An exclusion process with dynamic roadblocks*

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We study an exclusion process with multiple dynamic roadblocks. Each roadblock can move diffusively forward or backward with different rates, as well as unbind from/rebind to a free site. By Monte Carlo simulations, the two moving types are investigated in combination of roadblock number. The case of only diffusive roadblocks shows an asymmetric current-density relation. The case of only long-range jumping roadblocks presents that flux decreases with increasing roadblock number.

Keywords: exclusion process, roadblocks, diffusion, unbinding/rebinding

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1. Introduction

Recently, the study of non-equilibrium system has attracted considerable attention in many research fields, ranging from large complex networks to microscopic living organisms, by theoretical analysis and simulation.[1–4] Many models have been used to reproduce complex phenomena through numerous simple ingredients. The asymmetric simple exclusion process can represent fundamental aspects of phase transition, so it has been widely applied to traffic flow,[5–8] translation and transcription[9–12] processes in protein synthesis, molecular motors,[13–15] growing interfaces,[16] and quantum spin chains.[17]

In asymmetric simple exclusion process (ASEP), particles move forward or backward along a one-dimensional (1D) lattice. Periodic boundary and open boundary condition are two kinds of setups, and their steady-state currents are dependent on particle density and boundary reservoirs respectively. In the periodic totally asymmetric exclusion process, particles only move in one direction with rate ε, and the steady state current is

$$J_{\mathrm{TASEP}} = \varepsilon\rho(1-\rho).$$

The typical ASEP should be modified when utilized in different real-world transport processes, such as particles occupying multiple lattices,[10,18,19] coupling to a reservoir through a binding/unbinding process,[14,15] different types of particles.[8,20] The obstacles or roadblocks are often encountered in transport processes. Some bottlenecks are dynamic,[21,22] such as microtubule-associated proteins in cytoskeletal transport or DNA-binding proteins in transcription. Since binding energies are of the same order of magnitude as thermal energy in systems, proteins blocking the progression powered by molecular motors are mobile and can diffuse or unbind from the track of motor. Specifically, DNA-bound proteins can become roadblocks for RNA polymerase.[23–25] The proteins can also diffuse along DNA.[26,27] In addition, they may unbind from DNA, so blocked RNA polymerases can pass.

Sahoo *et al.*[28] investigated the blocking phenomenon by adding a roadblock in the totally asymmetric simple exclusion process (TASEP). But in the non-equilibrium system, such as DNA-binding proteins in transcription, more roadblocks may exist. Besides, local diffusive move forward or backward can have different rates. In the present work, we add more dynamic roadblocks with different jumpings, forward and backward rates in the TASEP.

The remainder of this paper is organized as follows. In Section 2 we describe the improved model. In Section 3, we present the simulation results of diffusive roadblocks with different forward and backward rates. In Section 4 we give the simulation results with multiple unbinding/rebinding roadblocks. In Section 5 these two conditions are combined together. In Section 6 some conclusions are drawn from the present studies.

2. Model

An ASEP with M roadblock particles is considered in the paper. The schematic of the model is shown in Fig. 1. A 1D lattice contains L sites with periodic boundary conditions. The series numbers of the sites are $1, 2, \ldots, L$ in sequence. The lattice is occupied by $N+M$ particles, in which N particles obey usual TASEP rules, and other M particles can diffuse or make long-range jumps that mimic the process of unbinding and rebinding. When the site $i+1$ is occupied by neither another normal particle nor one roadblock, the normal particle at site i

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can move forward into $i+1$ with rate ε. If the target site is not occupied by any particle, the roadblock can diffuse forward or backward with rate D_1 or D_2 respectively. Moreover, the roadblock may unbind from the site with rate $k_{\rm off}$ and rebind to one free site including the original one.

