Monte Carlo analysis of non-equilibrium steady states and relaxation kinetics in driven lattice gases

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We numerically investigate the long-time behavior of the density-density auto-correlation function in driven lattice gases, with particle exclusion and periodic boundary conditions in one, two, and three dimensions using precise Monte Carlo simulations of larger system sizes than previous studies. In the one-dimensional asymmetric exclusion process on a ring with half the lattice sites occupied, we find that correlations induce extremely slow relaxation to the asymptotic power law decay. We compare the crossover functions obtained from our simulations with various analytic results in the literature, and analyze the characteristic oscillations that occur in finite systems away from half-filling. As expected, correlations are weak in three dimensions and consequently the mean-field description is adequate. We also investigate the relaxation towards the non-equilibrium steady state in the two-time density-density auto-correlations, starting from strongly correlated initial conditions. We obtain simple aging scaling behavior in one, two, and three dimensions, with the expected power laws.

We numerically investigate the behavior of driven lattice gases with nearest neighbor interactions at half-filling with periodic boundary conditions below and at the critical temperature using Monte Carlo simulations of very large lattices in two dimensions. This work is one of few that explores the relaxation to a non-equilibrium steady state. We obtain data collapse for the finite-size scaling form of density-density auto-correlation function at the critical point. We achieve data collapse using finite-size scaling of the time-dependent order parameter during the transient regime starting from strongly correlated initial conditions. We present simple aging scaling of the density-density auto-correlation function at the critical point starting from strongly correlated initial conditions using Monte Carlo simulations of two different lattice anisotropies. We thus unambiguously confirm the critical exponents determined by renormalization group methods using measurement of dynamic quantities in the transient regime. Measuring these dynamic quantities in the transient regime provides more conclusive measurements of the critical exponents than previous studies measuring static quantities in the stationary state. We provide qualitative arguments that the lattice anisotropy determines the steady-state for sub-critical quenches.

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Dedication

I dedicate this work to my wife, Amanda.
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Chapter 1

Introduction

1.1 History

Non-equilibrium systems make up almost every part of our world. Nature has few, if any, true equilibrium systems. Our understanding and general theoretical framework for equilibrium systems is mature and well-established. We do not have the general analytical framework for non-equilibrium systems that we do for equilibrium systems. Following the work of Boltzmann and Gibbs [1], in equilibrium one can calculate most observables by means of the stationary probability distribution $e^{-\beta H}$, where $H$ is the Hamiltonian of the system and $\beta$ is the inverse temperature. Thus a generic way of calculating macroscopic observables from microscopic rules exists for equilibrium systems. Non-equilibrium systems have the property that they have a non-zero “current,” of particles, energy, etc. The cause of this “current” enters into the transition rates and generically cannot be accounted for in the probability distribution. Most studies focus on non-equilibrium “steady states.” Once the system has relaxed into a Non-Equilibrium Steady State, or NESS, the probability distributions become independent of time. The system has thus lost any memory of initial conditions and is time-translation invariant. There has been substantial work and progress devoted to NESSs, but we possess no generic theoretical framework for their description. Progress has been made towards a general classification of NESSs by Zia and Schmuitmann [2, 3]. Recently the approach to steady states has attracted interest [4]. In this transient regime, time translation invariance is broken and probability distributions depend on time. The transient regime is even less understood than NESSs. Understanding non-equilibrium behavior is extremely important to characterize real many-body systems in nature.

Simple models of non-equilibrium systems that share some of the properties of real systems are usually studied to gain understanding of the real system. The equilibrium Ising model introduced by Lenz [5] and Ising [6], to study ferromagnets became a standard for the study of equilibrium phenomena. The non-equilibrium version of the Ising model, a driven
version of a lattice gas [7] introduced by Katz, Lebowitz and Spohn [8, 9] can be used to model fast ionic conductors [10]. This model, which we will refer to as KLS, has been adopted as a simple system to study complex non-equilibrium behavior. It is related to the equilibrium Model B of critical dynamics, therefore it is sometimes referred to as Driven Model B. Model B is a system with a conservation law, i.e. the Ising model with spin exchange dynamics. Our conserved quantity is the number of particles. The Ising model with single spin flip dynamics is Model A, which does not have a conservation law. For a complete survey and definition of models A and B, see the review by Hohenberg and Halperin [11]. For the KLS model, theoretical models exist based on a coarse grained version of the microscopic model [12, 13, 14, 15, 16]. A theoretical model must be verified by experiment. No real system directly matches the microscopics of the KLS model. Therefore, our “experiment” is computer simulations. Using the microscopic rules that define the model [8, 9], one can perform numerical simulations, in which macroscopic observables can be measured. Therefore, the simulations bridge the gap between microscopic rules that define the model, and macroscopic observables that can be compared to macroscopic theories. Variations of the KLS model are used to model a variety of real life non-equilibrium systems such as traffic [17, 18] and protein synthesis [19, 20, 21].

A simplification of the KLS model is the driven lattice gas without nearest neighbor interactions called the Asymmetric Simple Exclusion Process or ASEP. Substantial work has been done on the ASEP which will be summarized in chapter 2. Notable are the field theoretic methods [12, 13, 14] where the scaling exponents were found exactly. Much of the theoretical understanding of the ASEP in one dimension is attributed to the model being mappable to Kardar-Parisi-Zhang (KPZ) surface growth [13], which has been extensively studied. A summary of the research will be done in chapter 2. Monte Carlo simulations have played a crucial role in verifying the exponents predicted by the field theories. These simulation results will be summarized in chapter 2. Additionally, there have been advances in exact results for the ASEP model. See Ref. [22] for a recent and thorough review of exact results. The use of the Bethe ansatz has yielded the dynamic exponent [23, 24, 25, 26, 27, 28]. Conditional probabilities were calculated using the Bethe Ansatz for both infinite lattices [29] and later generalized to finite lattices with periodic boundary conditions [30, 31]. The exact conditional probabilities however, are only tractable for very small systems. Considerable effort has been focused on determining scaling functions for correlations [32, 33, 34, 35, 36, 37, 38]. We attempt to confirm some of these results with our simulations.

Non-stationary properties for the ASEP have generated interest in the recent years. Calculating aging scaling exponents in the aging regime [4] has been done for KPZ surface growth [39, 40] and for the Edwards-Wilkinson surface growth [41, 42, 43, 44]. A notable result is the calculation of the initial slip exponent by Michael Krech. He shows the short time behavior is governed by known scaling exponents [45]. This property allows the exponents to be numerically determined using results in the transient regime. Limited exact results exist for correlated initial conditions which yield non-stationary properties. They are summarized in Ref. [22]. In principle, the conditional probabilities [29, 30, 31] can be used to calculate
temporal correlations starting from arbitrary initial conditions. This is only tractable for very small systems.

The critical exponents of the KLS model are still being debated in the literature; see Refs. [46, 47] for reviews of earlier work. The technicalities of the debate are examined in detail in chapter 2. The critical exponents were calculated using renormalization group methods in a \( \epsilon = 5 - d \) expansion by Janssen and Schmittmann [15], as well as by Leung and Cardy [16]. We call this Langevin equation and the corresponding set of critical exponents JSLC theory. These exponents did not agree with some simulation results [48, 49] while agreeing with others [50]. Finite-size effects in the KLS model must be carefully considered when performing simulations. Due to the anisotropic nature of the system, rectangular lattices with specific aspect ratios must be used [15, 16, 50]. The opposition to the JSLC theory believes an alternate field theory [51] obtained using a \( \epsilon = 3 - d \) expansion properly describes the KLS model with infinite drive [52, 53, 54]. The new field theory was shown to have flaws [55]. The opposition presents many simulation results which they claim support their position [56, 56, 57, 58, 59]. They do not adhere to the field theoretic predictions of JSLC that determine the correct lattice anisotropy, yet they claim to disprove JSLC. In each of the studies mentioned, static quantities are primarily used. Specifically, finite size scaling of the order parameter is used in most studies to measure the critical exponents, this method is sensitive to the “critical temperature” and the critical region used [60].

Dynamics in the steady state and non-stationary properties for the KLS model are far less studied. The initial slip exponent was calculated for Model A and B by Janssen, Schaub and Schmittmann [61], which dictates short time behavior. Zheng [62] performed simulations confirming the predictions of Janssen, Schaub and Schmittmann for Model A. Attempts to extend this formalism to the KLS model have been made [57, 58, 63].

The general understanding of sub-critical behavior is less developed than features at high or critical temperatures [46]. Below the critical point the system segregates into high and low density regions. For sub-critical temperatures in the KLS model, scaling of correlations has been elusive [49, 64, 65, 66]. The steady state of sub-critical temperatures is one stripe of high density and one of low density aligned parallel to the drive [46, 67]. It has been conjectured that the aspect ratio of the lattice determines the steady state of the system at sub-critical temperatures [67]. Moreover the steady state will be “stringy” if the system is square, with multiple stripes parallel to the drive [67].

1.2 Motivation

The static properties of the ASEP in the steady state are very well established. The steady state probability distribution is known to be constant [46, 68], making equal-time correlations trivial to calculate. Two-time correlations are non-trivial, and we do not possess an exact expression. It is known that the dynamic exponent that characterizes the power law
behavior of two-time correlations is \( z = 3/2 \). However, there are non-trivial scaling functions that modify the approach to the long-time power law behavior. We wish to characterize the approach to the asymptotic behavior by studying the local exponent of the two-time correlations and the scaling functions. We present extensive Metropolis Monte Carlo simulations of the ASEP at half-filling using much larger system sizes than previous studies [69, 70]. Away from half-filling, density fluctuations will transverse the system with a known velocity [68]. Using this velocity, we wish to characterize the recurrence oscillations of these density fluctuations.

Non-stationary properties of the ASEP in one dimension should be adequately described by previous studies of the KPZ surface growth model due to mapping between the two models. We will study the aging properties of the one-dimensional ASEP and confirm the aging exponents with our Monte Carlo simulations. To our knowledge there have been no previous studies on relaxation in the ASEP for two and three dimensions. We will present simple scaling arguments that yield the aging exponent and confirm the aging scaling with Monte Carlo simulations in one, two, and three dimensions.

It is known that a finite system is not actually critical. What we call the “Finite-size critical temperature” is not really a critical temperature. We will define the finite-size critical temperature as the temperature at which the fluctuations of the order parameter are maximum. We will carefully estimate this finite-size critical temperature of several systems. As discussed above and elaborated upon in chapters 2 and 5, most numerical studies of the KLS model at criticality have been fiercely disputed. Measurements of two-time quantities are absent in the literature. We will present finite-size scaling plots of the density-density auto-correlation function obtained from our Monte Carlo simulations of the KLS model at criticality to verify known critical exponents.

There have been few studies focused on transient properties of the critical KLS model [57, 58, 63]. These works focused on single-time quantities. We will measure the same single-time quantities as the previous studies in the transient regime, but for much larger system sizes. We wish to use simple scaling arguments to arrive at the value of the aging exponent for the density-density auto-correlation function and confirm this with Monte Carlo simulations of very large systems. We will present aging scaling plots of the density-density auto-correlation function from Monte Carlo simulation of the critical KLS model on lattices honoring both predicted anisotropy exponents. We will attempt to collapse both sets of data by using the critical exponents from both theories.

We will confirm the accepted value of the exponent for the power law growth of domains during sub-critical quenches. Based on our Monte Carlo simulations, we will provide qualitative arguments concerning the steady state of the KLS model at sub-critical temperatures for different lattice anisotropies. We will using simulation data to attempt to obtain aging scaling of the density-density auto-correlation function for sub-critical temperature quenches.
1.3 The Discrete Driven Lattice Gas

The KLS model is defined as $N$ particles on a $L_{\parallel} \times L_{\perp}^{d-1}$ lattice with periodic boundary conditions. A lattice site with location $i$ has occupation $n_i \in \{0, 1\}$, where 0, 1 represents an unoccupied, occupied site respectively. By definition only a single particle can occupy a site. The particle interaction energy is given by

$$H_{\text{inter}} = -J \sum_{\langle i,j \rangle} n_i n_j,$$

(1.1)

where $J$ is the interaction strength, and the angle brackets in the summation indicate the sum is over nearest neighbors. The parallel dimension “$\parallel$” is defined as the direction parallel to the external drive, which biases the particles to move in the direction of the drive. The rate to perform a hop evolving the system from state $X$ to state $Y$ in the KLS model is defined as

$$R(X \rightarrow Y) \propto e^{-\beta (H_{\text{inter}}(Y) - H_{\text{inter}}(X) + \ell E)},$$

(1.2)

where $\beta$ is the inverse temperature and $\ell = \{-1, 0, 1\}$ indicates hops against, transverse and parallel to the drive. For the majority of the results presented here, the drive $E$ is infinite, meaning that particles may not jump against the drive. Particle dynamics are symmetric perpendicular ($\perp$) to the drive. A figure representing these dynamics is shown in Fig. 1.1 for the $d = 2$ case.

![Figure 1.1: A two-dimensional lattice representing possible and forbidden transitions for the KLS model. The drive points to the right, parallel to the horizontal lattice direction.](image)

The periodic boundary conditions and the asymmetric hopping rates result in a non-zero average particle current. Asymmetric hopping rates combined with reflecting boundaries would result in all the particles being driven to one side of the lattice, and an equilibrium...
situation would arise. Conversely, symmetric hopping rates combined with periodic boundary conditions would yield the well-studied equilibrium Ising model solved by Onsager [71] in 1944. The periodic boundary conditions with the asymmetric hopping rates are the key ingredients to the non-equilibrium behavior of the KLS model. We will study two cases of the general KLS model. The ASEP is characterized by setting the interaction strength $J$ to zero, or letting the temperature and drive strength approach infinity while keeping the ratio $E/T$ constant. This has also been referred to as the “free” lattice gas.

1.3.1 ASEP

The ASEP is a simplified version of the KLS model. We will first focus on the one-dimensional case depicted in Fig. 1.2. The hopping rates with the drive are depicted by red arrows and have hopping rate $p$. Hopping rates against the drive are depicted by green arrows and have hopping rate $q$. The rates are normalized by $p + q = 1$. We define a bias

$$\Gamma = p - q = 2p - 1 = \begin{cases} 
0 & \text{SEP} \\
\in (0, 1) & \text{ASEP} \\
1 & \text{TASEP}
\end{cases}$$

which corresponds to the drive strength. The Simple Exclusion Process or SEP is a lattice gas with zero drive. The Totally Asymmetric Simple Exclusion Process or TASEP represents the ASEP for infinite drive. In the work presented here, we only simulate the dimensional lattice gas with finite drive, i.e. a non-zero hopping rate for hops against the drive. Therefore, the one-dimensional ASEP is accurately described by Fig. 1.2. Extension to higher dimensions is straightforward, Fig. 1.1 gives a pictorial representation of the TASEP in two dimensions.

1.3.2 KPZ surface growth

The one-dimensional TASEP can be mapped to the surface growth model in the KPZ universality class [13]. We first map the occupation at a site $n_i$ to a spin variable $\sigma_i(t) = 1 - 2n_i \in \{-1, 1\}$. We then map the spin variable to a height variable by adding all the spins from site 1 to site $i$, $h_i = \sum_{j \leq i} \sigma_j$. This mapping is shown for a sample configuration in Fig. 1.3.
The pink blocks in the figure represent active sites: places where the surface can grow. The KPZ surface growth model restricts the growth of the interface by only allowing growth at sites where the transition keeps the slope of the interface $\pm 1$. The active sites correspond to possible hops in the lattice gas representation, a dimer consisting of an occupied and unoccupied site. Fig. 1.4 shows the state of the system before and after a move. If a particle jumps from the last site on the lattice back to the first site, the entire height would decrease by 2. This scenario is depicted in the leftmost 2 configurations of Fig. 1.5. For our surface to actually grow we must account for the hops at the boundary. We denote of the number of hops from site $L$ to site 1 as $N_0$. We redefine our height as

$$h_i = \sum_{j=0}^{i} \sigma_j + 2N_0.$$ (1.4)
Using this definition of the height, we generate the rightmost configuration of Fig. 1.5, where the blue blocks represent the height added by the $2N_0$ term in Eq. 1.4. From the definition of surface height (Eq. 1.4), one can calculate the difference in surface height between two neighboring lattice sites as

$$\Delta h_i = h_i - h_{i-1} = \sigma_i.$$  \hspace{1cm} (1.5)

We see from the possible spin values that the slope of the surface is restricted to $\pm 1$. This restriction in the KPZ surface growth model directly parallels the particle exclusion in the lattice gas model.

