Shock of three-state model for intracellular transport of kinesin KIF1A

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Recently, a three-state model is presented to describe the intracellular traffic of unconventional (single-headed) kinesin KIF1A [Phys. Rev. Lett. 95, 118101 (2005)], in which each motor can bind strongly or weakly to its microtubule track, and each binding site of the track might be empty or occupied by one motor. As the usual two-state model, i.e. the totally asymmetric simple exclusion process (TASEP) with motor detachment and attachment, in steady state of the system, this three-state model also exhibits shock (or domain wall separating the high-density and low density phases) and boundary layers. In this study, using mean-field analysis, the conditions of existence of shock and boundary layers are obtained theoretically. Combined with numerical calculations, the properties of shock are also studied. This study will be helpful to understand the biophysical properties of the collective transport of kinesin KIF1A.

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I. INTRODUCTION

Molecular motors are biogenic force generators acting in the nanometer range. They are responsible for intracellular transport of wide varieties of cargo from one location to another in eukaryotic cells [1–6]. Linear motors produce sliding movements along filamentous structures called protein tracks; for example, myosin slides along actin filament [7–10], kinesin [11–15] and dynein [16–20] along microtubule. Microtubule and filamentary protein actin are protein filaments which form part of a dual-purpose scaffolding called cytoskeleton, act like struts or girders for the cellular architecture and, at the same time, also serve as tracks for the intracellular transportation networks.

However, experiments found, one single filamentary track is usually traveled along by multiple motors. Fundamental understanding of these collective physical phenomena may expose the causes of motor-related diseases (e.g., Alzheimer’s disease). In literatures, these phenomena are usually described by the totally asymmetric simple exclusion process (TASEP), which is originally proposed in [21], consists of particles hopping unidirectionally with hard-core exclusion along a 1D lattice. TASEP is one of many examples for driven systems with stationary nonequilibrium states, which cannot be described in terms of Boltzmann weights. To model the attachment and detachment of motors to and from tracks, Parmeggiani et al [22, 23] discussed a class of driven lattice gas obtained by coupling 1D TASEP to Langmuir kinetics, in which the attachment and detachment of motors is modeled as particle creation and annihilation respectively. Furthermore, Lipowsky et al [24, 25] suggested a more general model, in which the diffusion of motors in the cell is considered explicitly. However, in reality, a motor protein is not a mere particle, but an enzyme whose mechanical movement is coupled with its biochemical cycle. Therefore, recently, a three-state model is presented by Nishinari et al to describe the intracellular transport of single-headed kinesin KIF1A [26, 27]. In which, the microtubule (MT) binding motor might be in two states: strongly MT binding state and weakly MT binding state, denoted by $S, W$ respectively. Biochemically, the strongly binding state corresponds to bare
motor or ATP binding motor state, and the weakly binding state corresponds to ADP binding state.

One of the important feature of the collective motion of motors along one single track is the possible appearance of shock or domain wall, which is defined as the interface between the low-density and high density regions. For the usual two-state TASEP, using mean field method, the existence and properties of the shock have been discussed recently [28]. In this study, similar analysis to the Nishinari’s three-state model will be presented, the efficient and necessary conditions of the existence of shock will be given theoretically, and with the aid of numerical calculations the properties of the shock will also be discussed. The method used in this study can be regarded as a generalization of the one presented in [28].

In the next section, the three-state model and its mean field approximation will be briefly introduced, and then in Sec. III the conditions of the existence of shock will be presented. The existence of boundary layers and the properties of shock will be discussed in Sec. IV and V. Finally, this study will be shortly summarized in Sec. VI.

II. TASEP WITH THREE INTERNAL STATES

The three-state TASEP given in [28] can be mathematically described as follows. Let $S_i$ and $W_i$ denote the probabilities of finding a molecular motor in the states 1 and 2 at the lattice site $i$ at time $t$ respectively (states 1 and 2 correspond to strongly bound and weakly bound states of molecular motors). Then $S_i, W_i$ are governed by the following master equations

$$\frac{dS_i}{dt} = \omega_a (1 - S_i - W_i) - \omega_h S_i - \omega_d S_i + \omega_s W_i + \omega_f W_{i-1}(1 - S_i - W_i) + (1 - c)\omega_f W_i(S_{i+1} + W_{i+1}),$$

(R1)
\[
\frac{dW_i}{dt} = - (\omega_s + \omega_f)W_i(1 - S_{i+1} - W_{i+1}) + \omega_hS_i \\
- \omega_hW_i(2 - S_{i+1} - W_{i+1} - S_{i-1} - W_{i-1}) \\
+ \omega_b(W_i(1 - S_i - W_i),
\]

