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Theoretical investigation of totally asymmetric exclusion processes on lattices with junctions

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Abstract. Totally asymmetric simple exclusion processes on lattices with junctions, where particles interact with hard core exclusion and move on parallel lattice branches that at the junction combine into a single lattice segment, are investigated. A simple approximate theory, that treats the correlations around the junction position in a mean-field fashion, is developed in order to calculate stationary particle currents, density profiles and a phase diagram. It is shown that there are three possible stationary phases depending on the state of each of the lattice branches. At first-order phase boundaries, where the density correlations are important, a modified phenomenological domain wall theory, that accounts for correlations, is introduced. Extensive Monte Carlo computer simulations are performed to investigate the system, and it is found that they are in excellent agreement with theoretical predictions. The application of the theoretical method for other inhomogeneous asymmetric simple exclusion processes is outlined.

Keywords: driven diffusive systems (theory), stochastic particle dynamics (theory), molecular motors (theory)

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Contents

1. Introduction

Asymmetric simple exclusion processes (ASEPs) were introduced originally in 1968 as theoretical models for a description of the kinetics of biopolymerization [1]. Although in recent years the area of application of ASEPs has been significantly broadened [2]–[4], and it now includes road traffic flow analysis [5, 6], polymer dynamics in dense media [7] and many other problems, the major application of ASEPs remains the modelling of various biophysical transport phenomena. In particular, simple exclusion processes have been used successfully to describe protein synthesis [8, 9], mRNA translation phenomena [10], gel electrophoresis [11], motion of motor proteins along the cytoskeletal filaments [12] and the depolymerization of microtubules by special enzymes [13].

ASEPs are discrete non-equilibrium models that describe the stochastic dynamics of multi-particle transport along one-dimensional lattices. The lattices are finite and generally consist of $L \gg 1$ sites. Each site can be occupied by a single particle or be empty, and the particles interact only through the hard core exclusion potential. The dynamics of an ASEP is asymmetric, i.e., the particles can hop to the left or to the right but with different probabilities. In the simplest totally asymmetric simple exclusion process (TASEP) the particles move only in one direction. In this case the rules for the motion are the following. The particle at site $1 \leq i < L$ can move one step forward if the site $i + 1$ is empty. The particle can enter the lattice at the rate α if the first site is available, and it can leave the system from the last site $i = L$ at the rate β. In the stationary-state limit of the TASEP, the system can be found in one of three phases depending on whether entrance, exit or bulk processes dominate the overall dynamics.

The unusual dynamic properties and phase behaviour of ASEPs and a wide range of applications in chemistry, physics and biology have stimulated many theoretical studies of asymmetric exclusion processes [2]–[4]. There are several exact results for the steady-state properties of ASEPs for different update rules [3, 4], although most theoretical investigations utilize the approximate methods along with Monte Carlo computer simulations [8, 9, 14, 15]. The coupling of several exclusion processes has been considered in

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the study of parallel-chain ASEPs [16]–[18]. The combining of non-equilibrium exclusion processes with equilibrium particle association/dissociation phenomena led to unusual phenomena of localizations of density shocks [19]–[23]. However, despite the differences in specific dynamic rules and stationary properties of a specific ASEP, the microscopic origin of the unusual dynamic properties and phase behaviour can be well understood with the help of a phenomenological domain wall theory [24, 4].

The majority of the asymmetric exclusion processes investigated involve particle movement along the one-channel lattices. Although the one-channel approach describes many situations in biophysical processes, a more realistic description of cellular transport requires an extension of the original ASEP to include the possibility of transport on lattices with a more complex geometry. For example, consider the motor protein kinesins that move vesicles and organelles along the microtubules and play an important role in cellular transport [25, 12]. Microtubules are made of parallel linear polymers, called protofilaments, that are arranged circumferentially. It is known that kinesins walk only on single protofilaments. However, experiments [26] indicate that the number of protofilaments may vary, at least for *in vitro* conditions, and this indicates the existence of junctions and other lattice defects. Such defects might lead to motor protein crowding phenomena that are responsible for many human diseases [27]. These observations suggest the importance of investigation of the asymmetric exclusion processes on lattices with junctions as a model for these complex biological transport phenomena.

Recently Brankov *et al* [28] have investigated TASEP on chains with a double-chain section in the middle by using an approximate theory and computer simulations. This corresponds to having two consecutive junctions on the lattice. Several stationary phases, the existence of which had not been expected, are found. In addition, the density profiles at phase boundaries and strong correlations between different lattice branches have been observed, but this could not be explained because the theory neglected the correlations. In this paper, we present a theoretical investigation of a TASEP on a lattice with one junction. We develop a simple approximate theory that allows us to calculate particle currents, density profiles and a phase diagram at large times. At first-order phase boundaries, an extension of the domain wall theory [24] that accounts for correlations is developed. This approach is then applied in explicit calculations of density profiles. The theoretical predictions are compared with extensive Monte Carlo computer simulations. In addition, we briefly discuss the application of our method for TASEPs with two consecutive junctions [28].

The paper is organized as follows. In section 2 the model is introduced and theoretical calculations of stationary properties are presented. In section 3 theoretical predictions are discussed and compared with the results of Monte Carlo computer simulations. A final summary and conclusions are given in section 4.

2. Theoretical description

2.1. Model

We consider identical particles that move along the lattice with the junction positioned in the middle of the system, as shown in figure 1. The system is out of equilibrium, and it has three equal-size branches, each containing L sites. The particles can enter chain I

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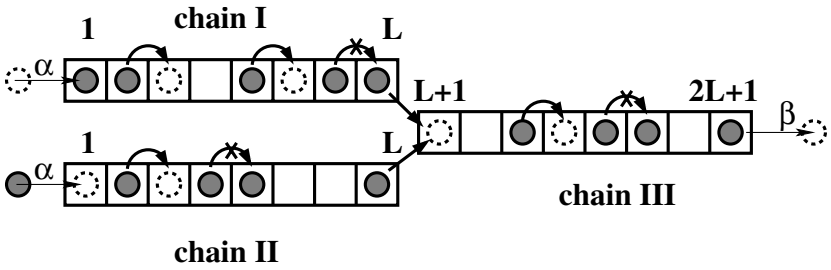

Figure 1. Schematic picture of the model for a TASEP on a lattice with a junction. Particles can enter chain I or chain II at the rate α. At the site $L+1$ two lattice branches coalesce into chain III, from which particles can exit at the rate β. Arrows indicate the allowed transitions, while crossed arrows correspond to the prohibited moves.

or chain II at the rate α if the first site at the corresponding branch is available. Two chains merge together at site $L+1$ and form chain III. The particle can leave the system at the rate β; see figure 1. Inside the lattice chains the particle can only move one step forward if the neighbouring site is empty.

