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Collective dynamics of an inhomogeneous two-channel exclusion process: Theory and Monte Carlo simulations

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ABSTRACT

This work is devoted to the development of a novel theoretical approach, named hybrid approach, to handle a localized bottleneck in a symmetrically coupled two-channel totally asymmetric simple exclusion process with Langmuir kinetics. The hybrid approach is combined with singular perturbation technique to get steady-state phase diagrams and density profiles. We have thoroughly examined the role played by the strength of bottleneck, binding constant and lane-changing rate in the system dynamics. The appearances of bottleneck-induced shock, a bottleneck phase and Meissner phase are explained. Further, the critical values of bottleneck rate are identified, which signify the changes in the topology of phase diagram. It is also found that an increase in lane-changing rate as well as unequal attachment, detachment rates weaken the bottleneck effect. Our theoretical arguments are in good agreement with extensively performed Monte Carlo simulations.

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1. Introduction

In protein synthesis, the genetic information is deciphered into proteins by molecular machines called ribosomes, which attach themselves at the start end of mRNA, move along the chain in a unidirectional manner and finally detach at the stop end [2]. Each translation step requires the binding of a freely diffusing transfer-RNA (tRNA) molecule, carrying the amino acid specific to each codon [2,31]. The important factor affecting the ribosome translation rate is relative concentrations of tRNA, which may vary from codon to codon. The codons with lower concentrations of tRNA reduce the protein synthesis rate and thus play the role of an inhomogeneity in a homogeneous system [33–35]. Apart from this, inhomogeneities also occur naturally in many other transport systems such as vehicular traffic [11], blood flow [25] and data flow in a Von Neumann architecture [21]. In traffic flow, the ongoing construction on roads, a slow moving vehicle or an accident can lead to slow down the flow rate on highways and produces congestion. Further, the separation of the CPU and the memory in computers creates Von Neumann bottleneck, which limits the performance of the computer via limited bandwidth between the CPU and the memory.

Totally asymmetric simple exclusion process (TASEP) [3,22] is well known to be a paradigmatic model for studying stochastic transport in many-particle systems. Both single-channel and multi-channel TASEPs have been well explored theoretically as well as using Monte Carlo simulations [5,9,20,28,29,32]. Further, one has to take into account the fact that the proteins as molecular motors can also attach from the bulk reservoir or detach from it (Langmuir Kinetics (LK)) [14]. In

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contrast to TASEP, where total number of particles remain conserved, the additional attachment–detachment dynamics (LK dynamics) violate the particle conservation and lead to many interesting phenomena [26]. In literature, the consequences of coupling of the two different dynamics: TASEP and LK have been well analyzed in single-channel [23,24,26] as well as two-channel homogeneous systems [6,10,18,37]. The idea of slowing down of particles at certain defect positions can be incorporated in the form of a set of inhomogeneous lattice sites (bottleneck), either as a single unit or randomly distributed over the whole lattice in TASEP. This type of disorder is known as site-wise disorder. Another type of disorder studied in literature is particle-wise, where a slow moving particle itself acts as an inhomogeneity in the system. The present work focuses on site-wise disorder which is suitable to model the inhomogeneities present in transport of molecular motors.

