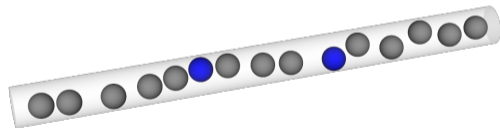


TAGGED PARTICLE(S) IN SINGLE-FILE SYSTEMS

IN AND OUT OF EQUILIBRIUM

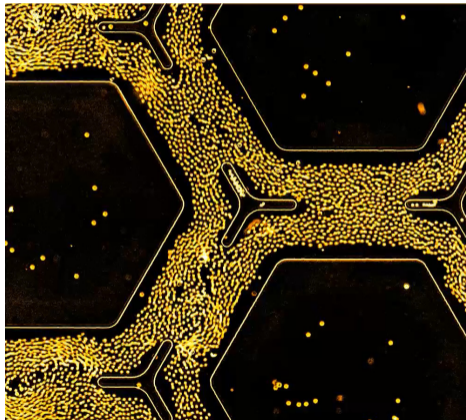
ALEXIS PONCET

ICTS / CNRS MEETING – BANGALORE
DECEMBER 2024



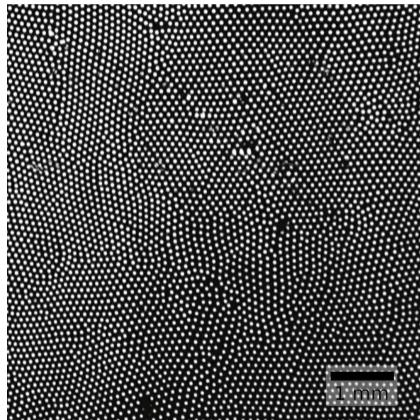
I CHOSE A TOPIC BUT...

Active hydraulics in trivalent networks



[Jorge, Chardac, **Poncet** & Bartolo, Nat. Phys. 2024.]

Melting of non-reciprocal hydrodynamic crystals



[Guillet, **Poncet**, Bartolo et al., under review]

SINGLE-FILE SYSTEMS





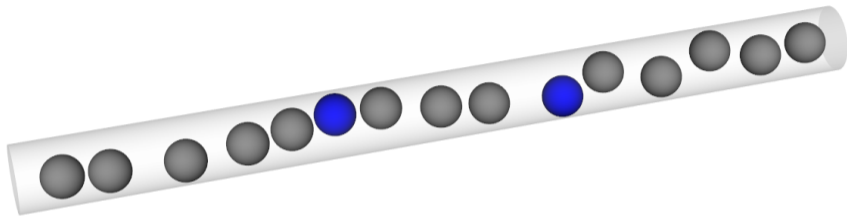
Olivier Bénichou

Aurélien Grabsch

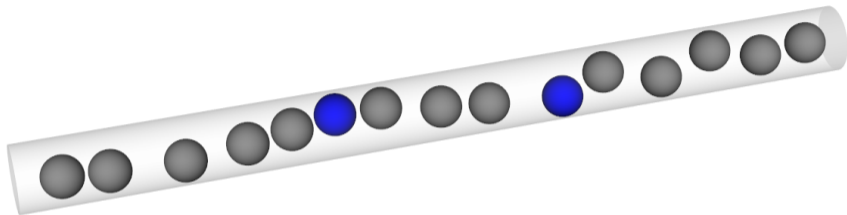
Pierre Illien



SINGLE-FILE SYSTEMS

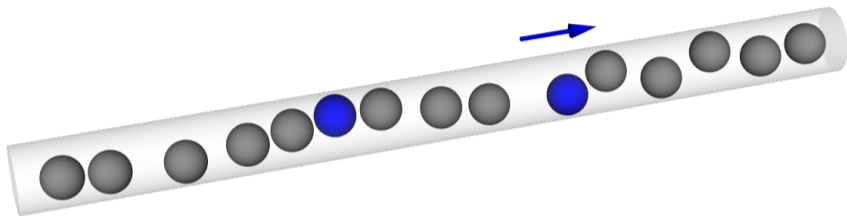


Diffusive particles that cannot pass one another.



