condensation, coarsening is not a spatial phenomenon but happens on the level of the occupancy of condensate sites, which is studied in detail in Chapter 6 for the zero range process.

The analog to (2.24) for systems without conservation law would be to require the $\mathcal{I}_e$ is a singleton. In one space dimension this condition can be violated for nonequilibrium systems due to the existence of one or more absorbing states [68], as for example percolation. In more than one dimension phase transitions can also occur in equilibrium systems such as the Ising model, which is shortly discussed below.

The phase diagram

The occurrence of a phase transition depends on the system parameters, summarized in the vector $\boldsymbol{\alpha} \in D_\alpha$, which determine the dynamics and thus the extremal measures $\mathcal{I}_e(\boldsymbol{\alpha})$ of the process. The *phase space* of a process with locally conserved number of particles is given by $[0, \eta_{max}] \times D_\alpha$, all possible tuples $(\rho, \boldsymbol{\alpha})$ of densities and system parameters. The *phase diagram* is a decomposition of this space into regions with qualitatively different behavior, called *phases*. This nomenclature is of course related, but should not be mixed up with the notion of pure phases $\mathcal{I}_e$. In particular, one phase of the phase diagram is the region of extremal measures,

$$\left\{(\rho, \boldsymbol{\alpha}) \,\middle|\, \exists\, \mu_\rho \in \mathcal{I}_e(\boldsymbol{\alpha})\right\}, \tag{2.25}$$

which is usually called *homogeneous phase*. In case of phase separation, its complement is non-empty corresponding to the so-called *phase separated phase*, which is illustrated in Figure 2.1 for the Ising model. This region is bounded above and below by the boundary of the homogeneous phase at the critical densities $\rho_+(\boldsymbol{\alpha})$ and $\rho_-(\boldsymbol{\alpha})$ respectively, and the stationary measures are mixtures of $\mu_{\rho_-(\boldsymbol{\alpha})}$ and $\mu_{\rho_+(\boldsymbol{\alpha})}$. In case of condensation, the condensate phase is unbounded from above and there are no stationary measures with density $\rho > \rho_c$, which can be seen in Figure 5.1 in Chapter 5 for the zero range process. In general, phase diagrams are used in various contexts to characterize critical phenomena, which do not always fit in the above picture for our context. In particular they can also be used to characterize the ergodic behavior of the system, as can be seen in Figure 3.1 for the asymmetric simple exclusion process.

Phases can be characterized by *order parameters*, averages of certain observables $f \in C(X, \mathbb{R})$, that show qualitatively different behavior depending on the phase. Generic choices are one-point or two-point correlation functions like $\langle \eta(0) \rangle$ or $\langle \eta(0)\eta(x) \rangle$, depending on the model under consideration. These order parameters usually show non-analytic behavior along phase boundaries, establishing the connection to the free energy approach mentioned in the beginning of this subsection. Depending on the degree of the non-analyticity, phase transition are called *first order*, if the order parameter is discontinuous, and *continuous* otherwise. An important example is the *correlation length* ξ defined as

$$\xi^{-1} = \lim_{x \to \infty} -1/x \log\left(\langle \eta(0)\eta(x) \rangle - \langle \eta(0) \rangle \langle \eta(x) \rangle\right), \tag{2.26}$$

giving the exponential decay rate of two-point correlation functions. At a phase boundary it usually diverges since this decay is subexponential, characterizing *long range order*. In general, the non-analytic behavior is governed by critical exponents which are independent of the model details and may be classified into *universality classes* (see e.g. [68, 108]).

A standard equilibrium example: The Ising model

For equilibrium models the above concept of phase transitions is well established, at least for non-conserving dynamics (see e.g. [129]). It can be applied in great generality since the reversible stationary measures can be characterized by the Gibbs measures $\mathcal{G}$, which is shortly discussed below. By identifying the symmetry of the system and the nature of the

order parameter involved in the phase transition one can usually find the universality class of the transition and even obtain a rough idea of the possible phase diagram.

We illustrate the above concept for the stochastic Ising model, the standard example in equilibrium statistical mechanics. For equilibrium systems in general, to each configuration $\boldsymbol{\eta}_\Lambda$ on a finite sublattice $\Lambda \subset \mathbb{Z}^d$ there is an associated energy $H(\boldsymbol{\eta}_\Lambda|\boldsymbol{\eta}_{\Lambda^c})$ which determines the interaction of the particles depending on the (fixed) outside configuration in $\Lambda^c = \mathbb{Z}^d \backslash \Lambda$ via boundary terms. A Gibbs measure μ on $X = E^{\mathbb{Z}^d}$ is defined by requiring that its conditional expectations are of the form

$$\mu(\boldsymbol{\eta}_\Lambda|\boldsymbol{\eta}_{\Lambda^c}) = \exp\big[-H(\boldsymbol{\eta}_\Lambda|\boldsymbol{\eta}_{\Lambda^c})\big]/Z(\Lambda)\,, \tag{2.27}$$

for all Λ and $\boldsymbol{\eta}_{\Lambda^c}$, where $Z(\Lambda)$ normalizes the right hand side to one (for details see e.g. [56]). The energy can be connected to the jump rates of a corresponding particle system via the condition of detailed balance (2.20). The Gibbs measures are given by the set $\mathcal{G}$ of all solutions to (2.27), called DLR equations (Dobrushin, Lanford, Ruelle), under variation of $\boldsymbol{\eta}_{\Lambda^c}$. For systems with no conserved quantity, it can be shown under very general conditions that for sufficiently small interaction the Gibbs measure is unique, i.e. $|\mathcal{G}| = 1$ (see e.g. Theorem II.1.8 in [129]). The interaction strength J is measured in some suitable norm of the interaction potential which determines the energy. For systems exhibiting a phase transition there exists a critical value J_c such that for $J > J_c$ it is $|\mathcal{G}| > 1$. This is equivalent to saying that the limit $\Lambda \to \mathbb{Z}^d$ of (2.27) depends on the boundary conditions $\boldsymbol{\eta}_{\Lambda^c}$.

A standard example is the ferromagnetic Ising model, with spin variables σ_x in $E = \{-1, 1\}$, no external field and attracting nearest neighbor interaction $J > 0$, i.e.

$$H(\boldsymbol{\eta}_\Lambda|\boldsymbol{\eta}_{\Lambda^c}) = J \sum_{x\in\Lambda} \sum_{|y|=1} \eta(x)\,\eta(x+y) \tag{2.28}$$

(see [99], Chapter IV or [28], Chapter VIII). If the interaction is strong enough, $J > J_c$, then for dimension $d = 2$ the extremal Gibbs measures $\mathcal{G}_e$ consist of two translation invariant measures μ_{m_+}, μ_{m_-} with positive and negative magnetization $m_+ = -m_- = \langle\sigma_x\rangle_{\mu_{m_+}}$ respectively, whereas for $J < J_c$ it is $\mathcal{G}_e = \{\mu_0\}$. This is true for (Glauber) spin-flip dynamics without conservation. If the dynamics is such that the magnetization is locally conserved (Kawasaki spin exchange), which is comparable to the systems in our interest, $\mu_m \in \mathcal{G}_e$ for every $m \in [-1, 1]$ in case of weak interaction. For $J > J_c$ there is no extremal Gibbs measure with magnetization $m \in (m_-, m_+)$, as can be seen in the phase diagram in Figure 2.1. Restricted on say $m = 0$, the equilibrium distribution is given by the mixture $\frac{1}{2}\mu_{m_-} + \frac{1}{2}\mu_{m_+}$ of two extremal measures. As mentioned above, this measure concentrates on phase separated configurations with domains of positive and negative magnetizations. Due to fluctuations in form and position of these domains, the measure is still translation invariant in two dimensions. For $d \geq 3$ there exist also non-translation invariant extremal distributions with a localized interface between the two domains, manifesting spontaneous symmetry breaking. In Figure 2.1 we also plot the grand canonical expectation value of the magnetization $m(h)$ as a function of the conjugate variable $h \in \mathbb{R}$. This is analogous to the chemical potential for lattice gases and can be interpreted as an external magnetic field, adjusting the average magnetization in the system.

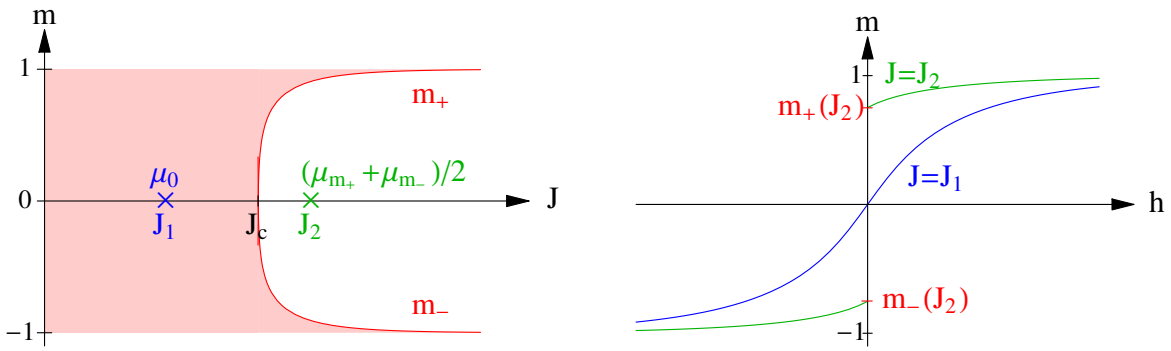


Figure 2.1: Phase separation in the two-dimensional Ising model with nearest neighbor interaction J and conserved magnetization m. **Left:** The phase diagram shows the region of pure states μ_m (shaded in red), which is bounded by the spontaneous magnetizations m_+ and m_- above the critical point J_c. At $m = 0$ there is a pure phase μ_0 for $J_1 < J_c$ (blue) and only a mixture at $J_2 > J_c$ (green). **Right:** Magnetization m as a function of the magnetic field h (conjugate variable) for $J = J_1$ (blue) and $J = J_2$ (green) as given on the left.

Boundary induced phase transitions

Consider a nonequilibrium system on a finite lattice $\Lambda_L = \{1, \dots, L\}$ with fixed bulk dynamics and open boundary conditions with rates denoted as a vector $\boldsymbol{\alpha} \in D_\alpha$. We concentrate on one space dimension for easier presentation. Due to the open boundary, the number of particles is not conserved and the process has a unique stationary measure $\mu_L^{\boldsymbol{\alpha}}$. By Theorem 2.2.d) we know that the limit $\lim_{L\to\infty} \tau_{k(L)}\mu_L^{\boldsymbol{\alpha}}$, shifted away from the (fixed) left boundary, is invariant for the process on $\Lambda = \mathbb{Z}$ for every sequence $k(L) \in \Lambda_L$ with $k(L)$, $L - k(L) \to \infty$ for $L \to \infty$. So the open boundary mechanism picks a stationary measure of the corresponding infinite system, which is known in the physics literature as *steady state selection*. Moreover, we expect that the above limit is independent of the specific sequence $k(L)$ and is an extremal invariant measure for the infinite process. Thus for every boundary mechanism $\boldsymbol{\alpha}$ it is

$$\lim_{L\to\infty} \tau_{k(L)}\mu_L^{\boldsymbol{\alpha}} = \mu_{\rho(\boldsymbol{\alpha})} \in \mathcal{I}_e \,, \tag{2.29}$$

where the limiting bulk density $\rho(\boldsymbol{\alpha}) = \lim_{L\to\infty}\langle \eta(k(L))\rangle_{\mu_L^{\boldsymbol{\alpha}}}$ serves as an order parameter and thus should be an analytic function of $\boldsymbol{\alpha}$. If this picture is violated, for example the limit in (2.29) may be non-extremal, the system exhibits a *boundary induced phase transition*. Note that this is not a phase transition in the sense (2.24), which is a pure bulk property. In fact boundary induced critical phenomena can be better understood in terms of the order parameter $\rho(\boldsymbol{\alpha})$. Since there is no conservation law, the appropriate phase space of the process is just D_α. Possible critical phenomena include phase separation, which is illustrated in detail for the asymmetric simple exclusion process in Section 2.2.2, and spontaneous symmetry breaking. Systems with open boundaries are not translation invariant, but since they do not have particle conservation either, they often exhibit other symmetries, such as CP-invariance which can be broken for two-species models as discussed in Section 2.2.4.

Note that for boundary induced critical phenomena a general classification similar to page 13 is not possible in lack of a conservation law. However, the notions can be applied to specific systems as will be illustrated for the examples mentioned above.

Boundary induced phase transitions do not have a direct counterpart in equilibrium systems. Their origin is the non-zero current, which can transport boundary effects into the bulk, and that for nonlinear current-density relations, the domain boundaries can be stable and well defined objects even in one dimension, as we discuss in Section 2.2.3.

2.1.4 Hydrodynamic limits

Interacting particle systems as models of real phenomena are of course always finite, but can consist of a very large number of components, for example a fluid or a gas. In this case one is neither interested nor able to give a precise description of the microscopic process $\boldsymbol{\eta}_t$. The primary interest lies in understanding the time evolution of quantities on a macroscopic scale. Mathematically such a situation is idealized by introducing a lattice constant of order $1/L$, i.e. rescaling the space variable as $x \to u = x/L$. The scale $L \sim |\Lambda_L|$ is proportional to the size of the lattice, so that in the limit $L \to \infty$ the volume of the system is some bounded subset $V \subset \mathbb{R}^d$. To see the driven motion of the particles on the rescaled space one has to look at large times $t \to t/L$, the so-called *Eulerian time scale*, whereas the appropriate time scale to see the diffusive motion in symmetric systems would be $t \to t/L^2$. In the limit $L \to \infty$ the stochastic fluctuations are usually averaged out and the time evolution of macroscopic observables can be described by deterministic equations. For the processes we consider, the hydrodynamic equation of the density profile $\rho(t,u)$ is given by

$$\partial_t \rho(t,u) + \nabla_u \cdot j\big(\rho(t,u)\big) = 0 \,, \quad \rho(0,u) = \rho(u) \,, \tag{2.30}$$

where $j(\rho) \in \mathbb{R}^d$ is the current density relation defined in (2.23). This is a *conservation law*, reflecting the fact that driven lattice gases locally conserve the number of particles. Using Stokes' theorem, this can be seen by the space integrated version of (2.30),

$$\partial_t \int_V \rho(t,u)\, du = \int_{\partial V} j\big(\rho(t,u)\big) \cdot dS(u) \,, \tag{2.31}$$

where $dS(u)$ denotes a vector valued surface element of ∂V. Particles can only enter or leave a volume $V \subset \mathbb{R}^d$ via boundary currents, and in any closed system, i.e. $j|_{\partial V} = 0$, the total mass is conserved. For questions on conservation laws on the level of the differential equation we refer the reader to [26] and references therein.

In the following we sketch a typical result on the rigorous derivation of (2.30). Consider a translation invariant process on $\Lambda_L = (\mathbb{Z}/L\mathbb{Z})^d$ with stationary product measures ν_α, $\alpha \in [0,1]$ and non-zero stationary current j. Suppose that $\rho : \mathbb{R}^d \to [0,\infty)$ is a reasonable function and the initial distribution μ of the process is close to a product measure with site dependent density

$$\langle \eta(x) \rangle_\mu = \rho(x/L) \quad \text{for all } x \in \Lambda \,, \tag{2.32}$$

a so-called *local equilibrium measure*. Then for large L, the distribution $\mu S(Lt)$ of the process at time $Lt \geq 0$ is approximately a product measure with density $\rho(t, x/L)$, where $\rho(t,u)$

is the solution of the hydrodynamic equation (2.30). This property is called *conservation of local equilibrium* and is a key point in the derivation. There has been a lot of work to rigorously prove this statement mostly for attractive particle systems (see e.g. [114, 93]), which is explained in detail in [84] (see also references therein). The first derivation in the context of exclusion processes was given in [115].

In general, the current density relation $j(\rho)$ is a nonlinear function and solutions to hyperbolic conservation laws develop discontinuities after finite time even for smooth initial data. So they have to be understood in the sense of distributions, but such weak solutions are not uniquely determined by the initial data (see e.g. [26], Chapter IV). However, the time evolution of the underlying particle system is of course well defined, and one possibility to single out the relevant solution that describes it is the entropy criterion. Define an *entropy entropy-flux pair* $S : \mathbb{R} \to \mathbb{R}$, $F : \mathbb{R} \to \mathbb{R}^d$ as a solution of the d relations $S'j' = F'$ for which S is convex. Then there is a unique weak solution $\rho(t,u)$ of (2.30) that fulfills

$$\partial_t S\big(\rho(t,u)\big) + \nabla_u \cdot F\big(\rho(t,u)\big) \leq 0\,. \tag{2.33}$$

for all entropy entropy-flux pairs. The name of this criterion comes from the fact that $-S$ can be interpreted as the physical entropy of the system. Indeed, the integrated version of (2.33) gives that the total entropy $-\int_V S\big(\rho(t,u)\big)\,du$ of the system should increase monotonic in time. This increase is due to discontinuities of weak solutions, for classical, differentiable solutions of (2.30) the entropy is conserved, i.e. equality holds in (2.33). In general there can be more than one solution to the defining relations of entropy entropy-flux pairs, which are purely technical and are not related to the physical entropy. For equation (2.30) for example the entropies are given by the one parameter family $S(u) = |u - c|$, $c \in \mathbb{R}$ [114].

Another uniqueness criterion is obtained by adding an artificial viscosity term to the right hand side of (2.30). This leads to the viscous equation

$$\partial_t \rho(t,u) + \nabla_u \cdot j\big(\rho(t,u)\big) = \epsilon \sum_{k,l=1}^{d} a_{k,l} \partial^2_{u_k,u_l} \rho(t,u), \quad \rho(0,u) = \rho(u)\,. \tag{2.34}$$

This equation is parabolic and thus has a unique solution $\rho_\epsilon(t,.) \in C^\infty\big(\mathbb{R}^d, [0,\infty)\big)$ for all $t > 0$, even if the initial data do not have this property [26]. If one can show that the limit $\lim_{\epsilon\to 0} \rho_\epsilon$ exists in an appropriate sense, which is in general very difficult (cf. [26], Chapter XV), it defines a unique solution of (2.30). In more than one space dimension this depends in general on the choice of the diffusion matrix $(a_{k,l})_{k,l=1,\dots,d}$, which one has to choose properly (cf. (4.59) in Section 4.4.1), to get the same solution as from the entropy criterion. On the equivalence of both criteria see also [26], Chapters VIII and IX.

If there is more than one conserved quantity in the system (e.g. several species of particles) the corresponding macroscopic description is given by a system of conservation laws. Up to now there is only little rigorous work on the hydrodynamic limit for systems with more than one particle species. For references see Chapter 4, where we address this question and derive the hydrodynamics of the zero range process with several particle species. In this case there are also very few results on existence and uniqueness of solutions of the macroscopic equation, in particular the equivalence of the above criteria is no longer certain. Thus

a general result corresponding to [114] cannot be obtained in this case and we explain the problems arising in Chapter 4.

Setting $\epsilon = 1/L$ in (2.34) it can be interpreted as the lattice constant and the viscous term as the first order correction in the derivation of (2.30) for $L \to \infty$. If the particles have no drift, the current vanishes, $j(\rho) \equiv 0$, and the second order term dominates the long time behavior. But this can be seen only on the diffusive time scale t/L^2 and the limit is given by the parabolic heat equation (see e.g. [127], Chapter 9). For rigorous hydrodynamic limits in this case see [84] and references therein.

2.2 Exclusion processes

In processes with exclusion interaction the maximum number of particles per site is restricted to one, i.e. $E = \{0, 1\}$. A jump to site y is only allowed if this site is empty, so $c(x, y, \boldsymbol{\eta}) = 0$ if $\eta(y) = 1$. In the following we concentrate on simple exclusion processes, where the particles only jump to nearest neighbor sites, i.e. $c(x, y, \boldsymbol{\eta}) = 0$ if $|x - y| > 1$, and we focus on one-dimensional lattices $\Lambda \subset \mathbb{Z}$. We collect basic results on stationary measures and explain the matrix product ansatz, an important technique in this context which is used in Chapter 3. We introduce the theory of boundary induced phase transitions and steady state selection, the main topics of Chapters 3 and 4. Finally we summarize results on phase separation in two-component systems which is one of the motivations for the analysis in Chapters 5 and 6.

2.2.1 The asymmetric simple exclusion process

The paradigmatic model of this class is the asymmetric simple exclusion process (ASEP), originally introduced in [102]. Particles jump to the right with rate p and to the left with rate q, i.e.

$$c(x, y, \boldsymbol{\eta}) = \eta(x)\big(1 - \eta(y)\big)\big(p\,\delta_{y,x+1} + q\,\delta_{y,x-1}\big)\ . \tag{2.35}$$

The bulk part of the generator is given by

$$\mathcal{L}_v f(\boldsymbol{\eta}) = \sum_{\substack{x\in\Lambda\\ x+1\in\Lambda}} \big[p\eta(x)\big(1-\eta(x+1)\big) + q\eta(x+1)\big(1-\eta(x)\big)\big]\big[f(\boldsymbol{\eta}^{x\leftrightarrow x+1}) - f(\boldsymbol{\eta})\big]\ . \tag{2.36}$$

To ease notation we introduce $\boldsymbol{\eta}^{x\leftrightarrow y}$ to be a symmetrized version of $\boldsymbol{\eta}^{x\to y}$, the configuration where the occupation numbers on x and y are interchanged, i.e.

$$\eta^{x\leftrightarrow y}(z) = \begin{cases} \eta(y)\,, & z = x \\ \eta(x)\,, & z = y \\ \eta(z)\,, & \text{otherwise} \end{cases}\ . \tag{2.37}$$

First we consider the ASEP on the finite, periodic lattice $\Lambda_L = \mathbb{Z}/L\mathbb{Z}$. When the number of particles is fixed to $\Sigma_L = N$, one can show that all possible configurations have equal weight [105, 29], i.e. the canonical measure defined in Section 2.1.2 is given by

$$\mu_{L,N}(\boldsymbol{\eta}) = 1\Big/\binom{L}{N} = N!\,(L-N)!/L!\ . \tag{2.38}$$

The average number of particles per site is N/L and the corresponding grand canonical measures are the product measures ν_ρ with density $\rho \in [0,1]$. That means the one-point marginals are independent and given by

$$\nu_\rho^1(k) = \nu_\rho\big(\{\eta(x) = k\}\big) = \rho\, k + (1-\rho)(1-k)\,, \tag{2.39}$$

for all $x \in \Lambda_L$, $k \in \{0,1\}$. Thus, as defined in (2.23), the current density relation for the ASEP is given by

$$j(\rho) = (p-q)\rho(1-\rho)\,. \tag{2.40}$$

The system on the lattice $\Lambda_L = \{1,\dots,L\}$ with reflecting or closed boundary conditions is studied in detail in [124]. In this case the stationary measure is reversible and the current vanishes. The grand canonical version is of product form with site dependent density

$$\rho(x) = \frac{1}{2}\Big(1 + \tanh\big[1/2(x-n)\log(p/q)\big]\Big)\,. \tag{2.41}$$

This density profile has the shape of a step, extending over a region with length of order $1/\log(p/q)$ independent of L, and centered at $n \in \Lambda_L$, which determines the expected number of particles in the system. In analogy to phase separation in equilibrium systems, one may regard the region of the step as a domain wall separating an empty and a completely filled domain of the system. The canonical stationary distributions $\mu_{L,N}$ are lengthy to write down and can be found in [124] and [117, 123].

Another common choice is to couple the system on $\Lambda_L = \{1,\dots,L\}$ at both ends to particle reservoirs with density ρ_l and ρ_r respectively. Formally this is done by adding two sites $\eta(0)$ and $\eta(L+1)$ with fixed distributions $\nu_{\rho_l}^1$ and $\nu_{\rho_r}^1$. The boundary part of the generator is then given by

$$\begin{aligned}(\mathcal{L}_b f)(\boldsymbol{\eta}) = &\big[p\,\rho_l\big(1-\eta(1)\big) + q\,(1-\rho_l)\,\eta(1)\big]\big[f(\boldsymbol{\eta}^{0\leftrightarrow 1}) - f(\boldsymbol{\eta})\big] + \\ &\big[p\,\eta(L)(1-\rho_r) + q\,\big(1-\eta(L)\big)\rho_r\big]\big[f(\boldsymbol{\eta}^{L\leftrightarrow L+1}) - f(\boldsymbol{\eta})\big]\,.\end{aligned} \tag{2.42}$$

We discard the degenerate situations $q=0$, $\rho_l = (1-\rho_r) = 0$ and $p=0$, $\rho_l = (1-\rho_r) = 1$, which are analogous to special reflecting boundary conditions. If non-degenerate, the number of particles is no longer conserved and the process is irreducible on X_L with the unique stationary measure $\mu_L^{\rho_l,\rho_r}$, that depends on the boundary parameters ρ_l and ρ_r. Asymptotic properties of these measures for large L were first characterized in [97], using certain recursion relations on the system size. In [30, 122] such relations were used to give an exact solution in the totally asymmetric case $q=0$. The same idea independently led to formulate the stationary measures as a matrix product in [32], which is described in Section 2.2.2.

According to Theorem 2.2.d), invariant measures on the infinite lattice $\Lambda = \mathbb{Z}$ can be obtained from those on Λ_L in the limit $L \to \infty$ for various boundary conditions. The set $\mathcal{I}$ has been completely characterized in [98] and its extreme points are given by

$$\mathcal{I}_e = \big\{\nu_\rho,\ \rho \in [0,1]\big\} \cup \big\{\nu^{(n)},\ n \in \mathbb{Z}\big\}\,. \tag{2.43}$$

The so-called blocking measures $\nu^{(n)}$ are of product form with site dependent densities

$$\rho(x) = \big\langle \eta(x)\big\rangle_{\nu^{(n)}} = (p/q)^{x-n}\big/\big(1+(p/q)^{x-n}\big)\,. \tag{2.44}$$

The profile approaches exponentially fast the densities 0 and 1 to the left and right of $x = n$. The measures are reversible and can be characterized as the limiting measures for reflecting boundary conditions. In [52] they have been studied for asymmetric exclusion processes with more general transition probabilities and are mentioned again in Section 2.3.3.

2.2.2 The matrix product ansatz

The totally asymmetric simple exclusion process (TASEP) with $q = 0$ and open boundary conditions was solved in [32], using the *matrix product ansatz* (MPA). This technique was previously applied to the problems of directed lattice animals [65] and quantum antiferromagnetic spin chains [86]. For the ASEP this approach simplified the derivation of the previous results and could be generalized to the partially asymmetric case with $q > 0$. The idea is to represent the stationary weight of a configuration $\boldsymbol{\eta} \in \{0,1\}^{\Lambda_L}$ as a product of certain linear operators (matrices) E, D on some auxiliary space. The product is closed by two vectors $\langle w|$, $|v\rangle$,

$$W^L(\boldsymbol{\eta}) = \big\langle w\big| \prod_{x=1}^{L} \eta(x)\, D + (1-\eta(x))\, E\big| v\big\rangle \,. \tag{2.45}$$

We use Dirac's bra-ket notation familiar from quantum mechanics to denote the scalar product $\langle w|D|v\rangle = (w, Dv)$. D represents an occupied, E an empty site and the matrices are in general infinite and non-commuting. Let D, E, $\langle w|$ and $|v\rangle$ fulfill the algebraic relations

$$\begin{aligned} p\,DE - q\,ED &= D + E \\ \big\langle w\big|\,\big(\rho_l\, p\, E - (1-\rho_l)\, q\, D\big) &= \big\langle w\big| \\ \big(\rho_r\, p\, D - (1-\rho_r)\, q\, E\big)\big|\, v\big\rangle &= \big|\, v\big\rangle \,. \end{aligned} \tag{2.46}$$

If in addition $\boldsymbol{\eta}_t$ is irreducible, and if the expressions in (2.45) are normalizable, i.e.

$$Z(L) := \sum_{\boldsymbol{\eta}\in X_L} W(\boldsymbol{\eta}) = \langle w|(D+E)^L|v\rangle \neq 0 \,, \tag{2.47}$$

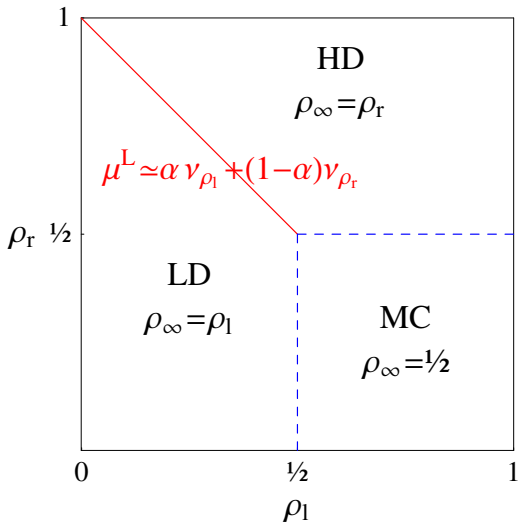
then the invariant measure is given by $\mu_L^{\rho_l,\rho_r}(\boldsymbol{\eta}) = W^L(\boldsymbol{\eta})/Z(L)$. A proof can be found in [100] Section III.3, using the same recursion relations on the system size, which were first noted in [97].

Typical quantities of interest are for example the density profile or two-point correlation functions. With $C = D + E$ they can be written as

$$\begin{aligned} \big\langle \eta(x)\big\rangle_{\mu_L^{\rho_l,\rho_r}} &= \big\langle w\big|\, C^{x-1}\, D\, C^{L-x}\big|\, v\big\rangle / Z(L) \\ \big\langle \eta(x)\,\eta(x+y)\big\rangle_{\mu_L^{\rho_l,\rho_r}} &= \big\langle w\big|\, C^{x-1}\, D\, C^{y-1}\, D\, C^{L-x-y}\big|\, v\big\rangle / Z(L) \,. \end{aligned} \tag{2.48}$$

For one-dimensional systems one can define a stationary, site independent current also for open boundary conditions (cf. discussion in Section 2.1.2) and with (2.35) it is given by

$$j_L^{\rho_l,\rho_r} = p\big\langle \eta(x)\big(1-\eta(x+1)\big)\big\rangle_{\mu_L^{\rho_l,\rho_r}} - q\big\langle \big(1-\eta(x)\big)\eta(x+1)\big\rangle_{\mu_L^{\rho_l,\rho_r}} = \frac{Z(L-1)}{Z(L)} \,, \tag{2.49}$$



- MC: Maximum current phase, bulk dominated with $\rho_\infty = \frac{1}{2}$ independent of the boundary conditions, maximal current $j = (p-q)/4$
- LD, HD: Low and high density phase, boundary dominated with $\rho_\infty = \rho_l$ and $\rho_\infty = \rho_r$ respectively
- ——: phase coexistence line first order phase transition between HD and LD with $\rho_r > \rho_l$
- – –: continuous phase transition between HD, LD and MC

Figure 2.2: Phase diagram for the bulk density of the ASEP with open boundaries.

which follows directly from the first relation of (2.46). As the matrices are in general infinite dimensional the evaluation of such quantities can still be a formidable task, but often it is at least possible to obtain asymptotic expressions. However, in certain regions of the parameter space the matrices can be chosen to be finite dimensional [104]. A simple example is the case of one-dimensional matrices for $\rho_l = \rho_r$, which leads to the product measure ν_{ρ_l}. See Proposition III.3.6 in [100] for general properties of the matrices.

In the totally asymmetric case $q = 0$ the relations (2.46) have a recursive structure that allows to calculate n-point functions without knowing D, E, $|v\rangle$ and $\langle w|$ explicitly. On the other hand, for $q > 0$ one has to find a representation for the matrices and vectors. This is possible using the close relation to creation and annihilation operators of the q-deformed harmonic oscillator. In [116, 38, 104] this idea was used to give exact solutions for special parameter values which allow finite dimensional representations, whereas in [120, 119, 22] the full solution is given for a slightly simplified model, where particles at the left boundary can only enter, at the right only exit the system. Those results show that the stationary measures have asymptotic product form in the bulk, i.e. $\tau_{k(L)}\, \mu^L \xrightarrow{w} \nu_{\rho_\infty}$ weakly for $L, k(L) \to \infty$ with $L - k(L) \to \infty$ (see [100], Theorem III.3.29). The bulk density ρ_∞ depends on the boundary conditions ρ_l and ρ_r and is explained in the phase diagram given in Figure 2.2. The only exception to this is for $\rho_l + \rho_r = 1$ and $\rho_l < \frac{1}{2}$ where the above weak limit is given by the mixture $\alpha\nu_{\rho_l} + (1-\alpha)\nu_{\rho_r}$ with $\alpha = \lim_{L\to\infty} k(L)/L \in [0,1]$ (see [100], Theorem III.3.41). So for these parameters, marked as a red line in the phase diagram, the system exhibits a boundary induced phase separation as explained in Section 2.1.3. The domain wall, separating the densities ρ_l and ρ_r, has the form of a shock as given in (2.41) with diffusively moving position. So in a typical configuration both phases with densities ρ_l and ρ_r are present, known as *phase coexistence*. The phase diagram can actually be understood by studying the motion of domain walls on a macroscopic level, as is explained in Section 2.2.3.

In [130, 131, 118] the MPA was used to find time dependent distributions of the ASEP. In the stationary case, it was generalized to the ASEP with impurities, such as a slow particle [103] or a slow bond introduced in [74], for which exact results have been obtained only for deterministic update with a stochastic defect in [69]. In [70] the MPA was used to recover solutions of certain integrable reaction-diffusion models. It also turned out that the MPA is not just an ansatz. The stationary measure of a one-dimensional stochastic model with finite interaction range and a finite number of different particle species can always be written as a matrix product [88, 85]. Generalized quadratic algebras resulting from nearest neighbor interactions have been studied systematically in [73, 111] and in [5, 6] or [82] (see also references therein) in the context of the multi-species ASEP. In this context the case with two species was studied extensively, which we discuss in section 2.2.4. The MPA was also applied to the ASEP with different update procedures, see [112] and references therein. It is not limited to finite lattices, in [35] it was shown that it can be used to calculate finite correlation functions for systems on an infinite one-dimensional lattice (see also Section 3.2). For a partial review on application of the MPA see [31] and [29].

2.2.3 Boundary induced phase transitions

Boundary conditions have decisive influence on the stationary measure of nonequilibrium systems, since the non-zero current can carry boundary effects into the bulk. As was shown before for the ASEP, stationary properties are the result of an interplay between bulk and boundary effects. It turned out that this behavior can be understood by analyzing the motion and stability of domain walls, that separate regions of different particle density. On a macroscopic scale, stable phase boundaries take the form of sharp edges (discontinuities) in the density profile and are therefore called shocks. On the microscopic scale of the lattice, a shock is still a rather smeared out object and it is not a priori clear how to define its position.

Consider the ASEP on $\Lambda = \mathbb{Z}$ with initial product distribution ν_{ρ_l,ρ_r} with densities ρ_l for $x \leq 0$ and ρ_r for $x > 0$. Assume that the particles are driven to the right, i.e. $p > q$. Then there exists a stable shock if $\rho_l < \rho_r$. Its position can be defined by coupling two processes with initial distributions ν_{ρ_l,ρ_r} such that the configurations differ only at site $X_0 = 0$. The location X_t of this defect then marks the shock location. This was first shown in [139, 4, 27] for special values of ρ_l and in [51] for the general case. In [47] it was shown for a similar coupling that X_t can be interpreted as the position of a second class particle. The precise statement is that there exists a measure μ_{ρ_l,ρ_r} of asymptotic product form ν_{ρ_l} and ν_{ρ_r} for $x \to \pm\infty$ respectively, which is stationary in the reference frame of the shock, i.e. for the process $\tau_{X_t}\boldsymbol{\eta}_t$. It was also shown that the position obeys a law of large numbers, i.e. $X_t/t \to v_s$ a.s. for $t \to \infty$ where $v_s = (p-q)(1-\rho_l-\rho_r)$ is the shock velocity. In the reference frame moving at constant speed v_s, the stationary measure is not given by μ but is rather a translation invariant mixture of ν_{ρ_l} and ν_{ρ_r} due to diffusive fluctuations of the shock position [4, 48]. This phenomenon was first studied in [139] and called *dynamical phase transition* (see also [100], Section III.2). As we see below, this is closely related to boundary induced phase transitions. A nice discussion of the direct analogy to phase separation in the 2D Ising model (cf. Section 2.1.3) can be found in [33]. Exact results for the shock measure μ_{ρ_l,ρ_r} were obtained in [33, 34, 35] using the MPA. In [49] the question of multiple shocks was addressed. A detailed review of this subject can be found in [100], Section III.2.

On the level of the hydrodynamic equation (2.30), the above phenomenon is well known as shock solutions of hyperbolic conservation laws. The shock velocity for general systems with current $j(\rho)$ is found to be

$$v_s = \frac{j(\rho_l) - j(\rho_r)}{\rho_l - \rho_r} , \tag{2.50}$$

as a simple consequence of the conservation of mass (see e.g. [26]). For the ASEP the current density relation is given by (2.40), leading to the result for v_s mentioned above. This was used in [89] for the ASEP on a finite lattice Λ_L with open boundary conditions $\rho_l \in [0,1]$ and $\rho_r = 0$ to establish a maximum principle for the stationary current j_L for $L \to \infty$. In [87, 109] this was generalized for all $\rho_r \in [0,1]$ to the extremal principle

$$\lim_{L\to\infty} j_L^{\rho_l,\rho_r} = \begin{cases} \max\limits_{\rho\in[\rho_l,\rho_r]} j(\rho) , & \text{for } \rho_l > \rho_r \\ \min\limits_{\rho\in[\rho_l,\rho_r]} j(\rho) , & \text{for } \rho_l < \rho_r \end{cases} , \tag{2.51}$$

in the case of positive drift $j(\rho) \geq 0$, and analogous for negative drift. The claim is that for large L the stationary current of the open system is selected from the current density relation for the bulk dynamics. (2.51) results from the analysis of the motion and stability of domain walls on the level of the hydrodynamic equation. These are given by stable shocks with speed (2.50) if the characteristic velocities satisfy $j'(\rho_l) > v_s > j'(\rho_r)$, i.e. the domains are drifting towards each other. If they are drifting apart the domain wall is unstable and given by a so-called rarefaction fan. The macroscopic time evolution consists of a combination of these two types of solutions and is a standard topic in the theory of hyperbolic conservation laws [26]. The stationary measure is then dominated by one of the boundary domains or by bulk domains with vanishing characteristic velocity and densities determined by the maxima and minima of the current density relation.

The main point of these studies is that the phase diagram for open boundary conditions of any driven diffusive system in one dimension (like Figure 2.2 for the ASEP) can be constructed from the knowledge of the current density relation alone. The microscopic details of the bulk interaction are therefore subsumed in the relation $j(\rho)$, while the boundaries set the range of the above extremal problem.

In general it is much easier to calculate $j(\rho)$ which is defined for periodic boundary conditions in (2.23), and then apply (2.51) rather than solving the model exactly with open boundary conditions. One example is the KLS model [80] (Katz, Lebowitz, Spohn), a generalized version of the TASEP with next nearest neighbor interactions given by the jump rates

$$0100 \xrightarrow{1+\delta} 0010 , \quad 1100 \xrightarrow{1+\epsilon} 1010 , \quad 0101 \xrightarrow{1-\epsilon} 0011 , \quad 1101 \xrightarrow{1-\delta} 1011 , \tag{2.52}$$

with parameters $\epsilon, \delta \in (-1,1)$. The model is exactly solvable for periodic boundary conditions and using (2.51) the phase diagram for the open system was constructed in [109]. In case of sufficiently strong repulsive interaction $\epsilon > 0$, $j(\rho)$ has a double hump structure with a minimum, leading to a minimal current phase. This is illustrated in Figure 2.3, where the parameter $\delta \neq 0$ accounts for the asymmetry of $j(\rho)$. Note that the extremal principle (2.51) is conjectured to hold in general, but this has not been proven rigorously. So far its validity

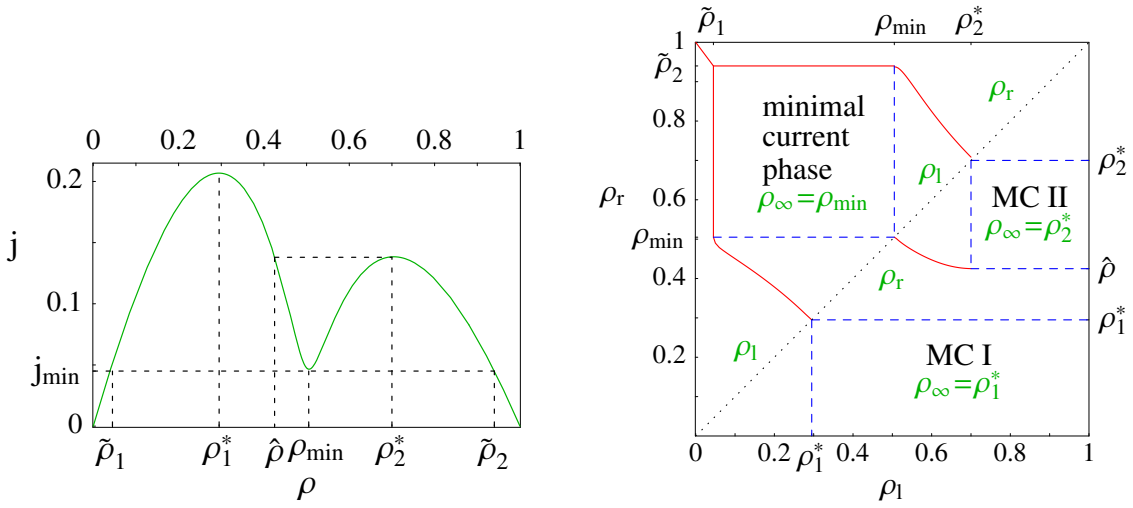


Figure 2.3: Boundary induced phase transitions for the KLS model (2.52) with repulsive interaction for parameters $\epsilon = 0.995$ and $\delta = 0.2$. **Left:** Fundamental diagram $j(\rho)$ defined in (2.23). **Right:** Corresponding phase diagram for the bulk density ρ_∞ with open boundary conditions ρ_l, ρ_r, via graphical construction from $j(\rho)$ using the extremal principle (2.51). MC I and MC II are maximal current phases, the phase boundaries are given by straight lines —— (first order), and broken lines – – (continuous).

is only assured for models like the ASEP which can be solved exactly for open boundary conditions. For the KLS model the validity of (2.51) is supported by phenomenological stability arguments and Monte Carlo simulations [109]. Rigorous results for a particular line in the phase diagram are given in [7]. An alternative strategy to prove (2.51) would be to derive hydrodynamic limit (cf. Section 2.1.4) for systems with open boundaries, since it is rigorously known on the level of the hydrodynamic equation.

It was also noticed in [7] that the role of the boundary conditions is crucial for the validity of (2.51). The generic choice is to couple the bulk with reservoirs of fixed distribution, like it was done in (2.42) for the ASEP. Apart from that, the dynamics for the reservoir boundaries is the same as in the bulk. But one can also specify arbitrary birth and death rates for particles in some finite region at the boundaries, which have nothing to do with the jump rates in the bulk. This causes a local perturbation and the boundary densities, important variables for the extremal principle (2.51), are no longer well defined. However one expects, that the bulk behavior of the system is still governed by (2.51), leading to the following conjecture [7, 64].

Conjecture. For any local boundary mechanism (however complicated) there exist *effective boundary densities* ρ_l and ρ_r, such that the stationary bulk properties are identical to a model with reservoir boundaries ρ_l and ρ_r.

Thus in these effective variables the phase diagram of the process is universal, i.e. independent of the details of the boundary mechanism. But it is possible that for certain mechanisms

not all effective densities $\rho_l, \rho_r \in [0,1]$ can be realized. Such an example was given in [63], where a part of the universal phase diagram is not accessible by the boundary mechanism.

The only rigorous results on the existence of an effective boundary density are given in [104, 22] for the partially asymmetric simple exclusion process with independent injection and exit rates at the boundaries. These lead to the same phase diagram as the coupling to reservoirs at specific densities, for which the rates are related by the bulk drive p/q. It is an open question if there is an effective density for more general systems and how it can be properly defined. We give a partial answer to this in Chapter 3, illustrated for a toy model on a semi-infinite lattice with a generalized boundary mechanism. Another related open question is if there is an equivalent extremal principle for systems with more than one species of particles. In this context we introduce the n-component zero range process in Chapter 4, and study the hydrodynamic conservation laws with open boundary conditions.

2.2.4 Phase transitions in two-component systems

A first example of a boundary induced phase transition in this context has been given in [41, 42] on the lattice $\Lambda_L = \{1, \dots, L\}$. The two species $+$ and $-$ move in different directions and pass each other with rate q.

$$\begin{aligned} &+0 \xrightarrow{1} 0+\,, \quad 0- \xrightarrow{1} -0\,, \quad +- \xrightarrow{q} -+\,; \\ &|0 \xrightarrow{\alpha} |+\,, \quad |- \xrightarrow{\beta} |0\,; \qquad 0| \xrightarrow{\alpha} -|\,, \quad +| \xrightarrow{\beta} 0|\,. \end{aligned} \tag{2.53}$$

The boundary rates are given in the second line, where the boundary is denoted by $|$, and they are assumed to be non-degenerate so that the process is irreducible and has a unique stationary measure $\mu_L^{\alpha,\beta}$. Due to the lacking conservation law the system is CP-invariant, i.e. symmetric under charge conjugation $+ \leftrightarrow -$ together with space inversion $x \leftrightarrow L - x + 1$. Therefore this is also true for the measure $\mu_L^{\alpha,\beta}$ and in particular it means that the expected numbers of $+$ and $-$ particles in the finite system are equal. But within a certain range of the parameters α, β and q the measure mainly concentrates on configurations with a pair of different particle densities, and its counterpart related by CP-inversion. Thus the limiting measure $\lim_{L\to\infty} \tau_{k(L)} \mu_L^{\alpha,\beta}$ is a CP-invariant mixture of two extremal stationary measures, which themselves are not CP-invariant. The existence of these measures alone is not surprising, since the infinite system is in general not CP-invariant due to local conservation of both particle species. The process exhibits boundary induced phase separation and in contrast to the ASEP discussed in Section 2.2.2 there is no phase coexistence but symmetry breaking in the following sense. The system shows only either one of the two density pairs and the above limit is independent of the sequence $k(L)$. So the domain wall is not fluctuating but rather pinned to one of the boundaries. For $\alpha = \infty$ or $\beta = 1$ the matrix product representation of the stationary measure can be solved exactly. In the limit $\beta \to 0$ exact results were obtained in [59] by mapping the process on a biased random walk model. For other parameter values the result is based on non-rigorous mean field calculations, corroborated by Monte Carlo simulation data [9, 24].

From the discussion in the previous subsection it becomes clear that phase separation in periodic systems with finite interaction range is not possible, since one of the two resulting domain boundaries is generically unstable. This situation can be avoided in the presence of

two or more species of particles. In such systems all phase boundaries can be stable and one can observe phase separation on periodic lattices. This can be interpreted to be the result of an effective long range interaction when the different particle species block each other and form clusters occupying a positive fraction of the volume.