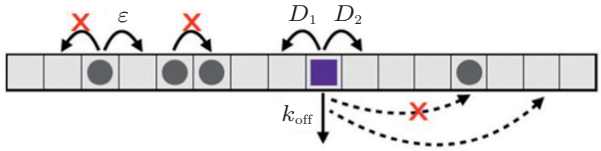


Fig. 1. (color online) Illustration of two types of particles, N active particles and M roadblock particles, occupying 1D lattice.

Monte Carlo method is used to simulate the dynamics. At each Monte Carlo step corresponding to a time interval δt, L moves are performed. In each move, a site is chosen randomly and updated obeying the rules discussed above. A normal particle on the chosen site i at time t can move to the neighboring site $i+1$ with probability $\varepsilon\delta t$, provided that site $i+1$ is not occupied. A roadblock on the chosen site i can diffuse to neighboring site $i-1$ or $i+1$ with probability $D_1\delta t$ or $D_2\delta t$, if the site $i-1$ or $i+1$ is vacant. Furthermore, the roadblocks can vacate the site i with probability $k_{\rm off}\delta t$ and jump to one free site randomly. The move probability $(D_1+D_2+k_{\rm off})\delta t$ should be no more than 1. 10^8 Monte Carlo steps are run in each simulation. In order to insure the steady state, data after 10^7 Mote Carlo steps are used.

3. Diffusive roadblocks without unbinding

In this section, we consider diffusing roadblocks which do not unbind ($k_{\rm off}=0$). Firstly, one roadblock with different D_1 and D_2 is investigated. When $D_2=0$, the diffusing roadblock corresponds to a stationary one, so the flux is always 0. When $D_1=0$, the model degenerates into TASEP with one slow particle (Fig. 2(a)). An asymmetry with maximal current at $\rho>0.5$ is found at different combinations of D_1 and D_2 (Figs. 1(b)–1(d)). Comparing with the scenario of TASEP with one slow particle, the diffusing rate D_2 leads to the asymmetry. With increasing D_1, the maximal current reduces. Figure 3 shows the relationships between the maximum current and relevant density different values of D_1 and D_2. With the enhancement of D_2, the maximum current enlarges, and the relevant density tends to 0.5.

Form Fig. 4, we can see that the asymmetry is independent of roadblock number M. But with enlarging M, the flux decreases. Moreover, in systems of different sizes with the same M roadblocks, fluxes are also different. Figure 4(c) shows that the same proportion of roadblocks in any system size results in similar fluxes.