Without chain I or chain II, the junction disappears and the system reduces to a totally asymmetric simple exclusion process on a one-channel lattice, for which the full description of the stationary properties, such as the phase diagram, particle currents and density profiles, is known [2]–[4]. This simplest model of a TASEP on a lattice without junctions has three stationary phases. When the entrance into the system is a rate-limiting process, for $\alpha < 1/2$ and $\alpha < \beta$, the system is found in a low density (LD) phase with the current and bulk density given by

$$J_{\mathrm{LD}} = \alpha(1-\alpha), \qquad \rho_{\mathrm{bulk,LD}} = \alpha. \tag{1}$$

If the exit controls the dynamics of the system, for $\beta < 1/2$ and $\beta < \alpha$, the stable stationary state for the system is a high density (HD) phase with the following current and bulk density:

$$J_{\mathrm{HD}} = \beta(1-\beta), \qquad \rho_{\mathrm{bulk,HD}} = 1-\beta. \tag{2}$$

Finally, for large entrance and exit rates ($\alpha > 1/2$ and $\beta > 1/2$), when the dynamics is determined by bulk processes, the system is in a maximal current (MC) phase with

$$J_{\mathrm{MC}} = 1/4, \qquad \rho_{\mathrm{bulk,MC}} = 1/2. \tag{3}$$

Full density profiles for systems of any size can be calculated explicitly [2].

The microscopic origin of the complex phase behaviour and unusual dynamic properties of asymmetric exclusion processes can be explained via a phenomenological domain wall (DW) theory [24]. According to this approach, the domain wall is the boundary region between two possible stationary phases, and it moves through the system as a random walker with a speed determined by the currents and densities in the two phases:

$$v_{\mathrm{DW}} = u_+ - u_- = \frac{J_+ - J_-}{\rho_+ - \rho_-}, \tag{4}$$

where '+' ('−') corresponds to the phase to the right (left) of the domain wall, and u_+ and u_- give the domain wall rates for hopping to the right or left. For $v_{\rm DW} > 0$ ($u_+ > u_-$) the domain wall moves to the right and the 'negative' phase becomes a stationary state of the system, while for $v_{\rm DW} < 0$ ($u_+ < u_-$) the domain wall travels to the left and the 'positive' phase wins over. On the phase boundaries the domain wall has equal probability of going forward or backward, i.e., $u_+ = u_-$ and $v_{\rm DW} = 0$. As a result, the density profiles are linear. This is due to the fact that the domain wall can be found with equal probability at any position in the system.

2.2. Theoretical calculations for stationary phases

The overall state of the system is specified by the nature of phases that might exist in each of the lattice branches. Since only three stationary phases can be found in each lattice chain (HD, LD or MC), the total number of possible stationary phases in the system with the junction is equal to $3^3 = 27$. However, because of the symmetry, chains I and II should have identical phases (see figure 1), and the overall state of the system is determined by phases in chain I (or II) and chain III. Then the number of possible stationary states reduces to just $3^2 = 9$.

The overall stationary current passing through the system can be written as

$$J_{\rm overall} = J_{\rm III} = J_{\rm I} + J_{\rm II} = 2J_{\rm I}. \tag{5}$$

This suggests that chains I and II cannot have the maximal current phase with $J = 1/4$, because the maximal possible current through the system is just equal to 1/4. Thus, there are only six possible stationary phases: (LD, LD), (LD, HD), (LD, MC), (HD, LD), (HD, HD) and (HD, MC), where, in the expression (A, B), A describes the phase in chains I and II, while B corresponds to the phase in chain III.

The junction introduces an inhomogeneity in the system and it makes it impossible to solve the large time dynamics exactly [14, 29]. However, the TASEP on the lattice with a junction can be mapped onto three coupled homogeneous asymmetric exclusion processes as shown in figure 2, for which an approximate description can be developed [14, 29]. In order to obtain the dynamic properties of the system explicitly, in the simplest approximation, we assume that there are no correlations of the occupations of the sites before and after the junction, i.e.,

$$J_{\rm overall} = 2J_{\rm junction} = 2\langle\tau_L(1-\tau_{L+1})\rangle \approx 2\langle\tau_L\rangle(1-\langle\tau_{L+1}\rangle), \tag{6}$$

where $\langle\tau_L\rangle = \rho_L$ is the probability of occupation of site L on chain I or II, and $\langle\tau_{L+1}\rangle = \rho_{L+1}$ is the average particle density at the site $L+1$ of chain III. The effective rates $\alpha_{\rm eff}$ and $\beta_{\rm eff}$ (see figure 2) can be expressed in terms of the particle densities at the sites near the junction,

$$\alpha_{\rm eff} = 2\rho_L, \qquad \beta_{\rm eff} = 1 - \rho_{L+1}. \tag{7}$$

Now we can investigate the existence of different stationary phases. Consider first the (LD, LD) phase, which can be specified by the following conditions:

$$\alpha < 1/2, \qquad \alpha < \beta_{\rm eff}; \qquad \alpha_{\rm eff} < 1/2, \qquad \alpha_{\rm eff} < \beta. \tag{8}$$

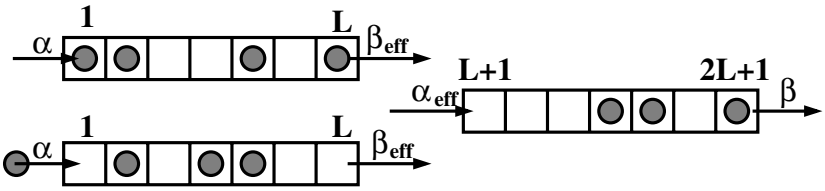

Figure 2. The totally asymmetric simple exclusion process on the lattice with the junction can be mapped onto three homogeneous TASEPs coupled at the ends. The effective rate $\beta_{\rm eff}$ describes the process of exiting from chains I or II, while the effective rate $\alpha_{\rm eff}$ corresponds to the entrance into chain III.

