Obstacle induced particle jamming in exclusion dynamics

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Particles in a strip
  model
  stationary state
  residence time

Strip without obstacles
  effect of lateral displacement
  mean field or macroscopic limit
  analogy with a not symmetric Random Walk
  results

Strip with obstacles
  mean field stationary state
  results on residence time
The problem

Propose a basic model to study the effect of obstacles in a strip in which particles are moving possibly in a preferred direction.

Question we address: effect of the obstacles on the *residence time*, that is to say, the typical time needed by the particles to walk along the whole lane?

In collaboration with A. Muntean, O. Krehel, R. van Santen, A. Sengar,


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Flux in a strip with obstacles

The motion of particles obeys the following rules:

- particle move randomly in any direction on a square lattice (the strip);
- particles enter the strip through the top boundary;
- particles exit the strip through the bottom boundary;
- top and vertical boundaries are reflecting for particles moving inside the strip;
- particle possibly experiences a downward drift.

Possible impediments to motion:

- obstacles in the core of the strip modeled by rectangles with reflecting boundaries;
- particles entering the strip through the bottom boundary.
Model

- \( (1-h)(1-\delta)/2 \)
- \( h/2 \)
- \( (1-h)(1+\delta)/2 \)

- \((y, x) \in \{1, \ldots, L_1\} \times \{1, \ldots, L_2\}\) lattice site
- simple exclusion in the bulk
- reflecting vertical boundaries
- reservoirs \( \rho_u = 1 \) and \( \rho_d \in [0, 1) \)
- \( h \in [0, 1) \) probability of horizontal motion
- \( \delta \in [0, 1] \) vertical drift
- black squares denote obstacles
Model

At each time step $t$ try to move a number of particles equal to the number of particles $n(t - 1)$ in the strip at $t - 1$ plus one.

For $n(t - 1) + 1$ times with probabilities

$$\frac{\varrho_u L_1}{\varrho_u L_1 + \varrho_d L_1 + n(t)}, \frac{\varrho_d L_1}{\varrho_u L_1 + \varrho_d L_1 + n(t)}, \frac{n(t)}{\varrho_u L_1 + \varrho_d L_1 + n(t)}$$

do the following: Top insert, Bottom insert, Bulk move.

Top insert: choose uniformly a site in row 1 and put there a new particle if empty: $n(t) = n(t) + 1$.

Bottom insert: choose uniformly a site in row $L_2$ and put there a new particle if empty: $n(t) = n(t) + 1$.

Bulk move: see the picture.
Let evolve the system for a sufficiently long time $\bar{t}$ and then for $t$ large the sum

$$\rho(y, x) = \frac{1}{t - \bar{t}} \sum_{t' = \bar{t}}^{t} \eta_{t'}(y, x)$$

becomes constant and provides the stationary occupation number profile.

Horizontal average:

$$\rho(x) = \frac{1}{L_1} \sum_{x=1}^{L_1} \rho(y, x)$$
Stationary state

Parameters: $L_1 = 80$, $L_2 = 400$, $\varrho_u = 1$, $\varrho_d = 0$, $h = 0.5$, and $\delta = 0.04$.
One obstacle on the left and three obstacles on the right.
Obstacle width: red 10, green 20, blue 40, and purple 70.
Residence time

The main quantity of interest is the *residence time* at stationarity:

\[ R = \text{typical time a particle needs to exit the strip at stationarity} \]

Computing the residence time:

- *Monte Carlo* estimate: we shall run long simulations and average *at stationarity* the time needed by each particle which entered the strip through the top boundary to exit through the bottom boundary;

- we shall develop two analytic arguments to estimate the residence time which will be called *Mean Field* (MF) and *Birth–and–Death* (BD) estimates.
Strip without obstacles
Effect of lateral displacement

In absence of obstacles we expected a trivial effect due to the two–dimensionality of the problem (positive $h$):

- consider a phenomenon taking time $T$ for the analogous one dimensional problem ($h = 0$);
- in the strip it will take the time $T'$ such that

$$T' = T + hT' \implies T' = \frac{T}{1 - h}$$

Numerically we find this trivial result in the cases $\delta = 1$ or $\varrho_d = 0$

Numerically we find not trivial results in the cases $\delta = 0$ and $\varrho_d > 0$

- absence of monotony with respect to $h$
- transition between two different analytic results
Macroscopic variables under diffusive scaling $\varepsilon \to 0$: 

$$y \to \varepsilon y, \quad x \to \varepsilon x, \quad t \to \varepsilon^2 t \quad \text{and} \quad \delta \to \varepsilon \delta$$

It is derived a macroscopic equation for the typical occupation number $m_t(y, x)$ for $\varepsilon \to 0$: 

$$\frac{\partial m_t}{\partial t} = \frac{1}{2} h \frac{\partial^2 m_t}{\partial y^2} + \frac{1}{2} (1 - h) \frac{\partial^2 m_t}{\partial x^2} - \delta (1 - h) \frac{\partial}{\partial x} [m_t(1 - m_t)]$$

Mean field stationary profile

In absence of obstacle: look for stationary solution of the macroscopic equation $\varrho = \varrho(x)$ not depending on the horizontal coordinate $y$.

