Canadian Journal of Physics
Revue canadienne de physique

Mean-field analysis of two-species TASEP with attachment and detachment

Journal:	<i>Canadian Journal of Physics</i>
Manuscript ID	cjp-2016-0644.R1
Manuscript Type:	Article
Date Submitted by the Author:	29-Oct-2016
Complete List of Authors:	Song, Minghua; Fudan University, School of Mathematical Sciences Zhang, Yunxin; Fudan University, School of Mathematical Sciences
Keyword:	two-species TASEP, domain wall, boundary layer, molecular motor, phase transition

SCHOLARONE™
Manuscripts

Only

Mean-field analysis of two-species TASEP with attachment and detachment

Minghua Song¹ and Yunxin Zhang^{1,2}

¹Shanghai Key Laboratory for Contemporary Applied Mathematics, Centre for Computational Systems Biology, School of Mathematical Sciences, Fudan University, Shanghai 200433, China.

²Kavli Institute for Theoretical Physics China, CAS, Beijing 10090, China.

E-mail: xyz@fudan.edu.cn

Abstract. In the field of statistical physics, unidirectional motion of large number of particles along a single track can be described by totally asymmetric simple exclusion process (TASEP). From which many meaningful properties, such as the appearance of domain wall (defined as the borderline of high particle density and low particle density along the motion track) and boundary layers, can be obtained. However, it is biologically general that a single track may be occupied by different particle species. For example, in cells each protofilament of microtubule is usually occupied by different species of motor protein. So previous studies about TASEP including only one particle species may not be reasonable enough to find more detailed properties of the particle motion process in real cell environment. To address this problem, TASEP including two particle species is discussed in this study. Theoretical methods to get particle densities of each species are provided. By which, phase transition related properties of particle densities are obtained. Our analysis show that domain wall and boundary layers of single species densities always appear simultaneously with those of the total particle density. The height of domain wall of total particle density is equal to the summation of those of single particle species. Phase diagrams for typical model parameters are also presented. The methods presented in this study can be generalized to analyze TASEP with more particle species.

PACS numbers: 87.16.Nn, 05.40.Jc, 87.16.A-, 82.39.-k

1. Introduction

In last decades, several theoretical models have been developed to describe the unidirectional motion of a large number of particles, including the motion of motor proteins along microtubule, the motion of RNA polymerases along DNA template during gene transcription, the motion of ribosomes along messenger RNA transcript during translation, as well as the bus traffic process in our daily life [1, 2, 3, 4]. In which, most of them can be regarded as generalizations of the one-dimensional totally asymmetric simple exclusion process (TASEP) [5, 6].

In TASEP, motion track of particles is simplified to a one-dimensional lattice with length $N + 1$, particles enter the track from the first site 0 provided this site is not occupied, and leave the track from the last site N . If lattice site $i + 1$ is empty, the particle at lattice site i will hop forward to site $i + 1$ with given rate. Generally, particles may also detach into environment and end their unidirectional motion from bulk lattice sites, and new particles may also attach to any one of unoccupied bulk sites. In recent years, TASEP has been studied extensively. Especially for its phase transition related properties, i.e., the appearance of domain wall (DW) and boundary layers (BLs), which are usually driven by boundary conditions [7, 8, 9, 10, 11, 12, 13, 14]. However, in most of previous studies, the self-propelled particles are usually assumed to be the same species, i.e., they all have the same properties, including the hopping rate, attachment/detachment rate, as well as the entering rate and leaving rate. But in real cells, one protofilament of microtubule (which is the main highway to transport the cargos in cells) is usually occupied by motor proteins from different species [15]. So, to know more detailed properties about the particle motion process in reality, the usual TASEP should be generalized to include particles from different species [16, 17, 18, 19].

The simplest generalization is the two-species ASEP, which has been discussed in recent studies [20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30]. However, to our knowledge, in most of the previous studies (except [24, 27, 28]), no particle attachment/detachment to/from bulk sites of the track (which is usually called the Langmuir kinetics) is included, here the bulk sites are all the sites except the first site 0 and the terminal site N . Furthermore, they usually assumed that one particle species enters the motion track from site 0 and leaves from site N , while the other one enters from site N and leaves from site 0. Meanwhile, it is also assumed that two-species pair $(P_1)_i(P_2)_{i+1}$ can change to $(P_2)_i(P_1)_{i+1}$, i.e. forward hopping of one species will never be blocked by the other species. For convenience, the two particle species are denoted by P_1 and P_2 respectively, and $(P_k)_i$ means there is a particle P_k at site i .

The TASEP discussed in this study also includes two particle species. But both of them enter the motion track from the first site 0 and leave from last site N , i.e. they not only travel along the same track, but also move to the same direction. Previous studies about one species TASEP have shown that nontrivial attachment/detachment (i.e. the Langmuir kinetics) is one of the key driven factors to the appearance of DW in particle density [31, 32, 9, 33, 3, 13]. So, in this study, both of the two particle species

are allowed to attach to (and detach from) bulk sites of the track. The same as in one species cases, we also called this process “TASEP-LK” process [9].

2. Models for two-species TASEP

Let n_i and m_i be occupation numbers of particle species P_1 and P_2 at site i , respectively. Specifically $n_i = 1$ means site i is occupied by a particle P_1 , while $n_i = 0$ means site i is not occupied by particle P_1 . Because of the hard-core exclusion, $n_i + m_i = 0$ or 1 . For $1 \leq i \leq N - 1$, the time evolution of n_i and m_i are governed by following equations

$$dn_i/dt = n_{i-1}(1 - n_i - m_i) - n_i(1 - n_{i+1} - m_{i+1}) + \omega_{1,A}(1 - n_i - m_i) - \omega_{1,D}n_i, \quad (1)$$

$$dm_i/dt = qm_{i-1}(1 - n_i - m_i) - qm_i(1 - n_{i+1} - m_{i+1}) + \omega_{2,A}(1 - n_i - m_i) - \omega_{2,D}m_i. \quad (2)$$

Where, for convenience, forward hopping rate of species P_1 is normalized to be unit, and forward hopping rate of species P_2 is assumed to be $q \leq 1$. The attachment rate of species P_k to any unoccupied bulk site i is denoted by $\omega_{k,A}$, and the detachment rate of species P_k from bulk sites is denoted by $\omega_{k,D}$. At the first site $i = 0$ (left boundary),

$$dn_0/dt = \alpha_1(1 - n_0 - m_0) - n_0(1 - n_1 - m_1), \quad (3)$$

$$dm_0/dt = \alpha_2(1 - n_0 - m_0) - qm_0(1 - n_1 - m_1). \quad (4)$$

Where α_k is the entry rate of particle P_k to the first site 0 . While at the last site $i = N$ (right boundary),

$$dn_N/dt = n_{N-1}(1 - n_N - m_N) - \beta_1n_N, \quad (5)$$

$$dm_N/dt = qm_{N-1}(1 - n_N - m_N) - \beta_2m_N, \quad (6)$$

with β_k the leaving rate of particle P_k from the last site N .

In cells, hopping rate of particles is usually determined by their biochemical properties. For example, forward hopping of motor proteins, such as conventional kinesin, is mechanochemically coupled with hydrolysis of adenosine triphosphate (ATP). Each forward mechanical step is tightly coupled with one ATP hydrolysis. Therefore, hopping rate is determined by the rate of ATP hydrolysis. Meanwhile, leaving rate of particles from motion track is also determined by their biochemical properties, or even the rate of ATP hydrolysis. Therefore it is biophysically reasonable to assume that the ratio of leaving rate of the two species $\beta_1 : \beta_2$ is equal to ratio of their forward hopping rate $1 : q$. Meanwhile, experiments found that, if the two heads of motor protein kinesin both bind adenosine diphosphate (ADP), then it will soon detach from microtubule. This means that detachment rate of motor proteins is also determined by their biochemical properties and the rate of ATP hydrolysis. So, for convenience of theoretical analysis, this study also assumes that $\omega_{1,D} : \omega_{2,D} = 1 : q$. However, except their biochemical properties, entry rate α_k and attachment rate $\omega_{k,A}$ of particle species P_k are also influenced by environmental conditions, especially their concentrations. So, the corresponding rate ratios, $\alpha_1 : \alpha_2$ and $\omega_{1,A} : \omega_{2,A}$ may be different from the ratio $1 : q$.