The stationary currents and bulk densities are given by

$$J_{\rm I} = \alpha(1-\alpha), \qquad \rho_{\rm I,bulk} = \alpha, \qquad J_{\rm III} = \alpha_{\rm eff}(1-\alpha_{\rm eff}), \qquad \rho_{\rm III,bulk} = \alpha_{\rm eff}. \tag{9}$$

Using the expression (5) for currents, the effective rate $\alpha_{\rm eff}$ can be expressed in terms of the entrance rate α:

$$\alpha_{\rm eff} = \frac{1-\sqrt{1-8\alpha(1-\alpha)}}{2}. \tag{10}$$

Thus $\alpha_{\rm eff}$ always satisfies the conditions (8); however, this equation yields physically reasonable values of the effective entrance rate only when the term in the square root is positive, i.e.,

$$\alpha < \frac{1}{2} - \frac{\sqrt{2}}{4} \approx 0.146. \tag{11}$$

Because $\rho_{L+1} = \alpha_{\rm eff}$ in the (LD, LD) phase, the effective exit rate, as follows from equation (7), is given by $\beta_{\rm eff} = 1 - \alpha_{\rm eff}$. Then the condition $\alpha < \beta_{\rm eff}$ holds for all values of the parameters. Thus the system is in the (LD, LD) phase when

$$\beta > \frac{1-\sqrt{1-8\alpha(1-\alpha)}}{2} \qquad \text{and} \qquad \alpha < \frac{1}{2} - \frac{\sqrt{2}}{4}. \tag{12}$$

For the (LD, HD) phase the conditions of existence can be written as

$$\alpha < 1/2, \qquad \alpha < \beta_{\rm eff}; \qquad \beta < 1/2, \qquad \beta < \alpha_{\rm eff}; \tag{13}$$

while the stationary currents and bulk densities are

$$J_{\rm I} = \alpha(1-\alpha), \qquad \rho_{\rm I,bulk} = \alpha, \qquad J_{\rm III} = \beta(1-\beta), \qquad \rho_{\rm III,bulk} = 1-\beta. \tag{14}$$

Because the particle current is stationary, equation (5) implies that

$$\beta = \frac{1-\sqrt{1-8\alpha(1-\alpha)}}{2}, \qquad \text{and} \qquad \alpha < \frac{1}{2} - \frac{\sqrt{2}}{4}. \tag{15}$$

These expressions describe the parameter's space for the (LD, HD) phase.

Similar analysis can be performed for the (LD, MC) phase. The allowed parameters for this phase are specified by

$$\alpha < 1/2, \qquad \alpha < \beta_{\rm eff}; \qquad \alpha_{\rm eff} > 1/2, \qquad \beta > 1/2. \tag{16}$$

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The currents and bulk densities have the following values:

$$J_{\mathrm{I}} = \alpha(1-\alpha), \qquad \rho_{\mathrm{I,bulk}} = \alpha, \qquad J_{\mathrm{III}} = 1/4, \qquad \rho_{\mathrm{III,bulk}} = 1/2. \tag{17}$$

Then the currents in chains I and II are $J_{\mathrm{I}} = J_{\mathrm{II}} = 1/8$, which implies that

$$\alpha = \frac{1}{2} - \frac{\sqrt{2}}{4}. \tag{18}$$

This equation along with the condition $\beta > 1/2$ fully determines the region of existence of the (LD, MC) phase.

The situation is very different for the (HD, LD) phase for which

$$\beta_{\mathrm{eff}} < 1/2, \qquad \alpha > \beta_{\mathrm{eff}}; \qquad \alpha_{\mathrm{eff}} < 1/2, \qquad \alpha_{\mathrm{eff}} < \beta. \tag{19}$$

The corresponding equations for the currents and bulk densities are

$$J_{\mathrm{I}} = \beta_{\mathrm{eff}}(1-\beta_{\mathrm{eff}}), \qquad \rho_{\mathrm{I,bulk}} = 1-\beta_{\mathrm{eff}}, \qquad J_{\mathrm{III}} = \alpha_{\mathrm{eff}}(1-\alpha_{\mathrm{eff}}), \qquad \rho_{\mathrm{III,bulk}} = \alpha_{\mathrm{eff}}. \tag{20}$$

It is known that in this phase $\rho_L = 1-\beta_{\mathrm{eff}}$ and $\rho_{L+1} = \alpha_{\mathrm{eff}}$. Then, from equation (7) it can be shown that

$$\alpha_{\mathrm{eff}} = 2(1-\beta_{\mathrm{eff}}), \qquad \text{and} \qquad \beta_{\mathrm{eff}} = 1-\alpha_{\mathrm{eff}}. \tag{21}$$

However, these two equations have no real solutions together, and therefore the (HD, LD) phase cannot exist for any value of the entrance rate α and the exit rate β.

The (HD, HD) phase is determined from the conditions

$$\beta_{\mathrm{eff}} < 1/2, \qquad \beta_{\mathrm{eff}} < \alpha; \qquad \beta < 1/2, \qquad \beta < \alpha_{\mathrm{eff}}; \tag{22}$$

The stationary properties of this phase are given by

$$J_{\mathrm{I}} = \beta_{\mathrm{eff}}(1-\beta_{\mathrm{eff}}), \qquad \rho_{\mathrm{I,bulk}} = 1-\beta_{\mathrm{eff}}, \qquad J_{\mathrm{III}} = \beta(1-\beta), \qquad \rho_{\mathrm{III,bulk}} = 1-\beta. \tag{23}$$

The stationary condition for the particle currents (see equation (5)) helps to determine the effective exit rate constant:

$$\beta_{\mathrm{eff}} = \frac{1-\sqrt{1-2\beta(1-\beta)}}{2}. \tag{24}$$

After combining this result with the set of phase existence requirements (22) we obtain the final conditions for the (HD, HD) phase:

$$\beta < \frac{1}{2}, \qquad \text{if } \alpha > \frac{1-\sqrt{1-2\beta(1-\beta)}}{2}. \tag{25}$$