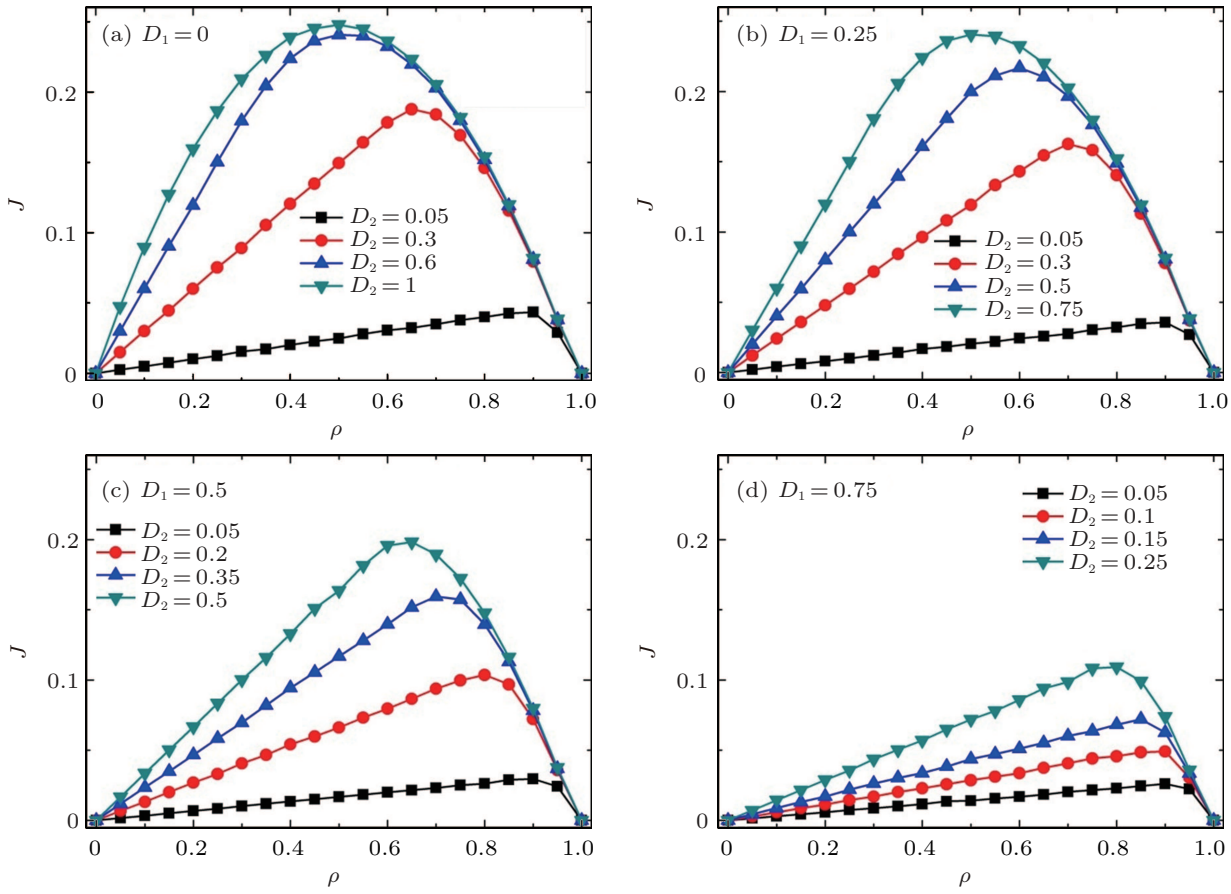


Fig. 2. (color online) Current–density relations for different values of D_1 and D_2, with $k_{\rm off}=0$, $\varepsilon=1$, $M=1$, and $L=1000$.

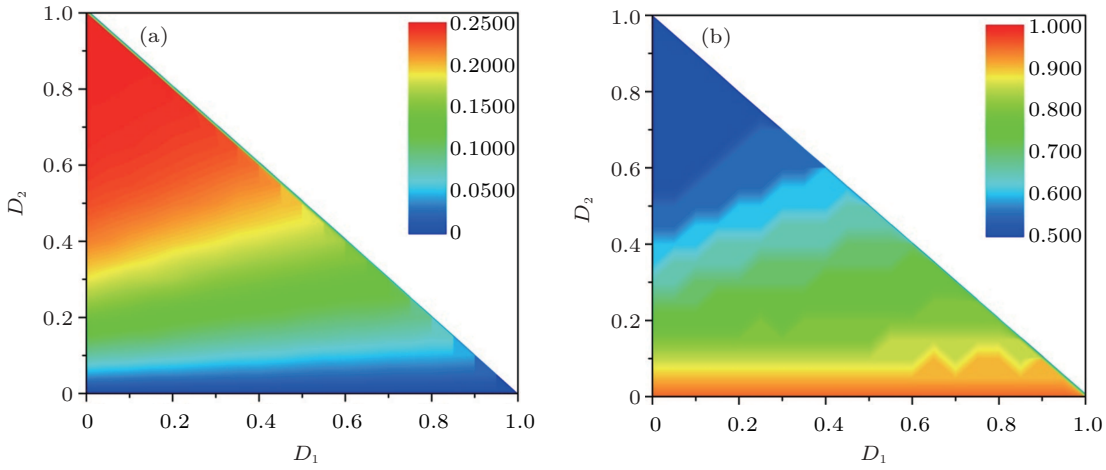


Fig. 3. (color online) (a) Maximum flux and (b) corresponding density against D_1 and D_2, respectively, with $k_{\rm off} = 0$, $\varepsilon = 1$, $M = 1$, and $L = 1000$.