Define $\rho_1(i) = \langle n_i \rangle$ and $\rho_2(i) = \langle m_i \rangle$. By mean-field approximation, for large N limit, equations for steady state values of particle densities ρ_1 and ρ_2 can be obtained from Eqs. (1,2),

$$\partial_x J_k = q^{1-k} \Omega_{k,A} (1 - \rho_1 - \rho_2) - \Omega \rho_k, \quad k = 1, 2, \quad (7)$$

where $J_k = \rho_k(1 - \rho_1 - \rho_2)$, $\Omega_{k,A} = N\omega_{k,A}$, $\Omega = N\omega_{1,D} = N\omega_{2,D}/q =: N\omega$, and $0 < x < 1$. Note, this study assumes that $\langle n_i m_{i+1} \rangle = \rho_1(i) \rho_2(i+1)$, and in the analysis of mean-field approximation (MFA), the length of motion track is normalized to 1. Meanwhile, this study also assumes that the unbinding/binding rate $\omega_{k,D/A}$ scales inversely with track length N , which is the most interesting cases. For other cases, one can discuss similarly as in [34, 35]. From Eq. (7), one can show that total particle density $\rho = \rho_1 + \rho_2$ satisfies

$$\partial_x J = K\Omega(1 - \rho) - \Omega\rho, \quad (8)$$

where $K = K_1 + K_2 = [\omega_{1,A} + \omega_{2,A}/q]/\omega$, and $J = \rho(1 - \rho)$. From Eqs. (3-6), one can obtain that at boundaries $x = 0, 1$, particle densities ρ_1, ρ_2 and ρ satisfy $\rho_1(0) = \alpha_1, \rho_2(0) = \alpha_2/q$, and $\rho(1) = \rho_1(1) + \rho_2(1) = 1 - \beta$ with $\beta = \beta_1 = \beta_2/q$.

We need to point out that, with notations defined previously, the density current of the first particle species is J_1 . However, the density current of the second particle species should be qJ_2 , and so the total density current is $J_1 + qJ_2 = (\rho_1 + q\rho_2)(1 - \rho)$, which is different from J .

Eq. (8) implies that the governing equation for total particle density ρ is the same as the one obtained for one-species ‘‘TASEP-LK’’ process [36], but with *effective* detachment rate $\Omega_D = \Omega$, *effective* attachment rate $\Omega_A = K\Omega$, initiation (entry) rate $\alpha = \alpha_1 + \alpha_2/q$, and termination (leaving) rate $\beta = \beta_1 = \beta_2/q$ (see Fig. 1). So total particle density ρ can be obtained by the same methods as described in one-species ‘‘TASEP-LK’’ process. But the main difficulty for two-species cases is how to get single species densities ρ_1 and ρ_2 . Actually, no reasonable boundary conditions at $x = 1$, i.e., values of $\rho_1(1)$ and $\rho_2(1)$, can be derived from Eqs. (5,6). Meanwhile, properties of densities ρ_1 and ρ_2 are different from the ones as in one-species cases. For example, in one-species ‘‘TASEP-LK’’ process, particle densities before and after DW location x_w satisfies $\rho(x_w^-) + \rho(x_w^+) = 1$ [37]. This is because that across DW location x_w , $J = \rho(1 - \rho)$ is conserved. But for two-species cases, particle densities ρ_1, ρ_2 do not satisfy this relation. However, the plots in Fig. 1 imply that DWs of density ρ, ρ_1, ρ_2 appear at the same location. Actually, further numerical calculations show that their BLs also appear simultaneously, see Fig. 6 below.

Along motion track, J_1, J_2 , and consequently J , always change continuously, even if corresponding densities ρ_1, ρ_2 and ρ are discontinuous. At any location x of the track, $\rho_k(x^-)[1 - \rho(x^-)] = J_k(x^-) = J_k(x^+) = \rho_k(x^+)[1 - \rho(x^+)]$ and $\rho(x^-)[1 - \rho(x^-)] = J(x^-) = J(x^+) = \rho(x^+)[1 - \rho(x^+)]$. Through simple analysis, we obtained $\rho_1(x^-)/\rho_2(x^-) = \rho_1(x^+)/\rho_2(x^+)$ and $\rho_k(x^-)/\rho(x^-) = \rho_k(x^+)/\rho(x^+)$. Particularly, this relation also holds at location x_w of DW.

As we have mentioned before, total particle density ρ can be obtained from Eq. (8) with boundary conditions $\rho(0) = \rho_1(0) + \rho_2(0) = \alpha_1 + \alpha_2/q$ and $\rho(1) = 1 - \beta$.

Figure 1. (Color online) Mean density profiles obtained from Eqs. (1-6) (black dotted line), and their mean-field approximations obtained from Eqs. (7,8) (solid lines for ρ , dashdot lines for ρ_1 , and dashed line for ρ_2). Parameter values used in calculations are **(a)** $\Omega_{1,A} = 0.01$, $\Omega_{2,A} = 0.14$, $\alpha_1 = 0.2$, $\alpha_2 = 0.09$, and **(b)** $\Omega_{1,A} = 0.1$, $\Omega_{2,A} = 0.05$, $\alpha_1 = 0.1$, $\alpha_2 = 0.18$. Other parameter values are $N = 10^3$, $q = 0.9$, $\Omega_{1,D} = \Omega_{2,D}/q = 0.1$, $\beta_1 = \beta_2/q = 0.3$. Total particle density ρ in both **(a)** and **(b)** is the same as the one in usual “TASEP-LK” process with $\alpha = \beta = 0.3$, and $\Omega_D = 0.1$, $\Omega_A = 0.15$. Locations of domain wall for total density ρ and single species densities ρ_1, ρ_2 are the same. Across domain wall location, $J = \rho(1 - \rho)$ and $J_k = \rho_k(1 - \rho)$ for $k = 1, 2$ are all conserved.

But, if there exists DW between boundaries $x = 0$ and $x = 1$, then without boundary value $\rho_k(1)$, single species density ρ_k cannot be obtained simply by Eq. (7). Actually, with boundary value $\rho_k(0)$, only the value of density ρ_k before DW location x_w , i.e. in interval $[0, x_w)$, can be directly obtained by Eq. (7). One of the main aims of this study is to find methods to get single species density ρ_k along the whole track, i.e. in interval $[0, 1]$, but using only boundary condition at $x = 0$.

Let $\Delta := \rho(x_w^+) - \rho(x_w^-)$, i.e. the DW height of total density ρ (see [37] for more detailed analysis about DW height). Then the DW height of single species density is $\Delta_k := \rho_k(x_w^+) - \rho_k(x_w^-) = [\rho_k(x_w^+)/\rho(x_w^+)]\rho(x_w^+) - [\rho_k(x_w^-)/\rho(x_w^-)]\rho(x_w^-) = [\rho_k(x_w^+)/\rho(x_w^+)]\Delta = [\rho_k(x_w^-)/\rho(x_w^-)]\Delta$. So, $\Delta_1 + \Delta_2 = \Delta$, and $\Delta_k > 0$ iff $\Delta > 0$. Therefore, DWs of total density ρ and single species densities ρ_1 and ρ_2 always appear at the same location, which is consistent with the finding through numerical calculations (see Fig. 1).

The value $\rho_k(x_w^+)$ can be obtained as follows, $\rho_k(x_w^+) = \rho_k(x_w^-) + \Delta_k = \rho_k(x_w^-) + [\rho_k(x_w^-)/\rho(x_w^-)][\rho(x_w^+) - \rho(x_w^-)] = \rho(x_w^+)\rho_k(x_w^-)/\rho(x_w^-)$. Using $\rho_k(x_w^+)$ as left boundary condition, the value of single species density ρ_k after DW location x_w , i.e. in interval $(x_w, 1)$, can be obtained from Eq. (7). Note, the above method to get single species density ρ_k is also available when there exists BLs at either boundary $x = 0$ or boundary $x = 1$. BLs of single species densities ρ_1, ρ_2 and total density ρ are also appear simultaneously.

3. Methods to obtain particle densities ρ_1, ρ_2 : special cases $K = 1$

The basic idea to obtain single species densities ρ_1, ρ_2 is to use Eq. (7) and the expression of total density ρ . Therefore, the first step is to get ρ from Eq. (8).

For $K = 1$, Eq. (8) is reduced to

$$(\partial_x \rho - \Omega)(2\rho - 1) = 0, \quad (9)$$

with boundary conditions $\rho(0) = \alpha$ and $\rho(1) = 1 - \beta$. The method to get density ρ from Eq. (9) has been discussed previously in [36]. For the sake of convenience, we introduced briefly as follows.

Eq. (9) has two general solutions, $\rho_l(x) \equiv 1/2$ and $\rho(x) = \Omega x + C$ with C an constant determined by boundary conditions. The constant solution $\rho(x) \equiv 1/2$ coincides with the density $\rho_l \equiv K/(K+1)$ given by Langmuir kinetics (LK), and corresponds to the maximal current (MC) phase. For convenience, the solution $\rho(x) = \Omega x + C$ which satisfies the left boundary condition $\rho(0) = \alpha$ is denoted by $\rho_\alpha(x) := \Omega x + \alpha$, and the solution $\rho(x)$ which satisfies the right boundary condition $\rho(1) = 1 - \beta$ is denoted by $\rho_\beta(x) := \Omega x + 1 - \beta - \Omega$.

