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Residence time estimates for asymmetric simple exclusion dynamics on strips

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HIGHLIGHTS

- We target at estimating the residence time of particles undergoing ASEP on a two-dimensional vertical strip.
- The asymmetry is given by different reservoir levels and a strong anisotropic drift.
- We focus on the effect of anisotropy on residence times.
- Our analysis relies on a Mean Field Model and a 1D Birth-and-Death Model.
- The topic is relevant for pedestrian flows and biological transport in crowded environments.

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ABSTRACT

The target of our study is to approximate numerically and, in some particular physically relevant cases, also analytically, the residence time of particles undergoing an asymmetric simple exclusion dynamics on a two-dimensional vertical strip. The sources of asymmetry are twofold: (i) the choice of boundary conditions (different reservoir levels) and (ii) the strong anisotropy from a drift nonlinear in density with prescribed directionality. We focus on the effect of the choice of anisotropy on residence time. We analyze our results by means of two theoretical models, a Mean Field and a one-dimensional Birth and Death one. For positive drift we find a striking agreement between Monte Carlo and theoretical results. In the zero drift case we still find agreement as long as particles can freely escape the strip through the bottom boundary. Otherwise, the two models give different predictions and their ability to reproduce numerical results depends on the horizontal displacement probability. The topic is relevant for situations occurring in pedestrian flows or biological transport in crowded environments, where lateral displacements of the particles occur predominantly affecting therefore in an essentially way the efficiency of the overall transport mechanism.

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1. Introduction

The efficiency of transport of active matter in microscopic systems is an issue of paramount importance in a number of fields of science including biology, chemistry, and logistics. Looking particularly at drug-delivery design scenarios [1], ion moving in molecular cytosol [2–4], percolation of aggressive acids through reactive porous media [5], the traffic of pedestrians in regions with drastically reduced visibility (e.g., in the dark or in the smoke) [6–8] (see also the problem of traffic of cars on single-lane highways [9]), we see that the efficiency of a medical treatment, the properties of ionic currents thorough cellular membranes, the durability of a highly permeable material, or the success of the evacuation of a crowd of humans, strongly depends on the time spent by the individual particle (colloid, ion, acid molecule, or human being) in the constraining geometry (body, molecule, fabric, or corridor).

In this framework, we focus our attention on the study of the simplest 2D scenario that mimics alike dynamics. The *Gedankenexperiment* we make is the following: we imagine a vertical strip whose top and bottom entrances are in touch with infinite particle reservoirs at constant densities. Assume particles are driven downwards by the boundary densities difference and/or an external constant and uniform field (electrical, gravitational, generally-accepted crowd opinion, …). Let the *residence time* be the typical time a particle entering the strip at stationarity from the top boundary needs to exit through the bottom one. In this framework, under the assumption that particles in the strip interact only via hard-core exclusion, we study the *ballistic-like* versus the *diffusion-like* dependence of the residence time on the external driving force (main source of anisotropy in the system), on the length of the strip, on the horizontal diffusion, and, finally, on the choice of the boundary condition at the bottom.

We recover the structure of the fluxes as well as the residence times proven mathematically by Derrida and co-authors in Ref. [10] for the asymmetric simple exclusion model on the line; see also Ref. [11] for a more recent approach. In chemistry single file diffusion has been demonstrated for zeolite catalysts [12] to dramatically reduce the rate of a reaction. This happens in particular when zeolitic microporous systems are used with linear micropores with dimensions that are similar as the size of the molecules that are converted. Since they cannot pass single file inhibition occurs (see, for instance, Ref. [13]).

Additionally, we discover new effects that are purely due to the choice of the 2D geometry and which are therefore absent in a 1D lattice. The most prominent, within the precision of our numerical simulations, is the non-monotonic behavior in changes in the horizontal displacement probability in the bouncing back regime reported in Section 6.3. Under certain conditions, particles start accumulating near the bottom exit of the strip. This crowding leads to a bouncing-back effect in which particles trying to escape are reflected in the bulk. We observe that, in such a case, increasing the frequency of horizontal movements help particles to overcome obstacles and to find their way to the exit.

To investigate this model, we employ several working techniques including Taylor series truncations for the derivation of the mean-field equations, ODE analysis of the stationary case, estimates involving the structure of the stationary measure for birth and death processes on a line, as well as Monte Carlo simulations to exploit the resources offered by the various parameter regimes. In 1D, this model has been widely studied both by the mathematical and physical communities, see e.g. Refs. [14,15,10,16,17,11]. In 2D, the situation is very much unexplored especially in the asymmetric case. We deal with this precise problem and we give a rather complete description of the phenomenon. Our results, which are based on a thorough study of two simplified models and extensive Monte Carlo simulations, open new mathematical problems concerning the typical time a particle need to cross a region in hard-core repulsion regime.

More precisely, in the paper we develop two analytic approaches to predict the mean residence time: a macroscopic Mean Field theory and a semi-microscopic approach in which the particle motion is imagined as that of a single particle against a prescribed background density profile borrowed from the macroscopic Mean Field theory. These two different predictions are very similar to each other but for the regime described above in which the non-monotonic effect is found. In this regime the horizontal displacement probability tunes the system behavior from the macroscopic prediction to the semi-microscopic one, with the two limits recovered, respectively, in the zero and one horizontal probability displacement cases.

The importance of the exclusion rule on the time dependence of the typical distance covered by a particle is not new in the scientific literature. Due to the exclusion rule, the asymmetric process on a square lattice that we discuss here can be considered to occur on a percolating lattice. The symmetric exclusion case has been widely explored for diffusion, as for instance the "ant in the labyrinth" by de Gennes [18]. The distance travelled by the ant is proportional to the square root of the time (random walk diffusion) as long as the site occupancy is low, but, when the critical 0.5928 site occupation is approached, this changes to a time dependence close to cubic root of time. Beyond this critical site occupancy the order in time rapidly drops. The excluded volume problem in several dimensions has not yet found however a satisfactory solution [19].

A related but similar phenomenon occurs in the symmetric 1D case. When site occupation increases the distance time relation becomes the fourth root of time [20]. The asymmetric problem in 2D, that we are interested in, can be more easily addressed as asymmetric exclusion with driven diffusion, see Ref. [21] for a paper and [22] for a complete review. In the 1D total asymmetric case (particles can move only from the top to the bottom), using a kinematic wave theory related approach and the method of maximum transported current [22], it is identified a three parameter space region as a function of the rates at which particles would enter (from the top) or exit (from the bottom) the strip. These regions closely relate to the particle density where percolation sets in (on a square lattice with stochastic bond formation the percolation threshold is 0.5). In this paper we will be mainly concerned with the case where the relative probability for a particle to enter the strip (from the top) is one. In this case the two situations than can be distinguished are the high density phase (exit probability

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