MIT 8.334 Final Project:
Density Profiles Near Critical Points in 1D Out-of-Equilibrium Systems

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Several 1D lattice models have become hallmarks for the study of non-equilibrium critical phenomena. One well-known example of such a system is a branching and annihilating random walk (BARW), which, in addition to equilibrium diffusion, produces offspring particles and annihilates with neighboring particles. BARWs exhibit an absorbing state phase transition for some branching rate below which the system enters an inescapable inert state. In this project, I study a BARW with biased motion and particles injected at a constant rate from the left boundary. The system therefore resembles another important non-equilibrium 1D system, an asymmetric simple exclusion process (ASEP), which is known to exhibit boundary-induced phase transitions in which the phase of the system is determined entirely by the rate of particle injection and removal rather than the the dynamics within the bulk. The biased and open-boundary BARW studied here is found to be dominated by bulk dynamics and therefore exhibits no boundary-induced phase transition. As such, it maintains the same critical point as the standard BARW. For branching rates near but below the absorbing state critical point, the system's density profile exhibits a power-law (rather than exponential) decay toward 0.

I. INTRODUCTION

Many out-of-equilibrium systems are known to exhibit critical phenomena with scaling laws similar to those observed in equilibrium systems. Crucially, however, these phase transitions are caused by explicitly non-equilibrium processes and therefore have no equilibrium equivalents.

Even simple 1-dimensional lattice models can demonstrate a rich variety of critical phenomena and therefore serve as tractable starting points for the study of non-equilibrium phase transitions more generally. For instance, branching and annihilating random walks (BARWs) [1, 2] are non-equilibrium extensions of simple diffusive random walks with the additional ability to produce "offspring" particles and annihilate with neighboring particles. These systems are often used to model simple chemical reaction networks such as

$$\begin{aligned} A + A &\to 0 \\ A &\to 2A \end{aligned} \tag{1}$$

where here 0 denotes an "inert" species. BARWs are well studied and have been shown to exhibit absorption state phase transitions [3], in which the system converges to an inescapable state consisting only of inert particles.

Another example of a fundamentally non-equilibrium phase transition is observed in open-boundary asymmetric simple exclusion processes (ASEPs) [4, 5]. ASEPs model random walks undergoing simple diffusion subject to an external drift, resulting in a random walk that undergoes biased hopping in one direction. Additionally, in open-boundary ASEPs, particles are injected into the system from a left reservoir of density ρ_L, corresponding to an injection rate $\alpha = \rho_L$; after diffusing the length of the system, particles exit into a second reservoir of density ρ_R, corresponding to a removal rate $\beta = 1 - \rho_R$. The

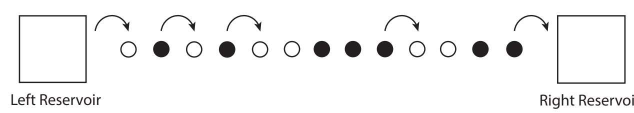

FIG. 1. Scematic of a TASEP. Arrows indicate eligible moves that can be made by particles within the system. Particles diffuse to the left at rate 1, jump into the system from the left reservoir at rate α, and jump out of the system into the right reservoir at rate β.

process is illustrated in figure 1. This system exhibits boundary-induced phase transitions, wherein the properties of the bulk are determined entirely by the state of the right and left reservoirs, rather than by the diffusive dynamics within the bulk of the system itself. I will limit my focus to Total ASEPs (TASEPs), which hop to the right with probability 1 and to the left with probability 0; I will further limit the study to the case $\rho_R = 0$, such that $\beta = 1$.

I first provide an overview of the critical phenomena observed in these two systems. I review each system in the mean-field limit, which provides a qualitative view of the critical phenomena in each of the systems, before refining the critical point locations and scaling behaviors of each using rejection-free kinetic Monte Carlo simulations. I then consider a system that combines properties of both BARWs and TASEPs. Specifically, I consider a BARW following the reaction network in eq. (1), but with totally biased motion, in addition to particle injection and removal, according to the above TASEP setup. The result is a system that exhibits a continuous phase transition at the same critical point for which an absorbing state appears in the BARW. However, because of the constant injection of particles into the system, what is observed is neither an absorbing state nor a boundary-induced phase transition. Rather, for a given branching rate, the density profile of the system converges to the average density of the standard BARW with the same branching rate. Its convergence to this average density is exponential far from the critical point. However, close to the critical point, where the correlation length of the system diverges, I instead observe power-law convergence.

The report is structured as follows: in the next section, I review the properties of the absorbing state phase transition in the BARW mentioned above. Then, in section 3, I discuss the boundary-induced phase transition observed in TASEPs. I then discuss the critical phenomena and density profiles of the proposed open-boundary and biased BARW in section 4, and I show that it exhibits power law decay toward the average BARW density near the absorbing state critical point.