Such a phenomenon was observed for the first time in [44, 45] on the lattice $\Lambda_L = \mathbb{Z}/L\mathbb{Z}$ with three particle species A, B and C, where one of them can be regarded as empty sites. The rates are cyclic in A, B and C and given by

$$AB \underset{1}{\overset{q}{\rightleftarrows}} BA\,, \quad BC \underset{1}{\overset{q}{\rightleftarrows}} CB\,, \quad CA \underset{1}{\overset{q}{\rightleftarrows}} AC\,. \tag{2.54}$$

For $q = 1$ the particles undergo symmetric diffusion and the system is homogeneous, i.e. in the limit $L \to \infty$ the extremal stationary measures are given by translation invariant distributions $\mu_{\rho_A,\rho_B,\rho_C}$, with densities ρ_A, ρ_B, $\rho_C \in [0,1]$ and $\rho_A + \rho_B + \rho_C = 1$. For $q \neq 1$ the particle exchange rates are biased. Since the model is invariant under the exchange $A \leftrightarrow B$, $q \to 1/q$ it is sufficient to consider $q < 1$. It is shown that in this case phase separation occurs due to an effective long range interaction. For large systems typical stationary configurations are of the form $\ldots AAABBBBBCCCCCCAA\ldots$ with vanishing current. The boundaries fluctuate only locally, indicating also spontaneous breaking of translation invariance. Exact calculations are presented in the case of equal particle numbers, where the current vanishes and the model satisfies detailed balance with respect to a long-range asymmetric Hamiltonian. For general non-zero particle numbers the statements are confirmed by heuristic arguments. Note that in contrast to boundary induced phenomena this result strongly indicates phase separation for the infinite system. One expects $\mu_{1,0,0}$, $\mu_{0,1,0}$ and $\mu_{0,0,1}$ to be the only translation invariant extremal measures, besides a series of blocking measures analogous to the ASEP (2.43). However in this model breaking of translation invariance is not a trivial phenomenon, since blocking configurations occur also for periodic boundary conditions.

In [10, 12] the first model (2.53) was considered with periodic boundary conditions, with the additional jump $-+ \to +-$ at rate 1 and with equal particle numbers. This system is also CP-invariant and for $q < 1$ strong phase separation with vanishing current occurs, just as in the previous model (2.54). For large q the system is homogeneous, confirmed by Monte Carlo simulations and exact results via MPA [11] for $q = 3$ (product measure) and $q = 4$. The authors also claimed the existence of a mixed phase for $1 < q < q_c \approx 1.4$, where the system shows phase separation with a non-vanishing current. This result was only based on Monte Carlo simulations, mean field calculations and a phenomenological extension of Yang-Lee theory for this system [8]. In [13] the previous results were heuristically extended to general particle numbers, studying the macroscopic equivalent Burgers equation corroborated by Monte Carlo simulations. However, in [113, 121] the mixed phase was not found in exact calculations for the grand canonical ensemble. The previous observations leading to its postulation are due to a sharp crossover with an anomalously large but finite correlation length. This was proven in [76, 78] using a mapping to the zero range process (see Section 2.3.3) and exact results on a condensation transition for this model, which is the main topic of Chapter 5. In view of this result, a system showing phase separation with a non-vanishing current has only recently been introduced in [77]. For a recent review on critical phenomena in one-dimensional two-component systems see [125].

2.3 Zero range processes

The zero range process (ZRP) is an interacting particle system without exclusion interaction and was originally introduced in [128]. Besides being of interest on its own as a model for bosonic lattice gases, it has gained much attention due to its close relation to the ASEP, explained in section 2.3.3 Other important features are that the stationary measures are of product form under very general conditions, and the possibility of condensation transitions, which are the topic of Chapters 5 and 6.

2.3.1 Definition and construction

The local state space of the zero range process is $E = \mathbb{N}$, so the number of particles per site is unbounded. At a given site $x \in \Lambda$, the number of particles $\eta(x)$ decreases by one with rate $g(\eta(x))$ and the leaving particle jumps to site $x + y$ with probability $p(y)$. So the transition rates are given by

$$c(x, x+y, \boldsymbol{\eta}) = g\big(\eta(x)\big)\, p(y)\ , \tag{2.55}$$

depending only on the configuration at site x, which can be interpreted as a particle interaction of range zero. In general, the functions g and p could also depend on the site x (cf. Section 2.3.4), but here we focus on translation invariant systems. The jump probability $p : \mathbb{Z} \to [0, 1]$ is normalized and assumed to be of finite range $R \in \mathbb{Z}^+$,

$$\sum_{y\in\Lambda} p(y) = 1\ , \quad p(0) = 0 \quad \text{and} \quad p(y) = 0 \text{ for } |y| > R\ . \tag{2.56}$$

To exclude hidden conservation laws p should be irreducible on finite periodic lattices, so that every particle can reach any site with positive probability. For the dynamics to be well defined on infinite lattices and to be non-degenerate, the rate function $g : \mathbb{N} \to [0, \infty)$ has to satisfy

$$\sup_{k\in\mathbb{N}} |g(k+1) - g(k)| =: \bar{g} < \infty\ , \quad g(k) > g(0) = 0 \text{ for all } k > 0. \tag{2.57}$$

Since the generic state space $X = \mathbb{N}^\Lambda$ would not be compact, the construction of the dynamics for general lattices given in section 2.1.1 has to be modified. In [3, 96] this is done on the restricted state space

$$X = \big\{\boldsymbol{\eta} \in \mathbb{N}^\Lambda \big|\, \|\boldsymbol{\eta}\|_\alpha < \infty\big\}\ , \quad \text{where} \quad \|\boldsymbol{\eta}\|_\alpha = \sum_{x\in\Lambda} |\eta(x)|\, \alpha(x) \tag{2.58}$$

for some $\alpha : \Lambda \to (0, \infty)$ with

$$\sum_{y\in\Lambda} \alpha(y) < \infty \quad \text{and} \quad \sum_{y=-R}^{R} p(y)\, \alpha(x+y) \le M\, \alpha(x) \tag{2.59}$$

for all $x \in \Lambda$ and a constant $M > 0$. Such an α can easily be found, for instance $\alpha(x) = b^{|x|}$ for $b \in (0, 1)$. The measurable structure on X is given by the smallest σ-algebra so that the

map $\boldsymbol{\eta} \to \eta(x)$ is measurable for each $x \in \Lambda$. Note that if $\{\eta(x), x \in \Lambda\}$ are nonnegative random variables with uniformly bounded means, then $\boldsymbol{\eta} \in X$ with probability one. Thus X is large enough to contain many distributions of interest. For $\boldsymbol{\eta}, \boldsymbol{\zeta} \in X$ the distance $\|\boldsymbol{\eta}-\boldsymbol{\zeta}\|_\alpha$ as defined in (2.58) provides the topology on X. Let $L(X,\mathbb{R})$ be the set of Lipshitz continuous functions $f : X \to \mathbb{R}$, i.e. for all $f \in L(X,\mathbb{R})$ there exists an $l(f) \in [0,\infty)$ such that

$$|f(\boldsymbol{\eta}) - f(\boldsymbol{\zeta})| \le l(f)\|\boldsymbol{\eta}-\boldsymbol{\zeta}\|_\alpha \quad \text{for all } \boldsymbol{\eta},\boldsymbol{\zeta} \in X\ . \tag{2.60}$$

The next theorem was proved in [3] and shows that the formal generator

$$(\mathcal{L}f)(\boldsymbol{\eta}) = \sum_{x\in\Lambda}\sum_{y=-R}^{R} g(\eta(x))\,p(y)\big(f(\boldsymbol{\eta}^{x\to x+y}) - f(\boldsymbol{\eta})\big), \tag{2.61}$$

for $f \in L(X,\mathbb{R})$ defines a Markov process on X.

Theorem 2.3 (Andjel) *Under the above conditions on g and p (2.56) - (2.59), $\mathcal{L}$ generates a semigroup $S(t)$ of operators on $L(X,\mathbb{R})$ with*

$$\big|S(t)\,f(\boldsymbol{\eta}) - S(t)\,f(\boldsymbol{\zeta})\big| \le l(f)\,e^{\bar{g}(M+2)t}\|\boldsymbol{\eta}-\boldsymbol{\zeta}\|_\alpha \tag{2.62}$$

for all $\boldsymbol{\eta}, \boldsymbol{\zeta} \in X$ and $f \in L(X,\mathbb{R})$.

Proof. See [3], Theorem 1.4.

This defines the process $\boldsymbol{\eta}_t$ analogously to (2.2) with a restricted set $L(X,\mathbb{R}) \subset C(X,\mathbb{R})$ of observables. In fact $S(t)$ is not strongly continuous on $C(X,\mathbb{R})$, so no direct application of the Hille-Yosida Theorem (see Appendix A.1, Theorem A.2) is possible. Nevertheless, all results of section 2.1.1 can be obtained without general semigroup theory [3, 101]. The inequality (2.62) assures that $\mathbb{P}^{\boldsymbol{\eta}}\big[\{\boldsymbol{\eta}_t \in X\}\big] = 1$ for all $\boldsymbol{\eta} \in X$, so the process does not leave the restricted state space during time evolution. The above construction is also possible if p and g are not translation invariant, as long as p is irreducible and (2.57) is fulfilled uniformly in x. For further details on the construction of the dynamics see [3] and references therein.

2.3.2 Stationary measures

In the following we summarize results on stationary measures for the ZRP which are well known and can be found for example in [3, 40, 84]. Under very general conditions there are stationary product measures with one-point marginals

$$\nu^1\big(\{\eta(x) = k\}\big) \propto W(k)\,\phi_x^k \quad \text{with weight} \quad W(k) = \prod_{i=1}^{k} 1/g(i)\ . \tag{2.63}$$

The $\phi_x \in [0,\infty)$ can be interpreted as site dependent fugacities of grand canonical measures in the context of open boundary conditions (see below). They have to fulfill the stationarity condition (2.18), which becomes

$$\sum_{y\in\Lambda}\big\langle c(y,x,\boldsymbol{\eta}) - c(x,y,\boldsymbol{\eta})\big\rangle_\nu = \sum_{|y|\le R} p(y)\,\phi_{x-y} - \phi_x = 0 \tag{2.64}$$

for all $x \in \Lambda$, since with the weight in (2.63) it is $\langle g(\eta(x)) \rangle_\nu = \phi_x$. This is the most general ansatz for stationary product measures for the bulk generator (2.61) (see e.g. Theorem 1.8 in [3]). The problem is now to find solutions $(\phi_x)_{x\in\Lambda}$ to (2.64) on a given lattice Λ, such that (2.63) can be properly normalized. Note that the equation depends only on the jump probabilities p, whereas the jump rates g determine the allowed range of the solution, as we see in the following.

Periodic boundary conditions

On the periodic lattice $\Lambda_L = (\mathbb{Z}/L\mathbb{Z})^d$ the only solution to (2.64) is the constant function $\phi_x \equiv \phi$. Thus (2.63) defines a translation invariant grand canonical product measure $\bar\nu_\phi^L$ (cf. Section 2.1.2) with one-point marginals

$$\bar\nu_\phi^1(k) = W(k)\,\phi^k/Z(\phi)\;, \tag{2.65}$$

with the (one site) normalizing partition function

$$Z(\phi) = \sum_{k=0}^{\infty} W(k)\,\phi^k\;. \tag{2.66}$$

The expected particle density as a function of ϕ is denoted as $R : D_\phi \to D_\rho$ and given by

$$R(\phi) = \sum_{k=0}^{\infty} k\,\bar\nu_\phi^1(k) = \phi\,\partial_\phi \log Z(\phi) \qquad \text{with} \quad \rho_c = \lim_{\phi\nearrow\phi_c} R(\phi)\;. \tag{2.67}$$

The measures are well defined on the domain D_ϕ, which is determined by the radius of convergence $\phi_c \in [0,\infty]$ of $Z(\phi)$. It is easy to see that $\phi_c \geq \liminf_{i\to\infty} g(i)$, whereas equality holds in many interesting cases, for instance if $\lim_{i\to\infty} g(i) \in [0,\infty]$ exists. Often $D_\phi = [0,\phi_c)$ and R has full range $D_\rho = R(D_\phi) = [0,\infty)$, i.e. the critical density ρ_c diverges. This is for example the case if $g(i)$ is non-decreasing (see [40] and Lemma 5.1). But depending on the weight $W(k)$, $\rho_c < \infty$ is also possible and in this case we have $D_\phi = [0,\phi_c]$, $D_\rho = [0,\rho_c]$ and the system exhibits a condensation transition as discussed in Chapter 5. It is $R(0) = 0$ and $R(\phi)$ is monotonic increasing on D_ϕ and thus invertible. We denote the inverse function $\Phi : D_\rho \to D_\phi$ by $\Phi(\rho)$.

With (2.16) the corresponding canonical measures are given by $\mu_{L,N} = \bar\nu_\phi^L(.\,|\Sigma_L = N)$ with arbitrary $\phi \in [0,\infty)$ which is canceled by the normalization. It is

$$\mu_{L,N}(\boldsymbol{\eta}) = \frac{1}{Z(L,N)} \prod_{x\in\Lambda_L} W\big(\eta(x)\big)\,\delta(\Sigma_L(\boldsymbol{\eta}),N) \tag{2.68}$$

where the canonical partition function is given by

$$Z(L,N) = \sum_{\boldsymbol{\eta}\in X_L} \prod_{x\in\Lambda_L} W\big(\eta(x)\big)\,\delta(\Sigma_L(\boldsymbol{\eta}),N)\,. \tag{2.69}$$

In the limit of large system size $L, N = [\rho L] \to \infty$ with fixed particle density $\rho \in D_\rho$, the canonical measure (2.68) is expected to be equivalent to the grand canonical measure (2.65) with $\phi = \Phi(\rho)$. A rigorous result on this equivalence is available in [84], Appendix 2, but it only covers the case $\rho_c = \infty$. In Chapter 5, we generalize this result to densities $\rho \in [0,\infty)$ even if $\rho_c < \infty$, and explain the precise meaning of the term 'equivalence'.

Closed or reflecting boundary conditions

In this case (2.64) is altered when x is within range R of the boundary. For every finite, connected lattice, it can be interpreted as the master equation of a random walker with occupation probability ϕ_x. Since p is assumed to be irreducible, there is a unique stationary distribution $(\tilde{\phi}_x)_{x\in\Lambda_L}$ and every positive solution of (2.64) has the form $\phi\,(\tilde{\phi}_x)_{x\in\Lambda_L}$ for some $\phi > 0$. To get a well defined grand canonical measure with fugacity ϕ it is necessary that $\phi\,\tilde{\phi}_x \in D_\phi$ for all $x \in \Lambda_L$. In this case the grand canonical product measure has site dependent marginals

$$\bar{\nu}_\phi\big(\{\eta(x) = k\}\big) = \bar{\nu}^1_{\tilde{\phi}_x\,\phi}(k) = W(k)\,\tilde{\phi}_x^k\,\phi^k/Z(\tilde{\phi}_x\,\phi)\;. \tag{2.70}$$

This leads to site dependent densities $R_x(\phi) = R(\tilde{\phi}_x\,\phi)$ with R given in (2.67), and the canonical measures are also analogous to (2.68) and (2.69), where the weights $W\big(\eta(x)\big)$ have to be replaced by $W\big(\eta(x)\big)\tilde{\phi}_x^{\eta(x)}$.

Open boundary conditions

Consider the ZRP on the lattice $\Lambda_L = \{1,\dots,L\}^d$. For non-degenerate open boundary conditions there is a unique stationary measure, but in contrast to the previous lattices, this is in general not of product form. We take boundary conditions which are compatible with the bulk dynamics, i.e. we fix boundary values ϕ_x for all $x \notin \Lambda_L$ with $|x - \Lambda_L| \le R$. If these are non-degenerate (2.64) has a unique solution, but this is positive only under special conditions. See [2] and references therein for a discussion of boundary value problems of linear difference equations. If there is no positive solution, then the stationary measure is not of product form. The case of general open boundary conditions or dimensions $d > 1$ has not been studied so far, but we expect a similar situation as for the ASEP (Section 2.2.2), namely that in the limit $L \to \infty$ the measures are asymptotically product.

Note that for every solution ϕ_x of (2.64), $a\phi_x + b$ is also a solution for all $a, b \in \mathbb{R}$, so there are at least two degrees of freedom for the boundary conditions. This can be used to get an explicit solution for the most basic example. Consider the one-dimensional lattice $\Lambda_L = \{1,\dots,L\}$ and nearest neighbor jump probabilities $p(y) = p\,\delta_{y,1} + q\,\delta_{y,-1}$ with $p, q \ge 0$, $p + q = 1$. In this case one can specify $\phi_0 = \phi_l$ and $\phi_{L+1} = \phi_r$ independently to get the unique solution

$$\phi_x = \phi_l + (\phi_r - \phi_l)\frac{(p/q)^x - 1}{(p/q)^{L+1} - 1}\;. \tag{2.71}$$

Thus there exists a stationary product measure ν with site dependent marginals

$$\nu\big(\{\eta(x) = k\}\big) = W(k)\,\phi_x^k/Z(\phi_x)\;, \tag{2.72}$$

if and only if $\phi_l, \phi_r \in D_\phi$, since (2.71) is monotonic in x. For large L the fugacity profile ϕ_x is essentially constant except for the neighborhood of one of the boundaries. Depending on the drift direction the bulk value is equal to ϕ_r if $p < q$ or to ϕ_l if $p > q$. For $p = q$ the solution to (2.64) is a linear profile, which has been studied in [18, 19]. For jump probabilities $p(y)$ with range $R > 1$ one has to specify more than two boundary values of ϕ. But to get a solution to (2.64) they can in general not be chosen independently.

The infinite lattice

The translation invariant product measures $\bar\nu_\phi$, $\phi \in D_\phi$ defined in (2.65) are also stationary for the process on the infinite lattice $\Lambda = \mathbb{Z}^d$. If $g(k)$ is non-decreasing, a sufficient condition for $D_\phi = [0, \phi_c)$ and $D_\rho = [0, \infty)$ (see [40] and Lemma 5.1), it was shown in [3] (Theorem 1.9) that these are all translation invariant elements of $\mathcal{I}_e$. If in addition p is symmetric and not positive recurrent (e.g. symm. random walk on $\mathbb{Z}$ or $\mathbb{Z}^2$), the complete characterization $\mathcal{I}_e = \{\bar\nu_\phi | \phi \in [0, \phi_c)\}$ is given in [3], Theorem 1.10. But in general, just as for the ASEP, there exist also non-translation invariant stationary measures, which can be obtained as limit solutions to open boundary problems. Consider the example $p(y) = p\,\delta_{y,1} + q\,\delta_{y,-1}$ from above with $\Lambda = \mathbb{Z}$. Then, for $\phi_c = \infty$, $\phi_x = (p/q)^x$ gives a non-translation invariant stationary product measure for asymmetric jump probabilities $p \neq q$. On the other hand, for $\phi_c < \infty$ these solutions are ruled out and $\mathcal{I}_e = \{\bar\nu_\phi | \phi \in [0, \phi_c)\}$ if $g(k)$ is non-decreasing (see [3] Theorem 1.11). A crucial idea of the above results is to use attractivity, defined in the appendix (A.6). For the ZRP this is equivalent to non-decreasing jump rates (see [84], Theorem II.5.2), and if this is not fulfilled there are basically no other results on the infinite lattice than the existence of the product measures $\bar\nu_\phi$, $\phi \in D_\phi$.

The stationary current

As discussed in section 2.1.2 the microscopic current is in general hard to write down, but the drift takes the easy form $d(x, \boldsymbol{\eta}) = \sum_{|y| \le R} y\, p(y)\, g\big(\eta(x)\big)$. For the translation invariant product measures $\bar\nu_\phi$ we have $\big\langle g\big(\eta(x)\big)\big\rangle_{\bar\nu_\phi} = \phi$ and with $\phi = \Phi(\rho)$ defined after (2.67), this leads to the current-density relation (2.23)

$$j(\rho) = m(p)\,\Phi(\rho) \ \in \mathbb{R}^d\,. \tag{2.73}$$

Here $m(p) = \sum_{y=-R}^{R} y\, p(y) \in \mathbb{R}^d$ denotes the first moment of p. For non-symmetric jump probabilities this is in general non-zero and determines the direction of the current. The absolute value $|j(\rho)|$ is monotonic increasing in ρ with $j(0) = 0$, approaching its maximum $|m(p)|\phi_c$ for $\rho \to \rho_c$. The ZRP is reversible if and only if p is symmetric and in this case it is $j(\rho) = 0$.

The grand canonical measures (2.65) can easily be generalized to inhomogeneous jump rates g_x [40]. They keep the same form with fugacity ϕ, site dependent weights $W_x(k)$, partition function $Z_x(\phi)$ and densities $\rho_x(\phi)$ (2.67). The current is of course site independent and still given by $j = m(p)\,\phi$. They are well defined for all $\phi < \phi_c$, where ϕ_c is now the minimal radius of convergence of the Z_x. A special case for non-translation invariant jump probabilities p is discussed in (2.74) in the next subsection.

Note that due to monotonicity of $|j(\rho)|$, there are no boundary induced phase transitions for the ZRP. But since the local state space is infinite there are condensation transitions which we discuss in Section 2.3.4 and Chapter 5.

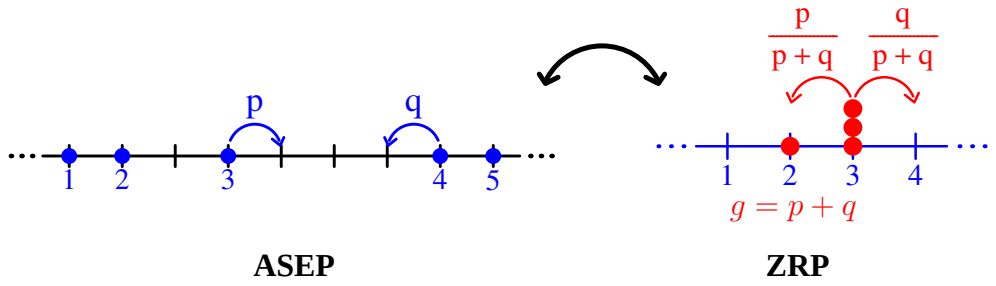


Figure 2.4: Equivalence of the dynamics of the ASEP and the ZRP.

2.3.3 Relation to the asymmetric simple exclusion process

On translation invariant one dimensional lattices, the ASEP seen from a tagged particle is equivalent to the ZRP with nearest neighbor jumps and constant jump rate $g(k) \equiv \Theta(k)g$. This was first noticed in [46, 83] and is shortly explained in the following. Consider the ASEP on $\Lambda_L = \mathbb{Z}/L\mathbb{Z}$ with $N \leq L$ particles, each labeled with a number $i \in \{1, \dots, N\}$ in consecutive order. Take $x_i \in \Lambda_L$ to be the position of the i-th particle. We tag the particle $i = 1$, i.e. we choose a reference frame with $x_1 = 0$, leading to $x_1 < \dots < x_N$. This order is preserved, since the particles cannot pass each other. Every particle i in the ASEP is regarded as a lattice site of the ZRP, whose occupation number $\eta(i)$ is determined by the number of empty sites to the right of the ASEP particle. So the ZRP is defined on the lattice $\Lambda_N = \mathbb{Z}/N\mathbb{Z}$ with $L-N$ particles and the configurations are mapped via $\eta(i) = x_{i+1} - x_i - 1$. In the ASEP particles jump to the right with rate p (2.35), corresponding to a jump of an empty site to the left. So the choice $g = (p+q)$, $p(1) = q/(p+q)$ and $p(-1) = p/(p+q)$ in the ZRP maps the dynamics of both processes, which is illustrated in Figure 2.4. So the ASEP can be described in terms of the particle distances by a particular ZRP with nearest neighbor jumps. Since the ZRP has stationary product measures with fugacities $\phi < \phi_c = g$ this mapping can be used to find the stationary distribution of particle distances for the ASEP. As the above mapping works also for more general exclusion processes, it can be useful in situations where the stationary measure is not known.

First we would like to apply the mapping on the infinite lattice $\Lambda = \mathbb{Z}$. If the particle positions $x_i \in \mathbb{Z}$ are not bounded above or below the ZRP is also defined on $\mathbb{Z}$. If the x_i are bounded below, i.e. there is a first particle with position tagged to $x_1 = 0$, the corresponding ZRP is defined on the semi-infinite lattice $\Lambda = \mathbb{Z}^+$. To fix ideas we take $p > q$, so the ASEP particles are driven to the right. For simplicity we assume $p + q = 1$ without loss of generality. Then the blocking measures for the ASEP described in (2.43) correspond to a stationary product measure $\bar{\nu}$ for the ZRP given in (2.72) with boundary conditions $\phi_0 = p + q = 1$ and $\lim_{x\to\infty} \phi_x = 0$. The solution to (2.64) in this case is $\phi_x = (q/p)^x$ and the density is given by $\rho(x) = (q/p)^x / \big(1-(q/p)^x\big)$. We have $\sum_{x\in\mathbb{Z}^+} \rho(x) < \infty$ for all $q < p$ since the ZRP particles are driven to the left out of the system. The one-point marginals of $\bar{\nu}$ decay exponentially (cf. (2.72)), so there are only finitely many particles in the ZRP with probability one, corresponding to finitely many empty sites between the ASEP particles in a blocking configuration.

The mapping also works, when each particle i in the ASEP has individual jump rates p_i to the right and q_i to the left. In the ZRP this leads to site dependent jump rates $g_i(k) = \Theta(k)(p_i + q_{i+1})$ and jump probabilities $p(i, i+y) = q_{i+1}\,\delta_{y,1} + p_i\,\delta_{y,-1}$ which are not translation invariant. On a periodic lattice, the analogue to (2.64),

$$\sum_{|y|\leq 1} p(i-y,i)\,\phi_{i-y} - \phi_i = 0 \quad \text{for all } i \in \{1,\dots,N\}\,, \tag{2.74}$$

has constant solutions $\phi_x \equiv \phi$ if and only if p is doubly stochastic. This is equivalent to $p_{i-1}q_{i+2} = p_{i+1}q_i$ for all i, which is fulfilled for example in the totally asymmetric case where $q_i = 0$ for all i. Then the stationary measure of the ZRP still has simple product structure with site dependent jump rates g_i, as discussed at the end of the previous subsection. This mapping was used in [91] to study phase transitions for a disordered ASEP on a periodic lattice, where the p_i are quenched random variables. In [17] the case $q_i \neq 0$ with $p_i + q_i = 1$ for all i was studied on $\Lambda = \mathbb{Z}$, involving a non-constant solution of (2.74). We give more details on this phase transition in Section 2.3.4.

Note that there exists a similar mapping in the theory of reaction-diffusion models, stochastic particle systems without conserved bulk dynamics. Under certain conditions on the transition rates, one has closed equations for the time evolution of the size distribution of empty intervals between particles. This is known as empty interval method or interparticle distribution function method, described in [106, 81] and references therein.

2.3.4 Condensation transitions

Condensation transitions in the ZRP have been studied the first time in the context of phase transitions in exclusion models with particle-wise disorder. The particles move at individual random rates with a common drift direction on a one-dimensional lattice with periodic boundary conditions. Since particles cannot overtake, the one with the slowest drift can cause an obstruction. This is not the case as long as the particle density exceeds a critical value, $\rho > \rho^*$, because for high densities the mobility of all particles is reduced anyway due to the exclusion interaction. In this laminar phase, disorder causes only local perturbations and on a macroscopic scale the stationary distribution looks uniform with a product distribution for interparticle distances. For small densities particles can move almost freely, and if $\rho < \rho^*$ they pile up behind the slowest particle, which has macroscopic region of empty sites ahead. In this jammed phase, disorder causes a global effect and the interparticle distances have a stationary distribution which is not of product form. This result was obtained in [91] for the disordered totally asymmetric exclusion process and in [17] for partial asymmetry by calculating the stationary distribution of interparticle distances. Due to the mapping explained in Section 2.3.3 this is given by the stationary distribution of a corresponding zero range process with site-wise disorder. An independent analysis using the matrix product ansatz (cf. Section 2.2.2) is given in [39], where also the close relation to the corresponding condensation transition is pointed out.

On the level of the ZRP, the mechanism is the following. There are invariant product measures $\bar{\nu}_\phi$ as given in (2.65) for $\phi < \phi_c = \min_i \phi_c(i)$, the critical fugacity for the slowest site. These measures have the density $R(\phi) = \langle R_i(\phi) \rangle_i$ averaged over the quenched distribution $P(i)$ of site-wise disorder. Depending on the form of this distribution, $\rho_c = R(\phi_c) < \infty$ is possible, defining the critical density for the ZRP. For $\rho > \rho_c$ the product measure $\bar{\nu}_\phi$ is no longer well defined and an extensive fraction of particles piles up on the slowest site, forming a condensate. In the ASEP this corresponds to the free headway of the slowest particle in the jammed phase. The critical densities in both models are related via $\rho^* = 1/(1 + \rho_c)$ since the ZRP describes the interparticle distances of the ASEP. In the laminar phase the particle density in the ZRP is below ρ_c, resulting in product invariant measures. For a review on phase transitions in disordered exclusion models see [40, 90]. The hydrodynamics of this phenomenon has been studied in [126].

The analysis of condensation transitions in the ZRP is an interesting topic on its own and the above transition is closely related to Bose-Einstein condensation. A similar phenomenon can occur also for translation invariant systems which does not have a corresponding equivalent in finite range exclusion processes. The statics and dynamics of this type of condensation are studied in detail in Chapters 5 and 6.

Chapter 3

Boundary induced phase transitions and the effective density

3.1 Introduction

Stationary properties of nonequilibrium lattice gases with open boundaries are the result of an interplay between bulk and boundary effects. In Section 2.2.3 it is demonstrated that this behavior can be understood by analyzing the motion and stability of domain walls. This leads to the conjecture of an extremal principle for the stationary current (2.51), that characterizes bulk properties of the stationary measure for large system sizes. In this way it is possible to deduce the phase diagram of the model from the current-density relation of the process (2.23). One key ingredient for the extremal principle is that the effect of any boundary mechanism on the stationary bulk properties of an exclusion model can be summarized in a single variable, the effective boundary density $\rho_{\mathit{eff}} \in [0, 1]$. So apart from differences in the boundary region, the stationary system should behave as if it was coupled to reservoirs, for which there is only one degree of freedom, the density. In these effective variables the phase diagram is supposed to be independent of the particular boundary mechanism and is simply determined by the bulk dynamics that enter the current-density relation. The only rigorous results on the validity of this conjecture are given in [5, 22, 104] by the exact calculation of stationary measures for the partially asymmetric simple exclusion process. For independent injection and exit rates at the boundaries, the bulk properties of the stationary measures are found to be identical to reservoir coupling with an effective density (see Section 3.4.2). For more general models, the existence of an effective boundary density is still an open question, for which we present some progress in the forthcoming chapter.

In general, we expect ρ_{eff} to be the result of boundary as well as bulk properties of the system. The right context to isolate this interplay and study it for generalized boundary mechanisms is a semi-infinite system with only one boundary. This excludes for example boundary induced phase separation, and the boundary of a semi-infinite system always selects a pure phase of the bulk dynamics. In [7] it is suggested that ρ_{eff} is given by the stationary bulk density of such a semi-infinite system. As we see in the next section, this has to be further specified and only makes sense in a certain region of the phase diagram, since the stationary measure of a system with infinite state space and conservation law is not unique.

In Section 3.3 we define an effective boundary density and prove existence and uniqueness for ASEP bulk dynamics and general boundary mechanisms. It turns out that in this case the effects of boundary inhomogeneities remain localized in a finite region at the boundary, and the effective density ρ_{eff} can be directly computed by solving the stationarity conditions for a finite system. We illustrate this by using a toy model with a slightly generalized boundary mechanism. This method seems to be restricted to bulk dynamics with nearest neighbor hopping and stationary product measures. We shortly discuss these limitations towards the end of this chapter, and propose a less explicit definition of the effective boundary density for general bulk dynamics.

3.2 The semi-infinite ASEP

First we introduce the semi-infinite ASEP and characterize its stationary measures with a simple boundary reservoir. To use the matrix product method in an efficient way we restrict ourselves to the totally asymmetric case, which highly reduces the complexity of the calculations.

3.2.1 Stationary measures with the matrix product ansatz

In the following we consider the totally asymmetric simple exclusion process on the semi-infinite lattice $\Lambda = \mathbb{Z}^+ = \{1, 2, \ldots\}$. In the bulk particles jump to the right with rate 1,

$$c(x, y, \boldsymbol{\eta}) = \eta(x)\big(1 - \eta(y)\big)\, \delta_{y,x+1}\ , \tag{3.1}$$

and at the boundary they are injected with rate $\alpha \in \mathbb{R}^+$, which corresponds to a reservoir of density α if $\alpha \leq 1$. For $\alpha > 1$ the system shows the same stationary behavior as for $\alpha = 1$, as we see below. The full generator is given by

$$\begin{aligned}\mathcal{L}f(\boldsymbol{\eta}) = &\sum_{x=1}^{\infty} \eta(x)\big(1 - \eta(x+1)\big)\big[f(\boldsymbol{\eta}^{x\to x+1}) - f(\boldsymbol{\eta})\big] \\ &+\alpha\big(1 - \eta(1)\big)\big[f(\boldsymbol{\eta}^{0\to 1}) - f(\boldsymbol{\eta})\big]\ .\end{aligned} \tag{3.2}$$

In contrast to systems with two boundaries the state space $X = \{0,1\}^{\mathbb{Z}^+}$ is infinite and uniqueness of the stationary measure is no longer assured. In fact it was noticed in [97] that there can be several asymptotic densities for $x \to \infty$, summarized in the following ergodic theorem:

Theorem 3.1 (Liggett) *Let π be a product measure on $\mathbb{Z}^+$ for which $\rho = \lim_{x\to\infty} \langle \eta(x) \rangle_\pi$ exists. For $\alpha = 0$, $\rho = 1$ the additional assumption $\sum_{x=1}^{\infty} \langle 1 - \eta(x) \rangle_\pi = \infty$ is required.*

$$\textit{If } \alpha \geq 1/2 \textit{ then } \lim_{t\to\infty} \pi S(t) = \begin{cases} \mu_\rho^\alpha & \textit{, if } \rho \geq 1/2 \quad \textit{(bulk dominated)} \\ \mu_{1/2}^\alpha & \textit{, if } \rho \leq 1/2 \quad \textit{(maximum current)}\ . \end{cases}$$

$$\textit{If } \alpha \leq 1/2 \textit{ then } \lim_{t\to\infty} \pi S(t) = \begin{cases} \mu_\rho^\alpha & \textit{, if } \rho > 1 - \alpha \quad \textit{(bulk dominated)} \\ \nu_\alpha & \textit{, if } \rho \leq 1 - \alpha \quad \textit{(boundary dominated)}\ . \end{cases}$$

The stationary measures are asymptotically product with density ρ, i.e. $\lim_{x\to\infty} \tau_x \mu_\rho^\alpha = \nu_\rho$ denoted by $\mu_\rho^\alpha \simeq \nu_\rho$, and $\mu_\alpha^\alpha = \nu_\alpha$. The limits are understood in a weak sense with test functions $f \in C(X, \mathbb{R})$.

Proof. See [97], Theorem 1.8.

We summarize the statement of the theorem in a phase diagram for the ergodic behavior in Figure 3.1 (bottom right) on page 44, where we plot the stationary bulk density ρ_∞ as a function of α and the initial density ρ. In the boundary dominated phase the stationary bulk density $\rho_\infty = \alpha$ is determined by the boundary rate and the measures are product. They are independent of the initial density ρ, which is also true in the maximum current phase with $\rho_\infty = 1/2$, whereas in the bulk dominated phase ρ_∞ is equal to the initial density ρ. Note that in contrast to systems with two boundaries the bulk extends to infinity in the semi-infinite context. The bulk dominated measures are determined by the density of the bulk, whereas the maximum current phase is a result of the bulk dynamics. This information can also be obtained on a hydrodynamic level by analyzing the motion and stability of shocks as was explained in Section 2.2.3.

So far, the measures were only characterized asymptotically. In the following we derive exact expressions for arbitrary correlation functions of the stationary measure using the matrix product ansatz (MPA), which is shortly explained in Section 2.2.2. Although a direct application to infinite lattices is not possible, one can make the ansatz

$$W\big(\eta(1),\dots,\eta(L)\big) = \big\langle w\big| \prod_{x=1}^{L} \eta(x)\, D + (1-\eta(x))\, E \big|v\big\rangle \tag{3.3}$$

for the weight of all finite cylinder configurations of length $L \in \mathbb{Z}^+$ (cf. [35]). With these weights one can calculate any finite correlation function of the measure, which is thus uniquely determined. The normalization for the above weights depends on L and is given by $Z(L) = \langle w|(D+E)^L|v\rangle$.

Theorem 3.2 *Let the matrices D, E and the vectors $\langle w|$ and $|v\rangle$ fulfill the algebraic relations*

$$\begin{aligned} &a) \quad DE = c\,(D+E) \\ &b) \quad \alpha\langle w|E = c\langle w| \\ &c) \quad (D+E)|v\rangle = |v\rangle\ . \end{aligned} \tag{3.4}$$

Then the measure μ_c^α defined by the above weights (3.3) is stationary for the process (3.2) with boundary rate α if and only if

$$\alpha < 1/2\,,\ c \le \alpha(1-\alpha) \quad \textit{or} \quad \alpha \ge 1/2\,,\ c \in [0, 1/4]\ . \tag{3.5}$$

The normalization is $Z(L) = \langle w|v\rangle = 1$ for all $L \in \mathbb{Z}^+$ and the parameter c determines the stationary current, i.e.

$$j = \big\langle \eta(x)\big(1-\eta(x+1)\big)\big\rangle_{\mu_c^\alpha} = c \quad \textit{for all } x \in \Lambda\ . \tag{3.6}$$

For $c = \alpha(1-\alpha)$ the measure is product with constant density α, i.e. $\mu_{\alpha(1-\alpha)}^\alpha = \nu_\alpha$.

Remark. Note that with $\hat{D} = D/c$ and $\hat{E} = E/c$ the algebra (3.4) can be written as $\hat{D}\hat{E} = \hat{D} + \hat{E}$, $\alpha\langle w|\hat{E} = \langle w|$ and $c(\hat{D} + \hat{E})|v\rangle = |v\rangle$. So in fact only the third relation differs from the system with two boundaries, and the parameter c accounts for the freedom in the asymptotic density, which is not fixed in the semi-infinite system. Thus we use the same notation μ_c^α as in Theorem 3.1, where it is clear that c is not a density. The form (3.4) of the algebra is more convenient, since the matching condition (3.4.c) removes the L-dependence from the normalization.

In contrast to finite lattices, where it is obvious that the expressions (3.3) defining the measure are positive (see e.g. [100], Section III.3), this has to be shown in our case. Moreover, it is only this positivity requirement that yields the constraints on the parameters c and α given in (3.5), as can be seen in the following proof.

Proof. Due to (3.4.c) it is obvious that for every L the normalization is given by $Z(L) = \langle w|(D+E)^L|v\rangle = \langle w|v\rangle$ which can be chosen to 1 by scaling the vectors $\langle w|$ and $|v\rangle$ appropriately. Using (3.4.a) the stationary current (3.6) calculated at some bond $(x, x+1)$ is given by

$$j = \big\langle w\big|(D+E)^{x-1}DE\big|v\big\rangle = c\,\big\langle w\big|(D+E)^{x}\big|v\big\rangle = c\,. \tag{3.7}$$

It is easy to see that there is a one-dimensional representation of (3.4) with matrices $D = \alpha$ and $E = 1-\alpha$ if and only if $c = \alpha(1-\alpha)$. In this case the measure is product with density $\big\langle w\big|(D+E)^{x-1}D\big|v\big\rangle = \alpha$ for all $x \in \mathbb{Z}^+$.

Next we show that with (3.4) the stationarity condition for the process (3.2) is fulfilled, i.e. $\big\langle \mathcal{L}f\big\rangle_{\mu_c^\alpha} = 0$ for any continuous cylinder function $f \in C_0(X, \mathbb{R})$. The argument is kept rather short, since it follows along standard lines given in [35]. Suppose f concentrates on sites $\{1, \dots, L\}$. Then using (3.2) for the generator and the shorthand $\eta(x) = \eta_x$ for better reading we have after a rearrangement of terms,

$$\begin{aligned}\big\langle \mathcal{L}f\big\rangle_{\mu_c^\alpha} = \sum_{\boldsymbol{\eta}} f(\boldsymbol{\eta}) \Bigg\{ &\sum_{x=1}^{L-1} \Big[(1-\eta_x)\,\eta_{x+1}\,\mu_c^{\alpha,L}(\boldsymbol{\eta}^{x+1\to x}) - \eta_x\,(1-\eta_{x+1})\,\mu_c^{\alpha,L}(\boldsymbol{\eta})\Big] \\ &+\Big[(1-\eta_L)\,\eta_{L+1}\,\mu_c^{\alpha,L+1}\big((\boldsymbol{\eta},\eta_{L+1})^{L+1\to L}\big) - \eta_L\,(1-\eta_{L+1})\,\mu_c^{\alpha,L+1}\big((\boldsymbol{\eta},\eta_{L+1})\big)\Big] \\ &+\alpha\Big[\eta_1\,\mu_c^{\alpha,L}(\boldsymbol{\eta}^{1\to 0}) - (1-\eta_1)\,\mu_c^{\alpha,L}(\boldsymbol{\eta})\Big]\Bigg\}\,,\end{aligned} \tag{3.8}$$

where $\boldsymbol{\eta}$ denotes a configuration on $\{1, \dots, L\}$ and $\mu_c^{\alpha,L}$ the corresponding measure. For the term $x = L$ one site is added to the configurations and the measures with obvious notation. Every configuration can be seen as a finite sequence of empty and occupied blocks. Suppose $\boldsymbol{\eta} = \underbrace{E\dots E}_{\tau_1}\underbrace{D\dots D}_{\tau_2}\dots\underbrace{E\dots E}_{\tau_n}$ consists of n such blocks of lengths τ_i, $i = 1, \dots, n$, starting and ending with an empty block without restriction. We denote a configuration as $\boldsymbol{\tau} = (\tau_i)_{i=1,\dots,n}$ and at the boundary between a full block i and an empty one $i+1$ we can apply the bulk rule (3.4.a) of the algebra to get $\boldsymbol{\tau} = c(\boldsymbol{\tau}^i + \boldsymbol{\tau}^{i+1})$. Here $\boldsymbol{\tau}^i$ results from $\boldsymbol{\tau}$ by deleting one site in block i, and denotes a configuration in $\{0,1\}^{\{1,\dots,L-1\}}$. Noting that

it has non-zero values only at the block boundaries, the sum over x in (3.8) is found to be telescoping,

$$\sum_{\substack{i=1\\ i\ odd}}^{n-2} c\big[\big(\mu_c^{\alpha,L-1}(\boldsymbol{\tau}^i)+\mu_c^{\alpha,L-1}(\boldsymbol{\tau}^{i+1})\big)-\big(\mu_c^{\alpha,L-1}(\boldsymbol{\tau}^{i+1})+\mu_c^{\alpha,L-1}(\boldsymbol{\tau}^{i+2})\big)\big] = \\ = c\,\mu_c^{\alpha,L-1}(\boldsymbol{\tau}^1)-c\,\mu_c^{\alpha,L-1}(\boldsymbol{\tau}^n)\,. \tag{3.9}$$

The remaining terms are exactly canceled by the boundary terms, which is easy to see by applying (3.4.a) and (3.4.c) to the second, and (3.4.b) to the third line of (3.8). If the first or last block of $\boldsymbol{\eta}$ are different, the same argument works analogously. Thus for the sum over $\boldsymbol{\eta}$ in (3.8) every term vanishes individually and it is $\langle \mathcal{L}f\rangle_{\mu_c^\alpha}=0$ for every $f\in C_0(X,\mathbb{R})$.

It remains to show that the expressions are positive. With the rules (3.4) the probability of any cylinder set can be directly transformed into a sum with terms of the form $\langle w|D^k|v\rangle$, $k\in\mathbb{N}$, with positive prefactors. Thus it suffices to show that these terms are positive. They can be calculated by using the recursion

$$\langle w|D^{k+2}|v\rangle = \langle w|D^{k+1}(D+E)|v\rangle-\langle w|D^kDE|v\rangle = \\ = \langle w|D^{k+1}|v\rangle - c\langle w|D^k|v\rangle \tag{3.10}$$

with initial values $\langle w|D^0|v\rangle = 1$ and $\langle w|D|v\rangle = 1-c/\alpha$. The eigenvalues of this linear recursion are given by

$$\lambda_{1,2} = 1/2 \pm \sqrt{1/4-c}\,, \tag{3.11}$$

which are real numbers if and only if $c\in[0,1/4]$. In principle the imaginary part could be non-zero, corresponding to oscillating solutions which then have to become negative, as a consequence of (3.10). But for obtaining a probability measure the solution has to be a monotonic decreasing positive sequence. For $c<1/4$ it is given by

$$\langle w|D^k|v\rangle = \frac{\lambda_1-c/\alpha}{\sqrt{1-4c}}\,\lambda_1^k - \frac{\lambda_2-c/\alpha}{\sqrt{1-4c}}\,\lambda_2^k\,, \tag{3.12}$$

which is positive if and only if the prefactor of $\lambda_1^k>\lambda_2^k$ is positive, i.e. $\alpha\lambda_1-c>0$. Since $c<1/4$ and thus $\lambda_1>1/2$, this is equivalent to

$$\alpha<1/2\,,\ c\le\alpha(1-\alpha) \quad \text{or} \quad \alpha\ge 1/2\,,\ c\in[0,1/4)\,. \tag{3.13}$$

For $c=1/4$ it is $\lambda_1=\lambda_2=1/2$ and the solution to (3.10) is given by

$$\langle w|D^k|v\rangle = \Big(1+\frac{\alpha-1/2}{\alpha}\,k\Big)(1/2)^k\,, \tag{3.14}$$

which is positive if and only if $\alpha\ge 1/2$. Thus in addition to (3.13) the measure is also well defined for $\alpha\ge 1/2$, $c=1/4$. □

3.2.2 Correlation functions and the phase diagram

Using the algebra (3.4) one can find recursion relations to calculate correlation functions. In the following we demonstrate this for the density profile $\rho(x) = \langle \eta(x) \rangle_{\mu_c^\alpha}$ (one-point function) and analyze the asymptotic behavior of the profiles and higher order correlation functions.

