TASEP on parallel tracks: effects of mobile bottlenecks in fixed segments

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We study the flux of totally asymmetric simple exclusion processes (TASEPs) on a twin coaxial square tracks. In this biologically motivated model the particles in each track act as mobile bottlenecks against the movement of the particles in the other although the particle are not allowed to move out of their respective tracks. So far as the outer track is concerned, the particles on the inner track act as bottlenecks only over a set of fixed segments of the outer track, in contrast to site-associated and particle-associated quenched randomness in the earlier models of disordered TASEP. In a special limiting situation the movement of particles in the outer track mimic a TASEP with a “point-like” immobile (i.e., quenched) defect where phase segregation of the particles is known to take place. The length of the inner track as well as the strength and number density of the mobile bottlenecks moving on it are the control parameters that determine the nature of spatio-temporal organization of particles on the outer track. Variation of these control parameters allow variation of the width of the phase-coexistence region on the flux-density plane of the outer track. Some of these phenomena are likely to survive even in the future extensions intended for studying traffic-like collective phenomena of polymerase motors on double-stranded DNA.

I. INTRODUCTION

Totally asymmetric simple exclusion process (TASEP) is one of the simplest models of non-equilibrium systems of interacting self-driven particles [1]. Properties of TASEP and its various extensions have been analyzed to get insight into the spatio-temporal organization in wide varieties of physical and biological systems [2–5]. In the simplest version of this model particles hop forward, with rate $p$, from one site to the next on a one-dimensional lattice of equi-spaced sites; however, a particle successfully executes the forward hop if, and only if, the target site is empty.

Effects of two types of quenched (time-independent) defects on the spatio-temporal organization of the particles have been explored extensively [2–5]. (A) In one class of models of quenched defect the randomness is associated with the lattice: particles hop at the rate $p$ from all sites except from the “point defect” from where the hopping rate is $p' < p$. Such a single defect site can give rise a nontrivial macroscopic phase segregation of the particles into high-density and low-density regions [5]. Two types of extensions of this model have been reported: (i) $r (> 1)$ successive sites are occupied by defects so that the defect may be regarded as a single extended object of length $r$; (ii) $r (> 1)$ point defects are distributed randomly over the entire lattice [6, 7] so that the lattice can be viewed as “disordered” rather than merely defective. In the latter case time-independent random hopping rates, drawn from a probability distribution $P(p)$, are assigned to each lattice site. From now onwards we refer to this class of models as random-site TASEP (RST). (B) In the second class of models with quenched defect, the randomness is associated with the particles: a single “impurity” particle is allowed to hop at a rate $p' < p$ whereas the hopping rate of all the other particles is $p$. The growth of platoons of particles behind the impurity is reminiscent of coarsening phenomena and the steady state of the system can be expressed formally in terms of a Bose-Einstein-like condensate of the vacancies (absence of particles) in front of the impurity particle [10–12]. In the more general version of this model the particles are assigned time-independent hopping rates randomly drawn from a probability distribution [10–13]. From now onwards we refer to this class of models as random-particle TASEP (RPT).

In this paper we introduce a biologically-motivated quasi-one dimensional TASEP with two parallel tracks of lattice sites. Although the particles are not allowed to shift from one track to the other, the flow in each influences that in the other through a prescription that we define in the next section. We shall refer to this model as TASEP with mobile bottlenecks (TMB). As we’ll explain in the next section, in one special limit this TMB reduces to RST. We also indicate possible extensions of the model for potential applications in traffic-like collective phenomena in biological systems [5, 7]. Using a combination of approximate analytical arguments and highly accurate numerical simulations, we demonstrate the rich varieties of spatio-temporal organizations, including phase segregations, in this model.

II. THE MODEL AND ITS COMPARISON WITH OTHER MODELS OF DISORDERED TASEP

Dynamic blockage against directed (albeit stochastic) movement of proteins and macromolecular complexes along filamentous tracks is well known [8]. For example, a class of molecular motors walk along the surface of stiff tubular filaments called microtubules [8, 14]. Microtubule-associated proteins, which act as blockage against the forward stepping of these motors, can detach from the microtubule thereby opening up the blockage.