II. ABSORBING STATE PHASE TRANSITIONS IN BRANCHING AND ANNIHILATING RANDOM WALKS

In a BARW diffusing and interacting via the reaction network proposed in eq. (1), a particle can either a) hop along the integer lattice, or b) produce an offsping particle, which is placed either to its left or to its right, chosen randomly. Either of these processes can lead a particle to annihilate with neighboring particles. In the mean-field limit, the assumption is made that the density profile of the system is uniform, $\rho(\mathbf{x}, t) = \rho(t)$, and thus spatial gradients (diffusion terms) can be ignored. The mean-field dynamics for the density of particles in a BARW in the continuum limit are then governed by [6]

$$\frac{d\rho}{dt} = \sigma\rho - 2\lambda\rho^2 \tag{2}$$

where σ is the branching rate and λ is the annihilation rate. The steady state solution to this ODE is obtained by setting $\partial_t \rho = 0$, in which case for $\sigma > 0$,

$$\rho(t \to \infty) = \frac{2\lambda}{\sigma} \tag{3}$$

which implies that in the mean-field limit, the system will always be in the active phase ($\rho > 0$). Returning to eq. (2) and setting $\sigma = 0$ (no branching), we find that the steady-state solution is $\rho(t \to \infty) = 0$, which corresponds to the absorbing state in which annihilation is the dominant interaction and drives the system to an inert state.

The mean-field theory is sufficient for a qualitative understanding of the phases that can emerge in the 1D system. However, it only provides correct quantitative predictions for dimensions $d > d_c = 2$. In the case of $d = 1$, it has been shown that fluctuations are sufficiently large that even for a range of non-zero branching rates, $0 < \sigma < \sigma_c$, the annihilation processes in the system are sufficient to produce an absorbing steady-state [1].

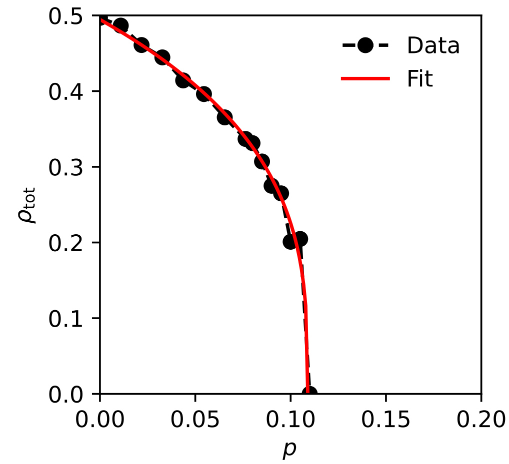

FIG. 2. BARW steady-state density as a function of diffusion probability p (where branching then has probability $1 - p$). The system undergoes a phase transition into an absorbing state at $p_c \approx 0.109$.

This result is confirmed in numerical simulations. I perform a rejection-free kinetic Monte Carlo simulation in which particles diffuse with rate $\Gamma_D = 1$ and branch with rate Γ_B. As a result, for each time step, a particle diffuses or branches with probability p and $1 - p$, respectively, where

$$p = \frac{\Gamma_D}{\Gamma_D + \Gamma_B} \tag{4}$$

Shown in figure (2) are the simulation results for the average steady-state density of a BARW with periodic boundary conditions as a function of diffusion probability p. From fits to the simulation data, the absorbing state phase transition occurs at $p_c \approx 0.109$, and converges to $\rho = 0$ with a scaling of

$$\rho \sim (p_c - p)^{\beta}, \qquad \beta \approx 0.314 \tag{5}$$

The result agrees with other numerical work [7]. It has been shown using tools from Doi-Peliti field theory [8] that a BARW that produces a single offspring particle belongs to the directed percolation (DP) universality class [2, 9], from which we expect $\beta \approx 0.277$, in relatively good agreement with the above simulation results.

III. BOUNDARY-INDUCED PHASE TRANSITIONS IN ASYMMETRIC SIMPLE EXCLUSION PROCESSES

In this section, I discuss the emergence of boundary-induced phase transitions in TASEPs [4, 5]. For simplicity, I consider the case where $\rho_R = 0$ ($\beta = 1$), and study the density profiles in the bulk of the system for different injection rates of $\alpha = \rho_L$.