If expanding solution domain $[0, 1]$ to the whole space, i.e., $(-\infty, \infty)$, then both $\rho_\alpha(x)$ and $\rho_\beta(x)$ cross the line $\rho = \rho_l \equiv 1/2$. Denote corresponding intersection points by x_α and x_β , respectively. It can be easily get that $x_\alpha = (1 - 2\alpha)/(2\Omega)$ and $x_\beta = (2\beta + 2\Omega - 1)/(2\Omega)$. The solution ρ of Eq. (9) is obtained by the following process. If $x_\alpha < x_\beta$, then $\rho_\alpha(x)$ is on the left of $\rho_\beta(x)$. So a maximal current phase appears between x_α and x_β . For such cases,

$$\rho(x) = \begin{cases} \rho_\alpha(x), & 0 < x \leq x_\alpha, \\ 1/2 & x_\alpha \leq x \leq x_\beta, \\ \rho_\beta(x), & x_\beta \leq x < 1. \end{cases} \quad (10)$$

On the other hand, if $x_\alpha > x_\beta$ then $\rho_\alpha(x)$ is on the right of $\rho_\beta(x)$. For these cases, a domain wall will appear between x_β and x_α . Based on the continuity of $J = \rho(1 - \rho)$, i.e. $J_\alpha(x_w) = J_\beta(x_w)$, the location of domain wall can be obtained as follows,

$$x_w = (\Omega + \beta - \alpha)/(2\Omega). \quad (11)$$

The solution $\rho(x)$ of Eq. (9) can then be obtained,

$$\rho(x) = \begin{cases} \rho_\alpha(x), & 0 < x < x_w, \\ \rho_\beta(x), & x_w < x < 1. \end{cases} \quad (12)$$

Note, x_α, x_β, x_w may not lie in interval $[0, 1]$. For those cases, corresponding boundary layers will appear. For example, if $x_w < 0$ then there will exist left boundary layer.

After getting total density ρ , single species densities ρ_1 and ρ_2 can be obtained by four steps. **(1)** Get left solutions $\rho_{\alpha,1}(x)$ and $\rho_{\alpha,2}(x)$ in interval $(-\infty, x_\alpha]$ from Eq. (7) by matching left boundary conditions $\rho_{\alpha,1}(0) = \alpha_1$ and $\rho_{\alpha,2}(0) = \alpha_2/q$, respectively; **(2)** Get solutions $\rho_1(x)$ and $\rho_2(x)$ in interval $[\min\{x_\alpha, x_\beta\}, \max\{x_\alpha, x_\beta\}]$ from Eq. (7) by matching boundary conditions $\rho_k(x_\alpha) = \rho_{\alpha,k}(x_\alpha)$; **(3)** Get solutions $\rho_1(x)$ and $\rho_2(x)$

in interval $[x_\beta, \infty)$ by matching $\rho_k(x_\beta^+) = \rho_k(x_\beta^-)$; (4) Get single species densities by confining the above obtained ρ_1 and ρ_2 in interval $[0, 1]$. Note, if $x_\alpha > x_\beta$, and $0 < x_w < 1$, there will exist domain wall for both ρ_1 and ρ_2 at x_w , see detailed discussion below.

If the solution $\rho(x)$ of Eq. (9) is $\rho(x) = \Omega x + C$, then from Eq. (7), single species density ρ_k can be obtained as follows,

$$\rho_1 = \Omega_{1,A}x + C_1, \quad (13)$$

$$\rho_2 = \frac{\Omega_{2,A}}{q}x + C_2. \quad (14)$$

On the other hand, if the solution $\rho(x)$ of Eq. (9) is $\rho_l(x) \equiv 1/2$, then ρ_1 and ρ_2 satisfy

$$\partial_x \rho_1 = \Omega_{1,A} - 2\Omega \rho_1,$$

$$\partial_x \rho_2 = \frac{\Omega_{2,A}}{q} - 2\Omega \rho_2.$$

Their solutions are

$$\rho_1 = \frac{\Omega_{1,A} - \exp(c_1 - 2\Omega x)}{2\Omega}, \quad (15)$$

$$\rho_2 = \frac{\frac{\Omega_{2,A}}{q} - \exp(c_2 - 2\Omega x)}{2\Omega}. \quad (16)$$

Constants C_k and c_k are determined by boundary conditions.

By matching boundary conditions at $x = 0$, left solutions $\rho_{\alpha,1}(x)$ and $\rho_{\alpha,2}(x)$ in interval $(-\infty, x_\alpha]$ are given as follows,

$$\rho_{\alpha,1}(x) = \Omega_{1,A}x + \alpha_1, \quad (17)$$

$$\rho_{\alpha,2}(x) = (\Omega_{2,A}x + \alpha_2)/q. \quad (18)$$

Then values of $\rho_{\alpha,1}(x_\alpha)$ and $\rho_{\alpha,2}(x_\alpha)$ can be obtained. Using $\rho_{\alpha,k}(x_\alpha)$ as boundary conditions, single species density $\rho_{MC,k}(x)$ in interval $[\min\{x_\alpha, x_\beta\}, \max\{x_\alpha, x_\beta\}]$ can be obtained by Eqs. (15,16). Where constants c_1 and c_2 are

$$c_1 = 2\Omega x_\alpha + \ln [\Omega_{1,A} - 2\Omega \rho_{\alpha,1}(x_\alpha)],$$

$$c_2 = 2\Omega x_\alpha + \ln \left[\frac{\Omega_{2,A}}{q} - 2\Omega \rho_{\alpha,1}(x_\alpha) \right].$$

Using $\rho_{MC,k}(x_\beta)$ as boundary condition of $\rho_{\beta,k}(x)$, i.e., $\rho_{\beta,k}(x_\beta) = \rho_{MC,k}(x_\beta)$, the constant C_k in Eqs. (13,14) can be determined. Therefore, right solution $\rho_{\beta,k}$ of Eq. (7) can be obtained,

$$\rho_{\beta,1}(x) = \Omega_{1,A}(x - x_\beta) + \rho_{MC,1}(x_\beta), \quad (19)$$

$$\rho_{\beta,2}(x) = \frac{\Omega_{2,A}}{q}(x - x_\beta) + \rho_{MC,2}(x_\beta). \quad (20)$$

Finally, single species density $\rho_k(x)$ in the main body of motion track, i.e., for $0 < x < 1$, can be obtained from $\rho_{\alpha,k}$, $\rho_{MC,k}$, and $\rho_{\beta,k}$. If $x_\alpha < x_\beta$ then

$$\rho_k(x) = \begin{cases} \rho_{\alpha,k}(x), & 0 < x \leq x_\alpha, \\ \rho_{MC,k}(x), & x_\alpha \leq x \leq x_\beta, \\ \rho_{\beta,k}(x), & x_\beta \leq x < 1. \end{cases} \quad (21)$$

On the other hand, if $x_\beta < x_\alpha$ then

$$\rho_k(x) = \begin{cases} \rho_{\alpha,k}(x), & 0 < x < x_w, \\ \rho_{\beta,k}(x), & x_w < x < 1. \end{cases} \quad (22)$$

Similar as in the expression of total density ρ , see Eqs. (10,12), locations x_α, x_β, x_w may not lie in interval $[0, 1]$. For those cases, boundary layer will appear.

Except their boundary values, densities ρ, ρ_k are said to be in low density phase (LD) if they are less than $1/2$. On the contrary, if they are larger than $1/2$, then they are said to be in high density (HD) phase. If $0 < x_w < 1$ then density ρ will be in LD phase in $(0, x_w)$ and in HD phase in $(x_w, 1)$. For convenience, the phase of density for such cases is denoted by LD-DW-HD. Moreover, boundary layer is denoted by BL. In some cases, we also use $BL_{l/r}^\pm$ to denote left/right boundary layer in which density ρ sharply increases/decreases along the motion track.

Typical examples of densities ρ, ρ_1, ρ_2 are plotted in Fig. 2, where thick dotted lines are obtained by numerical iterations of Eqs. (1-6), and others are obtained from Eqs. (7,8) using the method discussed in this section. These plots show that for large initiation rate $\alpha = \alpha_1 + \alpha_2 > 0.5$, there exists left BL for both total density ρ and single species densities ρ_1 and ρ_2 . Meanwhile, there might exist right BL for either large or small values of leaving rate β . Again, we emphasize that DW of single species density ρ_k always exists at the same location as that of total density ρ , with domain wall height satisfies $\Delta_k = [\rho_k(x_w^-)/\rho(x_w^-)]\Delta$ and $\Delta = \Delta_1 + \Delta_2$. For special cases $K = 1$, the phase of single species densities ρ_1 and ρ_2 may not be the same as that of total density ρ . If ρ is in LD phase, then both ρ_1 and ρ_2 will be in LD phase. However, when ρ is in HD phase, one of the single species densities, or even both of them, may still remain in LD phase.