(2)

where \(\omega_a\) is the rate of a molecular motor binding to the empty lattice site \(i\), i.e. the transition rate of state 0 to state 1, \(\omega_h\) is the transition rate of state 1 to state 2, i.e. the rate of ATP hydrolysis, \(\omega_d\) is the transition rate of state 1 to state 0, i.e. the rate of detachment, \(\omega_b\) is the rate of random Brownian motion. After the release of ADP, the motor steps forward to the next binding site in front with rate \(\omega_f\), stays at the current location with rate \(\omega_s\). \(c\) is an interpolating parameter \((0 \leq c \leq 1)\). The corresponding equations for the left boundary \((i = 1)\) are given by

\[
\frac{dS_1}{dt} = \alpha(1 - S_1 - W_1) - \omega_hS_1 - \gamma_1S_1 + \omega_sW_1 + (1 - c)\omega_fW_1(S_2 + W_2),
\]

(3)

\[
\frac{dW_1}{dt} = - (\omega_s + \omega_f)W_1 + \omega_hS_1 + c\omega_fW_1(S_2 + W_2) \\
+ \omega_bW_2(1 - S_1 - W_1) - \omega_bW_1(1 - S_2 - W_2) - \gamma_2W_1,
\]

(4)

where \(\alpha\) is the rate of attachment of the motors at the left boundary (i.e. the lattice site \(i = 1)\), \(\gamma_1\), \(\gamma_2\) are the rates of detachment of motors in state 1 and state 2 at the left boundary respectively. The equations for the right boundary \((i = N)\) are given by

\[
\frac{dS_N}{dt} = \delta(1 - S_N - W_N) + \omega_fW_{N-1}(1 - S_N - W_N) \\
+ \omega_sW_N - \omega_hS_N - \beta_1S_N,
\]

(5)

\[
\frac{dW_N}{dt} = \omega_hS_N - \omega_sW_N - \beta_2W_N + \omega_bW_{N-1}(1 - S_N - W_N) \\
- \omega_bW_N(1 - S_{N-1} - W_{N-1}),
\]

(6)

where \(\delta\) is the rate of attachment of the motors at the right boundary (i.e. the lattice site \(i = N)\), \(\beta_1\), \(\beta_2\) are the rates of detachment of motors in state 1 and state 2 at the right boundary respectively.

It should be pointed out that the exclusion process described above is different from the one discussed in [29], where multiple occupancy of sites is allowed if particles are
in different internal states. Here, the multiple occupancy is unallowed. However, the particles bounding to the lattice site might be in two different states 1 and 2, corresponding to the strongly bound and weakly bound states. As in [22], attachment and detachment of a motor are modeled as, effectively, creation and annihilation of motors on the lattice. Moreover, the transition between states 1 and 2 is described by the rates $\omega_h$, $\omega_s$, $\omega_f$, the Brownian ratched mechanism is described by rate $\omega_b$.

**Mean Field Approximation:** In the large $N$ limit, we can make the continuum mean field approximation to Eqs. (1) and (2). Let $\Delta x = \frac{1}{N-1}$ and $x = (i - 1)\Delta x$. Obviously, $0 \leq x \leq 1$, since $1 \leq i \leq N$. Using the Taylor expansion

\[
S(x+\Delta x) = S(x) + \sum_{k=1}^{+\infty} \frac{(\pm \Delta x)^k }{k!} \frac{\partial^k S(x)}{\partial x^k}, \quad W(x+\Delta x) = W(x) + \sum_{k=1}^{+\infty} \frac{(\pm \Delta x)^k }{k!} \frac{\partial^k W(x)}{\partial x^k}.
\]

(7)

The continuum limits of Eqs. (1) and (2) are then

\[
\frac{\partial S(x,t)}{\partial t} = \omega_a(1 - S - W) + \omega_s W - (\omega_h + \omega_d) S \\
+ \omega_f \left( W - \Delta x \frac{\partial W(x,t)}{\partial x} \right) (1 - S - W) \\
+ (1 - c)\omega_f W \left( S + W + \Delta x \frac{\partial S(x,t)}{\partial x} + \Delta x \frac{\partial W(x,t)}{\partial x} \right)
\]

(8)

\[
\frac{\partial W(x,t)}{\partial t} = c\omega_f W \left( S + W + \Delta x \frac{\partial S(x,t)}{\partial x} + \Delta x \frac{\partial W(x,t)}{\partial x} \right)
\]

(9)

Thus, the probability density $\rho(x,t) = S(x,t) + W(x,t)$ of finding a molecular motor at lattice site $x$ at time $t$ satisfies [summing Eqs. (8) and (9)]

\[
\frac{\partial \rho(x,t)}{\partial t} = \omega_a(1 - \rho) - \omega_d S + \omega_f \frac{\partial W(\rho - 1)}{\partial x} \Delta x + O(\Delta x^2).
\]

(10)