### 1.3.3 KLS model

The ASEP model represents the infinite temperature regime of the KLS model. What we will refer to as the KLS model will mean finite values of temperature and non-zero interaction strength. Properties at the critical point have attracted much interest as well as two opposing theories. The model is basically the same as the d-dimensional ASEP. Rates for the KLS model depend on the change in energy in addition to the hopping direction. The rates are explicitly defined in chapter 3. The KLS model undergoes a phase transition like its equilibrium counterpart, the Ising model. The KLS model has no exact expression for the critical temperature $T_C$, in contrast to the equilibrium model $T_{eq}^C = 0.5673J$ [71], where $J$ is the interaction strength. The critical temperature for the KLS model is estimated using simulations. Each estimate of the critical temperature is a lower bound on the true critical temperature for an infinite system [72]. The critical temperature for the driven model is higher than for the equilibrium Ising model [46]. The accepted value of the critical temperature is $T_C = 1.41T_{eq}^C$ [46]. The negative interaction energy favors transitions that result in particles being nearest neighbors. In our simulations, we always set the interaction strength $J = 1$ and the drive strength $E = \infty$. Therefore, the only free parameter is the temperature. In one dimension with infinite drive, the KLS model becomes the TASEP, thus rendering the temperature irrelevant.
When starting from random initial conditions and quenching to a sub-critical temperature there are two transient time regimes for anisotropic lattices. First, the system coarsens into a multi-stripe configuration. Once the stripes form there is a regime where the stripes merge into one stripe. Multi-stripe metastable states can last very long. Simulations can become stuck in the metastable states forever. For sub-critical temperatures, we present results using continuous time Monte Carlo simulation [73]. This has advantages for this temperature regime that will be discussed in chapter 3.

We are interested in the two distinct time regimes for the KLS model: transient and stationary. Unlike the ASEP, the probability for a specific state $X$ is not simple, $P(X) \not\propto 1$. Thus, slow relaxation is observed when performing a quench from high temperature to low temperature, or to the critical point. Correlated initial conditions are not needed to observe aging in the KLS model as was true for the ASEP. Moreover, time-dependent quantities measured during quenches from high-temperature random states or alternating initial conditions to the critical point are only distinguishable at extremely short times.
Chapter 2
Theoretical Approaches

2.1 Quantities of Interest

There has been a great amount of impressive analytical work performed on both the ASEP and the KLS models, a few comprehensive reviews are refs. [46, 74, 68, 75, 22, 76]. Prior to explaining some of these methods we first need to define commonly measured quantities that these approaches attempt to calculate. In the last chapter we defined the occupation at a single site as $n_i(t)$ in the discrete description of the model. Some approaches use a coarse grained continuum version where the occupation is replaced by the density $\rho(\vec{x}, t)$. Similarly the discrete spin and height have continuum counterparts $\phi(\vec{x}, t)$ and $h(\vec{x}, t)$. The continuous height variable has the same name as the discrete counterpart, however it should be clear from the spatial parameter whether or not the description is discrete (lattice index $i$) or continuous (position $\vec{x}$). A quantity that has inspired a great amount of work is the density-density correlation function, defined as

$$S(\vec{x}, \vec{y}, t, s) = \langle \rho(\vec{x}, t)\rho(\vec{x} + \vec{y}, t + s) \rangle - \langle \rho(\vec{x}, t) \rangle \langle \rho(\vec{x} + \vec{y}, t + s) \rangle. \quad (2.1)$$

Using the spin mapping $\phi(\vec{x}, t) = 2\rho(\vec{x}, t) - 1$, this can also be written as

$$S(\vec{x}, \vec{y}, t, s) = \frac{1}{4} (\langle \phi(\vec{x}, t)\phi(\vec{x} + \vec{y}, t + s) \rangle - \langle \phi(\vec{x}, t) \rangle \langle \phi(\vec{x} + \vec{y}, t + s) \rangle), \quad (2.2)$$

where $\langle \cdot \rangle$ denotes an ensemble average over stochastic realizations. This spin mapping differs by a sign from the one presented in chapter 1 for the KPZ mapping, the choice is arbitrary and we follow the common convention used for both systems. In the stationary state, a periodic system becomes translationally invariant in both space and time. Therefore the correlation function depends only on coordinate $(\vec{x} - \vec{y})$ and time $(t - s)$ differences, therefore we set $\vec{y} = -\vec{x}$ and $s = -t$. In the stationary state, two time correlations will only have one time variable, time difference. Defining the average density $\bar{\rho} = \langle \rho(\vec{x}, t) \rangle = N/L$, we then obtain

$$S(\vec{x}, t) = \langle \rho(\vec{x}, t)\rho(0, 0) \rangle - \bar{\rho}^2. \quad (2.3)$$
Two limits are static or equal-time spatial correlations i.e. \( t = 0 \),
\[
S(\vec{x}, t = 0) = \langle \rho(\vec{x}, 0)\rho(0, 0) \rangle - \rho^2,
\] (2.4)
and temporal correlations or auto correlation i.e. \( \vec{x} = 0 \),
\[
S(\vec{x} = 0, t) = \langle \rho(0, t)\rho(0, 0) \rangle - \rho^2.
\] (2.5)

In the transient state time translational invariance is broken and the correlation function, namely the auto-correlation function explicitly depends on two times, \( t \) and \( s \). We study the relaxation of the system from a strongly correlated initial state that considerably differs from any non-equilibrium steady-state configuration. As we shall explain in more detail in Sec. 2.3.5 below, one expects that the physical aging scaling regime \( s \ll t \) is governed by the simple aging scaling form \[4\]
\[
S(0, t, s) = s^{-\zeta}h_S(t/s).
\] (2.6)

Indeed, we shall see that this scaling ansatz yields satisfactory data collapse. We remark that in the literature on glassy systems, an alternate so-called sub-aging fitting, \( S(0, t, s) = h_S(t/s^\mu) \) with \( \mu < 1 \), has been popular \[4\].

### 2.2 General Langevin Equation for the Driven Lattice Gas

A starting point for many studies is a continuous coarse grained equation of motion. Following the method outlined by Schmittmann and Zia \[46\], we derive a general mesoscopic Langevin equation by starting with the continuity equation
\[
\partial_t \rho(\vec{x}, t) = -\vec{\nabla} \cdot \vec{j}(\vec{x}, t),
\] (2.7)
which honors particle conservation. The current density has three terms
\[
\vec{j}(\vec{x}, t) = -\lambda \vec{\nabla} \mu(\vec{x}, t) + \vec{j}_E(\vec{x}, t) + \vec{\xi}(\vec{x}, t).
\] (2.8)

The first term is the systematic current, which dampens density fluctuations via a change in the chemical potential. Here \( \lambda \) is the transport coefficient. The chemical potential is defined as
\[
\mu(\vec{x}, t) = \frac{\delta H[\rho(\vec{x}, t)]}{\delta \rho(\vec{x}, t)} = 2\frac{\delta H[\phi(\vec{x}, t)]}{\delta \phi(\vec{x}, t)}
\] (2.9)

Following the standard treatment of the Ising model, we now take the functional \( H[\phi(\vec{x}, t)] \) as the Ginzburg-Landau Hamiltonian
\[
H[\phi(\vec{x}, t)] = \int d^d x \left\{ \frac{1}{2} \left( \nabla \phi(\vec{x}, t) \right)^2 + \frac{1}{2} \tau \phi^2(\vec{x}, t) + \frac{u}{4!} \phi^4(\vec{x}, t) \right\},
\] (2.10)
where $\tau$ is the reduced temperature. The integrand in Eq. 2.10, which we will denote as $F(\phi(\vec{x}, t), \nabla \phi(\vec{x}, t))$ is only a function of $\nabla \phi(\vec{x}, t)$ and $\phi(\vec{x}, t)$, therefore the functional derivative is evaluated

$$\frac{\delta H[\phi(\vec{x}, t)]}{\delta \phi(\vec{x}, t)} = \frac{\partial}{\partial \phi(\vec{x}, t)} F(\phi(\vec{x}, t), \nabla \phi(\vec{x}, t)) - \nabla \left[ \frac{\partial}{\partial (\nabla \phi(\vec{x}, t))} F(\phi(\vec{x}, t), \nabla \phi(\vec{x}, t)) \right],$$

(2.11)

and we arrive at the chemical potential in terms of the magnetization density

$$\mu(\vec{x}, t) = 2\tau \phi(\vec{x}, t) + \frac{u}{3} \phi^3(\vec{x}, t) - 2\nabla^2 \phi(\vec{x}, t).$$

(2.12)

The second term in Eq. 2.8 is due to the external drive imposed upon the system. This term must be invariant under particle-hole exchange, vanish if the density is 0 or 1 and be proportional to the external drive $\vec{E}$. The accepted form to satisfy these constraints is

$$\vec{j}_E(\vec{x}, t) = \rho(\vec{x}, t)(1 - \rho(\vec{x}, t))\vec{E} = \frac{1}{4}(1 - \phi^2(\vec{x}, t))\vec{E},$$

(2.13)

where $\vec{E}$ is a coarse-grained form of the drive $\vec{E}$ which saturates to a constant as $\vec{E} \to \infty$.

The final term in Eq. 2.8 is the stochastic zero-mean white noise which can be anisotropic

$$\langle \xi(\vec{x}, t) \rangle = 0$$

(2.14)

$$\langle \xi_i(\vec{x}, t) \xi_j(\vec{x}', t') \rangle = n_{ij} \delta(\vec{x} - \vec{x}') \delta(t - t')$$

(2.15)

$$\langle \xi_i(\vec{x}, t) \xi_j(\vec{x}', t') \rangle = n_{ij} \delta(\vec{x} - \vec{x}') \delta(t - t') \delta_{i,j},$$

(2.16)

where $i$ and $j$ represent different directions transverse to the drive. Inserting Eqs. 2.12 and 2.13 into Eq. 2.8 and then into the continuity equation 2.7 yields

$$\partial_t \rho(\vec{x}, t) = 4\lambda \left\{ (\tau_\parallel \nabla_\parallel^4 - \nabla_\parallel^4 + \tau_\perp \nabla_\perp^4 - \nabla_\perp^4 - 2\nabla_\parallel^2 \nabla_\perp^2) \phi(\vec{x}, t) \right\}$$

$$+ \frac{1}{3} \left( u_\parallel \nabla_\parallel^4 + u_\perp \nabla_\perp^4 \right) \phi^3(\vec{x}, t) + \frac{\xi}{2} \nabla_\parallel \phi^2(\vec{x}, t) - \nabla_\parallel \xi(\vec{x}, t) - \nabla_\perp \cdot \xi(\vec{x}, t),$$

(2.17)

where we have distinguished between directions transverse and parallel to the drive with different gradient and constant subscripts to introduce the anisotropic noise and drive direction. This is the full Langevin equation valid at any temperature. Now we will consider specific temperature regimes.

### 2.3 The Asymmetric Simple Exclusion Process

The model for the Asymmetric Simple Exclusion Process or ASEP was explained in chapter 1. Other common names are the “free” lattice gas and it is also the infinite temperature limit.
of the nearest neighbor interacting case. The only interaction between particles is exclusion, therefore the functional Hamiltonian takes the form

$$H[\phi(\vec{x}, t)] = \int d^d x \frac{1}{2} \phi^2(\vec{x}, t). \quad (2.18)$$

Following the same procedure using to derive Eq. 2.17 except now with the above Hamiltonian we arrive at the Langevin equation,

$$\frac{\partial}{\partial t} \phi(\vec{x}, t) = \lambda \left( \nabla^2 + \vec{\nabla}^2 \right) \phi(\vec{x}, t) + \frac{\xi}{4} \nabla || \phi^2(\vec{x}, t) - \nabla || \xi(\vec{x}, t) - \nabla \cdot \vec{\xi}(\vec{x}, t), \quad (2.19)$$

this is an anisotropic generalization of the isotropic noisy Burgers equation [12].

### 2.3.1 Relation to the KPZ equation

In chapter 1 we showed how to map the discrete version of the the simple exclusion process in one dimension to the discrete surface growth model. For \(d = 1\) Eq. 2.19 can be mapped to the well known KPZ equation [13]. The KPZ equation is a non-linear equation to describe surface growth with surface tension. The linear counterpart is the Edwards-Wilkinson equation [77]. The continuous height variable \(h(x, t)\) is related to the spin density \(\phi(x, t)\) by the continuous version of Eq. 1.5

$$\nabla h(x, t) = \phi(x, t), \quad (2.20)$$

where the position and gradient are scalar quantities for \(d = 1\). Using Eq. 2.20 in Eq. 2.19 we arrive at the KPZ equation

$$\frac{\partial}{\partial t} h(x, t) = \lambda \nabla^2 h(x, t) + [\nabla h(x, t)]^2 \xi - \xi(x, t). \quad (2.21)$$

Thus the ASEP is in the same universality class as KPZ and they will share the same exponents for \(d = 1\).

### 2.3.2 Analytically obtainable quantities

This subsection directly follows our publication [78]. For the ASEP in the stationary state, it is well known that each possible particle configuration \(C\) occurs with equal probability \(P^*(C)\), namely the inverse of the number \(N(C) = \binom{L}{N}\) of possible states [79]

$$P^*(C) = \frac{1}{N(C)} = \frac{N!(L - N)!}{L!}. \quad (2.22)$$

If nearest-neighbor interactions were added, the stationary probabilities would depend on the particles’ relative positions. From the simple product measure (2.22), we can readily obtain
the equal-time stationary density-density correlation function $S(\vec{x} - \vec{x} \neq 0, t' - t = 0)$. The probability to find a particle at a given site $\vec{x}$ is just the average density $\bar{\rho}$, and given that site $\vec{x}$ is occupied the density at a different site $\vec{x}' \neq \vec{x}$ is $(N - 1)/(L - 1)$, which yields $\langle n(\vec{x}, t)n(\vec{x}', t) \rangle = \sum_{C} P^*(C)n(\vec{x})n(\vec{x}') = \sum_{C'} P^*(C')N(N - 1)/L(L - 1)$. The sum now extends over configurations $C'$, which encompass all possible states of $N - 2$ particles in the remaining $L - 2$ sites, whose stationary probability $P^*(C')$ is again given by Eq. (2.22). But the summation gives us a multiplicative factor $N(C') = 1/P^*(C')$, which is the number of possible configurations of the remaining $N - 2$ particles placed in the remaining $L - 2$ sites. Hence we arrive at the simple result $\langle n(\vec{x}, t)n(\vec{x}', t) \rangle = N(N - 1)/L(L - 1)$, and the equal-time correlation function becomes

$$S(\vec{x} - \vec{x} \neq 0, 0) = \frac{N(N - 1)}{L(L - 1)} \left( \frac{N}{L} \right)^2. \quad (2.23)$$

Taking the thermodynamic limit $N, L \to \infty$ while keeping $\rho = N/L$ constant, the correlation function (2.23) vanishes for $\vec{x} \neq \vec{x}'$. However, in a finite system, Eq. (2.23) yields a negative value

$$S_{\text{min}} = \rho \left( \frac{\rho L - 1}{L - 1} \right) - \bar{\rho}^2 = - \bar{\rho}(1 - \bar{\rho}) \frac{L}{L - 1}, \quad (2.24)$$

reflecting the particle anti-correlations induced by site exclusion. An expression for the average current can be derived using our knowledge of spatial correlations. The current from site $i$ to site $i + 1$ can be written as

$$j_i(t) = pn_i(t)(1 - n_{i+1}(t)) - qn_{i+1}(t)(1 - n_i(t)), \quad (2.25)$$

where the left term accounts for hopping right across the bond which can only be non-zero if site $i$ is occupied and site $i + 1$ is unoccupied. Likewise the right term corresponds to hopping left across the bond, and site $i + 1$ must be occupied and $i$ must be unoccupied for this term to be non-zero. Taking the ensemble average of this quantity yields

$$\langle j_i(t) \rangle = p \left( \langle n_i(t) \rangle - \langle n_i(t) n_{i+1}(t) \rangle \right) - q \left( \langle n_{i+1}(t) \rangle - \langle n_{i+1}(t) n_i(t) \rangle \right). \quad (2.26)$$

Assuming again we are in the stationary state where spatial and temporal translational invariance holds, the average occupation is $\langle n_i(t) \rangle = \bar{\rho}$ and equal time correlations from Eq. 2.23 are $\langle n_i(t) n_{i+1}(t) \rangle = \bar{\rho}^2$ in the thermodynamic limit. Averaging over all lattice sites yields the total current

$$J(t) = \frac{1}{L} \sum_{i=1}^{L} j_i(t) = (p - q)\bar{\rho}(1 - \bar{\rho}). \quad (2.27)$$

In a finite one-dimensional system with periodic boundary conditions, i.e., a ring with $L$ sites, another notable quantity is the velocity of a single “tagged” particle [68]

$$v_t = \frac{L - N}{L - 1}. \quad (2.28)$$
Note that $v_t = 1 - \bar{\rho}$ in the thermodynamic limit. Since our numerical data are obtained in finite systems, the typical return time $t_r = L/v_t$ for a specific particle to traverse the entire ring and come back to its original site posits an upper limit to the argument $t < t_r$ for a meaningful analysis of the time-dependent auto-correlation function $S(0, t)$. We remark that the tagged particle velocity has to be carefully distinguished from the propagation speed of a collective density fluctuation \cite{75}

$$v_c = 1 - 2\bar{\rho},$$  \hspace{1cm} (2.29)

which vanishes only at half-filling $\bar{\rho} = 1/2$.