Using similar method as in [36], typical examples of phase diagram of density ρ , for special cases $K = 1$, are given in Fig. 3. Generally, density ρ may be in any one of the seven possible phases, including all possible combinations of LD, MC, and HD. The lines in Figs. 3(b,c,e,f) are obtained by $\alpha_2 = q(\alpha - \alpha_1)$, since density ρ depends only on the summation $\alpha = \alpha_1 + \alpha_2/q$.

4. Maximal current phase of total density ρ for special cases $K = 1$

In this section, we will show that if *effective* initiation rate α and leaving rate β satisfy

$$\alpha > 1/2 - \Omega, \quad \beta > 1/2 - \Omega, \quad \text{and} \quad \alpha + \beta > 1 - \Omega, \quad (23)$$

then total particle density ρ will be in maximal current (MC) phase near right boundary $x = 1$, in which $\rho = 1/2$ and $J = J_1 + J_2 = 1/4$.

The MC phase of density ρ may appear in four cases: “LD-MC”, “LD-MC-HD”, “MC-HD”, and “MC”, see Fig. 3(a,d). Based on the continuity of J and J_k at locations $x_\alpha = (1 - 2\alpha)/(2\Omega)$ and $x_\beta = (2\beta + 2\Omega - 1)/(2\Omega)$, we have the following conclusions.

Figure 2. (Color online) Typical examples of densities ρ, ρ_1, ρ_2 for $K = 1$. Parameter values used in calculations are $q = 0.9$, $\Omega_1 = 0.2$, $\Omega_2/q = 0.1$. The phase of density ρ is as follows. (a) LD-MC-BL $^-$; (b) LD-MC-HD; (c) LD-HD; (d) LD-DW-HD; (e) BL $^+$ -HD; (f) LD-BL $^-$; (g) LD-BL $^+$; (h) LD-DW-HD; (i) MC; (j) BL $^-$ -MC-BL $^-$; (k) BL $^-$ -MC-HD; (l) BL $^-$ -HD. Line types in this figure are the same as in Fig. 1.

Figure 3. (Color online) Phase diagrams of total density $\rho = \rho_1 + \rho_2$ obtained from stationary mean-field Eq. (8) with $K = 1$, $\Omega = 0.3$ in (a,b,c), and $\Omega = 0.5$ in (d,e,f). (b,e) and (c,f) are phase diagrams in (α_1, α_2) plane, which correspond to $\beta = 0.4$ and $\beta = 0.6$, respectively (see the horizontal dotted and dashed lines in (a,d)).

(1) If MC appears at left boundary $x = 0$, i.e. in phase “MC-HD”, or “MC”, then $x_\alpha \leq 0$ and $x_\beta > 0$. Which means that $\alpha \geq 1/2$, and $\beta > 1/2 - \Omega$.

(2) If MC appears at right boundary, i.e. in phase “LD-MC” or “MC”, then $x_\alpha < 1$ and $x_\beta \geq 1$. Which means $\beta \geq 1/2$, and $\alpha > 1/2 - \Omega$.

(3) If MC appears only in part of the main body of motion track, i.e. in “LD-MC-HD” phase, then $0 < x_\alpha < x_\beta < 1$. Which means $\alpha < 1/2$, $\beta < 1/2$, and $\alpha + \beta > 1 - \Omega$.

Based on the above three conclusions (1,2,3), we then obtain conditions listed in Eq. (23) for the existence of MC phase.

From Eqs. (15-16), one can verify that in MC phase, derivatives of single species density ρ_1 and ρ_2 are as follows,

$$\begin{aligned}\partial_x \rho_1(x) &= e^{2\Omega(x_\alpha - x)}(\Omega_{1,A} - 2\Omega\rho_{\alpha,1}(x_\alpha)), \\ \partial_x \rho_2(x) &= e^{2\Omega(x_\alpha - x)}(\Omega_{2,A}/q - 2\Omega\rho_{\alpha,2}(x_\alpha)).\end{aligned}$$

By substituting expressions of x_α and $\rho_{\alpha,k}(x)$, see Eqs. (17, 18), we obtain

$$\begin{aligned}\partial_x \rho_1(x) &= 2e^{2\Omega(x_\alpha - x)}(\Omega_{1,A}\alpha_2 - \Omega_{2,A}\alpha_1)/q, \\ \partial_x \rho_2(x) &= 2e^{2\Omega(x_\alpha - x)}(\Omega_{2,A}\alpha_1 - \Omega_{1,A}\alpha_2)/q.\end{aligned}$$

Which implies that, if total density ρ is in MC phase, i.e., $\rho \equiv 1/2$ (see Fig. 4), the value of $\Omega_{1,A}\alpha_2 - \Omega_{2,A}\alpha_1$ is essential to determine the monotonicity of single species densities ρ_1 and ρ_2 .

Depends on values of rates α_k and $\Omega_{k,A}$, even if the total density ρ is constant in certain interval, single species density ρ_k may not be, and they may increase or decrease in this interval. This is different from the cases in which density ρ is in LD or HD phase. For those cases, both ρ_1 and ρ_2 increase with x , and with slopes $\Omega_{1,A}$ and $\Omega_{2,A}/q$, respectively, see Eqs. (13,14). For the cases in which total density ρ is constant, if $\Omega_{1,A}\alpha_2 - \Omega_{2,A}\alpha_1 > 0$ then ρ_1 has positive slope, i.e. increases along the motion track, while ρ_2 has negative slope. Both ρ_1, ρ_2 are all constants iff $\Omega_{1,A}\alpha_2 - \Omega_{2,A}\alpha_1 = 0$, see Fig. 4. Finally, previous analysis shows that, for $K = 1$, there exists DW iff $|\alpha - \beta| < \Omega$ and $\alpha + \beta + \Omega < 1$. The DW lies at $x_w = (\Omega + \beta - \alpha)/(2\Omega)$ with height $\Delta = 1 - \alpha - \beta - \Omega$. The DW height of single species density ρ_k can be obtained by $\Delta_k = [\rho_k(x_w^-)/\rho(x_w^-)]\Delta$, see Eqs. (10,11,13,14).

5. Methods to obtain particle densities ρ_1, ρ_2 : general cases $K > 1$

As mentioned in [9], due to particle-hole symmetry, this study only discusses the “TASEP-LK” process with $K \geq 1$. For these general cases, the idea used in the special cases with $K = 1$ can also be employed to get the single special density ρ_k . Roughly speaking, the method of obtaining densities ρ_1, ρ_2 of the two particle species is to use Eq. (7) and the solution of total density ρ , as well as the key relationship $\rho_1(x_w^-)/\rho_2(x_w^-) = \rho_1(x_w^+)/\rho_2(x_w^+)$ at locations x_w of domain wall or boundary layers.

After the total density $\rho(x)$ has been obtained, there are also four steps needed to get single species density $\rho_{\alpha,k}(x)$. (1) Get left solutions $\rho_{\alpha,1}$ and $\rho_{\alpha,2}$ in interval

Figure 4. (Color online) Typical examples of densities ρ, ρ_1, ρ_2 , in which maximal current (MC) phase appears in total density ρ . In the MC phase of ρ , i.e., $\rho = 1/2$, densities ρ_1, ρ_2 of single particle species may be constants, or increase/decrease along the motion track, which depends on the sign of $\Omega_{1,A}\alpha_2 - \Omega_{2,A}\alpha_1$. For $\Omega_{1,A}\alpha_2 - \Omega_{2,A}\alpha_1 > 0$, ρ_1 increases along the track (a). While for $\Omega_{1,A}\alpha_2 - \Omega_{2,A}\alpha_1 < 0$, ρ_1 decreases along the track (b). For special cases, $\Omega_{1,A}\alpha_2 - \Omega_{2,A}\alpha_1 = 0$, both ρ_1 and ρ_2 are constants when total density ρ is in the MC phase (c,d). Line types in this figure are the same as in Fig. 1.