As the discussion in [30], in the thermodynamic limit $N \to \infty$, there are three regimes to be distinguished. If $\omega_a$ and $\omega_d$ are of order $[1/(N-1)]^\alpha$ with $\alpha < 1$, then at the steady state, the system, Eqs. (9) and (10), reduces to

\[
\begin{cases}
\omega_a(1 - W - S) - \omega_d S = 0, \\
c\omega_f W (S + W) - (\omega_s + \omega_f)W + \omega_h S = 0.
\end{cases}
\]

(11)
So the probability $S$ satisfies

$$ck(k + 1)S^2 + [(k + 1)(l + 1) + n − c(2k + 1)]S + (c − l − 1) = 0,$$  

(12)

and $W = 1 − (k+1)S$, $ρ = S+W$, where $l = ω_s/ω_f$, $n = ω_h/ω_f$, $k = ω_d/ω_a$ (because of the particle-hole symmetry, we restrict the discussion to the case $ω_a ≥ ω_d$, i.e. $0 ≤ k ≤ 1$).

For the cases that $ω_a$ and $ω_d$ are of order $[1/(N − 1)]^α$ but with $α > 1$, the local kinetics is negligible and the system will be

$$\begin{cases} 
W(W + S − 1) = C, \\
cω_f(W(S + W) − (ω_s + ω_f)W + ω_hS = 0
\end{cases}$$

(13)

where the constant $C$ is determined by the left or right boundary conditions. The case of the local rates $ω_a$ and $ω_d$ being of the order $1/(N − 1)$ is the most interesting one, and will be investigated further in this study. In the following, we always assume that the local rates $ω_a$ and $ω_d$ are of the order $1/(N − 1)$.

**III. THE EXISTENCE OF SHOCK**

Let

$$\Omega_a = \frac{ω_a}{Δx}, \quad \Omega_d = \frac{ω_d}{Δx},$$

(14)

then at steady state, the leading terms of $Δx$ of Eqs. (9), (10) are

$$\begin{cases} 
ω_f \frac{∂W(ρ − 1)}{∂x} + Ω_a(1 − ρ) − Ω_dS = 0 \\
cω_f(W(S + W) − (ω_s + ω_f)W + ω_hS = 0
\end{cases}$$

(15)

or

$$\begin{cases} 
ω_f \frac{∂W(ρ − 1)}{∂x} + Ω_a(1 − ρ) − Ω_d(ρ − W) = 0, \\
cω_fWρ − (ω_s + ω_f)W + ω_h(ρ − W) = 0.
\end{cases}$$

(16)

The second equation implies

$$W = \frac{nρ}{n + l + 1 − cρ},$$

(17)
The steady state flux is then proportional to

\[ J = W(1 - \rho) = \frac{n\rho(1 - \rho)}{n + l + 1 - c\rho}. \] (18)

The same as in [27], at the steady state, we can obtain the left boundary conditions

\[ S(0) = \frac{\alpha - [c\alpha(\alpha - \omega_s)/\omega_f]}{c\alpha + \omega_h}, \quad W(0) = \frac{\alpha}{\omega_f}, \] (19)

and the right boundary conditions

\[ S(1) = \frac{\omega_s + \beta}{\omega_h} \left[ \frac{\omega_h}{\omega_h + \omega_s + \beta} - \frac{\beta}{\omega_f} \right], \quad W(1) = \frac{\omega_h}{\omega_h + \omega_s + \beta} - \frac{\beta}{\omega_f}. \] (20)

One can find that Eqs. (16) involves only the first-order derivatives of \( \rho \) and \( W \) with respect to \( x \) whereas there are two sets of boundary conditions (19) and (20). Therefore, if we integrate the equations (16) with the left boundary conditions (19), the solution (denoted by \( \rho_l, W_l, S_l \) respectively) may not, in general, match smoothly with the solution (denoted by \( \rho_r, W_r, S_r \) respectively) obtained for the same equations but with the right boundary conditions (20). This discontinuity corresponds to a shock or domain wall. However, at any position \( x \), the continuity condition of motor flux, or equivalently \( J_l(x) = J_r(x) \), should be satisfied, where \( J_l(x) = W(x-)[1 - \rho(x-)] \) and \( J_r(x) = W(x+)[1 - \rho(x+)] \). At the shock position \( x_s \),

\[
\begin{cases}
W(x_s-) = W_l(x_s), & \rho(x_s-) = \rho_l(x_s), \\
W(x_s+) = W_r(x_s), & \rho(x_s+) = \rho_r(x_s).
\end{cases}
\] (21)

So the continuity condition \( J_l(x_s) = J_r(x_s) \) implies

\[ \frac{n\rho_l(x_s)(1 - \rho_l(x_s))}{n + l + 1 - c\rho_l(x_s)} = J(x_s) = \frac{n\rho_r(x_s)(1 - \rho_r(x_s))}{n + l + 1 - c\rho_r(x_s)}, \] (22)

or

\[ \rho_l(x_s) + \rho_r(x_s) = 1 + \frac{c}{n}J(x_s) = 1 + \gamma\rho_l(x_s)\rho_r(x_s), \] (23)

where \( \gamma = \frac{c}{n+l+1} < 1 \).