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Major impact of confinement: **subdiffusion**, $\langle X(t)^2 \rangle \propto t^{1/2}$



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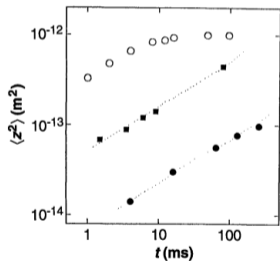
Major impact of confinement: **subdiffusion**, $\langle X(t)^2 \rangle \propto t^{1/2}$

For a driven particle: **sub-ballistic motion**, $\langle X(t) \rangle \propto t^{1/2}$

EXPERIMENTAL EVIDENCE OF ANOMALOUS BEHAVIOR

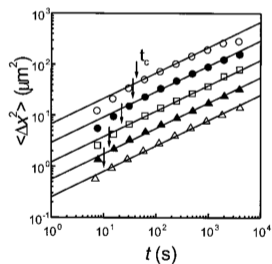
Zeolites

[Kukla et al., Science (1996)]



Colloids

[Wei et al., Science (2000)]



SYMMETRIC EXCLUSION PROCESS (SEP)

Paradigmatic model at equilibrium (and out-of-equilibrium if forced)



Exponential clock and hard core exclusion

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Exponential clock and hard core exclusion

Long-history in physics and mathematics

1983 $\langle X^2(t) \rangle = \frac{1-\rho}{\rho} \sqrt{\frac{2t}{\pi}}$ [Arratia, Ann. Probab.]

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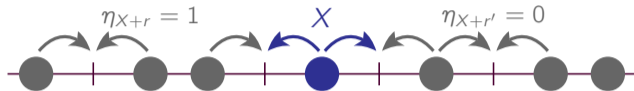
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Connection with larger issues

- ▶ Mapping on XXX quantum spin chain [Alexander & Holstein 1978; de Gier & Essler 2006]
- ▶ Test for Macroscopic Fluctuation Theory [Bertini, RMP 2015]

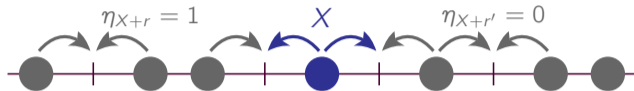
1. Tagged particle at equilibrium



How to close the hierarchy of density-displacement correlations ?

Method: Generalized density profiles

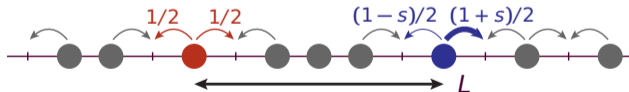
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Method: Generalized density profiles

2. Out-of-equilibrium effects at high density



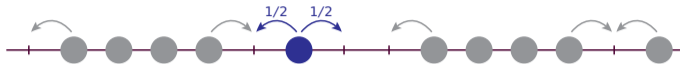
How to probe the effects of a driven particle?

Method: Vacancy motion at high density

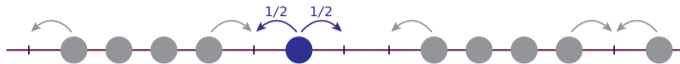
1. TAGGED PARTICLE AT EQUILIBRIUM



ONE PARTICLE IN THE SEP



ONE PARTICLE IN THE SEP

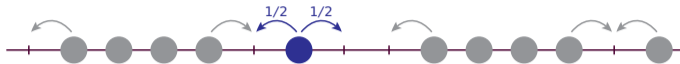


1. The variance

$$\langle X(t)^2 \rangle_{t \rightarrow \infty} \sim \frac{1-\rho}{\rho} \sqrt{\frac{2t}{\pi}} \quad [\text{Arratia 1983}]$$

$$\langle X(t)^2 \rangle_{t \rightarrow \infty} \sim \frac{S(\rho)}{\rho} \sqrt{\frac{4D(\rho)t}{\pi}} \quad [\text{Kollmann, PRL 2003}]$$

ONE PARTICLE IN THE SEP



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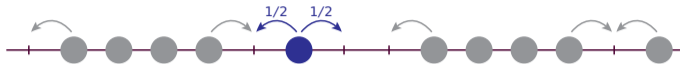
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[Krapivsky, Mallick & Sadhu, PRL 2014; Hedge, Sabahpandit & Dhar, PRL 2014; Sadhu & Derrida, J. Stat. Mech. 2015]

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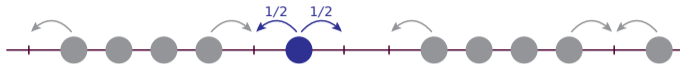
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But what is the underlying structure?