In the TASEP, particles can jump to lattice site i on the condition that it is not already occupied, and out of site i on the condition that site $i+1$ is not occupied. In the mean-field limit, site i has probability ρ_i of being occupied (and therefore a probability $1-\rho_i$ of being vacant), where ρ_i is the site's ensemble-averaged density. The mean-field equation governing the dynamics of the density profile ρ_i at site i is therefore

$$\frac{\partial \rho_i}{\partial t} = \rho_{i-1}(1-\rho_i) - \rho_i(1-\rho_{i+1}) \tag{6}$$

The continuum limit is the continuity equation

$$\frac{\partial \rho}{\partial t} + a\frac{\partial J}{\partial x} = 0 \tag{7}$$

where a is the lattice spacing and the current is given by

$$J = j_0(\rho) - D\frac{\partial \rho}{\partial x} \tag{8}$$

where $j_0(\rho) = \rho(\rho-1)$ and $D = a/2$. In the steady state, J is a constant and has been shown to take on the value $J = j_0(\rho^*)$, where ρ^* is the value of the density that maximizes $j_0(\rho)$ over the interval $\rho \in [0, \alpha]$ [4], and is therefore given by

$$\rho^* = \min\left(\alpha, \frac{1}{2}\right) \tag{9}$$

The system undergoes a continuous phase transition at $\alpha = 1/2$, at which point it reaches a maximal current $J = 1/4$.

The mean-field theory captures the correct bulk density in each regime (it can be shown that the upper critical dimension is $d_c = 2$ for this system as well [4]). To obtain accurate density profiles near the boundary of the system, I again perform a rejection-free kinetic Monte Carlo simulation: particles are inserted stochastically with rate α at the first lattice site, hop between bulk lattice sites at rate 1, and exit via the last lattice site with rate $\beta = 1$. The resulting steady-state density profiles are shown in figure (3) and agree with the analytic profiles derived in [10]. These computations reveal specific behaviors for the density profile near the boundaries, showing that for $\alpha < 1/2$, the density profile converges to ρ^* exponentially, while for $\alpha > 1/2$, it converges as a power law. The phase transition is characterized by the divergence of the correlation length [10]

$$\xi^{-1} = -\log\left(4\alpha(1-\alpha)\right) \tag{10}$$

The numerically computed density profile for each regime is shown in figure 3.

Note that the bulk behavior of the density profile is entirely determined by the rates at which particles are entering the system and not on the diffusive dynamics within the bulk itself. It is this property that makes the observed phase transition unique to non-equilibrium systems.

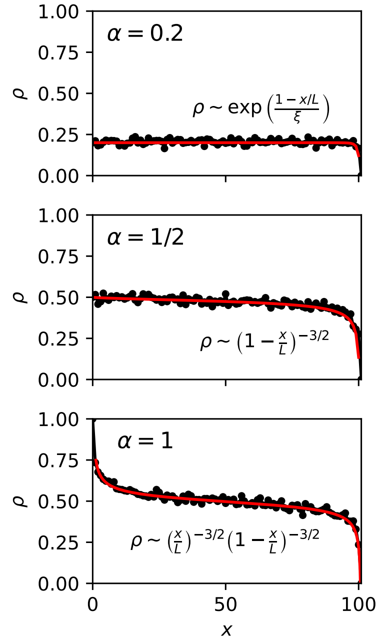

FIG. 3. The numerically computed density profiles for systems in the regions $\alpha < 1/2$ (top), which converges exponentially to its bulk density; $\alpha = 1/2$ (middle), which converges as a power law; and $\alpha > 1/2$ (bottom), which converges as a power law as well. Analytic profiles are shown in red and derived in [10].

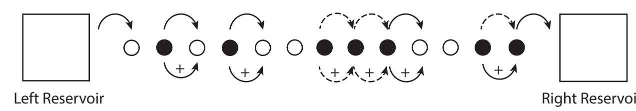

FIG. 4. Schematic for the process considered in section 4. Top arrows indicate hopping to the right, while bottom arrows with a plus sign indicate branching, with the placement of an additional offspring particle to the right. Dashed arrows indicate moves that would result in annihilation between the particle currently at lattice site i and the new particle being place there.

IV. ASEPS WITH BRANCHING AND ANNIHILATION

I now consider a system that combines the above two processes. In particular, I consider a 1D BARW with the same reaction network as in section 2 (eq. (1)). Additionally, the system is connected to a left reservoir of particles with density ρ_L from which particles diffuse into the system at rate α and a right reservoir with density 0 via which particles leave the system at rate $\beta = 1$. A schematic of the system is shown in figure (4).