From Eqs. (16), one can show the probability \( \rho \) satisfies

\[ (\gamma\rho^2 - 2\rho + 1)\rho_x = \Omega_{ah}(1 - \gamma\rho) \left[ (k + 1)c\rho^2 - \left( \frac{c}{\gamma} + c + k(l + 1) \right) \rho + \frac{c}{\gamma} \right], \] (24)
with \(\Omega_{ah} = \Omega_a/\omega_h\). It can be proved that, for \(0 \leq c \leq 1\) and \(l \geq 0\), the discriminant
\[
\Delta := \left[ \frac{c}{\gamma} + c + k(l + 1) \right]^2 - \frac{4(k + 1)c^2}{\gamma} \geq 0.
\]
So the equation (24) can be reformulated as
\[
(\rho - \rho_3)(\rho - \rho_4)\rho_x = -\Omega_{ah}(k + 1)c(\rho - \rho_0)(\rho - \rho_1)(\rho - \rho_2),
\] (25)
where
\[
\rho_0 = \frac{1}{\gamma}, \quad \rho_{3,4} = \frac{1 \mp \sqrt{1 - \gamma}}{\gamma},
\]
\[
\rho_{1,2} = \frac{\left[ \frac{c}{\gamma} + c + k(l + 1) \right] \mp \sqrt{\left[ \frac{c}{\gamma} + c + k(l + 1) \right]^2 - \frac{4(k + 1)c^2}{\gamma}}}{2(k + 1)c}.
\] (26)
One can easily show that, for \(0 \leq c \leq 1\), \(l \geq 0\) and \(k \geq 0\),
\[
\rho_0 \geq 1, \quad \rho_4 \geq 1, \quad \rho_2 \geq 1, \quad \rho_1 \leq \frac{1}{2} \leq \rho_3 \leq 1.
\] (27)
Particularly,
\[
\rho_1 = \frac{\frac{2c}{\gamma}}{\left[ \frac{c}{\gamma} + c + k(l + 1) \right] \mp \sqrt{\left[ \frac{c}{\gamma} + c + k(l + 1) \right]^2 - \frac{4(k + 1)c^2}{\gamma}}} = \rho_3.
\] (28)
Moreover, one can easily show that the function \(f(x) = x - \sqrt{x^2 - x}\) decreases with \(x \geq 1\) monotonously. So, for \(c \leq (1 - k)(l + 1) + n\),
\[
\rho_1 = \frac{\left[ \frac{c}{\gamma} + c + k(l + 1) \right] - \sqrt{\left[ \frac{c}{\gamma} + c + k(l + 1) \right]^2 - \frac{4(k + 1)c^2}{\gamma}}}{2(k + 1)c} \\
= \frac{(k + 1)(l + 1) + n + c}{2(k + 1)c} - \sqrt{\left( \frac{(k + 1)(l + 1) + n + c}{2(k + 1)c} \right)^2 - \frac{l + n + 1}{(k + 1)c}} \\
\geq \frac{(k + 1)(l + 1) + n + c}{2(k + 1)c} - \sqrt{\left( \frac{(k + 1)(l + 1) + n + c}{2(k + 1)c} \right)^2 - \frac{(k + 1)(l + 1) + n + c}{2(k + 1)c}} \\
\geq \frac{l + n + 1}{c} - \sqrt{\left( \frac{l + n + 1}{c} \right)^2 - \frac{l + n + 1}{c}} = \rho_3.
\] (29)
Therefore, in the following, we always assume that \( \rho_0, \rho_2, \rho_4 \geq 1 \), and \( \frac{1}{2} \leq \rho_3 \leq \rho_1 \leq 1 \).

The general solutions of Eq. (25) are

\[
F(\rho) = x + C, \tag{30}
\]

where \( C \) is an arbitrary constant and

\[
F(\rho) = \frac{1}{\Omega_{ah}(k + 1)c} [A \ln |\rho - \rho_0| + B \ln |\rho - \rho_1| + D \ln |\rho - \rho_2|], \tag{31}
\]

with

\[
A = \frac{\rho_0(\rho_0 - 1)}{\rho_0(\rho_2 - \rho_0)(\rho_2 - \rho_0)}, \quad B = \frac{\rho_1^2 - 2\rho_0\rho_1 + \rho_0}{\rho_0(\rho_1 - \rho_1)(\rho_1 - \rho_2)}, \quad D = \frac{\rho_2^2 - 2\rho_0\rho_2 + \rho_0}{\rho_0(\rho_2 - \rho_1)(\rho_1 - \rho_2)}. \tag{32}
\]