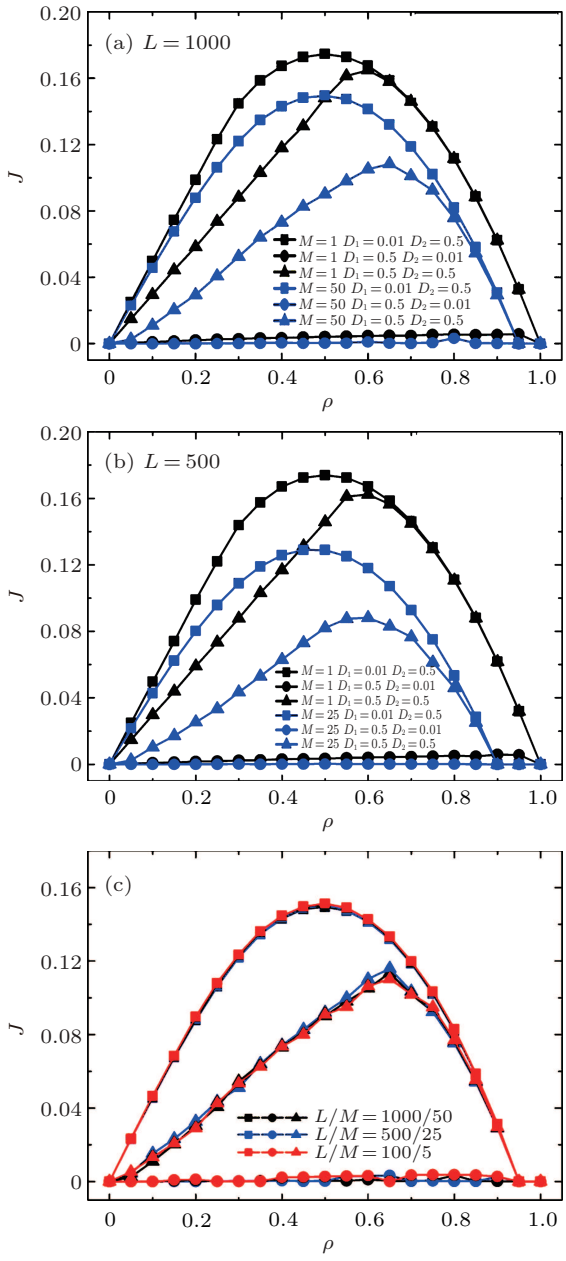


Fig. 4. (color online) Current-density relations with no-jumping roadblocks at system size $L = 1000$ (a), 500 (b), and at the same L/M (c), respectively, with $k_{\rm off} = 0$ and $\varepsilon = 1$.

4. Non-diffusive roadblocks

In this section, we investigate non-diffusive roadblocks that can only move through the unbinding-rebinding process ($D_1 = D_2 = 0$). Figures 5 and 6 show that the relationships between particle flux and density are qualitatively consistent with that in TASEP without roadblocks.

The particle flux is intensely dependent on system size, when $k_{\rm off}$ is very small as shown in Figs. 5(a) and 5(b). With increasing roadblock number M, the particle flux decreases in the same system (Fig. 5(c)). Movements of roadblocks are very rare because of small $k_{\rm off}$. Therefore, in the average condition, the system segregates into M subregions of length N/M, i.e., containing N/M particles behind one roadblock. The waiting time before a roadblock unbinds is $k_{\rm off}^{-1}$, and it can chooses a free site randomly. M subregions of particles lead to M subregions of free sites. If the roadblock chooses one free site from the closest forward subregion, the blocked particles can move a distance $(L-N-M)/2M$ on average. If the roadblock chooses one free site from any other subregions, the blocked particles move $(L-N-M)/M$ sites on average.