We find that branching and annihilation processes in the system supersede the boundary-induced effects, and the bulk density in the system is set by the BARW density in figure (2). In particular, the density profile is

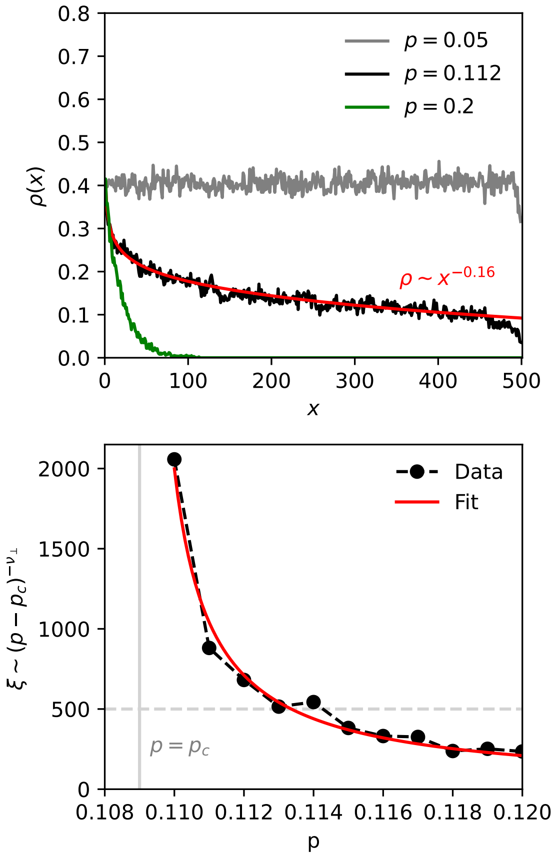

FIG. 5. (*Top*) Density profiles for a range of p values, where p denotes the probability of diffusion vs branching for a particle, as defined in eq. (4). The qualitative behavior of the density profiles can be divided into region $p < p_c$ and $p > p_c$, where p_c is the same critical point as found in the standard BARW problem. The density profiles converge to their bulk values (which are the same as those expected for a given p in figure (2)). Far from $p = p_c$ (gray and green curves), this convergence is exponential; near $p = p_c$ (black curve), the convergence is power law, indicating the divergence of the system's correlation length. (*Bottom*) The correlation length for values of p close to the critical point. The correlation length diverges as $\xi \sim (p - p_c)^{-\nu_\perp}$, where the fit to the data suggests $\nu_\perp \approx 0.94$. The dashed gray line indicates the system size, beyond which estimates of ξ are less reliable.

independent of the injection rate α, and depends only on the diffusion/branching rates. Figure (5) shows density profiles for systems on each side of the critical point $p = p_c \approx 0.109$. For $p < p_c$, the bulk of the density profile converges to its BARW value shown in the top panel of figure (2); for $p > p_c$ (the absorbing state), the bulk converges to 0, as expected. The injection rate α affects the density profile only transiently for $p < p_c$, quickly settling into its bulk density; moreover, the density profiles decay exponentially for $p \gg p_c$. However, as the critical point is approached, the correlation length diverges, and the density profile exhibits a power law decay to the bulk density as $p \to p_c$.

Because the bulk converges to the steady-state density of the BARW with the same p, figure (2) also applies to the system described here, and it can be conjectured that the system remains in the DP universality class despite non-equilibrium boundary effects. For additional evidence of this, a fit of the density profile to the form $\rho(x) \sim (p - p_c)^{-\nu_\perp}$ for various values of p (see the bottom panel of Figure (5)) yields an estimate for the correlation length critical exponent of

$$\nu_\perp \approx 0.94 \tag{11}$$

which is again in relatively good agreement with the DP universality class exponent of $\nu_\perp \approx 1.096$ [11].

The phases of the system are therefore dominated by the bulk behavior, rather than by the boundary conditions, as in standard TASEPs. The result is a system that has neither an absorbing state phase transition (which is by definition destroyed because of the constant injection of particles into the system) nor a boundary-induced phase transition, but nonetheless maintains the critical point and scaling behaviors of the DP universality class and exhibits power-law decay toward its bulk density near the absorbing state critical point.

V. DISCUSSION

In this project, I considered the density profiles of non-equilibrium 1D lattice systems near their critical points. Several of systems—branching and annihilating random walks (BARWs) and totally asymmetric simple exclusion processes (TASEPs)—are well studied in the literature. These are two scenarios in which non-equilibrium processes lead to unique behaviors in the systems' density profiles. Inspired by these two systems, I considered a BARW that undergoes the same external forcing as a TASEP. I found that the critical point is the same as that of the unbiased and periodic BARW and leads to power-law density profiles near this critical point. This study can be immediately extended in several ways. First, I considered only the simplest implementation of both the BARW and the TASEP. However, it is known that BARWs exhibit different critical behaviors depending on whether an even or odd number of offspring are considered [12]. Furthermore, increasingly complex multi-species BARWs can be considered that could reveal novel critical phenomena [13]. It is also known that ASEPs have a rich phase diagram when, in addition to the injection rate α, the removal rate β is also allowed to vary [5, 10].

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