Can we quantify density-displacement correlations?

GENERALIZED DENSITY PROFILES FRAMEWORK



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Sublinear cumulants

$$\langle \chi^{2n}(t) \rangle_c = K_{2n} \sqrt{2t}$$

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$$\Phi'(\lambda, 0^\pm) + \frac{\psi(\lambda)}{e^{\pm\lambda} - 1} \Phi(\lambda, 0^\pm) = 0$$

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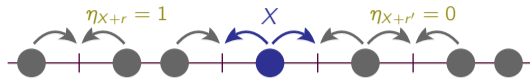
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Our goal is to find a closed bulk equation

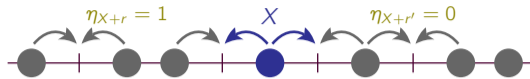
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At the lowest order, the bulk equation is closed!

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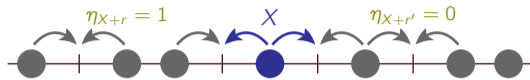
Also works for an arbitrary single-file system

structure factor $S(\rho)$ and diffusion coefficient $D(\rho)$

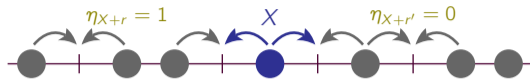
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2. LOW DENSITY LIMIT ($\rho \rightarrow 0$)



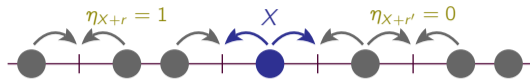
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Closure relation at all orders

[Poncet, Grabsch, Illien & Bénichou, PRL 2021]

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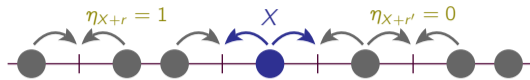
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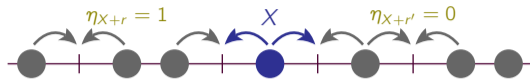
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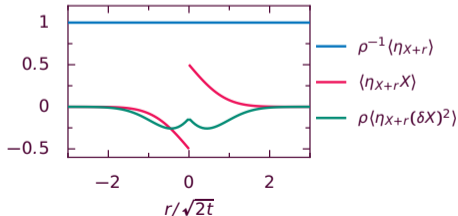
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Closure relation found iteratively

[Grabsch, **Poncet**, Rizkallah, Illien & Bénichou, Sci. Adv. 2021 / PRE 2023]

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$$\ln \langle e^{\lambda X} \rangle \sim \Psi(\lambda) \sqrt{2t}$$

Generalized density profiles

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Solution as Wiener-Hopf equation

$$\Omega(v) + \int_{-\infty}^0 dz K(v-z)\Omega(z) = K(v)$$

$$\text{with } K(v) = \omega \frac{e^{(v+\Psi')^2}}{\sqrt{\pi}},$$

ω such that $\Omega(0) = 2\Psi$,

and boundary conditions.

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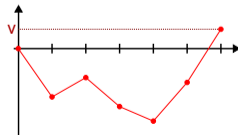
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Link with a simple random walk

$$\Omega(v) = -\sum_{n \geq 1} (-\omega)^n p_n(v)$$

$$p_n(v) = \mathbb{P}(X_0 = 0, X_1 < 0, \dots, X_{n-1} < 0, X_n = v)$$

$$P(X_{n+1} - X_n = \eta) = \frac{e^{-(\eta+\Psi')^2}}{\sqrt{\pi}}$$



ANALYTICAL EXPRESSIONS FOR THE MOMENTS AND CORRELATIONS

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Moments

$$\langle X^2(t) \rangle \underset{t \rightarrow \infty}{\sim} \frac{1-\rho}{\rho} \sqrt{\frac{2t}{\pi}}$$

$$\langle X^4(t) \rangle_c \underset{t \rightarrow \infty}{\sim} \frac{1-\rho}{\rho^3} (12(1-\rho)^2 - \pi(2 - 3(4 - \sqrt{2})\rho) + (8 - 3\sqrt{2})\rho^2) \sqrt{\frac{2t}{\pi^3}}$$