Get the equation:

$$\frac{1}{2} \frac{d^2}{dx^2} \varrho - \delta \frac{d}{dx} \varrho(1 - \varrho) = 0 \quad \text{with} \quad \varrho(0) = \varrho_u, \varrho(L_2 + 1) = \varrho_d$$

Parameters: $L_1 = 100$, $L_2 = 200$, $h = 0.5$, and $\delta = 0.8$. Left: $\varrho_u = 1$, $\varrho_d = 0$. Right: $\varrho_u = 0.8$, $\varrho_d = 0.55$. 
Mean Field residence time prediction

The Mean Field equation is a continuity equation for the flux

$$\tilde{J}_t = -\frac{1}{2} h \frac{\partial m_t}{\partial y} \vec{e}_1 + \left( -\frac{1}{2} (1 - h) \frac{\partial m_t}{\partial x} + \delta(1 - h)m_t(1 - m_t) \right) \vec{e}_2$$

At stationarity the density $\varrho$ depends only on $x$, thus the flux reads

$$J = -\frac{1}{2} (1 - h) \frac{\partial \varrho}{\partial x}(x) + \delta(1 - h)\varrho(x)[1 - \varrho(x)] = -\frac{1}{2} (1 - h)\varrho'(0)$$

Assume that the typical velocity $v(x)$ of a particle occupying a position with vertical coordinate $x$ is such that

$$\varrho(x)v(x) = J$$

A simple integration gives the residence time

$$R = \int_0^{L_2+1} \frac{\varrho(x)}{J} \, dx = -\frac{2}{(1 - h)\varrho'(0)} \int_0^{L_2+1} \varrho(x) \, dx$$
Analogy with a not symmetric Random Walk

Jump probabilities are chosen as follows:

\[ q_i = \frac{1 - h}{2} (1 + \delta) [1 - \varrho(L_2 + 1 - i + 1)] \quad \text{for } i = 1, \ldots, L_2 \]

\[ p_i = \frac{1 - h}{2} (1 - \delta) [1 - \varrho(L_2 + 1 - i - 1)] \quad \text{for } i = 0, \ldots, L_2 - 1 \]
Analogy with a not symmetric Random Walk

\[
\begin{array}{cccccc}
0 & 1 & q_x & p_x & L_2 & L_2+1 \\
\bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\
\downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow \\
\text{boundary } \varrho_d & i & \text{boundary } \varrho_u
\end{array}
\]

Residence time

\[ R = \mathbb{E}[T] \]

where

\[ T = \text{first hitting time to } 0 \text{ for a walker started at } L_2 \]

It is well known that

\[
\mathbb{E}[T] = \frac{1}{q_{L_2}} + \sum_{i=1}^{L_2-1} \frac{1}{q_i} \left( 1 + \sum_{j=i+1}^{L_2} \prod_{k=i+1}^{j} \frac{p_{k-1}}{q_k} \right)
\]

A general explicit expression cannot be provided, but one can compute the above sum numerical for any choice of the parameters.
Results: $\varrho_d = 0$

Parameters: $\varrho_d = 0$, $L_1 = 100$, and $L_2 = 200$; the symbols $\bullet$, $\bigtriangleup$ and $\blacksquare$ refer to the cases $h = 0, 0.4, 0.8$.

Solid curves are the random walk prediction, open disks represent the Mean Field prediction.
Parameters: $h = 0.4$, and $L_1 = 100$; ⬤, ▲ and ■ refer to $\varrho_d = 0, 0.4, 0.8$. Solid curves and open disks represent the BD and the MF predictions. Open squares denotes the MF and BD result for $L_2$ large:

$$R_{MF} = R_{BD} \approx \frac{L_2}{(1 - h)(1 - \varrho)(\delta)}$$
Results: $\delta = 0$ and $\varrho_d > 0$

Parameters: $\delta = 0$, $L_1 = 100$, and $L_2 = 200$; the symbols $\bullet$, $\Delta$ and $\blacksquare$ refer to the cases $h = 0, 0.4, 0.8$.