Corollary 3.3 *The density profile for $x \geq 2$ of the measure μ_c^α defined in Theorem 3.2 is given by*

$$\rho(x) = c^x \sum_{k=2}^{x} \frac{(k-1)\big(2(x-1)-k\big)!}{(x-1)!\,(x-k)!} \left[\frac{\lambda_1/\lambda_2^k - \lambda_2/\lambda_1^k}{\lambda_1 - \lambda_2} - \Big(\frac{1}{\alpha}\Big)^k \right], \tag{3.15}$$

for $c < 1/4$ and by

$$\rho(x) = (1/4)^x \sum_{k=2}^{x} \frac{(k-1)\big(2(x-1)-k\big)!}{(x-1)!\,(x-k)!} \left[(1+k)\,2^k - \Big(\frac{1}{\alpha}\Big)^k \right]. \tag{3.16}$$

for $c = 1/4$. It is $\rho(1) = 1 - c/\alpha$ and λ_1 and λ_2 are given in (3.11) as eigenvalues of a linear recursion.

Proof. Using (3.4.c) and (3.4.b) we have $\rho(1) = \langle w|D|v\rangle = 1 - c/\alpha$. In general it is $\rho(x+1) = \langle w|C^x D|v\rangle$ and we use the relation

$$C^x D = \sum_{k=1}^{x} \frac{k\,(2x-1-k)!}{x!\,(x-k)!} \sum_{i=0}^{k} E^i\, D^{k+1-i}\, c^{x-k} \tag{3.17}$$

for all $x \in \mathbb{Z}^+$. This can be shown by induction using only the bulk relation (3.4.a), as it is done in [32], relation (A.5). Multiplying with $\langle v|$, $|w\rangle$ and using (3.4.b) we obtain

$$\langle w|C^x D|v\rangle = \sum_{k=1}^{x} \frac{k\,(2x-1-k)!}{x!\,(x-k)!}\, c^{x-k} \Big[Q_{k+1} - \Big(\frac{c}{\alpha}\Big)^{k+1} \Big], \tag{3.18}$$

where $Q_k = \sum_{i=0}^{k} \big(\frac{c}{\alpha}\big)^i \langle w|D^{k-i}|v\rangle$. For the sum Q_k, $k \in \mathbb{Z}^+$ one can derive the same recursion relation as (3.10), so that

$$Q_{k+2} = Q_{k+1} - c\,Q_k\,, \quad \text{with} \quad Q_0 = Q_1 = 1\,. \tag{3.19}$$

The solution is given in terms of the same eigenvalues $\lambda_{1,2} = 1/2 \pm \sqrt{1/4 - c}$ from (3.11) and for $c < 1/4$ we have

$$Q_k = \frac{\lambda_1}{\lambda_1 - \lambda_2}\,\lambda_1^k - \frac{\lambda_2}{\lambda_1 - \lambda_2}\,\lambda_2^k\,. \tag{3.20}$$

Inserting this into (3.18) and using $\lambda_1\lambda_2 = c$ we get (3.15). For $c = 1/4$ and $\lambda_1 = \lambda_2 = 1/2$ the solution is $Q_k = (1+k)(1/2)^k$ leading to (3.16). □

For $x \to \infty$ the density tends to a constant value ρ_∞ with the asymptotic behavior

$$\rho(x) \simeq \rho_\infty + B(\alpha, c)\, x^{-\beta} \exp[-x/\xi] \,, \tag{3.21}$$

for some constant $B(\alpha, c) \in \mathbb{R}$. The correlation length $\xi \in (0, \infty]$ may be infinite and characterizes the exponential part of the decay of $\rho(x) - \rho_\infty$. For long range correlations, i.e. $\xi = \infty$, the approach to the asymptotic bulk density ρ_∞ is given by a pure power law with exponent $\beta \in \mathbb{R}$. The values of these parameters depend on α and c and can be computed using the asymptotic form for $x \to \infty$ of the sum

$$\begin{aligned} \sum_{k=2}^{x+1} \frac{(k-1)\,(2x-k)!}{x!\,(x+1-k)!}\,(1/z)^k &\simeq \frac{1}{\sqrt{\pi}\,(2z-1)^2}\,\frac{4^x}{x^{3/2}} && \text{for } z > 1/2 \\ &\simeq \frac{2}{\sqrt{\pi}}\,\frac{4^x}{x^{1/2}} && \text{for } z = 1/2 \\ &\simeq (1-2z)\Big(\frac{1}{z(1-z)}\Big)^{x+1} && \text{for } z < 1/2 \,. \end{aligned} \tag{3.22}$$

These relations can be found in [100], Lemma III.3.2.4 and were first given in [32]. Using $\lambda_1 \geq 1/2$ and $\lambda_2 \leq 1/2$ one can determine the parameter values in (3.21) as a function of α and c. The bulk density is given by

$$\rho_\infty = \begin{cases} \alpha & , \text{ for } c = \alpha(1-\alpha) \\ \lambda_1 = 1/2 + \sqrt{1/4 - c} & , \text{ for all other parameter values of (3.5)} \,. \end{cases} \tag{3.23}$$

The values for ξ and β are summarized in the phase diagram in Figure 3.1 (top), which shows all stationary measures characterized by α and ρ_∞. The results are compatible with Theorem 3.1. and of course closely related to the phase diagram of the ASEP with two boundaries, given in Section 2.2.2. There one has a unique stationary measure which depends on the two boundary variables α and β, while here we only have one boundary and the set of existing stationary measures is indexed by the asymptotic bulk density ρ_∞. Note that for $\rho_\infty = \alpha$ (red) the measure is product everywhere and thus the density profiles are flat. For the bulk dominated measures (blue) with $\rho_\infty > \alpha$ the profiles are increasing, i.e. $B(\alpha, c) < 0$, and decreasing for $\rho_\infty < \alpha$. The current is always given by $c = \rho_\infty(1 - \rho_\infty)$, indicating that the measures are asymptotically product, which is proved below. We also show the corresponding phase diagram where the measures are indexed by the current $j = c$ in Figure 3.1 (bottom left), since it is the original parameter in Theorem 3.2.

Using the recursion (3.10), higher order correlation functions can be easily calculated as a function of the density. This is only interesting away from the line of product measures where $\rho_\infty = \lambda_1$ and leads to

$$\big\langle \eta(x) \dots \eta(x+k) \big\rangle_{\mu_c^\alpha} - \rho_\infty^{k+1} = \begin{cases} \frac{\rho(x) - \rho_\infty}{2\rho_\infty - 1} \left(\rho_\infty^{k+1} - (1-\rho_\infty)^{k+1} \right) & , \text{ for } j < 1/4 \\ \big(2\rho(x) - 1\big)\, k (1/2)^{k+1} & , \text{ for } j = 1/4 \,. \end{cases} \tag{3.24}$$

So all truncated correlation functions with fixed k vanish for $x \to \infty$ with the same asymptotic behavior as the density profile $\rho(x)$, and the measures are asymptotically product. Thus

$$\mu_c^\alpha \simeq \nu_{\rho_\infty} \quad \text{for } x \to \infty \,, \tag{3.25}$$

with ρ_∞ defined in (3.23), recovering the result of Theorem 3.1.

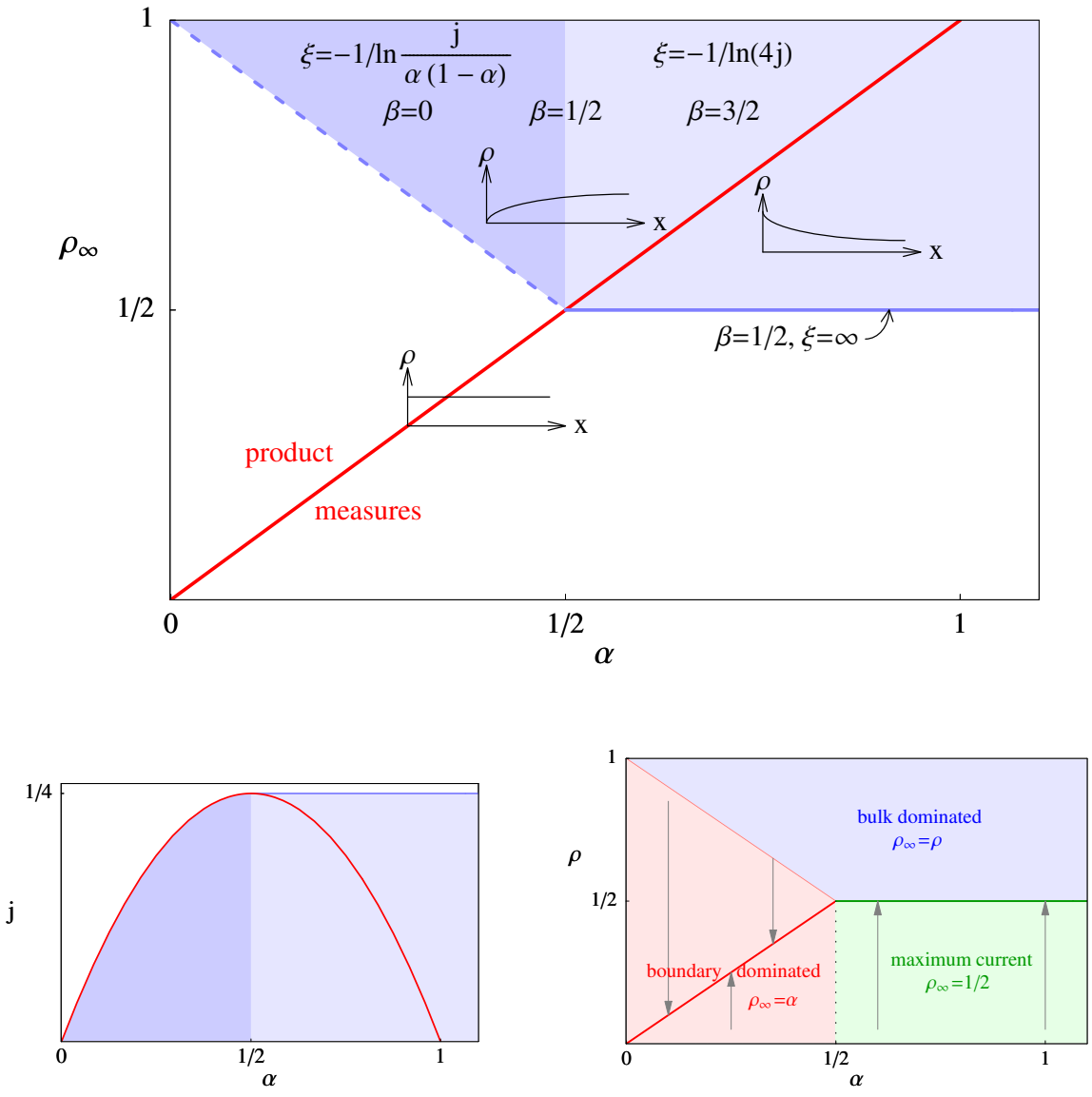


Figure 3.1: Phase diagram for the semi-infinite ASEP. **Top:** The set of stationary measures is given by the blue region and along the red line of product measures as a function of the boundary rate α and the bulk density ρ_∞. Values of the exponent β and the correlation length ξ (3.21) are given in the various regions. **Bottom left:** Corresponding phase diagram in terms of the current $j = \rho_\infty(1-\rho_\infty)$. **Bottom right:** Ergodic behavior according to Theorem 3.1, giving the stationary bulk density ρ_∞ as a function of α and initial density ρ.

3.3 Generalized boundary mechanisms

Following the exact solution of the semi-infinite TASEP with a simple reservoir boundary, we now analyze the effect of a generalized boundary mechanism. For that purpose we consider a toy model with a slightly more complicated injection mechanism, which serves as an example throughout this section. Its generator is

$$\begin{aligned}\mathcal{L}f(\boldsymbol{\eta}) = &\sum_{x=1}^{\infty} \eta(x)\big(1-\eta(x+1)\big)\big[f(\boldsymbol{\eta}^{x\to x+1}) - f(\boldsymbol{\eta})\big] \\ &+\big(1-\eta(1)\big)\big[\alpha_1\eta(2) + \alpha_2\big(1-\eta(2)\big)\big]\big[f(\boldsymbol{\eta}^{0\to 1}) - f(\boldsymbol{\eta})\big]\ ,\end{aligned} \tag{3.26}$$

so the entrance rate of particles at site one depends also on the occupation of site two, namely it is α_1 if site two is occupied and α_2 if it is empty.

3.3.1 Matrix product ansatz for the toy model

The most direct way to see the effect of the above boundary mechanism on the stationary measure would of course be an exact computation. As shown in [85], the stationary measures of any lattice gas with finite range interactions can be written in matrix product form. Moreover, specific rules are given how to construct the algebra relations from the generator. But of course the larger the interaction range, the more complicated are the algebraic rules. Besides the matrices E and D, these relations contain 4 new unknown operators X_{00}, X_{01}, X_{10} and X_{11} in our case, as a result of the next nearest neighbor interaction at the boundary. Following [85], the relations for the boundary are given by

$$\begin{aligned} \alpha_2\langle w|EE &= -\langle w|X_{10} & \alpha_1\langle w|ED &= -\langle w|X_{11} \\ \alpha_2\langle w|EE &= \langle w|X_{00} & \alpha_1\langle w|ED &= \langle w|X_{01} \end{aligned} \tag{3.27}$$

The new operators arising from the boundary interactions also change the bulk relations,

$$\begin{aligned} DEE &= X_{01}E - EX_{10} & DED &= X_{01}D - EX_{11} \\ DEE &= DX_{00} - X_{10}E & DED &= DX_{01} - X_{10}D \end{aligned}$$

$$X_{00}E = EX_{00}\ , \quad X_{11}D = DX_{11}\ , \quad X_{00}D = EX_{01}\ , \quad X_{11}E = DX_{10}\ . \tag{3.28}$$

This demonstrates that a priori the effects of the boundary mechanism might also effect the bulk dynamics. For the original system there were only two unknown operators, which one could choose to be real numbers, $X_0 = -X_1 = c$ (cf. Section 3.2 and [32]). Here the boundary relations (3.27) suggest $X_{00} + X_{10} = 0$ and $X_{11} + X_{01} = 0$, and moreover $X_{01} + X_{00} = c(D+E)$ from (3.28) by comparison with (3.4). Under these assumptions the relation at the right boundary is given, as in (3.4), by $(D+E)|v\rangle = |v\rangle$. To use these matrix relations for a solution a representation of X_{00} and X_{01} at least in terms of E and D is needed, which we could not identify. Simple choices like linear combinations led to contradictions when the algebraic rules were applied in different order.

There have been several systematic approaches (see e.g. [73, 111] or [5, 6]) concerning the classification and representations of quadratic algebras, as they arise for nearest neighbor

interactions. But the above algebra contains a product of three operators and the methods that have been used so far to find representations for such algebras are more improvised rather than systematic [85] and work only if the boundary rates are bulk compatible, i.e. for coupling to a reservoir. In particular, so far there has been no exact solution with the MPA for a system with a lattice inhomogeneity similar to our case. Some deeper systematic understanding of the algebra structure analogous to the quadratic case seems to be necessary. This is of course an intricate problem, but out of scope for this thesis since the MPA is only used as a tool to determine stationary measures, which is the main interest here. To achieve this, we pursue a different strategy in the following, which gives less complete results but in a much more general context.

3.3.2 Product measures and the effective density

In this section we consider the ASEP with partial asymmetry on $\Lambda = \mathbb{Z}^+$ and show that for any boundary mechanism with a finite range there exists a stationary measure, which is product outside the boundary range. The density of this measure provides a properly defined effective boundary density ρ_{eff}. In general the existence of such measures is restricted to systems which have nearest neighbor hopping and stationary product measures in the bulk. We discuss this point and a possible alternative definition for other models in Sections 3.4.2 and 3.5.

In the partially asymmetric simple exclusion process particles jump to the right with rate p and to the left with rate q (cf. (2.35)). To fix ideas and avoid lengthy distinctions of cases we take $p > q$ for the rest of this section. The results can be used directly for the case $p < q$ with a particle-hole transformation $\eta(x) \to 1 - \eta(x)$. The bulk part of the generator of the ASEP is given in (2.36) and the boundary mechanism should be of finite range $R \in \mathbb{Z}^+$, where

$$\boldsymbol{\eta} = \big(\eta(1), \dots, \eta(R)\big) \longrightarrow \boldsymbol{\eta}' = \big(\eta'(1), \dots, \eta'(R)\big) \quad \text{with rate } d_{\boldsymbol{\eta},\boldsymbol{\eta}'} \,. \tag{3.29}$$

Note that all possible transitions are allowed, for example also simultaneous movement of particles. On top of that, particles in $\{1, \dots, R\}$ are subject to the bulk dynamics. In this description, the toy model (3.26) corresponds to $R = 2$ with $d_{(0,1),(1,1)} = \alpha_1$, $d_{(0,0),(1,0)} = \alpha_2$ and $d_{\boldsymbol{\eta},\boldsymbol{\eta}'} = 0$ otherwise.

Now consider the same process restricted to the boundary range $\Lambda_R = \{1, \dots, R\}$, coupled to a reservoir with density $\rho_r \in [0, 1]$ at the right boundary. The boundary part of the generator for this finite process is thus given by

$$\begin{aligned} \mathcal{L}_b f(\boldsymbol{\eta}) = &\sum_{\boldsymbol{\eta}'} d_{\boldsymbol{\eta},\boldsymbol{\eta}'} \big[f(\boldsymbol{\eta}') - f(\boldsymbol{\eta})\big] + \\ &\big[p\,\eta(R)(1-\rho_r) + q\,\big(1-\eta(R)\big)\rho_r\big]\big[f(\boldsymbol{\eta}^{R\leftrightarrow R+1}) - f(\boldsymbol{\eta})\big] \,. \end{aligned} \tag{3.30}$$

Due to the finite state space the process has a unique stationary measure $\mu_{\rho_r}^{d_{\boldsymbol{\eta},\boldsymbol{\eta}'}}$ for every $\rho_r \in [0, 1]$. In the following we fix the left boundary mechanism $d_{\boldsymbol{\eta},\boldsymbol{\eta}'}$ and denote the measure by μ_{ρ_r}. We consider the density at site R as a function of ρ_r, writing simply

$$\rho(\rho_r) = \big\langle \eta(R) \big\rangle_{\mu_{\rho_r}} \,. \tag{3.31}$$

The boundary rates $d_{\boldsymbol{\eta},\boldsymbol{\eta}'}$ should be non-degenerate such that the process on Λ_R is irreducible for every $\rho_r \in [0,1]$, to guarantee uniqueness of the measure. Possible problems can arise through absorbing states for $\rho_r \in \{0,1\}$ and total asymmetry, but these cases can be identified and treated easily for specific systems (cf. the example in the next subsection), so we exclude them from the general considerations.

Theorem 3.4 *If there exists a fixed point $\rho^* = \rho(\rho^*) \in [0,1]$ of (3.31), the process on $\Lambda = \mathbb{Z}^+$ has a stationary measure which is of product form with density ρ^* for all $x \geq R$. For every non-degenerate boundary mechanism, there exist at least one and at most two such fixed points. In the second case one of them is $\rho^* = 1$ ($\rho^* = 0$ for $p < q$) and corresponds to fully occupied configurations with zero current.*

This suggests the following definition of the effective boundary density, which we also formulate for negative drift.

Definition. For every non-degenerate boundary mechanism $d_{\boldsymbol{\eta},\boldsymbol{\eta}'}$ we define the *effective boundary density* ρ_{eff} to be the unique fixed point $\rho^* \in (0,1)$ of Theorem 3.4. If the latter does not exist it is $\rho_{\mathit{eff}} = 0, 1$ depending on the drift, i.e.

$$\rho_{\mathit{eff}} = \begin{cases} \rho^* \ , \text{ if } \rho^* = \rho(\rho^*) \in (0,1) \text{ exists,} \\ 1 \\ 0 \end{cases} \ , \text{ otherwise if } \begin{matrix} p > q \\ p < q \end{matrix} . \tag{3.32}$$

Remark. Note that this is not only an abstract definition of ρ_{eff}, but gives also the recipe to compute it explicitly. Since the state space $X_R = \{0,1\}^{\{1,\dots,R\}}$ of the model used for its definition is finite, $|X_R| = 2^R$, the stationarity relations can be solved explicitly. The complexity of this calculation depends of course on the range R of the boundary mechanism, but for small R this is straightforward, as is illustrated in the next subsection.

Proof of Theorem 3.4. Let μ_{ρ^*} be a stationary measure with $\rho(\rho^*) = \rho^*$ of the finite process. We extend this measure to $\mathbb{Z}^+$ in the following sense. Let $\boldsymbol{\eta}_{x_1,\dots,x_k} = \big(\eta(x_1),\dots,\eta(x_k)\big)$ be any cylinder configuration based on sites $x_1,\dots,x_k \in \mathbb{Z}^+$ with $x_1,\dots,x_l \leq R$ and $x_{l+1},\dots,x_k > R$ for some $l \in \{0,\dots,k\}$. Then we define

$$\mu\big(\boldsymbol{\eta}_{x_1,\dots,x_k}\big) = \mu_{\rho^*}\big(\boldsymbol{\eta}_{x_1,\dots,x_l}\big) \prod_{i=l+1}^{k} \nu^1_{\rho^*}\big(\eta(x_i)\big) \ . \tag{3.33}$$

Since ν_{ρ^*} is stationary for the bulk dynamics of the process and $\rho(\rho^*) = \rho^*$ with matching current $j = (p-q)\rho^*(1-\rho^*)$, it is evident that this product continuation of μ_{ρ^*} is stationary for the process on $\mathbb{Z}^+$.

Fix some non-degenerate boundary rates $d_{\boldsymbol{\eta},\boldsymbol{\eta}'}$. For the process on Λ_R, the stationary current as a function of ρ_r is given by

$$j(\rho_r) = p\,\rho(\rho_r)\big(1-\rho_r\big) - q\,\big(1-\rho(\rho_r)\big)\,\rho_r \ . \tag{3.34}$$

Note that although $p > q$, the current of the finite system on Λ_R can still be negative as an effect of the left boundary mechanism, spanning the whole system. In case of a fixed point $\rho_r = \rho^*$, (3.34) reduces to the current density relation for the ASEP given in (2.40), $j^*(\rho^*) = (p-q)\rho^*(1-\rho^*) \geq 0$. Thus fixed points are characterized by the intersection points of j and j^*. With (3.34) we have

$$j(0) = p\,\rho(0) > 0 = j^*(0) \quad \text{and} \quad j(1) = -q\,\big(1-\rho(1)\big) \leq 0 = j^*(1)\,, \tag{3.35}$$

where positivity of $j(0)$ is ensured, since the boundary is supposed to be non-degenerate. Since $j(\rho_r)$ is continuous for a finite system, there is at least on fixed point $\rho^* \in (0,1]$.

Now we assume that there are two fixed points $\rho^* \neq \rho^{**} \in (0,1)$ for some boundary rates $d_{\boldsymbol{\eta},\boldsymbol{\eta}'}$. Then one can construct a corresponding mechanism for the right boundary with the same effective densities by using that the bulk dynamics is particle hole symmetric under space inversion. Consider the process with these boundary mechanisms on a finite lattice Λ_L with $L > 2R$. Due to non-degeneracy of $d_{\boldsymbol{\eta},\boldsymbol{\eta}'}$ it is irreducible and has a unique stationary measure. This is in contradiction to $\rho^* \neq \rho^{**}$, yielding two different stationary measures. □

At this point the reader might have a look at Figure 3.3 where the fixed point relations for the toy model (3.26) are plotted, illustrating the arguments in the proof and the discussion below. For partial asymmetry in the bulk with $p > q > 0$ and for the boundary mechanism it is $\rho(1) < 1$ and with (3.35) we have $\rho_{\mathit{eff}} \in (0,1)$. The extreme values $\rho_{\mathit{eff}} \in \{0,1\}$ only occur in the case of total asymmetry of the boundary rates $d_{\boldsymbol{\eta},\boldsymbol{\eta}'}$ or the bulk rates or in case of other degeneracies as a result of zero rates. This leads to the question if models with totally asymmetric bulk or boundary rates can have effective boundary densities $\rho_{\mathit{eff}} \in (0,1)$. The answer is part of the next proposition that specifies the range of the effective densities under variation of the boundary rates.

Proposition 3.5 *Consider a fixed collection of allowed transitions in the boundary region Λ_R, denoted by the set of pairs $B = \{(\boldsymbol{\eta},\boldsymbol{\eta}')\}$. So $\rho_{\mathit{eff}} : [0,\infty)^{|B|} \to [0,1]$ as defined in (3.32) can be regarded as a function of the corresponding rates $\big(d_{\boldsymbol{\eta},\boldsymbol{\eta}'}\big)_{(\boldsymbol{\eta},\boldsymbol{\eta}')\in B}$ and we take $\rho_{\mathit{eff}}{}^* = \sup \rho_{\mathit{eff}}$ to be the supremum on $[0,\infty)^{|B|}$. Then for every $\rho \in [0, \rho_{\mathit{eff}}{}^*)$ there exists a set of rates $\big(d_{\boldsymbol{\eta},\boldsymbol{\eta}'}\big)_{(\boldsymbol{\eta},\boldsymbol{\eta}')\in B}$ such that $\rho_{\mathit{eff}} = \rho$. If the set B is non-degenerate, in the sense that particles should be allowed to enter the system, we have $\rho_{\mathit{eff}}{}^* > 0$.*

Remark. In particular this ensures the existence of non-degenerate effective densities for every boundary mechanism as long as particles are allowed to enter the system, which is of course a minimal requirement. In fact, for most 'reasonable' systems the boundary mechanism has full range, i.e. $\rho_{\mathit{eff}}{}^* = 1$. But there are also counterexamples, for instance in [63] where part of the generic phase diagram is not accessible due to degeneracies in the deterministic bulk dynamics. An analogous result can be formulated if the allowed rates only vary on a connected subset of $[0,\infty)^{|B|}$ with non-zero volume.

Proof. We keep the notation of the proof of Theorem 3.4. The key point is that due to the finite system size $j(\rho_r)$ and $\rho(\rho_r)$ and thus also ρ_{eff} as defined in (3.32) are continuous functions of ρ_r and the boundary rates $\big(d_{\boldsymbol{\eta},\boldsymbol{\eta}'}\big)_{(\boldsymbol{\eta},\boldsymbol{\eta}')\in B}$. If those vanish altogether it is clearly

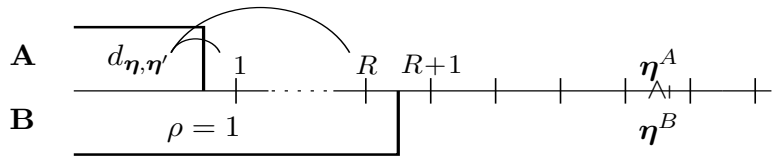


Figure 3.2: The coupling used in the proof of Proposition 3.6.

$j(\rho_r) = 0$ for all $\rho_r \in [0,1]$ and also $\rho_{\mathit{eff}} = 0$. If particle injection is allowed, take the rate d_i for this process positive (but small) and all other rates equal to zero. Then we have $j(0) > 0 = j^*(0)$ but if d_i is small enough, the maximum of the current j (a continuous function of d_i) is still smaller than the maximum of the fixed point current j^*. The latter depends only on the bulk rates p and q and is given by $(p-q)/4$ at $\rho_r = 1/2$. So there has to be a fixed point in $(0, 1/2)$ and thus ${\rho_{\mathit{eff}}}^* > 0$. The existence of intermediate fixed points $\rho_{\mathit{eff}} \in (0, {\rho_{\mathit{eff}}}^*)$ follows by continuity of ρ_{eff} as a function of the boundary rates. □

3.3.3 The bulk dominated phase

So far we only showed that there exist measures which are product outside the range of the boundary mechanism, i.e. we identified a set of product measures which is equivalent to the red line in Figure 3.1 (top). We still have to show the existence of the bulk dominated measures (blue region in Figure 3.1) for $\rho_{\mathit{eff}} > 1/2$ and that in this case the boundary can still be described by an effective density. Heuristically this is clear, since in this phase the characteristic velocity of the bulk given by $j'(\rho)$ is negative and therefore the boundary mechanism causes only perturbations which decay for $x \to \infty$. But in contrast to the boundary dominated phase, we expect that the effect of generalized boundary mechanisms is not restricted to a finite region and that the effective description of the boundary can only be valid asymptotically.

Proposition 3.6 *For every boundary mechanism $d_{\eta,\eta'}$ and all $\rho \in [1/2, 1]$ there exists a stationary measure $\mu^{d_{\eta,\eta'}}$ of the semi-infinite ASEP which is asymptotically dominated from above by the product measure ν_ρ.*

Proof. The proof uses the coupling method explained in the Appendix A.3. The process of interest with generalized boundary rates $d_{\eta,\eta'}$ of range R on the lattice $\Lambda = \mathbb{Z}^+$ is called process A in the following. We couple it with process B, the usual semi-infinite ASEP as defined in (3.2) with left boundary reservoir of density 1, defined on the lattice $\mathbb{Z}^+ \backslash \Lambda_R = \{R+1, R+2, \ldots\}$. Its generator is given by

$$\begin{aligned}\mathcal{L}f(\boldsymbol{\eta}) = \sum_{x=R+1}^{\infty} &\left[p\,\eta(x)\big(1-\eta(x+1)\big) + q\,\big(1-\eta(x)\big)\,\eta(x)\right]\left[f(\boldsymbol{\eta}^{x\leftrightarrow x+1}) - f(\boldsymbol{\eta})\right] \\ &+p\,\big(1-\eta(R+1)\big)\left[f(\boldsymbol{\eta}^{R\to R+1}) - f(\boldsymbol{\eta})\right]. \end{aligned} \tag{3.36}$$

We know from Theorem 3.1 that this process has stationary measures $\mu^1_\rho \simeq \nu_\rho$, which are asymptotic product measures with densities $\rho \in [1/2, 1]$. We use the basic coupling for

which the bulk jump rates are given in (A.5) in Appendix A.3. The boundary of the coupled process is given by the bond $(R, R+1)$, where we have the rates

$$\begin{array}{cccccccccc} A & 1\,0 & \xrightarrow{p} & 0\,1 & \times 1 & \xrightarrow{p} & \times 1 & 0\,0 & \xrightarrow{p} & 0\,0 \\ B & \times & & 1 & 0 & & 1 & 0 & & 1 \end{array} \qquad \begin{array}{cccccc} 0\,1 & \xrightarrow{q} & 1\,0 \\ \times & & \times \end{array} . \tag{3.37}$$

In each case the wildcard $\times$ can be either 0 or 1 without changing the corresponding rate. In the region $\{1, \dots, R\}$ the process A evolves according to its definition independent of process B. This situation is illustrated in Figure 3.2. From (3.37) it is clear that both marginal processes are Markovian with the same jump rates as process A and B respectively. It is also obvious that only discrepancies of the type $\begin{smallmatrix}0\\1\end{smallmatrix}$ can be created at the boundary. Take the initial measure π for the coupled process to have the marginal $\pi_B = \mu_\rho^1$, which is stationary for the B process for some $\rho \in [1/2, 1]$, and $\pi_A \leq \pi_B$ on $x > R$. Thus the configuration of the A process is dominated by $\boldsymbol{\eta}_t^A \leq \boldsymbol{\eta}_t^B$ on $\mathbb{Z}^+ \backslash \Lambda_R$ for all times $t \geq 0$ and the stationary measure of the coupled process concentrates on such configurations. With Theorem A.4 there exists a stationary measure of process A with $\mu^{d_{\boldsymbol{\eta},\boldsymbol{\eta}'}} \leq \mu_\rho^1$ on $x > R$. The statement of the theorem follows, since $\mu_\rho^1 \simeq \nu_\rho$ for $x \to \infty$ with Theorem 3.1. □

This is general statement ensures the existence of at least one stationary measure which is dominated by $\nu_{1/2}$, independent of the boundary rates $d_{\boldsymbol{\eta},\boldsymbol{\eta}'}$. Dominating the measures from below in a suitable range of ρ_{eff} would show that they are asymptotically product and exist for every density in that range. Thus one would have to prove the following conjecture.

Conjecture. *For every $\rho \in (1 - \rho_{\mathit{eff}}, 1]$ there exists a stationary measure which is asymptotically dominated from below by a product measure ν_ρ.*

We are not able to prove this in general, but one can try to show this for specific systems using coupling arguments similar to the one above. This is done below for the toy model (3.26) in Proposition 3.7. Another strategy might be to show a law of large numbers for the time evolution of initial shock measures as it was done for translation invariant systems (see [100], Section III.2 and references therein).

3.4 Applications

3.4.1 The toy model

For the toy model defined in (3.26) the range of the boundary dynamics is $R = 2$ and we have total asymmetry $p = 1$, $q = 0$. On the finite lattice $\Lambda = \{1, 2\}$ coupled to a right reservoir of density ρ_r one has to solve the following $2^R = 4$ relations, resulting from the stationarity condition $\langle \mathcal{L} f \rangle_{\mu_{\rho_r}} = 0$ and the normalization,

$$\begin{aligned} \mu_{\rho_r}(0,0)\,\alpha_2 &= \mu_{\rho_r}(0,1)\,(1-\rho_r) \\ \mu_{\rho_r}(1,0) &= \mu_{\rho_r}(0,0)\,\alpha_2 + \mu_{\rho_r}(1,1)(1-\rho_r) \\ \mu_{\rho_r}(1,1)\,(1-\rho_r) &= \mu_{\rho_r}(0,1)\,\alpha_1 \\ 1 &= \mu_{\rho_r}(0,0) + \mu_{\rho_r}(1,0) + \mu_{\rho_r}(0,1) + \mu_{\rho_r}(1,1)\,. \end{aligned} \tag{3.38}$$

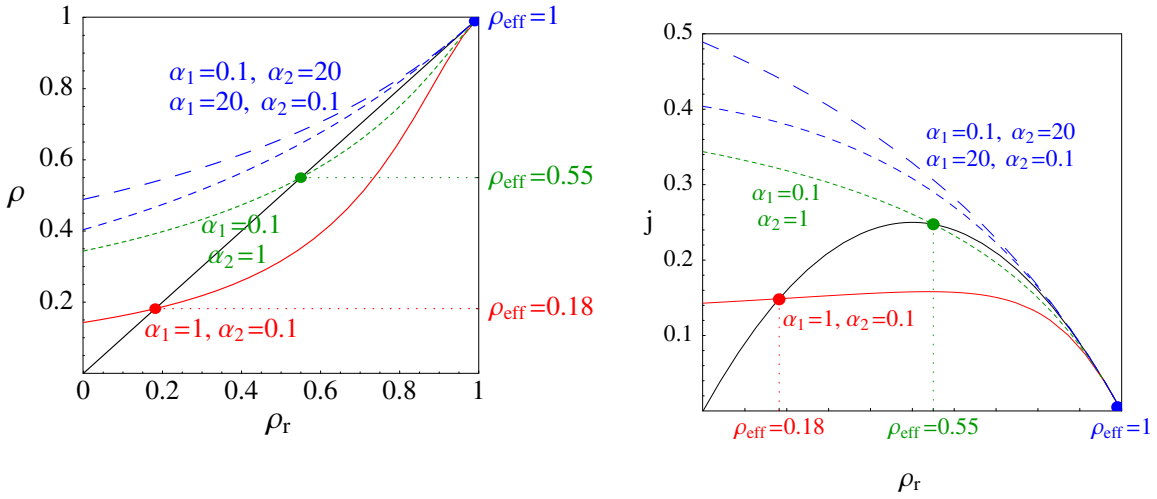


Figure 3.3: Fixed point relation for the toy model. **Left:** $\rho(\rho_r)$ as given in (3.31) for several values of α_1 and α_2. **Right:** Corresponding relation for the stationary current (3.34), as used in the proof of Theorem 3.4.

A straightforward calculation leads to

$$\rho_2(\rho_r) = \mu_{\rho_r}(0,1) + \mu_{\rho_r}(1,1) = \frac{\alpha_2(1+\alpha_1-\rho_r)}{(1-\rho_r)^2 + \alpha_2(1+\alpha_1-\rho_r)(2-\rho_r)} \,. \tag{3.39}$$

The effective boundary density is determined by the fixed points of this equation,

$$\rho_{\mathit{eff}} = \begin{cases} (1+\alpha_1)\,\alpha_2/(1+\alpha_2) & , \text{ for } \alpha_1\alpha_2 < 1 \\ 1 & , \text{ for } \alpha_1\alpha_2 \geq 1 \end{cases} . \tag{3.40}$$

This is illustrated in Figure 3.3 (left), where the fixed point relation (3.39) and the effective densities are plotted for several values of α_1 and α_2. The fixed points correspond to intersections of the current $j(\rho_r) = \rho_2(\rho_r)(1-\rho_r)$ with $j^* = \rho_r(1-\rho_r)$, which are both plotted in Figure 3.3 (right) to illustrate the argument in the proof of Theorem 3.4. Due to the total asymmetry of the model, $j(\rho_r)$ is nonnegative and the fixed point $\rho(1) = 1$ exists for any α_1, α_2 corresponding to the fully occupied configuration as an absorbing state. Non-degenerate fixed points only exist for $\alpha_1\alpha_2 < 1$.

For $\alpha_1 = \alpha_2 = \alpha$ we have $\rho_{\mathit{eff}} = \alpha \wedge 1$, with $\wedge$ denoting the miminum, so (3.40) is of course compatible with the results of Section 3.2. Another special case is $\alpha_2 = 0$, for which the empty configuration is an absorbing state independent of α_1 and ρ_r, which is due to the total asymmetry of the bulk. As soon as the first two lattice sites are empty, which happens with probability one during time evolution, no particle can enter the system any more. Thus the system is degenerate in the sense of Section 3.3.2 and for every α_1 there are two absorbing states with density 0 and 1.

For $\alpha_1 = 0$ the situation is different. We have $\rho_{\mathit{eff}} = \alpha_2/(1+\alpha_2) < 1$ and the system can be solved exactly on the lattice $\mathbb{Z}^+$. Whenever a particle enters site 1 with rate α_2, site 2

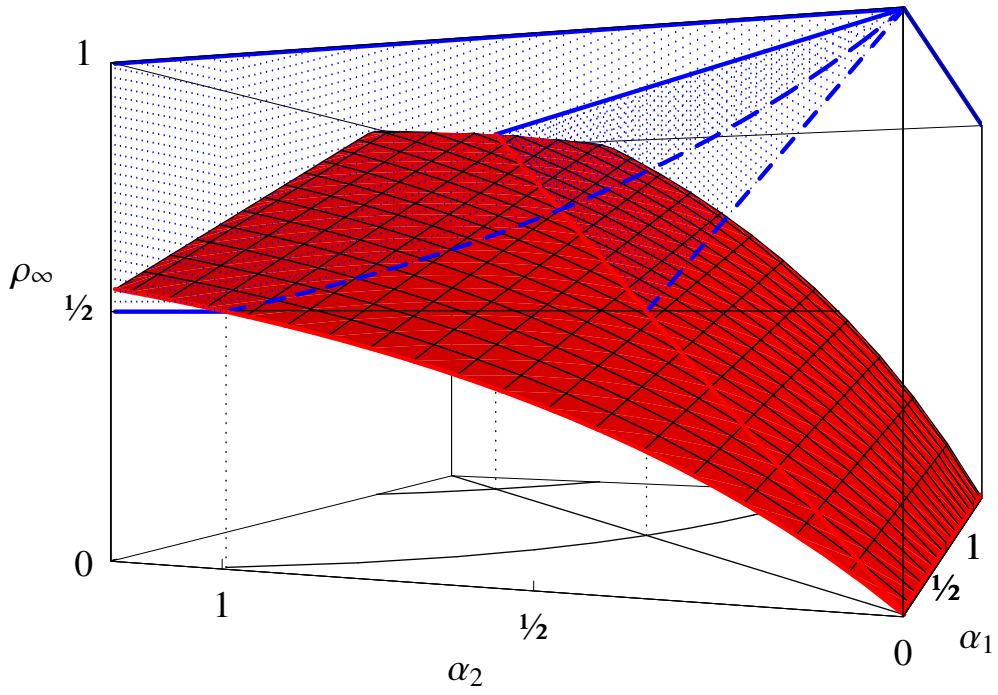


Figure 3.4: Exactly known stationary measures of the toy model, characterized by the bulk density ρ_∞. The red surface represents the measures which are product for $x \geq 2$ with density $\rho_{\mathit{eff}} = (1+\alpha_1)\alpha_2/(1+\alpha_2)$. The model is exactly solvable for $\alpha_1 = 0$, $\alpha_2 = 0$ and $\alpha_1 = \alpha_2$ and the corresponding bulk dominated measures are shown in blue.

is empty and it jumps there with rate 1 independent of the system configuration on the rest of $\mathbb{Z}^+$. So the arrival process of particles at site 2 is independent and Poisson with effective rate $(1/\alpha_2 + 1/1)^{-1} = \alpha_2/(1+\alpha_2)$. In this case the toy model is equivalent to an effective model on $\Lambda = \{2, 3, \ldots\}$ with boundary density ρ_{eff} even on the level of the dynamics. In particular this implies of course that all stationary measures are exactly identical to the ones computed in Section 3.2 in terms of the effective rate. This can be seen in the $\alpha_1 = 0$ plane in Figure 3.4, where we plot all stationary measures that are known exactly in the phase diagram of the toy model.

To show existence of other bulk dominated measures with asymptotic density ρ_∞ we have to find measures asymptotically equal to ν_{ρ_∞} that dominate the process from below, since domination from above is given by Proposition 3.6. This can be done by coupling the general process to one of the exactly solvable cases mentioned above. This is enough in order to obtain all expected measures at least for $\alpha_1 \wedge \alpha_2 \geq 1/2$.

Proposition 3.7 *For $\alpha_1 \neq \alpha_2$ the process (3.26) has stationary measures which are asymptotic product with densities*

$$\rho_\infty \geq 1/2 \quad \textit{if } \alpha_1 \wedge \alpha_2 \geq 1/2 \quad \textit{and} \quad \rho_\infty > 1 - \alpha_1 \wedge \alpha_2 \quad \textit{if } \alpha_1 \wedge \alpha_2 < 1/2. \tag{3.41}$$

Proof. We couple the process A with boundary rates α_1, α_2 to process B with simple boundary rate $\alpha_1 \wedge \alpha_2$, which was solved exactly in Section 3.2. For the basic coupling the bulk rates are given in (A.5) and for $\alpha_2 > \alpha_1$ the boundary rates at sites $x = 1, 2$ are

$$\begin{array}{llll} A & 0\,0 \overset{\alpha_1}{\longrightarrow} 1\,0 & 0\,0 \overset{\alpha_2-\alpha_1}{\longrightarrow} 1\,0 & 0\,1 \overset{\alpha_1}{\longrightarrow} 1\,1 \\ B & 0\,0 \qquad 1\,0 & 0\,0 \qquad 0\,0 & 0\,\times \qquad 1\,\times \end{array}$$

$$\begin{array}{llll} A & 0\,0 \overset{\alpha_2}{\longrightarrow} 1\,0 & 0\,1 \overset{\alpha_1}{\longrightarrow} 1\,1 & 1\,\times \overset{\alpha_1}{\longrightarrow} 1\,\times \\ B & 1\,\times \qquad 1\,\times & 1\,\times \qquad 1\,\times & 0\,\times \qquad 1\,\times \end{array}, \tag{3.42}$$

where $\times$ denotes 0 or 1. In the case $\alpha_1 > \alpha_2$ the rates can be specified analogously. Starting the coupled process with a configuration $\boldsymbol{\eta}_0^A = \boldsymbol{\eta}_0^B$ leads to $\boldsymbol{\eta}_t^A \geq \boldsymbol{\eta}_t^B$ for all times $t > 0$ as a simple consequence of the coupled boundary rates. For the initial measure of process B we can take any stationary measure $\mu_{\rho_\infty}^{\alpha_1 \wedge \alpha_2}$ from Section 3.2 with asymptotic densities ρ_∞ as given in (3.41). Thus for every such density there exists a stationary measure of process A which is asymptotically dominated from below by ν_{ρ_∞}. Together with Proposition 3.6 this proves the statement. □

The above coupling argument can be generalized to other systems as long as there are exactly solvable cases with special rates. For our particular model one could still slightly improve the statement for $\alpha_1 \wedge \alpha_2 < 1/2$, by distinguishing various cases. But the full phase diagram cannot be derived without some deeper insight. A possible strategy for this has been mentioned at the end of the previous subsection.

3.4.2 Other applications and limitations

First we would like to apply the above results to the partially asymmetric simple exclusion process on the lattice $\Lambda = \mathbb{Z}^+$, where particles jump with rate p to the right and with rate q to the left. At site 1 particles enter with rate α and exit with rate β,

$$\begin{aligned} \mathcal{L}f(\boldsymbol{\eta}) = &\sum_{x=1}^{\infty} \big[p\eta(x)(1-\eta(x+1)) + q(1-\eta(x))\eta(x+1)\big]\big[f(\boldsymbol{\eta}^{x\leftrightarrow x+1}) - f(\boldsymbol{\eta})\big] \\ &+ \big[\alpha(1-\eta(1)) + \beta\eta(1)\big]\big[f(\boldsymbol{\eta}^{0\leftrightarrow 1}) - f(\boldsymbol{\eta})\big] \,. \end{aligned} \tag{3.43}$$

If these rates are related such that $\alpha = p\rho_l$, $\beta = q(1-\rho_l)$, this corresponds to the coupling to a reservoir of density $\rho_l \in [0,1]$. But in general the boundary rates can be chosen independently with range $[0,\infty)$ and in this case the effective boundary density is a nontrivial function of α, β, p and q. This is of course already known through the exact solution of this model via the MPA which is, however, rather involved and was addressed in a series of publications listed in Section 2.2.2. Using Theorem 3.4 we obtain the existence of stationary product measures on $\mathbb{Z}^+$, since the range of the boundary mechanism is $R = 1$. To get ρ_{eff} one has to solve a single site system coupled to a reservoir with density ρ_r at the right boundary,

$$\mu_{\rho_r}(1)\big(\beta + p(1-\rho_r)\big) = \mu_{\rho_r}(0)\big(\alpha + q\rho_r\big) \,, \quad \mu_{\rho_r}(0) + \mu_{\rho_r}(1) = 1 \,. \tag{3.44}$$

This leads to

$$\rho_{\mathit{eff}} = \frac{\alpha+\beta+p-q-\sqrt{(\alpha+\beta+p-q)^2-4\alpha(p-q)}}{2(p-q)}\,, \tag{3.45}$$

recovering the previous results. The same could be done for a toy model with partial asymmetry, but the formulas become long and the qualitative behavior is the same as for the totally asymmetric case, so we skip this discussion.

Although applicable for any kind of boundary mechanism the method is restricted to systems with nearest neighbor bulk dynamics that have stationary product measures. If either of the two conditions is violated, the effect of the boundary mechanism is in general not localized in a finite region and the ansatz does not work. We demonstrate this for two models with more general bulk dynamics, which have been analyzed in the context of boundary induced phase transitions. They include three site interactions with a generalized fundamental diagram, as mentioned in Section 2.2.3.