The last possible phase in the system is the (HD, MC) phase, which is specified by the following conditions:

$$\beta_{\mathrm{eff}} < 1/2, \qquad \beta_{\mathrm{eff}} < \alpha; \qquad \beta > 1/2, \qquad \alpha_{\mathrm{eff}} > 1/2. \tag{26}$$

The particle currents and bulk densities in this phase are given by

$$J_{\mathrm{I}} = \beta_{\mathrm{eff}}(1-\beta_{\mathrm{eff}}), \qquad \rho_{\mathrm{I,bulk}} = 1-\beta_{\mathrm{eff}}, \qquad J_{\mathrm{III}} = 1/4, \qquad \rho_{\mathrm{III,bulk}} = 1/2. \tag{27}$$

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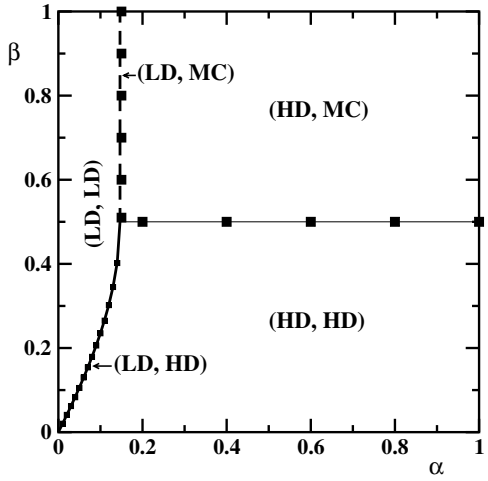

Figure 3. Phase diagram for the totally asymmetric exclusion system on the lattice with the junction. Lines are calculated from theoretical predictions for phase boundaries, while symbols are from Monte Carlo computer simulations. The thick solid line corresponds to a non-equilibrium first-order phase transition between the (LD, LD) and (HD, HD) phases. The thin solid line shows a continuous phase transition between the (HD, HD) and (HD, MC) phases. Meanwhile, the thick dashed line describes a mixed phase transition between the (LD, LD) and (HD, MC) phases: a first-order transformation in chains I and II, and the continuous phase transition in chain III. The sizes of the symbols reflect the statistical error of the computer simulations.

From equation (5) it can be easily shown that

$$\beta_{\text{eff}} = \frac{1}{2} - \frac{\sqrt{2}}{4}. \tag{28}$$

Comparing this result with the conditions (26), we finally derive

$$\alpha > \frac{1}{2} - \frac{\sqrt{2}}{4}, \qquad \text{and} \qquad \beta > \frac{1}{2}. \tag{29}$$

These expressions describe the phase space for the (HD, MC) phase.

Thus the analysis that considers TASEPs on lattices with junctions as coupled asymmetric exclusion systems suggests the existence of five phases. The calculated phase diagram is shown in figure 3. It can be seen that two phases, namely, (LD, MC) and (LD, HD), correspond to stationary phase boundaries. This result is due to the neglect of correlations around the junction point. However, for these conditions, the domain wall that separates two phases can move with equal probability to the right and to the left [24]. Thus the density profiles will be different from the one predicted from the simplest theory, that treats the correlations around the junction in a mean-field manner. The density profile can be expected to be linear in chain I and chain II segments for the (LD, MC) phase, extrapolating between coexisting low density and high density phases, while the density profile in chain III still corresponds to the maximal current phase. For the (LD, HD) phase the linear density profiles can be found in all lattice segments, although the slopes strongly depend on intersegment density correlations.

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2.3. Phase boundaries

The qualitative domain wall arguments presented above indicate that particle density changes linearly for some phase coexistence lines. However, exact linear density profiles might differ significantly from the densities obtained within the simplest approximate theory that neglects the correlations near the junction. Here we utilize the domain wall approach [24] to account for these correlations in order to derive the phase boundary density profiles explicitly.

The line specified by $\alpha = 1/2 - \sqrt{2}/4$ for $\beta > 1/2$ (see figure 3) describes the mixed phase coexistence of (LD, LD) and (HD, MC). When crossing this line, the density jumps in the lattice segments I and II, while the change is continuous in chain III. At the phase boundary the domain wall in chain I or II moves randomly with equal forward and backward rates between the low density ($\rho_{\rm LD} = 1/2 - \sqrt{2}/4$) and high density ($\rho_{\rm HD} = 1 - \beta_{\rm eff} = 1/2 + \sqrt{2}/4$) regions. The domain wall picture cannot be used in lattice chain III when the maximal current phase appears [24], and the intersegment correlations are not significant. Then the resulting density profiles in the left lattice segments are expected to be linear, connecting the low density and high density values.

Determining the density profiles at the phase boundary between the (LD, LD) and (HD, HD) phases is a much more complicated problem because of the strong correlations around the junction. This phase coexistence line is given by the following conditions:

$$\alpha < \frac{1}{2} - \frac{\sqrt{2}}{4}, \qquad \beta = \frac{1 - \sqrt{1 - 8\alpha(1-\alpha)}}{2}, \tag{30}$$

as shown in figure 3. The domain wall separates the coexisting stationary phases and it can be found in any lattice segment. Here we assume that a single domain wall can only be found in the lattice chain III, or two domain walls are at the same time in the segments I and II. Because the lattice chains I and II are identical and the stationary properties of the system are the results of averaging over many positions of the domain wall, only the dynamics of the single domain wall in one of the channels I or II should be monitored. The situation when one domain wall in lattice chain I and/or chain II coexists with the domain wall in the lattice segment III is not stable and it cannot contribute to the stationary properties of the system. In this case, the strong current at the junction quickly eliminates one of the domain walls.

