Two dimensional exclusion process between rough interfaces

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Abstract. Driven flow between rough walls is studied in the framework of the two-dimensional exclusion process by using continuous-time Monte Carlo simulations. In particular we consider the effect of the roughness and other characteristics of the walls on the current and current profiles at different types of locations along the channel.

1. Introduction
Technological advances have made it possible to miniaturize devices down to submicrometric sizes and has enabled manufacturing of numerous devices used for manipulation and transport of matter. Especially the field of microfluidics has obtained a growing amount of interest since it was born about twenty years ago [1]. Microfluidics has been used to answer fundamental questions in physics such as the behavior of single molecules or particles in fluid flows. Transport in some dynamical environment can also be used to probe the properties of the environment. It is a well known fact that the structure, e.g. the roughness, of the surface does not cause any significant deviation in the properties of the flow if the system size is big enough. However, surface roughness becomes relevant if typical length scales of the system are comparable to the scale of its variation as is the case of microfluidic setups concerning fluids in rough or structural microchannels [2, 3, 4].

The asymmetric exclusion process is one of the simplest lattice models describing transport far from equilibrium [5, 6]. In one dimension it has been extensively studied during the past decades while its extension to higher and possible more physical (higher) dimensions are almost neglected. Furthermore, the studies on exclusion models in two dimensions are usually studies with semi infinite lattices [7] without any geometrical constraint. When considering transport in realistic environments the geometry is usually restricted. Examples of realistic transport processes vary from fluid flow in channels to vehicular traffic. In addition, from numerous diffusion studies made in past decades we have learned that even the most simple geometrical constraints can cause significant changes in mass transport [8].

Even though the hydrodynamic equations corresponding to the asymmetric exclusion process are not the Navier-Stokes equations, analysis of exclusion process can produce relevant insight in transport in rough channels especially in situations, where the system is far from equilibrium and inertia is not a major factor, but the underlying microscopy can not be forgotten. In this work we consider the two dimensional asymmetric exclusion process (ASEP) in rough channels. The channel walls are provided by interfaces produced by a discrete interface model.
2. Models

2.1. Models for the rough channels

We first consider stationary channel walls $h_l$ and $h_u$, i.e. lower wall and upper wall obeying body-centered solid-on-solid (BCSOS) statistics [9]. For comparison, we also have considered the exclusion process between two BCSOS interfaces driven against each other [10, 11]. The location or the ‘height’ of a single BCSOS interface [9] is described by a function $h_i(x, t)$ such that, for every site $x = 1, \ldots, L$, $h_i(x + 1, t) - h_i(x, t) = \pm 1$, where we without loss of generality assume that the possible values of $h_i$ are integers and $i = l, u$. Only two kinds of processes, adsorption ($h_i$ locally increases) and desorption ($h_i$ locally decreases), are available. The stationary state of a single interface is totally disordered, i.e. every configuration allowed by periodic boundary conditions has the same probability to occur.

2.2. Exclusion process

The exclusion process differs from independent random walkers because in it only one particle is allowed to be in a lattice site at any given instant of time. All particles are identical and independently moving in the channel, i.e. between walls $h_u(x, t)$ and $h_l(x, t)$, on a lattice $(x, y)$, where the lattice point coordinates in the horizontal direction $(x)$ are the same $x = 1, \ldots, L$ as for the channel model above, again with periodic boundary conditions and the values of the vertical coordinate $(y)$ coincide with the possible locations of the walls at $h_i(x, t)$.

By denoting the location of the particles by $(x_p, y_p)$, the requirement that particles move inside the channel is equivalent to the condition $h_u(x_p, t) \leq y_p \leq h_l(x_p, t)$. For the moves of the particle, the following exclusion rule is imposed in all cases: Only one particle can be at each site at instant of time so that for a jump $(x_p, y_p) \rightarrow (x_p', y_p')$ to be possible, the arrival site must be empty.

For moves on the square lattice there are a few natural choices for the possible particle jumps $(x_p, y_p) \rightarrow (x_p', y_p')$. Here we concentrate on the case where only nearest-neighbor jumps are allowed such that the particle jumps in the horizontal direction $(x_p, y_p) \rightarrow (x_p + 1, y_p)$ with the attempt rate $\alpha$ and in the vertical direction $(x_p, y_p) \rightarrow (x_p, y_p \pm 1)$ with rate $\beta$. The dynamics used in this study is sequential, i.e. one particle jumps at a time.

For tracer diffusion of independent particles between similar walls the diffusion coefficient for different choices of dynamics do not differ significantly [11]. The same is found for dispersion around the flow in the present case. However, for lattice gas models of fluid flow with parallel dynamics including particle collisions, it is well known that in two dimension the number of jump directions must be at least eight in order to retain the conservation laws. Collision phenomena could also be included in exclusion models by allowing longer jumps of the particles. Our model best describes the strongly dissipative case.