First we consider a modification of the toy model where the jump rates in the bulk also depend on the occupation of the second site to the right, just as the boundary rates. The bulk generator is

$$\begin{aligned}\mathcal{L}_v f(\boldsymbol{\eta}) = \sum_{x\in\Lambda} & p_1\eta(x)\big(1-\eta(x+1)\big)\eta(x+2)\big[f(\boldsymbol{\eta}^{x\to x+1})-f(\boldsymbol{\eta})\big] \\ & +p_2\eta(x)\big(1-\eta(x+1)\big)\big(1-\eta(x+2)\big)\big[f(\boldsymbol{\eta}^{x\to x+1})-f(\boldsymbol{\eta})\big],\end{aligned} \tag{3.46}$$

with rates $p_1, p_2 \in \mathbb{R}^+$. This is a special case of the KLS model introduced in [80], where it was shown that on a periodic lattice for every density $\rho \in [0,1]$ there exists a stationary measure which is in general non-product. In [7] the model was studied with open boundaries in the context of boundary induced phase transitions and a solution in terms of the MPA was given in [85]. In both cases the boundary rates α_1, α_2 are chosen such that they correspond to a bulk like reservoir, leading to a translation invariant stationary measure. For other choices of the boundary rates, the stationary statistics of the first lattice site is certainly changed. But since the measure is not product this effect is not localized in a finite region but decays only asymptotically.

In the next model we would like to mention, a particle can also hop two sites to the right if both sites ahead are empty. The bulk dynamics is given by the generator

$$\begin{aligned}\mathcal{L}_v f(\boldsymbol{\eta}) = \sum_{x\in\Lambda} & p_1\eta(x)\big(1-\eta(x+1)\big)\big[f(\boldsymbol{\eta}^{x\to x+1})-f(\boldsymbol{\eta})\big] \\ & +p_2\eta(x)\big(1-\eta(x+1)\big)\big(1-\eta(x+2)\big)\big[f(\boldsymbol{\eta}^{x\to x+2})-f(\boldsymbol{\eta})\big]\end{aligned} \tag{3.47}$$

with rates $p_1, p_2 \in \mathbb{R}^+$. On a periodic lattice this process has stationary product measures for all densities $\rho \in [0,1]$ with current $j(\rho) = \rho(1-\rho)[p_1 + 2p_2(1-\rho)]$ as shown in [85]. It was also found that these product measures remain for the open system, if the boundary rates

$$|0,\ldots \to |1,\ldots \text{ with } \alpha_1 \quad \text{and} \quad |0,0,\ldots \to |0,1,\ldots \text{ with } \alpha_2\,, \tag{3.48}$$

are chosen as $\alpha_1 = \rho_l p_2(p_1/p_2 + 1 - \rho_l)$, $\alpha_2 = \rho_l p_2$, corresponding to a reservoir of density ρ_l. Using the ansatz of Theorem 3.4 for the semi-infinite system with general α_1 and α_2 there

are now two matching conditions that have to be fulfilled, due to the next nearest neighbor jumps. The extra relation $\langle \eta(1)(1-\eta(2)) \rangle_{\mu_{\rho_r}} = \rho_r(1-\rho_r)$ imposes a condition on the system parameters, which turns out to be exactly the condition for the coupling to a reservoir given above. But in this case the existence of product measures with density ρ_l is a priori clear and moreover, the system can be solved exactly.

3.5 Discussion

As a result of the last section, the definition of the effective boundary density given in Section 3.3.2 is limited to systems with nearest neighbor bulk dynamics and stationary product measures. However the analysis of this chapter suggests an alternative for general lattice gases which is, roughly speaking, the asymptotic density of the boundary dominated measures. We shortly specify this idea more precisely in the following using non-rigorous arguments, which are inspired by the well established theory for the corresponding hydrodynamic equation.

We consider lattice gases that have translation invariant stationary measures for every density, i.e. for all $\rho \in [0,1]$ in case of exclusion models. This excludes systems with bulk phase transitions that are studied in Chapters 5 and 6, since our focus here is on boundary induced phenomena. For such systems there exists a well defined current-density relation $j(\rho)$, which is generically (at least) a C^1-function, except for degenerate cases involving for example some zero rates, which we want to exclude. Then it is natural to define

$$M_l = \{\rho \,|\, j'(\rho) > 0\} \quad \text{and} \quad M_r = \{\rho \,|\, j'(\rho) < 0\} \tag{3.49}$$

to be the set of densities which are accessible by the left and right boundary respectively, since j' determines the characteristic velocity of density fluctuations. This means that for all $\rho \in M_l$ there exists a translation invariant, boundary dominated stationary measure of the semi-infinite process coupled to a reservoir with density ρ. For a general boundary mechanism fix an initial distribution with density $\rho \in M_l$, for simplicity we just take the product measure ν_ρ. This determines a unique stationary measure with some asymptotic density ρ_∞ as a function of ρ. Take

$$M_l^* = \{ \underbrace{\lim_{x\to\infty}\lim_{t\to\infty} \langle \eta(x) \rangle_{\nu_\rho S(t)}}_{\rho_\infty(\rho)} \,|\, \rho \in M_l \} \tag{3.50}$$

to be the set of all possible ρ_∞, under variation of the initial density ρ. It is $M_l^* \subset \overline{M}_l$ since densities in M_r are not accessible from the initial condition. Moreover M_l^* and M_l have at most one value in common, defining the effective boundary density, i.e.

$$M_l^* \cap M_l \neq \emptyset \;\Rightarrow\; M_l^* \cap M_l = \{\rho_{\mathit{eff}}\}. \tag{3.51}$$

On the other hand if $M_l^* \cap M_l = \emptyset$ there is in general no well defined effective density for the boundary mechanism under consideration. In this case one can only identify one of the intervals $I \subset [0,1]\backslash M_l$ via $\left|I \cap \left(M_l^* \cup \{1\}\right)\right| = 2$. This characterization is unique since for all other intervals $J \subset [0,1]\backslash M_l$ it is $\left|J \cap \left(M_l^* \cup \{1\}\right)\right| \leq 1$. The interpretation is that

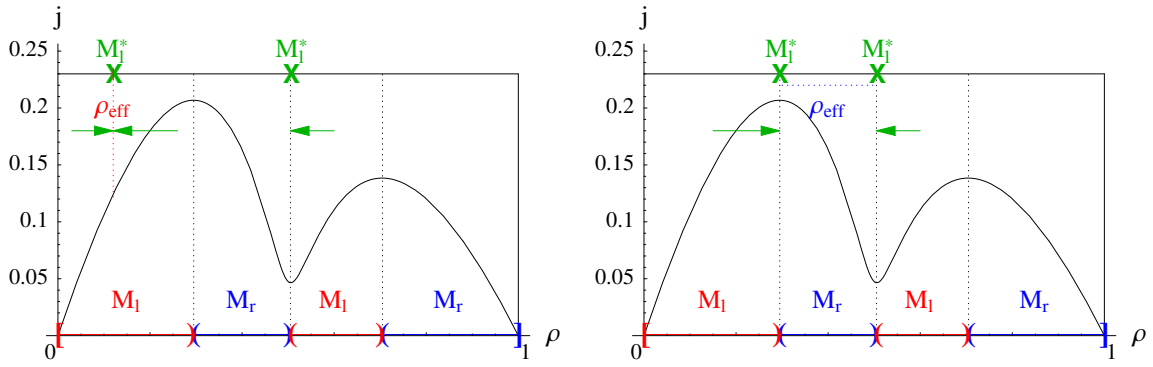


Figure 3.5: Definition of the effective boundary density ρ_{eff} for the KLS model introduced in Section 2.2.3, using the fundamental diagram. ρ_{eff} is well defined in M_l (left) and arbitrary in M_r (right).

for initial densities $\rho \in M_l$ the system evolves towards I as far as possible, no matter if ρ is larger or smaller than the densities in I. These ideas are illustrated in Figure 3.5 for the KLS model introduced in Section 2.2.3. All choices $\rho_{\mathit{eff}} \in I$ lead to asymptotically equivalent measures, which can also be seen directly in the phase diagram since it is independent of the left boundary density in the intervals I of $[0,1]\backslash M_l$ (cf. Figure 2.3 or 3.1). In general, deviations of the real and the effective measure for finite x decay with the correlation length of the system which is a pure bulk property and thus independent of ρ_{eff}.

However in special cases, there might be a certain generic choice of ρ_{eff} also outside M_l, as for example in Section 3.3.2 through the existence of stationary product measures for ASEP type bulk dynamics. But it is important to note that in the bulk dominated phase, these measures only exist for the special bulk density $\rho_\infty = \rho_{\mathit{eff}}$ (red line in Figure 3.1). For all other bulk dominated measures (blue region in Figure 3.1) deviations due to a boundary inhomogeneity decay asymptotically as explained above.

In contrast to the situation in Section 3.3 the above generalization is of course a rather academic definition, since the exact computation of ρ_{eff} still involves the solution of the semi-infinite system. But the description can be used at least in simulations to numerically determine ρ_{eff} in an efficient way.

Chapter 4

Zero range processes with several species of particles

4.1 Introduction

For one-component systems the analysis of the hydrodynamic limit equation led to the theory of boundary induced phase transitions, which provides a general framework for a quantitative description of the steady state selection in systems which are in contact with particle reservoirs (see Section 2.2.3). In systems with more than one conserved quantity interesting new phenomena have been found such as phase separation and spontaneous symmetry breaking as explained in Section 2.2.4, for a recent review see [125]. Again it is natural to ask for principles governing steady state selection and the resulting phase diagram in systems with many species of particles. The macroscopic behavior of such systems has been examined to some extent only recently [110] and there are very few rigorous results [132, 133, 134].

In the next section we generalize the zero range process to n different types of particles. The jump rate g_i of the i-th component depends on the occupation numbers of all n species at a given site. It turns out, that for the process to have stationary product measures, the rates of the different species cannot be chosen independently. In general these measures are nontrivial and do not factorize with respect to the different components. Our goal is the derivation of the hydrodynamic equations on the Euler scale (cf. Section 2.1.4), which are given by a system of n conservation laws. For this purpose we use the relative entropy method of Yau [141], which was previously applied to the one-component ZRP, summarized in [84], Chapter 6. While directly applicable to the present case, this method has the disadvantage of yielding the desired result only up to the first shock. So far we did not attempt to extend our result to all times following the lines in [114]. The derivation is given in Section 4.3, where we also show that the system of conservation laws is hyperbolic and the thermodynamic entropy of the stationary measure is a Lax entropy. This property follows from certain reciprocity relations for the steady currents of the components. Such relations have been established for special ZRPs in [53, 54] and recently in the more general context of so-called bricklayer models [133]. In Section 4.4 we analyze the system of conservation laws with open boundary conditions in terms of entropy variables [135] where it takes a particular simple form. For stationary solutions the system decouples, and we are able to derive stationary

density profiles under very general conditions, which we state explicitly for one-dimensional geometry. The contents of this chapter have been published in [62].

4.2 The n-component zero range process

In the following we introduce the n-component zero range process and construct the dynamics analogously to Section 2.3.1. We identify necessary and sufficient conditions for the existence of stationary product measures.

4.2.1 Definition of the dynamics

Consider a zero range process on the periodic lattice $\Lambda_L = (\mathbb{Z}/L\mathbb{Z})^d$ with n different species of particles. Let $\eta_i(x) \in \mathbb{N}$ denote the number of particles of component $i \in \{1,\dots,n\}$ on site $x \in \Lambda_L$. The state space is given by $X_L = (\mathbb{N}^n)^{\Lambda_L}$ and for a particle configuration we use the notations $\boldsymbol{\eta} = \big(\boldsymbol{\eta}(x)\big)_{x\in\Lambda_L} = \Big(\big(\eta_1(x),\dots,\eta_n(x)\big)\Big)_{x\in\Lambda_L}$. At a given site $x \in \Lambda_L$, the jump rate of i-type particles is given by $g_i\big(\boldsymbol{\eta}(x)\big)$ and the leaving particle jumps to site $x+y$ with (translation invariant) probability $p_i(y)$. The jump probabilities $p_i : \mathbb{Z} \to [0,1]$ are normalized and assumed to be of finite range $R \in \mathbb{Z}^+$, i.e. we assume (2.56) for every $i = 1,\dots,n$

$$\sum_{y\in\Lambda_L} p_i(y) = 1\,, \quad p_i(0) = 0 \quad \text{and} \quad p_i(y) = 0 \text{ for } |y| > R\,. \tag{4.1}$$

To exclude hidden conservation laws the p_i should also be irreducible and since we are interested in the hydrodynamic limit on the Euler scale, the first moments should not vanish, i.e. $m(p_i) = \sum_{y\in\Lambda_L} y\, p_i(y) \neq 0$. For each i, the rate function $g_i : \mathbb{N}^n \to [0,\infty)$ vanishes for all $\mathbf{k} = (k_1,\dots,k_n) \in \mathbb{N}^n$ with $k_i = 0$ and is otherwise positive, i.e.

$$g_i(\mathbf{k}) \geq 0 \quad \text{and} \quad g_i(\mathbf{k}) = 0 \;\Leftrightarrow\; k_i = 0\,. \tag{4.2}$$

The generator is given by

$$(\mathcal{L}f)(\boldsymbol{\eta}) = \sum_{x,y\in\Lambda_L} \sum_{i=1}^{n} g_i\big(\boldsymbol{\eta}(x)\big)\, p_i(y) \Big(f(\boldsymbol{\eta}^{i;x\to x+y}) - f(\boldsymbol{\eta}) \Big). \tag{4.3}$$

The configuration $\boldsymbol{\eta}^{i;x\to x+y}$ results from $\boldsymbol{\eta}$ after one particle of component i has jumped from x to $x+y$, i.e. $\eta_j^{i;x\to x+y}(z) = \eta_j(z) + \delta_{i,j}(\delta_{z,(x+y)} - \delta_{z,x})$ for all $z \in \Lambda_L$, $j = 1,\dots,n$. The number of particles $\Sigma_L^i(\boldsymbol{\eta}) = \sum_{x\in\Lambda_L} \eta_i(x)$ of each species i is conserved, and these are the only conserved quantities. They divide the configuration space into canonical subsets $X_{L,\mathbf{N}} = \{\boldsymbol{\eta} \in X_L \big| \Sigma_L^i(\boldsymbol{\eta}) = N_i,\ i = 1,\dots,n\}$ with fixed particle numbers $\mathbf{N} = (N_1,\dots,N_n) \in (\mathbb{Z}^+)^n$, cf. Section 2.3.2. Restricted to such a subset the process is well defined and irreducible.

However, to show the hydrodynamic limit we also need existence of the dynamics in the limit $L \to \infty$, i.e. on the infinite lattice $\mathbb{Z}^d$. Thus we assume the extra condition

$$\sup_{i\in\{1,\dots,n\}} \sup_{\mathbf{k}\in\mathbb{N}^n} |g_i(\mathbf{k}^i, k_i+1) - g_i(\mathbf{k})| < \infty\,, \tag{4.4}$$

analogous to (2.57). We use the shorthand $(\mathbf{k}^i, k_i \pm 1) = (k_1, \dots, k_{i-1}, k_i \pm 1, k_{i+1}, \dots, k_n)$ here and in the following. Similarly to (2.58) and (2.59), X has to be restricted to configurations with $\|\boldsymbol{\eta}\|_\alpha < \infty$, where we set $\|\boldsymbol{\eta}\|_\alpha = \sum_{x\in\Lambda} \sum_{i=1}^n |\eta_i(x)|\alpha(x)$ in this case. With these assumptions the result (2.62), proving the existence of the dynamics, can be readily generalized to the multi-species case with the same techniques as used in [3, 101].

To ensure the existence of nontrivial stationary product measures with positive particle densities, we tighten the positivity requirement on the jump rates in (4.2) such that they are uniformly bounded away from zero. The relevant quantity for later analysis is the limit inferior

$$g_i^* := \liminf_{\substack{|\mathbf{k}|\to\infty \\ k_i>0}} g_i(\mathbf{k}) > 0 \qquad \text{for all } i = 1, \dots, n\,. \tag{4.5}$$

4.2.2 Stationary product measures

For the one-component process with $n = 1$ there exists the family $\bar\nu_\phi$ of translation invariant stationary product measures (cf. Section 2.3.2). Instead of using the fugacity $\phi \in (0, \infty)$, the notation with the chemical potential $\mu = \log\phi \in \mathbb{R}$ turns out to be more convenient in this chapter, so we write

$$\bar\nu_\mu^L(\boldsymbol{\eta}) = \prod_{x\in\Lambda_L} \frac{1}{Z(\mu)}\, e^{\mu\,\eta_1(x)} \prod_{k=1}^{\eta_1(x)} \frac{1}{g_1(k)} \quad \text{with } Z(\mu) = \sum_{l=0}^{\infty} e^{\mu\, l} \prod_{k=1}^{l} \frac{1}{g_1(k)}\,. \tag{4.6}$$

The only difference to the description with fugacities is that the degenerate case $\phi = 0$, corresponding to zero particle densities, is not covered by $\mu \in \mathbb{R}$. We also keep the superscript L for the product measures to explicitly denote the system size. This should not lead to confusion although the lattice actually consists of L^d sites. In the case $n > 1$, the stationary measures are of product form only under the following condition on the jump rates:

Assumption. For every $i, j \in \{1, \dots, n\}$, $\mathbf{k} = (k_1, \dots, k_n) \in \mathbb{N}^n$ with $k_i, k_j > 0$ let

$$g_i(\mathbf{k})\, g_j(\mathbf{k}^i, k_i - 1) = g_j(\mathbf{k})\, g_i(\mathbf{k}^j, k_j - 1)\,. \tag{4.7}$$

This assumption is equivalent to the existence of a potential $G : \mathbb{N}^n \to \mathbb{R}$ for the logarithm of the jump rates such that

$$\log g_i(\mathbf{k}) = G(\mathbf{k}) - G(\mathbf{k}^i, k_i - 1)\,. \tag{4.8}$$

Given G, the jump rates defined via (4.8) clearly satisfy (4.7) by construction. On the other hand for given jump rates g_i obeying (4.7) one can define G recursively via (4.8) by fixing $G(0, \dots, 0) = 0$. This construction does not depend on the order of summation, since by (4.7) the sum over closed loops of indices vanishes. For example one can choose

$$\begin{aligned} G(\mathbf{k}) = &\sum_{j_1=1}^{k_1} \log g_1(j_1, 0, \dots, 0) + \\ &\sum_{j_2=1}^{k_2} \log g_2(k_1, j_2, 0, \dots, 0) + \dots + \sum_{j_n=1}^{k_n} \log g_n(k_1, \dots, k_{n-1}, j_n)\,. \end{aligned} \tag{4.9}$$

The stationary weight is given by $W(\mathbf{k}) = \exp[-G(\mathbf{k})]$ and the grand canonical measures are of product form, as formulated in the next theorem.

Theorem 4.1 (Stationary product measures)
The zero range process defined on Λ_L in (4.3) with more than one component, $n > 1$, has stationary product measures if and only if the condition (4.7), or equivalently (4.8), is fulfilled. In this case the grand canonical family of stationary measures can be written as

$$\bar{\nu}^L_{\boldsymbol{\mu}}(\boldsymbol{\eta}) = \prod_{x\in\Lambda_L} \frac{1}{Z(\boldsymbol{\mu})} \exp\Big[- G\big(\boldsymbol{\eta}(x)\big) + \sum_{i=1}^{n} \mu_i\, \eta_i(x)\Big] \tag{4.10}$$

with the chemical potentials $\boldsymbol{\mu} = (\mu_1, \dots, \mu_n) \in D_\mu$. D_μ is the open domain of convergence of the partition function

$$Z(\boldsymbol{\mu}) = \sum_{\mathbf{k}\in\mathbb{N}^n} \exp\Big[- G(\mathbf{k}) + \sum_{i=1}^{n} \mu_i\, k_i\Big] \,. \tag{4.11}$$

Proof. See Section 4.2.4.

Remark. If the jump rates are site dependent and satisfy (4.8) with potential G_x for every site x, the measure defined analogously to (4.10) is still stationary, since the terms in the proof (4.26) cancel for each site individually. However, it is not clear how to generalize the reverse argument to space-dependent rates.

4.2.3 Properties of the stationary measures

We denote the particle density of component $i \in \{1, \dots, n\}$ as a function of the chemical potentials by R_i. Due to translation invariance it is site independent and given by (cf. (2.15))

$$R_i(\boldsymbol{\mu}) = \big\langle \eta_i(0) \big\rangle_{\bar{\nu}^L_{\boldsymbol{\mu}}} = \partial_{\mu_i} \log Z(\boldsymbol{\mu}) > 0 \,. \tag{4.12}$$

Note that in this chapter we define $\mathbf{R} = (R_1, \dots, R_n) : D_\mu \to D_\rho = \mathbf{R}\big(D_\mu\big) \subset (0,\infty)^n$ only on the open domain D_μ of convergence of Z. Therefore, unlike in Section 2.3.2 and Chapter 5, we neglect a possible extension to the boundary of D_μ.

Lemma 4.2 *$D_\mu \subset \mathbb{R}^n$ is a convex region with infinite volume measure, and if $\boldsymbol{\mu}^* \in D_\mu$ then $\big\{\boldsymbol{\mu} \,\big|\, \mu_i \le \mu_i^*,\ i = 1, \dots, n\big\} \subset D_\mu$. For $\boldsymbol{\mu} \in D_\mu$ the measure $\bar{\nu}^L_{\boldsymbol{\mu}}$ has some finite exponential moments. The function $\mathbf{R} : D_\mu \to D_\rho$ is invertible, i.e. its derivative (called compressibility)*

$$D\mathbf{R}(\boldsymbol{\mu}) := \Big(\partial_{\mu_j} R_i(\boldsymbol{\mu})\Big)_{i,j} = D^2 \log Z(\boldsymbol{\mu}) = \Big(\partial^2_{\mu_i\mu_j} \log Z(\boldsymbol{\mu})\Big)_{i,j} \tag{4.13}$$

is a symmetric, positive definite $n \times n$ matrix and $\log Z(\boldsymbol{\mu})$ is strictly concave. D_ρ is simply connected and there exists an $\alpha > 0$ such that $\boldsymbol{\rho} \in D_\rho$ for all $|\boldsymbol{\rho}| < \alpha$.

Proof. With condition (4.5) D_μ is non-empty. The convexity of D_μ easily follows from the concavity of $\log Z(\boldsymbol{\mu})$ given below in (4.15), and the monotonicity of the logarithm. This implies $Z(q\boldsymbol{\mu}^1 + (1-q)\boldsymbol{\mu}^2) \leq Z(\boldsymbol{\mu}^1)^q Z(\boldsymbol{\mu}^2)^{1-q} < \infty$ for all $\boldsymbol{\mu}^1, \boldsymbol{\mu}^2 \in D_\mu$ and $q \in [0,1]$, thus D_μ is convex. For every $\boldsymbol{\mu}^* \in D_\mu$ we have $\left\{\boldsymbol{\mu} \,\middle|\, \mu_i \leq \mu_i^*,\, i = 1, \dots, n\right\} \subset D_\mu$ due to monotonicity (4.12) and D_μ has infinite volume measure.

The existence of some finite exponential moments on D_μ follows from $\langle e^{\boldsymbol{\theta}\cdot\boldsymbol{\eta}(\mathbf{0})}\rangle_{\bar\nu^L_{\boldsymbol{\mu}}} = Z(\boldsymbol{\mu}+\boldsymbol{\theta})/Z(\boldsymbol{\mu}) < \infty$ for sufficiently small $\boldsymbol{\theta} \in \mathbb{R}^n$. Therefore the density $\mathbf{R}$ is well defined on D_μ and the compressibility is given by the matrix of second derivatives as

$$D\mathbf{R}(\boldsymbol{\mu}) = \left(\left\langle \eta_i(0)\, \eta_j(0) \right\rangle^c_{\bar\nu^L_{\boldsymbol{\mu}}} \right)_{i,j}, \tag{4.14}$$

where $\left\langle \eta_i(0)\, \eta_j(0) \right\rangle^c_{\bar\nu^L_{\boldsymbol{\mu}}} := \left\langle \eta_i(0)\, \eta_j(0) \right\rangle_{\bar\nu^L_{\boldsymbol{\mu}}} - \left\langle \eta_i(0) \right\rangle_{\bar\nu^L_{\boldsymbol{\mu}}} \left\langle \eta_j(0) \right\rangle_{\bar\nu^L_{\boldsymbol{\mu}}}$. Thus $D\mathbf{R}(\boldsymbol{\mu})$ is symmetric and positive definite, because

$$\mathbf{a}^T \cdot \left(D^2 \log Z(\boldsymbol{\mu}) \right) \mathbf{a} = \left\langle \Big(\sum_{i=1}^n a_i\, \eta_i(0) \Big)^2 \right\rangle^c_{\bar\nu^L_{\boldsymbol{\mu}}} > 0 \tag{4.15}$$

for all $\mathbf{a} \in \mathbb{R}^n$ with $|\mathbf{a}| = 1$. Hence the eigenvalues of $D^2 \log Z(\boldsymbol{\mu})$ are real and positive, which ensures that $\log Z(\boldsymbol{\mu})$ is strictly concave and $\mathbf{R}$ is invertible on D_μ.
Since $\mathbf{R}$ and its inverse are continuous, D_ρ is diffeomorphic to the convex set D_μ and thus simply connected. The existence of $\alpha > 0$ in the last statement is a direct consequence of the properties of D_μ and the regularity of $D\mathbf{R}$. □

We denote the inverse of $\mathbf{R}$ by $\mathbf{M} = (M_1, \dots, M_n) : D_\rho \to D_\mu$ and define the measure $\nu^L_{\boldsymbol{\rho}} := \bar\nu^L_{\mathbf{M}(\boldsymbol{\rho})}$, which is indexed by the particle densities $\boldsymbol{\rho}$. Due to Lemma 4.2, $\nu^L_{\boldsymbol{\rho}}$ is defined at least for small densities, and in many cases it is $D_\rho = (0,\infty)^n$ as for example under the assumption (4.35) or (4.36) in Section 4.3.1. However, there are also cases where there is no stationary product measure for large densities and a condensation transition occurs, which is discussed in detail in Chapter 5. In this case the behavior of $Z(\boldsymbol{\mu})$ and $\mathbf{R}(\boldsymbol{\mu})$ at the boundary ∂D_μ is of importance, but in this chapter we do not discuss this point any further and restrict ourselves to open domains.

Analogous to (2.73) the stationary current of component i is given by

$$J_i(\boldsymbol{\rho}) = m(p_i)\, \langle g_i \rangle_{\nu^1_{\boldsymbol{\rho}}} = m(p_i)\, \exp\left[M_i(\boldsymbol{\rho})\right] \quad \in \mathbb{R}^d \tag{4.16}$$

as a function of the particle densities. We denote it by capital $\mathbf{J}$ in this chapter only, to avoid possible confusion with lowercase indices j. The first moment $m(p_i) \in \mathbb{R}^d$ determines the direction of the current, whereas the absolute value $|J_i| \propto \exp\left[M_i(\boldsymbol{\rho})\right]$ depends on the chemical potential of component i only and is thus monotonic increasing in ρ_i.

Definition. The *thermodynamic entropy* $S : D_\rho \to \mathbb{R}$ of the stationary measure (4.10) is the convex conjugate of $\log Z(\boldsymbol{\mu})$ given by the Legendre transform

$$S(\boldsymbol{\rho}) = \sup_{\boldsymbol{\mu} \in D_\mu} \left(\sum_{i=1}^n \rho_i \mu_i - \log Z(\boldsymbol{\mu}) \right) = \boldsymbol{\rho} \cdot \mathbf{M}(\boldsymbol{\rho}) - \log Z\big(\mathbf{M}(\boldsymbol{\rho})\big)\,. \tag{4.17}$$

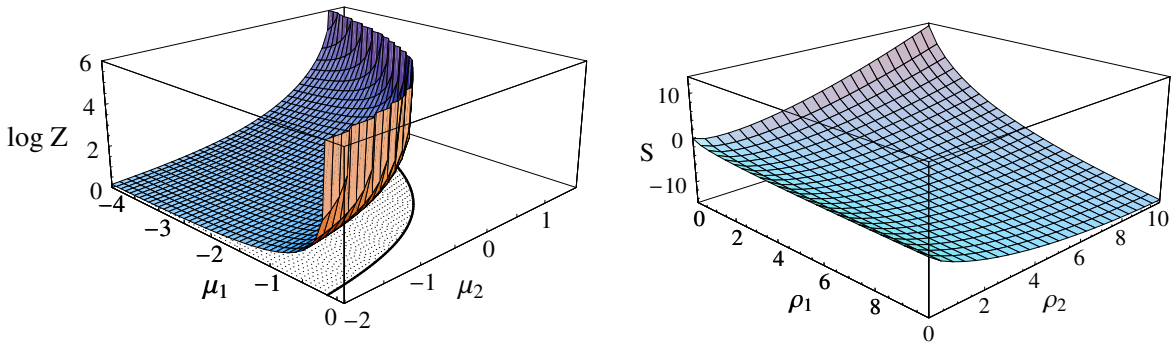


Figure 4.1: Illustration of example (4.21). **Left:** $\log Z$ as a (concave) function of the chemical potentials μ_1 and μ_2. The domain D_μ is given by the grey region in the μ_1, μ_2-plane with the black line (——) as boundary. **Right:** Entropy S as a function of the densities ρ_1 and ρ_2 with domain $D_\rho = (0,\infty)^2$.

In principle the Legendre transform is defined for all $\boldsymbol{\rho} \in [0,\infty)^n$. But for densities $\boldsymbol{\rho} \notin D_\rho$ the expression using $\mathbf{M}(\boldsymbol{\rho})$ is not valid and the supremum is attained at the boundary ∂D_μ, which is discussed in Section 5.4 in the context of phase transitions. For $\boldsymbol{\rho} \in D_\rho$ we have

$$\partial_{\rho_i} S(\boldsymbol{\rho}) = M_i(\boldsymbol{\rho}) \tag{4.18}$$

for all $i \in \{1,\dots,n\}$, and thus $D\mathbf{M}(\boldsymbol{\rho}) = D^2 S(\boldsymbol{\rho}) \in \mathbb{R}^{n\times n}$. This leads to the following relation for the determinants, denoted by $|.|$,

$$\left|D^2 S(\boldsymbol{\rho})\right| = \left|D\mathbf{M}(\boldsymbol{\rho})\right| = \left|D\mathbf{R}(\mathbf{M}(\boldsymbol{\rho}))\right|^{-1} = \left|D^2 \log Z(\mathbf{M}(\boldsymbol{\rho}))\right|^{-1} > 0\,. \tag{4.19}$$

Thus S is strictly concave on D_ρ. Note that due to the grand canonical structure of the stationary measure the densities are given as derivatives of the partition function with respect to the chemical potentials. With (4.16) this leads to $\log\langle g_i\rangle_{\nu_{\boldsymbol{\rho}}} = \partial_{\rho_i} S(\boldsymbol{\rho})$ and thus

$$\partial_{\rho_j} \log\langle g_i\rangle_{\nu^1_{\boldsymbol{\rho}}} = \partial_{\rho_i} \log\langle g_j\rangle_{\nu^1_{\boldsymbol{\rho}}}\,, \tag{4.20}$$

for all $i,j \in \{1,\dots,n\}$, which can be considered as the macroscopic analogue of condition (4.7) on the jump rates.

As an example we consider a two-component system with jump rates

$$g_1(k_1,k_2) = \Big(\frac{k_1}{1+k_1}\Big)^{k_2}\,, \quad g_2(k_1,k_2) = \frac{k_2}{1+k_1}\,. \tag{4.21}$$

They obviously fulfill conditions (4.2) to (4.4) and (4.7), so the stationary product measure (4.10) exists with weight $W(k_1,k_2) = (1+k_1)^{k_2}/k_2!$. The partition function (4.11) can be calculated explicitly as

$$Z(\mu_1,\mu_2) = \frac{\exp[e^{\mu_2}]}{1-\exp[e^{\mu_2}+\mu_1]}\,, \tag{4.22}$$

with domain of convergence $D_\mu = \{\boldsymbol{\mu} \,|\, \mu_1 < -\exp[\mu_2]\}$. In Figure 4.1 (left) we plot the logarithm of Z, which is concave and diverging at the boundary of D_μ. Writing $E_{\mu_1,\mu_2} = \exp[e^{\mu_2} + \mu_1]$, the particle densities are given by

$$R_1(\mu_1,\mu_2) = \frac{E_{\mu_1,\mu_2}}{1-E_{\mu_1,\mu_2}}\,, \quad R_2(\mu_1,\mu_2) = \frac{\exp[\mu_2]}{1-E_{\mu_1,\mu_2}}\,, \tag{4.23}$$

with full range $D_\rho = (0,\infty)^2$, since $E_{\mu_1,\mu_2} \to 1$ for $(\mu_1,\mu_2) \to \partial D_\mu$. These relations can be inverted to get

$$M_1(\rho_1,\rho_2) = \log\Big(\frac{\rho_1}{1+\rho_1}\Big) - \frac{\rho_2}{1+\rho_1}\,, \quad M_2(\rho_1,\rho_2) = \log\Big(\frac{\rho_2}{1+\rho_1}\Big)\,. \tag{4.24}$$

So the entropy (4.17) can be computed explicitly and is plotted in Figure 4.1 (right).

4.2.4 Proof of Theorem 4.1

First we assume that (4.7) and (4.8) are satisfied and show that $\bar\nu^L_{\boldsymbol{\mu}}$ defined in (4.10) is stationary. Since G exists by assumption, the measure $\bar\nu^L_{\boldsymbol{\mu}}$ is well defined on D_μ. This part of the proof is a straightforward generalization of the standard argument for $n = 1$, given for example in [84], Proposition II.3.2. To prove stationarity of $\bar\nu^L_{\boldsymbol{\mu}}$ we have to show that for all $f \in C(X_L,\mathbb{R})$

$$\langle \mathcal{L} f\rangle_{\bar\nu^L_{\boldsymbol{\mu}}} = \sum_{\boldsymbol{\eta}\in X_L}\sum_{x,y\in\Lambda_L}\sum_{i=1}^N g_i\big(\boldsymbol{\eta}(x)\big)\,p_i(y)\Big(f(\boldsymbol{\eta}^{i;x\to x+y}) - f(\boldsymbol{\eta})\Big)\bar\nu^L_{\boldsymbol{\mu}}(\boldsymbol{\eta}) = 0\,. \tag{4.25}$$

For every $x,y\in\Lambda_L$, $i = 1,\dots,n$ one has

$$\sum_{\boldsymbol{\eta}\in X_L} g_i\big(\boldsymbol{\eta}(x)\big) f(\boldsymbol{\eta}^{i;x\to x+y})\,\bar\nu^L_{\boldsymbol{\mu}}(\boldsymbol{\eta}) = \sum_{\boldsymbol{\eta}\in X_L} g_i\Big((\eta_1,..,\eta_i+1,..,\eta_n)(x)\Big) f(\boldsymbol{\eta})\,\bar\nu^L_{\boldsymbol{\mu}}(\boldsymbol{\eta}^{i;x+y\to x})\,,$$

with the shorthand $(\eta_1,...,\eta_n)(x) = \big(\eta_1(x),...,\eta_n(x)\big)$. Using this and a change of variables in the summation over x we can rewrite (4.25) as

$$\begin{aligned}\langle \mathcal{L} f\rangle_{\bar\nu^L_{\boldsymbol{\mu}}} = \sum_{\boldsymbol{\eta}\in X_L} f(\boldsymbol{\eta}) \sum_{i=1}^N \sum_{x,y\in\Lambda_L} & p_i(y)\,\bar\nu^1_{\boldsymbol{\mu}}\big(\boldsymbol{\eta}(x-y)\big)\,\bar\nu^1_{\boldsymbol{\mu}}\Big((\eta_1,..,\eta_i-1,..,\eta_n)(x)\Big) \\ & \Bigg[\frac{g_i\Big((\eta_1,..,\eta_i+1,..,\eta_n)(x-y)\Big)\,\bar\nu^1_{\boldsymbol{\mu}}\Big((\eta_1,..,\eta_i+1,..,\eta_n)(x-y)\Big)}{\bar\nu^1_{\boldsymbol{\mu}}\big(\boldsymbol{\eta}(x-y)\big)} \\ & - \frac{g_i\big(\boldsymbol{\eta}(x)\big)\,\bar\nu^1_{\boldsymbol{\mu}}\big(\boldsymbol{\eta}(x)\big)}{\bar\nu^1_{\boldsymbol{\mu}}\Big((\eta_1,..,\eta_i-1,..,\eta_n)(x)\Big)}\Bigg] \prod_{z\in\Lambda_L\setminus\{x-y,x\}} \bar\nu^1_{\boldsymbol{\mu}}\big(\boldsymbol{\eta}(z)\big) = 0\,.\end{aligned} \tag{4.26}$$

Analogous to a single species the crucial relation for the square brackets to vanish is

$$\bar\nu^1_{\boldsymbol{\mu}}(\mathbf{k}) = \frac{\bar\nu^1_{\boldsymbol{\mu}}(\mathbf{k}^i, k_i-1)}{g_i(\mathbf{k})}\,\exp[\mu_i] \tag{4.27}$$

for all $i = 1, \dots, n$, $\mathbf{k} = (k_1, \dots, k_n) \in \mathbb{N}^n$ with $k_i > 0$. In our case (4.27) easily follows from the assumption (4.8). Thus (4.26) vanishes for every $f \in C(X_L, \mathbb{R})$, (4.25) is shown and $\bar{\nu}^L_{\boldsymbol{\mu}}$ is stationary.

Assume now that ν is an arbitrary stationary product measure of the zero range process with generator $\mathcal{L}$ given in (4.3). Then

$$\langle \mathcal{L} f \rangle_\nu = 0 \quad \text{for all} \quad f \in C(X_L, \mathbb{R}) \tag{4.28}$$

and, by inserting special functions f, one can deduce conditions on the jump rates. Consider a configuration $\bar{\boldsymbol{\eta}}$ where there are $\mathbf{k} = (k_1, \dots, k_n) \in \mathbb{N}^n$ particles at a fixed site x and the rest of the lattice is empty, i.e. $\bar{\boldsymbol{\eta}}(z) = \delta_{z,x}\mathbf{k}$ for all $z \in \Lambda_L$. From the stationarity condition (4.28) with the indicator function $f = \chi_{\bar{\boldsymbol{\eta}}}$ we obtain for the one-point marginal

$$\Big[g_1(\mathbf{k}) + \ldots + g_n(\mathbf{k}) \Big] \, \nu^1(\mathbf{k}) = \sum_{i=1}^{N} \nu^1(\mathbf{k}^i, k_i - 1) \, , \tag{4.29}$$

where we set $\nu^1(\mathbf{k}) = 0$ if $k_i < 0$ for some $i \in \{1, \dots, n\}$. To get (4.29) we used

$$\nu^1(0, .., 0, k_i, 0, .., 0) = \nu^1(\mathbf{0}) \prod_{l=1}^{k_i} \frac{1}{g_i(0, .., 0, l, 0, .., 0)} \, , \tag{4.30}$$

which is known from the stationary measure of the one component system (2.65). Now let f be the indicator function of $\bar{\boldsymbol{\eta}}^{i;x \to x+y}$, with $\bar{\boldsymbol{\eta}} = \big(\delta_{z,x}\mathbf{k}\big)_{z \in \Lambda_L}$ as above and $k_i > 0$. Using (4.28) to (4.30) we obtain

$$\begin{aligned} & p_i(y) \nu^1(\mathbf{0}) \Big[g_i(\mathbf{k}) \, \nu^1(\mathbf{k}) - \nu^1\big(\mathbf{k}^i, k_i - 1\big) \Big] = \\ & \quad = - \sum_{j \neq i} p_j(-y) \, \nu^1\big(\mathbf{k}^{i,j}, k_i - 1, k_j - 1\big) \Big[g_j(\mathbf{e}_i + \mathbf{e}_j) \, \nu^1(\mathbf{e}_i + \mathbf{e}_j) \; - \nu^1(\mathbf{e}_j) \Big] \end{aligned} \tag{4.31}$$

with the shorthand $(\mathbf{k}^{i,j}, k_i - 1, k_j - 1) = \mathbf{k} - \mathbf{e}_i - \mathbf{e}_j$, where $\mathbf{e}_i \in \mathbb{R}^n$ is the unit vector in direction i. (4.31) holds for all $y \in \Lambda_L$ and is obviously fulfilled if the two square brackets vanish individually. Under the assumption that the brackets do not vanish, one can easily construct a contradiction to (4.31) or (4.29). Thus we obtain

$$\nu^1(\mathbf{k}) = \nu^1(\mathbf{k}^i, k_i - 1) / g_i(\mathbf{k}) \tag{4.32}$$

for all $i \in \{1, \dots, n\}$. Applying (4.32) twice in different order for arbitrary $i \neq j$ we get

$$\nu^1(\mathbf{k}) = \frac{\nu^1(\mathbf{k}^{i,j}, k_i - 1, k_j - 1)}{g_i(\mathbf{k}) \, g_j(\mathbf{k}^i, k_i - 1)} = \frac{\nu^1(\mathbf{k}^{i,j}, k_i - 1, k_j - 1)}{g_j(\mathbf{k}) \, g_i(\mathbf{k}^j, k_j - 1)} \, , \tag{4.33}$$

and (4.7) immediately follows.

4.3 Hydrodynamics

In this section we derive the hydrodynamic limit for the n-component zero range process and analyze the properties of the resulting system of conservation laws.

4.3.1 The hydrodynamic limit

Analogous to the outline given in Section 2.1.4 we show that under Eulerian scaling $t \to t/L$, $x \to u = x/L$ in the limit $L \to \infty$ the time evolution of the local particle densities $\boldsymbol{\rho}(t,u)$ is given by the following system of conservation laws:

$$\partial_t \rho_i(t,u) + \sum_{k=1}^{d} \partial_{u_k} J_i^k\big(\boldsymbol{\rho}(t,u)\big) = 0\;, \quad i = 1,\dots,n\;, \tag{4.34}$$

where $J_i^k\big(\boldsymbol{\rho}\big)$ is the k-th spatial component of the current $J_i(\boldsymbol{\rho})$ of species i defined in (4.16), and $u = (u_1,\dots,u_d) \in \mathbb{T}^d = \big(\mathbb{R}/\mathbb{Z}\big)^d$ is the continuous space variable on the d-dimensional unit torus. To prove convergence to (4.34), the dynamics of the zero range process has to be well defined in the limit $L \to \infty$ which is guaranteed by (4.4). We also need to impose an extra condition on the stationary measure, which is needed for the one-block estimate as one important part of the convergence proof (see Lemma 4.6 in Section 4.3.3). There are two alternatives. The first one is to require that the partition function $Z(\boldsymbol{\mu})$ is finite for all $\mu \in \mathbb{R}^n$, which is equivalent to the existence of finite exponential moments, i.e.

$$\big\langle \exp[\boldsymbol{\theta}\cdot\boldsymbol{\eta}(0)]\big\rangle_{\bar\nu_{\boldsymbol{\mu}}} = Z(\boldsymbol{\mu}+\boldsymbol{\theta})/Z(\boldsymbol{\mu}) < \infty \text{ for all } \boldsymbol{\theta}\in\mathbb{R}^n \quad \Leftrightarrow \quad D_\mu = \mathbb{R}^n\;. \tag{4.35}$$

Note that this implies $D_\rho = (0,\infty)^n$, avoiding possible problems in case $\boldsymbol{\rho}(t,u)$ reaches the boundary of D_ρ. Alternatively, we can impose sublinearity of the jump rates, i.e. for all $i \in \{1,\dots,n\}$

$$\lim_{n\to\infty} \sup_{\substack{|\mathbf{k}|\ge n\\ k_i>0}} g_i(\mathbf{k})/k_i = 0 \quad \text{and} \quad \lim_{\boldsymbol{\mu}\to\boldsymbol{\mu}^*} Z(\boldsymbol{\mu}) = \infty \text{ for all } \boldsymbol{\mu}^* \in \partial D_\mu\;. \tag{4.36}$$

The second statement is needed to ensure $D_\rho = (0,\infty)^n$, since sublinearity does not rule out $D_\mu \subsetneq \mathbb{R}^n$. Given a solution $\boldsymbol{\rho}(t,u)$ of (4.34) we denote the corresponding local equilibrium measure by $\nu^L_{\boldsymbol{\rho}(t,.)}$, which is compared to the time dependent distribution π_t^L of the zero range process:

$$\nu^L_{\boldsymbol{\rho}(t,.)} := \prod_{x\in\Lambda_L} \nu^1_{\boldsymbol{\rho}(t,x/L)} \qquad \text{and} \qquad \pi_t^L = \pi_0^L S_{tL}\;, \tag{4.37}$$

where S_{tL} is the semi-group S_t associated to the generator $\mathcal{L}$ speeded up by L. The proof of the following theorem is an application of Yau's relative entropy method [141], which requires some regularity of the solution $\boldsymbol{\rho}(t,u)$. Since the solutions of (4.34) in general develop shocks after a finite time even for smooth initial data (cf. Section 2.1.4), the convergence proof is valid only up to the time T of the appearance of the first discontinuity.

Theorem 4.3 (Hydrodynamic limit)
Let $\boldsymbol{\rho} \in C^2\big([0,T]\times\mathbb{T}^d, [0,\infty)^n\big)$ be a solution of (4.34) for some $T \in (0,\infty)$ with smooth and bounded initial profile $\boldsymbol{\rho}(0,.)$, satisfying $\rho_i(0,u) \ge \rho_i^* > 0$, $i = 1,\dots,n$. Under the assumption (4.35) or (4.36) let π_0^L be a sequence of probability measures on X_L, whose entropy $H\big(\pi_0^L\big|\nu^L_{\boldsymbol{\rho}(0,.)}\big)$ relative to $\nu^L_{\boldsymbol{\rho}(0,.)}$ is of order $o(L^d)$. Then

$$H\big(\pi_t^L\big|\nu^L_{\boldsymbol{\rho}(t,.)}\big) = o(L^d) \quad \textit{for all } \; t\in[0,T]\;. \tag{4.38}$$

Proof. The proof of Theorem 4.3 is close to the ones given in [84, 133] and its most important steps are sketched in Section 4.3.3.

Applying the entropy inequality (A.11) in the standard way, Theorem 4.3 implies the following.

Corollary 4.4 *Under the assumptions of Theorem 4.3, for any continuous test function $f \in C(\mathbb{T}^d)$, $t \in [0,T]$ and $i = 1,\dots,n$, we have the limit*

$$\lim_{L\to\infty} \left\langle \left| \frac{1}{L^d} \sum_{x\in\Lambda_L} f(x/L)\,\eta_i(x) - \int_{\mathbb{T}^d} f(u)\,\rho_i(t,u)\,d^d u \right| \right\rangle_{\pi_t^L} = 0\,. \tag{4.39}$$

Proof. See [84], Corollary 6.1.3.

This shows convergence of the density profiles, but in principle $\eta_i(x)$ could also be replaced by any bounded cylinder function h, and $\rho_i(t,u)$ by $\langle h\rangle_{\nu^L_{\boldsymbol{\rho}(t,u)}}$ respectively.