Let us define a position of the domain wall in the system via the relative coordinate x:

$$x = \frac{i}{L}, \tag{31}$$

where i is the site index and L is the length of one lattice segment. Therefore, the case of $0 < x \leq 1$ describes chains I and II, while $1 < x \leq 2$ corresponds to chain III. When the domain wall is in chain I (and simultaneously in chain II) it can move at the same rate $u_{\rm I}$ to the left or to the right, while in chain III it travels forward or backward at the rate $u_{\rm III}$; see figure 4. These rates can be determined by utilizing expression (4):

$$u_k = \frac{J_k}{\rho_+^k - \rho_-^k}, \qquad \text{for } k = \text{I}, \text{III}, \tag{32}$$

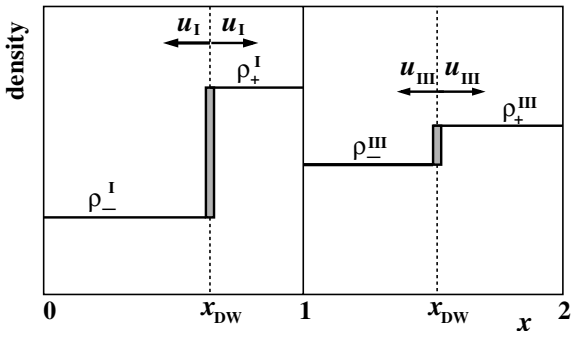

Figure 4. Schematic picture of the domain wall dynamics at the phase coexistence line of the (LD, LD) and (HD, HD) phases. The domain wall in chains I and II hops to the right or left at the rate $u_{\rm I}$, while in chain III it moves at the rate $u_{\rm III}$.

where

$$\rho_-^{\rm I} = \alpha, \qquad \rho_+^{\rm I} = 1-\alpha, \qquad \rho_-^{\rm III} = \beta, \qquad \rho_+^{\rm III} = 1-\beta, \tag{33}$$

and

$$J_{\rm I} = \alpha(1-\alpha), \qquad J_{\rm III} = 2J_{\rm I}. \tag{34}$$

As a result, we obtain the following expressions for the rates $u_{\rm I}$ and $u_{\rm III}$:

$$u_{\rm I} = \frac{\alpha(1-\alpha)}{1-2\alpha}, \tag{35}$$

$$u_{\rm III} = \frac{2\alpha(1-\alpha)}{1-2\beta} = \frac{2\alpha(1-\alpha)}{\sqrt{1-8\alpha(1-\alpha)}}. \tag{36}$$

To calculate the density profiles we introduce a probability $P_{\rm I}$ of finding the domain wall at any position in the chain I or II, and $P_{\rm III}$ gives the probability that the domain wall is in the lattice chain III. These probabilities are obviously normalized:

$$P_{\rm I} + P_{\rm III} = 1. \tag{37}$$

The probability that the domain wall occupies a specific site i is equal to $P_{\rm I}/L$ or $P_{\rm III}/L$ for $i < L$ and $i > L$, respectively. Then, at the junction,

$$u_{\rm I}P_{\rm I}/L = u_{\rm III}P_{\rm III}/L. \tag{38}$$

This relation reflects the fact that the domain wall has equal probabilities of travelling between different lattice segments. By combining the last two equations we obtain

$$P_{\rm I} = \frac{u_{\rm III}}{u_{\rm I}+u_{\rm III}}, \qquad P_{\rm III} = \frac{u_{\rm I}}{u_{\rm I}+u_{\rm III}}. \tag{39}$$

These expressions have a simple physical explanation. The domain wall spends less time in the lattice segments where it fluctuates faster. All lattice chains have the same length L, and the domain wall in the lattice segment where it fluctuates faster is able to diffuse to the junction point quicker. As a result, it will jump to another lattice chain more

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frequently. This is a reason for strong intersegment density correlations at the first-order phase transitions.

We can determine the probabilities of having the domain wall at any position less then a certain value of x. If the domain wall is in channels I and II at the coordinate $x_{\rm DW}$, then this probability is given by

$$\mathrm{Prob}(x_{\rm DW} < x) = P_{\rm I} x, \qquad 0 < x \leq 1, \tag{40}$$

Similarly, for the domain wall in the lattice chain III,

$$\mathrm{Prob}(x_{\rm DW} < x) = P_{\rm I} + P_{\rm III}(x-1), \qquad 1 < x \leq 2. \tag{41}$$

Then the density at any position can be calculated as

$$\rho(x) = \rho_-^k \mathrm{Prob}(x_{\rm DW} > x) + \rho_+^k \mathrm{Prob}(x_{\rm DW} < x), \qquad k = \mathrm{I}, \mathrm{III}. \tag{42}$$

Finally, combining equations (33), (35), (36), (39), (40) and (41), we obtain

$$\rho(x)_{\rm I} = \alpha + \frac{2(1-2\alpha)^2}{2(1-2\alpha) + \sqrt{1-8\alpha(1-\alpha)}} x, \qquad 0 < x \leq 1; \tag{43}$$

and

$$\rho(x)_{\rm III} = \frac{1-\sqrt{1-8\alpha(1-\alpha)}}{2} + \frac{2(1-2\alpha)\sqrt{1-8\alpha(1-\alpha)}}{2(1-2\alpha) + \sqrt{1-8\alpha(1-\alpha)}} + \frac{1-8\alpha(1-\alpha)}{2(1-2\alpha) + \sqrt{1-8\alpha(1-\alpha)}}(x-1), \tag{44}$$

for $1 < x \leq 2$. At the entrance sites we have, as expected, $\rho(x=0)_{\rm I} = \alpha$, while at the last site, $\rho(x=2)_{\rm III} = (1+\sqrt{1-8\alpha(1-\alpha)})/2 = 1-\beta$. At the junction, the densities are equal to

$$\rho(x=1)_{\rm I} = \alpha + \frac{2(1-2\alpha)^2}{2(1-2\alpha) + \sqrt{1-8\alpha(1-\alpha)}},$$
$$\rho(x=1)_{\rm III} = \frac{1-\sqrt{1-8\alpha(1-\alpha)}}{2} + \frac{2(1-2\alpha)\sqrt{1-8\alpha(1-\alpha)}}{2(1-2\alpha) + \sqrt{1-8\alpha(1-\alpha)}}. \tag{45}$$

It is important to note that the densities at the junction are not equal to the values $1-\alpha$ for chains I and II, and $\beta = (1-\sqrt{1-8\alpha(1-\alpha)})/2$ for chain III, respectively, as expected from the simplest approximate theory that assumes an independent coupling between the lattice segments. The domain wall approach allows us to take into consideration the correlations in the densities around the junction.