### 2.3.3 General scaling relations the ASEP and KPZ

The scaling form for the density-density correlation function for the ASEP in the stationary state can be written as \cite{46}

$$S(\vec{x}_\perp, x_\parallel, t) = b^{d+\Delta} S(b\vec{x}_\perp, b^{1+\Delta}x_\parallel, b^z t),$$  \hspace{1cm} (2.30)

$$\hat{S}(\vec{k}_\perp, k_\parallel, t) = \hat{S}(b^{-1}\vec{k}_\perp, b^{-(1+\Delta)}k_\parallel, b^z t),$$  \hspace{1cm} (2.31)

$$\hat{S}(\vec{k}_\perp, k_\parallel, \omega) = b^{-z} \hat{S}(b^{-1}\vec{k}_\perp, b^{-(1+\Delta)}k_\parallel, b^{-z} \omega),$$  \hspace{1cm} (2.32)

where the $\vec{k}$'s are wave vectors and $\omega$ is the frequency. The anisotropic behavior is included by separating the distances or momenta into the component parallel to the drive ($\parallel$) and the transverse components ($\perp$). These relations define the anisotropy exponent $\Delta$ and dynamic exponent $z$. Janssen and Schmittmann obtained the exact scaling relation using renormalization group in a $\epsilon = d - 2$ expansion, with the critical dimension $d_c = 2$ \cite{14},

$$\hat{S}(\vec{k}_\perp, k_\parallel, \omega) = \omega^{-1} \hat{f}(\omega^{-1/2}k_\perp, \omega^{-\frac{1}{2}}(b-d)k_\parallel).$$  \hspace{1cm} (2.33)

Setting $b = \omega^{1/z}$ in Eq. 2.32 we obtain

$$\hat{S}(\vec{k}_\perp, k_\parallel, \omega) = \omega^{-1} \hat{f}(\omega^{-1/z}k_\perp, \omega^{-(1+\Delta)/z}k_\parallel).$$  \hspace{1cm} (2.34)

Comparing Eqs. 2.33 and the theory fixes the values for the the exponents $z = 2$ and $\Delta = \frac{2-d}{3}$ for $d \leq d_c$, for $d > d_c$ mean field accurately determines the exponents. It is useful at this point to define the parallel and perpendicular dynamic exponents as $z_\parallel = \frac{z}{1+\Delta}$ and $z_\perp = z$ which allows us to rewrite Eq. 2.34 as

$$\hat{S}(\vec{k}_\perp, k_\parallel, \omega) = \omega^{-1} \hat{f}(\omega^{-1/z_\perp}k_\perp, \omega^{-1/z_\parallel}k_\parallel).$$  \hspace{1cm} (2.35)

Now the exponent values can be summarized in table 2.1 below.

To obtain the long time behavior of the steady-state auto correlation function, we first set $b = t^{-1/z}$ in Eq. 2.30,

$$S(\vec{x}_\perp, x_\parallel, t) = t^{-(d+\Delta)/z} \hat{f}(t^{-1/z}\vec{x}_\perp, t^{-(1+\Delta)/z}x_\parallel).$$  \hspace{1cm} (2.36)
Table 2.1: List of exponents for the ASEP

<table>
<thead>
<tr>
<th>d</th>
<th>1</th>
<th>2†</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>ℓ⊥</td>
<td>2</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>ℓ∥</td>
<td>3/2</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>Δ</td>
<td>1/3</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

† logarithmic corrections are present at $d_c = 2$

In taking the $\vec{x}_\perp, x_\parallel \to 0$ limit we obtain the asymptotic limit for the auto correlation function,

$$S(t) \sim t^{-\zeta}, \quad \zeta = \frac{d + \Delta}{z} = \frac{d + \Delta}{(1 + \Delta)z_\parallel}.$$  \hfill (2.37)

In order to carefully characterize the approach to the asymptotic regime in our Monte Carlo simulations, we shall utilize a corresponding local (effective) exponent defined via

$$-\zeta_{\text{eff}}(t) = \frac{\log S(0, t) - \log S(0, t - 1)}{\log t - \log(t - 1)}.$$  \hfill (2.38)

The expected finite-size scaling form is readily obtained from the general expression 2.30 by setting $L_\parallel = b^{-(1+\Delta)}$, and $\vec{x}_\perp, x_\parallel \to 0$ we find for the auto-correlation function

$$S(0, t) = L_\parallel^{-1}S_{FS}\left(t/L_\parallel^{z_\parallel}\right).$$  \hfill (2.39)

A more detailed discussion of each dimension is in order at this point.

$d = 1$:

The transverse spatial directions become obsolete, and with the exact renormalization group result $\Delta = 1/3$ we obtain $z_\parallel = 3/2$ and $\zeta = 1/z_\parallel = 2/3$. As mentioned above, the scaling behavior for the equivalent surface growth model falls into the KPZ universality class \cite{13}.

The central quantity in this description is the height-height correlation function

$$C(x, t) = \left\langle[h(x, t) - h(0, 0)]^2\right\rangle.$$  \hfill (2.40)

Asymptotically, it takes the scaling form

$$C(x, t) = b^{-2\alpha}C(bx, b^{z_\parallel}t),$$  \hfill (2.41)

with the roughness exponent $\alpha$ (note that in the growth model literature, the dynamical exponent $z_\parallel$ is usually labeled $z$). The height-height correlation is closely related to the density-density correlation function by \cite{36}

$$S(x, t) = \frac{1}{8} \frac{\partial^2}{\partial x^2}C(x, t),$$  \hfill (2.42)
which gives the scaling form

\[ S(x, t) = b^{-2\alpha+2}S(bx, b^{z\parallel}t). \]  

(2.43)  

According to Eqs. (2.42) and (2.41), we can therefore identify \( 2 - 2\alpha = (d + \Delta)z\parallel/z = 1 \) in one dimension, or \( \alpha = 1/2 = 2 - z\parallel \) [12, 13, 14]. Historically three different scaling functions are studied. First setting \( b = 1/|x| \), and recalling \( \alpha = 1/2 \) and \( z\parallel = 3/2 \), Eq. (2.41) becomes [34]

\[ C(x, t) \propto |x|F(\xi), \quad \xi = t/|x|^{3/2}, \]  

(2.44)  

whereas equivalently the matching condition \( b = t^{-1/z\parallel} \) leads to [36]

\[ C(x, t) \propto t^{2/3}g(y), \quad y = x/t^{1/3}. \]  

(2.45)  

Consistency then requires that

\[ F(\xi) \propto \xi^{3/3}, \quad g(y) \propto |y| \]  

(2.46)  

for large arguments \( \xi \gg 1 \) and \( y \gg 1 \). Letting \( b = t^{-1/z} \) in Eq. 2.43 yields

\[ S(x, t) = t^{2(\alpha-2)/z\parallel}f(t^{-1/z\parallel}x), \]  

(2.47)  

\[ S(x, t) = t^{-2/3}f(t^{-2/3}x), \]  

(2.48)  

\[ S(0, t) = t^{-2/3}, \]  

(2.49)  

where the second line agrees with the result in Eq. 2.36. The scaling function \( f(y) \) is often called \( g''(y) \) in the KPZ language because it is the second spatial derivative of \( g(y) \). The scaling form for \( d = 1 \) (Eq. 2.48) has been calculated by renormalization group applied to the noisy Burgers equation [12, 14]. Determining the scaling function \( F(\xi) \) has been approached using mode coupling techniques [32, 33, 34] and the crossover to the asymptotic scaling carefully studied. In particular we will compare our Monte Carlo data directly to the results of Frey, Täuber and Hwa [34]. To determine the scaling function \( f(y) \) several mode coupling approximations [80, 81, 82, 83] have been utilized along with numerical integration [35, 36, 37, 38]. The most notable are the results of Prähöfer and Spohn [36], who determined \( f(y) \) exactly; in Sec. 4 we directly compare our Monte Carlo data to their result

\[ f(y) \propto e^{-0.295|y|^3}. \]  

(2.50)  

\( d = d_c = 2 \):  

At the upper critical dimension, logarithmic corrections arise. The simple power law (2.37) is replaced with [12, 32, 14]

\[ S(0, 0, t) \sim \frac{1}{t((\log t)^{1/2}}. \]  

(2.51)  

Accordingly, in order to capture the approach to the asymptotic scaling limit we need to redefine the local exponent in this case as

\[ S(0, 0, t)(\log t)^{1/2} \propto t^{-\zeta_\pi(t)}. \]  

(2.52)
It turns out though that the mean-field approximation
\[ S_{\text{MF}}(0, 0, t) \sim t^{-1} \] (2.53)
provides reasonable agreement with our simulation data as well.

\[ d > 2: \]
Above the critical dimension, the mean-field predictions for the scaling exponents \( \Delta = 0 \) and \( z = 2 = z_{\parallel}, \zeta = d/2 \) should provide an adequate description of the density auto-correlation function data.

### 2.3.4 Exact Analytic Results

The ASEP in one dimension has many exact analytic results, for a thorough review see ref. [22]. Here we will highlight some important results. The Bethe ansatz [84] is applicable to the ASEP as shown by Dhar [23]. Several authors [23, 24, 25, 26] obtained the dynamic exponent \( z_{\parallel} = 3/2 \) for half-filling using the Bethe ansatz. This was later generalized for arbitrary filling [27, 28] and shows density oscillations away from half-filling. Another impressive result using the Bethe ansatz is the calculation of conditional probabilities
\[ p(n'_1, n'_2, ..., n'_L; t'|n_1, n_2, ..., n_L; t), \] (2.54)
which specifies the probability to have the set of occupations \( n'_1, n'_2, ..., n'_L \) at time \( t' \) given the occupations \( n_1, n_2, ..., n_L \) at time \( t \). The conditional probability was calculated first for a finite number of particles on an infinite lattice by Schütz [29], which for long times reduces to non-interacting particles. This was adapted for a finite number of particles on a finite lattice with periodic boundary conditions by Priezzhev [30]. The conditional probabilities can be used to calculate the auto correlation function [31], however the expressions for the exact probabilities [29, 30] are only tractable for very small system sizes.

### 2.3.5 Aging behavior from general scaling forms

Let us consider transient relaxation properties of driven lattice gases with exclusion. For example, starting from a steady state obtained with a specified set of hopping probabilities \( p \) and \( q = 1 - p \), we may wish to understand how the system responds to a sudden change of these probabilities to new values \( p' \) and \( q' = 1 - p' \). However, recall that the non-equilibrium steady state probability distribution (2.22) is independent of the hopping probabilities. This means that statistically the stationary configurations before and after the sudden bias change are indistinguishable. As a consequence, no slow relaxation processes follow the change of hopping probabilities. As we have confirmed with our Monte Carlo simulations, any macroscopic observables such as the mean particle current assume their new stationary values essentially instantaneously after the bias reset.
In order to construct initial conditions that generate non-stationary relaxation with broken time translation invariance, we consider the mapping of the TASEP to a surface growth problem in the KPZ universality class [85]. In the growth model, one obtains slow relaxation towards the stationary state if the process is initiated with a flat surface $h(x, 0) = 0$ everywhere, and roughening subsequently commences on small length scales $\sim t^{1/z_\parallel}$. In the TASEP picture, this initial state is accomplished at half-filling $\rho = 1/2$ by placing the particles alternately on every other site. The mean-square interface width of the corresponding finite one-dimensional growth model can be obtained from our TASEP Monte Carlo data on a ring of length $L$ via the mapping presented in section 1.3.2

$$w(L, t)^2 = \left\langle h_i(t)^2 \right\rangle_L = \frac{1}{L} \sum_{i=1}^{L} \left[ i - 2 \sum_{j=1}^{i} n_j(t) \right]^2,$$  

(2.55)

where $w(L, 0)^2 = 0$. The standard finite-size scaling relation for the interface width reads [86]

$$w(L, t) = L^{\alpha} W(t/L^{z_\parallel}),$$  

(2.56)

which implies the initial growth law $w(L, t) \sim t^{\alpha/z_\parallel} = t^{1/3}$, valid up to times $t \approx L^{z_\parallel}$ [13]. The width is a good indicator of when the steady state is reached as will be shown in our results.

We wish to obtain the aging scaling form given by Eq. 2.6. To motivate this form we first provide the initial slip scaling form for the density-density correlation function given by Krech [87]

$$C_{IS}(x, t, s \ll t) = \left( \frac{s}{t} \right)^\theta |x|^{2\alpha} F(t/x^{z_\parallel}),$$  

(2.57)

where Krech found the initial slip exponent to be $\theta = (d + 4)/z_\parallel - 2$, which is dependent on the standard dynamics scaling exponent $z$. With this result we assume that both times $t$ and $s$ would scale the same, thus we can generalize Eq. 2.30 by adding the waiting time $s$

$$S(\vec{x}_\perp, x_\parallel, t, s) = b^{d+\Delta} S(b\vec{x}_\perp, b^{1+\Delta} x_\parallel, b^\gamma t, b^\gamma s),$$  

(2.58)

$$S(t, s) = b^{d+\Delta} S(b^\gamma t, b^\gamma s).$$  

(2.59)

Setting the scaling parameter to be $b = s^{-1/z}$, we arrive at the aging scaling form

$$S(t, s) = s^{-(d+\Delta)/z} f_{C}(t/s),$$  

(2.60)

which gives the aging exponent $\zeta = (d + \Delta)/z$. For the $d = 1$ case the aging exponent for the height-height correlation has been shown to be $\lambda = -2\alpha/z_\parallel$ [39, 40] and Monte Carlo simulations confirm this[40, 39, 88, 44]. The aging exponent can be found from the scaling form for the height-height correlation Eq. 2.41 and adding the second time quantity $s$ and following the same procedure above used to arrive at Eq. 2.60 yields

$$C(t, s) = s^{2\alpha/z_\parallel} h_{C}(t/s).$$  

(2.61)
Similarly we can write down the density-density aging scaling starting from Eq. 2.43
\[ S(t, s) = s^{(2\alpha - 2)/z_\parallel} f_C(t/s), \] (2.62)
which yields \( \zeta = (2 - 2\alpha)/z_\parallel \). By comparing Eqs. 2.61 and 2.62 we can relate the two aging exponents
\[ \zeta = \lambda + 2/z_\parallel. \] (2.63)
Simple aging has been observed for a variety of quantities in the Edwards-Wilkinson model [41, 42, 43, 44]. There have been limited exact results [89, 90, 91] for correlated initial conditions and short times, most of which are again only tractable for very small system sizes.