So the solution of Eq. (25), which satisfies the left boundary condition \( \rho(0) = S(0) + W(0) \), see Eq. (19), is

\[
F(\rho_l) = x + F_0, \quad \text{or} \quad \rho_l(x) = F^{-1}(x + F_0), \tag{33}
\]

where \( F_0 = F[\rho(0)] \). Similarly, the solution of Eq. (25), which satisfies the right boundary condition \( \rho(1) = S(1) + W(1) \), see Eq. (20), is

\[
F(\rho_r) = x + F_1 - 1, \quad \text{or} \quad \rho_r(x) = F^{-1}(x + F_1 - 1), \tag{34}
\]

where \( F_1 = F(\rho(1)) \). In the following, we assume \( \rho_l \neq \rho_r \) (otherwise, there would be no shock and boundary layers).

Combining (21) (23) (33) (34), one sees that, at the shock position \( x_s \)

\[
\begin{cases}
F(\rho_l(x_s)) - F(\rho_r(x_s)) + F_1 - F_0 - 1 = 0, \\
\rho_l(x_s) + \rho_r(x_s) = 1 + \gamma \rho_l(x_s) \rho_r(x_s).
\end{cases} \tag{35}
\]

These are the efficient and necessary condition of the existence of shock at the position \( x_s \). In other words, at the shock position \( x_s \), \( H(x_s, \Omega_a, k, \omega_f, l, n, c) := \)

\[
F(\rho_l(x_s)) - F\left(\frac{1 - \rho_l(x_s)}{1 - \gamma \rho_l(x_s)}\right) + F_1 - F_0 - 1 = 0. \tag{36}
\]

If there exists \( 0 < x_s < 1 \), such that \( H(x_s, \Omega_a, k, \omega_f, l, n, c) = 0 \), the shock will appear at \( x_s \), and the height of the shock is

\[
\varepsilon_s = |\rho_r(x_s) - \rho_l(x_s)| = \left|\frac{1 - 2\rho_l(x_s) + \gamma \rho_l^2(x_s)}{1 - \gamma \rho_l(x_s)}\right|. \tag{37}
\]
Let
\[ H(\rho) := F(\rho) - F\left(\frac{1 - \rho}{1 - \gamma \rho}\right) + F_1 - F_0 - 1 = 0, \quad (38) \]
then from \((31)\), one can obtain
\[ \frac{dH(\rho)}{d\rho} = \frac{dF(\rho)}{d\rho} - \frac{d}{d\rho} F\left(\frac{1 - \rho}{1 - \gamma \rho}\right) = \frac{\gamma \rho^2 - 2\rho + 1}{\Omega_{ah}(1 - \gamma \rho)} \times \frac{[(1 - \rho) - \rho_1(1 - \gamma \rho)][(1 - \rho) - \rho_2(1 - \gamma \rho)] + (\gamma - 1)(\rho - \rho_1)(\rho - \rho_2)}{(\rho - \rho_1)(\rho - \rho_2)[(1 - \rho) - \rho_1(1 - \gamma \rho)][(1 - \rho) - \rho_2(1 - \gamma \rho)]} \]
\[ = \frac{\gamma(1 - \rho)^2(1 - \gamma \rho_1)(\rho - \rho_3)(\rho - \rho_4)\left(\frac{1 - \rho_1}{1 - \gamma \rho_1} - \rho_2\right)}{\Omega_{ah}(1 - \gamma \rho)^3(\rho - \rho_1)(\rho - \rho_2)\left(\frac{1 - \rho_1}{1 - \gamma \rho_1} - \rho_2\right)} \]
\[
\begin{cases}
> 0 & \text{if } 0 \leq \rho < \frac{1 - \rho_1}{1 - \gamma \rho_1}, \\
< 0 & \text{if } \frac{1 - \rho_1}{1 - \gamma \rho_1} < \rho < \rho_1, \\
> 0 & \text{if } \rho_1 < \rho \leq 1.
\end{cases} \quad (39)
\]

Using this property of the function \(H(\rho)\), we can obtain the following results:

\textbf{(I)} For \(0 \leq \rho(0) < \rho_3\) and \(\rho_3 < \rho(1) \leq \rho_1\), the conditions of existence of shock in interval \((0, 1)\) is
\[ F\left(\frac{1 - \rho(1)}{1 - \gamma \rho(1)}\right) < F_0 + 1 \quad \text{and} \quad F\left(\frac{1 - \rho(0)}{1 - \gamma \rho(0)}\right) < F_1 - 1, \quad (40) \]
see Fig. 1 (a). From \((25)\) \((31)\), one can find the function \(F(\rho)\) increases with \(\rho\) for \(0 \leq \rho < \rho_3\) and \(\rho_1 < \rho < 1\), and decreases with \(\rho\) for \(\rho_3 < \rho < \rho_1\). Thus
\[ F\left(\frac{1 - \rho(1)}{1 - \gamma \rho(1)}\right) < F_0 + 1 \iff \rho_1^{-1}\left(\frac{1 - \rho(1)}{1 - \gamma \rho(1)}\right) < 1, \]
\[ F\left(\frac{1 - \rho(0)}{1 - \gamma \rho(0)}\right) < F_1 - 1 \iff \rho_r(0) < \frac{1 - \rho(0)}{1 - \gamma \rho(0)}. \quad (41) \]

Therefore, the conditions presented in \((40)\) are generalizations of the ones obtained in \([28]\) for the usual TASEP with motor detachment and attachment:

\[ \rho_1^{-1}(1 - \rho(1)) < 1, \quad \text{and} \quad \rho_r(0) < 1 - \rho(0). \quad (42) \]

In fact, if the parameter \(c = 0\) (i.e. \(\gamma = 0\)), the Eq. \((24)\) reduces to
\[ (1 - 2\rho)\rho_x = \Omega_{ah}[(l + n + 1) - [(l + n + 1) + k(l + 1)]\rho], \quad (43) \]
which is similar as the model discussed in [22] for the usual TASEP. For such reduced cases, $\rho_3 = 0.5$, and the conditions (40) of existence of shock is reduced to (42).

(II) For $0 \leq \rho(0) < \rho_3$ and $\rho_1 \leq \rho(1) \leq 1$, the conditions of existence of shock in interval $(0, 1)$ is

$$
F\left( \frac{1 - \rho(1)}{1 - \gamma \rho(1)} \right) < F_0 + 1, \quad \text{and} \quad F\left( \frac{1 - \rho(0)}{1 - \gamma \rho(0)} \right) > F_1 - 1,
$$

(44)

see Fig. 1(b). Similar as in (I),

$$
F\left( \frac{1 - \rho(1)}{1 - \gamma \rho(1)} \right) < F_0 + 1 \iff \rho_l^{-1}\left( \frac{1 - \rho(1)}{1 - \gamma \rho(1)} \right) < 1,
$$

$$
F\left( \frac{1 - \rho(0)}{1 - \gamma \rho(0)} \right) > F_1 - 1 \iff \rho_r^{-1}\left( \frac{1 - \rho(0)}{1 - \gamma \rho(0)} \right) > 0.
$$

(45)

Therefore, conditions (44) are also generalizations of the ones for the usual TASEP [28]:

$$
\rho_l^{-1}(1 - \rho(1)) < 1, \quad \text{and} \quad \rho_r^{-1}(1 - \rho(0)) > 0.
$$

(46)

(III) For $0 \leq \rho(0), \rho(1) \leq \rho_3$, the condition of the existence of shock in $(0, 1)$ is

$$
\rho_l^{-1}(\rho_3) < 1 \quad \text{and} \quad \tilde{\rho}_r(0) < \frac{1 - \rho(0)}{1 - \gamma \rho(0)}
$$

(47)

where $\tilde{\rho}_r(x)$ is one of the solutions of differential equation [24], which satisfies $\tilde{\rho}_r(1) = \rho_3$ and $\tilde{\rho}_r(0) > \rho_3$. See Fig. 1(c).

(IV) For $\rho(0), \rho(1) > \rho_3$, there exists no shock in $(0, 1)$. It can be readily verified that the function $f(\rho_l, \rho_r) = \rho_l + \rho_r - \gamma \rho_l \rho_r - 1$ increases monotonously with $0 \leq \rho_l, \rho_r \leq 1$, and $f(\rho_3, \rho_3) = 0$. For $\rho(0), \rho(1) > \rho_3$, one knows that $\rho_3 \leq \min(\rho_l, \rho_r) < \max(\rho_l, \rho_r)$ (note: we always assume $\rho_l \neq \rho_r$). Thus $f(\rho_l, \rho_r) = \rho_l + \rho_r - \gamma \rho_l \rho_r - 1 > 0$. It is to say that there exists no shock [see (35)].

(V) For $0 \leq \rho(1) < \rho_3$ and $\rho_l(0) > \rho_3$, there exists no shock in $(0, 1)$.

In conclusion, $\rho(0) < \rho_3$ is one necessary condition of the existence of shock in $(0, 1)$.