4.3.2 Properties of the limit equation

We introduce the matrices $D\mathbf{J}^k(\boldsymbol{\rho}) := \big(\partial_{\rho_j} J_i^k\big)_{i,j}$ giving the derivative of the current in direction $k \in \{1,\dots,d\}$,

$$D\mathbf{J}^k(\boldsymbol{\rho}) = \Delta^k(\boldsymbol{\rho})\, D\mathbf{M}(\boldsymbol{\rho}) \quad \text{with} \quad \Delta^k_{i,j}(\boldsymbol{\rho}) = \delta_{i,j}\, m_k(p_i)\, \exp\big[M_i(\boldsymbol{\rho})\big]\,, \tag{4.40}$$

where Δ^k is a diagonal matrix and $m_k(p_i)$ is the k-th space component of $m(p_i)$. Using this, one can rewrite (4.34) in the quasilinear form

$$\partial_t \boldsymbol{\rho}(t,u) + \sum_{k=1}^d D\mathbf{J}^k\big(\boldsymbol{\rho}(t,u)\big)\,\partial_{u_k}\boldsymbol{\rho}(t,u) = 0\,. \tag{4.41}$$

Definition. A system of conservation laws in quasilinear form (4.41) is called *hyperbolic*, if the matrix $\sum_{k=1}^d \omega_k D\mathbf{J}^k$ is diagonalizable for all $\boldsymbol{\omega} = (\omega_1,\dots,\omega_d) \in \mathbb{R}^d$ with $|\boldsymbol{\omega}| = 1$ (cf. [135]). The system is called *strictly hyperbolic*, if additionally all its eigenvalues $\lambda_i(\boldsymbol{\rho})$ are non-degenerate in the (strict) uniform sense

$$\big\{\lambda_i(\boldsymbol{\rho}) \,\big|\, \boldsymbol{\rho} \in D_\rho\big\} \cap \big\{\lambda_j(\boldsymbol{\rho}) \,\big|\, \boldsymbol{\rho} \in D_\rho\big\} = \emptyset \tag{4.42}$$

for all $i \neq j \in \{1,\dots,n\}$.

Definition. A strictly convex function $S \in C^1([0,\infty)^n, \mathbb{R})$ is called *Lax entropy* of the system (4.41), if there exists an *entropy flux* $F \in C^1([0,\infty)^n, \mathbb{R}^d)$ such that

$$\sum_{i=1}^n \partial_{\rho_i} S(\boldsymbol{\rho})\,\big(D\mathbf{J}^k\big)_{i,j}(\boldsymbol{\rho}) = \partial_{\rho_j} F_k(\boldsymbol{\rho})\,, \tag{4.43}$$

for all $j = 1,\dots,n$, $k = 1,\dots,d$.

For weak solutions of (4.34) the Lax entropies obey an inequality analogous to (2.33).

Proposition 4.5 *The limit system of conservation laws (4.41) is hyperbolic and the negative thermodynamic entropy $-S(\boldsymbol{\rho})$ defined in (4.17) is a Lax entropy for this system.*

The question of strict hyperbolicity, i.e. whether all eigenvalues of $\sum_{k=1}^{d} \omega_k D\mathbf{J}^k$ are non-degenerate, cannot be answered in general. It depends on the dynamics of the ZRP, in particular also on the moments of the jump probabilities as discussed below, and one has to check for each system separately. With (4.40) we also see that $D\mathbf{J}^k(\boldsymbol{\rho}) D^2 \log Z\big(\mathbf{M}(\boldsymbol{\rho})\big) = \Delta^k(\boldsymbol{\rho})$ is diagonal. In particular this means that the Onsager reciprocity relations, requiring the symmetry of this matrix (cf. [53, 133]), are fulfilled for our system.

Proof. Since $D\mathbf{M}(\boldsymbol{\rho}) = D^2 S(\boldsymbol{\rho})$ is symmetric and positive definite there exists a unique matrix $A \in \mathbb{R}^{n\times n}$ with the same properties and $A^2 = D^2 S$, so we write $A = (D^2 S)^{1/2}$. With (4.40) we have for all $k = 1, \dots, d$

$$D\mathbf{J}^k = \big(D^2 S\big)^{-1/2} \Big(\big(D^2 S\big)^{1/2} \Delta^k \big(D^2 S\big)^{1/2} \Big) \big(D^2 S\big)^{1/2} . \tag{4.44}$$

Thus $D\mathbf{J}^k$ is similar to the real symmetric matrix $\big(D^2 S\big)^{1/2} \Delta^k \big(D^2 S\big)^{1/2}$, which implies that $\sum_{k=1}^{d} \omega_k D\mathbf{J}^k$ is diagonalizable for all $|\boldsymbol{\omega}| = 1$ and that (4.41) is hyperbolic.

With (4.18) and (4.40) it is easy to see that $S(\boldsymbol{\rho})$ satisfies (4.43), provided we set $F(\boldsymbol{\rho}) = \sum_{j=1}^{n} \mathbf{m}(p_j)(M_j(\boldsymbol{\rho}) - 1) \exp[M_j(\boldsymbol{\rho})]$. □

The equations (4.43) are the dn defining relations for entropy entropy-flux pairs of hyperbolic systems (cf. (2.33) and [26, 135]). In the single species case $n = 1$ there can be many solutions for the $d + 1$ unknowns as discussed in Section 2.1.4. But for general systems with $n \geq 2$ these equations can be overdetermined and the existence of an entropy entropy-flux pair is not guaranteed. A special case is $n = 2$ and $d = 1$ for which $dn = d + 1$ and there is a well defined solution, as discussed in [133, 132]. However, as we just have shown, the hydrodynamic equation of the ZRP (2.30) has always a strictly convex entropy $-S$, defined in (4.17), with corresponding entropy flux F.

Systems of conservation laws with entropy are studied in detail in [135]. In general, by transformation to the so-called entropy variables the quasilinear equation (4.41) simplifies to a symmetric system. In our case these variables are given by the chemical potentials $\boldsymbol{\mu}(t,u) := \mathbf{M}\big(\boldsymbol{\rho}(t,u)\big)$ and the derivative of the current with respect to $\boldsymbol{\mu}$ is even diagonal,

$$D\mathbf{R}\big(\boldsymbol{\mu}(t,u)\big)\, \partial_t \boldsymbol{\mu}(t,u) + \sum_{k=1}^{d} \Delta^k\big(\boldsymbol{\mu}(t,u)\big)\, \partial_{u_k} \boldsymbol{\mu}(t,u) = 0 \,, \tag{4.45}$$

where $\Delta^k_{i,j}(\boldsymbol{\mu}) := \delta_{i,j}\, m_k(p_i)\, \exp[\mu_i]$ as defined in (4.40).

To summarize, we have shown that the limit equation (4.34) is a hyperbolic system with globally convex entropy. General results on the existence and uniqueness of solutions of such systems are rare, even for the simple form (4.45). So further results for systems with open boundaries are based on solid arguments rather than rigorous proofs and presented in Section 4.4. Existence and uniqueness of weak solutions for strictly hyperbolic systems has been established for $n = 1, 2$ in $d = 1$ dimensions under some additional assumptions involving the nonlinearity of the current ([26], Chapters XI and XII).

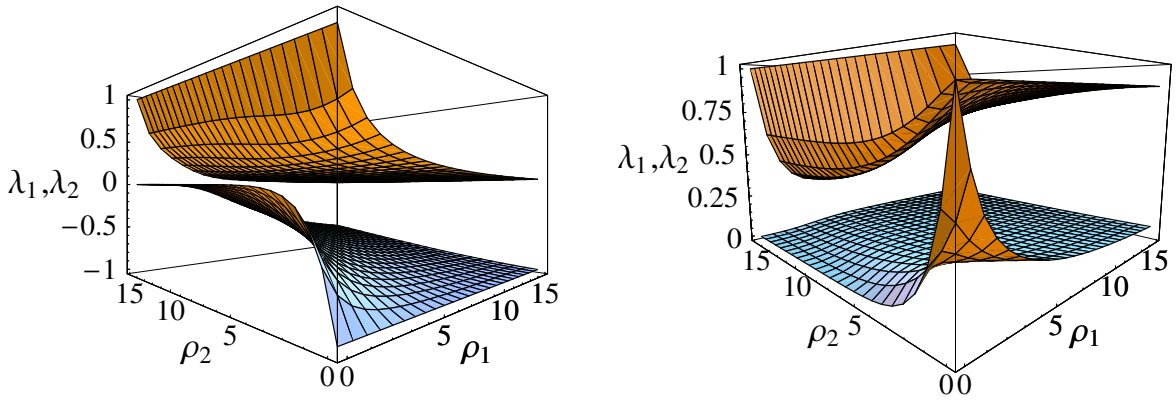


Figure 4.2: Eigenvalues λ_1, λ_2 of the current derivative $D\mathbf{J}$ (4.40) as a function of ρ_1 and ρ_2, for the model given by the partition function in (4.46). **Left:** $m(p_1) = -1$, $m(p_2) = 1$ and the system is strictly hyperbolic. **Right:** Strict hyperbolicity is violated for the choice $m(p_1) = 0.9$, $m(p_2) = 1$.

For two-component systems in one dimension strict hyperbolicity is guaranteed if the moments of the jump probabilities have different sign, for example $m(p_1) < 0 < m(p_2)$. The reason is that the determinant of the current matrix $D\mathbf{J}(\rho_1, \rho_2)$ (4.40) is proportional to the product $m(p_1)\, m(p_2) < 0$, and thus the eigenvalues also have different sign. But if both species are driven in the same direction strict hyperbolicity (4.42) is in general not satisfied. We illustrate this for example (4.21) with modified rate $g_1(k_1, k_2) = k_1 \left(\frac{k_1}{1+k_1}\right)^{k_2}$, where

$$\log Z(\mu_1, \mu_2) = \exp[\mu_2] + \exp\left[\mu_1 + e^{\mu_2}\right], \tag{4.46}$$

with $D_\mu = \mathbb{R}^2$, so (4.35) is fulfilled and Theorem 4.3 applies. The densities $\mathbf{R}(\boldsymbol{\mu})$ and their inverse can be computed in direct analogy to (4.23) and (4.24). Thus the current matrix $D\mathbf{J}$ with eigenvalues $\lambda_1(\rho_1, \rho_2)$, $\lambda_2(\rho_1, \rho_2)$ are given explicitly, but we omit the lengthy formulas. In Figure 4.2 we plot the eigenvalues as a function of the densities and see that they are well separated as long as $m(p_1)$ and $m(p_2)$ have different sign (left). This is not true if both have the same sign and can be seen especially well if they have similar absolute value (right). In general the eigenvalue surfaces can also intersect, which could be seen for the original example (4.21), although our proof of the hydrodynamic limit does not work in this case.

4.3.3 Proof of Theorem 4.3

The proof follows closely the one given in [84], Chapter 6, and [133] and we only sketch the main steps. The only part where we have to use the special structure of the stationary measures for n-component systems is (4.52), where additional terms cancel due to the symmetry of $D\mathbf{M}(\boldsymbol{\rho})$. Since π_t^L and $\nu^L_{\boldsymbol{\rho}(t,.)}$ are absolutely continuous with respect to each other and

with respect to an invariant reference measure $\nu^L_{\boldsymbol{\alpha}}$, $\boldsymbol{\alpha} \in (0,\infty)^n$, one can define the density

$$\psi^L_t(\boldsymbol{\eta}) := \frac{d\nu^L_{\boldsymbol{\rho}(t,.)}}{d\nu^L_{\boldsymbol{\alpha}}} = \prod_{x\in\Lambda_L} \frac{Z\big(\mathbf{M}(\boldsymbol{\alpha})\big)}{Z\big(\mathbf{M}(\boldsymbol{\rho}(t,x/L))\big)} \prod_{i=1}^n \frac{\exp\big[\eta_i(x) M_i\big(\boldsymbol{\rho}(t,x/L)\big)\big]}{\exp\big[\eta_i(x) M_i(\boldsymbol{\alpha})\big]} \,. \tag{4.47}$$

Let $H_L(t) := H\big(\pi^L_t \big| \nu^L_{\boldsymbol{\rho}(t,.)}\big)$ be the entropy of π^L_t relative to $\nu^L_{\boldsymbol{\rho}(t,.)}$. To establish the estimate (4.38), we prove a Gronwall type inequality

$$H_L(t) \le H_L(0) + C\int_0^t H_L(s)\, ds + o(L^d) \tag{4.48}$$

with uniform error bound for all $t \in [0,T]$. The entropy production is bounded above by

$$\partial_t H_L(t) \le \Big\langle \frac{1}{\psi^L_t(\boldsymbol{\eta})} \Big(L\mathcal{L}^*\psi^L_t(\boldsymbol{\eta}) - \partial_t \psi^L_t(\boldsymbol{\eta}) \Big) \Big\rangle_{\pi^L_t} \,, \tag{4.49}$$

where $\mathcal{L}^*$ is the adjoint of $\mathcal{L}$ in $L^2(\nu^L_{\boldsymbol{\alpha}})$, the set of square integrable functions w.r.t. $\nu^L_{\boldsymbol{\alpha}}$. This inequality is proved in [84], Lemma VI.1.4, under very general conditions covering our case. Using the regularity of $\mathbf{M}\big(\boldsymbol{\rho}(t,.)\big)$, the right hand side of (4.49) can be rewritten as

$$\begin{aligned}
\big(\psi^L_t(\boldsymbol{\eta})\big)^{-1} L\mathcal{L}^*\psi^L_t(\boldsymbol{\eta}) &= -\sum_{i=1}^n \sum_{x\in\Lambda_L} \sum_{k=1}^d \partial_{u_k} J^k_i\big(\boldsymbol{\rho}(t,x/L)\big) \\
&\quad - \sum_{i=1}^n \sum_{x\in\Lambda_L} \sum_{k=1}^d \partial_{u_k} M_i\big(\boldsymbol{\rho}(t,x/L)\big) \Big(m_k(p_i)\, g_i\big(\boldsymbol{\eta}(x)\big) - J^k_i\big(\boldsymbol{\rho}(t,x/L)\big)\Big) + O(L^{d-1}) \\
\big(\psi^L_t(\boldsymbol{\eta})\big)^{-1} \partial_t \psi^L_t(\boldsymbol{\eta}) &= \sum_{i=1}^n \sum_{x\in\Lambda_L} \partial_t\, M_i\big(\boldsymbol{\rho}(t,x/L)\big) \Big(\eta_i(x) - \rho_i(t,x/L)\Big) \,.
\end{aligned} \tag{4.50}$$

The right hand side of the first line is a telescoping sum and vanishes up to an error $O(L^{d-1})$. Because of the regularity of $\mathbf{M}(\boldsymbol{\rho})$ a summation by parts permits to replace the local variables by their block averages. Those are defined as

$$\eta^\ell_i(x) = \frac{1}{(2\ell+1)^d} \sum_{|x-y|\le\ell} \eta_i(y) \,, \quad g^\ell_i(\boldsymbol{\eta})(x) = \frac{1}{(2\ell+1)^d} \sum_{|x-y|\le\ell} g_i\big(\boldsymbol{\eta}(y)\big) \tag{4.51}$$

for $i = \{1,\dots,n\}$ and $\ell \in \mathbb{Z}^+$. Using the hyperbolic system (4.34) and the symmetry of $D\mathbf{M}$ we obtain

$$\partial_t M_i\big(\boldsymbol{\rho}(t,x/L)\big) = -\sum_{j=1}^n \sum_{k=1}^d \partial_{\rho_i} J^k_j\big(\boldsymbol{\rho}(t,x/L)\big)\, \partial_{u_k} M_j\big(\boldsymbol{\rho}(t,x/L)\big) \,. \tag{4.52}$$

Inserting (4.51) and (4.52) into (4.50), we get

$$\begin{aligned}
&\Big\langle \frac{1}{\psi^L_t} \Big(\partial_t\psi^L_t - L\mathcal{L}^*\psi^L_t \Big) \Big\rangle_{\pi^L_t} = \\
&\qquad = \Big\langle \sum_{i=1}^n \sum_{x\in\Lambda_L} \sum_{k=1}^d \partial_{u_k} M_i\big(\boldsymbol{\rho}(t,x/L)\big) \, \Big(m_k(p_i)\, g^\ell_i(\boldsymbol{\eta})(x) - J^k_i\big(\boldsymbol{\eta}^\ell(x)\big)\Big) \Big\rangle_{\pi^L_t} \\
&\qquad\quad + \Big\langle \sum_{i=1}^n \sum_{x\in\Lambda_L} \sum_{k=1}^d \partial_{u_k} M_i\big(\boldsymbol{\rho}(t,x/L)\big) \, f^k_i\Big(\boldsymbol{\eta}^\ell(x), \boldsymbol{\rho}(t,x/L)\Big) \Big\rangle_{\pi^L_t} \,,
\end{aligned} \tag{4.53}$$

where we define

$$f_i^k(\mathbf{a},\mathbf{b}) = J_i^k(\mathbf{a}) - J_i^k(\mathbf{b}) - \boldsymbol{\nabla} J_i^k(\mathbf{b})\cdot(\mathbf{a}-\mathbf{b}) \tag{4.54}$$

for all $\mathbf{a}, \mathbf{b} \in \mathbb{R}^n$. A bound for the second term on the right hand side of (4.53) can be derived from the entropy inequality given in the appendix (A.11). Dropping the argument of f_i^k

$$\left\langle \sum_{i=1}^{n}\sum_{x\in\Lambda_L}\sum_{k=1}^{d} \partial_{u_k} M_i\big(\boldsymbol{\rho}(t,x/L)\big)\,\big|f_i^k\big| \right\rangle_{\pi_t^L} \leq CH\big(\pi_t^L\big|\nu^L_{\boldsymbol{\rho}(t,.)}\big) + O(L^d\ell^{-1})\,. \tag{4.55}$$

The first term is estimated integrated over the compact time interval $[0,t]$, $t \leq T$, by using the so-called one-block estimate, which we quote in a slightly specialized version to fit our purposes.

Lemma 4.6 (One-block estimate)
With either one of the two regularity assumptions (4.35) or (4.36) on the stationary measure it is for all $t \in [0,T]$

$$\lim_{\ell\to\infty}\lim_{L\to\infty} L^{-d}\left\langle \sum_{i=1}^{n}\sum_{x\in\Lambda_L}\sum_{k=1}^{d}\Big|m_k(p_i)\,g_i^\ell(\boldsymbol{\eta})(x) - J_i^k\big(\boldsymbol{\eta}^\ell(x)\big)\Big| \right\rangle_{\pi_t^L} = 0\,. \tag{4.56}$$

Proof. A proof in a more general context can be found in [84], Lemma V.3.1.

Inserting (4.55) and (4.56) into (4.53) we obtain (4.48) via (4.49) and Theorem 4.3 follows.

4.4 Stationary solutions for systems with open boundaries

We turn to one of the motivations of this chapter and apply the results of the previous sections to determine stationary density profiles of multicomponent systems with open boundary conditions. The following results are based on solid arguments rather than rigorous proofs, since general results on hyperbolic conservation laws like (4.34) are rare. They have to be analyzed from case to case and we explicitly state our assumptions, which one would have to prove to make the arguments rigorous.

4.4.1 Uniqueness criterion for the physical solution

Although (4.34) is derived only up to the first discontinuity, we assume in the following the validity of the hydrodynamic equation in the sense of weak solutions. They are in general not unique and we have to use a criterion to single out the physical solution, as explained in Section 2.1.4. One possibility is to add a viscosity term with a small parameter ϵ to the right hand side of (4.34). A natural choice is the diffusive first order correction term which was neglected in the derivation, where the small parameter is interpreted as the lattice constant $\epsilon = O(1/L)$. This is of the form $\sum_{k,l=1}^{d} D^i_{k,l}\partial^2_{u_k u_l}$ where for every species

$i = 1, \dots, n$ the coefficients of the mixed spatial derivatives are given by the bulk diffusion matrix $D^i \in \mathbb{R}^{d\times d}$ which is a function of $\boldsymbol{\rho}$. This can be calculated by the Green-Kubo formula for the corresponding reversible ZRP with symmetric jump probabilities (see [129], Prop. II.2.1). Since the symmetric ZRP is a gradient system, the dynamic part of the formula, involving current-current correlations, vanishes and the viscosity is already determined by the stationary measure itself. The diffusion matrix is given by

$$D^i_{k,l}(\boldsymbol{\rho}) = \sum_{j=1}^{n} \big(D\mathbf{M}(\boldsymbol{\rho})\big)_{i,j} \exp\big[M_j(\boldsymbol{\rho})\big]\sigma_{k,l}(p_j)\,, \tag{4.57}$$

for $i = 1, \dots, n$, with $\sigma_{k,l}(p_i) = \sum_{x\in\Lambda_L} x_k x_l\, p_i(x)$. Since this involves the inverse of the compressibility $D\mathbf{M} = D\mathbf{R}^{-1}$ the viscosity decouples with respect to the particle species in (4.45) in terms of the entropy variables μ_i,

$$\sum_{j=1}^{n} \big(D\mathbf{R}(\boldsymbol{\mu}^\epsilon)\big)_{i,j}\, \partial_t \mu^\epsilon_j + \sum_{k=1}^{d} m_k(p_i)\, \partial_{u_k} \exp[\mu^\epsilon_i] = \epsilon \sum_{k,l=1}^{d} \sigma_{k,l}(p_i)\, \partial^2_{u_k u_l} \exp[\mu^\epsilon_i]\,. \tag{4.58}$$

The solution $\boldsymbol{\mu}^\epsilon(t,u)$ of this equation is unique and globally well defined (see e.g. [26]), since the second derivatives on the right hand side are positive definite, since they can be written as $\sigma_{k,l}(p_i)\,\partial^2_{u_k u_l} = \big\langle \big(x_1\partial_{u_1} + \ldots + x_n\partial_{u_n}\big)^2\big\rangle_{p_i}$. If $\boldsymbol{\mu}^\epsilon(t,u)$ converges in a proper sense for $\epsilon \searrow 0$, the limit $\boldsymbol{\mu}^0(t,u)$ is a weak solution of (4.45). This convergence is in general very hard to show (see e.g. [135] Chapter 3.8 or [26] Chapter XV and references therein), and in the following we just assume that it holds.

In general, for $d, n > 1$ the limit solution $\boldsymbol{\mu}^0(t,u)$ depends on the choice of the diffusion matrix. A hint that (4.57) singles out the right physical solution is given by comparison with the alternative entropy criterion. Since $D^2S(\boldsymbol{\rho})\Big(\delta_{i,j}\sigma_{k,l}(p_i)\partial_{\rho_j} \exp\big[M_i(\boldsymbol{\rho})\big]\Big)_{i,j}$ is similar to a symmetric, positive definite matrix (analogous to (4.44)), we have for some $\delta > 0$ and arbitrary $\mathbf{a}_k \in \mathbb{R}^n$, $k = 1, \dots, d$,

$$\sum_{k,l=1}^{d} \mathbf{a}_k^T D^2 S(\boldsymbol{\rho})\Big(\delta_{i,j}\sigma_{k,l}(p_i)\,\partial_{\rho_j} \exp\big[M_i(\boldsymbol{\rho})\big]\Big)_{i,j} \mathbf{a}_l \geq \delta \sum_{k=1}^{d} |\mathbf{a}_k|^2 \geq 0\,. \tag{4.59}$$

This expresses the viscous dissipation for the entropy and ensures (see [135], Chapter 3.8) that $\boldsymbol{\mu}^0(t,u)$ satisfies the inequality

$$\partial_t S\big(\mathbf{R}(\boldsymbol{\mu}^0(t,u))\big) + \sum_{k=1}^{d} \partial_{u_k} F_k\big(\boldsymbol{\mu}^0(t,u)\big) \leq 0\,, \tag{4.60}$$

as to be expected for a physical solution (cf. (2.33) in Section 2.1.4). Thus we expect that the zero viscosity limit $\boldsymbol{\mu}^0(t,u)$ describes the macroscopic chemical potential profiles of the zero range process. Note that for time independent solutions, the system (4.58) decouples and stationary profiles can be obtained very easily. They are only determined by the first and second moment of the jump probabilities and the boundary conditions, whereas they are independent of the jump rates. The rates only enter the partition function $Z(\boldsymbol{\mu})$ and thus the transformation to density profiles via $\mathbf{R}(\boldsymbol{\mu}) = D\log Z(\boldsymbol{\mu})$, which is illustrated in the next subsection.

4.4.2 Stationary profiles for one-dimensional systems

There has been considerable activity to understand the structure of the nonequilibrium steady state of systems with open boundaries as discussed in Sections 2.2.3 and 2.2.4. Here we study this issue in one dimension on the level of the hydrodynamic equations, where the space variable is no longer defined on the torus, but $u \in [0,1]$. For the rest of this chapter, we switch to the fugacity variables $\phi_i := \exp[\mu_i]$, since they are more convenient in the following.

The analysis of the previous subsection suggests, that for one-dimensional open systems coupled to reservoirs with densities $\boldsymbol{\rho}(0)$ at the left and $\boldsymbol{\rho}(1)$ at the right, the stationary fugacity profile ϕ_i^0 for every $i \in \{1,\dots,n\}$ is given by the limit solution for $\epsilon \searrow 0$ of the equation

$$m(p_i)\,\partial_u \phi_i^\epsilon(u) = \epsilon\,\sigma(p_i)\,\partial_u^2 \phi_i^\epsilon(u)\;, \tag{4.61}$$

where $\sigma(p_i) = \sum_{x\in\Lambda_L} x^2 p_i(x) > 0$. The boundary conditions are given by the fugacities $\phi_i(0) = \exp\big[M_i(\boldsymbol{\rho}(0))\big]$ and $\phi_i(1)$ respectively. Note that the equations are decoupled and the solution is easily found to be

$$\phi_i^\epsilon(u) = \phi_i(0) + \big(\phi_i(1) - \phi_i(0)\big)\big(r_i^{u/\epsilon} - 1\big)\big/\big(r_i^{1/\epsilon}) - 1\big)\;, \tag{4.62}$$

with the asymmetry ratio $r_i = \exp\big[m(p_i)/\sigma(p_i)\big]$. The profiles (4.62) have a very simple structure. They are bounded above and below by $\phi_i(0)$ and $\phi_i(1)$ respectively, so the solution lies within the domain D_ϕ as long as the boundary values do. For $\epsilon \searrow 0$ they converge pointwise to flat curves $\phi_i^0(u)$ with a discontinuity at one boundary, if $\phi_i(0) \neq \phi_i(1)$. The location of the jump depends only on the sign of $m(p_i)$, which corresponds to the direction of the current. The coupled transformation to the stationary density profile $\rho_i^0(u)$ involves the fugacities of all components and is given by $\rho_i^0 = R_i\big(\log\phi_1^0,\dots,\log\phi_n^0\big)$ defined in (4.12).

Note the similarity of (4.62) to exact density profiles for the ZRP with nearest neighbor jumps $p(y) = p\,\delta_{y,1} + q\,\delta_{y,-1}$ with $p+q=1$ given in (2.71). In this case $r_i = \exp[2p-1]$ for the hydrodynamic solution as compared to the asymmetry parameter $p/(1-p)$ for the exact expression. Both coincide in the symmetric case $p = 1/2$, where the solution would be a linear profile rather than (4.62). For $p \neq 1/2$ the profiles are different for non-zero $\epsilon = 1/L$, but ϕ_i^0 gives the correct profile in the limit $L\to\infty$ and it can be applied to systems with completely general jump probabilities, whereas the exact solution is only available for nearest neighbor jumps. Although there is no quantitative agreement, we expect that the hydrodynamic profile qualitatively shows the correct behavior also for finite L.

We illustrate this result for the two-component system with rates

$$g_1(k_1,k_2) = k_1\left(\frac{k_1}{1+k_1}\right)^{k_2}\;,\quad g_2(k_1,k_2) = \frac{k_2}{1+k_1}\;, \tag{4.63}$$

which has been studied before at the end of Section 4.3.2. The partition function is given by $Z(\phi_1,\phi_2) = \exp\big[\phi_2 + \phi_1 e^{\phi_2}\big]$ (cf. (4.46)) and the densities can be calculated explicitly

$$R_1(\phi_1,\phi_2) = \phi_1\,\exp[\phi_2]\;,\quad R_2(\phi_1,\phi_2) = \phi_2\big(1+\phi_1\,\exp[\phi_2]\big)\;. \tag{4.64}$$

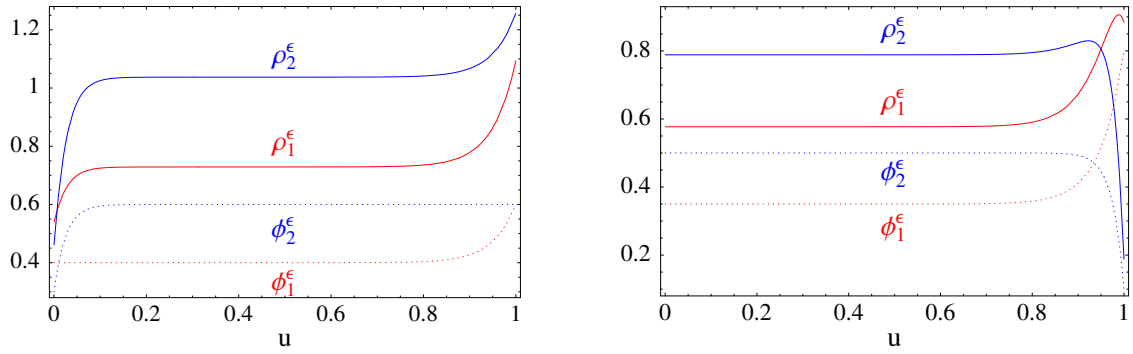


Figure 4.3: Stationary fugacity profiles ϕ_1^ϵ (···), ϕ_2^ϵ (···) and density profiles ρ_1^ϵ (——), ρ_2^ϵ (——) with $\epsilon = 0.05$ for an open system with jump rates (4.63).
Left: $m(p_1) = 1$, $m(p_2) = -2$, $\phi_1(0) = 0.4$, $\phi_2(0) = 0.3$, $\phi_1(1) = 0.6$, $\phi_2(1) = 0.6$.
Right: $m(p_1) = 1$, $m(p_2) = 2$, $\phi_1(0) = 0.35$, $\phi_2(0) = 0.5$, $\phi_1(1) = 0.8$, $\phi_2(1) = 0.1$.

The jump probabilities are chosen such that $\sigma(p_1) = \sigma(p_2) = 1$ and $m(p_1) = 1$. Therefore the bulk value $\phi_1^0(u)$, $u \in (0,1)$ is equal to the left boundary $\phi_1(0)$. For $m(p_2) = 2$ the same is true for ϕ_2 and also the density profiles are determined by their left boundary value. This can be seen in Figure 4.3 (right), where we plot the profiles for small $\epsilon = 0.05$, for better illustration. The only peculiarity in this case is that the density profiles do not have to be monotonic, in contrast to the fugacity profiles. For $m(p_2) = -2$ the particle species are driven in opposite directions, leading to a combination of fugacities in the bulk, which is not present at either of the two boundaries. So the bulk densities do no longer agree with their boundary values, as shown in Figure 4.3 (left).

4.5 Concluding remarks on steady state selection

We have seen in (4.40) that the current derivative $D\mathbf{J}(\boldsymbol{\rho}) \in \mathbb{R}^{n\times n}$ is a regular matrix and thus the mapping $\boldsymbol{\rho} \mapsto \mathbf{J}(\boldsymbol{\rho})$ is invertible. So coexistence of two phases with different densities $\boldsymbol{\rho}^1 \neq \boldsymbol{\rho}^2$ but equal currents $\mathbf{J}(\boldsymbol{\rho}^1) = \mathbf{J}(\boldsymbol{\rho}^2)$ is not possible and there are no boundary induced phase transitions for the n-component ZRP, as have been explained in Section 2.2.3 for exclusion models. This also includes that the eigenvalues of $D\mathbf{J}(\boldsymbol{\rho})$ which determine the characteristic velocities are non-zero for all $\boldsymbol{\rho} \in D_\rho$, so that there are no bulk dominated phases. The steady state selection in open systems is particularly simple in terms of chemical potentials or fugacities. In these variables the stationary viscous equation decouples (4.61) and the solutions ϕ_i^ϵ have the form (4.62) for every process. The bulk value, given by the zero viscosity limit ϕ_i^0, is selected from one of the boundaries, and depends only on the sign of the first moment $m(p_i)$ but not on the boundary values. The jump rates g_i only enter the transformation to density profiles $\mathbf{R}(\boldsymbol{\mu}) = D \log Z(\boldsymbol{\mu})$ through the partition function.

To summarize, the qualitative behavior of the stationary measure of multi-component zero range processes is fixed by the particle drift alone and is independent of the boundary conditions. This is in contrast to one-dimensional driven lattice gases with exclusion dynam-

ics, where a change of sign of the characteristic velocities is the key ingredient for boundary induced phase transitions as explained in Section 2.2.3. But despite the absence of boundary induced critical phenomena, the zero range process is a very important interacting particle system, last but not least due to its close relation to exclusion models (cf. Section 2.3.3). As has been shown in this chapter, it is one of the few examples of multi-species systems, where the selection of stationary states is well understood under very general conditions.

Chapter 5

Condensation transition in the zero range process

5.1 Introduction

In [21, 40] it was noticed that for translation invariant zero range processes a condensation phenomenon can occur, which is similar to the one induced by disorder explained in section 2.3.4. The idea is to choose the jump rates such that the critical density (2.67) is finite, i.e. $\rho_c < \infty$, which characterizes a condensation transition according to Section 2.1.3. This can be realized, if the jump rates $g(k)$ have a slowly decaying tail for $k \to \infty$, inducing an effective attraction between particles. In [40] the borderline case was identified to be $g(k) \simeq a + b/k^\gamma$ with parameters $a, \gamma > 0$ and $b \in \mathbb{R}$. For $0 < \gamma < 1$ and $b > 0$, or for $\gamma = 1$ and $b > 2$ one has $\rho_c < \infty$, whereas for $\gamma > 1$ or faster decaying rates there is no condensation. Mapping such a ZRP to an exclusion model, this form of g would correspond to a long range dependence of the jump rates. So there is no equivalent for this condensation mechanism in finite range exclusion processes, in contrast to the one induced by disorder. However, in [76] it was noticed that the finite size correction of the current of particles leaving a cluster of size k in phase separated two-species exclusion models is just of the form $j(k) \simeq j_0 + b/k^\gamma$ for $k \to \infty$. So this type of (one-component) ZRP can be used as an effective model for the domain wall dynamics of two-species exclusion processes. Depending on the coefficient b and the exponent γ of the first order correction of the current, the results for the ZRP can be used as a criterion for the occurrence of phase separation, discussed in Section 2.2.4.

In addition to its applications to exclusion models this condensation transition is an intriguing phenomenon already for the ZRP itself. In this chapter we study it on the level of the stationary measure, the question of the relaxation dynamics is addressed in Chapter 6. In the next section we establish rigorous results for the condensation transition in the context of the equivalence of ensembles (cf. Section 2.1.2). For general rates $g(k)$, imposing only the regularity assumptions of Section 2.3.1, we prove that in case of condensation the canonical measures are asymptotically equivalent to product measures with critical density ρ_c. This is consistent with the non-rigorous results obtained for special jump rates in [21, 40]. Under additional assumptions we further show that, besides the homogeneous background phase

with density ρ_c, the condensed phase typically consists of a single, randomly located site, where any additional mass is concentrated. This is based on results for large deviations of independent, subexponentially distributed random variables [14, 136] and closely follows a similar proof given in [75]. For the model introduced in [40] with parameter $\gamma = 1$ we analyze the critical behavior and statistical properties of the background phase in detail in Section 5.3. Up to this point, the results have been published in [61]. In Section 5.4 we generalize the rigorous result on the equivalence of ensembles to systems with two species of particles, and discuss a generic example, which has been studied non-rigorously in [43, 66].

5.2 Stationary measures above criticality

Consider a ZRP on the periodic lattice $\Lambda_L = (\mathbb{Z}/L\mathbb{Z})$, with jump rates $g(k)$ and jump probabilities $p(x)$, that fulfill the regularity assumptions (2.56) and (2.57) in Section 2.1.3. We restrict ourselves to one space dimension only for simplicity of the presentation. In fact, the results in this chapter do not depend on the structure of the lattice at all, as long as the stationary measures exist as discussed below. On Λ_L the process has translation invariant, grand canonical stationary measures $\bar{\nu}_\phi$ with fugacity $\phi \in D_\phi$ as defined in (2.65). We recall that D_ϕ is the domain of the particle density $R(\phi)$, given in (2.67) with range $D_\rho = R(D_\phi)$. It can be either $D_\phi = [0, \phi_c)$ or $D_\phi = [0, \phi_c]$, where ϕ_c is the radius of convergence of the partition function $Z(\phi)$ defined in (2.66). In contrast to Chapter 4 we are especially interested in the behavior at the boundary of D_ϕ. We recall the definitions in this context,

$$\bar{\nu}_\phi^1(k) = W(k)\,\phi^k/Z(\phi)\;, \quad W(k) = \prod_{i=1}^{k} 1/g(i)\;, \quad Z(\phi) = \sum_{k=0}^{\infty} W(k)\,\phi^k\;. \tag{5.1}$$

If the particle density exceeds $\rho_c = \lim_{\phi\to\phi_c} R(\phi)$, which could also be infinite, there are no stationary product measures and the system exhibits a condensation transition. In addition to the grand canonical measures there are the canonical stationary measures

$$\mu_{L,N}(\boldsymbol{\eta}) = \frac{1}{Z(L,N)} \prod_{x\in\Lambda_L} W\big(\eta(x)\big)\,\delta(\Sigma_L(\boldsymbol{\eta}), N)\;, \tag{5.2}$$

given in (2.68) for every fixed number of particles $N \in \mathbb{N}$.

5.2.1 Equivalence of ensembles

To formulate our results we have to impose some (mild) regularity conditions on the jump rates $g(k)$. In order to avoid the degenerate case $\phi_c = 0$ we assume that the $g(k)$ are uniformly bounded away from zero, analogous to (4.5). We further require the existence of the Cesaro limit

$$\lim_{k\to\infty} \frac{1}{k} \sum_{i=1}^{k} \log g(i) \quad \in (-\infty, \infty]\;. \tag{5.3}$$

For example, this is fulfilled if the rates are uniformly bounded from above or if $\lim_{k\to\infty} g(k)$ exists in $(0,\infty]$, which could also be infinite. The next lemma summarizes an important relation between the critical values ϕ_c and ρ_c and elementary properties of the corresponding grand canonical measures.

Lemma 5.1 *Given the above assumptions, if $\phi_c = \infty$ it is necessarily $\rho_c = \infty$, whereas for $\phi_c < \infty$, ρ_c can be either infinite or finite. In the second case the partition function is also finite, $Z(\phi_c) < \infty$, and $\bar\nu^1_{\phi_c}$ is a well defined probability measure with finite first moment ρ_c. It decays only subexponentially*

$$\lim_{k\to\infty} \frac{1}{k} \log \bar\nu^1_{\phi_c}(k) = 0 \; . \tag{5.4}$$

On the other hand, for each $0 \le \phi < \phi_c$ the measure $\bar\nu^1_\phi$ has an exponential tail.
If the jump rates $g(k)$ are non-decreasing in k, then $\rho_c = \infty$.

Proof. The first part is shown in [84], Lemma 2.3.3. The tail behavior of $\bar\nu^1_{\phi_c}$ follows directly from assumption (5.3), since with (5.1)

$$\frac{1}{k} \log W(k) = -\frac{1}{k} \sum_{i=1}^{k} \log g(i) \; . \tag{5.5}$$

This ensures existence of the limit (5.4), which vanishes by the definition of ϕ_c. For $\phi < \phi_c$ the asymptotic behavior is given in Chapter 4, Lemma 4.2. If $g(i)$ is a non-decreasing function of i, then $\phi_c = \lim_{i\to\infty} g(i) \in (0,\infty]$ exists and $W(k)\,\phi_c^k = \prod_{i=1}^k \frac{\phi_c}{g(i)} \ge 1$ for all $k \in \mathbb{N}$. Thus $Z(\phi_c)$ diverges and necessarily $\rho_c = \infty$ by the first statement. □

Thus a condensation transition, which is defined by $\rho_c < \infty$ in Section 2.1.3, is only possible if the jump rates are not non-decreasing (see e.g. the model studied in Section 5.3). In this case we have $D_\phi = [0, \phi_c]$ with $\phi_c < \infty$, and the inverse of the density, $\Phi : [0, \rho_c] \to [0, \phi_c]$ is not defined for $\rho > \rho_c$. We extend its definition for all $\rho \in [0,\infty)$ in the following way,

$$\bar\Phi(\rho) = \begin{cases} \Phi(\rho) \;, & \text{for } \rho < \rho_c \quad (\text{inverse of } R(\phi) \text{ given in } (2.67)) \\ \phi_c \;, & \text{for } \rho \ge \rho_c \end{cases} \; . \tag{5.6}$$

Consider the ZRP on Λ_L with $\rho_c < \infty$ and supercritical canonical measures $\mu_{L,\lfloor \rho L \rfloor}$ with $\rho > \rho_c$. The heuristic picture developed in [21] and [40], is that for large L most sites of the system are distributed according to $\bar\nu_{\phi_c}$ with homogeneous density ρ_c, called *background phase* or simply *bulk*. The $(\rho - \rho_c)L$ excess particles presumably condense in a region with vanishing volume fraction, the *condensed phase* or *condensate*. If so, locally one observes the grand-canonical ensemble with $\phi = \phi_c$, justifying the above definition. Consequently, we define the asymptotic bulk density as

$$\rho_{bulk}(\rho) = R\big(\bar\Phi(\rho)\big) = \begin{cases} \rho \;, & \text{if } \rho < \rho_c \\ \rho_c \;, & \text{if } \rho \ge \rho_c \end{cases} \; , \tag{5.7}$$

which serves as an order parameter for the condensation transition (cf. Figure 5.1) in the following sense. For $\rho > \rho_c$, ρ_{bulk} is independent of ρ and gives the density of the background

phase in large, finite systems. For $\rho \leq \rho_c$ there is no condensate and the whole system is homogeneously distributed with density $\rho_{bulk} = \rho$.

These considerations are made precise in Corollary 5.3 and the next theorem, where we use the relative entropy (see appendix (A.7)) as a convenient characterization of the distance between canonical and grand canonical measure (cf. [25]).

Theorem 5.2 *Let $\bar{\Phi}(\rho)$ be defined as in (5.6). Then the relative entropy of the n-point marginals $\mu^n_{L,[\rho L]}$ and $\bar{\nu}^n_{\bar{\Phi}(\rho)}$ asymptotically vanishes, i.e.*

$$\lim_{L\to\infty} H\left(\mu^n_{L,[\rho L]} \,\middle|\, \bar{\nu}^n_{\bar{\Phi}(\rho)}\right) = 0 \,, \tag{5.8}$$

for every $n \in \mathbb{Z}^+$ and $\rho \in [0,\infty)$. The canonical partition functions (2.69) converge as

$$\lim_{L\to\infty} \frac{1}{L} \log Z\big(L,[\rho L]\big) = \log Z(\bar{\Phi}(\rho)) - \rho \log \bar{\Phi}(\rho) = -S(\rho) \,, \tag{5.9}$$

where $S(\rho)$ is the thermodynamic entropy defined in (4.17).

Proof. The proof is given in Section 5.2.3.

Remarks. For every $\mathbf{x} = (x_1,\dots,x_n) \in \Lambda_L^n$ with $x_i \neq x_j$ for $i \neq j$, the n-point marginal is defined as $\mu^n_{L,N}(\mathbf{k}) := \mu_{L,N}(\{\eta_{x_1} = k_1,\dots,\eta_{x_n} = k_n\})$. Since the measure $\mu_{L,N}$ is permutation invariant, the marginals do not depend on the sites x_i individually, but only on their number n. The same is of course true for the translation invariant product measures $\bar{\nu}_\phi$, which are uniquely determined by the one-point marginal $\bar{\nu}^1_\phi$.
Note that the thermodynamic entropy is defined in (4.17) by the Legendre transform

$$S(\rho) = \sup_{\phi\in D_\phi} \big(\rho \log\phi - \log Z(\phi)\big) \,. \tag{5.10}$$

Equality on the right hand side of (5.9) holds even for $\phi_c < \infty$ and $\rho > \rho_c$, where the supremum is attained at the boundary of D_ϕ. This connection will be used in Section 5.4 for two-component systems to get a proper definition of $\bar{\Phi}$ analogous to (5.6).
There are different definitions for the notion 'equivalence of ensembles' in the literature (see e.g. [55]), one of which corresponds to the convergence of the partition functions as given in (5.9). A direct consequence of the first statement (5.8) is the equivalence of ensembles in the following (probabilistic) sense.

Corollary 5.3 (Equivalence of ensembles)
Under the assumptions of Theorem 5.2, for all $\rho \in [0,\infty)$ the canonical measures (5.2) weakly converge to the product measure (5.1),

$$\mu_{L,[\rho L]} \xrightarrow{w} \bar{\nu}_{\bar{\Phi}(\rho)} \,, \quad \text{for } L\to\infty \,, \tag{5.11}$$

for all bounded cylinder test functions in $C_{0,b}(X,\mathbb{R})$.

Proof. Pointwise convergence of finite dimensional marginals follows directly from (5.8) and positivity of the relative entropy (A.8), and this is equivalent to weak convergence for bounded, local test functions. □

In the subcritical case, $\bar{\nu}^1_{\bar{\Phi}(\rho)}$ has some finite exponential moments due to Lemma 5.1. A direct application of the relative entropy inequality (A.11) ensures convergence also for unbounded cylinder functions, which grow at most linearly, such as the particle density. With a different, more complex argument [84] the class of functions can be further generalized.

Proposition 5.4 *For subcritical densities $\rho \in [0, \rho_c)$ the canonical measures $\mu_{L,\lfloor \rho L \rfloor}$ weakly converge to the product measure $\bar{\nu}_{\Phi(\rho)}$ in the limit $L \to \infty$ as in (5.11) for cylinder test functions $f \in C_0(X, \mathbb{R})$ with finite second moment $\langle f^2 \rangle_{\bar{\nu}_{\Phi(\rho)}}$.*

Proof. See [84], Appendix 2.1.

This ensures weak convergence for basically all local observables. But in the supercritical case $\rho > \rho_c$ a weak limit of the canonical measures in this generality does not exist. With Corollary 5.3 the only candidate would be $\bar{\nu}_{\phi_c}$. But this is clearly only the limit for bounded observables, since for instance $\langle \eta(0) \rangle_{\mu_{L,\lfloor \rho L \rfloor}} = \rho > \rho_c$ for every $L \in \mathbb{Z}^+$. In this sense our result is a generalization of the statement for the subcritical case.