### 2.4 Critical Langevin equation for the KLS model

We now motivate a Langevin equation for critical DDS [15, 16]. This model will be referred to as KLS model at criticality or critical DDS, for infinite values of drive it is also referred to as the infinitely driven lattice gas (IDLG). Critical DDS is described by the transverse dimension becoming critical and thus the reduced temperature in the transverse direction becomes zero and the parallel reduced temperature remains finite and positive,
\[ \tau_\perp = \frac{T - T_{\perp,C}}{T_{\perp,C}} = 0 \] (2.64)
\[ \tau_\parallel = \frac{T - T_{\parallel,C}}{T_{\parallel,C}} > 0. \] (2.65)
Although the two other cases \((\tau_\perp > 0, \tau_\parallel = 0)\) and \((\tau_\perp = 0, \tau_\parallel = 0)\) have been analyzed [15, 16] but we do not study them. The driving field term is the most relevant in the parallel direction, higher order terms are not needed because the parallel reduced temperature is non-zero. When we refer to the reduced temperature \(\tau\) without a subscript, it represents the transverse critical temperature. We also set the parallel noise strength equal to zero, \(n_\parallel = 0\). Applying these changes to Eq. 2.17 we arrive at the critical DDS Langevin equation:
\[ \partial_t \rho(\vec{x}, t) = 4\lambda \left\{ (\tau_\parallel \vec{\nabla}_\parallel^2 + \tau_\perp \vec{\nabla}_\perp^2 - \vec{\nabla}_\perp^4) \phi(\vec{x}, t) + \frac{1}{3} u_\perp \vec{\nabla}_\perp^2 \phi^3(\vec{x}, t) \right\} + \frac{\xi}{2} \vec{\nabla}_\parallel \phi^2(\vec{x}, t) - \vec{\nabla}_\perp \cdot \vec{\xi}_\perp(\vec{x}, t). \] (2.66)

The critical temperature has been estimated by many groups over the years for \(d = 2\). The critical temperature is typically given in units of the equilibrium two-dimensional critical temperature for the Ising model found by Onsager [71] to be \(T_{C}^{\text{eq}} = 0.5673 J\), where we set the Boltzmann constant equal to 1. Previous studies [8, 9, 49, 50, 72, 56, 57, 92, 93] all give the critical temperature around \(T_C \approx 1.47T_{C}^{\text{eq}}\) for the KLS model.
2.4.1 General scaling relations

The general scaling form near the critical point in real space is [46]
\[ S(\vec{x}_\perp, x_\parallel, t, \tau) = b^{d+\Delta-2+\eta} S(\vec{x}_\perp b, x_\parallel b^{1+\Delta}, t b^z, \tau b^{-1/\nu}), \] (2.67)
and for momentum space
\[ \tilde{S}(\vec{k}_\perp, k_\parallel, t, \tau) = b^{-2+\eta} \tilde{S}(\vec{k}_\perp b^{-1}, k_\parallel b^{-(1+\Delta)}, t b^z, \tau b^{-1/\nu}). \] (2.68)

Exact exponents for \( d < d_c = 5 \) have been found by Janssen and Schmittmann [15] and Leung and Cardy [16] using renormalization group methods in an \( \epsilon = 5 - d \) expansion to be
\[ \Delta = \frac{8 - d}{3}; z_\perp = z = 4; z_\parallel = \frac{12}{11 - d}; \eta = 0; \nu = \frac{1}{2}; \beta = \frac{1}{2} \] (2.69)

where \( \eta, \nu \) and \( z \) assume mean field values [15, 16]. We will refer to this set of exponents which describe Eq. 2.66 as JSLC (Janssen, Schmittmann, Leung and Cardy). As defined in the previous subsection the parallel dynamic exponent is defined by \( z_\parallel = z/(1+\Delta). \) Here the anisotropic exponent \( \Delta \) is very important for simulations. It determines how the transverse and longitudinal lengths scale. If finite-size scaling is to be performed on simulation data one must strictly adhere to anisotropic scaling by choosing proper lattice proportions, which follow
\[ L_\parallel \propto L_\perp^{1+\Delta}. \] (2.70)

Now we will define all anisotropic exponents. Unlike the ASEP model, in the KLS model the equal time correlation function is not trivial and therefore there are four \( \eta \) exponents. Two corresponding to momentum space which, we define from Eq. 2.68 and taking \( t = \tau = 0, \)
\[ \tilde{S}(\vec{k}_\perp, k_\parallel) = |\vec{k}_\perp|^{-2+\eta_\perp} S_\perp(k_\parallel/|\vec{k}_\perp|^{1+\Delta}), \] (2.71)
\[ \tilde{S}(\vec{k}_\perp, k_\parallel) = k_\parallel^{-2+\eta_\parallel} S_\parallel(|\vec{k}_\perp|/k_\parallel^{1/(1+\Delta)}), \] (2.72)
where
\[ \eta_\perp = \eta \text{ and } \eta_\parallel = \frac{\eta + 2\Delta}{1 + \Delta}. \] (2.73)

Similarly, real space functions and \( \eta \) exponents can be defined from Eq. 2.67,
\[ S(\vec{x}_\perp, x_\parallel) = |\vec{x}_\perp|^{-d+2-\eta_{RS}^{\perp}} g_\perp(x_\parallel/|\vec{x}_\perp|^{1+\Delta}), \] (2.74)
\[ S(\vec{x}_\perp, x_\parallel) = x_\parallel^{-d+2-\eta_{RS}^{\parallel}} g_\parallel(|\vec{x}_\perp|/x_\parallel^{1/(1+\Delta)}), \] (2.75)
where
\[ \eta_{RS}^{\perp} = \eta + \Delta \text{ and } \eta_{RS}^{\parallel} = \frac{\eta - \Delta(d - 3)}{1 + \Delta}. \] (2.76)
Finally we come to the two correlation length exponents, defined by letting $b = \tau^\nu$ in Eq. 2.68 which yields
\[
\tilde{S}(\vec{k}_\perp, k_\parallel, t, \tau) = \tau^{\nu(\eta-2)} \tilde{S}(\vec{k}_\perp \tau^{-\nu_\perp}, k_\parallel \tau^{-\nu_\parallel}, t \tau^{\nu_\parallel}),
\]
(2.77)
where
\[
\nu_\perp = \nu \text{ and } \nu_\parallel = \nu(1 + \Delta).
\]
(2.78)

We wish to examine temporal properties of our Monte Carlo simulations, therefore we need to perform careful finite-size scaling analysis. Starting from the general real space scaling form, we can generalize Eq. 2.67 by adding the lattice sizes,
\[
S(\vec{x}_\perp, x_\parallel, t, \tau, L_\perp, L_\parallel) = b^{d+\Delta-2+\eta} S(\vec{x}_\perp b, x_\parallel b^{1+\Delta}, t b^\nu, \tau b^{-1/\nu}, L_\perp b, L_\parallel b^{1+\Delta}),
\]
(2.79)
letting $b = L_\parallel^{-1/(1+\Delta)}$ we arrive at the finite-size scaling form for the auto correlation function at the critical point,
\[
S(t, L_\perp, L_\parallel) = L_\parallel^{-\frac{d+\Delta-2+\eta}{1+\Delta}} S_{FS}(t/L_\parallel^{z/(1+\Delta)}),
\]
(2.80)
and letting $L_\parallel \to \infty$ we arrive at the asymptotic power law
\[
S(t) \propto t^{-\frac{d+\Delta-2+\eta}{z}}.
\]
(2.81)

Several authors have made the claim [51, 94] that Eq. 2.66 does not describe the infinitely driven lattice gas. They claim the drive term is irrelevant and the randomly driven lattice gas (RDLG) model accurately describes the model. The RDLG and its critical exponents will be discussed in the next subsection. This was disputed [55] by several authors, including the authors of the original field theory (JSLC) who pointed out flaws in the new approach. This spurred the authors to correct a flaw [95] in refs. [51, 94] and argue further [56, 57] that the RDLG is the accurate description of the critical IDLG. An extremely careful finite-size scaling analysis was performed in refs. [92, 93] that agreed with the JSLC field theory. Work was done at the same time which supported the RDLG description [58], however the results were not nearly as conclusive. The work which supported JSLC [92, 93] inspired a “comment” [59] which attempted to discredit the results. This “comment” [59] was dismissed by the authors of [92, 93] as containing irrelevant information in a response [96] criticizing the “comment.” So the proper description of the IDLG is still unsettled in the published literature.

A quantity commonly studied in this debate is the anisotropic order parameter [50, 72]
\[
m(t, \tau, L_\perp, L_\parallel) = \frac{\sin(\pi/L_\perp)}{2L_\parallel} \left| \sum_{j,k} \sigma_{j,k}(t) e^{i\frac{2\pi j}{L_\perp}} \right|, \quad (2.82)
\]
which is sensitive to stripes of high and low density parallel to the drive. The order parameter has the finite-size scaling form \cite{15, 16}

\[ m(\tau, L_{||}) = L_{||}^{-\beta/\nu} \tilde{m}(\tau L_{||}^{1/\nu}), \]  

(2.83)

and the asymptotic behavior

\[ m(\tau) \propto \tau^\beta, \]  

(2.84)

which defines the order parameter exponent \( \beta \). The common way to arrive \cite{46} at the order parameter exponent is to start from the scaling form for the density-density correlation which is proportional to \( \phi(\vec{x}, t)^2 \) and has the scaling form Eq. 2.67. The order parameter is proportional to \( \phi(\vec{x}, t) \) so one can assume it scales with \( b(d+\Delta-2+\eta)/2 \). Setting \( b = \tau^\nu \) yields

\[ \beta = \left( \nu/2 \right)(d + \Delta - 2 + \eta). \]  

(2.85)

This is shown not to be true in arbitrary dimensions for the KLS model by JSLC \cite{15, 16}, they find \( \beta \) takes its mean field value of \( 1/2 \). By coincidence, in two dimensions Eq. 2.85 does in fact yield \( 1/2 \). The scaling form in Eq. 2.83 has been used to determine the values of the critical exponents \( \nu_{||, \perp}, \beta \) in studies which agree with the JSLC predictions \cite{50, 72} and studies that disagree \cite{56}. There are a few drawbacks of this approach. First one needs to accurately determine the critical temperature for a finite system. As stated in the introduction, this is not really a critical temperature because the system is finite, it is the temperature at which the variance of the order parameter is maximum. This is difficult in simulations, and normally accomplished by finding the peak of the susceptibility or specific heat curves or analysis of the Binder cumulant \cite{97}. The reduced temperature \( \tau_{\perp} \) plays an absolutely crucial role in the data collapse using Eq. 2.83. Small changes in the critical temperature generate large variations in the data collapse of the steady state order parameter. Another problem is even with an accurate value of \( T_c \) the system needs to relax to the steady state, which can take a very long time in simulations. Performing a quench from the disordered state (high-temperature) to near the critical point can avoid the complications of relaxing to the steady state at the correct temperature. We simulate a very large system for a shorter time and extract the critical exponents. The anisotropic scaling form of the order parameter at \( T_c \) starting from a high temperature state by virtue of the aging scaling laws is \cite{61}

\[ m(t, \tau, L_{\perp}, L_{||}) = b^{-\beta/\nu_{||}} \tilde{m}(b^{-\Delta} t, b^{1/\nu_{||}} \tau, b^{-1/(1+\Delta)} L_{\perp}, b^{-1} L_{||}). \]  

(2.86)

By setting \( b = L_{||} \) and keeping \( \tau \) constant yields the scaling form

\[ m(t) = L_{||}^{-\beta/\nu_{||}} \tilde{m}(t/L_{||}^{\Delta}). \]  

(2.87)

The studies in refs. \cite{57, 63} use these scaling forms to obtain numerical values for the critical exponents which agree with the RDLG exponents, however they did not adhere to the anisotropic exponent \( \Delta = 2 \) predicted by JSLC theory, yet they claim to refute the JSLC theory with their results.
The approach we use is to add a second time variable to Eq. 2.67 akin to what we did for the ASEP in Eq. 2.58. Janssen, Schaub and Schmittmann demonstrated that for Model B there is no new short-time exponent due to the conserved particle density [61]. We therefore assume that the waiting time \( s \) scales the same as \( t \). Adding the waiting time \( s \) to Eq. 2.67 and setting \( b = s^{-1/z} \) yields the simple aging scaling relation at the critical point

\[
S(t, s, \tau = 0) = s^{-(d+\Delta-2+\eta)/z} S(t/s),
\]

therefore \( \zeta = (d + \Delta - 2 + \eta)/z \) is the aging exponent.

We find that this form with the JSLC exponents give outstanding data collapse for extremely large lattices in the vicinity of the critical point. We use \( T = 1.41 T_C^{eq} \) for the critical temperature of the very large lattices.

**2.5 The Randomly Driven Lattice Gas**

We introduce the RDLG and its critical exponents here to compare with those of the JSLC theory. By eliminating the drive term \( \frac{\xi_\parallel}{2} \nabla_\parallel \phi^2(\vec{x}, t) \) in Eq. 2.66 results in a well studied Langevin equation,

\[
\partial_t \rho(\vec{x}, t) = 4\lambda \left\{ \left( \tau_\parallel \vec{\nabla}_\parallel^2 + \tau_\perp \vec{\nabla}_\perp^2 - \vec{\nabla}_\perp^4 \right) \phi(\vec{x}, t) + \frac{1}{3} u_\perp \vec{\nabla}_\perp^2 \phi^3(\vec{x}, t) \right\} - \nabla_\parallel \xi_\parallel(\vec{x}, t) - \nabla_\perp \cdot \vec{\xi}_\perp(\vec{x}, t),
\]

which describes the randomly driven lattice gas (RDLG), which has critical dimension \( d_c = 3 \) [52, 53, 54]. The most important feature of this system is the anisotropic noise. The exponents associated with the scaling relation Eq. 2.68 for the randomly driven lattice gas were found to be

\[
\Delta = 1 - \frac{\eta}{2}, z_\perp = z = 4 - \eta, z_\parallel = \frac{8 - 2\eta}{4 - \eta},
\]

where \( \eta \) and \( \nu \) are the only independent exponents. Using renormalization group methods Schmittmann and Zia found [52] \( \eta = 4\epsilon^2/243 + O(\epsilon^3) \) and then Schmittmann later obtained [53]

\[
\nu = \frac{1}{2} + \frac{\epsilon}{12} + \frac{e^2}{18} \left( \frac{10}{27} + \frac{1}{4} + \ln \frac{2}{\sqrt{3}} \right) + O(\epsilon^3),
\]

with the details of the analysis given in ref. [54]. The argument that the order parameter would scale as \( b^{(1/2)(d+\Delta-2+\eta)} \) is valid in this case, therefore Eq. 2.85 gives the correct exponent for \( \beta \) for the RDLG. In our results section we will simulate the KLS model for \( d = 2 \), and we will use both sets of critical exponents to attempt data collapse. We thus make a list of exponents for the DLG and RDLG below in table 2.2.
Table 2.2: List of exponents for KLS and RDLG for \( d = 2 \)

<table>
<thead>
<tr>
<th></th>
<th>JSLC (exact)</th>
<th>RDLG (( \approx ))</th>
<th>JSLC (exact)</th>
<th>RDLG (( \approx ))</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Delta )</td>
<td>2</td>
<td>1</td>
<td>( \eta )</td>
<td>0</td>
</tr>
<tr>
<td>( z(z_{\perp}) )</td>
<td>4</td>
<td>4</td>
<td>( \eta_{\perp} )</td>
<td>0</td>
</tr>
<tr>
<td>( z_{\parallel} )</td>
<td>4/3</td>
<td>2</td>
<td>( \eta_{\parallel} )</td>
<td>4/3</td>
</tr>
<tr>
<td>( \nu(\nu_{\perp}) )</td>
<td>1/2</td>
<td>0.62</td>
<td>( \eta^{RS}_{\perp} )</td>
<td>2</td>
</tr>
<tr>
<td>( \nu_{\parallel} )</td>
<td>3/2</td>
<td>1.25</td>
<td>( \eta^{RS}_{\parallel} )</td>
<td>2/3</td>
</tr>
<tr>
<td>( \zeta )</td>
<td>1/2</td>
<td>0.25</td>
<td>( \beta )</td>
<td>1/2</td>
</tr>
</tbody>
</table>

† approximate \( \epsilon \) expansion

2.6 Sub-critical driven lattice gas

We conclude the theory chapter with the driven lattice gas at temperatures below the critical point. The theoretical results for the ASEP and critical KLS model are impressive and there are many conclusive simulation results that we will explore in the next two chapters to support them. Many of these results utilize dynamical scaling, which has been elusive for sub-critical temperatures [49, 64, 65]. It is well known that below the critical point the system separates into high and low density regions called stripes, with the true ground state being one high density region and one low density region. One result that is standard is exponent for power law growth of domains \( R \sim t^{1/3} \), where \( R \) is the domain size. An accepted way to measure domain size is by the inverse number of broken bonds [64] in the transverse and parallel directions denoted as \( R_{\perp}(t) \) and \( R_{\parallel}(t) \) respectively, a broken bond is two adjacent lattice sites where one is occupied and one is not. Combining these two length scales we arrive at the isotropic length scale [64]

\[
R(t) = \frac{2L_{\parallel}L_{\perp}}{1/R_{\perp}(t) + 1/R_{\parallel}(t)}.
\]

Another way to determine domain size is to measure where the isotropic spatial density-density correlation function becomes negative for the first time [65]. Both of these methods yielded algebraic growth. Yeung et al. [64] obtain \( R(t) \propto t^{1/3} \). Alexander et al. [65] obtain \( R_{\perp}(t) \propto t^{1/5} \), although the authors conjecture that the true exponent is 1/3. Using the scaling ansatz for the spatial density-density correlation function (Eq. 2.4)

\[
S(x_{\perp}, x_{\parallel}, t) = S \left( \frac{x_{\perp}}{R_{\perp}(t)}, \frac{x_{\parallel}}{R_{\parallel}(t)} \right)
\]

attempts at dynamical scaling were made [49, 64, 65], however conclusive data collapse was never achieved. Somewhat more promising scaling results came from Levine, Kafri and Mukamel [66] by using more anisotropic lattice sizes than previous studies, but still rather
small transverse lengths $L_\perp = 8, 16, 32$. Levine et al. proposed the scaling form

$$S(x_\perp, x_\parallel = 0, t) = g_\perp \left( \frac{x_\perp}{(t/L_\perp)^{1/3}} \right),$$

and achieve reasonable data collapse using this form. The absence of clear dynamical scaling has been attributed to very long lived metastable states [49] which consist of multiple regions of high and low density. More recently Zia, Shaw and Schmittmann proposed [67] that there may be a new “phase” which explains the long lived metastable state with multiple stripes as the true long time limit for square lattice geometries and the single stripe configuration as the asymptotic limit for geometries that respect Eq. 2.70 with $\Delta = 2$. The arguments and simulations in ref. [66] support this result. Zia et al. [67] also propose that this could be the cause for the discrepancy between the two competing descriptions for the critical KLS properties, arguing that different geometries cause the system to relax to different states. For sub-critical temperatures starting from the fully ordered state (1 stripe of density 1) Zia et al. [67] observed relaxation into the multiple stripe state for square lattices, clearly signifying that the single stripe configuration is not the steady state. We will explore relaxation from a disordered state to the ordered state in the results chapter and argue that for sub-critical temperatures, if the system is not sufficiently long in the direction parallel to the drive, the system does in fact evolve into multi-stripe states. For sufficiently large systems with $\Delta = 2$, multiple stripes are very likely to intersect during early domain growth and form a single stripe rather than wrap around the system in the parallel direction forming multiple stripes.