3. Monte Carlo simulations and discussion

In order to check the validity of our approximate theory we performed extensive computer Monte Carlo simulations. Since the computer calculations for the cases of phase transitions are very time-consuming, especially for small values of entrance and exit rates, we utilized one of the continuous-time Monte Carlo algorithms, the so-called BKL algorithm, first introduced by Bortz, Kalos and Lebowitz almost 30 years ago [30]. The main idea of the

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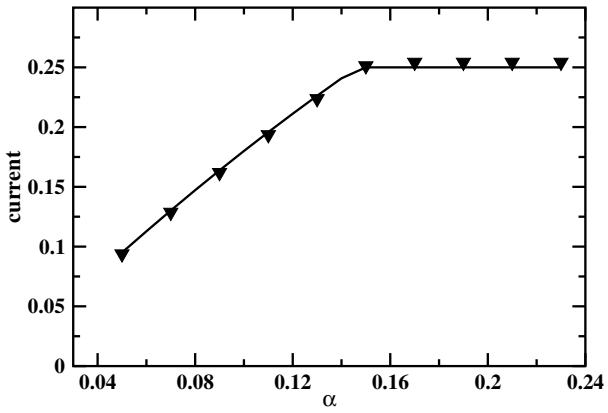

Figure 5. The particle current as a function of the entrance rate α. The exit rate is fixed; $\beta = 1$. The current saturates at $\alpha \approx 0.15$ which corresponds to the phase transition between the (LD, LD) and (HD, MC) phases. A solid line describes theoretical predictions, while symbols are the results of computer simulations.

BKL algorithm is the creation of an event-driven update scheme, so that the rejected, 'eventless' steps are skipped. The method is simple to implement, and with the latest improvements [31] it is also very efficient and fast.

In our simulations the number of effective steps per site was typically around 10^7. At phase transitions we ran simulations much longer, and the number of effective steps per site was 10^8–10^9. For all simulations we neglect the first 3% of Monte Carlo steps to account for the time that the system takes to achieve a stationary state. Our theoretical calculations assume infinite size lattice segments; however, in our simulations we used $L = 100$ and we checked that for larger sizes of lattice segments the results do not deviate from the ones presented here.

A phase diagram obtained from Monte Carlo simulations is shown in figure 3. The boundaries between the stationary phases have been determined by considering the saturation in the currents and comparing qualitative changes in the density profiles. Specifically, the phase coexistence line between the (LD, LD) and (HD, HD) phases is found when the density profiles become linear. The boundary between the (LD, LD) and (HD, MC) phases is determined when the linear density profile is observed in the chains I and II, and the overall particle current saturates. Similarly, the current saturation method allows one to specify the phase boundary between the (HD, HD) and (HD, MC) phases. The overall error in the determination of the phase boundaries is less than 5% [18]. To illustrate our approach, the dependence of the current on the entrance rate α (for fixed exit rate $\beta = 1$) is plotted in figure 5. It can be clearly seen that the current saturates at $\alpha \approx 0.15$.

Monte Carlo simulations allowed us also to calculate explicitly the particle densities. The resulting density profiles for different stationary phases are shown in figure 6. Since the stationary properties in chains I and II are essentially the same, we investigated in detail only one of two equivalent lattice segments. The computer simulations for the densities in the bulk phases are well described by the theoretical predictions. Note, however, the deviations near the junction that grow as the system approaches the phase boundaries.

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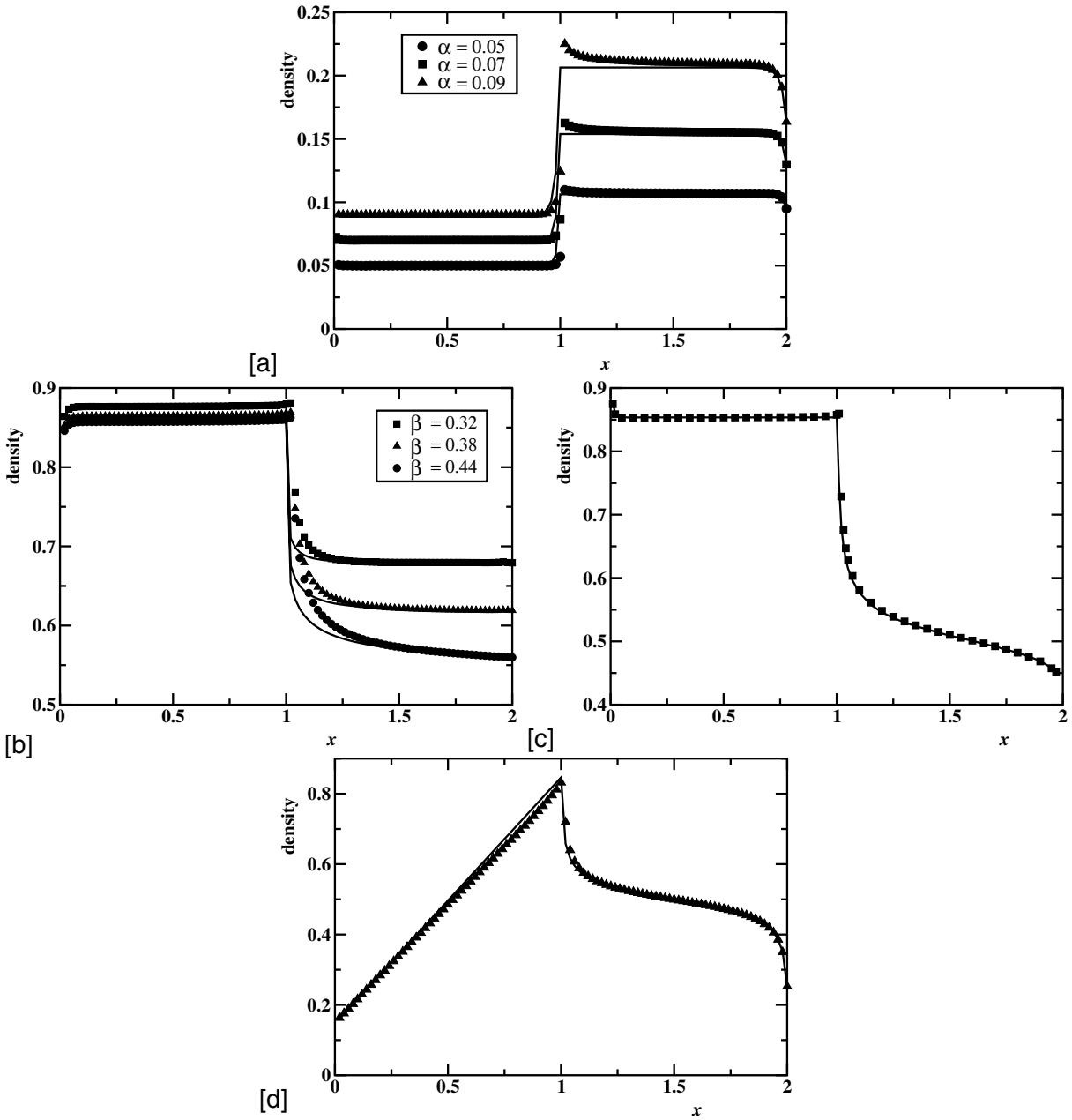