$(-\infty, x_w)$ from Eq. (7) with boundary conditions $\rho_{\alpha,1}(0) = \alpha_1$ and $\rho_{\alpha,2}(0) = \alpha_2/q$, respectively. (2) Use $\rho_{\beta,k}(x_w^+) = \rho_{\alpha,k}(x_w^-) + \Delta_k = \rho(x_w^+) \rho_{\alpha,k}(x_w^-) / \rho(x_w^-)$ to get the value of density $\rho_{\beta,k}(x)$ at $x = x_w^+$. (3) Use $\rho_{\beta,k}(x_w^+)$ as the boundary condition to get the right solutions $\rho_{\beta,1}$ and $\rho_{\beta,2}$ in interval $(x_w, 1)$. (4) Get single species density by confining $\rho_{\alpha,k}$ and $\rho_{\beta,1}$ in interval $[0, 1]$, and connect them at location x_w .

The method to get total particle density ρ is similar to that used in special cases $K = 1$, but with the help of Lambert W function, see Fig. 5 and for details see [36]. In brief, left solution $\rho_\alpha(x)$ and right solution $\rho_\beta(x)$, which satisfy Eq. (8) with left and right boundary conditions respectively, should be obtained firstly. Then based on the continuity of J and J_k , location x_w of domain wall can be determined (x_w may lie outside the interval $[0, 1]$). Finally total density ρ is obtained by linking $\rho_\alpha(x)$ and $\rho_\beta(x)$ at location x_w , and restricting the new linked function in interval $[0, 1]$.

For general cases $K > 1$, the equation of total density reads

$$-\partial_x[\rho(1 - \rho)] + K\Omega(1 - \rho) - \Omega\rho = 0, \quad (24)$$

with boundary conditions $\rho(0) = \alpha$ and $\rho(1) = 1 - \beta$. On the other hand, densities of the two single species satisfy

$$-\partial_x[\rho_1(1 - \rho)] + K_1\Omega(1 - \rho) - \Omega\rho_1 = 0, \quad (25)$$

$$-\partial_x[\rho_2(1 - \rho)] + K_2\Omega(1 - \rho) - \Omega\rho_2 = 0, \quad (26)$$

Figure 5. (Color online) The real branches $W_0(\xi)$ and $W_{-1}(\xi)$ of Lambert W function.

where $K_1\Omega = \Omega_{1,A}$ and $K_2\Omega = \Omega_{2,A}/q$. From Eq. (24), we get

$$\partial_x \rho = \frac{K - (K+1)\rho}{1 - 2\rho} \Omega. \quad (27)$$

Substituting Eq. (27) into Eqs. (25,26) we then obtain

$$\partial_x \rho_1 + P(x)\rho_1 = K_1\Omega,$$

$$\partial_x \rho_2 + P(x)\rho_2 = K_2\Omega,$$

where $P(x) = \frac{(K-1)\Omega}{2\rho-1}$. So the general solutions of ρ_1 and ρ_2 are

$$\rho_1 = e^{-\int P(x)dx} \left[c_1 + \int K_1\Omega e^{\int P(x)dx} \right], \quad (28)$$

$$\rho_2 = e^{-\int P(x)dx} \left[c_2 + \int K_2\Omega e^{\int P(x)dx} \right], \quad (29)$$

where constant c_k can be determined by the boundary condition at $x = 0$ or $x = 1$.

Similar as in [36], to obtain the total density $\rho(x)$, a rescaled density $\sigma(x)$ is introduced as follows,

$$\sigma(x) = \frac{K+1}{K-1} [2\rho(x) - 1] - 1. \quad (30)$$

It can be easily verified that $\sigma(x)$ satisfies

$$\partial_x \sigma(x) + \partial_x \ln |\sigma(x)| = \Omega \frac{(K+1)^2}{K-1}.$$

By integration we get

$$|\sigma(x)| \exp\{\sigma(x)\} = Y(x), \quad (31)$$

where the function $Y(x)$ is

$$Y(x) = |\sigma(x_0)| \exp \left\{ \Omega \frac{(K+1)^2}{K-1} (x - x_0) + \sigma(x_0) \right\}.$$

In which, x_0 is usually chosen as $x_0 = 0$ or $x_0 = 1$, where the density $\rho(x_0)$ and consequently $\sigma(x_0)$ is known. By matching left or right boundary condition, corresponding expression of $Y(x)$ can be obtained, denoted by $Y_\alpha(x)$ or $Y_\beta(x)$ respectively. Then the function $\sigma(x)$, denoted by $\sigma_\alpha(x)$ and $\sigma_\beta(x)$ correspondingly, can be obtained from Eq. (31). Note that the special case $\sigma(x) = 0$ corresponds to the Langmuir isotherm $\rho(x) = \rho_l = K/(K+1)$.

Equation like Eq. (31) is known to have an explicit solution written in terms of a special function called W function, see Refs. [38, 36] and Fig. 5. The W function, obtained by $W(\xi) \exp[W(\xi)] = \xi$, is a multivalued function with two real branches, which are usually denoted as $W_0(\xi)$ and $W_{-1}(\xi)$. The first branch, $W_0(\xi)$, is defined for $\xi \geq -1/e$; it diverges at infinity sublogarithmically. The second branch, $W_{-1}(\xi)$, is always negative and defined in the domain $-1/e \leq \xi \leq 0$. Using these properties of Lambert W function, the branch of W is selected according to the value of rescaled density σ .

As have been discussed in [13, 36], there exists left boundary layer if $\alpha > 1/2$. Therefore, we have the following left rescaled solution only when $0 \leq \alpha \leq 1/2$,

$$\sigma_\alpha(x) = W_{-1}(-Y_\alpha(x)) < 0. \quad (32)$$

For the right rescaled solution $\sigma_\beta(x)$, we have

$$\sigma_\beta(x) = \begin{cases} W_0(Y_\beta(x)) > 0, & 0 \leq \beta < 1 - \rho_l, \\ 0, & \beta = 1 - \rho_l, \\ W_0(-Y_\beta(x)) < 0, & 1 - \rho_l < \beta \leq 1/2, \\ W_0(-Y_{\beta=1/2}(x)) < 0 & \beta > 1/2. \end{cases} \quad (33)$$

We note that, due to the existence of right boundary layer, when $\beta > 1/2$, the right solution $\sigma_\beta(x)$ is only an approximation.

So far, total densities $\rho_\alpha(x)$ and $\rho_\beta(x)$, which satisfy left and right boundary conditions respectively, can be obtained from Eq. (32) and Eq. (33). The domain wall location x_w can be determined by the continuity of J and J_k , which implies $\rho_\alpha(x_w) + \rho_\beta(x_w) = 1$, or equivalently $\sigma_\alpha(x_w) + \sigma_\beta(x_w) = -2$. If there exists left boundary layer, especially when $\alpha > 0.5$, we set $x_w = 0$. Meanwhile, if there exists right boundary layer, especially in low density phase, we set $x_w = 1$.

The continuity of J at x_w gives

$$\rho_\alpha(x_w)[1 - \rho_\alpha(x_w)] = J_\alpha(x_w) = J_\beta(x_w) = \rho_\beta(x_w)[1 - \rho_\beta(x_w)].$$

While the continuity of J_k at x_w means

$$\rho_{\alpha,k}(x_w)[1 - \rho_\alpha(x_w)] = J_{\alpha,k}(x_w) = J_{\beta,k}(x_w) = \rho_{\beta,k}(x_w)[1 - \rho_\beta(x_w)].$$

Therefore,

$$\frac{\rho_{\alpha,k}(x_w)}{\rho_\alpha(x_w)} = \frac{\rho_{\beta,k}(x_w)}{\rho_\beta(x_w)}, \quad (34)$$

and the height of domain walls Δ, Δ_k of total density and single species density satisfy

$$\begin{aligned}\Delta_k &= \rho_k(x_w^+) - \rho_k(x_w^-) = \rho_{\beta,k}(x_w) - \rho_{\alpha,k}(x_w) \\ &= \frac{\rho_{\alpha,k}(x_w)}{\rho_{\alpha}(x_w)} [\rho_{\beta}(x_w) - \rho_{\alpha}(x_w)] = \frac{\rho_k(x_w)}{\rho(x_w)} [\rho(x_w^+) - \rho(x_w^-)] \\ &= \frac{\rho_k(x_w)}{\rho(x_w)} \Delta = \frac{\rho_{\alpha,k}(x_w)}{\rho_{\alpha}(x_w)} \Delta = \frac{\rho_{\beta,k}(x_w)}{\rho_{\beta}(x_w)} \Delta = \frac{\rho_k(x_w)}{\rho(x_w)} \Delta.\end{aligned}\quad (35)$$