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the outer and inner tracks are labelled by the symbols $T_o$ and $T_i$, respectively. Often these bound proteins either slide along the same track diffusively or, occasionally, detach from the track itself. Thus, most of the blockages against the movement of molecular motors are dynamic in nature. Our generic model here has been motivated by molecular motor traffic on DNA strands [15] which began receiving serious attention after Brewer [16] summarized the earlier experimental observations scattered in the literature. During DNA replication, the replication machine, called DNA polymerase (DNAP) moves along one of the two strands of a double-stranded DNA. Often a DNAP and a RNAP approach each other head-on along DNA. Often a DNAP and a RNAP approach each other head-on along DNA or RNA strands face hindrance caused by proteins bound to the respective tracks [6]. These bound proteins either slide along the same track diffusively or, occasionally, detach from the track itself. The model developed here has been motivated by molecular motor traffic in the two tracks.

Our model is shown schematically in Fig. 1. It consists of two square tracks with a common center where the outer and inner tracks are labelled by the symbols $T_o$ (outer) and $T_i$ (inner), respectively. Each track consists of equi-spaced discrete sites; the lengths of the outer and inner tracks, denoted by $L_o$ and $L_i$, respectively, are the total number of sites of the respective tracks. Particles on both tracks have identical size and each covers $r$ consecutive lattice sites simultaneously (For $r > 1$, it might be more appropriate to regard these particles as hard rods). The number of particles on $T_i$ and $T_o$ are $N_i$ and $N_o$, respectively; the corresponding number densities being $N_i/L_i = \rho_i$ and $N_o/L_o = \rho_o$, respectively. We also define the coverage densities $\rho_i^{cov} = r N_i/L_i$ and $\rho_o^{cov} = r N_o/L_o$; for $r = 1$, coverage densities are identical to the corresponding particle densities.

Just as in TASEP the particles hop forward by one single lattice spacing (i.e., from one lattice site to the next on the same track) provided the target site is not covered by the leading particle. In the outer and inner tracks the hopping rates are $Q^{(o)}$ and $Q^{(i)}$, respectively provided the adjacent site on the other track is not covered by a particle; however, if the adjacent site on the other track is covered by a particle, the hopping is possible at the corresponding reduced rates $q^{(o)}$ and $q^{(i)}$, respectively. Thus, as we mentioned in the introduction, flow in the two tracks are affected by the mutual hindrance although no direct transfer of particles from one track to the other is allowed. We have studied both co-directional traffic and counter-moving traffic in the two tracks.

**III. RESULTS AND DISCUSSION**

In the following subsections, wherever possible, we provide theoretical estimates of the quantities of our interest based on either mean-field approximation or heuristic arguments. We also compute these quantities numerically by carrying out computer simulations. In order to ensure that the data are collected, indeed, in the steady state of the system we discard the data for the...
first **five million** time steps. Throughout this paper we consider the limits \( L_o \to \infty \). So far as the inner track is concerned, we’ll pay special attention to the two limits \( L_i \to 0 \) and \( L_i \to \infty \), in addition to more general cases. Our primary interest will be the flux \( J_o \) in the outer track although we’ll also present the results for the inner track. The three main characteristic parameters of the inner track that control the nature of the flux \( J_o \) in the outer track are (i) the length \( L_i \), (ii) the density \( \rho_i \), and (iii) \( q^{(o)} \) which is a measure of the strength of the hindrance created by the inner-track particles for the outer-track flow (and, vice-versa).

### A. \( L_i \) comparable to \( L_o \)

In order to test the validity and accuracy of the approximate analytical expressions that we derive here for \( J_o \) and \( J_i \), we also collect corresponding numerical data by direct computer simulations of the model. The chosen parameter values \( L_o = 8000 \) and \( L_i = 7996 \) not only ensure that the tracks are sufficiently long but also allow minimal difference in the lengths of the two tracks preserving their square shapes. \( P_j^{(i)} \) denotes the probability of finding a particle at site \( j \) on \( T_i \) (the inner track). Similarly \( P_m^{(o)} \) is the probability of finding a particle at site \( m \) on \( T_o \) (the outer track).