5.2.2 Typical configurations

Corollary 5.3 ensures that the volume fraction of the condensed phase vanishes in the limit $L \to \infty$. In principle the condensate phase could still consist of an infinite number of sites, and the question remains, how many such cluster sites exist in a typical configuration for large lattice size L. The answer depends on the large-k behavior of the critical one-point marginal $\bar{\nu}^1_{\phi_c}(k)$, which has a subexponential decay (5.4). If it is a power law, one can show that the excess particles condense on a single, randomly located site. This was first done in [75] for exponents $b > 3$ and we give a straightforward extension of this result to $b > 2$. However, we believe that the result holds also for other subexponential decays, and there is some hope to extend the proof to a wider class of distributions. For a detailed description and results on subexponential distributions we refer the reader to [14, 60].

Theorem 5.5 *Let $\bar{\nu}^1_{\phi_c}(k) \simeq k^{-b}$ have a monotonic decreasing power law tail with $b > 2$ and finite first moment ρ_c. Then for every $\rho > \rho_c$ the normalized maximum occupation number satisfies a weak law of large numbers, namely it converges in probability as*

$$\frac{1}{(\rho - \rho_c)L} \max_{s \in \Lambda_L} \eta(x) \overset{\mu_{L,\lfloor \rho L \rfloor}}{\longrightarrow} 1 \,, \quad \text{for } L \to \infty \,. \tag{5.12}$$

Remarks. By Corollary 5.3 we already know that the condensed phase typically contains of order $(\rho - \rho_c)L + o(L)$ particles in the limit $L \to \infty$, since almost all sites are distributed according to $\bar{\nu}_{\phi_c}$. Theorem 5.5 ensures, that all these excess particles are located on a single site, which is thus the typical volume of the condensed phase.

This interpretation is only valid for typical configurations of large but finite systems. For the process on the infinite lattice $\mathbb{Z}^d$ the canonical measures are not defined and statements like Theorems 5.2 and 5.5 are not possible. But we could ask for the ergodic behavior of the infinite system with initial distribution ν_ρ, $\rho > \rho_c$, and we expect $\nu_\rho S(t) \xrightarrow{w} \nu_{\rho_c}$ for $t \to \infty$ with bounded local test functions, analogous to Corollary 5.3. However it is far from obvious how one could prove such a statement. Ergodic theorems proved by Liggett, such as Theorem 3.1 in Chapter 3, used coupling techniques based on attractivity of the process (cf. Appendix A.2). But the ZRP is attractive if and only if the rates $g(k)$ are non-decreasing (see [84], Theorem 2.5.2), so this method cannot be used in case of a condensation transition according to Lemma 5.1. Moreover, an ergodic statement similar to Theorem 5.5 cannot be true after all. Although reducing due to the coarsening process, the number of cluster sites is certainly infinite for all times and the system does not saturate (cf. Chapter 6).
Theorem 5.5 does not give information on the order of the fluctuations of the condensate. Since this is closely related to the fluctuations of the number of particles in the bulk (discussed in Section 5.3.2), we expect it to be of the order $L^{1/(b-1)}$ for $2 < b < 3$ and $L^{1/2}$ for $b \geq 3$ (where b is the power law exponent in Theorem 5.5). In principle one could refine the statement of the theorem to get a rigorous bound on the rate of convergence which determines the fluctuations. However, for the proof we present below the expected behavior stated above cannot be shown due to technical reasons. So we stick to the weaker but concise formulation which covers the basic behavior in a general setting.

The proof of Theorem 5.5 uses large deviation results on the asymptotic distribution of $\Sigma_L(\boldsymbol{\eta})$ for $L \to \infty$, which we summarize in the following Lemma for our purpose.

Lemma 5.6 *Let $\omega_1, \omega_2, \ldots \in \mathbb{Z}$ be i.i.d. random variables with mean ρ_c and probability distribution $\pi(k) \simeq k^{-b}$ with $b > 2$. Then for every $\rho > \rho_c$ and some constant c,*

$$\begin{aligned} \pi^L\left(\left\{\sum_{i=1}^{L}\omega_i \geq \rho L\right\}\right) &\simeq L\,\pi\big(\{\omega_1 \geq (\rho-\rho_c)L\}\big)\,, \\ \pi^L\left(\left\{\sum_{i=1}^{L}\omega_i = [\rho L]\right\}\right) &\gtrsim c\,L\,\pi\big(\{\omega_1 = [(\rho-\rho_c)L]\}\big) \qquad \text{for } L\to\infty\,. \end{aligned} \tag{5.13}$$

Proof of Lemma 5.6 The first statement is shown in [136] Chapter 1, Corollary 1.1.1 to 1.1.3, the second in [75], Theorem 2.2.

The first line states that under the distribution π the rare event $\{\sum_{i=1}^{L}\omega_i \geq \rho L\}$ in the limit $L \to \infty$ is typically realized by the deviation of a single variable. Note that this has been shown for general subexponential distributions with integrated tail $\mu\big(\{\eta\,|\,\eta \geq k\}\big) \gtrsim \exp[-k^\alpha]$, $\alpha \in (0, 1/2)$ and finite second moment in [14], indicating a possible generalization of the Theorem.

Proof of Theorem 5.5. The proof follows closely the one given in [75], Theorem 2.2 and we only sketch the most important steps. In the following we denote $M_L(\boldsymbol{\eta}) = \max_{x\in\Lambda_L}\eta(x)$.

For convergence in probability (5.12) we have to show that

$$\lim_{L\to\infty} \mu_{L,[\rho L]}\Big(\Big\{\big|M_L/L - (\rho-\rho_c)\big| > \epsilon\Big\}\Big) = 0 \tag{5.14}$$

for every $\epsilon > 0$. By Corollary 5.3 we already know that $\mu_{L,[\rho L]}\big(\{M_L/L > \rho - \rho_c + \epsilon\}\big) \to 0$, since the bulk contains of order $\rho_c L$ particles. So it remains to show that for every $\epsilon > 0$

$$\mu_{L,[\rho L]}\big(\{M_L < r_\epsilon L\}\big) = \frac{\bar\nu^L_{\phi_c}\Big(\Big\{M_L < r_\epsilon L\,,\,\Sigma_L = [\rho L]\Big\}\Big)}{\bar\nu^L_{\phi_c}\big(\{\Sigma_L = [\rho L]\}\big)} \stackrel{L\to\infty}{\longrightarrow} 0\,, \tag{5.15}$$

where we use the shorthand $r_\epsilon = \rho - \rho_c - \epsilon$ and (2.16) to write the canonical measure in the conditional form.We split the event

$$\big\{M_L < r_\epsilon L\big\} = \big\{[L^\sigma] \le M_L < r_\epsilon L\big\} \cup \big\{M_L < [L^\sigma]\big\} \tag{5.16}$$

for some $\sigma \in (0,1)$ which is chosen below. A basic estimate in [75] shows that the probability of the second event on the right hand side vanishes for all $\sigma \in (0,1)$, whereas the first one is the crucial part. Using asymptotic monotonicity of $\bar\nu^1_{\phi_c}$ we obtain with some $C \in \mathbb{R}$

$$\begin{aligned}\bar\nu^L_{\phi_c}\Big(\Big\{[L^\sigma] \le M_L < r_\epsilon L\,,\,\Sigma_L = [\rho L]\Big\}\Big) \le \\ \le C\,L\,\bar\nu^1_{\phi_c}\big([L^\sigma]\big)\,\bar\nu^{L-1}_{\phi_c}\Big(\Big\{\Sigma_{L-1} \ge (\rho_c+\epsilon)(L-1)\Big\}\Big)\,.\end{aligned} \tag{5.17}$$

With the first statement of Lemma 5.6 the right hand side is of order

$$C\,L^2\,\bar\nu^1_{\phi_c}\big([L^\sigma]\big)\,\bar\nu^1_{\phi_c}\big(\{\eta \ge (\rho_c+\epsilon)L\}\big) = O\big(L^{3-b(1+\sigma)}\big)\,. \tag{5.18}$$

On the other hand the denominator of (5.15) is at least of order L^{1-b} due to the second statement of the lemma. Thus if we choose $\sigma \in (2/b, 1)$, (5.15) vanishes for $L \to \infty$ which finishes the proof. □

5.2.3 Proof of Theorem 5.2

We recall the shorthand $\{\boldsymbol{\eta}\,|\,\Sigma_L(\boldsymbol{\eta}) = N\} = \{\Sigma_L = N\}$ and that $\Sigma_L(\boldsymbol{\eta}) = \sum_{x\in\Lambda_L}\eta(x)$ denotes the number of particles. By definition (2.68) of the canonical measure, one has for every $\boldsymbol{\eta} \in X_L$ and $N \in \mathbb{N}$

$$\mu_{L,N}(\boldsymbol{\eta}) = \frac{W^L(\boldsymbol{\eta})\,\delta\big(\Sigma_L(\boldsymbol{\eta}), N\big)}{Z(L,N)}\,, \tag{5.19}$$

where W^L denotes the product measure $W^L(\boldsymbol{\eta}) = \prod_{x\in\Lambda_L} W(\eta(x))$. Thus, using (A.7), for every $\phi \in [0, \phi_c]$, the relative entropy takes the form

$$H\left(\mu_{L,N}\,\middle|\,\bar\nu^L_\phi\right) = \sum_{\boldsymbol{\eta}\in X_{L,N}} \mu_{L,N}(\boldsymbol{\eta})\,\log\frac{W^L(\boldsymbol{\eta})}{\bar\nu^L_\phi(\boldsymbol{\eta})\,Z(L,N)}\,, \tag{5.20}$$

since $\mu_{L,N}$ is absolutely continuous with respect to $\bar\nu_\phi^L$. From (2.65) and (2.69) we conclude

$$\bar\nu_\phi^L(\boldsymbol{\eta})\, Z(\phi)^L = W^L(\boldsymbol{\eta})\, \phi^N \qquad \text{for all } \boldsymbol{\eta} \in X_{L,N} \quad \text{and}$$
$$\bar\nu_\phi^L\big(\{\Sigma_L = N\}\big)\, Z(\phi)^L = Z(L,N)\, \phi^N\,. \tag{5.21}$$

Inserting in (5.20) this yields

$$H\left(\mu_{L,N} \,\middle|\, \bar\nu_\phi^L\right) = -\log \bar\nu_\phi^L\left(\{\Sigma_L = N\}\right). \tag{5.22}$$

At this point we use the sub-additivity of H given in (A.9) to get

$$H\left(\mu_{L,N}^n \,\middle|\, \bar\nu_\phi^n\right) \le -\frac{1}{[L/n]} \log \bar\nu_\phi^L\left(\{\Sigma_L = N\}\right)\,, \tag{5.23}$$

for every $n \in \{1,\dots,L\}$ and $\phi \in [0,\phi_c]$.

Now we set $N = [\rho L]$ with $\rho \in [0,\infty)$. The key point is to maximize $\bar\nu_\phi^L\left(\{\Sigma_L = [\rho L]\}\right)$ by appropriately adjusting $\phi = \bar\Phi(\rho)$ as defined in (5.6). To ensure that the right hand side of (5.23) vanishes we need a subexponential lower bound, which we identify in the following depending on the criticality of ρ.

- In the subcritical case, $\rho < \rho_c$, we have $\bar\Phi(\rho) = \Phi(\rho) < \phi_c$ and according to Lemma 5.1 $\bar\nu_{\Phi(\rho)}$ has exponential moments. Then the variance σ^2 of $\bar\nu_\phi$ is finite and the limit distribution of $(\Sigma_L - (\rho L))/(\sigma\sqrt{L})$ is given by the normal distribution $\mathcal{N}(0,1)$ (cf. (5.40)). By the local limit theorem (see e.g. [57], Chapter 9) we get $\bar\nu_{\Phi(\rho)}^L\big(\{\Sigma_L = [\rho L]\}\big) \simeq 1/\sqrt{L}$ for large L.

- For $\rho = \rho_c$ the decay of $\bar\nu_{\phi_c}$ is subexponential (Lemma 5.1), so its second moment could be infinite, leading to a non-normal limit distribution (cf. (5.41)). Since the first moment of $\bar\nu_{\phi_c}$ is $\rho_c < \infty$, by the local limit theorem for non-normal limit distributions (see also [57], Chapter 9) we obtain the lower bound $\bar\nu_{\phi_c}^L\big(\{\Sigma_L = [\rho_c L]\}\big) \gtrsim 1/L$.

- The supercritical case $\rho > \rho_c$, where $\bar\Phi(\rho) = \phi_c$, can be reduced to the critical one via

$$\bar\nu_{\phi_c}^L\Big(\Big\{\Sigma_L = [\rho L]\Big\}\Big) \ge \bar\nu_{\phi_c}^L\Big(\Big\{\eta(0) = [\rho L] - [\rho_c(L-1)]\,, \Sigma_{L-1} = [\rho_c(L-1)]\Big\}\Big) =$$
$$= \bar\nu_{\phi_c}^1\Big([\rho L] - [\rho_c(L-1)]\Big)\, \bar\nu_{\phi_c}^{L-1}\Big(\Big\{\Sigma_{L-1} = [\rho_c(L-1)]\Big\}\Big)\,. \tag{5.24}$$

  Both terms decay subexponentially, the first one using (5.4) and the second one as in.

Thus in all cases we have a subexponential lower bound on $\bar\nu_{\phi(\rho)}^L\left(\{\Sigma_L = [\rho L]\}\right)$ and the first part (5.8) of the theorem follows for all $\rho \in [0,\infty)$ from (5.23),

$$\lim_{L\to\infty} H\Big(\mu_{L,[\rho L]}^n \,\Big|\, \bar\nu_{\phi(\rho)}^n\Big) \le -\lim_{L\to\infty} \frac{1}{[L/n]} \log \bar\nu_{\phi(\rho)}^L\big(\{\Sigma_L = [\rho L]\}\big) = 0\,. \tag{5.25}$$

To establish (5.9) we use the second line of (5.21) and immediately get

$$\frac{1}{L}\log Z(N,L) - \frac{1}{L}\log \bar\nu_\phi^L\left(\{\Sigma_L = N\}\right) = \log Z(\phi) - \frac{N}{L}\log\phi\,, \tag{5.26}$$

for all N, L. With $N = [\rho L]$ and $\phi = \bar\Phi(\rho)$ we can use the above estimates, so that the second term on the left vanishes in the limit $L \to \infty$ and assertion (5.9) follows. □

In this proof we basically exploit the permutation invariance of the measures so that the relative entropy takes the simple form (5.22), which was first noticed in the context of information theory [25]. In the supercritical case $\rho > \rho_c$ this is the negative logarithm of a large deviation probability. In contrast to the proof of Theorem 5.3, we only need a subexponential lower bound, which can be obtained without restrictions on ν_{ϕ_c}.

5.3 Analysis of a generic example

In this section we analyze and apply the previous results to the generic model introduced in [40]. The jump rates are

$$g(k) = \Theta(k)\big(1 + b/k^{\gamma}\big) \,, \tag{5.27}$$

where $\Theta(0) = 0$ and $\Theta(k) = 1$ for $k > 0$.

5.3.1 Stationary measures and the phase diagram

The stationary weight for this process is given by

$$W(k) = \prod_{i=1}^{k} \frac{1}{g(i)} = (k!)^{\gamma} \Big/ \prod_{i=1}^{k} (i^{\gamma} + b) \tag{5.28}$$

The radius of convergence of the grand canonical partition function $Z(\phi) = \sum_k W(k)\phi^k$ (2.66) is $\phi_c = \lim_{k\to\infty} g(k) = 1$. Thus the critical grand canonical measure $\nu_{\phi_c}(k)$ is just given by $W(k)$ modulo normalization.

For $\gamma = 1$ the weight can be written as

$$W(k) = \frac{k!}{(1+b)_k} = \frac{k!\,\Gamma(1+b)}{\Gamma(1+b+k)} \simeq \Gamma(1+b)\, k^{-b} \,, \quad \text{for } k \to \infty \,, \tag{5.29}$$

where $(a)_k = \prod_{i=0}^{k-1}(a+i)$ is the Pochhammer symbol. Thus for large k, $\nu_{\phi_c}(k)$ decays like a power law with exponent b. The grand canonical partition function is given by

$$Z(\phi) = {}_2F_1(1,1;1+b;\phi) := \sum_{k=0}^{\infty} \frac{(1)_k (1)_k}{(1+b)_k} \frac{\phi^k}{k!} \,, \tag{5.30}$$

where ${}_2F_1$ denotes the hypergeometric function (see e.g. [1]). The particle density (2.67) is given by

$$R(\phi) = \frac{\phi\, {}_2F_1(2,2;2+b;\phi)}{(1+b)\, {}_2F_1(1,1;1+b;\phi)} \quad \text{for } \phi < 1, \tag{5.31}$$

and the critical density can be calculated exactly (cf. next subsection) to be

$$\rho_c = \lim_{\phi\to 1} R(\phi) = \begin{cases} \infty & , \text{ for } b \le 2 \\ 1/(b-2) & , \text{ for } b > 2 \end{cases} . \tag{5.32}$$

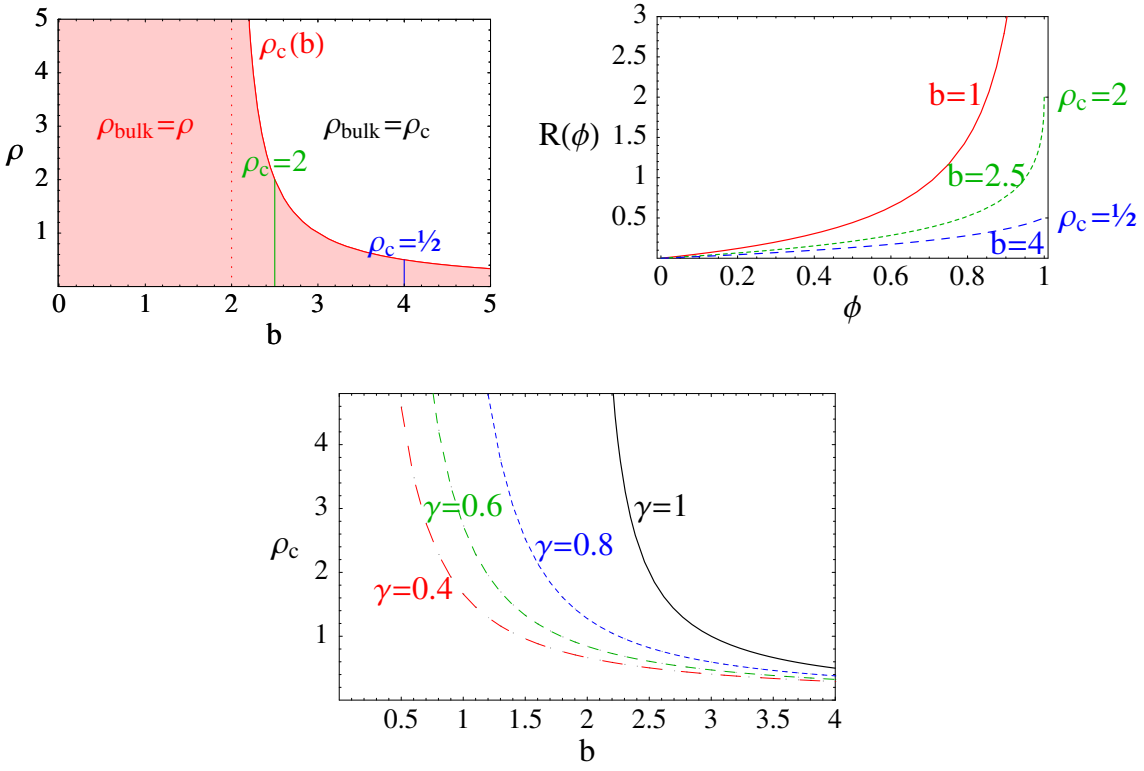


Figure 5.1: Condensation transition for the process (5.27). **Top left:** Phase diagram for $\gamma = 1$. The red region denotes the set of grand canonical product measures (homogeneous phase) bounded by the critical density $\rho_c(b)$ for $b > 2$. For canonical measures in the white region with $\rho > \rho_c$ the background density is given by $\rho_{bulk} = \rho_c$ (5.7) and the excess particles condensate. **Top right:** Density $R(\phi)$, setting the range of the homogeneous phase for several values of b. **Bottom:** Critical density $\rho_c(b)$ for several values of γ.

Thus for $b > 2$ the system exhibits a condensation transition and the phase diagram is given in Figure 5.1 (left).

For $\gamma \neq 1$ the asymptotic behavior of the critical measure for $k \to \infty$ is

$$\nu^1_{\phi_c}(k) = \frac{C_{k_0}}{Z(1)} \exp\Big[-\sum_{i=k_0}^{k} \log(1+b/i^\gamma)\Big] \sim \exp\Big[-\sum_{i=k_0}^{k} b/i^\gamma\Big] \sim \exp\Big[-\frac{b\,k^{1-\gamma}}{1-\gamma}\Big], \quad (5.33)$$

with some arbitrary constant $k_0 \gg 1$. For $\gamma \in (0,1)$ this corresponds to a stretched exponential decay, leading to a finite critical density $\rho_c < \infty$ for all $b > 0$, and the system exhibits a condensation transition. On the other hand, if $\gamma > 1$ or $b < 0$ there is no asymptotic decay and therefore no condensation.

In principle the stretched exponential tail (5.33) is not covered by Theorem 5.5. Nevertheless we expect condensation on a single site as for $\gamma = 1$, and the restriction should be only due to technical reasons. This is confirmed in Chapter 6 by a numerical study of the condensation dynamics. In contrast to the case $\gamma = 1$, the critical density cannot be deter-

mined explicitly for general γ. The approximation in (5.33) gives the correct behavior of $\nu_{\phi_c}(k)$ for large k but rather poor results for the critical density. Especially if γ is close to 1 and $b < 2$ the results are also qualitatively wrong. On the other hand it is straightforward to compute ρ_c numerically with good precision which is plotted in Figure 5.1 (bottom). Using (5.28) it is easy to see that ρ_c is monotonic increasing in γ and monotonic decreasing in b.

5.3.2 Stationary properties near criticality

Our goal in this section is to study the properties of the invariant measures of the process with $\gamma = 1$ for any $b > 0$. In the previous subsection the partition function and the density are expressed in terms of the hypergeometric function ${}_2F_1$ given in (5.30), (5.31). Around $\phi = 1$ it has the expansion

$$\begin{aligned} {}_2F_1(k,k;k+b;\phi) = \frac{\Gamma(k+b)\Gamma(k-b)}{\Gamma(k)^2}\,(1-\phi)^{b-k}\Big[1+O(1-\phi)\Big] + \\ \frac{\Gamma(k+b)\Gamma(b-k)}{\Gamma(b)^2}\left[1+\frac{k^2}{1+k-b}(1-\phi)+O(1-\phi)^2\right]. \end{aligned} \tag{5.34}$$

We analyze the grand canonical single site measure $\bar{\nu}^1_\phi$ in the limit $\phi \nearrow 1$, i.e. near the critical density ρ_c. According to (5.28) the large-k behavior of $\bar{\nu}^1_1$ is given by the power law $W(k) \simeq \Gamma(1+b)\,k^{-b}$, which determines the background phase for supercritical systems. These distributions have moments up to order $b-1$ and thus different scenarios are encountered under variation of b, which we discuss in the following.

The case $0 < b \leq 1$

For $b \in (0,1)$ the leading order in the asymptotic expansion for $Z(\phi)$ and $R(\phi)$ is given by

$$\begin{aligned} Z(\phi) &\simeq \Gamma(1+b)\Gamma(1-b)\,(1-\phi)^{b-1} \;\to\; \infty\,, \\ R(\phi) &\simeq \frac{\phi}{(1+b)^2(1-b)}\,(1-\phi)^{-1} \;\to\; \rho_c = \infty\,, \end{aligned} \tag{5.35}$$

as $\phi \nearrow 1$. Thus $R(\phi)$ has full range $D_\rho = [0,\infty)$ and for every density there exists a grand canonical product measure $\bar{\nu}^L_{\Phi(\rho)}$ (see Figure 5.2 (left)). The probability of having a fixed number of particles on a given site vanishes with increasing density, as is shown for the example of an empty site in Figure 5.2 (right). Thus in the limit $\phi \nearrow 1$ the number of particles per site diverges with probability one, as one might expect for homogeneous systems with $\rho \to \infty$.

For $b = 1$ this picture does not change qualitatively, but there are logarithmic corrections

$$\begin{aligned} Z(\phi) &= -\frac{\log(1-\phi)}{\phi} \;\to\; \infty\,, \\ \rho(\phi) &= \frac{\phi}{(\phi-1)\log(1-\phi)} - 1 \;\to\; \rho_c = \infty\,, \end{aligned} \tag{5.36}$$

as $\phi \nearrow 1$.

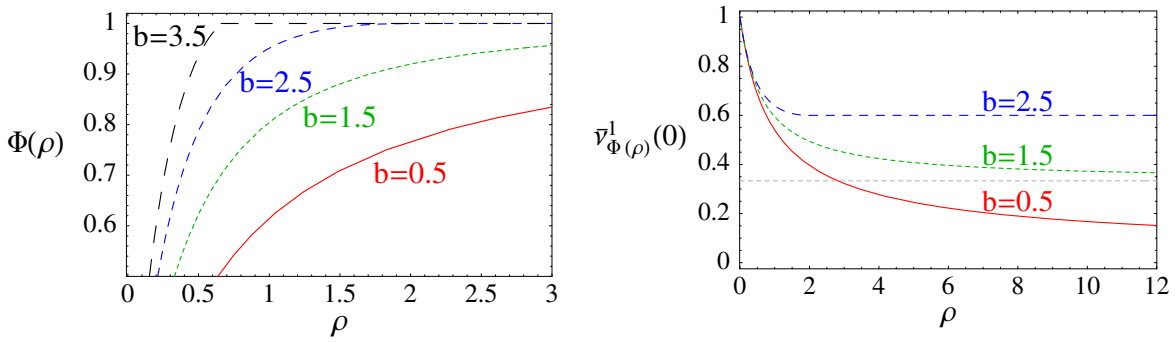


Figure 5.2: Stationary properties of the process (5.27) for $\gamma = 1$ and several values of b. **Left:** Fugacity $\Phi(\rho)$ as a function of the particle density. Note that this is proportional to the current $j(\rho) = m(p)\,\Phi(\rho)$ as given in (2.73). **Right:** Probability of an empty site $\bar\nu^1_{\Phi(\rho)}(0)$ as a function of the density ρ.

The case $1 < b \leq 2$

For $1 < b < 2$ the terms of leading order change, and

$$\begin{aligned} Z(\phi) &\simeq \frac{b}{b-1} + \Gamma(1+b)\,\Gamma(1-b)\,(1-\phi)^{b-1} \;\to\; Z(1) = \frac{b}{b-1}\,, \\ R(\phi) &\simeq \phi\,(b-1)\Gamma(b)\,\Gamma(2-b)\,(1-\phi)^{b-2} \;\to\; \rho_c = \infty\,, \end{aligned} \tag{5.37}$$

as $\phi \nearrow 1$. As before, for $b = 2$ the first order terms have logarithmic corrections but the qualitative behavior does not change. In particular, $D_\rho = [0, \infty)$ and there is a grand canonical stationary measure for every density (see Figure 5.2 (left)).

However, somewhat surprisingly, the character of this distribution for large ρ differs from the case $b \leq 1$. Since $Z(1) < \infty$, $\bar\nu_1^L$ is well defined and there is a non-zero probability of having a fixed number of particles at a given site,

$$\begin{aligned} \bar\nu_1^1(0) &= \frac{1}{Z(1)} = \frac{b-1}{b}\,, \\ \bar\nu_1^1(k) &= \frac{W(k)}{Z(1)} \simeq \Gamma(b)\,(b-1)\,k^{-b} \quad \text{for large } k. \end{aligned} \tag{5.38}$$

For example the probability of an empty site, given by $\bar\nu^1_{\phi(\rho)}(0) = 1/Z(\phi(\rho))$, decreases monotonic with increasing density ρ. In contrast to the case $b \leq 1$, it does not vanish in the limit $\rho \to \infty$, but approaches the non-zero value $\bar\nu_1^1(0) = (b-1)/b$ (see Figure 5.2 (right)). So no matter how large the density is, the fraction of empty sites in a typical configuration is always greater than $(b-1)/b$.

This is a well known phenomenon for distributions with power law tails (see e.g. [15] and references therein). A typical configuration $\boldsymbol{\eta} = \big(\eta(x)\big)_{x\in\Lambda_L}$ for this distribution $\bar\nu_1^1$ is known to have a hierarchical structure. The n-th largest value of $\boldsymbol{\eta}$ scales as $(\Gamma(b-1)L/n)^{1/(b-1)}$, which holds for every $b > 1$. In this particular case, $1 < b \leq 2$, it means that the particle

number $\Sigma_L(\boldsymbol{\eta})$ also scales as $L^{1/(b-1)}$ and thus grows faster than the number of summands L. Therefore the average particle density $\langle \Sigma_L \rangle_{\bar{\nu}_1^1}/L$ diverges as $L^{(2-b)/(b-1)}$ and the highest occupied site contains a non-zero fraction of the particles in the system. This hierarchical structure of typical configurations can be understood as a precursor for the condensation phenomenon to be discussed in the next part.

The case $b > 2$

In this case b is large enough such that besides the normalization also the first moment of the grand canonical distribution converges in the limit $\phi \nearrow 1$,

$$\begin{aligned} Z(\phi) &\simeq \frac{b}{b-1} - \frac{b}{(b-1)(b-2)}\,(1-\phi) && \to\ Z(1) = \frac{b}{b-1}\,, \\ R(\phi) &\simeq \frac{1}{b-2} + \phi(b-1)\Gamma(b)\Gamma(2-b)(1-\phi)^{b-2} && \to\ \rho_c = \frac{1}{b-2}\,. \end{aligned} \tag{5.39}$$

We note that for $b > 3$ also the second moment σ^2 of the distribution $\bar{\nu}_1^1$ exists and the number of particles satisfies the usual central limit theorem

$$\lim_{L\to\infty} \bar{\nu}_1^L \left(\xi_1 \le \frac{\Sigma_L - \rho_c L}{\sigma\sqrt{L}} \le \xi_2 \right) = \int_{\xi_1}^{\xi_2} G(\xi)\, d\xi, \tag{5.40}$$

where G denotes the Gaussian probability density with zero mean and unit variance. The density for $b > 3$ is of order $R(\phi) = 1/(b-2) + O(1-\phi)$ and its first derivative is finite at $\phi = 1$ leading to a kink in the function $\Phi(\rho)$, as can be seen in Figure 5.2 (left) for $b = 3.5$.

As explained already above the highest occupied site contains of order $L^{1/(b-1)}$ particles, and for $b < 3$ this fluctuation is larger than $\sqrt{L}$. Therefore the scaling limit leads to a self-similar distribution, which is given by the completely asymmetric Lévy distribution $\mathcal{L}_{(b-1)}$ (for details see [15] or [57]),

$$\lim_{L\to\infty} \bar{\nu}_1^L \left(\xi_1 \le \frac{\Sigma_L - \rho_c L}{\left(b\,\Gamma(b-1)\,L\right)^{1/(b-1)}} \le \xi_2 \right) = \int_{\xi_1}^{\xi_2} \mathcal{L}_{(b-1)}(\xi)\, d\xi. \tag{5.41}$$

With (5.39) we have $R'(1) = \infty$ for $b < 3$, leading to a differentiable function $\Phi(\rho)$, as shown in Figure 5.2 (left).

5.4 Generalization to two-component systems

As explained in the introduction, critical phenomena in systems with two or more species of particles are of particular interest. In this context a ZRP with two different kinds of particles has been introduced in [43, 66] to study condensation for this process. This is a special case of the n-component system introduced in Chapter 4 with state space $X = (\mathbb{N}\times\mathbb{N})^{\mathbb{Z}}$. The dynamics is defined by the jump rates $g_1,\ g_2 : \mathbb{N}\times\mathbb{N} \to [0,\infty)$, which should fulfill the conditions (4.1) to (4.5) given in Section 4.2.1. In the following, we generalize the rigorous

equivalence result of Section 5.2 on the condensation transition to the two component system. To prepare this we first review the most important properties of the stationary product measures and introduce the notion of condensation for two-component systems.

To concentrate on the main issues, we formulated the following results only for two particle species, but the main ideas can readily be generalized to n-component systems.

5.4.1 Properties of the condensation transition

We consider the process on the periodic lattice $\Lambda_L = (\mathbb{Z}/L\mathbb{Z})$ where the state space is given by $X_L = (\mathbb{N} \times \mathbb{N})^{\Lambda_L}$. It was shown in Section 4.2.2 that there exist stationary product measures if the jump rates fulfill

$$\frac{g_1(k_1, k_2)}{g_1(k_1, k_2 - 1)} = \frac{g_2(k_1, k_2)}{g_2(k_1 - 1, k_2)} \tag{5.42}$$

for all $k_1, k_2 \geq 1$, and in this case the stationary weight can be written as

$$W(k_1, k_2) = \prod_{i_1=1}^{k_1} \big[g_1(i_1, 0)\big]^{-1} \prod_{i_2=1}^{k_2} \big[g_2(k_1, i_2)\big]^{-1} . \tag{5.43}$$

Unlike in Chapter 4, we only use the chemical potentials μ_i within some of the proofs to simplify the notation. But the main parts of this chapter are formulated using the fugacity variables $\phi_i = \exp[\mu_i]$ and the one-point marginals of the grand canonical measures are

$$\bar{\nu}^1_{\boldsymbol{\phi}}(k_1, k_2) = \frac{1}{Z(\phi_1, \phi_2)} W(k_1, k_2)\, \phi_1^{k_1} \phi_2^{k_2} , \tag{5.44}$$

where $\boldsymbol{\phi} = (\phi_1, \phi_2)$ are the fugacities for each species. The grand canonical partition function is given by $Z(\boldsymbol{\phi}) = \sum_{k_1,k_2=0}^{\infty} W(k_1, k_2)\, \phi_1^{k_1} \phi_2^{k_2}$, and we recall the definition (2.67) of the densities $R_i(\boldsymbol{\phi}) = \phi_i \partial_{\phi_i} \log Z(\boldsymbol{\phi})$. In contrast to Chapter 4 we are especially interested in the behavior at the boundary of D_ϕ, the domain of definition of $\mathbf{R}(\boldsymbol{\phi})$. The range of densities is denoted by $D_\rho := \mathbf{R}(D_\phi) \subset [0, \infty)^2$.

Definition. Analogous to the criterion for single species systems in Section 2.1.3, we say that the two-component ZRP exhibits a *condensation transition* if $D_\rho \subsetneq [0, \infty)^2$.

The canonical measures for the two-component systems are given by

$$\mu_{L,N_1,N_2}(\boldsymbol{\eta}) = \frac{1}{Z(L, N_1, N_2)} \prod_{x \in \Lambda} W\big(\eta_1(x), \eta_2(x)\big)\, \delta\big(\Sigma^1_L(\boldsymbol{\eta}), N_1\big)\, \delta\big(\Sigma^2_L(\boldsymbol{\eta}), N_2\big) , \tag{5.45}$$

where the number of particles $\Sigma^i_L(\boldsymbol{\eta}) = \sum_{x \in \Lambda_L} \eta_i(x)$ is locally conserved for each species i. In this framework it is possible to fix any pair of densities $\boldsymbol{\rho} \in [0, \infty)^2$ and investigate the equivalence of $\mu_{L,\lfloor \rho_1 L \rfloor, \lfloor \rho_2 L \rfloor}$ to the corresponding product measure with fugacity $\boldsymbol{\Phi}(\boldsymbol{\rho})$ in the limit $L \to \infty$. Here $\boldsymbol{\Phi} : D_\rho \to D_\phi$ is the inverse of $\mathbf{R}(\boldsymbol{\phi})$, analogous to $\mathbf{M}(\boldsymbol{\rho})$ used in Chapter 4. In case of condensation it has to be extended to $[0, \infty)^2$ as it was done in Section 5.2 for a single species. There, the boundaries of D_ϕ and D_ρ were just single points

leading to a rather obvious extension. But for two species the situation is more complicated and it turns out that one has to use the thermodynamic entropy defined in (4.17) to get a unique extension.

Lemma 5.7 *In case of a phase transition we have $D_\phi \subsetneq [0,\infty)^2$ with $\partial D_\phi \cap D_\phi \neq \emptyset$ and $\partial D_\rho = \mathbf{R}\big(\partial D_\phi \cap D_\phi\big)$. For every $\boldsymbol{\rho} \in [0,\infty)^2$ there exists a unique maximizer $\bar{\boldsymbol{\Phi}}(\boldsymbol{\rho}) \in D_\phi$ for the thermodynamic entropy (4.17),*

$$S(\boldsymbol{\rho}) = \sup_{\boldsymbol{\phi}\in D_\phi} \boldsymbol{\rho}\cdot\log\boldsymbol{\phi} - \log Z(\boldsymbol{\phi}) = \boldsymbol{\rho}\cdot\log\bar{\boldsymbol{\Phi}}(\boldsymbol{\rho}) - \log Z\big(\bar{\boldsymbol{\Phi}}(\boldsymbol{\rho})\big)\,, \tag{5.46}$$

and $R_i\big(\bar{\boldsymbol{\Phi}}(\boldsymbol{\rho})\big) \leq \rho_i$, $i = 1,2$. $\bar{\boldsymbol{\Phi}}$ is a continuous function of $\boldsymbol{\rho}$, where for $\boldsymbol{\rho} \in D_\rho$ we have $\bar{\boldsymbol{\Phi}}(\boldsymbol{\rho}) = \boldsymbol{\Phi}(\boldsymbol{\rho})$ and for $\boldsymbol{\rho} \notin D_\rho$ it is $\bar{\boldsymbol{\Phi}}(\boldsymbol{\rho}) \in \partial D_\phi$. Moreover, $\bar{\boldsymbol{\Phi}}\big([0,\infty)^2\backslash D_\rho\big) = \partial D_\phi \cap D_\phi$.

Proof. The first statement is a direct generalization of Lemma 2.3.3 in [84] for the single species case. Since $D_\rho \subsetneq [0,\infty)^2$, there has to be a $\boldsymbol{\phi}^* \in \partial D_\phi$ with $\lim_{\boldsymbol{\phi}\to\boldsymbol{\phi}^*} R_i(\boldsymbol{\phi}) < \infty$ for $i = 1,2$, and thus by continuity of Z it is $Z(\boldsymbol{\phi}^*) < \infty$ and $\partial D_\phi \cap D_\phi \neq \emptyset$. Due to the regularity of $\mathbf{R}(\boldsymbol{\Phi})$, D_ρ is diffeomorphic to D_ϕ and thus $\partial D_\rho = \mathbf{R}\big(\partial D_\phi \cap D_\phi\big)$.

For $\boldsymbol{\rho} \in D_\rho$ (5.46) is obvious with $\bar{\boldsymbol{\Phi}}(\boldsymbol{\rho}) = \boldsymbol{\Phi}(\boldsymbol{\rho})$, as already given in the definition (4.17) of the thermodynamic entropy. For $\boldsymbol{\rho} \notin D_\rho$ we switch to the notation with chemical potentials in order to use regularity properties of D_μ from Lemma 4.2, such as convexity. By slight abuse of notation we write

$$F(\boldsymbol{\mu}) = \boldsymbol{\rho}\cdot\boldsymbol{\mu} - \log Z(\boldsymbol{\mu}) \tag{5.47}$$

for the function to be maximized in (5.46). It is strictly convex, i.e. D^2F is negative definite, and the level sets $L_F(c) = \big\{\boldsymbol{\mu} \in D_\mu \,\big|\, F(\boldsymbol{\mu}) \geq c\big\}$ are convex and closed relative to D_μ. For fixed $\boldsymbol{\rho}$ the derivatives

$$\partial_{\mu_i} F(\boldsymbol{\mu}) = \rho_i - R_i(\boldsymbol{\mu}) \tag{5.48}$$

are both positive for small $|\boldsymbol{\mu}|$ and so the level sets are also bounded for every $c \in \mathbb{R}$. For c small enough $L_F(c)$ is non-empty and since F is continuous it has a maximum $\bar{F}$ on D_μ. Since we consider $\boldsymbol{\rho} \notin D_\rho$, there is no local maximum in the interior of D_μ and thus $\bar{F}$ is obtained at the boundary $\partial D_\mu \cap D_\mu$. So $L_F(\bar{F}) \subset \partial D_\mu \cap D_\mu$ but it is also convex by definition. Moreover, since F is strictly convex $L_F(\bar{F})$ cannot be a straight line and thus there exists a unique $\bar{\boldsymbol{\mu}} \in \partial D_\mu \cap D_\mu$ with $L_F(\bar{F}) = \{\bar{\boldsymbol{\mu}}\}$.

At $\bar{\boldsymbol{\mu}}$ the derivatives of F are nonnegative, i.e. $\partial_{\mu_i} F(\bar{\boldsymbol{\mu}}) = \rho_i - R_i(\bar{\boldsymbol{\mu}}) \geq 0$. Otherwise, using the structure of D_μ given in Lemma 4.2, this would be in contradiction to the maximality of $F(\bar{\boldsymbol{\mu}})$. By strict convexity and continuity of F, its maximizer $\bar{\boldsymbol{\mu}}$ is a continuous function of $\boldsymbol{\rho}$, and with this and $\mathbf{M}(\partial D_\rho) = \partial D_\mu \cap D_\mu$ the last statement follows. □

In the next subsection we will see that the choice $\bar{\boldsymbol{\Phi}}(\boldsymbol{\rho})$ is the right one in the sense of the equivalence of ensembles. So far Lemma 5.7 just ensures that $\mathbf{R}\big(\bar{\boldsymbol{\Phi}}(\boldsymbol{\rho})\big)$ is a well defined, continuous projection of any density pair $\boldsymbol{\rho} = (\rho_1,\rho_2) \in [0,\infty)^2$ onto densities in D_ρ. If one of them is smaller than its original value ρ_i, this indicates a condensation of this species.

Definition. For every $\boldsymbol{\rho} \notin D_\rho$, $\boldsymbol{\rho}_c(\boldsymbol{\rho}) = \mathbf{R}\big(\bar{\boldsymbol{\Phi}}(\boldsymbol{\rho})\big) \in \partial D_\rho$ is called the *critical (background) density*. We say that *species* i *condensates* if $\rho_{c,i}(\boldsymbol{\rho}) < \rho_i$.

Note that the critical density depends on $\boldsymbol{\rho}$, in contrast to single species systems where there is only one critical density ρ_c defined in Section 2.3.2. Analogous to (5.7) the asymptotic bulk density is given by

$$\boldsymbol{\rho}_{bulk}(\boldsymbol{\rho}) = \mathbf{R}\big(\bar{\boldsymbol{\Phi}}(\boldsymbol{\rho})\big) = \begin{cases} \boldsymbol{\rho} & , \text{ if } \boldsymbol{\rho} \in D_\rho \\ \boldsymbol{\rho}_c(\boldsymbol{\rho}) & , \text{ if } \boldsymbol{\rho} \notin D_\rho \end{cases} \tag{5.49}$$

which can be considered as the order parameter of the condensation.

With the previous definition, $[0,\infty)^2 \backslash D_\rho$ can be partitioned into sets A, B and C, where only species 1, only species 2 or both species condensate. Depending on the specific model, each of these regions might also be empty, but in case of a condensation transition at least one has to be non-empty. For the images under $\bar{\boldsymbol{\Phi}}$ we have $\bar{\boldsymbol{\Phi}}(A) \cup \bar{\boldsymbol{\Phi}}(B) \cup \bar{\boldsymbol{\Phi}}(C) = \partial D_\phi \cap D_\phi$. Since D_μ is convex the boundary ∂D_ϕ is continuous, and furthermore we assume that

$$\partial D_\phi \quad \text{is a piecewise differentiable curve.} \tag{5.50}$$

Under this natural regularity condition we summarize some generic properties of the above partitions and their images under $\bar{\boldsymbol{\Phi}}$ in the next Lemma. An example illustrating these features is given in Section 5.4.3.

Lemma 5.8 *Suppose (5.50). If $A \neq 0$, $\bar{\boldsymbol{\Phi}}(A)$ is a straight line parallel to the ϕ_2-axis, i.e.*

$$\exists_{\phi_{c,1}>0}\ \bar{\boldsymbol{\Phi}}(A) = \big\{(\phi_{c,1},\phi_2)\big|0 \le \phi_2 < \bar{\phi}_2\big\} \quad \textit{for some } \bar{\phi}_2 \in (0,\infty]\,, \tag{5.51}$$

and in particular $\bar{\boldsymbol{\Phi}}(A)$ is a simply connected subset of $\partial D_\phi \cap D_\phi$. If $\boldsymbol{\rho} \in A$ then $(\rho_1^*,\rho_2) \in A$ and $\bar{\boldsymbol{\Phi}}(\rho_1^*,\rho_2) = \bar{\boldsymbol{\Phi}}(\boldsymbol{\rho})$ for all $\rho_1^* \ge \rho_1$. We can write $\boldsymbol{\rho}_c(\boldsymbol{\rho}) = (\rho_{c,1}(\rho_2),\rho_2)$ and

$$A = \bigcup_{0\le\phi_2<\bar{\phi}_2} \Big\{\big(\rho_1, R_2(\phi_{c,1},\phi_2)\big)\Big|\rho_1 > R_1(\phi_{c,1},\phi_2)\Big\}\,. \tag{5.52}$$

In particular A is simply connected and bounded below by the critical densities $\boldsymbol{\rho}_c(A) = \partial A \cap D_\rho$. Analogous statements hold for set B.
If $\boldsymbol{\rho} \in C$ then $\boldsymbol{\rho}^* \in C$ for all $\boldsymbol{\rho}^* \ge \boldsymbol{\rho}$. $\bar{\boldsymbol{\Phi}}(C)$ cannot be parallel to one of the axes but it is still simply connected, as well as C is.

Remarks. If $\bar{\phi}_2 < \infty$ the range in (5.51) might also be given by $0 \le \phi_2 \le \bar{\phi}_2$, namely if regime C is non-empty (cf. examples of Section 5.4.3). $\boldsymbol{\rho}^* \ge \boldsymbol{\rho}$ has the obvious meaning that $\rho_i^* \ge \rho_i$ for $i = 1,2$.

Proof. We return to the notation of the proof of Lemma 5.7 with chemical potentials. Let $\boldsymbol{\mu}(t)$, $t \in T$ be a parametrization of ∂D_μ. Then for $\boldsymbol{\rho} \notin D_\rho$ the maximizer $\bar{\boldsymbol{\mu}}$ of $F(\boldsymbol{\mu})$ defined in (5.47) is characterized by

$$\boldsymbol{\nabla}_\mu F(\boldsymbol{\mu}) \cdot \dot{\boldsymbol{\mu}}(t)\big|_{\boldsymbol{\mu}=\bar{\boldsymbol{\mu}}} = 0\,. \tag{5.53}$$

For $\boldsymbol{\rho} \in A$ it is $\partial_{\mu_1} F(\bar{\boldsymbol{\mu}}) = \rho_1 - R_1(\boldsymbol{\mu}) > 0$ and $\partial_{\mu_2} F(\bar{\boldsymbol{\mu}}) = 0$ according to (5.48) and thus necessarily $\dot{\mu}_1(t) = 0$. This (local) property together with the regularity of D_μ shown in Lemma 4.2 implies the global statement (5.51). With this and (5.47) an increase of ρ_1

corresponds to a constant increase of F on $\bar{\mathbf{\Phi}}(A)$ and thus $\bar{\boldsymbol{\mu}}$ does not change, and still $\boldsymbol{\rho} \in A$ which follows immediately from (5.48). (5.52) is a direct consequence of the previous statements and the regularity of the function $\mathbf{R}(\boldsymbol{\phi})$. An analogous proof works for $\boldsymbol{\rho} \in B$.

