Theoretical investigation of total-asymmetric simple exclusion processes with attachment and detachment*

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In this paper, traffic systems with attachment and detachment have been studied by total-asymmetric simple exclusion processes (TASEPs). Attachment and detachment in a one-dimensional system is a type of complex geometry that is relevant to biological transport with the random update rule. The analytical results are presented and have shown good agreement with the extensive Monte Carlo computer simulations.

Keywords: total-asymmetric simple exclusion process, attachment and detachment, mean-field approach, Monte Carlo simulations

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1. Introduction

The total-asymmetric simple exclusion process (TASEP) is an important tool for understanding different complex phenomena in chemistry, physics, and biology.[1−5] TASEPs have been widely used to describe biological transport, kinetics of protein synthesis and biopolymers, car traffic, and hopping of quantum dots.[6−18] Most theoretical studies of exclusion processes concentrate on single-lane systems where some important exact solutions have been obtained in several cases.[1,4]

Recently, an extension of the basic asymmetric simple exclusion processes was proposed in Ref. [12] to describe some experimental observations, such as frequent irreversible detachments of particles in biological transport phenomena.[19] The effects of dissociation from linear tracks are important for the motion of motor proteins.[20] The attachment–detachment kinetics are widely used to describe the absorption–desorption process in surface chemistry. In biophysics, it is used to describe particles randomly attached to and detached from a lattice.[14,17] In vehicular traffic, the detachment (attachment) may correspond to an off-ramp (on-ramp). TASEPs in a parallel update have been used to describe traffic flow on a single-lane highway with ramps.[21] For a single ramp (either an on-ramp or an off-ramp), in the model,[21] the bottleneck phenomenon does not exist. Traffic jams before the ramp and free flow after the ramp are not observed. For two consecutive ramps, in particular, when the on-ramp is placed before the off-ramp, the bottleneck effect occurs and the flow between two ramps saturates. These predictions are obtained from the model. No real traffic experiments have been reported to either confirm or reject these predictions. However, the effects of irreversible attachments on the dynamics of a multi-particle system with random update have been little understood theoretically and via simulations.

In this paper, TASEP with attachment and detachment, random update, and an open boundary will be studied. Both numerical and analytical results are presented. This paper is organized as follows. In Section 2, a detailed description of the model is given, and exact theoretical solutions are presented. In Section 3, we discuss Monte Carlo computer simulations and compare them with theoretical predictions. Finally, Section 4 provides a summary and conclusion.

2. Model and theoretical analysis

The system configuration of a simple attachment and detachment in one-dimensional (1D) system is shown in Fig. 1. The dynamics is prescribed by the total-asymmetric simple exclusion process.

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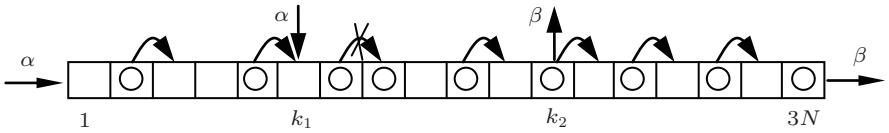


Fig. 1. System configuration of total-asymmetric simple exclusion processes with attachment and detachment. Particles are injected to the system on sites 1 and sites k_1 at rate α and ejected from the system on sites k_2 and $3N$ at rate β.

The system includes $3N$ sites where particles are injected to the system at rate α, if there is no particle on the first site and ejected from the system at rate β if there is a particle on the last site. In this model, each site has only two states, i.e., empty and occupied. On site k_1, a particle can be injected to the system at the same rate α, if there is no particle on site k_1 (it can be considered that particles attach to the system); and on site k_2, a particle can be ejected from the system at the same rate β, if there is a particle on the site k_2 (it can be considered that particles detach from the system), which are far away from boundaries (see Fig. 1).

To simplify the calculations we assume that the lattice sites $3N$ are a large number and the specific site k_1 (k_2) is of the one third (two third) of the lattice, i.e., $k_1 = N$ ($k_2 = 2N$). Firstly, we review some results for the TASEP model without attachments and detachments, which will be used in the present theory.