After getting total density ρ and its domain wall location x_w , single species density ρ_1 and ρ_2 can be obtained by the following process. The left solution $\rho_{\alpha,k}(x)$ in domain $[0, x_w]$ can be obtained from Eqs. (28,29) by matching left boundary conditions,

$$\begin{aligned}\rho_{\alpha,1}(x) &= e^{-\int_0^x P_{\alpha}(x)dx} \left[\alpha_1 + \int_0^x K_1 \Omega e^{\int_0^x P_{\alpha}(x)dx} \right], \\ \rho_{\alpha,2}(x) &= e^{-\int_0^x P_{\alpha}(x)dx} \left[\frac{\alpha_2}{q} + \int_0^x K_2 \Omega e^{\int_0^x P_{\alpha}(x)dx} \right].\end{aligned}$$

Substituting the expression of $P_{\alpha}(x)$ into the above two equations, and using Eq. (27), we obtain that, for $0 \leq \alpha < 0.5 \neq \rho_l$,

$$\rho_{\alpha,1}(x) = \frac{K_1}{K} \rho_{\alpha}(x) + \gamma_1 |\rho_{\alpha}(x) - \rho_l|^{\frac{1-K}{1+K}}, \quad (36)$$

$$\rho_{\alpha,2}(x) = \frac{K_2}{K} \rho_{\alpha}(x) + \gamma_2 |\rho_{\alpha}(x) - \rho_l|^{\frac{1-K}{1+K}}, \quad (37)$$

where

$$\gamma_1 = |\alpha - \rho_l|^{\frac{K-1}{K+1}} \left[\alpha_1 - \frac{K_1}{K} \alpha \right], \quad \gamma_2 = |\alpha - \rho_l|^{\frac{K-1}{K+1}} \left[\frac{\alpha_2}{q} - \frac{K_2}{K} \alpha \right].$$

Now, using $\rho_{\beta,k}(x_w) = \frac{\rho_{\alpha,k}(x_w)}{\rho_{\alpha}(x_w)} \rho_{\beta}(x_w)$ as boundary condition, the right solution $\rho_{\beta,k}(x)$ in interval $[x_w, 1]$ can be obtained. For $\beta \neq 1 - \rho_l$, we obtain that

$$\rho_{\beta,1}(x) = \frac{K_1}{K} \rho_{\beta}(x) + \delta_1 |\rho_{\beta}(x) - \rho_l|^{\frac{1-K}{1+K}}, \quad (38)$$

$$\rho_{\beta,2}(x) = \frac{K_2}{K} \rho_{\beta}(x) + \delta_2 |\rho_{\beta}(x) - \rho_l|^{\frac{1-K}{1+K}}, \quad (39)$$

where

$$\begin{aligned}\delta_1 &= |\rho_{\beta}(x_w) - \rho_l|^{\frac{K-1}{K+1}} \left[\rho_{\beta,1}(x_w) - \frac{K_1}{K} \rho_{\beta}(x_w) \right], \\ \delta_2 &= |\rho_{\beta}(x_w) - \rho_l|^{\frac{K-1}{K+1}} \left[\rho_{\beta,2}(x_w) - \frac{K_2}{K} \rho_{\beta}(x_w) \right].\end{aligned}$$

When $\beta = 1 - \rho_l$, the right solution in domain $[x_w, 1]$ will be

$$\rho_{\beta,1}(x) = \frac{K_1}{K} \rho_l + e^{(K+1)\Omega(x_w-x)} \times \left[\rho_{\beta,1}(x_w) - \frac{K_1}{K} \rho_l \right], \quad (40)$$

$$\rho_{\beta,2}(x) = \frac{K_2}{K} \rho_l + e^{(K+1)\Omega(x_w-x)} \times \left[\rho_{\beta,2}(x_w) - \frac{K_2}{K} \rho_l \right]. \quad (41)$$

Finally, we want to point out that the relationship presented in Eq. (34) also holds at left boundary layer, which is needed to get single species density ρ_k when there exist left boundary layer in total density ρ . To get intuitive impressions of properties of the

Figure 6. (Color online) Typical examples of densities ρ, ρ_1 and ρ_2 for general cases $K > 1$. In all calculations $K_1 = 1, K_2 = 0.5, \Omega = 0.1$ are used. The four figures in the first row show that, with the decrease of leaving rate β , densities ρ, ρ_1 and ρ_2 change from LD phase to phase with domain wall. The figures in the second row show that, with the decrease of β , the location x_w of domain wall moves to the left, see [37]. The last row includes examples with effective entrance rate $\alpha > 0.5$. The phase of density ρ in each figure is as follows. (a) LD-BL $_r^-$, (b,c) LD-BL $_r^+$, (d) LD-DW-HD $_1$, (e) LD-DW-HD $_2$ -BL $_r^-$, (f,g) LD-DW-HD $_2$, (h) LD-DW- ρ_l , (i) BL $_l^-$ -M-BL $_r^-$, (j) BL $_l^-$ -M, (k) BL $_l^-$ - ρ_l , (l) BL $_l^+$ -HD $_1$. Line types in this figure are the same as in Fig. 1.

two-species TASEP for general cases $K > 1$, typical examples of density ρ, ρ_1 and ρ_2 are plotted in Fig. 6.

In summary, the main process to obtain single species densities $\rho_1(x), \rho_2(x)$ is as follows. Total density ρ , as well as locations of its DW and BLs, can be obtained from Eq. (8) with boundary conditions $\rho(0) = \alpha = \alpha_1 + \alpha_2/q$ and $\rho(1) = 1 - \beta = 1 - \beta_1 = 1 - \beta_2/q$. Then single species density ρ_1 and ρ_2 in interval $[0, x_w)$ can be obtain from Eq. (7) with left boundary condition $\rho_1(0) = \alpha_1$ and $\rho_2(0) = \alpha_2/q$ respectively. Finally, density ρ_k in interval $(x_w, 1]$ can be obtained from Eq. (7) with left boundary condition $\rho_k(x_w^+)$, which is given by $\rho_k(x_w^+) = \rho_k(x_w^-) + \Delta_k$. The main difference from that in special cases $K = 1$ is that Lambert function [38] should be employed to help to get densities ρ and ρ_k .

For $K > 1$, properties of total density ρ are similar as those of the one-species “TASEP-LK” process [9, 13], i.e. there may exist left or right boundary layer, domain wall, or “Meissner” (M) phase. Here “Meissner” phase means that density ρ satisfies $1/2 < \rho < \rho_l = K/(K + 1)$, and is independent of initiation rate α and leaving rate β , see Fig. 6(i,j). Properties of single species density ρ_k may be different from ρ . For example, if ρ lies in $[0, 1/2]$ or $[\rho_l, 1]$, it will increase along the track. Otherwise, ρ will

decrease along the track. This is because that $\partial_x \rho = (K+1)\Omega(\rho - \rho_l)/(2\rho - 1)$, see Eq. (27). Therefore, if there exists DW in $(0, 1)$ and the leaving rate $1 - \rho_l < \beta < 1$, then after DW location x_w , density ρ decreases monotonically. Otherwise, if $0 < \beta < 1 - \rho_l$, ρ will increase after DW location x_w . However, the numerical results show that, after DW location x_w , the monotonicity of ρ_k may be different from those of ρ .

6. Monotonicity of single species density ρ_1 and ρ_2 when total density $\rho \equiv \rho_l$ is constant for general cases $K > 1$

Previous analysis about special cases $K = 1$ has shown that, if total density ρ is in MC phase, i.e. $\rho \equiv 1/2$ is constant, then single species density ρ_k may not be constant. Similar results hold for the general $K > 1$ cases. For $K > 1$, if $\beta = 1 - \rho_l$ then total density $\rho(x) = \rho_\beta(x)$ is constant in interval $[x_w, 1]$, $\rho \equiv \rho_l$ with $\rho_l = K/(K+1)$. But, similar as those in special cases $K = 1$, the corresponding single species densities ρ_1 and ρ_2 may not be constant. From Eqs. (40,41), we have

$$\partial \rho_{\beta,1}(x)/\partial x = -(K+1)\Omega \left[\rho_{\beta,1}(x_w) - \frac{K_1}{K}\rho_l \right] e^{(K+1)\Omega(x_w-x)}, \quad (42)$$

and

$$\partial \rho_{\beta,2}(x)/\partial x = -(K+1)\Omega \left[\rho_{\beta,2}(x_w) - \frac{K_2}{K}\rho_l \right] e^{(K+1)\Omega(x_w-x)}. \quad (43)$$