IV. THE EXISTENCE OF BOUNDARY LAYER

Generally speaking, if $\rho_l \neq \rho_r$ and there is no shock in $(0, 1)$, boundary layer will appear at least at one of the boundaries 0 and 1. Similar as in [28], we have the
following results:

**(I)** For $0 \leq \rho(0) < \rho_3$ and $\rho_3 < \rho(1) \leq \rho_1$: if

\[
F\left(\frac{1 - \rho(1)}{1 - \gamma \rho(1)}\right) > F_0 + 1 \quad \text{and} \quad F\left(\frac{1 - \rho(0)}{1 - \gamma \rho(0)}\right) < F_1 - 1,
\]

there exists boundary layer at the right boundary $x = 1$, see Fig. 1(d); if

\[
F\left(\frac{1 - \rho(1)}{1 - \gamma \rho(1)}\right) < F_0 + 1 \quad \text{and} \quad F\left(\frac{1 - \rho(0)}{1 - \gamma \rho(0)}\right) > F_1 - 1,
\]

there exists boundary layer at the left boundary $x = 0$ (in these cases, the shock position $x_s < 0$), see Fig. 2(b).

In view of the property (39) of function $H(\rho)$, the conditions (48) can be simplified as

\[
F\left(\frac{1 - \rho(1)}{1 - \gamma \rho(1)}\right) > F_0 + 1,
\]

and the conditions (49) can be simplified as

\[
F\left(\frac{1 - \rho(0)}{1 - \gamma \rho(0)}\right) > F_1 - 1.
\]

**(II)** For $0 \leq \rho(0) < \rho_3$ and $\rho_1 \leq \rho(1) \leq 1$: if

\[
F\left(\frac{1 - \rho(0)}{1 - \gamma \rho(0)}\right) < F_1 - 1,
\]

there exists boundary layer at the left boundary $x = 0$ (i.e. the shock position $x_s < 0$), see Fig. 2(c); if

\[
F\left(\frac{1 - \rho(1)}{1 - \gamma \rho(1)}\right) > F_0 + 1,
\]

there exists boundary layer at the right boundary $x = 1$ (i.e. the shock position $x_s > 0$), see Fig. 2(a).

**(III)** For $0 \leq \rho(0), \rho(1) \leq \rho_3$ and $\rho_1(1) \neq \rho(1)$, there exists boundary layer at $x = 1$. See Fig. 1(c), Fig. 2(d) and Fig. 3(a). If

\[
\tilde{\rho}_l^{-1}(\rho_3) < 1 \quad \text{and} \quad \tilde{\rho}_r(0) > \frac{1 - \rho(0)}{1 - \gamma \rho(0)},
\]

there is also the boundary layer at the left boundary $x = 0$. 
(IV) For $\rho_3 \leq \rho(0) < 1, 0 \leq \rho(1) \leq \rho_3$ and $\rho(0) \neq \tilde{\rho}_r(0)$, there exist boundary layers at both $x = 0$ and $x = 1$, see Fig. 3 (b) and Fig. 3 (c). For these cases, $\rho(x) = \tilde{\rho}_r(x)$ for $0 < x < 1$.

(V) For $\rho_3 \leq \rho(0), \rho(1) \leq 1$ and $\rho(0) \neq \rho_r(0)$, there exists boundary layer at $x = 0$. For these cases, $\rho(x) = \rho_r(x)$ for $0 < x \leq 1$, see Fig. 3 (d) and Fig. 4.

V. THE PROPERTIES OF SHOCK

Finally, we discuss the properties of shock briefly. From the discussion in Sec. III, one knows that $\rho(0) < \rho_3$ is necessary for the existence of shock. So, at the shock position $x_s, \rho_l(x_s) < \rho_r(x_s)$, see Eq. (23), and the height of the shock is [see Eq. (37)]

$$\varepsilon_s = \rho_r(x_s) - \rho_l(x_s) = \frac{1 - 2\rho_l(x_s) + \gamma\rho_l^2(x_s)}{1 - \gamma\rho_l(x_s)}. \tag{55}$$

The derivative of the height $\varepsilon_s$ with respect to $\rho_l(x_s)$ is

$$\frac{\partial \varepsilon_s}{\partial \rho_l(x_s)} = \frac{\gamma - 1}{(1 - \gamma\rho_l(x_s))^2} - 1 < 0. \tag{56}$$

At the same time, $\rho_l(0) = \rho(0) < \rho_3$ means $\frac{\partial \rho_l(x_s)}{\partial x_s} > 0$ [see (24)]. So

$$\frac{\partial \varepsilon_s}{\partial x_s} = \frac{\partial \varepsilon_s}{\partial \rho_l(x_s)} \frac{\partial \rho_l(x_s)}{\partial x_s} < 0, \tag{57}$$

which means, the shock height $\varepsilon_s$ decreases with the shock position $x_s$. Therefore, we only need to give the relations between shock position $x_s$ and the model parameters $\Omega_a, \Omega_d, \omega_f, \omega_s, \omega_h, \omega_b, c$.