First we consider the simpler case of \( r = 1 \). In the mean-field approximation, the master equations for the probabilities \( P_j^{(o)} \) and \( P_j^{(i)} \) are given by

\[
\frac{dP_j^{(o)}}{dt} = [Q^{(o)}(1 - P_{j-1}^{(i)}) + q^{(o)}P_{j-1}^{(i)}]P_j^{(o)}(1 - P_j^{(o)}) - [Q^{(o)}(1 - P_j^{(i)}) + q^{(o)}P_j^{(i)}]P_j^{(o)}(1 - P_{j+1}^{(o)}),
\]

\[
\frac{dP_j^{(i)}}{dt} = [Q^{(i)}(1 - P_{j-1}^{(o)}) + q^{(i)}P_{j-1}^{(o)}]P_j^{(i)}(1 - P_j^{(i)}) - [Q^{(i)}(1 - P_j^{(o)}) + q^{(i)}P_j^{(o)}]P_j^{(i)}(1 - P_{j+1}^{(i)}).
\]

Consequently, in the steady state the corresponding fluxes are given by

\[
J_o = \omega_m^{(o)} \rho_o (1 - \rho_o), \quad J_i = \omega_m^{(i)} \rho_i (1 - \rho_i)
\]

where the effective hopping rates under naive mean-field approximation would be

\[
\omega_m^{(o)} = Q^{(o)}(1 - \rho_i) + q^{(o)} \rho_i,
\]

\[
\omega_m^{(i)} = Q^{(i)}(1 - \rho_o) + q^{(i)} \rho_o.
\]

A comparison of the mean-field predictions with the corresponding simulation data revealed that the mean-field argument presented above leads to significant overestimate of both the fluxes \( J_o \) and \( J_i \).

![FIG. 3: (a) \( J_o \) is plotted against \( \rho_o \) for a few values of \( \rho_i \). (b) \( J_i \) is plotted against \( \rho_i \) for a few values of \( \rho_o \). The discrete data points have been obtained from computer simulations of the model with parameter values \( L_o = 8000 \), \( L_i = 7996 \), \( Q^{(o)} = 0.75 \) and \( q^{(o)} = 0.25 \). The continuous curves are obtained from the SBA outlined above with the value of \( \mu \) adjusted so as to get the best fit with the simulation data.](image)

Our mean-field estimate could be improved by extending the concept of single-bottleneck approximation (SBA) that was developed for randomly distributed static defects on the track. If \( \ell \) consecutive lattice sites are occupied by static defects and have defect-free sites at the two neighboring sites at the two ends of these \( \ell \) sites, the \( \ell \)-site “cluster” acts a single bottleneck of length \( \ell \). From the distribution of the lengths of such bottlenecks created by the independently distributed random defects one can calculate the size \( \ell \) of the longest bottleneck. The effect of the defects on the flux is overwhelmingly dominated by the longest bottleneck. For the purpose of our calculation we replace the probability \( \phi \) of the presence of a static defect at a lattice site by that of a mobile particle on the neighboring track. More specifically, for the calculation of \( J_o \) we treat \( \rho_o \) as the counterpart of \( \phi \). Similarly, for the calculation of \( J_i \) we replace \( \phi \) by \( \rho_o \). Based on these heuristic arguments
FIG. 4: Dependence of the flux on the relative direction of hopping of the particles in the two tracks is shown by plotting $J_o$ against $\rho_i$ for fixed $\rho_o = 0.5$. The letters ‘S’ and ‘O’ correspond to the same direction and opposite direction of flow in the two tracks. The hopping rates are $Q^{(o)} = 0.75 = Q^{(i)}$ and $q^{(o)} = 0.25 = q^{(i)}$ and the lengths of the tracks are $L_o = 8000$, $L_i = 7996$.

The fluxes $J_o$ and $J_i$ are given by expressions that are identical to those in (3) except that the effective hopping rates $\omega_{mf}^{(o)}$ and $\omega_{mf}^{(i)}$ are replaced by the expressions

$$\omega_{SBA}^{(o)} = Q^{(o)} e^{-\mu<\ell_i>} + q^{(o)} (1 - e^{-\mu<\ell_i>})$$

$$\omega_{SBA}^{(i)} = Q^{(i)} e^{-\mu<\ell_o>} + q^{(i)} (1 - e^{-\mu<\ell_o>})$$

where, utilizing the SBA [17], we have

$$<\ell_i> = \frac{\ln L_i + \ln (1 - \rho_i) + \gamma_e}{\ln (1/\rho_i)} - \frac{1}{2}$$

$$<\ell_o> = \frac{\ln L_o + \ln (1 - \rho_o) + \gamma_e}{\ln (1/\rho_o)} - \frac{1}{2}$$

Note that $\mu$ is a free parameter that is varied to get the best fit with the simulation data. The best fit to the simulation data are shown in fig.3. It is worth pointing out that in spite of the increase of $<\ell_i>$ and $<\ell_o>$ with $L_i$ and $L_o$, respectively, the exponentials in equations (5) do not vanish in the thermodynamic limit because, as we verified, $\mu$ decreases with increasing lengths of the tracks.