For $\alpha < \beta$ and $\alpha < 1/2$, the system is in the low-density (LD) phase, for which

$$\begin{aligned} &J = \alpha\,(1-\alpha)\,, \quad \rho = \alpha, \\ &\rho_1 = \alpha, \quad \rho_N = \frac{\alpha\,(1-\alpha)}{\beta}. \end{aligned} \tag{1}$$

For $\beta < \alpha$ and $\beta < 1/2$, the system is in the high-density (HD) phase, for which

$$\begin{aligned} &J = \beta\,(1-\beta)\,, \quad \rho = 1-\beta, \\ &\rho_1 = 1 - \frac{\beta\,(1-\beta)}{\alpha}, \quad \rho_N = 1-\beta. \end{aligned} \tag{2}$$

For $\alpha > 1/2$ and $\beta > 1/2$, the system is in the maximal current (MC) phase, for which

$$J = \frac{1}{4}, \quad \rho = \frac{1}{2}, \quad \rho_1 = 1 - \frac{1}{4\alpha}, \quad \rho_N = \frac{1}{4\beta}. \tag{3}$$

Following the idea, we can use three coupled chains without detachment and attachment to express the system. Segment 1 will have the injection rate α and the effective exit rate β_{eff1}, which can be defined as

$$\beta_{\text{eff1}} = 1 - \rho_{k_1+1}. \tag{4}$$

The particles can be injected into segment 2 in two ways: they can come from segment 1 to rate 1 (if there are no particles on the site $k_1 + 1$) or they can attach irreversibly at rate α. Similarly, segment 2 will have the effective injection rate α_{eff2} and the exit rate β_{eff2}, which can be defined as

$$\alpha_{\text{eff2}} = \alpha + \rho_{k_1}, \quad \beta_{\text{eff2}} = \beta + (1 - \rho_{k_2+1})\,. \tag{5}$$

Similarly, segment 3 will have the effective injection rate α_{eff3} and the exit rate β, which can be defined as

$$\alpha_{\text{eff3}} = \rho_{k2}. \tag{6}$$

It is assumed that the probabilities at which particles occupy sites k_1 and $k_1 + 1$ or sites k_2 and $k_2 + 1$ simultaneously are equal. However, since particles can be injected to the system at site k_1, the current in segment 1 cannot reach its maximum. Similarly, the current in segment 3 cannot reach its maximum, too, since particles can be ejected from the system at site k_2. The properties of TASEPs model and expressions (4), (5), and (6) are used to analyse the conditions for possible existence of phases.

The LD/LD/LD phase is determined by the following general conditions

$$\begin{aligned} &\alpha < \beta_{\text{eff1}}, \quad \alpha < \frac{1}{2}; \\ &\alpha_{\text{eff2}} < \beta_{\text{eff2}}, \quad \alpha_{\text{eff2}} < \frac{1}{2}; \\ &\alpha_{\text{eff3}} < \beta, \quad \alpha_{\text{eff3}} < \frac{1}{2}. \end{aligned} \tag{7}$$

In addition, densities at site k_1 (k_2) and k_1+1 (k_2+1) are given by

$$\begin{aligned} &\rho_{k_1} = \frac{\alpha\,(1-\alpha)}{\beta_{\text{eff1}}}, \quad \rho_{k_1+1} = \alpha_{\text{eff2}}, \\ &\rho_{k_2} = \frac{\alpha_{\text{eff2}}\,(1-\alpha_{\text{eff2}})}{\beta_{\text{eff2}}}, \quad \rho_{k_2+1} = \alpha_{\text{eff3}}. \end{aligned} \tag{8}$$