Thus the average velocity is average steps a particle moves in a time $1/k_{\rm off}$, and given as

$$v = \left(\frac{1}{M}\cdot\frac{L-N-M}{2M} + \frac{M-1}{M}\cdot\frac{L-N-M}{M}\right)\Big/\frac{1}{k_{\rm off}}. \quad (1)$$

The total flux is

$$J_{\rm ave} = v\rho = k_{\rm off}\cdot\frac{N}{L}\cdot\frac{(L-N-M)\cdot(2M-1)}{2M^2}. \quad (2)$$

Alternatively, we write $N = \rho L$, then

$$J_{\rm ave} = v\rho = k_{\rm off}\cdot\rho L\cdot\frac{(1-\rho-M/L)\cdot(2M-1)}{2M^2}. \quad (3)$$

System size L has an effect on the particle flux.

From Eq. (2), in a system with the same size L and particle number N, the flux reduces as roadblocks increase. Figure 5(c) shows the variations of flux at density $\rho = 0.5$ with variable M for different system sizes. The simulation result is in qualitative agreement with the analysis result.

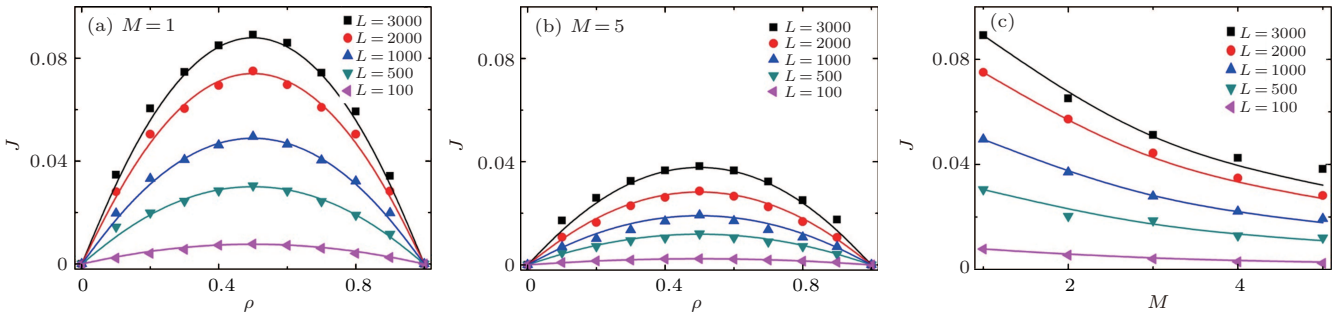


Fig. 5. (color online) Current–density relations at different system sizes with $M = 1$ (a) and 5 (b), respectively. (c) The maximum flux versus roadblock number M with $k_{\rm off} = 0.0007$, $D_1 = D_2 = 0$, and $\varepsilon = 0.7$. The discrete points are simulation results, and the solid lines are analysis results.

For large $k_{\rm off}$, the system behaves almost as a normal TASEP, which is independent of system size (Fig. 6(a)). However, if roadblock number M is not far less than system size L (Fig. 6(b)), the particle flux will present a significant decline, since roadblocks reduce the movement space of particles.