To conclude this section we briefly discuss properties of the interface between the high and low density regions. There is an analytic result for the Fourier transform of the height-height correlation function of the interface for the RDLG below criticality [98]. There are only simulation results for the driven lattice gas below criticality [99, 100]. The most striking result is that the roughness of the interface is suppressed by the drive [99] and becomes flat as the temperature is lowered.
Chapter 3

Monte Carlo Simulation

The theoretical treatments of Chapter 2 provide impressive results, however these theories need to be verified by direct numerical simulation. Exact solutions are limited, and usually only tractable for very small system sizes. The complexity of the problem due to the number of possible states and non-trivial transition rates makes exact results extremely difficult to obtain. Likewise, simulation of all possible trajectories in state space is unfeasible as well. There are simply too many possible configurations and trajectories to sample them all. For smaller systems ($L < 8$) I have directly generated every possible initial condition and simulated every possible trajectory for a few time steps. This provided basically no insight due to the time window being very small and most theoretical models are only valid in the large system size and long time limits. In order to intelligently sample relevant areas of state space for reasonable system sizes and times we turn to Monte Carlo simulations.

3.1 Master equation

The Monte Carlo method is a way to simulate the discrete version of the driven lattice gas introduced in section 1.3.1. Therefore we will use the site occupations, $n_i \in \{0, 1\}$ is \{unoccupied, occupied\}, and $i$ could be a multidimensional index. We define the probability for the system to be in a specific configuration $X$ which would specify all occupation numbers at time $t$ as $P(X, t)$. The probabilities must satisfy the master equation

$$\frac{\partial}{\partial t} P(X, t) = \sum_Y \left[ R(Y \to X) P(Y, t) - R(X \to Y) P(X, t) \right], \quad (3.1)$$

where we have introduced the rates $R(X \to Y)$ as the rates to go from state $X$ to state $Y$. Assuming the system is ergodic we may define the unique stationary probability distribution $P^*(X) = P(X, t \to \infty)$, which does not change in time. Ergodicity implies that $P^*(X)$ is independent of the initial condition. We can now distinguish between equilibrium and
non-equilibrium steady states. By definition, for a system in equilibrium each term in the sum in Eq. 3.1 must be equal to zero, therefore satisfying the detailed balance criterion,

\[
\frac{R(Y \rightarrow X)}{R(X \rightarrow Y)} = \frac{P_{eq}(X)}{P_{eq}(Y)},
\]

where the stationary probability distribution in equilibrium is denoted \(P_{eq}(X)\). When the system is in thermal equilibrium with an external reservoir at the temperature \(1/\beta\), it is known that

\[
\frac{P_{eq}(X)}{P_{eq}(Y)} = e^{\beta(H(Y)-H(X))},
\]

where \(H\) is the Hamiltonian of the system. Moving away from equilibrium, detailed balance is no longer satisfied and each term in the sum in the master equation is no longer zero in the stationary state. Thus we have a non-zero probability current [101] between states \(X\) and \(Y\) defined as

\[
K(X, Y) = R(Y \rightarrow X)P(Y, t) - R(X \rightarrow Y)P(X, t).
\]

The stationary probability distribution is still independent of time, so the sum of these probability currents will equal zero. Introducing an external drive \(E\) combined with periodic boundary conditions does not permit the energy associated with the drive to be represented by a potential in the Hamiltonian and 3.3 is not valid. Our non-equilibrium model is defined by the rates,

\[
\frac{R(Y \rightarrow X)}{R(X \rightarrow Y)} = e^{-\beta(H(X)-H(Y)+\ell E)},
\]

where \(\ell E\) is the work term caused by the drive and \(\ell = \{-1, 0, 1\}\) indicates hops against, transverse and parallel to the drive. When \(E \rightarrow 0\), the equilibrium condition is recovered, and detailed balance is restored Eq. 3.3. The most commonly used rates that satisfy Eq. 3.5 are Metropolis rates [102], which we will define in the subsequent section.

3.2 Discrete time Monte Carlo Simulations

3.2.1 General algorithm

To start the discrete time Monte Carlo simulation [103] we need to specify the initial state. Two extreme options we chose are uncorrelated (random) or strongly correlated. For the uncorrelated state the \(N\) particles are randomly placed on the \(N_L\) lattice sites, an example is shown in Fig. 3.1a. For the strongly correlated initial condition we place the particles in specified locations, namely for alternating initial conditions in \(d = 1\) we place the particles
only on odd numbered sites, for \( d = 2 \) the alternating initial condition looks like a checkerboard as shown in Fig. 3.1b. The dynamics is achieved by randomly selecting a particle, and then one of the \( 2d \) directions for a potential nearest-neighbor hop is randomly chosen. This is equivalent to randomly choosing a bond between two sites, in which one is occupied. A hop has a predetermined probability \( R_i \in [0,1] \). A random number \( r \in [0,1] \) is generated; if \( r < R_i \) then hop \( i \) is performed. Particle exclusion is realized in this simulation by setting \( R_i = 0 \) for any hop that attempts to move a particle into an occupied site. One Monte Carlo time step is defined as \( N \) hopping attempts. Thus on average the algorithm attempts to hop each particle once per Monte Carlo time step. Our choice of rates to move from state \( X \) to \( Y \) are Metropolis rates as stated in the previous section which are of the form,

\[
R(X \rightarrow Y) = \min(1, e^{-\beta(H(Y)-H(X)) + \ell E}).
\] (3.6)

### 3.2.2 Simulation of the ASEP

For the “free” lattice gas (\( T = \infty \)) all states have equal “energy” and as shown in section 2.3.2 all states are equally likely. Thus the rates going from state to state only depend on the external drive \( E \). For a \( d \)-dimensional system there are two sets of rates. First, rates parallel to the drive, \( p_\parallel \) for hop with the drive and \( q_\parallel \) for hops opposite the drive. Second, hops transverse to the drive have rate \( p_\perp \). If \( p_\parallel \neq q_\parallel \) then with the imposed periodic boundary conditions this prescription generates a (fluctuating) particle current along the drive direction. For the \( d = 1 \) case it is standard to impose \( p + q = 1 \) and specific choices of rates have well known names. The case of \( p = 1, q = 0 \) is known as the Totally Asymmetric Simple Exclusion Process (TASEP). When \( p \neq q \) and \( p, q > 0 \) this is known as both the Partially Asymmetric Simple Exclusion Process (PASEP) or Asymmetric Simple Exclusion Process (ASEP). Finally, when \( p = q \) this is called the Symmetric Simple Exclusion Process (SSEP) which is equivalent to an equilibrium system because the drive vanishes and detailed balance is recovered.
3.2.3 Simulation of the KLS model

The rates for the KLS model are more complicated due to the interaction energy between particles. Using the $d = 2$ case as an example, there are 7 possible energy differences from a single hop due to the interaction and 4 different directions to jump. For infinite drive using Metropolis rates, this reduces to only 4 unique rates. Due to the infinite drive, hops against the drive have rate zero and hops along the drive have rate unity. For hops transverse to the drive the change in energy determines the rates. A more specific set of rates can be defined for the $d = 2$ KLS model by defining the number of nearest neighbors in a state $X$ as

$$\Pi(X) = \sum_{\langle (i,j),(n,m) \rangle} n_{i,j} n_{n,m}, \quad (3.7)$$

where $n_{i,j}$ is occupation at site $(i,j)$ and the angle brackets in the summation denote nearest neighbor pairs of $(i,j),(n,m)$ only. For a larger lattice this quantity would be expensive to calculate. A useful and numerically cheap quantity to calculate is the change in nearest neighbor pairs between two different states $X$ and $Y$, defined as $\Delta \Pi(X \rightarrow Y) = \Pi(Y) - \Pi(X)$. We can now rewrite the Hamiltonian for a given state $X$ as

$$H(X) = -J \Pi(X), \quad (3.8)$$

and the change in energy as

$$H(Y) - H(X) = -J(\Pi(Y) - \Pi(X)) = -J \Delta \Pi(X \rightarrow Y). \quad (3.9)$$

A particle that is eligible to hop can have at most 3 nearest neighbors and the new position also can have at most 3 nearest neighbors. This imposes the restriction, $\Delta \Pi(X \rightarrow Y) \in \{-3,-2,-1,0,+1,+2,+3\}$. The Metropolis rates now reduce to 5 unique rates summarized below:

$$R(X \rightarrow Y) = \begin{cases} 0 & \ell = -1 \ \forall \Delta \Pi \\
1 & \ell = +1 \ \forall \Delta \Pi \\
1 & \ell = 0 \ \Delta \Pi \geq 0 \\
1 & \ell = 0 \ \Delta \Pi = -1 \\
1 & \ell = 0 \ \Delta \Pi = -2 \\
1 & \ell = 0 \ \Delta \Pi = -3 \end{cases} \quad (3.10)$$

Calculating and saving these rates in a look up table saves computation time by eliminating the need to calculate the exponential at each time step.
3.3 Continuous time Monte Carlo Simulation

3.3.1 General algorithm

The preparation of the system is the same as with the discrete time algorithm. We start with our choice of initial conditions. The crucial difference is that in the continuous time algorithm [73, 103] we use the knowledge of the rates to choose where to hop, conversely in the discrete time version we randomly choose a place to hop and then look at the rates. The advantage of this algorithm is that jumps are chosen at the correct rates and time is adjusted accordingly. In the discrete time algorithm the rejected hops are needed to obtain correct dynamics. This rejectionless algorithm comes at a cost of tedious bookkeeping which will be shown for the $d = 2$ KLS model. All possible hops from the current state $X$ must be stored at all times. The sum of the rates to exit a state $X$

$$\mathcal{R}(X) = \sum_{Y} R(X \rightarrow Y),$$

(3.11)

determines how much time is spent in the state $X$ which is defined as

$$\Delta t = \frac{1}{\mathcal{R}(X)}.$$  

(3.12)

The system “spends” more time in states with fewer transitions out of it because the sum of the rates Eq. 3.11 is small. The discrete time algorithm accomplishes this by rejecting hops, which uses CPU time.

3.3.2 Simulation of the ASEP

For a system with very few transition rates such as the “free” lattice gas in $d = 1$, the algorithm is simple to implement. I will outline it before diving into the complexities that arise when Ising interactions are introduced. There are only two unique rates for the free gas in $d = 1$, $p$ for jumps with the drive and $q$ for jumps against the drive. For any state, the number of hops against and with the drive are equal. This is because if two particles are next to each other there is a blocked jump in both directions. So two lists are maintained of lengths $N_p$ and $N_q$ of the location of possible hops with the drive and against the drive respectively. A random number $r \in [0, p + q]$ is generated, if $r < p$ then we are choosing to hop with the drive, otherwise we are choosing to hop against the drive. We then generate a random integer to choose the specific hop $m \in [0, N_{p,q}]$. The simulation clock is updated by via Eq. 3.12, the chosen particle is moved and the possible hop lists updated. This algorithm gives a speed increase approximately proportional to the density. The discrete time algorithm rejects all hops that try to move a particle into an occupied site, the probability for that neighbor to be occupied (which means this move will be rejected) is $(N - 1)/(L - 1) \approx \rho$. 
The continuous time algorithm does not waste time generating the random numbers for moves that will be rejected. This yields such an impressive speed increase in this simple case because the lists of possible hops are simple to update. Specifically, Fig. 3.2 shows a hop to the right (dark blue arrow), only 3 neighbors moves need to be checked and updated (light blue arrows). The case is similar for hops to the left.

Figure 3.2: Diagram of a hop in the $d = 1$ free lattice gas, the red particle is hopping to the right (blue arrow). The light red particles are possible particle locations and the 2 light blue arrows are possible jumps that would need checked and updated.

### 3.3.3 Simulation of the KLS model

The algorithm becomes far more complex when nearest neighbor interactions are added. As an example, a possible hop in the KLS model with infinite drive for $d = 2$ is shown in Fig. 3.3s, the solid red circle in the middle has been chosen to hop right (blue arrow). The 15 pink particles have a total of 29 possible hops (light blue arrows) that need to be checked and updated. This is computationally expensive to do. For the continuous time algorithm to be beneficial the time spent updating these possible hops must be less than the time the discrete time algorithm would spend attempting and rejecting hops.

Figure 3.3: Diagram of a hop in the $d = 2$ KLS model, the red particle is hopping to the right (blue arrow). The light red particles are possible particles locations and the 29 light blue arrows are possible jumps that would need checked and updated.
As shown in Eq. 3.10 there are four unique non-zero rates for the KLS model in two dimensions. We now need four lists to keep track of the moves from a state $X$. Let’s call these lists $L_n(X)$, which have lengths $N_n(X)$ where $n \in \{0, 1, 2, 3\}$ denotes the 4 different rates which we will call $R_n$. The sum of the rates, Eq. 3.11 becomes

$$\mathcal{R}(X) = \sum_n R_n N_n(X) \quad (3.13)$$

Sampling the all possible hops with the correct probabilities is done by drawing a random number $r \in [0, \mathcal{R}(X)]$. The next jump is chosen by first selecting which list we will draw the hop from using the rules

$$L_{\text{pick}}(X) = \begin{cases} 
L_0(X) & \text{if } 0 < r < R_0 N_0 \\
L_1(X) & \text{if } R_0 N_0 < r < R_0 N_0 + R_1 N_1 \\
L_2(X) & \text{if } R_0 N_0 + R_1 N_1 < r < R_0 N_0 + R_1 N_1 + R_2 N_2 \\
L_3(X) & \text{if } R_0 N_0 + R_1 N_1 + R_2 N_2 < r < \mathcal{R}(X)
\end{cases} \quad (3.14)$$

Once we have chosen a list $L_n(X)$ we then draw a random integer $m \in [1, N_n(X)]$ which chooses the specific hop in that list. The time is updated, the chosen hop is performed and the jump lists are updated. The continuous time algorithm gives a speed increase below $T_c$ where there are stripes of high density and many blocked hops. Above the critical point the algorithm is slower than the discrete time counterpart because the number of rejected jumps is not high and the bookkeeping takes more time than the discrete time would spend rejecting blocked hops.

### 3.4 Measurement of Quantities of interest

The general form for measuring the expectation value of a single time observable $O(i,t)$ in a Monte Carlo simulation is

$$\langle O(i,t) \rangle = \frac{1}{N} \sum_c O_c(i,t), \quad (3.15)$$

where the angular brackets denote an average over $N$ configurations $C$ generated by the Monte Carlo simulation, and $i$ is the multidimensional lattice index. For measuring single time quantities in the stationary state we can average over the time once the steady state is reached in a single realization to gain improved statistics,

$$\langle O(i) \rangle = \frac{1}{NT} \sum_c \sum_t O_c(i,t), \quad (3.16)$$
where $T$ is the total number of times we measured the quantity in one realization. Measuring correlations (two point connected cumulant) is done by extending Eq. 3.15:

$$S_O(i, j, t, s) = \langle O(i, t)O(j, s) \rangle - \langle O(i, t) \rangle \langle O(j, s) \rangle$$

$$= \frac{1}{N} \sum_{\{C, C'\}} O_C(i, t)O_{C'}(j, s) - \langle O(i, t) \rangle \langle O(j, s) \rangle,$$

where now $C$ is a configuration at time $t$ and $C'$ is a configuration at time $s$ in the same simulation realization, now the angular brackets denote an average over many pairs of configurations $\{C, C'\}$ in different realizations. The auto-correlation function is the correlation at two different time points but the same space point. Assuming spatial translational invariance we average over all points on the lattice to improve statistics. The auto-correlation is defined as

$$S_C(t, s) = \frac{1}{NN_L} \sum_{\{C, C'\}} \sum_i O_C(i, t)O_{C'}(i, s) - \langle O(t) \rangle \langle O(s) \rangle,$$

where $\langle O(t) \rangle = \sum_i O(i, t)$, and again $N_L$ is the total number of lattice points. Eq. 3.18 is the general auto-correlation function used to measure correlation in either a stationary or non-stationary state. It explicitly depends on two times and therefore it can be used when we are not in the stationary state. When the system is in the stationary state we have time translation invariance and the auto-correlation depends only on the difference in times $t - s$. In the stationary state we will denote the change in time as simply $t$. No confusion should arise, because if an auto-correlation function only has one time argument, we can assume we are in the stationary state. For example, the density-density auto-correlation function will be denoted $S(t)$ in the steady state, for determining aging properties it will be $S(t, s)$ where the explicit two time dependence is manifest.
Chapter 4

Monte Carlo results for the ASEP

This chapter is focused on our Monte Carlo results for the ASEP model defined in Chapter 1. We compare our results with the theoretical results summarized in Chapter 2. The results are divided into two sections, in section 4.1 we present results in the steady state and in section 4.4 we present results in the transient regime. Almost all of these results, with the exception of the data presented in figs. 4.3, 4.4 and 4.21, have been presented in our paper [78]. We will largely follow our presentation in Ref. [78].