From Eqs. (4), (5), (6), and (8), we can obtain the effective exit rate and the effective injection rate for each segment, namely

$$\begin{aligned} \alpha_{\text{eff2}} &= \frac{1+\alpha-\sqrt{(1-\alpha)\,(1-5\alpha)}}{2}, \\ \beta_{\text{eff1}} &= \frac{1-\alpha+\sqrt{(1-\alpha)\,(1-5\alpha)}}{2}, \end{aligned}$$

$$\alpha_{\text{eff3}} = \frac{1+\beta-\sqrt{(1+\beta)^2-4\alpha_{\text{eff2}}(1-\alpha_{\text{eff2}})}}{2},$$
$$\beta_{\text{eff2}} = \frac{1+\beta+\sqrt{(1+\beta)^2-4\alpha_{\text{eff2}}(1-\alpha_{\text{eff2}})}}{2}. \quad (9)$$

Comparing these expressions with the inequalities (7), we obtain

$$\alpha < \frac{3-\sqrt{5}}{4},$$
$$\frac{3\alpha(1-\alpha)-\alpha\sqrt{(1-\alpha)(1-5\alpha)}}{2} < \beta. \quad (10)$$

Similar calculations can be performed for the LD/LD/HD phase, which exists when

$$\alpha < \beta_{\text{eff1}}, \quad \alpha < \frac{1}{2}; \quad \alpha_{\text{eff2}} < \beta_{\text{eff2}}, \quad \alpha_{\text{eff2}} < \frac{1}{2};$$
$$\beta < \alpha_{\text{eff3}}, \quad \beta < \frac{1}{2}. \quad (11)$$

Particle densities at special site k_1 (k_2) and k_1+1 (k_2 + 1) are given by

$$\rho_{k_1} = \frac{\alpha(1-\alpha)}{\beta_{\text{eff1}}}, \quad \rho_{k_1+1} = \alpha_{\text{eff2}},$$
$$\rho_{k_2} = \frac{\alpha_{\text{eff2}}(1-\alpha_{\text{eff2}})}{\beta_{\text{eff2}}},$$
$$\rho_{k_2+1} = 1-\frac{\beta(1-\beta)}{\alpha_{\text{eff3}}}. \quad (12)$$

We can perform similar calculations and find that this phase exists when

$$\alpha < \frac{3-\sqrt{5}}{4},$$
$$\alpha < \beta < \frac{3\alpha(1-\alpha)-\alpha\sqrt{(1-\alpha)(1-5\alpha)}}{2}. \quad (13)$$

The case with the LD/MC/LD phase can be generally described by the following conditions

$$\alpha < \beta_{\text{eff1}}, \quad \alpha < \frac{1}{2}; \quad \alpha_{\text{eff2}} > \frac{1}{2}, \quad \beta_{\text{eff2}} > \frac{1}{2};$$
$$\alpha_{\text{eff3}} < \beta, \quad \alpha_{\text{eff3}} < \frac{1}{2}. \quad (14)$$

Particle densities at special site k_1 (k_2) and k_1+1 (k_2 + 1) are given by

$$\rho_{k_1} = \frac{\alpha(1-\alpha)}{\beta_{\text{eff1}}}, \quad \rho_{k_1+1} = 1-\frac{1}{4\alpha_{\text{eff2}}},$$
$$\rho_{k_2} = \frac{1}{4\beta_{\text{eff2}}}, \quad \rho_{k_2+1} = \alpha_{\text{eff3}}. \quad (15)$$

Combining Eq. (15) with Eqs. (4), (5), and (6) leads to the following expressions for the effective rates

$$\alpha_{\text{eff2}} = \frac{\alpha}{1-4\alpha(1-\alpha)},$$
$$\beta_{\text{eff1}} = \frac{1-4\alpha(1-\alpha)}{4\alpha}, \quad (16)$$
$$\alpha_{\text{eff3}} = \frac{1}{2\left[(1+\beta)+\sqrt{\beta^2+2\beta}\right]},$$
$$\beta_{\text{eff2}} = \frac{1+\beta+\sqrt{\beta^2+2\beta}}{2}. \quad (17)$$