Figure 6. Density profiles for different bulk stationary phases: (a) the (LD, LD) phase with $\beta = 1$ and three different entrance rates $\alpha = 0.05$, 0.07 and 0.09; (b) the (HD, HD) phase with $\alpha = 0.8$ and three different exit rates $\beta = 0.32$, 0.38 and 0.44; (c) the (HD, MC) phase with $\alpha = 1$ and $\beta = 0.58$; (d) the phase coexistence line between the (LD, LD) and (HD, MC) phases with $\alpha = 0.146$ and $\beta = 1$. Lines are our theoretical predictions for the full-length density profiles calculated from α, $\beta_{\rm eff}$, $\alpha_{\rm eff}$ and β by using the exact expressions derived in [2]. Symbols are obtained from the Monte Carlo computer simulations.

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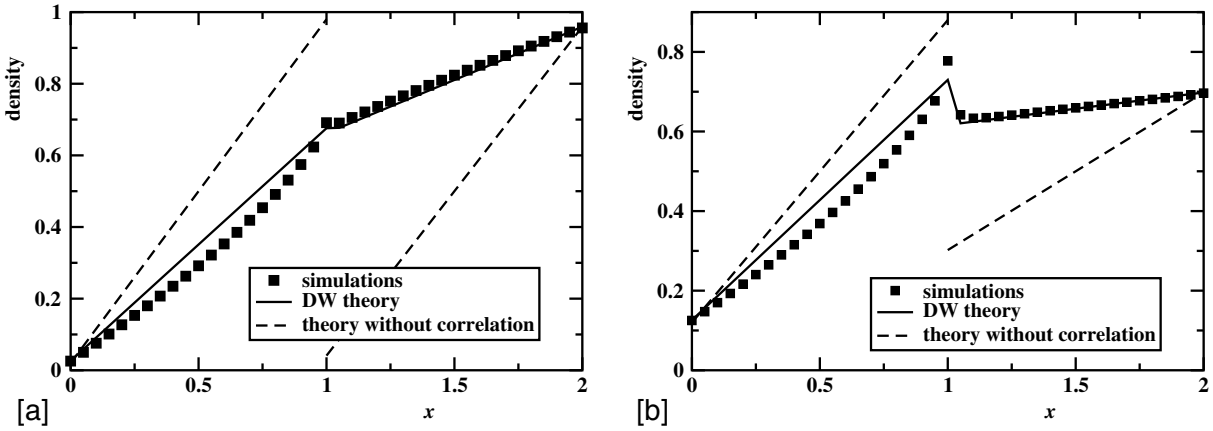

Figure 7. Density profiles for the phase coexistence line between the (LD, LD) and (HD, HD) phases for different parameters: (a) $\alpha = 0.02$, $\beta = 0.0408$; (b) $\alpha = 0.12$, $\beta = 0.3020$. Solid lines are theoretical predictions from the modified domain wall theory, namely, equations (43) and (44). Dashed lines correspond to the predictions of the simplest theory of independent motion of domain walls in each lattice segment without correlations. Symbols are obtained from the Monte Carlo computer simulations.

The situation is very different for the phase coexistence line between the (LD, LD) and (HD, HD) phases. As shown in figure 7, the density profiles that might be expected from the simplest picture of independent motion of the domain wall in each lattice segment without correlations are far away from the density profiles obtained in computer simulations. Our theoretical approach also predicts linear density profiles in all lattice segments, although with different slopes that are strongly affected by correlations. The extensive computer simulations (see figure 7) mainly confirm these suggestions, although the density profiles in chains I and II deviate slightly from linearity. There are several possible sources of these deviations: (1) the errors in the determination of the exact position of this phase boundary; and/or (2) the cross-correlation between the particles in chains I and II, as was observed for a related system [28].

The analysis of the stationary properties of the TASEP on the lattice with a junction indicates an excellent agreement with the theoretical predictions; see figures 3, 5, 6 and 7. Although the simplest approximate theory neglects the correlations around the junction, it does not strongly affect the positions of the phase boundaries, stationary currents and bulk density profiles. However, the effect of correlations is important at the first-order phase transitions between the (LD, LD) and (HD, HD) phases. An extension of the domain wall phenomenological approach, that argues that the domain wall fluctuates with different rates in the different lattice segments, is able to account for density correlations as compared with the results from the computer simulations (figure 7).