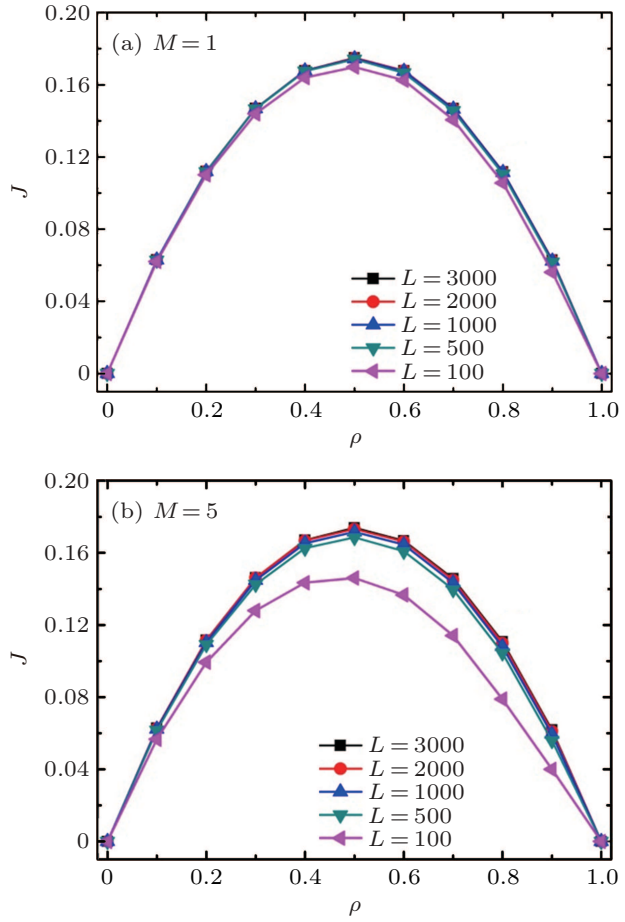


Fig. 6. (color online) Current–density relations for different system sizes, with $M = 1$ (a) and 5 (b). $k_{\rm off} = 0.7$, $D_1 = D_2 = 0$, and $\varepsilon = 0.7$.

5. Diffusive roadblocks with unbinding

Roadblocks with both diffusive and unbinding movements are also discussed. When $D_1 \gg D_2$, the roadblocks can be regarded as the only diffusive ones, so the particle flux is always asymmetric in the parameter space $(k_{\rm off}, D_1)$. When $D_1 \approx D_2$, the simulation result is similar to that given by Sahoo *et al.*[28] The roadblock number has no effect on symmetry qualitatively. When $D_1 \ll D_2$, $k_{\rm off} > D_2$ leads to the symmetric current–density relation with the maximum at $\rho = 0.5$. At $k_{\rm off} < D_2$, too small D_2 results in obstructing particle movement. Therefore the asymmetric relation appears (Fig. 7).

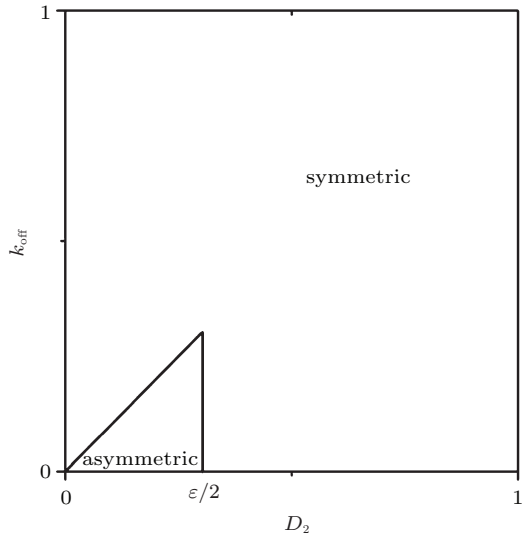


Fig. 7. A symmetric summary with dynamic behaviors of roadblocks at $D_1 \ll D_2$.

6. Conclusions

An exclusion process with multiple roadblocks on 1D lattice is investigated. Roadblocks exhibit two different types of dynamic moves, i.e., diffusive motion with different forward and backward rates, and long-range unbinding/rebinding. The case of only diffusive roadblocks shows an asymmetric current–density relation, and the particle flux increases with enhancing D_2. The case of only long-range jumping roadblocks presents that flux decreases with increasing roadblock number M. Combining two types of movements does not generate qualitatively new behavior, but phase diagram in $(k_{\rm off}, D_2)$ parameter space can be delineated. Despite the fact that the simple model reveals some interesting dynamics, additional work is needed to better understand biological systems, such as open boundary. More dynamic behaviors can be observed from variant models.

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