Substituting these results into Eq. (14) yields the following parameter ranges for the LD/MC/LD phase

$$\frac{3-\sqrt{5}}{4} < \alpha < \frac{1}{4}, \quad \beta > \frac{1}{4}. \quad (18)$$

Similar calculations can be performed for the LD/MC/HD phase, which exists when

$$\alpha < \beta_{\text{eff1}}, \quad \alpha < \frac{1}{2}; \quad \alpha_{\text{eff2}} > \frac{1}{2}, \quad \beta_{\text{eff2}} > \frac{1}{2};$$
$$\alpha_{\text{eff3}} > \beta, \quad \beta < \frac{1}{2}. \quad (19)$$

Particle densities at special sites k_1 (k_2) and k_1+1 (k_2+1) are given by

$$\rho_{k_1} = \frac{\alpha(1-\alpha)}{\beta_{\text{eff1}}}, \quad \rho_{k_1+1} = 1-\frac{1}{4\alpha_{\text{eff2}}},$$
$$\rho_{k_2} = \frac{1}{4\beta_{\text{eff2}}}, \quad \rho_{k_2+1} = 1-\frac{\beta(1-\beta)}{\alpha_{\text{eff3}}}. \quad (20)$$

We can perform similar calculations and find that this phase exists when

$$\frac{3-\sqrt{5}}{4} < \alpha < \frac{1}{4}, \quad \frac{3-\sqrt{5}}{4} < \beta < \frac{1}{4}. \quad (21)$$

The LD/HD/HD phase can be generally described by the following conditions

$$\alpha < \beta_{\text{eff1}}, \quad \alpha < \frac{1}{2}; \quad \alpha_{\text{eff2}} > \beta_{\text{eff2}}, \quad \beta_{\text{eff2}} < \frac{1}{2};$$
$$\alpha_{\text{eff3}} > \beta, \quad \beta < \frac{1}{2}. \quad (22)$$

Particle densities at special sites k_1 (k_2) and k_1+1 (k_2+1) are given by

$$\rho_{k_1} = \frac{\alpha(1-\alpha)}{\beta_{\text{eff1}}},$$
$$\rho_{k_1+1} = 1-\frac{\beta_{\text{eff2}}(1-\beta_{\text{eff2}})}{\alpha_{\text{eff2}}} \cdot \rho_{k_2} = 1-\beta_{\text{eff2}},$$
$$\rho_{k_2+1} = 1-\frac{\beta(1-\beta)}{\alpha_{\text{eff3}}}. \quad (23)$$

Combining Eq. (22) with Eqs. (4), (5), and (6) leads to the following expressions for the effective rates

$$\alpha_{\text{eff2}} = \frac{\beta_{\text{eff2}}(1-\beta_{\text{eff2}})\left[\beta_{\text{eff2}}(1-\beta_{\text{eff2}})-\alpha(1-\alpha)\right]}{\alpha},$$
$$\beta_{\text{eff1}} = \frac{\alpha}{\beta_{\text{eff2}}(1-\beta_{\text{eff2}})-\alpha(1-\alpha)},$$
$$\alpha_{\text{eff3}} = \frac{1-\beta+\sqrt{(1-\beta)(1-5\beta)}}{2},$$

$$\beta_{\rm eff2} = \frac{1+\beta-\sqrt{(1+\beta)(1-5\beta)}}{2}. \quad (24)$$

Substituting these results into Eq. (21) yields the following parameter ranges for the LD/HD/HD phase

$$\beta < \frac{3-\sqrt{5}}{4},$$
$$\beta < \alpha < \frac{3\beta(1-\beta)-\beta\sqrt{(1-\beta)(1-5\beta)}}{2}. \quad (25)$$

For the HD/MC/LD phase, that is given by

$$\alpha > \beta_{\rm eff1}, \quad \beta_{\rm eff1} < \frac{1}{2}; \quad \alpha_{\rm eff2} > \frac{1}{2}, \quad \beta_{\rm eff2} > \frac{1}{2};$$
$$\alpha_{\rm eff3} < \beta, \quad \alpha_{\rm eff3} < \frac{1}{2}. \quad (26)$$