Because of the complexity of the function $F$ [see (31)], it is difficult to get theoretical results as in [28]. From numerical calculations, we find that, the shock position $x_s$ decreases with parameters $\Omega_a, \alpha, \omega_b, \omega_s$, but increases with parameters $\Omega_d, \beta, \omega_f, \omega_h, c$, see Fig. 5 In the calculations, $x_s$ is obtained by (36) and (33).

VI. CONCLUDING REMARKS

In this study, the three-state process, which is presented in [26, 27] to model the intracellular transport of single-headed kinesin KIF1A, is theoretically analyzed.
using mean field approximation. By similar methods as for the usual TASEP \cite{28}, the conditions of the existence of shock or domain wall, which is defined as the interface of low-density and high-density phases, are obtained. With the aid of numerical calculations, the parameters dependent properties of the shock are also discussed. The results obtained in this study will be helpful to understand the real biophysical properties of motor traffic in eukaryotic cells.

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FIG. 1: There exists shock in (0,1) if $0 \leq \rho(0) < \rho_3$, $\rho_3 < \rho(1) \leq \rho_1$ and $F \left( \frac{1-\rho(1)}{1-\gamma \rho(1)} \right) < F_0 + 1$ (a); Or $0 \leq \rho(0) < \rho_3$, $\rho_1 \leq \rho(1) \leq 1$ and $F \left( \frac{1-\rho(1)}{1-\gamma \rho(1)} \right) < F_0 + 1$, $F \left( \frac{1-\rho(0)}{1-\gamma \rho(0)} \right) > F_1 - 1$ (b). There exists shock in (0,1) and boundary layer at $x = 1$ if $0 \leq \rho(0), \rho(1) \leq \rho_3$ and $\rho_1^{-1}(\rho_3) < 1$, $\tilde{\rho}_r(0) < \frac{1-\rho(0)}{1-\gamma \rho(0)}$ (c). There exists boundary layer at $x = 1$ if $0 \leq \rho(0) \leq \rho_3$, $\rho_3 \leq \rho(0) \leq \rho_1$ and $F \left( \frac{1-\rho(1)}{1-\gamma \rho(1)} \right) > F_0 + 1$ (d).
FIG. 2: There exists boundary layers at $x = 1$ if $0 \leq \rho(0) \leq \rho_3, \rho_1 \leq \rho(1) \leq 1$ and $F \left( \frac{1-\rho(1)}{1-\gamma \rho(1)} \right) > F_0 + 1$ (a); Or $0 \leq \rho(0), \rho(1) \leq \rho_3$ and $\rho_l(1) > \rho(1)$ (d). There exists boundary layers at $x = 0$ if $0 \leq \rho(0) < \rho_3, \rho_3 < \rho(1) \leq \rho_1$ and $F \left( \frac{1-\rho(0)}{1-\gamma \rho(0)} \right) > F_1 - 1$ (b); Or $0 \leq \rho(0) \leq \rho_3, \rho_1 \leq \rho(1) \leq 1$ and $F \left( \frac{1-\rho(0)}{1-\gamma \rho(0)} \right) < F_1 - 1$ (c).
FIG. 3: There exists boundary layers at $x = 1$ if $0 \leq \rho(0), \rho(1) \leq \rho_3$ and $\rho_l(1) < \rho(1)$ (a).

There exist boundary layers at both $x = 0$ and $x = 1$ if $\rho_3 \leq \rho(0) < 1, 0 \leq \rho(1) \leq \rho_3$ and $\rho(0) < \tilde{\rho}_r(0)$ (b); Or $\rho_3 \leq \rho(0) < \rho_1, 0 \leq \rho(1) \leq \rho_3$ and $\rho(0) > \tilde{\rho}_r(0)$ (c). There are boundary layers at $x = 0$ if $\rho_3 \leq \rho(0), \rho(1) \leq \rho_1$ and $\rho(0) < \rho_r(0)$ (d).
FIG. 4: There are boundary layers at $x = 0$ if $\rho_3 \leq \rho(1) \leq \rho_1, \rho_1 \leq \rho(0) \leq 1$ (a); Or $\rho_3 \leq \rho(0), \rho(1) \leq 1$ and $\rho(0) > \rho_r(0)$ (b); Or $\rho_3 \leq \rho(0) \leq \rho_1, \rho_1 \leq \rho(1) \leq 1$ (c); Or $\rho_3 \leq \rho(0), \rho(1) \leq 1$ and $\rho(0) < \rho_r(0)$ (d).
FIG. 5: The shock position $x_s$ decreases with parameters $\Omega_a, \alpha, \omega_b, \omega_s$, but increases with parameters $\Omega_d, \beta, \omega_f, \omega_h, c$. In the calculations, $x_s$ is obtained by Eqs. (36) and (33).