The magnitude of the flux $J_o$ depends on the relative direction of motion of the particles in the two tracks. For a fixed set of parameter values, we have carried out computer simulations of the model in two different situations: (a) when particles move in the same direction in the two tracks (corresponding data are labelled by the letter ‘S’ in fig.4), and (b) when the particles move in opposite directions in the two tracks (corresponding data are labelled by the letter ‘O’ in fig.4). $J_o$ is higher in case of co-directional motion than that for counter-directional motion on the two tracks. This difference is caused by the phase segregation of the particles into high-density and low-density regions. In case of opposite movements on the two tracks, a particle on the outer track has to overcome the full length of a high-density region on the inner track whereas the same particle need not face the full stretch of the same region if it moves co-directionally with the inner-track particles.

B. $L_i$ vanishingly small compared to $L_o$

Since $L_o \to \infty$ and, since in this section we are assuming $L_i \to 4$ (the smallest allowed value of $T_i$ that preserves its shape is 4), the inner track effectively acts as a “point” defect for the particles moving on the outer track.

First let us consider the special case $\rho_i = 1$. In this case the inner track acts effectively as a static “point-like” defect. It is well known that macroscopic phase segregation takes place in a TASEP with a single point
defect, where the density profile exhibits coexistence of a high-density and low-density regimes. Since each of the four sides of the outer track in our model sees a point-like defect, the profile consists of four segments each of which is similar to that of a TASEP with a single point-defect (see fig.5). The flat symmetric plateaus observed on the plots of \(J_o\) against \(\rho_o\) correspond to the coexistence of the high-density and low-density regimes. This qualitatively similar to the corresponding flux-density diagrams for TASEPs with point defects. Moreover, as shown also in the fig.4, lower is the value of \(q^{(o)}\), the stronger is the effect of the bottleneck and the smaller is the flux \(J_o\).

Next, in order to demonstrate the more general situations, in fig.6 we have plotted \(J_o\) as a function of \(\rho_o\) for five values of the parameter \(\rho_i\) = 0.0, 0.25, 0.5, 0.75, 1.0. As the data in this figure show, the higher is the density \(\rho_i\), longer is longest bottleneck and, consequently, the wider is the plateau region. This is consistent with the fact that a single bottleneck of longer size lowers the flux to a small value [2]. Finally, as expected intuitively, the flux-density curve for the outer track approaches the parabolic form \(Q^o\rho_o(1 - \rho_o)\) in the limit \(\rho_i \to 0\).

C. Flux-density relation for particles of size \(r > 1\)

Keeping in mind the possible future application of extensions of our model to the biophysical phenomena mentioned in the introduction, we have also studied the model for particle size \(r\) larger than 1. As a typical example, the flux \(J_o\) is plotted against the corresponding coverage density \(\rho_{cov}^o\) in fig.7 in those situations where all the particles on both the tracks have the same length \(r = 30\). The plateau observed in the special case \(r = 1\) survives also for all \(r > 1\). However, as is well known for TASEP with hard rods [2, 3], the maximum of the flux shifts to increasingly higher densities with increasing \(r\).

FIG. 6: \(J_o\) is plotted against \(\rho_o\) for several different values of \(\rho_i\). The values of the other parameters used for this figure are \(L_o = 8000, L_i = 80, Q^{(o)} = 0.75 = Q^{(i)}, q^{(o)} = 0.25 = q^{(i)}\).

FIG. 7: \(J_o\) of particles with \(r = 30\) is plotted against \(\rho_{cov}^o\) for three different values of \(\rho_{cov}^i\); the hopping rates are \(Q^{(o)} = 0.75 = Q^{(i)}\) and \(q^{(o)} = 0.25 = q^{(i)}\).

IV. SUMMARY AND CONCLUSIONS

In this paper we have developed a generic model for the TASEP on two co-axial square tracks that influence each other without any transfer of particles from one to another. In spite of its extreme simplicity, the model exhibits rich variety of phenomena in different parameter regimes. In the limit \(L_i/L_o \to 0\), the model reproduces the known properties of a TASEP with a single “point-like” defect on the track. In particular, it exhibits macroscopic phase segregation of the particles on the outer track. In general, our model the width of the coexistence region can be tuned by varying three distinct control parameters which we have clearly identified. Extensions of this model, incorporating further details, are likely to find use in modeling the traffic-like collective biological phenomena mentioned in section [II]

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