3. Results

In figure 1 we show snapshots of the scaled occupation probability between the walls for different average particle densities $\rho$. The spatial inhomogeneity decreases for increasing $\beta$, which is the rate of diffusion in the vertical direction. With flat (in the BCSOS sense) walls, spatial homogeneity is achieved in the simulation for all values of $\beta > 0$, while for increasing roughness the value of $\beta$ required for approximate homogeneity is larger. Homogeneity gets broken because the particles tends to drift towards the wall at locations with long slopes. Spatial homogeneity, or deviations from it, becomes a particularly important explaining factor for understanding the properties of the current through the system.

In Fig. 2 we show the expected value of the particle current $I$ crossing a lattice site as a function of the wall roughness $W = \langle (h_i - \bar{h}_i)^2 \rangle$, where the average $\bar{h}_i$ is taken over the configuration. The value of the current for a given wall roughness depends strongly also on other properties of the walls. Wall configurations corresponding to the extrema of the current
Figure 1. Probability to find particle at location \((i, j)\) with several values of the parameter \(\beta\) values. Here the red color indicates highest density and blue color lowes density. The average density is \(\rho = 0.2\) and the drift \(\alpha = 1\). The system size is \(L = 100\) and the width of the channel four lattice units. The parameter \(\beta\) controlling diffusion in the vertical direction increases from top to bottom from 0.25 to 20.

Figure 2. In the figure on the left we show average current through the cross-section measured at \(x = L\) as a function of the wall roughness \(W\) with \(\rho = 0.20\) for individual wall configurations. In the figure on the right we show the averaged current over configurations corresponding to a given wall roughness as a function of density. The system size is \(L = 100\) and the jump rates are \(\alpha = 1\) and \(\beta = 0.5\).
were created by running variations of the usual BCSOS dynamics for a while starting from certain initial configurations, a disordered one, a flat one and a faceted one. For example, the smallest currents were obtained by generating the wall configurations by depositing 'particles' anywhere on the interface [9] such that they slide down to the closest wall height minimum. The maximum current for a given roughness was obtained by producing walls such that the BCSOS dynamics corresponds to one-dimensional ASEP (one-to-one mapping where a particle corresponds to upward step), where in the ASEP interpretation particle a chosen randomly hops to a location as far as possible from the closest particles with conserving the order of particles in the system. This way it was possible to achieve wall configurations with very different topography and efficiently scan the available phase space for this plot. In Fig. 2 we show also the expected current averaged over the different configurations corresponding to the same roughness. For spatially homogeneous density the mean-field prediction $I(\rho) = \alpha \rho (1 - \rho) d$ for the averaged current works well, and increasing deviations are observed for increasing the wall roughness. The amount of this deviation decreases for increasing $\beta$.

In Fig. 3 we show the ensemble averaged current profiles at special points of the wall

Figure 3. The time-averaged current profile in $y$ direction at locations in $x$ direction corresponding to max $\{h_i\}$ (left) and mean $\{h_i\}$ (middle) and at any location (right) for several values of the density $\rho$. Here $L = 100$, $\alpha = 1$ and $\beta = 0.5$.

Figure 4. The time-averaged current profile in $y$ direction at locations in $x$ direction corresponding to max $\{h_i\}$ (left) and mean $\{h_i\}$ (middle) and at any location (right) for several values of the wall roughness $W$. Here $L = 100$, $\alpha = 1$ and $\beta = 0.5$. 

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\[ I(\rho) = \alpha \rho (1 - \rho) d \]
configurations and also averaged over the system for different values of the particle density \( \rho \). At the locations corresponding to the extrema, i.e. \( \max(h_1) \) and \( \min(h_1) \), the current tends to have a monotonic profile. The general shape of the profiles on those locations is easily understood by looking at Fig. 1. The particles tend to crowd at the slope leading to the extreme of a wall, leading to a smaller density right after it. At more typical locations the profile is symmetric. In Fig. 4 we show the ensemble averaged current profile at special points of a given configurations with each curve corresponding to a given value of the wall roughness \( W \). At the extremal locations the current goes to zero at one side of the tube because of the micro roughness of an BCSOS interface. The roughness alone does not explain the current profile, as evident also from figure 2, where the values of \( I \) spread widely for small and intermediate values of \( W \). This spread can be attributed to the dispersion of the current induced by the wall configuration. The distribution of the current (not shown) is found to be approximately gaussian.

4. Conclusions

The particle current in the two-dimensional exclusion process in a channel with rough walls was found to depend strongly on the configurations of the walls. Not only the roughness of the walls but also their overall shape determines the current. The regions close to the extrema (in the transverse direction) of the channels have a prominent effect on the transport. The channel profile in the highly dissipative case turns out to have a much greater impact on the particle flow and its dispersion than it does in the case of laminar flow previously considered in the literature. Work including interactions in both directions between fluctuating walls and the exclusion process is in progress.

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