# Single File escape dynamics in microfluidic channels 

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## Theory



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## Experiments

In collaboration with Dr. Stefano Pagliara
Prof. Ulrich Keyser group


UNIVERSITY OF
CAMBRIDGE
Cavendish
Laboratory BS

## Single File Diffusion



SFD ingredients:

- Order preservation

Free diffusion between collision events

## SFD - examples

## Diffusion in micro/nanoporous materials

Hahn, Karger, Kukla, Phys. Rev. Lett., (1996)

Mukherjee, et al., ACS Nano (2010)


## SFD - examples

## Transport of ions through nanopores

Hodgkin, Keynes,
J. Physiol., (1955)

Jensena, et al., PNAS (2010)


## SFD of colloidal particles

620 nm particles diffusing in the baths


Trapping and dragging particles with HOTs


Array of particle single files, $t=0$


Single file escape processes, $t=18 \mathrm{~s}$ (laser off) d)


## Experimental data

$$
N=3
$$



## Experimental data



## Emptying process


$-L / 2 \quad \boldsymbol{x}$ (MD units) $L / 2$
absorbing boundary
absorbing boundary
We want to characterize the probability of having at least one particle inside the channel $\left[-\mathrm{L}_{c} / 2, \mathrm{~L}_{c} / 2\right] \quad S_{1}\left(t \mid N, L_{c}, L_{0}\right)$

Mean First Passage Time $\longrightarrow$ Characteristic survival time

$$
T_{1}\left(N, L_{c}, L_{0}\right)=\int_{0}^{\infty} S\left(t \mid N, L_{c}, L_{0}\right) d t
$$

## Emptying process


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For Single File systems we can reconstruct this process exactly, using the Reflection Principle Method

## Reflection principle method

Mapping of the Single File into a non-interactive system
Interacting
$t=t_{1}$

Reflection Principle


## Reflection principle method

Mapping of the Single File into a non-interactive system

Interacting
$t=t_{1}$
$t=t_{2}$

Reflection Principle


## Reflection principle method

Mapping of the Single File into a non-interactive system

Interacting

$$
t=t_{1}
$$

$$
t=t_{2}
$$

$$
t=t_{3}
$$

$\square$
1

Reflection Principle


1

## Reflection principle method

Mapping of the Single File into a non-interactive system


Essential ingredients:

- Identical particles
- Elastic collisions


## Reflection principle method

Mapping of the Single File into a non-interactive system


## SFD - Emptying probability

Using the Reflection Principle method, it is possible to map a Single File system to the non-interactive equivalent

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Single File of point-like particles (uniform initial conditions):

$$
1-\frac{S_{1}\left(t \mid N, L_{c}, L_{0}\right)}{\downarrow}=\left[1-\frac{\left.S_{1}\left(t \mid 1, L_{c}, L_{0}\right)\right]^{N}}{\downarrow}\right.
$$

N particles survival probability

## SFD - Emptying probability



## SFD - Mean Emptying Time

It is possible to integrate the last formula to obtain an analytical expression for the Mean Emptying Time, valid for point-like particles

$$
T_{1}\left(N, L_{c}, L_{0}\right)=\frac{L_{c}^{2}}{D_{1}} g\left(N, \frac{L_{0}}{L_{c}}\right)
$$

Valid in presence of small forces $\quad k_{B} T \gg F_{e} L_{c}$

## SFD - Mean Emptying Time



## SFD - Mean Emptying Time

It is also possible to include excluded volume contributions to the Mean Emptying Time using an effective theory, defining an effective channel length

$$
L_{e f f}\left(N, L_{c}, L_{0}, \Gamma, R\right)=\frac{\sum_{k=1}^{N}\left[T_{k}-T_{k+1}\right]\left(L_{c}-2(k-1) R\right)}{T_{1}}
$$

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$$

and substituting it into the analytical expression valid for point-like particles

$$
T_{1}\left(N, L_{c}, L_{0}, R\right)=\frac{L_{e f f}\left(N, L_{c}, L_{0}, R\right)^{2}}{D_{1}(R, \Phi)} g\left(N, \frac{L_{0}}{L_{c}}\right)
$$

## SFD - Mean Emptying Time



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## SFD - Mean Emptying Time



## Conclusions

$\checkmark$ We studied the escape properties of Single File systems of colloidal particles in presence of absorbing boundaries
$\checkmark$ We studied the emptying process, finding an analytical solution for the Mean Emptying Time either in the presence and in the absence of an external force
$\checkmark$ We provided an effective theory to account for excluded volume contributions to the Mean Emptying Time
$\checkmark$ These results are in excellent agreement with experimental data of colloidal particles in microfluidic channels

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My supervisors Fulvio Baldovin
Enzo Orlandini
Matteo Pierno

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Dr. Pagliara and Prof. Keyser @ Cavendish Lab, Cambridge

## SFD - MSD sketch



Jepsen, D., (1965)
Harris, T. E., (1965)
Levitt, D., (1973)
Kollmann, M., (2003)

## Ballistic

## SFD - MSD sketch



Jepsen, D., (1965)
Harris, T. E., (1965)
Levitt, D., (1973)
Kollmann, M., (2003)

Ballistic + Early time diffusion

## SFD - MSD sketch



Jepsen, D., (1965)
Harris, T. E., (1965)
Levitt, D., (1973)
Kollmann, M., (2003)

Ballistic + Early time diffusion + Subdiffusion

## SFD - MSD sketch



Ballistic +Early time diffusion $\boldsymbol{+}$ Subdiffusion $\boldsymbol{+}$ Long time diffusion

## First passage statistics

## Survival probability



Probability that a particle, started from $x_{0}$, is still inside $[-L / 2, L / 2]$ at time $t$

## First passage statistics

Survival probability


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Mean First Passage Time $\longrightarrow$ Characteristic survival time

$$
T_{1}\left(\mathbf{x}_{0}, L\right)=\int_{0}^{\infty} S\left(t \mid \mathbf{x}_{0}, L\right) d t
$$

## SFD of colloidal particles - experimental setup


from Pagliara, Schwall, Keyser (2012)

## SFD of colloidal particles - experimental setup


from Pagliara, Schwall, Keyser (2012)

- PDMS chip is obtained by replica molding
- Chamber is made of two reservoires connected by eight sub-micrometric channels

from Pagliara, et.al (2011)


## Experimental data



## Experimental data



## Experimental data



## Experimental data