Although a lot of work has been done on homogeneous TASEPs, the effect of disorder on the steady-state dynamics of such systems is not well understood. Several studies have been performed on single-channel inhomogeneous TASEPs with [27,30] as well as without LK [2,7,8,15,16,19,31,36]. While investigating the role of a bottleneck in a closed TASEP [15,16], it was found that even the presence of a single bottleneck site can produce shock profile and a plateau in the fundamental current-density relation. Later, Kolomeisky [19] examined even richer case of single-channel open system and explored the consequences of the inhomogeneity with both faster and slower transition rates. He divided the system into two homogeneous TASEPs coupled at the single bottleneck site (defect mean-field theory (DMFT)) and proved analytically that a fast site has no effect on the phase diagram; whereas a slow site leads to shifting of the phase boundaries only. He also tested the theoretical results with Monte Carlo simulations and found a good agreement in low density (LD) and high density (HD) phases; while a little deviation was observed in maximal current (MC) phase. Another analytical approach namely finite-segment mean-field theory (FSMFT) was introduced by Chou and Lakatos [2] to study clusters of slow codons in protein synthesis. They found that ribosome density profiles near neighboring clusters of slow codons suppress the proteins synthesis. Dong et al. [7] generalized the DMFT to study the effect of two bottlenecks on the protein production rate and also performed extensive Monte Carlo simulations to conclude that the location as well as spacing between the bottlenecks affect the production rate and pointed out an important phenomenon namely *edge effect*. The investigation into edge effects was further carried out by Greulich and Schadschneider [8] to generate the phase diagrams of inhomogeneous TASEP using interacting subsystem approximation (ISA). They could successfully explain the interactions of defects with the boundaries of the single-channel system. The more complex case of inhomogeneous TASEP in the presence of Langmuir kinetics was studied by Qiu et al. [30]. They calculated phase diagrams and density profiles by adopting the concept of DMFT and also studied the effect of slow hopping rate and detachment rate on the phase diagram. Pierobon et al. [27] provided a detailed study on the role of a bottleneck in a TASEP with LK, using an effective mean-field theory and Monte Carlo simulations. They introduced the concept of carrying capacity to identify various novel phases called bottleneck phases. Importantly, all of the above studies focused on single-channel inhomogeneous systems.

Parallel to the inhomogeneous single-channel systems, particles in multi-channel transport systems [6,9,10,17,29,32] may also confront a bottleneck, present in either one or in more than one channels. The importance of studying the multi-channel system lies in the fact that it can act as a framework for extending the analysis to networks. Due to the complexity in dynamics generating from the interactions between different channels, it is difficult to examine the effects of inhomogeneity in a multi-channel open system. Up to our knowledge, the only contribution in this direction has been made by Wang et al. [38], which explored the effect of a local inhomogeneity in one of the lanes of a two-lane TASEP with LK under a symmetric lane changing rule. They extended the DMFT to a two-channel system by incorporating the concept of effective injection and removal rates at the inhomogeneous lattice site. Despite a good agreement between the solution of the mean-field equations and Monte Carlo simulations in Ref. [38], this approach fails to produce the steady-state phase diagrams of the two-channel system. Moreover, it is not feasible to analyze the role played by various parameters such as lane-changing rate, attachment–detachment rate and strength of bottleneck on the steady-state dynamics. One can infer from here that though DMFT is capable to provide analytic solutions for single-channel inhomogeneous TASEPs with [27,30] as well as without LK [19], it lacks some important ingredients to generate a complete picture of the dynamics of the corresponding two-channel system as discussed in section 3. This motivates us to develop a new approach to handle the bottleneck in a two-channel TASEP with LK, which not only overcomes the existing limitations, but also demonstrates the unexplored dynamics of two-channel inhomogeneous systems.

The objective of the proposed study is two-fold, first is to develop a general theoretical approach, which is capable to produce the phase diagrams and second is to study the effect of various system parameters on the steady-state phases. In this paper, we attempt to provide a complete picture of the dynamics of two-channel symmetrically coupled TASEP with LK in the presence of a single localized bottleneck in one of the two channels by adopting a new and simplified approach, called the *hybrid approach*. We have also validated the theoretical results with Monte Carlo simulations. The paper is organized as follows. In section 2, we define the model under examination and the governing dynamical rules. We briefly discuss the limitations of the earlier approaches in section 3. The theoretical hybrid approach and Monte Carlo simulations are covered in section 4 and section 5, respectively. A thorough analysis of the stationary properties of the model is discussed in section 6. In the concluding section 7, we summarize the results and future perspectives of our work.

2. Two-channel inhomogeneous TASEP with LK

We define our model in a two-channel $(L, 2)$ lattice, where L is the length of a channel. The two channels are denoted by A and B, in which particles are distributed under hard-core exclusion principle (see Fig. 1). We adopt random-sequential

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