For these special cases, $\rho(x_w^+) = \rho_l = K/(K+1)$, $\rho(x_w^-) = 1 - \rho(x_w^+) = 1 - \rho_l = 1/(K+1)$. So $\rho_{\beta,k}(x_w) = \rho_{\alpha,k}(x_w)\rho(x_w^+)/\rho(x_w^-) = K\rho_{\alpha,k}(x_w)$. From Eqs. (36,37), we get

$$\begin{aligned} \rho_{\alpha,k}(x_w) &= \frac{K_k}{K}\rho_{\alpha}(x_w) + \gamma_k |\rho_{\alpha}(x_w) - \rho_l|^{\frac{1-K}{1+K}} \\ &= \frac{K_k}{K(K+1)} + \left[\frac{\alpha_k}{q^{k-1}} - \frac{K_k}{K}\alpha \right] \left| \frac{\alpha - \rho_l}{\rho_{\alpha}(x_w) - \rho_l} \right|^{\frac{K-1}{1+K}} \\ &= \frac{K_k}{K(K+1)} + \left[\frac{\alpha_k}{q^{k-1}} - \frac{K_k}{K} \left(\alpha_1 + \frac{\alpha_2}{q} \right) \right] \times \left| \frac{K-(K+1)\alpha}{K-1} \right|^{\frac{K-1}{1+K}}. \end{aligned} \quad (44)$$

Therefore,

$$\begin{aligned} \rho_{\beta,k}(x_w) - \frac{K_k}{K}\rho_l &= K\rho_{\alpha,k}(x_w) - \frac{K_k}{K+1} \\ &= K \left[\frac{\alpha_k}{q^{k-1}} - \frac{K_k}{K} \left(\alpha_1 + \frac{\alpha_2}{q} \right) \right] \left| \frac{K-(K+1)\alpha}{K-1} \right|^{\frac{K-1}{1+K}} \\ &= \left[(K_1 + K_2) \frac{\alpha_k}{q^{k-1}} - K_k \left(\alpha_1 + \frac{\alpha_2}{q} \right) \right] \left| \frac{K-(K+1)\alpha}{K-1} \right|^{\frac{K-1}{1+K}} \\ &=: \left[(K_1 + K_2) \frac{\alpha_k}{q^{k-1}} - K_k \left(\alpha_1 + \frac{\alpha_2}{q} \right) \right] C(\alpha, K), \end{aligned} \quad (45)$$

where $C(\alpha, K) > 0$ for $K > 1$ and $\alpha < \rho_l = K/(K+1)$. So

$$\rho_{\beta,1}(x_w) - \frac{K_1}{K}\rho_l = \left[K_2\alpha_1 - \frac{K_1\alpha_2}{q} \right] C(\alpha, K) = \frac{\Omega_{2,A}\alpha_1 - \Omega_{1,A}\alpha_2}{q\Omega} C(\alpha, K), \quad (46)$$

and

$$\rho_{\beta,2}(x_w) - \frac{K_2}{K}\rho_l = \left[\frac{K_1\alpha_2}{q} - K_2\alpha_1 \right] C(\alpha, K) = \frac{\Omega_{1,A}\alpha_2 - \Omega_{2,A}\alpha_1}{q\Omega} C(\alpha, K). \quad (47)$$

Finally, from Eqs. (42,46) and Eqs. (43,47), we concluded that, when total density $\rho \equiv \rho_l$ is constant, the monotonicity of ρ_1 and ρ_2 depends on the value of $\Omega_{1,A}\alpha_2 - \Omega_{2,A}\alpha_1$.

The same as in the special $K = 1$ cases, if $\Omega_{1,A}\alpha_2 - \Omega_{2,A}\alpha_1 > 0$ then ρ_1 increases while ρ_2 decreases along the motion track. In contrast, if $\Omega_{1,A}\alpha_2 - \Omega_{2,A}\alpha_1 < 0$ then ρ_1 decreases while ρ_2 increases. Both ρ_1 and ρ_2 are constants iff $\Omega_{1,A}\alpha_2 - \Omega_{2,A}\alpha_1 = 0$, and in such cases $\rho_1 = K_1/(K + 1)$ and $\rho_2 = K_2/(K + 1)$ in interval $[x_w, 1]$, see Fig. 7.

Figure 7. (Color online) Typical examples of densities ρ, ρ_k for $\beta = 1 - \rho_l$. For these cases, near right boundary $x = 1$, total density ρ is constant. Besides parameter values given in the legends, we set $\Omega = 0.1$ and $K = 1.5$, therefore $\rho_l = K/(K + 1) = 0.6$. Although total density ρ is constant, single species densities ρ_1 and ρ_2 may not be. In the same way as in special cases $K = 1$, the monotonicity of ρ_k is determined by the sign of $\Omega_{1,A}\alpha_2 - \Omega_{2,A}\alpha_1$. For a positive value of it, ρ_1 will increase, while ρ_2 will decrease, along the track (when ρ is constant). In (a,b,c), ρ_1 increases while ρ_2 decreases. In (d,e), the same as the total density ρ , both ρ_1 and ρ_2 are also constants. In contrast, in (f), ρ_1 decreases while ρ_2 increases. (c,e) are examples with domain wall, and (b) is an example where there exists boundary layer. Line types in this figure are the same as in Fig. 1

For these general cases $K > 1$, examples of phase diagram of total density ρ in (α, β) plane are plotted in Fig. 8(a,b,c). The same as in the one-species “TASEP-LK”, BL may appear at one or both of the two boundaries. DW may appear in interval $(0, 1)$, and density ρ may be in LD phase ($\rho < 1/2$) or HD phase ($\rho > 1/2$). To show more details about the “TASEP-LK” process, in Fig. 8 the HD phase is divided into two different cases, HD₁ phase ($1/2 < \rho < \rho_l = K/(K + 1)$) and HD₂ phase ($\rho > \rho_l$). From the phase diagram in (α, β) plane, phase diagrams in any planes of parameter pair (σ_1, σ_2) can be easily obtained, where $\sigma_k = \alpha_1, \alpha_2, \beta_1, \beta_2$. Examples of phase diagram in (α_1, α_2) plane are plotted in Fig. 8(d,e,f), which are corresponding to the dotted horizontal lines in Fig. 8(a,b,c) respectively. The above discussion about the relationship between total density ρ and single species density ρ_k implies that phase diagrams of density ρ_k are topologically equivalent to those of the total density ρ .

Figure 8. (Color online) Phase diagrams of total density ρ obtained by stationary mean-field Eq. (8) for $K > 1$. Parameter values used in calculations are $\Omega = 0.1$, $K = 1.5$ for (a,d); $\Omega = 0.15$, $K = 1.5$ for (b,e); and $\Omega = 0.1$, $K = 4$ for (c,f). (d,e,f) are phase diagrams in (α_1, α_2) -plane with leaving rate $\beta = 0.45, 0.7, 0.3$, i.e., corresponding to horizontal dotted lines in (a,b,c), respectively. The meanings of Roman numerals in each connected area of figures are as follows. (1) I:=LD-BL $_r^+$, which means that density ρ is in LD phase, and there exists *right* boundary layer (BL) in which ρ *increases* sharply, i.e. $\rho(1) > \rho(1 - \epsilon)$ for small real number ϵ . (2) II:=LD-BL $_r^-$, i.e., ρ is in LD phase, and it *decreases* sharply at right boundary. (3) III:=LD-DW-HD $_1$, near left boundary density ρ is in low density phase, while near right boundary ρ is in high density phase, and there exists DW between these two phases. Here “HD $_1$ ” means $\rho > \rho_l$, i.e., $\beta < 1 - \rho_l$. (4) IV:=LD-DW-HD $_2$, where HD $_2$ means that density ρ is between 0.5 and ρ_l , i.e., $1 - \rho_l < \beta < 0.5$. (5) V:=LD-DW-M $_r$, where M $_r$ means that density ρ is between 0.5 and ρ_l but its value is independent of right boundary condition, therefore right BL appears. M $_r$ can be regarded as the right half part of “Meissner” phase. For this phase, $\beta > 0.5$. (6) VI:=BL $_l^+$ -HD $_1$, i.e., $\rho > \rho_l$ and ρ increases in left BL. (7) VII:=BL $_l^+$ -HD $_2$. (8) VIII:=M $^+$, which means that ρ is in “Meissner” phase and it increases in left BL. (9) IX:=BL $_l^-$ -HD $_1$. (10) X:=BL $_l^-$ -HD $_2$. (11) XI:=BL $_l^-$ -M. VIII and XI are two species cases of “Meissner” phase. For examples of density ρ which is in one of the above eleven phases, see Fig. 6.

7. Conclusions

In summary, “TASEP-LK” process with two particle species is discussed in this study. Unlike the previous studies about two-species TASEP, particle attachment/detachment to/from bulk sites of motion track is allowed. Both of the two particle species enter into the track from the same boundary, and move unidirectionally to the same direction. The two particle species do not change to each other, and do not exchange their locations even if they are adjacent to each other [20, 21, 23, 29].