4.1 Steady-state results

4.1.1 Recurrence oscillations in small systems

We begin with a discussion of small-scale properties of the driven lattice gas on a one-dimensional ring of length $L$. When the total density $\bar{\rho} = N/L \neq 1/2$, collective density fluctuations travel around the system with mean velocity $v_c$ defined in Eq. 2.29. This causes characteristic oscillations in the time-dependent density auto-correlation function $S(0,t)$, with peaks at multiples of the return time

$$T_c = L/v_c$$

as can be seen clearly in Figs. 4.1 and 4.2, which show data obtained for $L = 100$ and $L = 2000$, respectively, both at low density $\bar{\rho} = 0.1$. A plot of densities $\bar{\rho} \in \{0.2, 0.99\}$ is shown in Fig. 4.3, the peaks at locations from Eq. 4.1 can be seen as well in this graph for densities away from half filling. There is a maximum in the peak height at $\bar{\rho} \approx 0.35, 0.65$ that we do not know the cause of. The contour plot from of the autocorrelation for $\bar{\rho} \in \{0.2, 0.99\}$ is shown in Fig. 4.4, where we have overlayed lines corresponding to multiples of the return time from Eq. 4.1 of the density fluctuations which coincide with the maxima of the autocorrelation.
Figure 4.1: Characteristic recurrence oscillations in the density auto-correlation function $S(0, t)$ for a one-dimensional driven lattice gas at low density $\rho = 0.1$ and $L = 100$ (close-up). The (red) line indicates the minimum value $S_{\text{min}} = -0.909 \times 10^{-3}$ (red line), see Eq. 2.24. The inset has been included to show the actual magnitude of the oscillations. The data are averaged over 8,000,000 realizations.

Figure 4.2: Recurrence oscillations in the driven lattice gas auto-correlation function $S(0, t)$, again for $\rho = 0.1$, but a larger one-dimensional ring of length $L = 2000$; here $S_{\text{min}} = 0.45 \times 10^{-4}$, indicated by the dashed (red) line. The inset has been included to show the actual magnitude of the oscillations. The data are averaged over 8,000,000 realizations.
Figure 4.3: Characteristic recurrence oscillations in the density auto-correlation function $S(0, t)$ for a one-dimensional driven lattice gas at densities $\bar{\rho} \in \{0.2, 0.99\}$ at 0.01 intervals for a lattice of size $L = 100$, each density is averaged over 4 million realizations.

Figure 4.4: The contour plot of the data presented Fig. 4.3. The solid lines correspond to multiples of the return time defined in Eq. 4.1. The maxima are red and fade to bright yellow, the minima are blue and fade to green, matching Fig. 4.3.
Observe the flat section in Fig. 4.1 at a negative value $S_{\text{min}} = -0.9 \times 10^{-3}$ in the first minimum. Invoking the fact that in the steady state, all configurations carry the same statistical weight, we can understand this lower bound on the density auto-correlation function as follows: Consider a single occupied site $i$ at time $t$, hence $n_i(t) = 1$. At time $t' > t$, assume that the particle has left the site $i$, but has not yet traversed the entire system and returned: this situation will give the lowest average possible value for the correlation function. While the new location of the particle previously at $i$ can be inferred from the tagged particle velocity $v_t$, Eq. (2.28), the other $N - 1$ particles are left to fill any of the remaining $L - 1$ sites with equal likelihood, which gives a probability $(N - 1)/(L - 1)$ for site $i$ to become occupied at $t'$. Averaging over all $L$ sites, we thus arrive at the same average minimum value (2.24) for the auto-correlation function $S(0, t > 0)$ when the original particle has traveled away that we derived earlier for the equal-time density cumulant: After a brief decorrelation time, typical configurations at any given site at later time $t'$ are statistically correlated to the reference configuration at $t < t'$ in the same manner as different sites are at equal time in the stationary state. The amplitude of the recurrence oscillations naturally decreases with increasing system size. Note, however, that the mean negative value $S_{\text{min}} = 0.45 \times 10^{-4}$ is still clearly visible in Fig. 4.2 for $L = 2000$.

In order to extract the period of the recurrent density fluctuations, we Fourier transform the auto-correlation function, $S(\omega) = \int S(0, t) e^{i\omega t} dt$. The first peak in $|S(\omega)|$ is caused by the movement of a density fluctuation at a frequency $\omega_c = 2\pi/T_c$, see Fig. 4.5. At low densities, higher harmonics are also visible. The characteristic frequency $\omega_c$ vanishes as the density approaches 1/2. We finally note that previous work by Adams et al. studied in detail density oscillations in the open TASEP [104].
4.1.2 Finite-size scaling

The finite-size scaling form (2.39) produces satisfactory data collapse with $\eta = 3/2$ for our simulation results for vastly different lattice sizes ranging from $L = 64$ to $L = 2,097,152$ as can be seen in Fig 4.6. At $t/L^{3/2} \approx 0.1$ one observes the expected finite-$L$ cutoff from the scaling form (2.39), as the return time $T_c$ is approached. We note that earlier work has studied the finite-size scaling properties of the TASEP with open boundaries in the maximum current phase which is equivalent to the periodic case; however much smaller system sizes of respectively $L = 50$ and $L = 257$ were utilized by Pierobon et al. [69] and Juhasz and Santen [70].

4.2 Scaling functions

We now address the stationary height-height correlation function (2.40) in one dimension, and numerically determine associated scaling functions. Figures 4.7 and 4.8 depict the scaling functions $F(\xi)$ and $g(y)$ defined in eqs. 2.44 and 2.45 obtained from our simulations for a driven periodic lattice gas with exclusion on a ring of length $L = 2000$. The Monte Carlo data nicely confirm the relations (2.46). The crossover from $F(\xi) = \text{const}$ for small arguments $\xi$ to the asymptotic behavior $\sim \xi^{2/3}$ visible in Fig. 4.7 can be compared with the numerical solution of the mode-coupling equations depicted in Fig. 2 of Ref. [34]. The mode-coupling approximation appears to predict sharper crossover features, with $F(\xi)$ remaining constant.

Figure 4.6: Finite-size scaling for the density auto-correlation function for $L = 64$ (data averaged over 80,000 realizations), $L = 256$ (10000 realizations), $L = 2048$ (40,000 realizations), and $L = 2,097,152$ (60 realizations).
Figure 4.7: Double-logarithmic plot of the scaling function $F(\xi)$, defined in Eq. (2.44), obtained from Monte Carlo simulations in a driven lattice gas on a ring of length $L = 2000$, with $x \in [0, 64]$ and $t \in [0, 64]$. The data are averaged over 200 realizations.

until $\xi \approx 0.5$, where our data already indicate a noticeable curvature in the scaling function $F$. Fig. 4.8 shows a similar crossover features in the inset.

Our Monte Carlo simulation data for the scaling function $f(y)$ defined in Eq. 2.48, measured by averaging over a very large number of realizations, are plotted in Fig. 4.9. Our data are in reasonable agreement with the stretched exponential function $f(y) \propto \exp(-cy^3)$, where $c = 0.295(5)$, that was computed in Ref. [36] by numerical integration. The divergence of simulation data and the theoretical prediction at values of $y$ greater than 1.5 in Fig. 4.9 is presumably due to systematic errors caused by finite-size effects that are difficult to estimate in Monte Carlo simulation.

4.3 Slow relaxation

4.3.1 Local exponent for TASEP (d=1,2,3)

In Fig. 4.10 we plot the density auto-correlation function $S(0, t)$ as obtained from our simulations for a one-dimensional driven lattice gas with exclusion with $L = 2048$ (see also Fig. 4.6). From Eq. (2.37) with $\zeta = 1/z_{ll} = 2/3$, we expect the asymptotic long-time power law $S(0, t) \sim t^{-2/3}$, which fits the Monte Carlo data well for $t > 100$ on the double-logarithmic plot. The approach to the expected asymptotic power law auto-correlation decay can be carefully probed by studying the local effective exponent $\zeta_{\text{eff}}(t)$ defined in Eq. (2.38).

Figure 4.11 shows that the local exponent increases with time and in fact surpasses the
Figure 4.8: The scaling function $g(y)$ defined in Eq. (2.45), from the same data as in Fig. 4.7. The inset is the same scaling function on a double-logarithmic plot. ($L = 2000$, $x \in [0, 64]$, and $t \in [0, 64]$, averaged over 200 realizations)

Figure 4.9: Logarithmic plot of the scaling function $f(y)$, defined in Eq. (2.48), for $L = 2000$, with $x \in [0, 256]$ and $t \in [0, 256]$, with the data averaged over 400,000 realizations. Each data point is averaged over 200 $y$ values. The error bars representing the standard error are smaller than the symbols.
Figure 4.10: Double-logarithmic plot of the stationary auto-correlation function $S(0, t)$ for a one-dimensional driven lattice gas with exclusion for length $L = 2048$. The data are averaged over 40,000 realizations. The light green line represents a power law with exponent $-2/3$.

Figure 4.11: The local auto-correlation exponent (2.38) obtained from Monte Carlo simulation data for a one-dimensional driven lattice gas with length $L = 2048$ and for $\rho = 1/2$. The data are averaged over 40,000 realizations. Each point is averaged over 10 time steps. The error bars represent the standard error of the mean local exponent during the 10 time steps.
Figure 4.12: Time dependence of the local exponent $\zeta_{\text{eff}}(t)$ for one-dimensional driven lattice gases with $L = 2048$ (black circles, data averaged over 40,000 realizations) and $L = 2097152$ (red squares, 60 realizations). The corresponding straight lines are power law fits to the data.

The asymptotic value $2/3$, indicated by the horizontal line. In order to demonstrate that this is actually a finite-size effect, albeit a quite unusual one, we display in Fig. 4.12 a comparison of simulation data for the time dependence of the effective exponent for systems of sizes $L = 2048$ and $L = 1024 \times 2048 = 2097152$ on a logarithmic time scale. Even in the much larger lattice, $\zeta_{\text{eff}}(t)$ still rises beyond the asymptotic exponent value $\zeta = 2/3$ of the infinite system, yet at later time. Since we have not observed this overshooting in unbiased lattice gases with exclusion, it is clearly a consequence of the non-equilibrium drive. We note that the extremely slow crossover towards the asymptotic temporal power law has been recorded before in a model of reconstituting dimers that can be mapped to the TASEP [105].

In figs. 4.13 and 4.15 we plot the auto-correlation functions in two and three dimensions respectively. In each case, the system is half-filled ($\rho = 1/2$), and the hopping rates are equal in each direction transverse to the drive, but set totally asymmetric parallel to the drive. For a two-dimensional driven lattice gas ($L_x = L_y = 100$), we depict the effective exponent as defined in Eq. (2.52) in Fig. 4.14, and analogous results for the three-dimensional case are shown in Fig. 4.16. Since we are at or above the critical dimension $d_c = 2$, respectively, the asymptotic value is $\zeta = d/2$, Eq. (2.53). Indeed, the local exponent $\zeta_{\text{eff}}(t)$ quickly relaxes to 1 for $d = 2$ and $3/2$ for $d = 3$, and never surpasses these expected asymptotic values. The anomalously slow convergence and unusual finite-size behavior in one dimension are consequently caused by the strong out-of-equilibrium correlations present only for $d < d_c$. 
Figure 4.13: The auto-correlation function for a two-dimensional driven lattice gas with $L_x = L_y = 100$ and $\rho = 1/2$. The data are averaged over 600,000 realizations. The line is the power law $t^{-1}$.

Figure 4.14: The effective exponent $\zeta_{\text{eff}}(t)$, defined in Eq. (2.52), for a two-dimensional driven lattice gas with $L_x = L_y = 100$ and $\rho = 1/2$. The data are averaged over 600,000 realizations. Each point is averaged over 8 time steps. The error bars represent the standard error of the mean local exponent of the 8 measurements. The (red) horizontal line indicates the asymptotic value 1.
Figure 4.15: The auto-correlation function for a three-dimensional driven lattice gas with $L_x = L_y = L_z = 50$ and $\rho = 1/2$. The data are averaged over 1,320,000 realizations. The line is the power law $t^{-3/2}$.

Figure 4.16: The local exponent $\zeta_{\text{eff}}(t)$ for a three-dimensional driven lattice gas with $L_x = L_y = L_z = 50$ and $\rho = 1/2$. The data are averaged over 1,320,000 realizations. Each data point is averaged over 20 time steps, the error bars represent the standard error of the mean effective exponent during the 20 time steps. The (red) horizontal line indicates the asymptotic value 3/2.
Figure 4.17: The auto-correlation function for one-dimensional driven lattice gases (ASEP) with different hopping biases $\Gamma = 1.0$ (TASEP), 0.6, 0.4, 0.2 (all ASEP), and 0.0 (vanishing drive, SEP); $L = 4096$ and $\rho = 1/2$. The data are averaged over 5,000,000 realizations each.

Figure 4.18: Local auto-correlation exponent $\zeta_{\text{eff}}(t)$ for one-dimensional driven lattice gases (ASEP) with different hopping biases $\Gamma = 1.0$ (TASEP), 0.6, 0.4, 0.2 (all ASEP), and 0.0 (vanishing drive, SEP); $L = 4096$ and $\rho = 1/2$. The data are averaged over 5,000,000 realizations each.
4.3.2 Local exponent for ASEP (d=1)

Up to this point, we have provided results only for driven lattice gases with zero backward hopping rate along the drive direction (TASEP in one dimension). Assigning the forward hopping probability \( p \) and backward probability \( q \), we can define the bias \( \Gamma = p - q = 2p - 1 \). As long as \( 1/2 < p < 1 \) and \( 0 < \Gamma < 1 \) (ASEP), a macroscopic particle current persists, the system remains out of equilibrium, and one expects qualitatively the same behavior as for maximum bias or drive, \( p = \Gamma = 1 \). Thus, at long times, the temporal decay of the density auto-correlation function should be described by a power law with exponent \( \zeta = 2/3 \) in one dimension, for any non-zero value of the hopping bias \( \Gamma \). However, note that this statement is valid at asymptotically long times for sufficiently large systems, and a simple power-law decay will not necessarily be observable in finite systems with weak bias. Monte Carlo simulation data for one-dimensional driven lattice gases with various bias values are shown in figs. 4.17 and 4.18. As can be seen, the local exponent \( \zeta_{\text{eff}}(t) \) relaxes increasingly slowly towards its asymptotic value \( 2/3 \) as the bias is reduced. Figure 4.18 illustrates that for low bias and at short times, the density auto-correlation decay rather follows the symmetric exclusion process (SEP) relaxation, for which \( \zeta = 1/2 \). For example, for \( \Gamma = 0.2 \) a distinct decrease in the local exponent is observed for \( t < 30 \), later followed by a very slow increase.

4.4 Aging Dynamics

As discussed in chapter 2, when transitioning from one steady state characterized by a set of hopping rates \( p, q \) to another set \( p', q' \) all observables change instantly. This includes the auto-correlation function. If system is in a steady state with parameters \( p, q \) and at time 0 we change those parameters to \( p', q' \) and then record the densities at the waiting time \( s \) and a later time \( t \), the auto-correlation based on these measurements is time translationally invariant, thus only depends on \( t - s \). This scenario is depicted in Fig. 4.19 and discussed in section 2.3.5.

![Figure 4.19](image)

Figure 4.19: Time arrow for changing ASEP parameters at time \( t = 0 \) and measuring the auto-correlation function at times \( s \) and \( t \) after.