Particle densities at special sites k_1 (k_2) and k_1+1 (k_2+1) are given by

$$\rho_{k_1} = 1-\beta_{\rm eff1}, \quad \rho_{k_1+1} = 1-\frac{1}{4\alpha_{\rm eff2}},$$
$$\rho_{k_2} = \frac{1}{4\beta_{\rm eff2}}, \quad \rho_{k_2+1} = \alpha_{\rm eff3}. \quad (27)$$

Combining Eq. (26) with Eqs. (4), (5), and (6) leads to the following expressions for the effective rates

$$\alpha_{\rm eff2} = \frac{1+\alpha+\sqrt{\alpha^2+2\alpha}}{2},$$
$$\beta_{\rm eff1} = \frac{1+\alpha-\sqrt{\alpha^2+2\alpha}}{2},$$
$$\alpha_{\rm eff3} = \frac{1+\beta-\sqrt{\beta^2+2\beta}}{2},$$
$$\beta_{\rm eff2} = \frac{1+\beta+\sqrt{\beta^2+2\beta}}{2}. \quad (28)$$

Substituting these results into Eq. (25) yields the following parameter ranges for the HD/MC/LD phase

$$\alpha > \frac{1}{4}, \quad \beta > \frac{1}{4}. \quad (29)$$

Similar calculations can be performed for the HD/MC/HD phase, which exists when

$$\alpha > \beta_{\rm eff1}, \quad \beta_{\rm eff1} < \frac{1}{2}; \quad \alpha_{\rm eff2} > \frac{1}{2}, \quad \beta_{\rm eff2} > \frac{1}{2};$$
$$\alpha_{\rm eff3} > \beta, \quad \beta < \frac{1}{2}. \quad (30)$$

Particle densities at special sites k_1 (k_2) and k_1+1 (k_2+1) are given by

$$\rho_{k_1} = 1-\beta_{\rm eff1}, \quad \rho_{k_1+1} = 1-\frac{1}{4\alpha_{\rm eff2}},$$
$$\rho_{k_2} = \frac{1}{4\beta_{\rm eff2}}, \quad \rho_{k_2+1} = 1-\frac{\beta(1-\beta)}{\alpha_{\rm eff3}}. \quad (31)$$

We can perform similar calculations and find that this phase exists when

$$\alpha > \frac{1}{4}, \quad \frac{3-\sqrt{5}}{4} < \beta < \frac{1}{4}. \quad (32)$$

The last possible phase in the system is the HD/HD/HD phase, which is specified by the following conditions

$$\alpha > \beta_{\rm eff1}, \quad \beta_{\rm eff1} < \frac{1}{2}; \quad \alpha_{\rm eff2} > \beta_{\rm eff2}, \quad \beta_{\rm eff2} < \frac{1}{2};$$
$$\alpha_{\rm eff3} > \beta, \quad \beta < \frac{1}{2}. \quad (33)$$

Particle densities at special sites k_1 (k_2) and k_1+1 (k_2+1) are given by

$$\rho_{k_1} = 1-\beta_{\rm eff1}, \quad \rho_{k_1+1} = 1-\frac{\beta_{\rm eff2}(1-\beta_{\rm eff2})}{\alpha_{\rm eff2}},$$
$$\rho_{k_2} = 1-\beta_{\rm eff2}, \quad \rho_{k_2+1} = 1-\frac{\beta(1-\beta)}{\alpha_{\rm eff3}}. \quad (34)$$