Our theoretical method can be used successfully to analyse other inhomogeneous asymmetric exclusion processes. To illustrate it, consider a TASEP with two consecutive junctions [28] as shown in figure 8(a). The phase diagram and stationary properties of the bulk phases can be easily obtained via mean-field arguments similar to the one presented above [28]. However, the density profiles at the phase boundary line ($\alpha = \beta < 1/2$) can

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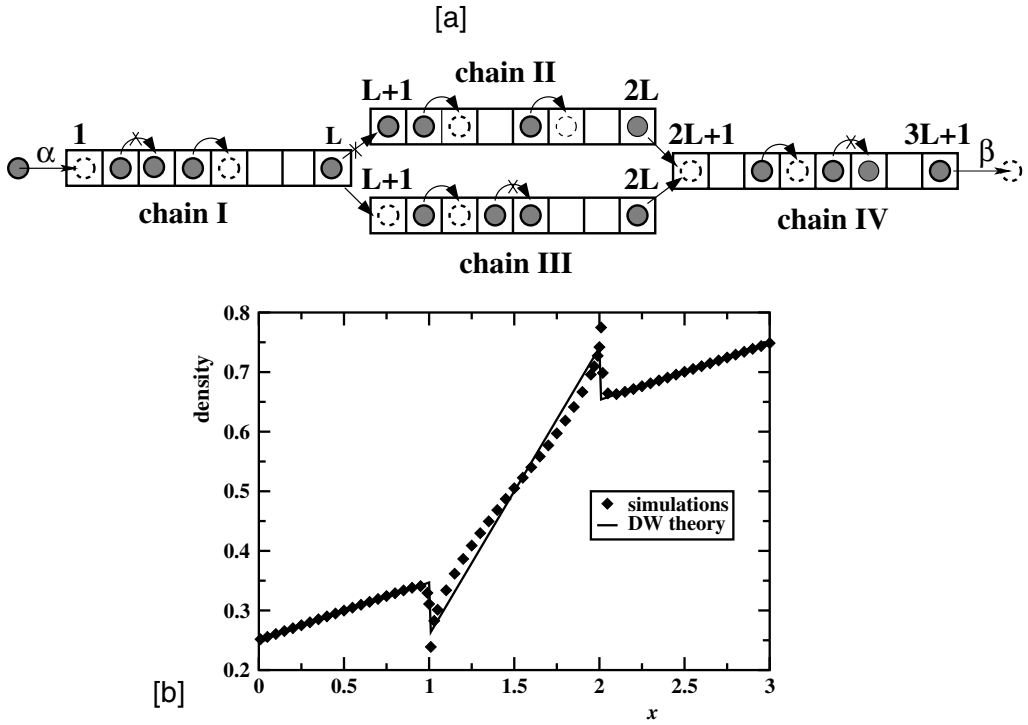

Figure 8. TASEP on the lattice with two consecutive junctions. (a) Schematic picture of the model; (b) density profiles at the phase coexistence line [28] (for $\alpha = \beta = 0.25$). Solid lines are theoretical predictions from the modified domain wall theory; symbols are from Monte Carlo computer simulations. The values $0 < x < 1$ correspond to chain I, $1 < x < 2$ describes chains II and III, and $2 < x < 3$ corresponds to chain IV.

only be calculated explicitly using the modified domain wall approach. The results are shown in figure 8(b) for the phase boundary between the high density and low density phases. Our theoretical calculations predict that for $\alpha = \beta = 0.25$ the slope in the lattice segments I and IV is equal to 0.0969, and for the segments II and III the slope is 0.484, which is in excellent agreement with the computer simulations, which give the values 0.0976 and 0.463, respectively.

4. Summary and conclusions

The stationary properties of totally asymmetric simple exclusion processes on lattices with junctions are investigated with the help of a simple approximate theory and by analysing extensive computer Monte Carlo simulations. It is found that the phase diagram of the system consists of three stationary phases. This behaviour is similar to the asymmetric exclusion processes on lattices without junctions, although the maximal current phase cannot be sustained in the lattice branches before the junction due to the stationary current limitations.

There are three different types of phase transition in this system. On the coexistence line between the (LD, LD) and (HD, HD) phases there are density jumps in all lattice

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segments that correspond to the first-order phase transitions. On the phase boundary between (HD, HD) and (HD, MC) the density profile changes continually in the lattice chain III. However, the phase transition between (LD, LD) and (HD, MC) has a quite unusual mixed character: a first-order transformation in the lattice chains I and II, and a continuous change in lattice chain III. This phase behaviour differs significantly from that of the TASEP on the lattices without junctions.

To analyse the dynamics of asymmetric exclusion processes on the lattice with a junction an approximate theoretical approach has been developed. According to this theory the system of particles moving on the lattice with the junction can be viewed as three TASEPs on the lattices without defects that couple at the junction. In the simplest approximation, the correlations near the junction position are neglected. This method allows us to calculate explicitly all stationary properties and the phase diagram. It is found that the theoretical predictions are in excellent agreement with Monte Carlo computer simulations for all phase regions except for the phase coexistence line between the (LD, LD) and (HD, HD) phases.

For the first-order phase boundary, where the intersegment density correlations are important, the modified domain wall approach is developed. We argue that the domain wall, that separates the low density and high density phases in each lattice segment, fluctuates with different rates in the different lattice branches. This means that the domain wall does not spend the same time in all lattice segments, and this leads to the correlations observed in the system. The computer Monte Carlo simulations fully support the predictions from the modified domain wall theory. It is suggested that this approach is general enough to be used successfully to account for correlations in other inhomogeneous asymmetric exclusion processes. For example, for TASEPs on lattices with double-chain sections [28], i.e., systems with two junctions, it can explicitly predict the density profiles and it can explain the observed density correlations.

One of the important properties of asymmetric exclusion processes is particle–hole symmetry [4]. The transport of particles from the left to the right is identical to the motion of 'holes' in the opposite direction. Thus the model presented above (see figure 1) can be easily mapped onto a system where particles move along one channel that splits into two branches at a junction point.

There are several extensions of the system that could be explored in the future. It is fairly straightforward to generalize our approach to the partially asymmetric exclusion process with a junction, for which a qualitatively similar phase diagram and stationary properties are expected. In the original model, the particle dynamics in the lattice segments before the junction were identical. It will be interesting to investigate a system where the two lattice branches before the junction are dynamically different. More complex dynamics is also expected for a system where more than three lattice branches are joined together at the same junction point. It is suggested that our approximate theory without correlations and the modified domain wall approach, supported by computer Monte Carlo simulations, will provide a reasonable way of analysing these complex non-equilibrium systems.

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