However, if we decide to record the densities at a “waiting time” \( s = 0 \) while the rates are \( p, q \), then changing the rates to \( p', q' \) at a later time \( r > s \) and then record the densities at an even later time \( t > r \), a timeline shown in Fig. 4.20, this yields the interesting behavior
shown in Fig. 4.21. To explain the behavior, we start with a state $C_0$ in the steady state for the TASEP ($\Gamma = 1$), this is time $s = 0$. The auto-correlation follows the blue line if the parameters are never changed, meaning all subsequent transitions to a new state $C_t$ were rates corresponding to $\Gamma = 1$. The green line however, where the rates were changed to ASEP ($\Gamma = 0$) rates at $r = 50$ displays a kink starting at $r$. This kink is caused by the evolution of the system up to time $r$ being governed by rates from $\Gamma = 1$ and then the system suddenly starts evolving with rates $\Gamma = 0$. The system itself has no memory of the transition, but the auto-correlation function does in this case, resulting in the strange behavior seen in Fig. 4.21. To arrive at a state $C_{t>r}$ starting at the state $C_0$ in the steady state we can define the transition probability (rate) as a product of the rates $\gamma \in \{p, q\}$ and $\gamma' \in \{p', q'\}$ as

$$R(C_0 \rightarrow C_{t>r}) = \gamma_0 \gamma_1 \cdots \gamma_{r-1} \gamma_r \gamma_{r+1} \cdots \gamma_{t-1} \gamma_t.$$  \hspace{1cm} (4.2)

The kink and slow relaxation is because the evolution starting from the state $C_0$ is interrupted and modified by different transition rates. For infinite time the auto-correlation acts as if the system always evolved according to the current rates. This lack of relaxation in the system when changing the drive value does not allow access to the aging scaling regime.

Starting from the highly correlated initial configuration of alternatingly occupied sites in the TASEP that corresponds to a flat surface in the growth model representation, time translation invariance is broken during the slow approach to the stationary regime. To properly differentiate the transient state from the steady state we measure the width defined in Eq. 2.55. Our Monte Carlo simulation results nicely confirm the scaling relation (2.56), as evidenced in Fig. 4.22 by the satisfactory data collapse for various system sizes with the expected scaling exponents (compare also the analogous mode-coupling results in Fig. 3 of Ref. [34], and the simulation data shown in Fig. 1 of Ref. [106]). Our measurements yield an initial growth exponent $0.30$, slightly different from the expected value $1/3$, likely caused by sizeable corrections to scaling in our data. Our finite-size scaling plot of the width matches the simulation data of Ref. [106]. Time translational invariance is broken while the width of the interface is growing ($t/L^z < 1$). Past this point, the system is in the stationary state and time translational invariance holds and aging would not be observeable. When time translational invariance is broken the density-density or height-height correlation functions then depend explicitly on both time arguments $t$ and $t'$. Henceforth we shall refer to the second argument as waiting time $s$, and consider the short-time scaling limit $s \ll t$ [4]. By means of a careful renormalization group analysis, Krech [87] established Eq. 2.57 which
Figure 4.21: A plot of the auto-correlation function for the 1-d driven lattice gas. The black line is $\Gamma = 0$, blue line $\Gamma = 1$. The red line is $\Gamma = 0$ and then changes to $\Gamma = 1$ at $t = 50$. The green line is $\Gamma = 1$ and then at $t = 50$ the rates change to $\Gamma = 0$. The system size is $L = 2000$, each curve is averaged over 20000 runs.

Figure 4.22: Finite-size scaling for the interface width of the one-dimensional growth model that corresponds to the TASEP, for system sizes $L = 600$, 800, and 1000, see Eq. (2.56). The data are averaged over 50,000 realizations each.
generalizes Eq. (2.44) that is valid in the stationary regime. Here, the initial slip exponent \( \theta = (d + 4)/z - 2 \) can be expressed in terms of the standard dynamic scaling exponent \( z \). This follows since the initial-time surface does not induce any novel singularities, as a consequence of the momentum dependence of the nonlinear vertex in the KPZ problem, and thus no additional renormalizations are required. In one dimension, the renormalization group predicts \( \theta = 4/3 \). For the TASEP density-density correlation function, we obtain by means of eqs. 2.42 and 2.57

\[
S_{IS}(x, t, s \ll t) = \left( \frac{8}{t} \right)^{\theta} |x|^2 \alpha^{-2} f(t/x^{z}) = \left( \frac{8}{t} \right)^{4/3} |x|^{-1} f(t/x^{3/2}).
\]

(4.3)

In order to arrive at the temporal behavior of the auto-correlation function, we must require that the scaling function \( f(\xi) \sim \xi^{-2/3} \) as its argument \( \xi \to \infty \), whence

\[
S_{IS}(0, t, s \ll t) = \left( \frac{8}{t} \right)^{4/3} t^{-2/3}.
\]

(4.4)

Our Monte Carlo auto-correlation data displayed in Fig. 4.23, obtained for various waiting times \( s \), convincingly confirm the scaling predicted by Eq. (4.4) for \( s \ll t \).

As shown for the KPZ growth model, no additional renormalizations, and hence no independent new scaling exponents are required in the non-stationary relaxation regime in one dimension [87]. In a similar vein, for the density-density auto-correlation function in the driven lattice gas, via matching \( b = s^{-1/z} \) we obtain Eq. (2.6), with the scaling exponent \( \zeta \) given in Eq. (2.37). Figure 4.24 confirms the simple aging scenario according to Eq. (2.6) through the nice data collapse of our Monte Carlo simulation results for various waiting times in one dimension, where \( \zeta = 2/3 \). We have also performed driven lattice gas simulations in two and three dimensions with alternating particle initial conditions on periodic lattices. As demonstrated in Figs. 4.25 and 4.26, we obtain simple-scaling data collapse with the expected scaling exponent \( \zeta = 1 \) for \( d = 2 \) and \( \zeta = 3/2 \) for \( d = 3 \), respectively.

Strongly correlated initial conditions are needed to access the aging scaling regime for the ASEP. As we discussed, there is no relaxation from a steady state specified by a set of rates \( \gamma \in \{p, q\} \) to a steady state specified by \( \gamma \in \{p', q'\} \). This is a consequence of the probability of a given state \( C \) in the steady state being independent of the parameter being changed (drive).
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Figure 4.23: Scaling plot for the density auto-correlation function for a one-dimensional driven lattice gas (TASEP) with length $L = 1000$ and density $\rho = 1/2$ in the non-equilibrium relaxation regime, see Eq. (4.4), measured for waiting times $s = 100, 160, \text{and} 220$. The data are averaged over 60,000 realizations.

Figure 4.24: Simple aging scaling plot, see Eq. (2.6), for the density-density auto-correlation function for a one-dimensional driven lattice gas (TASEP) of length $L = 1000$, at density $\rho = 1/2$, obtained from Monte Carlo simulation data with different waiting times $s = 100, 160, \text{and} 220$. The inset is the unscaled curves plotted against $t - s$ to show that time-translation invariance is broken. The data sets are averaged over 60,000 realizations each.
Figure 4.25: Density auto-correlation function for a two-dimensional driven lattice gas of size $L_x = L_y = 128$ for density $\rho = 1/2$ in the aging scaling regime for waiting times $s = 50, 100, \text{ and } 350$. The inset is the unscaled curves plotted against $t - s$ to show that time-translation invariance is broken. Each data set is averaged over 160,000 realizations.

Figure 4.26: Density auto-correlation function for a three-dimensional driven lattice gas of size $L_x = L_y = L_z = 20$ for density $\rho = 1/2$ in the aging scaling regime for waiting times $s = 10, 20, \text{ and } 30$. The inset is the unscaled curves plotted against $t - s$ to show that time-translation invariance is broken. Each data set is averaged over 4,200,000 realizations.
Chapter 5

Monte Carlo results for the KLS model

5.1 Critical Monte Carlo results

5.1.1 Stationary Results

As mentioned in chapter 2, steady state Monte Carlo results for the finite-size scaling of the order parameter have been inconclusive [50, 72, 56]. Our attempts to obtain finite-size scaling of the order parameter via Eq. 2.87 have been inconclusive as well. Scaling using Eq. 2.87 is sensitive to small changes in the critical temperature as was discussed in detail by Leung and Zia [60] and Wang [72]. Leung and Zia [60] elaborate further that care must be taken when choosing the critical region to fit the order parameter. If done carelessly one can obtain incorrect results. They prove this point by simulating the equilibrium counterpart of the KLS model, the equilibrium Ising model. Leung and Zia perform finite-size scaling of the order parameter at the critical point and obtain an incorrect value of the order parameter exponent following the methodologies of Ref. [107]. Due to the ambiguity of the finite-size scaling of the order parameter in the steady state we present measurements of different quantities.

Here a few steady state results from our Metropolis Monte Carlo simulations are shown. The relaxation towards the steady state at the critical point is very slow. We monitor this relaxation using the order parameter defined in Eq. 2.82. As the system size is increased, the time it takes to relax to the steady state increases as well, which is known as critical slowing down. This is a major problem due to there being finite-size effects to the critical temperature and scaling of correlations. We first present measurements of the variance of
the order parameter $m$,

$$
\vartheta(\tau, L_\perp, L_\parallel) = \langle m^2 \rangle - \langle m \rangle^2.
$$

(5.1)

This is commonly referred to as the “susceptibility” $\chi$. $\tau$, again is the reduced temperature in the transverse dimension. Due to the violation of the fluctuation response theorem in the KLS model [46] the correlations are not linearly related to the susceptibility, thus we will call this variance $\vartheta$ and not $\chi$. Since only infinite systems are actually critical, what we refer to as the critical temperature means the maximum of the variance defined in Eq. 5.1. Fig. 5.1 contains the variance data of 3 system sizes over a wide range of temperatures following Eq. 2.70, specifically $L_\parallel/L_\perp^{1+\Lambda} = 1/256$, where $\Lambda = \Delta = 2$ where $\Delta = 2$ is the JSLC value of the anisotropy exponent. Note here we distinguish between the anisotropy exponent $\Delta$ defined in chapter 2, with $\Lambda$ which will stand for the exponent used to define the lattice dimensions for simulations. When performing simulations one should use $\Lambda = \Delta$ so that the proportionality factor $A$ defined by

$$
L_\parallel = AL_\perp^{1+\Delta}
$$

remains constant. If $A$ is not constant, it will enter scaling forms as a relevant variable when performing finite-size scaling. Fig. 5.1 uses $A = 1/256$ and agrees with Fig. 1 of Ref. [72] which uses similar parameters. We will use $T_C = 1.41T_{eq}^{\infty}$, as this is the accepted asymptotic critical temperature of an infinite system [8, 9, 49, 50, 72, 56, 57, 92, 93] based on simulations. There is a clear peak around $T/T_C \approx 1$ in Fig. 5.1 indicating this is a good approximation of the critical temperature. Using the peaks of the variance curves we determined the critical

![Graph](image_url)

Figure 5.1: Plot of the variance defined in Eq. 5.1 for system sizes $(L_\parallel, L_\perp)$ of (16,16), (54,24) and (128,32) with each data point in each curve averaged over 100, 100 and 240 runs respectively. The critical temperature is defined as $T_C = 1.41T_{eq}^{\infty}$.
temperature for several system sizes by fitting a parabola to the variance close to the critical point similar to Ref. [72]. The results are shown in Figs. A.1, A.2, A.3 and A.4 for various system sizes in appendix A. We will refer to these numerical values of the critical temperature using $T_C(L_\parallel, L_\perp)$, which approaches $T_C$ from below as the system size is increased. We summarize our system size dependent critical temperatures in table 5.1.

Table 5.1: Numerical values of the critical temperature

<table>
<thead>
<tr>
<th>$L_\parallel$</th>
<th>$L_\perp$</th>
<th>$T_C(L_\parallel, L_\perp)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>16</td>
<td>0.755021 ± 0.00007†</td>
</tr>
<tr>
<td>54</td>
<td>24</td>
<td>0.772975 ± 0.00003†</td>
</tr>
<tr>
<td>128</td>
<td>32</td>
<td>0.782417 ± 0.00008†</td>
</tr>
<tr>
<td>250</td>
<td>40</td>
<td>0.787917 ± 0.00002†</td>
</tr>
</tbody>
</table>

† The errors obtained from the fit are highly optimistic. There are much larger systematic errors.

The finite-size scaling form from Eq. 2.79 produces satisfactory data collapse as evidenced by Fig. 5.2 using the exact exponents from JSLC theory summarized in table 2.2 and the numerical values of the critical temperature summarized in table 5.1. Note that due to the finite-size effects the asymptotic power law from Eq. 2.81 is inaccessible. Much larger systems and much longer times would be needed to measure this asymptotic power law. The system sizes needed to probe the asymptotic limit in the auto-correlation function take too long to reach the steady state, for this reason we turn to short-time dynamics.

5.1.2 Transient Results

As discussed in chapter 2, obtaining accurate values of the critical temperature is difficult. We determined the critical temperature for a few smaller systems by measuring the variance of the order parameter in our Metropolis Monte Carlo simulations. However system sizes this small yield finite-size effects in the temporal correlations as can be seen in Fig 5.2. Thus taking data in the asymptotic limit is impossible for the system sizes studied in the previous section. Increasing the system size and obtaining the finite-size cutoff at a later time is desirable. However, the size of the system needed is very large and the waiting time to reach the stationary state at the critical point is very long. We discussed in chapter 2 circumventing this problem by studying short time properties quenching from a high-temperature (disordered) to critical temperatures. We use the simple aging scaling form is $S(t, s) = s^{-\zeta} S(t/s)$, where $\zeta = (d + \Delta - 2 + \eta)/z$ at the critical point, which was obtained in chapter 2 using simple scaling arguments (Eq. 2.88). The predicted aging exponent from JSLC exponents is $\zeta^{\text{JSLC}} = 0.5$ and from RDLG exponents is $\zeta^{\text{RDLG}} \approx 0.25$. We perform two sets of simulations at $T = T_C$ for two different aspect ratios obeying Eq. 5.2 with $\mathcal{A} = 1$,
JSCL theory: \( \Lambda = \Delta^{\text{JSCL}} = 2 \) and RDLG theory: \( \Lambda = \Delta^{\text{RDLG}} = 1 \). We use \( A = 1 \), which gives extremely anisotropic systems, i.e. considerably longer in the dimension parallel to the drive than the transverse dimension. We attempt to collapse each set of data using both aging exponents. In both cases, \( \Lambda = \Delta^{\text{JSCL}} \) or \( \Lambda = \Delta^{\text{RDLG}} \), the aging exponent from JSCL theory, \( \zeta^{\text{JSCL}} \) gives outstanding data collapse which is evidenced in Figs. 5.3 and 5.5. Data collapse is not achieved using the aging exponent from the RDLG theory, \( \zeta^{\text{RDLG}} \), the clear lack of scaling is evident in Figs. 5.4 and 5.6.

Albano et al. [57, 63] studied the short time evolution of the order parameter \( m \). Using a slightly different order parameter, Albano et al. attempt scaling using a scaling ansatz and assuming that fluctuations parallel to the drive are of the order \( L_{\parallel}^{-1/2} \) [57]. Compare our Fig. 5.7 to Fig. 1 of Ref. [57], Fig. 3 of Ref. [58] and Fig. 10 of Ref. [63]. First we derive the scaling form used in a clear way. Starting from Eq. 2.86 we invert \( b^{-1} L_{\parallel} \) and \( b^{-1/(1+\Delta)} L_{\perp} \) which yields

\[
m(t, \tau, L_{\parallel}) = b^{-\beta/\nu} \tilde{m}(b^{-z_{\parallel}} t, b^{1/\nu} \tau, b^{1/(1+\Delta)} L_{\perp}^{-1}, b L_{\parallel}^{-1}).
\] (5.3)

Next setting \( b = t^{1/z_{\parallel}} \) and \( \tau = 0 \) yields

\[
m(t, L_{\parallel}) = t^{-\beta/2(z_{\parallel} \nu)} \tilde{m}(t^{1/z_{\parallel}} L_{\perp}^{-1}, t^{1/z_{\parallel}} L_{\parallel}^{-1}).
\] (5.4)

Now substituting \( L_{\perp} = A L_{\parallel}^{1/(1+\Delta)} \), where \( A \) is a constant, \( \tilde{m} \) is now only a function of \( t^{1/z_{\parallel}} L_{\parallel}^{-1} \). An important assumption is that \( t^{1/z_{\parallel}} L_{\parallel}^{-1} \) is small and following the same procedure
Chapter 5. Monte Carlo results for the KLS model

Figure 5.3: Aging scaling plot for the two-dimensional critical KLS model with infinite drive from our Metropolis Monte Carlo simulations, using $\Lambda = \Delta^{JSLC} = 2$. The system size is $L_\parallel = 125000$, $L_\perp = 50$. The data are collapsed using the scaling form in Eq. 2.88 with an aging exponent of $\zeta^{JSLC} = 0.5$. The inset is the unscaled curves plotted against $t - s$ to show that time-translation invariance is broken. Each curve is averaged over 200 runs.