Combining Eq. (33) with Eqs. (4), (5), and (6) leads to the following expressions for the effective rates,

$$\alpha_{\rm eff2} = \frac{1+\alpha+\sqrt{(1+\alpha)^2-4\beta_{\rm eff2}(1-\beta_{\rm eff2})}}{2},$$
$$\beta_{\rm eff1} = \frac{1+\alpha-\sqrt{(1+\alpha)^2-4\beta_{\rm eff2}(1-\beta_{\rm eff2})}}{2},$$
$$\alpha_{\rm eff3} = \frac{1-\beta+\sqrt{(1-\beta)(1-5\beta)}}{2},$$
$$\beta_{\rm eff2} = \frac{1+\beta-\sqrt{(1+\beta)(1-5\beta)}}{2}. \quad (35)$$

Substituting these results into Eq. (32) yields the following parameter ranges for the HD/MC phase

$$\beta < \frac{3-\sqrt{5}}{4},$$
$$\frac{3\beta(1-\beta)-\beta\sqrt{(1-\beta)(1-5\beta)}}{2} < \alpha. \quad (36)$$

The work stated above leads to the result that there are eight stationary phases in the system. The calculated phase diagram is presented in Fig. 2.

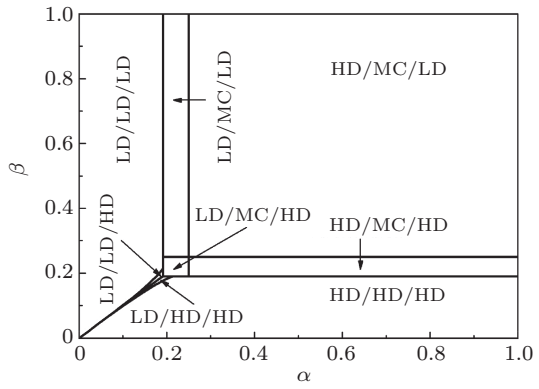


Fig. 2. The phase diagram for totally asymmetric simple exclusion processes with attachment and detachment.

3. Monte Carlo simulations and discussion

Extensive computer aided Monte Carlo simulations were carried out to check the validity of the approximate theory and the predictions. In the simulations, the number of effective steps per site was typically around 10^9. For all the simulations, the first 3% of Monte Carlo steps was neglected to account for the time that the system takes to reach a stationary state. The theoretical calculations were based on the lattice segments with infinite size. However, in the simulations presented in this paper, $3N = 300$ was used. For lattice segments with larger size, the results were checked and did not deviate from the ones presented here. Theoretical density profiles and Monte Carlo computer simulations are shown in Fig. 3. We can find that they agree well with each other.