Solid curves are the random walk prediction, dashed lines represent the Mean Field prediction.
Transition between the MF and BD regimes

Residence time vs. horizontal displacement probability \( h \) for \( L_1 = 100, L_2 = 200, \delta = 0, \varrho_d = 0.1 \) (left) and \( \varrho_d = 0.4 \) (right). Solid curves are the random walk prediction, dashed lines represent the Mean Field prediction.

Explicit formulas

\[
R^{\text{MF}} = \frac{1}{1 - h} \frac{1 + \varrho_d}{1 - \varrho_d} (L_2 + 1)^2 \quad \text{and} \quad R^{\text{BD}} = \frac{1}{1 - h} \frac{1}{1 - \varrho_d} L_2 (L_2 + 1)
\]
Non-monotonicity on $h$: $\delta = 0$, $L_1 = 100$, and $L_2 = 200$
Strip with obstacles
Solve the equation

\[
\frac{1}{2} h \frac{\partial^2 \rho}{\partial y^2} + \frac{1}{2} (1 - h) \frac{\partial^2 \rho}{\partial x^2} - \delta(1 - h) \frac{\partial}{\partial x} [\rho(1 - \rho)] = 0
\]

in the domain equal to the strip minus the region occupied by the obstacle

- with Neumann homogeneous boundary conditions on the vertical boundaries and on the boundaries of the obstacle
- with Dirichlet boundary conditions \( \rho_u \) and \( \rho_d \) on the top and on the bottom boundaries.

Remark: the solution will depend on the horizontal coordinate \( y \).
Mean Field stationary profile

Parameters: $\rho_d = 0.9$ (left), $\rho_d = 0.0$ (right), $W = 85$ (top), $W = 90$ (bottom), $L_1 = 100$, $L_2 = 400$, $h = 0.5$, $\delta = 0.05$, $\rho_u = 1$, $O_2 = 3$. 
Residence time estimate

As before we compare the Monte Carlo (labelled LA), the Mean Field (MF) and the Birth–and–Death (BD).

We use the horizontally averaged density profile

\[ \varrho(x) = \frac{1}{L_1} \sum_{x=1}^{L_1} \varrho(y, x) \]

We do not expect quantitative agreement, since in this case the horizontal translation invariance is lost.
Results: zero drift ($\delta = 0$)

Parameters: $L_1 = 100$, $L_2 = 400$, $O_2 = 3$, $h = 0.5$, $\rho_d = 0$ (left), and $\rho_d = 0.9$ (right).

We find the expected results: increasing with $W$, good agreement on the left for $W$ small enough (MF much better than BD), poor agreement on the right (BF better than MF).
Results: not zero drift ($\delta > 0$)

Parameters: $L_1 = 100$, $L_2 = 400$, $h = 0.5$, $O_2 = 3$, and $\delta = 0.1$.

Remarks:
- good agreement with MF (not reported on the picture);
- increasing with $W$ for $\varrho_d \leq 0.5$;
- not monotonic behavior with $W$ for $\varrho_d > 0.5$;
Focus on the case $\rho_d = 0.9$

Parameters: $L_1 = 100$, $L_2 = 400$, $h = 0.5$, $O_2 = 3$, and $\rho_d = 0.9$ (right).

The residence time $R$ is almost constant till a critical value of $W$ is reached, where it decreases abruptly. After that it starts to increase.

We can explain this effect in terms of the occupation number stationary profile.
Horizontally averaged occupation number profile

Parameters: lattice $100 \times 400$, $h = 0.5$, $\delta = 0.1$, $\rho_d = 0$ (left), $\rho_d = 0.4$ (center), $\rho_d = 0.9$ (right), and $O_2 = 3$. Remarks:

- left and center pictures are similar: nothing happens for $\varrho_d \leq 0.5$;
- at $\varrho_d = 0.9$ the average occupation number in the upper region is much higher and hence so it is the residence time;
- for $W = 80$ there is an abrupt change in the profile after the obstacle: the residence time decrease;
- the further increase of the occupation number in the upper part justifies the finale increase of the residence time.
Comments

- modeled the problem by means of a lattice exclusion process
- developed two analytical tools to estimate the residence time
- without obstacles: we found strange behaviors in the zero drift regime when particles are allowed to enter through the bottom boundary
- with obstacles: in the not zero drift regime we found a not monotonic behavior of the residence time with respect to the width of the obstacle
- explored the connection of such a behavior with the shape of the occupation number stationary profile
- what is the reason of the behaviors described above?
- what happens if other parameters of the obstacles are changed? Position? Height?
- last question is connect to Alessandro Ciallella’s poster: a similar problem in the framework of the Lorentz Gas system
Addenda