Figure 5.4: Aging scaling plot for the two-dimensional critical KLS model with infinite drive from our Metropolis Monte Carlo simulations, using $\Lambda = \Delta^{JSLC} = 2$. The system size is $L_\parallel = 125000$, $L_\perp = 50$. The data are collapsed using the scaling form in Eq. 2.88 with an aging exponent of $\zeta^{RDLG} \approx 0.25$. The inset is the unscaled curves plotted against $t - s$ to show that time-translation invariance is broken. Each curve is averaged over 200 runs.
Figure 5.5: Aging scaling plot for the two-dimensional critical KLS model with infinite drive from our Metropolis Monte Carlo simulations, using $\Lambda = \Delta^{RDLG} = 1$. The system size is $L_{\parallel} = 32400$, $L_{\perp} = 180$. The data are collapsed using the scaling form in Eq. 2.88 with an aging exponent of $\zeta_{JSLC} = 0.5$. The inset is the unscaled curves plotted against $t - s$ to show that time-translation invariance is broken. Each curve is averaged over 200 runs.

Figure 5.6: Aging scaling plot for the two-dimensional critical KLS model with infinite drive from our Metropolis Monte Carlo simulations, using $\Lambda = \Delta^{RDLG} = 1$. The system size is $L_{\parallel} = 32400$, $L_{\perp} = 180$. The data are collapsed using the scaling form in Eq. 2.88 with an aging exponent of $\zeta_{RDLG} = 0.25$. The inset is the unscaled curves plotted against $t - s$ to show that time-translation invariance is broken. Each curve is averaged over 200 runs.
outlined in [62], for alternating initial conditions (Fig. 3.1b) the initial value of the order parameter is zero. We expand the regular scaling function for small $t^{1/z_1} L^{-1}$,

$$\tilde{m}(t^{1/z_1} L^{-1}) = \tilde{m}_0 + \tilde{m}_1 t^{1/z_1} L^{-1} + \ldots$$

(5.5)

where $\tilde{m}_0$ is zero, $\tilde{m}_1$ is constant and we ignore higher order terms, therefore

$$m(t, L) \propto t^{1/z_1 - \beta/(z_1 \nu)}.$$  

(5.6)

Figure 5.7 demonstrates convincing data collapse using this form. Performing a fit to the $64000 \times 40$ data yields $1/z_1 - \beta/(z_1 \nu) \approx 0.487$, very close to 0.5 predicted by JSLC exponents. The JSLC power law $t^{0.5}$ and the power law from RDLG, $t^{0.37}$ are included in Fig. 5.7. Fig. 5.8 confirms the scaling relation in Eq. 2.87 using JSLC exponents. There is a short time at the beginning where the data do not collapse, $t < 500$ MCS, this is a small microscopic time $t_{mic}$ in which the order parameter depends on initial conditions [108]. Critical initial slip [61] occurs after $t_{mic} \approx 500$ MCS in Fig. 5.8. Using the RDLG exponents do not collapse the data as can be seen in Fig. 5.9.
Figure 5.8: Finite-size scaling according to Eq. 2.87 of the order parameter defined in Eq. 2.82. The data are rescaled using the JSLC exponents from table 2.2. The data collapse for large values of $t/L_{\parallel}^{4/3}$. Each curve is averaged over 500 realizations.

Figure 5.9: Finite-size scaling according to Eq. 2.87 of the order parameter defined in Eq. 2.82. The data are rescaled using the RDLG exponents from table 2.2. The data do not collapse for large $t/L_{\parallel}^2$. The appearance of data collapse at short times is due to all systems starting with $m(t) = 0$. Each curve is averaged over 500 realizations.
5.2 Sub-critical Monte Carlo results

In this section we present results for quenches from the disordered state \( T = \infty \) to below the critical point. The growth of domains has been shown to follow a power law, \( R \sim t^{1/3} \) [64, 65]. In Fig. 5.10 we present our Metropolis Monte Carlo measurements of domain sizes

\[
R_\parallel = \frac{L_\parallel L_\perp}{B_\parallel}
\]

(5.7)

\[
R_\perp = \frac{L_\parallel L_\perp}{B_\perp}
\]

(5.8)

where \( B_\parallel, B_\perp \) represent the number of broken bonds in the \( \parallel, \perp \) directions respectively. \( R_\parallel \) and \( R_\perp \) follow the expected behavior \( t^{1/3} \). Fig. 5.11 shows the time evolution of a smaller anisotropic system at infinite drive and \( T = 0.3T_C \). One can see that the interface between the high and low density regions is flat at late times. This agrees with Leung et al. [99] that the interface width is flat for high values of drive. The steady domain sizes are estimated from the data, \( R_{\perp,\text{steady}} \approx 17.5 \) and \( R_{\parallel,\text{steady}} \approx 53.6 \)

The typical evolution of non-equilibrium sub-critical stripe growth in the KLS model is, first, the system evolves into a multi-stripe state with many stripes of high and low density. Second, the stripes merge into the steady state configuration which is one stripe of high density and one stripe of low density. The multi-stripe state is an extremely long lived metastable state. This metastable state can be avoided however if the lattice is anisotropic. In Fig. 5.11 we present snapshots of the KLS

Figure 5.10: Parallel \( R_\parallel(t) \) and transverse \( R_\perp(t) \) lengths for the KLS model quenched from random initial conditions to \( T = 0.3T_C \). The dotted lines correspond to the steady state value of their respective lengths. The lattice size is \( L_\parallel = 64000 \) by \( L_\perp = 40 \). The data is averaged over 50 realizations, both curves come from the same data set.
model at different times during a quench from a disordered state to $T = 0.3T_C$, well into the sub-critical temperature regime. This evolution skips the multi-stripe metastable states and stripe merging regime. Lattices honoring $L_\parallel = L_\perp^{1+\Lambda}$, with $\Lambda = \Delta^{JS\text{LC}}$, are too long to fit on a single page. The smaller system in Fig. 5.11 behaves similarly. Fig. 5.11a shows the system after 1000 MCS have passed, we can see the stripes beginning to form parallel to the drive. The stripes fluctuate in the transverse direction and this causes stripes to merge during early times. The system is long enough that all stripes are “connected” during these early times. This really means there is one wildly fluctuating domain at early times. We can see at later times, Fig. 5.11c, that there exist 2 pronounced stripes. These two stripes are still connected and will merge into one stripe. Conversely, for an isotropic system, Fig. 5.12, the dynamics is completely different. For the $200 \times 200$ system multiple disconnected stripes form very early, evidenced by Fig. 5.12a. The structure of the system is clear (see Fig. 5.12d) by $t = 6000$ and does not qualitatively change in subsequent snapshots. It would take an enormous amount of time for the stripes to merge. Zia et al. [67] show that for isotropic systems that this multi-stripe phase is actually the steady state. They present simulations starting with a single stripe and it splits into multiple stripes for isotropic systems. This is a clear indication that the steady states are very different for different lattice aspect ratios.

Our attempts to obtain scaling of the auto-correlation function for sub-critical quenches have been unsuccessful. We have tried simple aging scaling, Eq. 2.6 which did not give convincing data collapse. We also attempted scaling for using the domain sizes similar to Ref. [109], this again did not result in data collapse.

These qualitative results raise many more questions. A proper way to characterize the multi-stripe phase is needed. What range of temperatures will result in a single stripe configuration for a given aspect ratio? It is encouraging that for a temperature as low as $0.3T_C$ we were able to reach a single stripe configuration starting from random initial conditions for an anisotropic lattice. There is a large parameter space to explore given that the lattice aspect ratio and temperature both change the steady state in drastic ways.
Figure 5.11: Snapshots of the lattice for a quench from a random state $T = \infty$ to $T = 0.3T_C$ at different times. The lattice size is $L_\parallel = 2000$ by $L_\perp = 20$. 
Figure 5.12: Snapshots of the lattice for a quench from a random state $T = \infty$ to $T = 0.3T_C$ at different times. The lattice size is $L_\parallel = 200$ by $L_\perp = 200$. 
Chapter 6

Conclusion

6.1 Summary

We presented simulation data for the ASEP model in one, two and three dimensions. The scaling exponents for the ASEP have been previously obtained from exact solutions and coarse grained field-theoretic renormalization group treatments. By measuring the density-density auto-correlation function in our Metropolis Monte Carlo simulations, we verified the scaling exponents. We carefully investigated the approach to the asymptotic power law using much larger systems than previously reported over many stochastic realizations. We found that this approach is extremely slow for finite drive values in one dimension at half-filling. At short times for weak drive, the auto-correlation behaves like the equilibrium lattice gas, and then very slowly approaches the asymptotic behavior expected for the driven system. For infinite drive (TASEP), the approach to the asymptotic power law is still slow. The effective exponent approaches its asymptotic value from below for all finite values of drive. Surprisingly, the effective exponent exceeds its asymptotic value for the TASEP. We demonstrated that these slow crossover features are not present in two and three dimensions and conclude that they must be a result of the strong non-equilibrium correlations in one dimension. We observe recurrence oscillations in the auto-correlation function away from half-filling in the TASEP. Standard finite-size scaling is performed for the one-dimensional case with expected results for a wide range of system sizes. We compare our numerical simulation data to analytic predictions of a few steady-state density-density and height-height scaling functions, and achieve excellent agreement. Non-stationary properties of the TASEP were studied through extensive simulations in the transient regime. Using simple scaling arguments, the aging exponent can be expressed by known exponents. The aging exponent is known for the equivalent KPZ surface growth model. By use of the mapping from the KPZ to TASEP, we are able to verify this exponent for the one-dimensional TASEP. We extend this simple scaling argument for the aging exponent to two and three dimensions and confirm it with our Monte Carlo simulations.
We provide simulation results for the KLS model at criticality that confirm JSLC critical exponents by measurement dynamic quantities simulating much larger lattices than previous studies. We show that the critical temperature is sensitive to finite-size effects as demonstrated in previous work. Finite-size scaling of the density-density auto-correlation function provides data collapse using JSLC exponents. By using simple scaling arguments, we arrive at an expression for the aging exponent in terms of known steady-state critical exponents. Monte Carlo simulations were performed in the transient regime and the density-density auto-correlation was measured at different waiting times. The aging exponent obtained using JSLC exponent values yielded convincing data collapse over a range of waiting times and different lattice anisotropies. We showed that the exponents from the RDLG theory did not provide data collapse for simple aging scaling. The time-dependent order parameter data at short times for different lattice sizes was collapsed using finite-size scaling and JSLC exponents. Using the same scaling form with RDLG exponents did not collapse our data. Our work provides further evidence using dynamic quantities, which were not previously accessed, that the KLS model with infinite drive is adequately described by JSLC theory and the corresponding coarse-grained Langevin equation.

We present Monte Carlo simulations of the KLS model during sub-critical quenches. We confirm the accepted exponent of power-law growth of domains. We were unable to obtain scaling of the density-density auto-correlation function during the quench. We provide qualitative arguments from our simulation results that the sub-critical steady state depends on the lattice aspect ratio. We present lattice configurations at different stages of evolution, illustrating that for an anisotropic lattice the steady state is indeed a single stripe with a flat interface. In a square lattice, the converse is true: the system quickly relaxes to a multi-stripe meta-stable state that is extremely long-lived. Previous work argued that this multi-stripe state is the steady-state of a square system. The multi-stripe configurations lasted for the length of our simulations.

The approach to the non-equilibrium steady states was studied and characterized using the KLS model in sub-critical, critical and infinite temperature regimes. We showed that simple aging scaling successfully collapses auto-correlation data for the ASEP in one, two and three dimensions. We were able to access the aging scaling regime using much larger system sizes than previous studies. Aging scaling was shown to be an extremely powerful tool. Aging scaling was previously unused for the critical KLS model for numerically confirming long-time critical exponents.

### 6.2 Outlook

For the ASEP model, our Monte Carlo results agreed well with the asymptotics of steady-state scaling functions. For non-stationary aging scaling, our results are very promising for our chosen initial conditions. Our data shows very clean, simple aging scaling for the ASEP in one, two, and three dimensions. There are many other choices for correlated initial
It would be useful to see how well the simple aging scaling form works for different correlated initial conditions. In principle, the scaling exponents should be independent of initial conditions, but the aging scaling time window may not be observable for every initial condition.

For the critical KLS model, a convincing direct measurement of the order parameter exponent $\beta$ is still lacking. For the many reasons discussed in chapters 2 and 5, a direct measurement is difficult in simulations. A more careful finite-size scaling analysis of the auto-correlation function using more system sizes would yield more convincing proof of the finite-size scaling at the critical point. The difficulty lies in obtaining accurate approximations of the finite-size critical temperatures. The steady-state asymptotic limit for the density-density auto-correlation function was unobtainable in the Monte Carlo simulations presented here. The long-time exponent of the steady-state auto-correlation should be the same as our aging exponent $\zeta$, as it was with the ASEP.

A clear understanding of the sub-critical regime of the KLS model is still lacking. We present qualitative arguments about the steady states at sub-critical temperatures. Aging scaling during sub-critical quenches would need to be investigated further. We attempted to collapse auto-correlation data using simple aging scaling but did not achieve scaling. Scaling the auto-correlation function using time-dependent domain sizes was unsuccessful at providing data collapse. This was only attempted for a few select temperatures. A more comprehensive study of many sub-critical temperatures may find a temperature range where scaling is achievable. Using anisotropic systems, like the one shown in Fig. 5.11, would allow a study of the evolution from a random initial state to the single stripe state without the long-lived multi-stripe meta-stable states. Square systems at sub-critical temperatures would be an interesting topic for further study. One could measure the size distribution of the stripes in the multi-stripe phase as a function of temperature and system size. Studying a range of lattice anisotropies could determine at what lattice anisotropy the system transitions from a multi-stripe to a single stripe steady-state.
Bibliography


Appendix A

Numerical determination of $T_C$ for finite systems

In this appendix we present the data used to generate the numerical estimates of $T_C(L_{\perp}, L_{\parallel})$. Each data set is fit with a parabola

$$f(T) = -A \left( T - T_C(L_{\perp}, L_{\parallel}) \right)^2 + B,$$

where $T_C(L_{\perp}, L_{\parallel})$, $A$ and $B$ are fit parameters. This is the same method used by Wang [72] to determine the critical temperatures. The estimates of the critical temperatures along with their errors are in table 5.1.

Figure A.1: Susceptibility curve for a $16 \times 16$ lattice with a parabolic fit. Each data point is averaged over 36000 realizations.
Figure A.2: Susceptibility curve for a $54 \times 24$ lattice with a parabolic fit. Each data point is averaged over 9000 realizations.

Figure A.3: Susceptibility curve for a $128 \times 32$ lattice with a parabolic fit. Each data point is averaged over 1000 realizations.
Figure A.4: Susceptibility curve for a $250 \times 40$ lattice with a parabolic fit. Each data point is averaged over 1000 realizations.
Appendix B

Computing resources utilized

In this appendix we will present approximations of the amount of computing resources used for some of our Monte Carlo results. The results presented here were obtained by running our independently developed Monte Carlo simulations. The simulation codes are written in C++ and were developed using emacs as an editor, the g++ (GCC) compiler and the GDB debugger. The majority of the results presented here came from simulations ran on the TBIRD cluster in the Virginia Tech Physics department. The TBIRD cluster has a variety of machines with different speed specifications, with a total of 1060 cores. The most used and powerful machines are:

**Quad-Core AMD Opteron Processor 8382:**
- 4 physical cores, 4 threads per physical core
- 2.6 GHz
- 12 Gb memory

**2× Intel Xeon CPU E5649:**
- 6 physical cores, 2 threads per physical core (two of these in the machine)
- 2.53 GHz
- 24 Gb memory.

**Intel Xeon CPU:**
- 4 physical cores
- 3.20 GHz
- 1 Gb memory

All time estimates presented here are based off of runtimes on TBIRD. I also utilized the TEMPEST cluster in the Virginia Tech Physics department which is comprised of 25 servers with the following specifications:

**Intel Xeon CPU**
- 4 physical cores
- 3.20 GHz
The ANANTHAM cluster from Advanced Research Computing at Virginia Tech was used for shorter simulations. ANANTHAM consists of 53 nodes with the specifications:

**AMD Opteron Processor 240**
- 2 physical cores
- 1.4 GHz
- 1 Gb memory.

Simulations of the ASEP model were relatively cheap compared to the KLS model. We will provide the resources used for a few data sets. The data presented in this dissertation are a subset of all the data. There are many more simulations that did not give presentable results due to incorrect parameter choices, e.g. small system sizes, temperature, number of realizations etc.

We present a table below of selected figures to give estimates of resources used in specific simulations. A dash means the amount was small enough to ignore. The “Time” is the average runtime, the “Cores” is the number of cores that were ran for that “Time” to generate the data in the figure. Similarly, “Memory” is the amount of memory used for each “Core.”

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