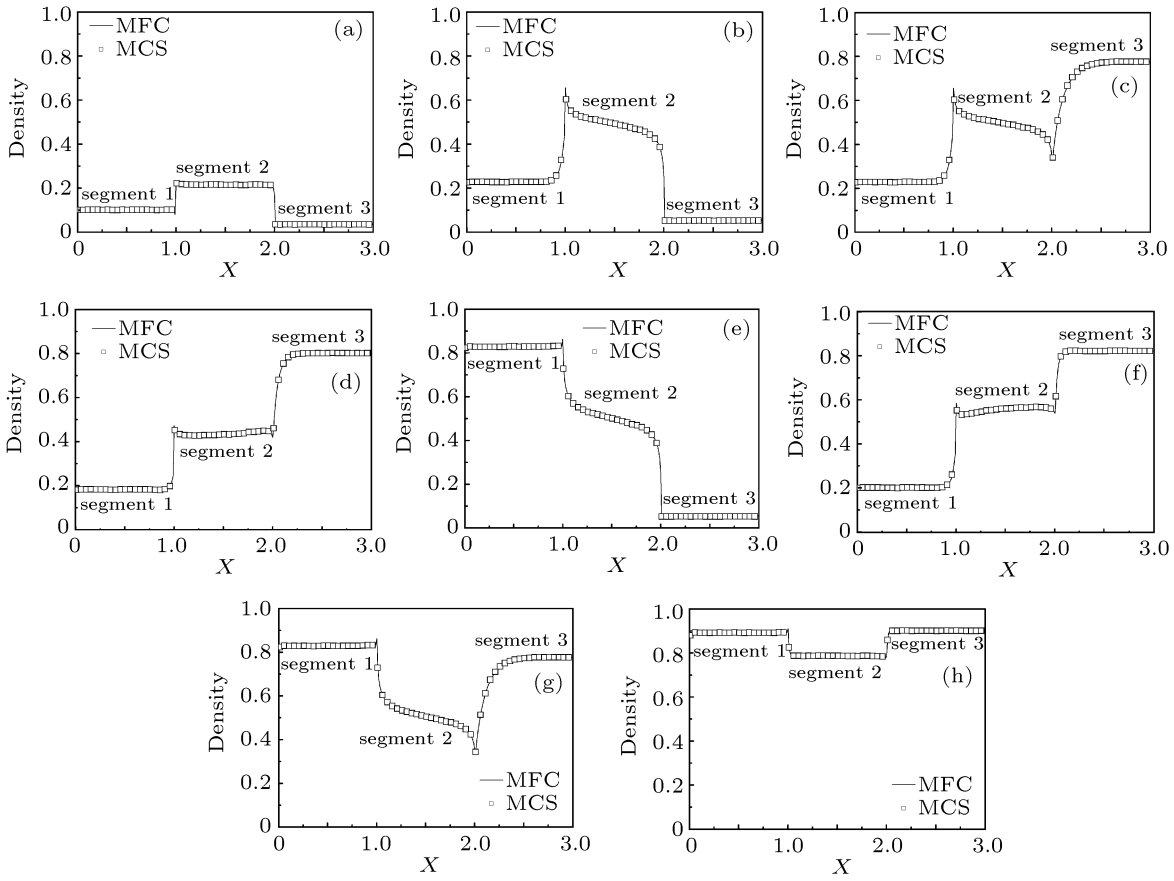


Fig. 3. Density profiles of different phases. Solid lines are for theoretical results of bulk densities, while symbols correspond to simulation results. Parameters are: (a) $\alpha = 0.1$, $\beta = 0.8$ for the (LD/LD/LD) phase; (b) $\alpha = 0.225$, $\beta = 0.8$ for the (LD/MC/LD) phase; (c) $\alpha = 0.225$, $\beta = 0.225$ for the (LD/MC/HD) phase; (d) $\alpha = 0.18$, $\beta = 0.2$ for the (LD/LD/HD) phase; (e) $\alpha = 0.8$, $\beta = 0.8$ for the (HD/MC/LD) phase; (f) $\alpha = 0.2$, $\beta = 0.18$ for the (LD/HD/HD) phase; (g) $\alpha = 0.8$, $\beta = 0.225$ for the (HD/MC/HD) phase; (h) $\alpha = 0.8$, $\beta = 0.1$ for the (HD/HD/HD) phase.

Our approximate theory is based on the representation of the system with attachment and detachment as three coupled totally asymmetric exclusion models. This suggests that there are 27 possible stationary phases; however, 15 phases cannot occur due to the fact that the particles can be injected to the system on site k_1, the current in segment 1 cannot reach its maximal current. Similarly, the current in the segment 3 cannot reach its maximal current, too, since particles can be ejected from the system on site k_2.

On segment 3 of the system, the density value is always in the LD phase, which implies that the particles can be ejected from the system on site k_2, since it can decrease the particle numbers that move forward into segment 3. Similarly, on segment 1 of the system, the density value is always in the HD phase, which implies that the particles can be injected to the system on site k_1, since this site becomes the bottleneck of the system.

4. Summary and conclusion

The work presented in this paper investigated totally asymmetric simple exclusion processes with attachment and detachment, and random update. The study shows that TASEP with attachment and detachment produces a system with eight possible phases.

On segment 3 of the system, the density value is always in the LD phase, which implies that the particles can be ejected from the system on site k_2, since it can decrease the particle numbers which move forward into the segment 3. Similarly, on the segment 1 of the system, the density value is always in the HD phase, which implies that the particles can be injected to the system on site k_1, since this site becomes the bottleneck of the system.

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