For $\boldsymbol{\rho} \in C$ it is $\partial_{\mu_i} F(\bar{\boldsymbol{\mu}}) > 0$ for both species $i = 1, 2$ and thus (5.53) implies that either $\dot{\mu}_i(t)$ both vanish such that $\bar{\mathbf{\Phi}}(C)$ is only a single point (cf. Section 5.4.3), or they are non-zero and have different sign. Again (5.48) implies that all $\boldsymbol{\rho}^* \in C$ with $\boldsymbol{\rho}^* \geq \boldsymbol{\rho}$ and $\boldsymbol{\rho} \in C$. Since A, B and D_ρ are simply connected also C is, and thus $\bar{\mathbf{\Phi}}(C)$ by continuity of $\bar{\mathbf{\Phi}}$. □

5.4.2 Equivalence of ensembles

According to (4.14) and (4.19) the covariance matrix $Cov(\boldsymbol{\phi})$ of the bivariate one-point distribution $\bar{\nu}^1_{\boldsymbol{\phi}}$ is given by

$$Cov_{i,j}(\boldsymbol{\phi}) = \left\langle \eta_i \eta_j \right\rangle^c_{\bar{\nu}^1_{\boldsymbol{\phi}}} = \phi_j \partial_{\phi_j} \left(\phi_i \partial_{\phi_i} \log Z(\boldsymbol{\phi}) \right) = \left((D^2 S)^{-1} \big(\mathbf{R}(\boldsymbol{\phi}) \big) \right)_{i,j} . \tag{5.54}$$

In particular it is given by the inverse of the second derivative matrix of the thermodynamic entropy S. Since $\bar{\nu}^1_{\boldsymbol{\phi}}$ has finite exponential moments for $\boldsymbol{\phi} \in \mathring{D}_\phi$, Cov is finite on $\mathring{D}_\phi$. To prove the theorem below we have to assume that it is finite also on $\partial D_\phi \cap D_\phi$, i.e.

$$Cov(\boldsymbol{\phi}) \in \mathbb{R}^{2\times 2} \quad \text{for all } \boldsymbol{\phi} \in \partial D_\phi \cap D_\phi \, . \tag{5.55}$$

This ensures that we have central limit theorems for a sum of i.i.d. $\bar{\nu}^1_{\boldsymbol{\phi}}$-random variables towards a bivariate Gaussian distribution, which are needed for the proof. This assumption is not necessary for the one-component case in Section 5.2, since there are central limit theorems towards Lévy distributions in the case $\phi = \phi_c$, which we are not aware of for the bivariate case.

Analogous to (5.3) we assume existence of the Cesaro limits

$$\begin{aligned} &\lim_{k_1 \to \infty} \frac{1}{k_1} \sum_{i_1=1}^{k_1} \log g_1(i_1, k_2) \in (-\infty, \infty] \quad \text{for all } k_2 \in \mathbb{N} \text{ and} \\ &\lim_{k_2 \to \infty} \frac{1}{k_2} \sum_{i_2=1}^{k_2} \log g_2(k_1, i_2) \in (-\infty, \infty] \quad \text{for all } k_1 \in \mathbb{N} \, , \end{aligned} \tag{5.56}$$

which could also be infinite. This includes regularity properties of the stationary weight $W(k_1, k_2)$, which are necessary for the proof of Lemma 5.10 formulated below.

Theorem 5.9 (Equivalence of ensembles)
Let $\bar{\mathbf{\Phi}}(\boldsymbol{\rho})$ be defined as in Lemma 5.7 and assume (5.55), (5.56). Then for every $\boldsymbol{\rho} \in [0, \infty)^2$ the canonical distribution (5.45) weakly converges to the product measure (5.44),

$$\mu_{L,[\rho_1 L],[\rho_2 L]} \xrightarrow{w} \nu_{\bar{\mathbf{\Phi}}(\boldsymbol{\rho})} \, , \quad \text{for } L \to \infty \, , \tag{5.57}$$

for all bounded cylinder test functions in $C_{0,b}(X, \mathbb{R})$. The canonical partition functions converge as

$$\lim_{L \to \infty} \frac{1}{L} \log Z(L, [\rho_1, L], [\rho_2 L]) = \log Z(\bar{\mathbf{\Phi}}(\boldsymbol{\rho})) - \rho_1 \log \bar{\Phi}_1(\rho) - \rho_2 \log \bar{\Phi}_2(\rho) \, . \tag{5.58}$$

Remarks. Unfortunately, we are not able to prove a result similar to Theorem 5.5 of Section 5.2.2, which would ensure that in a typical stationary configuration of a large finite system each species condensates only on a single site. However, we expect that such a statement holds and this intuition is supported by simulation results presented in Chapter 6. Moreover, in case of simultaneous condensation, both condensates can be on the same site under certain conditions, which we discuss further in the next subsection.
In analogy to Lemma 5.1 for a single species, we need a certain subexponential decay of $\bar{\nu}^1_{\boldsymbol{\phi}}$ on $\partial D_\phi \cap D_\phi$ for the proof of Theorem 5.9, which we summarize in the following lemma.

Lemma 5.10 *Assume (5.56). For $\boldsymbol{\phi} \in \bar{\boldsymbol{\Phi}}(A) \cup \bar{\boldsymbol{\Phi}}(C)$, i.e. species 1 condensates, we have*

$$\forall_{\epsilon>0}\, \exists_{k_2\in\mathbb{N}} \lim_{k_1\to\infty} -\frac{1}{k_1} \log \bar{\nu}_{\boldsymbol{\phi}}(k_1,k_2) < \epsilon\ . \tag{5.59}$$

Analogously, for $\boldsymbol{\phi} \in \bar{\boldsymbol{\Phi}}(B) \cup \bar{\boldsymbol{\Phi}}(C)$ we have

$$\forall_{\epsilon>0}\, \exists_{k_1\in\mathbb{N}} \lim_{k_2\to\infty} -\frac{1}{k_2} \log \bar{\nu}_{\boldsymbol{\phi}}(k_1,k_2) < \epsilon\ . \tag{5.60}$$

Proof of Lemma 5.10. Take $\boldsymbol{\phi} \in \bar{\boldsymbol{\Phi}}(A) \cup \bar{\boldsymbol{\Phi}}(C)$ with chemical potentials $\boldsymbol{\mu} = \log \boldsymbol{\phi}$ and define

$$\begin{aligned}\alpha(k_2) &:= -\lim_{k_1\to\infty} \frac{1}{k_1} \log \bar{\nu}^1_{\boldsymbol{\mu}}(k_1,k_2) = \\ &= \lim_{k_1\to\infty} \Big(-\frac{1}{k_1} \log W(k_1,k_2) - \mu_1 - \mu_2 \frac{k_2}{k_1} + \frac{1}{k_1} \log Z(\boldsymbol{\mu}) \Big) \geq 0\ ,\end{aligned} \tag{5.61}$$

where the limit exists for all $k_2 \in \mathbb{N}$ due to assumption (5.56). Thus there exists $K \in \mathbb{N}$ such that for all $k_1 > K$

$$\log Z(\boldsymbol{\mu}) \geq \big(\alpha(k_2)/2 + \mu_1\big)\, k_1 + \mu_2\, k_2 + \log W(k_1,k_2)\ . \tag{5.62}$$

Suppose now by contradiction that $\alpha(k_2) > 2\alpha$ for all $k_2 \in \mathbb{N}$ and some $\alpha > 0$, i.e. it is uniformly bounded away from zero. Then for every $\gamma_1, \gamma_2 \in (0,1)$ it is

$$e^{-\gamma_1\,\alpha\,k_1 - \gamma_2\,\mu_2\,k_2}\, Z(\boldsymbol{\mu}) \geq e^{(\mu_1 + (1-\gamma_1)\,\alpha)\,k_1 + (1-\gamma_2)\,\mu_2\,k_2}\, W(k_1,k_2) \tag{5.63}$$

Summing both sides over k_1 and k_2 we get with some constant $C > 0$

$$Z\Big(\big(\mu_1 + (1-\gamma_1)\,\alpha\big)\,,\, (1-\gamma_2)\,\mu_2\Big) \leq C\, Z(\boldsymbol{\mu}) < \infty\ . \tag{5.64}$$

This is in contradiction to $\boldsymbol{\phi} \in \bar{\boldsymbol{\Phi}}(A)$ for every choice of γ_1, γ_2 using the properties of $\bar{\boldsymbol{\Phi}}(A)$ given in Lemma 5.8. With this lemma, (5.64) is also in contradiction to $\boldsymbol{\phi} \in \bar{\boldsymbol{\Phi}}(C)$ by choosing γ_1 and γ_2 sufficiently small. Thus $\alpha(k_2)$ has to get arbitrarily close to zero and statement (5.59) follows. (5.60) can be shown analogously. □

Proof of Theorem 5.9. Using the same technique as for the one-component case presented in Section 5.2, it is enough to show that the relative entropy of the finite dimensional marginals vanishes. For the full measures it can be written as

$$H\big(\mu_{L,N_1,N_2} \,\big|\, \bar\nu^L_{\boldsymbol\phi}\big) = -\log \bar\nu^L_{\boldsymbol\phi}\big(\{\boldsymbol\eta \,|\, \Sigma^1_L(\boldsymbol\eta)=N_1,\, \Sigma^2_L(\boldsymbol\eta)=N_2\}\big)\;, \tag{5.65}$$

analogous to (5.22). With definitions (5.44) and (5.45) we have

$$\bar\nu^L_{\boldsymbol\phi}\big(\{\Sigma^1_L(\boldsymbol\eta)=N_1,\, \Sigma^2_L(\boldsymbol\eta)=N_2\}\big)\, Z(\boldsymbol\phi)^L = Z\big(L,N_1,N_2\big)\,\phi_1^{N_1}\phi_2^{N_2}\;, \tag{5.66}$$

analogous to (5.21). Using (5.46), where the thermodynamic entropy $S(\boldsymbol\rho)$ is defined by a Legendre transform, we immediately get from (5.65)

$$\begin{aligned}\inf_{\boldsymbol\phi\in D_\phi} H\big(\mu_{L,N_1,N_2} \,\big|\, \bar\nu^L_{\boldsymbol\phi}\big) &= -\log Z\big(L,N_1,N_2\big) - L\,S\big(N_1/L, N_2/L\big) = \\ &= H\big(\mu_{L,N_1,N_2} \,\big|\, \bar\nu^L_{\bar{\boldsymbol\Phi}(N_1/L,N_2/L)}\big)\;.\end{aligned} \tag{5.67}$$

We fix a pair of densities $\boldsymbol\rho$ and set $N_i = [\rho_i L]$. Then $\bar{\boldsymbol\Phi}\big(N_1/L, N_2/L\big)$ converges to $\bar{\boldsymbol\Phi}(\boldsymbol\rho)$ for $L\to\infty$ by continuity of $\bar{\boldsymbol\Phi}$, showing that this choice as defined in Lemma 5.7 minimizes the relative entropy (5.65).

It remains to show that the relative entropy of finite dimensional marginals indeed vanishes in the limit $L\to\infty$. Analogous to (5.23) it is bounded by

$$H\big(\mu^n_{L,[\rho_1 L],[\rho_2 L]} \,\big|\, \bar\nu^n_{\bar{\boldsymbol\Phi}(\boldsymbol\rho)}\big) \le -\frac{1}{[L/n]}\log \bar\nu^L_{\bar{\boldsymbol\Phi}(\boldsymbol\rho)}\big(\{\Sigma^1_L(\boldsymbol\eta)=[\rho_1 L], \Sigma^2_L(\boldsymbol\eta)=[\rho_2 L]\}\big) \tag{5.68}$$

for every $n\in\{1,\dots,L\}$ and $\boldsymbol\phi\in D_\phi$, and we have to find a subexponential lower bound to the probability on the right hand side.

For $\boldsymbol\rho\in D_\rho$ we have $\bar{\boldsymbol\Phi}(\boldsymbol\rho)=\boldsymbol\Phi(\boldsymbol\rho)\in D_\phi$ and $\bar\nu^1_{\boldsymbol\Phi(\boldsymbol\rho)}$ has finite covariance Cov by assumption (5.55). The limit distribution of $(\Sigma^1_L(\boldsymbol\eta),\Sigma^2_L(\boldsymbol\eta))$ is a bivariate Gaussian centered at $(\rho_1 L,\rho_2 L)$. Thus we get $\bar\nu^L_{\bar{\boldsymbol\Phi}}\big(\{\Sigma^1_L(\boldsymbol\eta)=N_1,\,\Sigma^2_L(\boldsymbol\eta)=N_2\}\big)\simeq 1/\sqrt{L}$ for $L\to\infty$ by the multivariate local limit theorem.

For $\boldsymbol\rho\in A$ we split the right hand side of (5.68) analogous to (5.24) and get the bound

$$\begin{aligned}H\big(\mu^n_{L,[\rho_1 L],[\rho_2 L]} \,\big|\, \bar\nu^n_{\bar{\boldsymbol\Phi}(\boldsymbol\rho)}\big) \le &-\frac{1}{[L/n]}\log \bar\nu^1_{\bar{\boldsymbol\Phi}(\boldsymbol\rho)}\Big(\big[\rho_1 L\big] - \big[\rho_{c,1}(\boldsymbol\rho)(L-1)\big]\;,\; k_2\Big) \\ &-\frac{1}{[L/n]}\log \bar\nu^{L-1}_{\bar{\boldsymbol\Phi}(\boldsymbol\rho)}\Big(\Big\{\Sigma^1_{L-1}(\boldsymbol\eta)=\big[\rho_{c,1}(\boldsymbol\rho)(L-1)\big]\;,\; \Sigma^2_{L-1}(\boldsymbol\eta)=[\rho_2 L]-k_2\Big\}\Big)\end{aligned} \tag{5.69}$$

for all $k_2\le[\rho_2 L]$. With Lemma 5.10 we can choose k_2 such that the first term is smaller than an arbitrary $\epsilon>0$ in the limit $L\to\infty$. Since k_2 depends only on ϵ the second term vanishes due to the local limit theorem for multivariate Gaussians like above. Thus for every $\epsilon>0$ we have

$$\lim_{L\to\infty} H\big(\mu^n_{L,[\rho_1 L],[\rho_2 L]} \,\big|\, \bar\nu^n_{\bar{\boldsymbol\Phi}(\boldsymbol\rho)}\big) < \epsilon\;, \tag{5.70}$$

and the relative entropy vanishes.

The case $\boldsymbol{\rho} \in B$ follows analogously. For $\boldsymbol{\rho} \in C$ we split

$$\begin{aligned} H\big(\mu^n_{L,[\rho_1 L],[\rho_2 L]} \,\big|\, \bar\nu^n_{\bar\Phi(\boldsymbol{\rho})}\big) \le & -\frac{1}{[L/n]} \log \bar\nu^1_{\bar\Phi(\boldsymbol{\rho})}\Big([\rho_1 L] - \big[\rho_{c,1}(\boldsymbol{\rho})(L-2)\big]\,,\; k_2\Big) \\ & -\frac{1}{[L/n]} \log \bar\nu^1_{\bar\Phi(\boldsymbol{\rho})}\Big(k_1\,,\; [\rho_2 L] - \big[\rho_{c,2}(\boldsymbol{\rho})(L-2)\big]\Big) \\ & -\frac{1}{[L/n]} \log \bar\nu^{L-2}_{\bar\Phi(\boldsymbol{\rho})}\Big(\Big\{\Sigma^1_{L-2}(\boldsymbol{\eta}) = \big[\rho_{c,1}(\boldsymbol{\rho})(L-2)\big] - k_1\,, \\ & \qquad\qquad \Sigma^2_{L-2}(\boldsymbol{\eta}) = \big[\rho_{c,2}(\boldsymbol{\rho})(L-2)\big] - k_2\Big\}\Big)\,, \end{aligned} \tag{5.71}$$

and apply Lemma 5.10 to the first two expressions. □

5.4.3 Generic examples

We close this chapter by applying the above results to some generic examples of two component systems. We mainly concentrate on the model introduced in [43, 66] with rates

$$\begin{aligned} g_1(k_1,k_2) &= \Theta(k_1)\Big(\frac{1+b/(k_1+1)}{1+b/k_1}\Big)^{k_2}\big(1+c/k_1\big)\,, \\ g_2(k_1,k_2) &= \Theta(k_2)\big(1+b/(k_1+1)\big)\,, \end{aligned} \tag{5.72}$$

where $b, c > 0$. It is easy to check that these rates fulfill condition (5.42), so there exists a stationary product measure. Moreover g_2 is independent of k_2 and $\log g_1$ is monotonic in k_1 so that (5.56) also holds and Theorem 5.9 applies. Following [43, 66] the grand canonical partition function and the densities can be calculated to be

$$\begin{aligned} Z(\boldsymbol{\phi}) &= \sum_{k_1=0}^{\infty} \phi_1^{k_1} \frac{1+k_1+b}{(1-\phi_2)(k_1+1)+b} \frac{k_1!}{(1+c)_{k_1}}\,, \\ R_1(\boldsymbol{\phi}) &= \frac{1}{Z(\boldsymbol{\phi})} \sum_{k_1=0}^{\infty} k_1\, \phi_1^{k_1} \frac{1+k_1+b}{(1-\phi_2)(k_1+1)+b} \frac{k_1!}{(1+c)_{k_1}}\,, \\ R_2(\boldsymbol{\phi}) &= \frac{1}{Z(\boldsymbol{\phi})} \sum_{k_1=0}^{\infty} (1+k_1)\, \phi_1^{k_1} \frac{\phi_2(1+k_1+b)}{[(1-\phi_2)(k_1+1)+b]^2} \frac{k_1!}{(1+c)_{k_1}}\,, \end{aligned} \tag{5.73}$$

Obviously it is $\phi_{c,1} = \phi_{c,2} = 1$ (cf. Lemma 5.8) and D_ϕ takes a particularly simple form. For $\phi_2 = 1$ we get for the corresponding densities

$$R_2(\phi_1, 1) = \big(1 + R_1(\phi_1,1)\big)/b < \infty \tag{5.74}$$

for all $\phi_1 \in [0,1)$. So species 2 condensates for all $b,\ c > 0$ if $\rho_2 > \rho_{c,2}(\rho_1) = (1+\rho_1)/b$, as was already noted in [43]. This corresponds to the set B as defined in Section 5.4.1 and the respective part of the boundary ∂D_ϕ, $\bar{\boldsymbol{\Phi}}(B)$, is given by $\phi_2 = 1$ as shown in Figure 5.3. Since g_2 is actually independent of k_2 the condensation is induced by particles of species 1, leading to interesting dynamical phenomena discussed in Section 6.4.1.

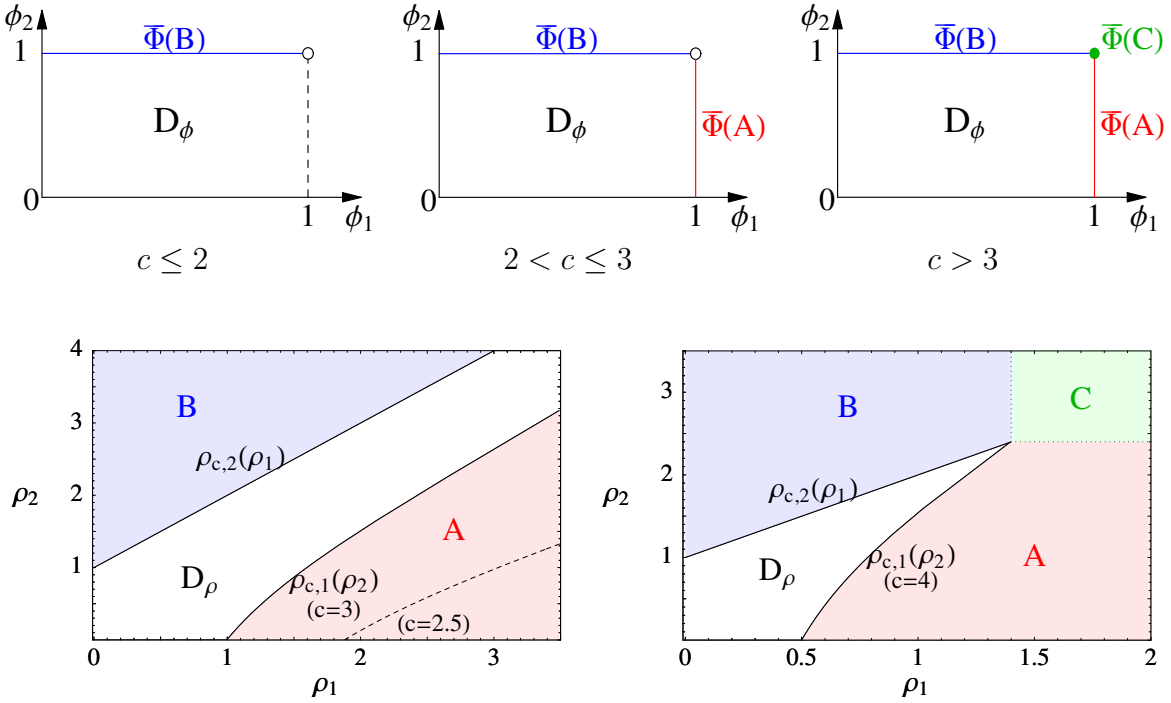


Figure 5.3: Critical behavior of the two-component system (5.72). **Top:** The structure of D_ϕ if only species 2 condensates (left), species 1 and 2 condensate but only separately (middle), species 1 and 2 can condensate also simultaneously (right). **Bottom:** Density phase diagram for $b = 1$ and $c = 3,\ 2.5$ (left), $c = 4$ (right). Region A: condensation of species 1, region B: condensation of species 2, region C: condensation of species 1 and 2.

If $\phi_1 = 1$ and $\phi_2 < 1$ the expressions in (5.73) only converge for $c > 2$, analogously to the one component model studied in Section 5.3. For the corresponding line of critical densities we only have the parametric expression $\{\mathbf{R}(1,\phi_2) \,|\, 0 \leq \phi_2 < 1\}$. This gives the boundary between D_ρ and region A, which is shown in red in Figure 5.3. For $\phi_1 = \phi_2 = 1$ convergence in (5.73) is given only for $c > 3$ and in this case the intersection point $\mathbf{R}(1,1)$ of $\rho_{c,2}(\rho_1)$ and $\rho_{c,1}(\rho_2)$ is found to be

$$R_1(1,1) = \frac{c(2+b) - 2 - 3b}{(c-3)\big(b(c-2)+c-1\big)}\ , \quad R_2(1,1) = \frac{(c-1)\big(b(c-3)+c-1\big)}{b(c-3)\big(b(c-2)+c-1\big)}\ . \tag{5.75}$$

This scenario is plotted in Figure 5.3 on the right. Condensation of both species takes place in region C (green), which does not exist for $c \leq 3$ as can be seen on the left.

As mentioned after Theorem 5.9 we expect the condensates to occupy only a single lattice site. Moreover, g_2 is obviously monotonically decreasing in k_1 and thus also g_1 in k_2, since both dependencies are linked by (5.42). So in region C it is favorable for both condensates to be on the same lattice site, which is supported by simulation results given in Chapter 6. While in this case the condensates 'attract' each other, their positions are of course independent if the rates have no mutual dependence, such as

$$g_1 = \Theta(k_1)\big(1 + b/k_1\big)\ , \quad g_2 = \Theta(k_2)\big(1 + c/k_2\big) \quad \text{with } b, c > 2\ . \tag{5.76}$$

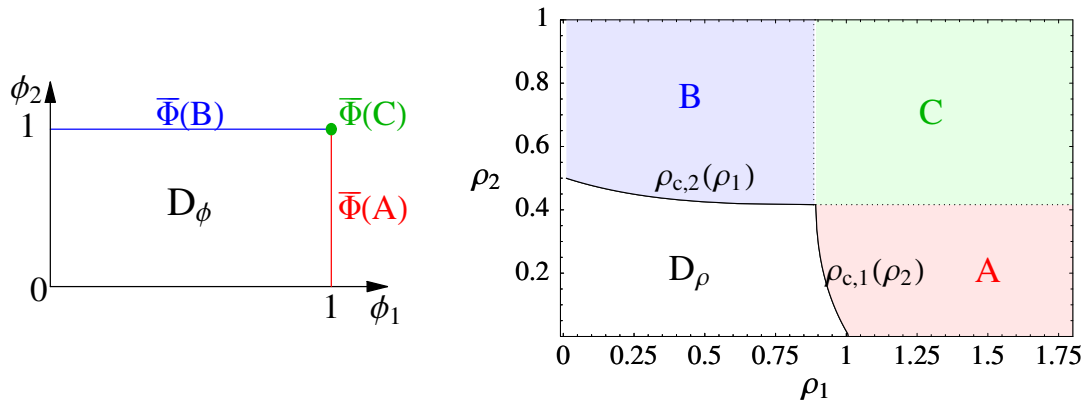


Figure 5.4: Critical behavior of the two-component system (5.77) with $b = 3$ and $c = 4$ where all regions A, B and C are non-empty. **Left:** The structure of D_ϕ. **Right:** Density phase diagram. For independent jump rates (5.76) $\rho_{c,2}(\rho_1)$ would be a straight horizontal and $\rho_{c,1}(\rho_2)$ a vertical line.

On the other hand, if we consider rates like

$$g_1 = \Theta(k_1)\big(1 + b/k_1\big)\big(k_2 + 1\big) \;, \quad g_2 = \Theta(k_2)\big(1 + c/k_2\big)\big(1 + 1/k_2\big)^{k_1} \;, \tag{5.77}$$

g_1 is increasing in k_2 and vice versa. Since (5.42) is fulfilled the analysis can be carried out completely analogously to the one above, and we find a phase diagram given in Figure 5.4 which indicates that both species condensate simultaneously if $b, c > 2$. But with rates (5.77) a double condensate is now less stable than two separate condensates of species 1 and 2 and so we expect them to be on different lattice sites.

In fact whenever g_1 is not decreasing in k_2, condensation of species 1 has to be induced by a decreasing dependence on k_1 and vice versa. So the mechanism in this case is the same as for independent species (5.76). With respect to condensation one observes just two copies of a single species system, with the only difference that the condensates cannot be on the same lattice site. This is of course much less interesting than the example (5.72) studied before, where condensation of species 2 is induced by the presence of particles of species 1.

In all the above examples D_ϕ has a very simple, rectangular structure. This considerably simplifies the analysis and suggests that there might be a simpler way of studying the phenomenon than described in the previous sections. It is, however, not obvious how to prove general statements more easily, since the form of D_ϕ can also be more complicated. Consider for example the rates

$$g_1 = \Theta(k_1)\Big(\frac{k_1}{1 + k_1}\Big)^{k_2}\big(1 + b/k_1\big) \;, \quad g_2 = \frac{k_2}{1 + k_1} \;, \tag{5.78}$$

which obey (5.42) and the partition function is found to be

$$Z(\boldsymbol{\phi}) = e^{\phi_2} \sum_{k_1=0}^{\infty} \frac{k_1!}{(1 + b)_{k_1}} \exp\big[(\phi_2 + \log \phi_1)k_1\big] \;. \tag{5.79}$$

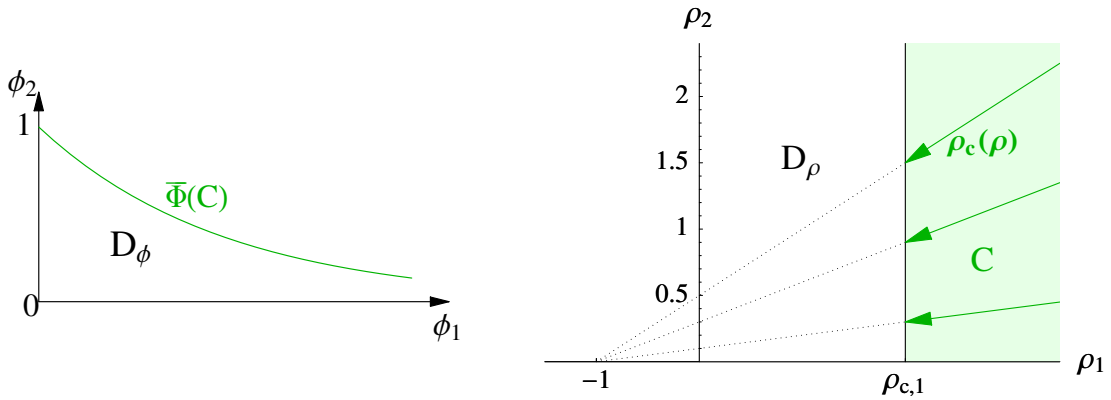


Figure 5.5: Critical behavior of the two-component system (5.78) for arbitrary $b > 2$, where both species condensate simultaneously. **Left:** Structure of D_ϕ where the corresponding D_μ would be convex. **Right:** Density phase diagram with $\rho_{c,1} = 1/(b-2)$. Arrows denote the projection $\boldsymbol{\rho}_c(\boldsymbol{\rho})$ on the critical (background) densities.

Thus $D_\phi = \left\{\boldsymbol{\phi} \in [0,\infty)^2 \,\middle|\, \phi_1 \leq \exp[-\phi_2]\right\}$ for $b > 2$ and according to Lemma 5.8 both species condensate simultaneously and regions A and B are empty. D_ϕ is shown in Figure 5.5 (left) and is not even convex, whereas the corresponding domain of chemical potentials D_μ is (not shown). As seen in Figure 5.5 (right) D_ρ has a rather simple structure and $\rho_{c,1} = 1/(b-2)$ is a constant, whereas $\rho_{c,2}(\boldsymbol{\rho}) = (1+\rho_{c,1})\rho_2/(1+\rho_1)$ is not. This example illustrates that $\boldsymbol{\rho}_c$ can depend nontrivially on $\boldsymbol{\rho}$ and the theory of Sections 5.4.1 and 5.4.2 is really necessary to understand the coarsening transition. Just by looking at D_ρ one would presumably think that only species 1 condensates.

5.5 Discussion

With Theorem 5.2 we provide a rigorous proof for the condensation transition in the ZRP which has been studied non-rigorously in [21, 40]. As a new result, we show in Theorem 5.5 that the condensed phase typically consists only of a single, randomly located site. This requires some technical assumptions on the tail behavior of the jump rates. These conditions should be not essential for the validity of the statement, and there are indications that a generalization is possible without substantial changes of the proof.

The analysis of the condensation in two-component systems reveals an interesting connection between the critical fugacities and the thermodynamic entropy of the system given in Lemma 5.7. We establish a rigorous result on the condensation in Theorem 5.9 under mild assumptions on the jump rates. A statement on the volume of the condensed phase would require large deviation estimates analogous to Lemma 5.6 for multivariate distributions, which we are not aware of so far. In contrast to one-component systems, where our results give a fairly complete picture, the two-component case is only partially understood. In particular we have only heuristic arguments but no rigorous statements concerning the structure of the condensed phase.

In comparison to previous chapters we would like to note that in contrast to boundary induced critical phenomena the condensation transition of the ZRP cannot be captured on a hydrodynamic level. Moreover, the description of the system with a hydrodynamic conservation law fails in case of condensation. On a macroscopic scale the particle density is no more a conserved quantity, since a non-zero fraction of the particles condensates on a region with vanishing volume fraction. This is consistent with the fact that the existence of a finite critical density contradicts the conditions of Section 4.3.1 for the derivation of the macroscopic equation.

Given the correspondence between the single-species ZRP and two-species exclusion processes [76], our results also provide new information on the stability of domain walls in such systems. As explained in Section 2.2.3, domain wall stability is a key ingredient in the theory of boundary induced phase transitions in one-component systems, and thus may shed light on steady state selection in the case of two particle species.

Chapter 6

Relaxation dynamics of the zero range process

6.1 Introduction

So far we investigated the condensation transition on the level of the stationary distribution, which carries no information on the kinetics of the phenomenon. A natural set-up is to start with particles uniformly distributed at some supercritical density $\rho > \rho_c$ on a large periodic lattice. The stationary measure determines the long-time behavior of the system, where a typical configuration consists of a uniform background phase at density ρ_c and one condensate site, containing the excess particles.

How does the system with uniform initial distribution relax to this configuration?

An intuitive picture can be obtained from computer simulation data for the density profile, shown in Figure 6.1. In an initial nucleation process, driven by density fluctuations, condensates rapidly evolve all over the system. Then a coarsening mechanism sets in, where the large condensates grow on the expense of smaller ones. The result of this is a typical stationary configuration with a single condensate site.

Domain coarsening is a well known phenomenon in the context of phase separation. The most famous example is probably given by domains of opposite magnetization in the Ising model, mentioned in Section 2.1.3. The coarsening dynamics usually takes place on a slow time scale, since it is only driven by boundary interactions between the domains, which are already relaxed to their stationary distribution. Due to this separation of time scales, the coarsening regime is expected to follow a universal scaling law, which is of particular interest. This has been studied in [16] for a disordered, symmetric ZRP and recently in [58] for the homogeneous, asymmetric case. There the time evolution of the probability distribution of the number of particles at a single site was analyzed numerically, with particular attention to the macroscopic component of that distribution. In view of our static result we pursue a somewhat different approach and investigate the effective dynamics of the condensates, using random walk arguments supported by Monte Carlo simulations.

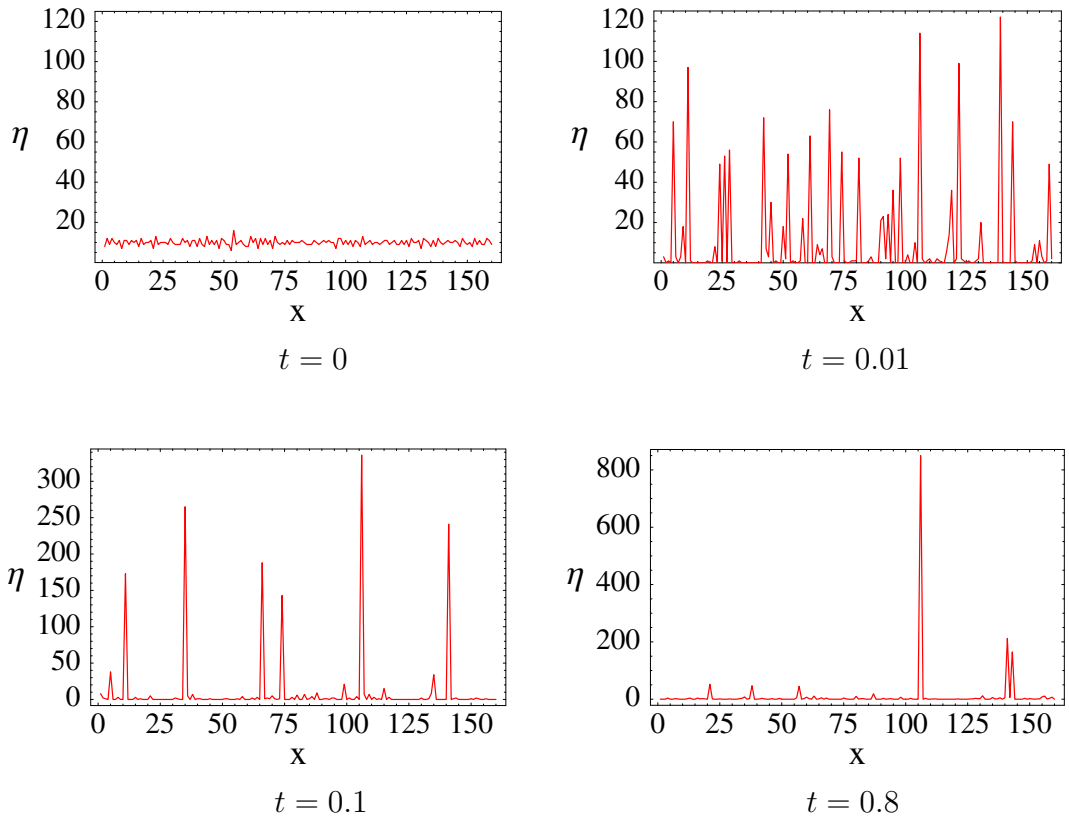


Figure 6.1: Configuration η_t at different times from simulation data with lattice size $L = 160$, jump rates $g(k) = \Theta(k)(1 + b/k)$ with $b = 2.5$ given in (5.27), asymmetric jump probabilities and uniform initial density $\rho = 10$. The time scale is normalized such that for $t = 1$ the system shows a typical stationary configuration.

In contrast to the stationary results of the previous Chapter, this analysis depends on the form of the jump rates and in particular on the symmetry of the jump probabilities, i.e. reversibility of the process. In the next two sections we study this in detail for the generic example (5.27) with rates $g(k) = \Theta(k)(1 + b/k^\gamma)$, introduced in [40]. We concentrate on one space dimension, with particular attention to the difference between symmetric and asymmetric jump probabilities. We derive a scaling law for the coarsening regime and an effective master equation for the late stage of relaxation, governing the occupation numbers of two remaining condensates. This part of the Chapter has been published in [62]. In Section 6.4 we generalize the analysis to two-component systems and study the effect of higher space dimensions. Unlike in previous chapters, we use heuristic considerations which are corroborated through comparison with simulation data instead of giving rigorous proofs.

6.2 Dynamics of the condensation

To describe quantitatively the relaxation dynamics we use the symbols '$\sim$' for proportional, '$\simeq$' for equivalent and '$O(L)$' for terms proportional to L, all asymptotically for $L \to \infty$.

6.2.1 Regimes of the relaxation dynamics

As indicated in the introduction, the dynamics leading from a uniform initial distribution with density $\rho > \rho_c$ to the stationary distribution can be divided into three regimes.

Nucleation: Driven by density fluctuations the excess particles condense in several random positions, which are called cluster sites. On the remaining lattice, the so-called bulk sites, the distribution relaxes to $\bar{\nu}_{\phi_c}$.

Coarsening: The condensates are essentially immobile, but they can exchange particles through the bulk. With increasing time the larger condensates gain particles at the expense of the smaller ones. The resulting decrease of the number of cluster sites and the increase of the mean condensate size are expected to follow a scaling law.

Saturation: Due to the finite system size, eventually only a single cluster site survives, containing all excess particles. This is a typical stationary configuration for large but finite systems, as has been discussed in Theorem 5.5.

Physically most interesting is the coarsening regime and in particular the expected scaling law and its universal properties, which we investigate in the following. Also of interest is the saturation regime, especially the case of two remaining condensates for which we find effective dynamical equations in Section 6.3.2. On the other hand the nucleation process takes only a very short time and is much harder to analyze since it depends on the initial condition, so we only discuss its influence on the other regimes very quickly.

In the following, we study these regimes and their dependence on system parameters in detail for the model with rates

$$g(k) = \Theta(k)(1 + b/k^\gamma) \,, \tag{6.1}$$

introduced in Section 5.3. We focus on the one dimensional lattices $\Lambda_L = \mathbb{Z}/L\mathbb{Z}$ with periodic boundary conditions and on nearest neighbor jumps. These are taken to be either totally asymmetric where particles only jump to the right, or symmetric, i.e.

$$p_a(y) = \delta_{1,y} \quad \text{or} \quad p_s(y) = \big(\delta_{-1,y} + \delta_{1,y}\big)/2 \,. \tag{6.2}$$

There are $(\rho - \rho_c)L$ excess particles in the system and we speak of a condensate if a site contains a non-zero fraction α of all excess particles. Since the bulk fluctuations grow only sublinearly with L (cf. Section 5.3.2), the cluster sites are well separated from the bulk for large L. The choice of α is therefore not critical as long as it is a small number in the interval $(0, 1)$. In simulations $\alpha = 1/40$ turned out to be a reasonable choice, requiring system sizes of about 200 sites minimum for the parameter values considered.

Definition. A site $x \in \Lambda_L$ is called a *cluster site*, if $\eta_t(x) \geq (\rho - \rho_c)L/40$. The set of cluster sites at a given time t is denoted by

$$\mathcal{C}_L(t) = \big\{x \in \Lambda_L \,\big|\, \eta_t(x) \geq (\rho - \rho_c)L/40\big\} \,, \tag{6.3}$$

and $M_L(t) = \sum_{x \in \mathcal{C}_L(t)} \eta_t(x)$ gives the total number of particles trapped in condensates.

Note that these quantities are defined for each realization $(\boldsymbol{\eta}_t)_{t\geq 0}$ of the process.

Our analysis is based on two simplifying assumptions, which we found to be good approximations comparing with numerical simulations.

Assumption (A1). Separation of time scales
The nucleation process is very fast so that at the beginning of the coarsening regime the bulk is already relaxed to $\bar{\nu}_{\phi_c}$.

So each bulk site loses particles at the average rate $\langle g\rangle_{\bar{\nu}^1_{\phi_c}} = \phi_c = 1$, cf. Section 5.3, resulting in a non-zero current for asymmetric jump probabilities. On top of that excess particles are exchanged between condensates. The bulk can be seen as a homogeneous medium where the excess particles move, and the cluster sites as boundaries where they enter and exit. A condensate of size $m \sim (\rho - \rho_c)L$ loses excess particles with rate $g(m) - 1 = b/m^\gamma$ and gains particles from neighboring condensates. The validity of this picture is confirmed by simulation data in the next subsection.

Assumption (A2). Independence of excess particles in the bulk
The excess particles can move independently through the bulk on their way to the next condensate and do not affect the bulk distribution $\bar{\nu}_{\phi_c}$.

This is a good approximation, since the number of excess particles in the bulk is small compared to L, as shown in the next subsection. So the motion through the bulk does not limit the coarsening time scale which is thus only determined by the effective rates at which particles leave cluster sites, as discussed in Section 6.3.

6.2.2 Validity of the basic assumptions

By definition a typical condensate has a size of order $m \sim \alpha(\rho - \rho_c)L$ and so there are of order $|\mathcal{C}_L| \sim 1/\alpha \sim 1$ cluster sites at the end of the nucleation process which have a typical distance of order L. The time scale for the formation of such condensates is expected to be of the same order as their distance, i.e. $O(L)$ for asymmetric jump rates, and $O(L^2)$ in the symmetric case due to diffusive motion of the particles. This is rather a lower bound on this time scale, but there is no reason to believe that it should be substantially larger. Also the dependence on the other system parameters ρ, b or γ is not obvious. However, it can be seen in simulations, that the nucleation process is very fast compared to the other regimes. This is illustrated in Figure 6.2 (left) for asymmetric jump rates. The time axis is scaled proportional to the time scale $\tau_a = (\rho-\rho_c)^2L^2/b$ of the coarsening regime (cf. Section 6.3). With this, the normalized ensemble average $\langle M_L(t)\rangle/((\rho - \rho_c)L)$ converges to 1 very quickly, indicating that most excess particles become trapped in a condensate and the bulk relaxes to $\bar{\nu}_1$. The coarsening regime starts when this number is sufficiently large and ends when the average number of cluster sites $\langle|\mathcal{C}(t)|\rangle$ becomes small (between 2 and 3) and the saturation regime sets in. This is plotted in Figure 6.2 (right), where we also see that with our definition the average number of cluster sites is independent of all system parameters. After a short time of growth, this number starts decreasing as a result of the beginning coarsening process.

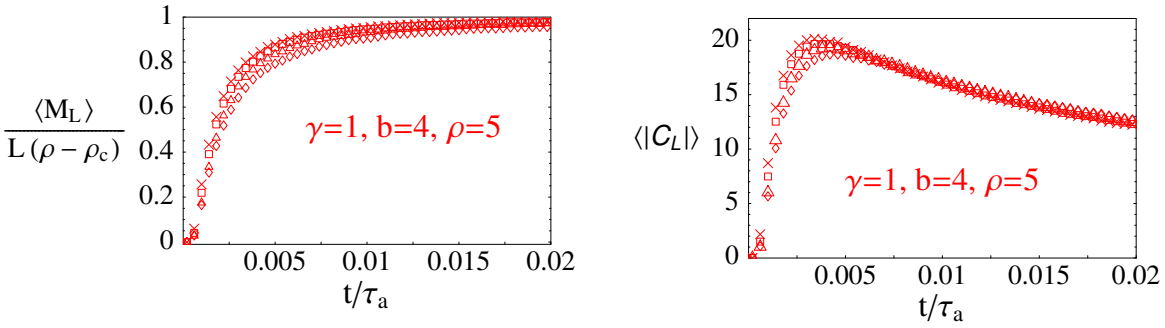


Figure 6.2: Separation of time scales. **Left:** Average fraction of particles in the condensed phase $\frac{\langle M_L(t)\rangle}{L(\rho-\rho_c)}$. **Right:** Average number of cluster sites $\langle|\mathcal{C}_L(t)|\rangle$. Both are plotted as a function of time in units of $\tau_a = (\rho-\rho_c)^2L^2/b$ (6.11) for $\gamma = 1$, $b = 4$, $\rho = 5$ and different values of L in the asymmetric case. Symbols: $L = 320(\diamond)$, $640(\triangle)$, $1280(\square)$, $2560(\times)$.