This study found that, domain walls and boundary layers of total particle density and single species densities always appear simultaneously. The height of domain wall of total density is equal to the summation of those of the two single species. More interestingly, the ratio of particle densities from different species does not change when coming across the domain wall. Which implies that the motion of different particle species along the same track will be jammed at the same position, and with the same probability. Based on these properties, theoretical methods to obtain steady state densities of the two particle species are presented. Our results show that properties of single species densities may be different from that of the total particle density.

In this study, phase diagrams of particle density in typical parameter planes are also presented. The methods presented in this study are also available to the analysis of “TASEP-LK” process including more than two particle species, since for any particle species, the domain wall of its density will always appear at the same position, and ratios of densities of any two particle species always hold unchanged before and after the position of domain wall. The results of this study are also helpful to further understandings of the biophysical process of cargo transportation in living cells, where one single protofilament of microtubule is actually occupied by various kinds of cargos and motor proteins [39, 15].

acknowledgments

This study was supported by the Natural Science Foundation of China (Grant No. 11271083), and the National Basic Research Program of China (National “973” program, project No. 2011CBA00804).

References

- [1] O. J. O’Loan, M. R. Evans, and M. E. Cates. Jamming transition in a homogeneous one-dimensional system: The bus route model. *Phys. Rev. E*, 58:1404–1418, 1998.
- [2] A. Nagar, A. Valleriani, and R. Lipowsky. Translation by ribosomes with mrna degradation: Exclusion processes on aging tracks. *J. Stat. Phys.*, 145:1385–1404, 2011.
- [3] Cécile Leduc, Kathrin Padberg-Gehle, Vladimír Varga, Dirk Helbing, Stefan Diez, and Jonathon Howard. Molecular crowding creates traffic jams of kinesin motors on microtubules. *Proc. Natl. Acad. Sci. USA*, 109:6100–6105, 2012.
- [4] Julien Racle, Flora Picard, Laurence Girbal, Muriel Coccagn-Bousquet, and Vassily Hatzimanikatis. A genome-scale integration and analysis of *lactococcus lactis* translation data. *PLOS Computational Biology*, 9:e1003240, 2013.
- [5] Paul C. Bressloff and Jay M. Newby. Stochastic models of intracellular transport. *Reviews of Modern Physics*, 85:135–196, 2013.
- [6] Debashish Chowdhury. Stochastic mechano-chemical kinetics of molecular motors: A multidisciplinary enterprise from a physicist’s perspective. *Physics Reports*, 529:1–197, 2013.
- [7] B. Derrida, E. Domany, and D. Mukamel. An exact solution of a one-dimensional asymmetric exclusion model with open boundaries. *Journal of Statistical Physics*, 69:667–687, 1992.
- [8] A. B. Kolomeisky, E. B. Kolomeisky G. M. Schütz, and J. P. Straley. Phase diagram of one-dimensional driven lattice gases with open boundaries. *J. Phys. A: Math. Gen.*, 31:6911–6919, 1998.

- [9] A. Parmeggiani, T. Franosch, and E. Frey. Phase coexistence in driven one-dimensional transport. *Phys. Rev. Lett.*, 90:086601, 2003.
- [10] Ekaterina Pronina and Anatoly B Kolomeisky. Theoretical investigation of totally asymmetric exclusion processes on lattices with junctions. *Journal of Statistical Mechanics: Theory and Experiment*, 7:P07010, 2005.
- [11] P. Greulich, A. Garai, K. Nishinari, A. Schadschneider, and D. Chowdhury. Intracellular transport by single-headed kinesin KIF1A: Effects of single-motor mechanochemistry and steric interactions. *Phys. Rev. E*, 75:041905, 2007.
- [12] R A Blythe and M R Evans. Nonequilibrium steady states of matrix-product form: a solver's guide. *Journal of Physics A: Mathematical and Theoretical*, 40:R333–R441, 2007.
- [13] Yunxin Zhang. Microtubule length dependence of motor traffic in cells. *Eur. Phys. J. E*, 35:101, 2012.
- [14] Chihiro Matsui. Multi-state asymmetric simple exclusion processes. *Journal of Statistical Physics*, 158:158–191, 2015.
- [15] R. D. Vale. The molecular motor toolbox for intracellular transport. *Cell*, 112:467–480, 2003.
- [16] F. C. Alcaraz, S. Damahapatra, and V. Rittenberg. n -species stochastic models with boundaries and quadratic algebras. *Journal of Physics A: Mathematical and General*, 31:845–878, 1998.
- [17] M. E. Fouladvand and F. Jafarpour. Multi-species asymmetric exclusion process in ordered sequential update. *Journal of Physics A: Mathematical and General*, 32:5845–5867, 1999.
- [18] P. Ferrari and J. Martin. Stationary distributions of multi-type totally asymmetric exclusion processes. *Ann. Probab.*, 35:807–832, 2007.
- [19] C. Arita and K. Mallick. Matrix product solution of an inhomogeneous multi-species TASEP. *Journal of Physics A: Mathematical and General*, 46:085002, 2013.
- [20] M. R. Evans, I. D. P. Foster, C. Godrèche, and D. Mukameil. Asymmetric exclusion model with two species: Spontaneous symmetry breaking. *Journal of Statistical Physics*, 80:69–102, 1995.
- [21] M. Mobilia and P.-A. Bares. Soluble two-species diffusion-limited models in arbitrary dimensions. *Physical Review E*, 63:036121, 2001.
- [22] P. F. Arndt and V. Rittenberg. Spontaneous breaking of translational invariance and spatial condensation in stationary states on a ring. II. the charged system and the two-component Burgers equations. *J. Stat. Phys.*, 107:989–1013, 2002.
- [23] G. M. Schütz. Critical phenomena and universal dynamics in one-dimensional driven diffusive systems with two species of particles. *Journal of Physics A: Mathematical and General*, 36:R339–R379, 2003.
- [24] S. Klumpp and R. Lipowsky. Phase transitions in systems with two species of molecular motors. *Europhys. Lett.*, 66:90–96, 2004.
- [25] R. Juhász. Weakly coupled, antiparallel, totally asymmetric simple exclusion processes. *Phys. Rev. E*, 76:021117, 2007.
- [26] E. Pronina and A. B Kolomeisky. Spontaneous symmetry breaking in two-channel asymmetric exclusion processes with narrow entrances. *J. Phys. A: Math. Theor.*, 40:2275–2286, 2007.
- [27] S. Muhuri and I. Pagonabarraga. Collective vesicle transport on biofilaments carried by competing molecular motors. *Europhys. Lett.*, 84:58009, 2008.
- [28] S. Muhuri and I. Pagonabarraga. Lattice-gas model for active vesicle transport by molecular motors with opposite polarities. *Phys. Rev. E*, 82:021925, 2010.
- [29] Somayeh Zeraati, Farhad H. Jafarpour, and Haye Hinrichsen. Phase transition in an exactly solvable reaction-diffusion process. *Physical Review E*, 87:062120, 2013.
- [30] S. Muhuri. Jamming transition in a driven lattice gas. *Europhys. Lett.*, 106:28001, 2014.
- [31] B. Derrida, S. A. Janowsky, J. L. Lebowitz, and E. R. Speer. Exact solution of the totally asymmetric simple exclusion process: Shock profiles. *Journal of Statistical Physics*, 73:813–842, 1993.
- [32] G. Schutz and E. Domany. Phase transitions in an exactly soluble one-dimensional exclusion process. *Journal of Statistical Physics*, 72:277–296, 1993.

- [33] K. Nishinari, Y. Okada, A. Schadschneider, and D. Chowdhury. Intracellular transport of single-headed molecular motors KIF1A. *Phys. Rev. Lett.*, 95:118101, 2005.
- [34] V. Popkov, A. Rakos, R. D. Willmann, A. B. Kolomeisky, and G. M. Schütz. Localization of shocks in driven diffusive systems without particle number conservation. *Phys. Rev. E*, 67:066117, 2003.
- [35] Y. Zhang. Theoretical analysis of kinesin KIF1A transport along microtubule. *J. Stat. Phys.*, 152:1207–1221, 2013.
- [36] A. Parmeggiani, T. Franosch, and E. Frey. Totally asymmetric simple exclusion process with langmuir kinetics. *Phys. Rev. E.*, 70:046101, 2004.
- [37] Yunxin Zhang. Domain wall of the totally asymmetric exclusion process without particle number conservation. *Chinese Journal of Physics*, 48:607–618, 2010.
- [38] R. Corless, G. Gonnet, D. Hare and D. Jeffrey, and D. Knuth. *Adv. Comput. Math.*, 5:329, 1996.
- [39] J. Howard. *Mechanics of Motor Proteins and the Cytoskeleton*. Sinauer Associates and Sunderland, MA, 2001.