Assumption (A.2) on the independence of excess particles, that are exchanged by the clusters through the relaxed bulk, is approved by showing that the number of such particles is small compared to bulk volume L. The mobility of excess particles in the bulk is characterized by the average exit rate from a site containing at least one particle, compared to average sites

$$v = \langle g(k)|k>0\rangle_{\bar\nu^1_{\phi_c}} - \langle g(k)\rangle_{\bar\nu^1_{\phi_c}} = \frac{1}{1-\bar\nu^1_{\phi_c}(0)} - 1 = \frac{\bar\nu^1_{\phi_c}(0)}{1-\bar\nu^1_{\phi_c}(0)} > 0\,, \tag{6.4}$$

as follows from (5.28). With this effective rate, the excess particles perform a random walk in the bulk, which is either biased or unbiased, depending on the first moment of the jump probabilities. The time it takes to reach the next condensate at a distance $m/(\rho-\rho_c) \sim L$ is given by the mean first passage time for a random walk [138]. For asymmetric jump probabilities in one dimension this is proportional to the distance and we can write the following balance equation for the number of excess particles $n(t)$ in the bulk

$$\tfrac{d}{dt}\, n(t) = \frac{b}{m^\gamma} - \frac{v\,(\rho-\rho_c)}{m}\, n(t)\,. \tag{6.5}$$

This equation has the stable fixed point

$$n^* = \frac{b}{v\,(\rho-\rho_c)} m^{1-\gamma} \sim \frac{b}{v\,(\rho-\rho_c)^\gamma} L^{1-\gamma}\,. \tag{6.6}$$

Thus the number of excess particles in the bulk grows sublinearly, so they occupy a vanishing fraction of the bulk volume for $L \to \infty$. Note that for $\gamma = 1$ it is $n^* = O(1)$, and the smaller γ the larger is the excess particle density

$$\rho_{bulk} - \rho_c = n^*/L \sim L^{-\gamma}\,, \tag{6.7}$$

where ρ_{bulk} is the total density of particles in the bulk. This results in finite size effects for simulation results, which is illustrated in Figure 6.3. For $\gamma = 0.4$ these effects are already

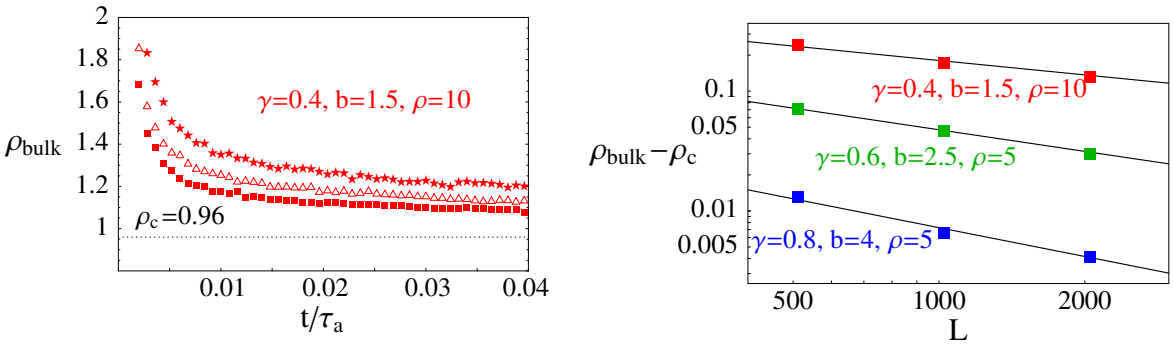


Figure 6.3: Independence of excess particles in the bulk. **Left:** Bulk density $\rho_{bulk}(t)$ as a function of time in units $\tau_a = (\rho - \rho_c)^2 L^2/b$ (6.11) for $\gamma = 0.4$, $b = 1.5$, $\rho = 10$ and $L = 512(\bigstar)$, $1024(\triangle)$, $1280(\blacksquare)$ in the totally asymmetric case. **Right:** Double logarithmic plot of the stationary excess particle density $\rho_{bulk} - \rho_c$ as a function of the system size L for $b = 1.5$, $\rho = 10$ and various values of γ, confirming the scaling of (6.7).

quite strong, and simulations for $\gamma = 0.2$ would require much larger lattice sizes to give reasonable results. On the other hand, for $\gamma = 1$ these finite size effects are completely negligible, as can be seen in Figure 6.2 (left).

In the case of symmetric jump probabilities p_s, excess particles perform an unbiased random walk and the mean first passage time to reach the next cluster site is proportional to the square of the distance, i.e. $O(L^2)$. On the other hand, most of the particles return to the cluster they just left and the probability of crossing the bulk to the next cluster is proportional to $1/L$ (see [138]). Since these are the only relevant events, also the time to enter the bulk effectively increases by a factor of L. So the right hand side of (6.5) is just multiplied with some factor, which does not affect the fixed point (6.6).

6.3 The single species system in one dimension

In this section we analyze the coarsening and the saturation regime of the model (6.1).

6.3.1 Coarsening dynamics

In the coarsening regime, the size $m(t)$ of a typical condensate in large systems is expected to grow according to a scaling law

$$m(t) \sim t^{\beta} \,, \tag{6.8}$$

with a scaling exponent β. Assuming (A1) and (A2) we estimate this exponent and its dependence on the system parameters in the following. First we note that the driving force for the exchange of excess particles is given by the derivative $(g(k) - 1)' = -\gamma\, b/k^{1+\gamma}$ in the following sense. Imagine two condensates of size m_1 and $m_2 > m_1$. The effective rate

at which condensate 1 loses a particle to condensate 2 is given by

$$b/m_1^\gamma - b/m_2^\gamma = g'(m_2)(m_1 - m_2) = \frac{\gamma\, b}{m_2^\gamma}\,\epsilon + O(\epsilon^2)\,. \tag{6.9}$$

The expansion parameter $\epsilon = \frac{m_2 - m_1}{m_2} \in (0,1)$ is a small number if both condensate sizes are similar, i.e. $m_1/m_2 \lesssim 1$. So the time scale of exchanging single excess particles is proportional to $m^\gamma/(\gamma\, b)$. But the coarsening time scale is determined by the time it takes to exchange of order m particles, which is thus given by

$$t = \int_0^m \frac{m'^\gamma}{\gamma\, b} dm' = \frac{m^{1+\gamma}}{\gamma(1+\gamma)b}\,. \tag{6.10}$$

Inserting $m \sim (\rho - \rho_c)L$ for the size of a typical condensate, this gives the expected coarsening time scale for asymmetric systems

$$\tau_a = \frac{(\rho - \rho_c)^{1+\gamma}}{\gamma(1+\gamma)b}\, L^{1+\gamma}\,. \tag{6.11}$$

By inverting (6.10) we obtain the expected scaling law for the normalized condensate size

$$\frac{m(t)}{(\rho - \rho_c)L} \simeq \big(t/\tau_a\big)^{\beta_a} \quad , \qquad \text{with } \beta_a = \frac{1}{1+\gamma}\,. \tag{6.12}$$

For a symmetric system there is an additional point. In contrast to the asymmetric case, it is very likely that particles return to the cluster site they just left, causing only fluctuation in the condensate size (see also Section 6.2.2). Particles which just left a condensate return to the same one with probability $1 - (\rho - \rho_c)/m$ close to one. Thus on average only every $m/(\rho - \rho_c)$-th excess particle reaches the next cluster, enlarging the time scale of exchanging single particles to $m^{1+\gamma}/\big((\rho - \rho_c)\gamma\, b\big)$. After integration analogous to (6.10) we obtain the coarsening time scale

$$\tau_s = \frac{(\rho - \rho_c)^{1+\gamma}}{\gamma(2+\gamma)b}\, L^{2+\gamma}\,. \tag{6.13}$$

The scaling law in this case is given by

$$\frac{m(t)}{(\rho - \rho_c)L} \simeq \big(t/t_s\big)^{\beta_s} \quad , \qquad \text{with } \beta_s = \frac{1}{2+\gamma}\,. \tag{6.14}$$

These predictions agree well with simulation data, shown in Figure 6.4. The typical cluster size is measured by the ensemble average $\langle \ldots \rangle$ of the mean cluster size $\bar{m}(t) = M_L(t)/|\mathcal{C}_L(t)|$. Using the time scales τ_a and τ_s respectively, and normalizing $\langle \bar{m} \rangle$ by the number of excess particles $(\rho - \rho_c)L$ the data for different system sizes collapse. The measured growth exponents from these data agree well with the above predictions. Independently, these exponents have been obtained numerically in [58] for $\gamma = 1$.

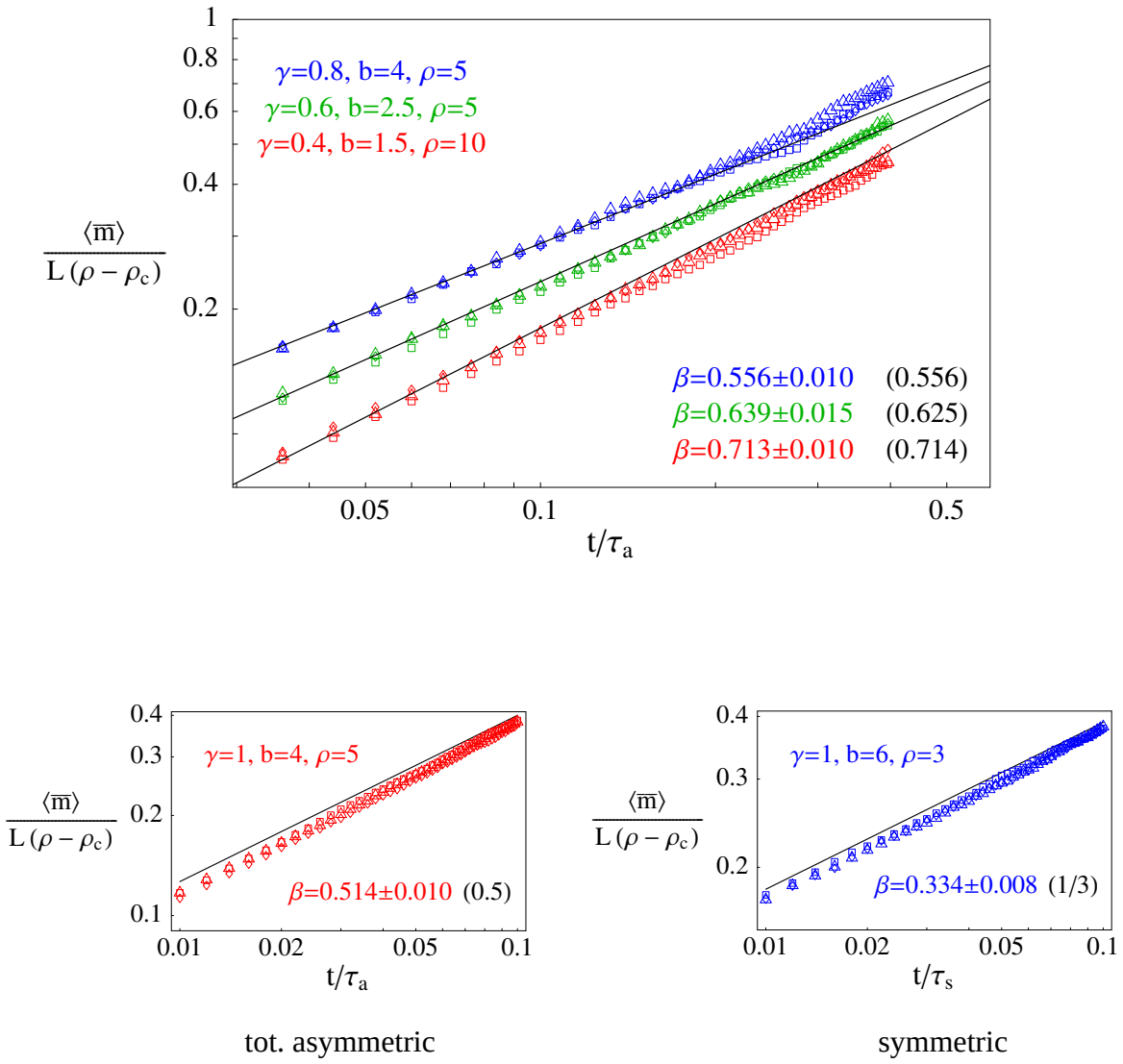


Figure 6.4: Verification of the predicted scaling laws (6.12), (6.14) denoted by straight lines in a double logarithmic plot of the normalized average cluster size $\frac{\langle \bar{m}(t) \rangle}{L(\rho-\rho_c)}$. The predicted scaling exponents are given in parentheses written in black. **Top:** Totally asymmetric case with time scale τ_a (6.11) for several values of γ. Symbols: $L = 512(\diamond)$, $1024(\triangle)$, $2048(\square)$. **Bottom:** The same plot with $\gamma = 1$ for asymmetric (left) and symmetric systems (right) and time scales τ_a (6.11) and τ_s (6.13), respectively. Symbols: (left) $L = 320(\diamond)$, $640(\triangle)$, $1280(\square)$; (right) $L = 160(\diamond)$, $320(\triangle)$, $640(\square)$.

6.3.2 Saturation

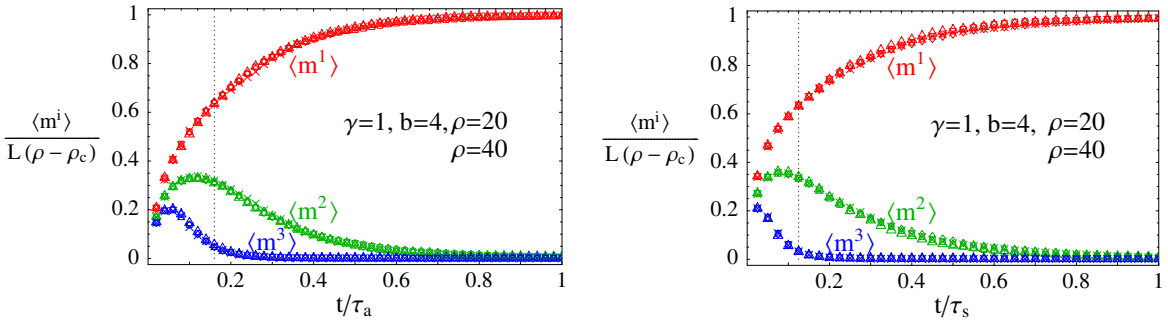
Eventually all condensates except for two disappeared and finite size effects become dominant. The scaling law (6.8) is no longer valid in this regime, since the mean condensate size $\bar{m}$ saturates towards its limiting value. The two condensates exchange particles until one of them vanishes or becomes very small, and the system has reached a typical stationary configuration, where all excess particles are concentrated at a single cluster site. In Figure 6.5 we plot the average size of the three largest condensates $\langle m^i(t)\rangle$, $i = 1, 2, 3$ normalized by the number of excess particles $(\rho - \rho_c)L$. Note that the coarsening regime ends at latest when the third largest condensate has disappeared, and thus takes only about a tenth of the total equilibration time. In the following, we focus on the totally asymmetric jump probabilities with $\gamma = 1$ for simplicity of notation. Symmetric jump probabilities would lead to an effective evolution equation of the same form and also the case $\gamma < 1$ leads to no further difficulties.

Let $M = m^1 + m^2$ be the total number of particles at the two largest cluster sites. In the following we switch to the time scale $t^* = t \,/\, ((\rho - \rho_c)L/b)$ on which the condensates exchange single particles with effective rates $(\rho - \rho_c)L/m^i = O(1)$, according to the discussion in the previous subsection. The fluctuations of M on this time scale are only $O(1)$. Thus it is $M = (\rho - \rho_c)L + O(1)$, since the bulk is relaxed to $\bar{\nu}_1$ and all other condensates have disappeared. Let $q(m, t^*)$ be the probability of having $m = 0, \ldots, M$ particles at one cluster site and $M - m$ at the other one. The dynamics is then governed by the effective master equation

$$\begin{aligned}\partial_{t^*} q(m,t^*) = &-q(m,t^*)\left[\frac{\theta(m)}{m/M} + \frac{\theta(M-m)}{1-m/M}\right] \\ &+q(m-1,t^*)\frac{\theta(m)}{1-(m-1)/M} + q(m+1,t^*)\frac{\theta(M-m)}{(m+1)/M}\,. \end{aligned} \tag{6.15}$$

The exchange rates on the right hand side depend only on the rescaled variable m/M and not on the system parameters ρ, L and b. For large M, m/M varies on the time scale $t^*/\,M \simeq t \,/\, ((\rho - \rho_c)^2 L^2/b)$, confirming that τ_a (6.11) is also the appropriate time scale for the saturation regime. Therefore the plots in Figure 6.5 are independent of the system parameters. However, in the following discussion we stick to the time scale t^* and the discrete variable m.

For any initial condition the solution of (6.15) tends to the inverse binomial distribution $q^*(m) \sim 1 \,/ \binom{M}{m}$. It is symmetric around $m = M/2$ and for small m we have $q^*(m) = O(M^{-m})$. Thus the two extreme occupation numbers $m = 0$ and $m = M$ are the most probable ones and in the limit $L \to \infty$ both have probability $1/2$, consistent with the results of Section 4.2. For $m = \alpha M$, $\alpha \in (0,1)$ it is $q^*(m) = O\left(\sqrt{M}\left(\alpha^\alpha (1-\alpha)^{1-\alpha}\right)^M\right)$ using Stirling's formula. Thus, for the stationary process the typical time for a macroscopic fluctuation of the condensate size diverges exponentially with the system size L.



tot. asymmetric symmetric

Figure 6.5: Normalized average size of the three largest condensates $\frac{\langle m^i(t)\rangle}{L(\rho-\rho_c)}$, $i=1,2,3$ as a function of time. **Left:** Asymmetric case with time scale τ_a (6.11). Symbols: $\rho=20$, $L=80(\diamond)$, $160(\triangle)$, and $\rho=40$, $L=80(\square)$, $160(\times)$. **Right:** Symmetric case with time scale τ_s (6.13). Symbols: $\rho=20$, $L=40(\diamond)$, $80(\triangle)$, and $\rho=40$, $L=40(\square)$, $80(\times)$.

To study the saturation dynamics, we write (6.15) in the canonical form, using the discrete derivative $\nabla_m f(m) := f(m+1)-f(m)$,

$$\begin{aligned}\partial_{t^*} q(m,t^*) &= -\nabla_m\Big(a(m)\,q(m,t^*)\Big) + \nabla_m^2\Big(d(m)\,q(m,t^*)\Big)\\ a(m) &= \frac{1}{(1-m/M)} - \frac{M}{m} = \frac{2m/M-1}{m/M(1-m/M)}\\ d(m) &= \frac{1}{2}\left(\frac{1}{(1-m/M)}+\frac{M}{m}\right) = \frac{1}{2m/M(1-m/M)}\,.\end{aligned} \tag{6.16}$$

For ease of notation, we take $0<m<M$ and ignore the boundary terms at $m=0,M$. Note that (6.16) is symmetric around $m=M/2$. It describes diffusive motion in a double well potential with drift $a(m)$ and diffusion coefficient $d(m)$, with the slightly unusual feature that the minima of the potential are located close to the boundaries at $m=1$ and $m=M-1$.

The master equation (6.16) must be supplied with a suitable initial condition $q(m,0)$, which, since resulting from a complex coarsening process, is not readily available. A rough estimate can be found by noting that $q(m,0)$ is roughly proportional to the lifetime of the two-condensate configuration $(m,M-m)$. It is determined by the inverse exit rate taken from equation (6.15), and thus we expect $q(m,0)\approx 6m/M\,(1-m/M)$. This is a symmetric single hump distribution with mean $M/2$ and standard deviation $M/(2\sqrt{5})\approx 0.22M$. Comparing with the simulation data at the time when the third largest condensate has just disappeared, $m^3(t)/M<0.01$, we indeed find a single hump distribution with mean $M/2$ and standard deviation $0.166M$. When solving equation (6.16) with this initial distribution, the expectation of the larger condensate size, given by $1/2+\langle|m/M-1/2|\rangle_{q(m,t)}$, is indistinguishable from $\langle m^1(t)\rangle$ in Figure 6.5. Note that, except for the time scales, the asymmetric (left) and symmetric plots (right) are almost identical, confirming that the effective master equation for the symmetric case is of the same form as (6.15).

6.4 Generalizations

6.4.1 Coarsening in the two-component system

In the following we extend the analysis of the coarsening regime to the two component zero range process introduced in Section 5.4. The jump rates (5.72) are given by

$$g_1(k_1,k_2) = \Big(\frac{1+b/(k_1+1)}{1+b/k_1}\Big)^{k_2}\big(1+c/k_1\big)\ , \quad g_2(k_1,k_2) = 1+b/(k_1+1)\ . \tag{6.17}$$

We concentrate on asymmetric, nearest neighbor jump probabilities, but the symmetric case could be treated analogously. The phase diagram of this model given in Figure 5.3 consists of three regimes.

In regime A, which exists for $c > 2$, only the first species condensates. Thus on cluster sites k_1 is of order L and the rates up to first order are given by

$$g_1(k_1,k_2) \simeq 1+c/k_1\ , \quad g_2(k_1,k_2) \simeq 1+b/k_1\ . \tag{6.18}$$

Thus the particles of species 2 do not influence the effective cluster dynamics of species 1 and we have

$$\tau_A = \frac{\big((\rho_1-\rho_{c,1})L\big)^2}{c}\ , \quad \frac{m_1(t)}{(\rho_1-\rho_{c,1})L} \simeq \big(t/\tau_A\big)^{1/2}\ . \tag{6.19}$$

This is completely analogous to the one component case (6.12) with $\gamma = 1$, where $m_i(t)$ denotes the typical size of a condensate of species i. However, on the cluster site the average jump rate of the second species has to be compatible with the bulk value $\phi_2 \in (0,1)$, because on the coarsening time scale the system is already stationary except for the cluster dynamics. Thus the distribution on this site, denoted by $\tilde\nu_2$ is slightly changed since

$$\phi_2 = \langle g_2\rangle_{\bar\nu^1_\phi} = (1+b/k_1)\,\tilde\nu_2\big(\{k_2>0\}\big)\ , \tag{6.20}$$

and thus for large k_1, $\tilde\nu_2(0) \simeq 1-\phi_2 > \nu^1_{(1,\phi_2),2}(0)$. We suspect $\tilde\nu_2(k_2) = (1-\phi_2)\phi_2^{k_2}$.

Regime B of the phase diagram (Figure 5.3) exists for all $b, c > 0$ and shows more interesting behavior for the condensation of species 2, since g_2 depends only on the number of particles of species 1. On a cluster site it is $k_2 \sim L$ and for fixed k_1 the rate g_1 vanishes in the limit $L\to\infty$ (see (6.17)). But its average has to be equal to the bulk value ϕ_1, and thus k_1 has to be of order $\sqrt{k_2} \sim \sqrt{L}$, as was first noticed in [43]. With this the rates on a cluster site are given by

$$\begin{aligned} g_1(k_1,k_2) &\simeq \exp\big[-bk_2/k_1^2\big]\,(1+c/k_1) \\ g_2(k_1,k_2) &\simeq 1+b/k_1 = 1+\frac{\sqrt{-b\log\phi_1}}{\sqrt{k_2}}\ , \end{aligned} \tag{6.21}$$

where the last identity is due to the compatibility relation $\phi_1 = \langle g_1\rangle = \exp[-bk_2/k_1^2]$. This ratio of k_1 and k_2 is stable, since on a cluster site

$$\partial_{k_1} g_1(k_1,k_2) \simeq \phi_1\Big(\frac{-2\log\phi_1}{k_1} - \frac{2\log\phi_1 + c}{k_1^2}\Big) > 0\ . \tag{6.22}$$

Thus fluctuations of k_1 are balanced by inflow and outflow of particles from the bulk. Since $\partial_{k_1} g_2(k_1, k_2) \simeq -b/k_1^2$, this mechanism is one order of magnitude faster than the dynamics of the condensate. So the coarsening is driven by the exchange of particles of species 2, the particles of species 1 quickly adjust on the cluster sites. With (6.21) the expected scaling law is of type (6.11), (6.12) with $\gamma = 1/2$, leading to

$$\tau_B = \frac{4\big((\rho_2 - \rho_{c,2})L\big)^{3/2}}{3\sqrt{-b \log \phi_1}} , \quad \frac{m_2(t)}{(\rho_2 - \rho_{c,2})L} \simeq \big(t/\tau_B\big)^{2/3} . \tag{6.23}$$

The predictions for regions A and B coincide with preliminary simulation data shown in Figure 6.6 (top).

In regime C, which exists only for $c > 3$, both species condensate. Since g_1 is decreasing with k_2 and vice versa, a site which contains both condensates of species 1 and 2 loses particles much more slowly than a single condensate site. Thus these double condensates are more stable and we expect that in a typical stationary configuration there is one cluster site containing both condensates. This intuition is supported by looking at the compatibility relation of regime B which has to hold in regime C, too. But here also $\phi_1 = 1$ and thus on a cluster site of species 2, k_1 has to scale larger than $\sqrt{k_2}$. In turn also the distribution of 2-particles on a cluster site of 1-particles (6.20) would become degenerate. The jump rates for a double condensate are of the order

$$g_1(k_1, k_2) \simeq 1 + \frac{c - b(k_2/k_1)}{k_1} , \quad g_2(k_1, k_2) \simeq 1 + \frac{b(k_2/k_1)}{k_2} . \tag{6.24}$$

k_2/k_1 is a number of order unity and close to $(\rho_2 - \rho_{c,2})/(\rho_1 - \rho_{c,1})$. Thus both clusters grow at the same time scale and we expect

$$\tau_C \sim L^2 , \quad \frac{m_1(t)}{(\rho_1 - \rho_{c,1})L} \sim \frac{m_2(t)}{(\rho_2 - \rho_{c,2})L} \sim \big(t/\tau_C\big)^{1/2} , \tag{6.25}$$

which is confirmed by simulation data given in Figure 6.6 (bottom). The dependence on the other system parameters appears to be more complicated and we could not yet identify it.

6.4.2 Comments on higher space dimension

We consider a typical configuration in the coarsening regime, with a relaxed bulk and condensates on the d-dimensional torus $\Lambda_L = (\mathbb{Z}/L\mathbb{Z})^d$. The space dimension influences the motion of excess particles in the bulk. As has been discussed in Section 6.2.2, they perform a random walk which is biased or unbiased, depending on the symmetry of the jump probabilities. The properties of a biased random walk are largely independent of the space dimension, in particular the expected number of distinct sites visited $\langle R_t \rangle$ is proportional to the time t. In the symmetric case the behavior changes qualitatively with the dimension (see e.g. [138]), where

$$\langle R_t \rangle \sim \begin{cases} \sqrt{t} & , \text{ for } d = 1 \\ t/\log t & , \text{ for } d = 2 \\ t & , \text{ for } d \geq 3 \end{cases} . \tag{6.26}$$

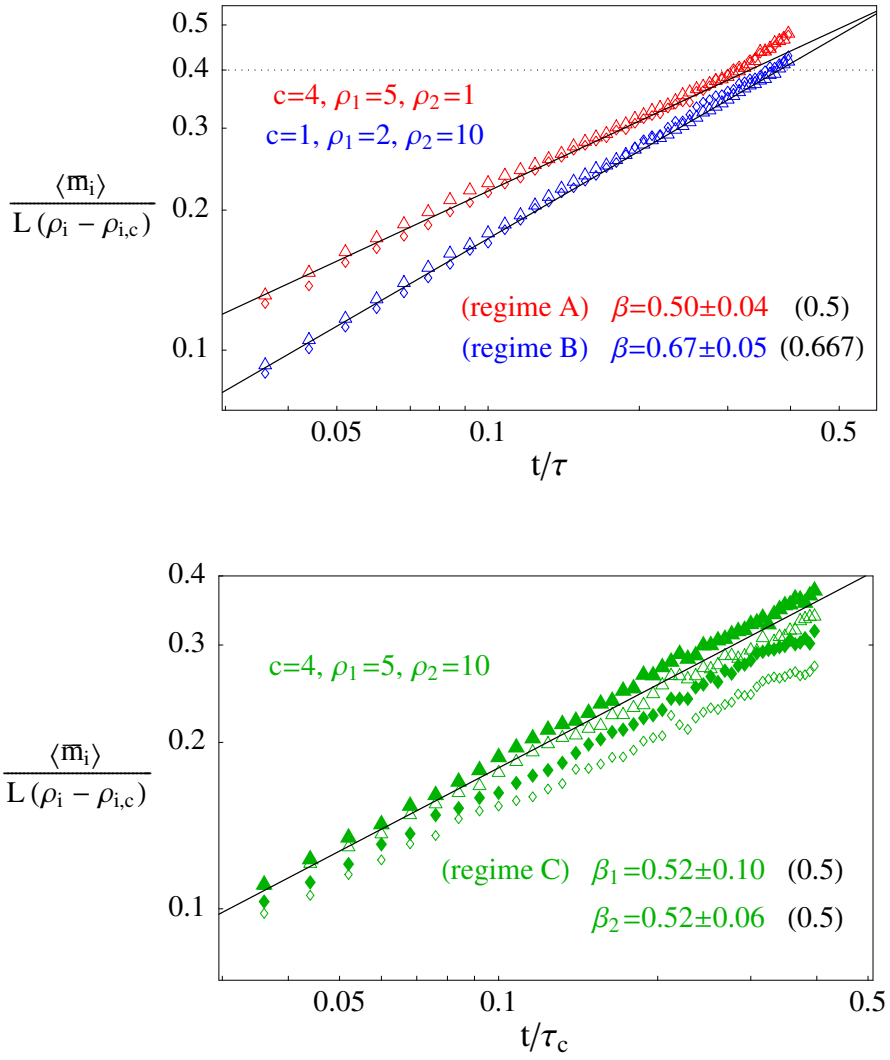


Figure 6.6: Verification of the predicted scaling laws (6.19), (6.23) and (6.25) denoted by straight lines in a double logarithmic plot of the normalized average cluster size $\frac{\langle \bar{m}(t) \rangle}{L(\rho - \rho_c)}$ for $b = 1$ and different values for c, ρ_1 and ρ_2. The predicted scaling exponents are given in parentheses written in black. **Top:** Regimes A and B with different time scales τ_A and τ_B respectively, and symbols $L = 512(\diamond)$, $1024(\triangle)$. The dotted line marks the end of the coarsening regime where the exponents are measured. **Bottom:** Regime C with symbols $L = 256(\diamond)$, $512(\triangle)$ for species 1 and filled symbols for species 2.

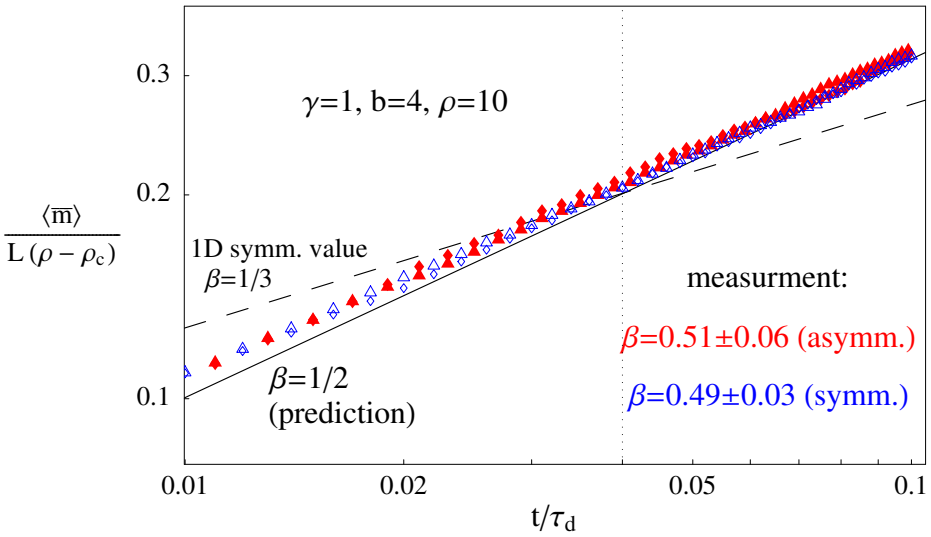


Figure 6.7: Comparison of symmetric and asymmetric jump probabilities for dimension $d = 2$ in a double logarithmic plot of the normalized average cluster size $\frac{\langle \bar{m}(t) \rangle}{L(\rho-\rho_c)}$. The predicted scaling (6.27) with $\beta = 1/2$ is denoted by a straight line and compared to the symmetric scaling $\beta = 1/3$ in dimension $d = 1$ given by a dashed line. The dotted line marks the beginning of the coarsening regime where the exponents are measured. Symbols: $L^2 = 256(\diamond), 1024(\triangle)$ for symmetric jumps and filled symbols for asymmetric jumps.

For $d = 1$, the range is only proportional to $\sqrt{t}$, leading to a large probability of excess particles to return to the condensate they left. This yields a coarsening scaling law which is different from the asymmetric case, as discussed in Section 6.3.1. However, for dimensions $d \geq 3$, unbiased random walkers show the same qualitative behavior as biased ones. The borderline case is given by dimension $d = 2$, where we expect the same behavior as for higher dimensions, up to logarithmic corrections. The above phenomenon is closely related to the question of recurrence and transience of random walks on infinite lattices.

Since the derivation of the scaling law in Section 6.3.1 is otherwise independent of space dimension, (6.12) should be valid for symmetric and asymmetric systems. Note that also the validity of the Assumptions (A1) and (A2) as discussed in Section 6.2.2 is not affected. So the typical condensate size is expected to grow as

$$\frac{m(t)}{(\rho-\rho_c)L^d} \simeq \left(t/\tau_d\right)^{\beta} \quad , \qquad \text{with } \beta = \frac{1}{1+\gamma} \, . \tag{6.27}$$

But since a condensate consists now of order $(\rho-\rho_c)L^d$ particles, the coarsening time scale changes and is given by

$$\tau_d = \frac{(\rho-\rho_c)^{1+\gamma}}{\gamma(1+\gamma)b} \, L^{d(1+\gamma)} \, . \tag{6.28}$$

This significantly increases the simulation time for systems in higher space dimension and data for reasonable system sizes are very hard to get. We have some preliminary results for

$d = 2$ shown in Figure 6.7, indicating the validity of the above conjecture. For the accessible system sizes, the quality of the data is slightly affected by the logarithmic corrections, and simulations for $d = 3$ are clearly exceeding our resources.

6.5 Discussion

The arguments used in Section 6.3.1 to derive the coarsening scaling law are applicable in a very general context, since they are only based on assumptions (A1) and (A2), which are rather generic in case of condensation phenomena. This leads to conjectures for the coarsening behavior of systems in higher space dimensions and with two species of particles. These statements are supported by preliminary simulations, but still have to be confirmed by thorough numerical data. In particular, simultaneous condensation in case of two particle species requires further analysis. To test the generality of our technique, one could also try to apply it to systems with different jump rates that also exhibit a condensation transition.

For the single species ZRP with rates (5.27) in one dimension our analysis given in Section 6.3 is largely complete. This process is an effective model for domain wall dynamics in multi-species exclusion models [76], and the condensation transition corresponds to phase separation in such systems. Thus our analysis provides new information on the coarsening behavior and the fluctuations in typical stationary configurations. Together with the static results of Chapter 5, this contributes to the understanding of phase transitions in systems with several particle species, which is currently a topic of major interest.

Appendix

A.1 Semigroup and generator

In the following we summarize some facts about the characterization of a Markov process using the Markov semigroup, used in Chapter 2. The material is taken from [99], Chapter I, and we refer the reader to this reference for more details.

Assume that X is a compact metric space with measurable structure given by the σ-algebra of Borel sets. Let $C(X,\mathbb{R})$ be the set of continuous functions $f : X \to \mathbb{R}$ considered as a Banach space with norm $\|f\| = \sup_{\boldsymbol{\eta}\in X} |f(\boldsymbol{\eta})|$.

Definition. A *Markov semigroup* is a collection of linear operators $\{S(t), t \geq 0\}$ on $C(X,\mathbb{R})$ with the following properties:

a) $S(0) = I$, the identity operator on $C(X,\mathbb{R})$.
b) The mapping $t \mapsto S(t)\, f$ is right continuous for every $f \in C(X,\mathbb{R})$.
c) $S(t+s)\, f = S(t)S(s)\, f$ for all $f \in C(X,\mathbb{R})$ and all $s,t \geq 0$.
d) $S(t)\, 1 = 1$ for all $t \geq 0$.
e) $S(t)\, f \geq 0$ for all nonnegative $f \in C(X,\mathbb{R})$.

The operators $S(t)$ determine the time evolution of observables. The importance of Markov semigroups lies in the fact that each one corresponds to a Markov process, as is formulated in the following theorem.

Theorem A.1 *Suppose $\{S(t), t \geq 0\}$ is a Markov semigroup on $C(X,\mathbb{R})$. Then there exists a unique Markov process $\{\mathbb{P}^{\boldsymbol{\eta}}, \boldsymbol{\eta} \in X\}$ such that*

$$S(t)\, f(\boldsymbol{\eta}) = \mathbb{E}^{\boldsymbol{\eta}} f(\eta_t) \tag{A.1}$$

for all $f \in C(X,\mathbb{R})$, $\boldsymbol{\eta} \in X$, and $t \geq 0$. On the other hand, if $\{\mathbb{P}^{\boldsymbol{\eta}}, \boldsymbol{\eta} \in X\}$ is a Feller Markov process on X, then the linear operators $\{S(t), t \geq 0\}$ defined via (2.2) are a Markov semigroup.

Proof. See [99], Theorem I.1.5.

Feller Markov processes have the additional property that $S(t)f \in C(X,\mathbb{R})$ for arbitrary

$f \in C(X, \mathbb{R})$ and $t \geq 0$. This is not clear for general Markov processes but the ones we study here have this property. Thus the problem of constructing a Feller Markov process is reduced to the construction of the corresponding semigroup, which is done using their generators.

Definition. A *Markov generator* is a linear, closed operator Ω on $C(X, \mathbb{R})$ with domain D_Ω which satisfies the following conditions:

a) $1 \in D_\Omega$ and $\Omega 1 = 0$.
b) D_Ω is dense in $C(X, \mathbb{R})$.
c) If $f \in D_\Omega$, $\lambda \geq 0$, and $f - \lambda\Omega\, f = g$, then $\min_{\boldsymbol{\eta} \in X} f(\boldsymbol{\eta}) \geq \min_{\boldsymbol{\eta} \in X} g(\boldsymbol{\eta})$.
d) The range $\mathcal{R}(I - \lambda\Omega) = C(X, \mathbb{R})$ for all sufficiently small $\lambda > 0$.

Theorem A.2 (Hille-Yosida) *There is a one-to-one correspondence between Markov generators and semigroups on $C(X, \mathbb{R})$ given by:*

$$
\begin{aligned}
a) \quad & D_\Omega = \left\{ f \in C(X, \mathbb{R}) : \lim_{t \searrow 0} \frac{S(t)\, f - f}{t} \text{ exists} \right\} \text{ , and} \\
& \Omega\, f = \lim_{t \searrow 0} \frac{S(t)\, f - f}{t} \text{ for } f \in D_\Omega \text{ ,} \\
b) \quad & S(t)\, f = \lim_{n \to \infty} \left(I - t\, \Omega / n \right)^{-n} f \quad \text{for } f \in C(X, \mathbb{R}) \text{ and } t \geq 0 \text{ .}
\end{aligned}
\tag{A.2}
$$

For $f \in D_\Omega$ it is $u(t) = S(t)\, f \in D_\Omega$ for all $t > 0$, given by the unique solution of the backward equation

$$
\frac{d}{dt} u(t) = \Omega u(t) \text{ ,} \quad u(0) = f \text{ .} \tag{A.3}
$$

Proof. See [99], Theorem I.2.9.

Suppose Ω is a Markov generator on $C(X, \mathbb{R})$ with domain D_Ω. A linear subspace $D \subset D_\Omega$ is said to be a *core* for Ω, if Ω is the closure of its restriction to D. Thus Ω is uniquely determined by its values on a core. The next theorem addresses the convergence of sequences of semigroups, which can be used for example to characterize processes on infinite lattices.

Theorem A.3 (Trotter Kurtz) *Let Ω and Ω_n, $n \in \mathbb{Z}^+$ be generators of the Markov semigroups $S(t)$ and $S_n(t)$. If there is a core D for Ω such that $D \subset D_{\Omega_n}$ for all n and $\Omega_n f \to \Omega f$ for all $f \in D$, then*

$$
S_n(t) f \to S(t) f \tag{A.4}
$$

for all $f \in C(X, \mathbb{R})$ uniformly for t in compact sets.

Proof. See [99], Theorem I.2.12.

A.2 Monotonicity and coupling

The state space X of an interacting particle system is a partially ordered set with $\boldsymbol{\eta} \leq \boldsymbol{\zeta}$ if $\eta(x) \leq \zeta(x)$ for all $x \in \Lambda$. A test function $f \in C(X, \mathbb{R})$ is called *increasing* if $\boldsymbol{\eta} \leq \boldsymbol{\zeta}$ implies $f(\boldsymbol{\eta}) \leq f(\boldsymbol{\zeta})$. This induces a partial order on the set of probability measures $P(X)$, namely $\mu_1 \leq \mu_2$ if $\langle f \rangle_{\mu_1} \leq \langle f \rangle_{\mu_2}$ for all increasing $f \in C(X, \mathbb{R})$. This property is called *stochastic monotonicity* and we say that μ_1 dominates μ_2 from below and μ_2 dominates μ_1 from above.

A *coupling* $(\boldsymbol{\eta}, \boldsymbol{\zeta}) \in X \times X$ of two random variables $\boldsymbol{\eta}, \boldsymbol{\zeta} \in X$ is a joint construction of them on a common probability space. The marginals of the coupling measure μ have to be the distributions μ_1 and μ_2 of $\boldsymbol{\eta}$ and $\boldsymbol{\zeta}$ respectively.

Theorem A.4 *For two probability measures $\mu_1, \mu_2 \in P(X)$ we have $\mu_1 \leq \mu_2$ if and only if there is a coupling $(\boldsymbol{\eta}, \boldsymbol{\zeta})$ such that $\boldsymbol{\eta}$ has distribution μ_1, $\boldsymbol{\zeta}$ has distribution μ_2, and $\boldsymbol{\eta} \leq \boldsymbol{\zeta}$ a.s., i.e. the coupling measure $\mu \in P(X \times X)$ concentrates on the set $\big\{(\boldsymbol{\eta}, \boldsymbol{\zeta}) \,\big|\, \boldsymbol{\eta} \leq \boldsymbol{\zeta}\big\}$.*

Proof. See [99], Theorem 2.4 page 72.

The coupling concept can also be applied to processes $\boldsymbol{\eta}_t$, $\boldsymbol{\zeta}_t$ with generators $\mathcal{L}_1$ and $\mathcal{L}_2$ and common state space X. The coupled process $(\boldsymbol{\eta}_t, \boldsymbol{\zeta}_t)$ with state space $X \times X$ has to be such that the marginal processes $\boldsymbol{\eta}_t$ and $\boldsymbol{\zeta}_t$ are Markovian and have generators $\mathcal{L}_1$ and $\mathcal{L}_2$ respectively. Due to the construction on the same probability space, the marginal processes $\boldsymbol{\eta}_t$ and $\boldsymbol{\zeta}_t$ have the same Poisson times for transitions. The idea of the so-called *basic coupling* in the context of interacting particle systems is that particles in $\boldsymbol{\eta}_t$ and $\boldsymbol{\zeta}_t$ move together whenever they can. There are many other ways of coupling two processes which are not used in this thesis, a comprehensive survey can be found in [50]. For exclusion models the basic coupling was first used in [98] (see also references therein) and can be analytically defined by writing down the generator of the coupled process which is done in [99], Section VIII.2. An alternative probabilistic way is to construct the processes using an underlying common Poisson process for the transition events. The latter approach is more intuitive and very much reminiscent of the construction of a single process. It is discussed in detail in [100], Section III.3. In the following we just give the jump rates when $\boldsymbol{\eta}_t$ and $\boldsymbol{\zeta}_t$ are two versions of the ASEP on $\Lambda = \mathbb{Z}$. Writing the configurations on top of each other we have for the jump rates of the $\boldsymbol{\eta}$ particles

$$\begin{array}{cccccc} \boldsymbol{\eta} & 1\,0 & \overset{p}{\underset{q}{\rightleftarrows}} & 0\,1 & 1\,0 \xrightarrow{p} 0\,1 & 1\,0 \overset{p}{\underset{q}{\rightleftarrows}} 0\,1 \quad 1\,0 \overset{p}{\underset{q}{\rightleftarrows}} 0\,1 \\ \boldsymbol{\zeta} & 1\,0 & & 0\,1 & 0\,1 \qquad 0\,1 & 1\,1 \qquad 0\,0 \end{array} . \tag{A.5}$$

For the $\boldsymbol{\zeta}$ particles the jump rates are analogous by exchanging top and bottom, and all other rates are equal to zero. It is easy to see that with these rules both marginal processes are Markovian, i.e. independent of the configuration of the other marginal. Completely analogously one could specify coupled rates for particle creation and annihilation for systems with open boundaries (c.f. Section 3.3.3). We say that $x \in \Lambda$ is a discrepancy at time t if $\eta_t(x) \neq \zeta_t(x)$, characterized by a local configuration $\binom{1}{0}$ or $\binom{0}{1}$. They can move according to

the last two rules of (A.5), whereas the first two rules state, that they can only disappear, but cannot be created. Thus for the ASEP on $\Lambda = \mathbb{Z}$ if $\boldsymbol{\eta}_0 \leq \boldsymbol{\zeta}_0$ we have

$$\boldsymbol{\eta}_t \leq \boldsymbol{\zeta}_t \quad \text{for all } t \geq 0 \,. \tag{A.6}$$

This property is called *attractivity*.

Stochastic monotonicity may not be conserved when the coupled processes are not the same, for instance if one of them has a local inhomogeneity, which can be the source of creation of discrepancies. However, if (A.6) is still true, this can be used to dominate (unknown) stationary measures of the perturbed process $\boldsymbol{\zeta}_t$ by known ones of the unperturbed process $\boldsymbol{\eta}_t$. The strategy is to start the coupled process $(\boldsymbol{\eta}_t, \boldsymbol{\zeta}_t)$ with initial distribution π concentrating on $\big\{(\boldsymbol{\eta}, \boldsymbol{\zeta}) \,\big|\, \boldsymbol{\eta} \leq \boldsymbol{\zeta}\big\}$, where the marginal $\pi_1 = \mu_1$ is a (known) stationary measure of $\boldsymbol{\eta}_t$. With (A.6) and the above Theorem, it immediately follows that there exists a stationary measure μ_2 of the perturbed process with $\mu_2 \leq \mu_1$. This strategy is used in Section 3.3.3, where we couple the ASEP on a semi-infinite lattice with different boundary mechanisms.

A.3 Relative entropy

In the following we summarize a few properties of relative entropy which are used in Chapter 5. Proofs and more detailed information can be found in [137], [84] Appendix 1.8 or [25], Chapter I.3.

For two arbitrary probability measures μ, ν on a countable set Ω it is defined as

$$H(\mu|\nu) = \begin{cases} \sum\limits_{\omega\in\Omega} \mu(\omega) \log \frac{\mu(\omega)}{\nu(\omega)} \;, & \text{if } \mu \ll \nu \\ \qquad\infty \qquad\quad , & \text{otherwise} \end{cases} \tag{A.7}$$

where $\mu \ll \nu$ means that μ is absolutely continuous with respect to ν. It has the properties

$$H(\mu|\nu) \geq 0 \,, \quad H(\mu|\nu) = 0 \Leftrightarrow \mu(\omega) = \nu(\omega) \text{ for all } \omega \in \Omega \,. \tag{A.8}$$

In the proof of Theorem 5.2 we use the sub-additivity of H, namely if two measures μ, ν have marginals μ_i, ν_i, $i = 1, 2$, then

$$H(\mu|\nu) \geq H(\mu_1|\nu_1) + H(\mu_2|\nu_2) \,. \tag{A.9}$$

The relative entropy can also be written as the solution of a variational problem

$$H(\mu|\nu) = \sup_{f\in C_b(\Omega,\mathbb{R})} \big\{ \langle f \rangle_\mu - \log \langle e^f \rangle_\nu \big\} \,, \tag{A.10}$$

where C_b denotes bounded, continuous functions. A direct consequence is the entropy inequality,

$$\langle f \rangle_\mu \leq \alpha^{-1} \big(\log \langle e^{\alpha f} \rangle_\nu + H(\mu|\nu) \big) \,, \tag{A.11}$$

for all $\alpha > 0$. This can be used to estimate the expectation of a function with respect to a probability measure μ in terms of exponential moments of a second measure ν.

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