ANALYTICAL EXPRESSIONS FOR THE MOMENTS AND CORRELATIONS

Moments

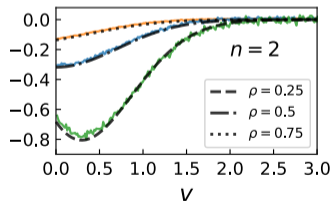
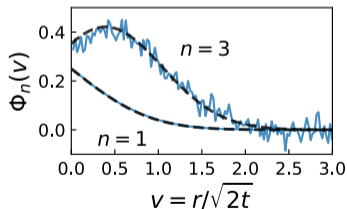
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Correlations

$$\langle X \eta_{X+r} \rangle(t) \underset{t \rightarrow \infty}{\sim} \operatorname{erfc}\left(\frac{r}{\sqrt{2t}}\right)$$

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LINK WITH MACROSCOPIC FLUCTUATION THEORY

Fluctuating hydrodynamics of the SEP

$$\partial_t \rho = \partial_x [D(\rho) \partial_x \rho + \sqrt{\sigma(\rho)} \eta]$$

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optimal path ρ^* between $t = 0$ and $t = T$

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MFT solution at final time = generalized density profile

$$\tilde{\rho}^*(x = v, t = T) = \Phi(v)$$

RECENT DEVELOPMENTS

- ▶ **Solution of the MFT equations for the SEP**

 - Non-local Cole-Hopf mapping gives AKNS integrable systems

 - Wiener-Hopf equation for final profile

 - [Mallick, Moriya, Sasamoto, PRL 2022]

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[Mallick, Moriya, Sasamoto, PRL 2022]

► Fourth cumulant of an arbitrary single-file system

[Grabsch & Bénichou, PRL 2024]

$$\begin{aligned} K_4 = & \frac{3\sigma(\rho)^3 (\rho D'(\rho) + D(\rho))}{\pi^{3/2} \rho^6 D(\rho)^{7/2}} - \frac{\sigma(\rho) (\sigma(\rho) \sigma'(\rho) (\rho D'(\rho) + 4D(\rho)) + 2\sigma(\rho)^2 D'(\rho) - \rho D(\rho) \sigma'(\rho)^2)}{4\sqrt{\pi} \rho^5 D(\rho)^{7/2}} + \frac{3\sigma(\rho)^3 (D'(\rho)^2 - D(\rho) D''(\rho))}{8\sqrt{\pi} \rho^4 D(\rho)^{9/2}} \\ & + \frac{3\sigma(\rho)^3 (2D(\rho) D''(\rho) - D'(\rho)^2)}{8\pi^{3/2} \rho^4 D(\rho)^{9/2}} + \frac{(3\sqrt{2} - 4) \sigma(\rho)^2 \sigma''(\rho)}{8\sqrt{\pi} \rho^4 D(\rho)^{5/2}} + \frac{3(\sqrt{2}\pi - 2\sqrt{3}) \sigma(\rho)^3 (2D(\rho) D''(\rho) - 3D'(\rho)^2)}{16\pi^{3/2} \rho^4 D(\rho)^{9/2}}. \end{aligned}$$

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► Interest of generalized density profiles beyond diffusive systems

run and tumble, Levy flights, etc.

[Grabsch, Berlioz, Rizkallah, Illien & Bénichou, PRL 2024]

The generalized density profiles $\langle \eta_{X+r} X^n \rangle$ encode the **non-stationary structure** associated with the **anomalous dynamics** of single-file systems.

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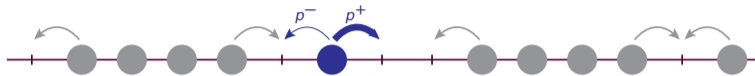
- ▶ Exact equations giving the variance of an arbitrary single-file
- ▶ Closure relation for the SEP at all densities
- ▶ Highlights the integrable nature of the problem
- ▶ Relevant beyond the diffusive case

OUT-OF-EQUILIBRIUM EFFECTS AT HIGH DENSITY



ONE DRIVEN PARTICLE IN THE SEP

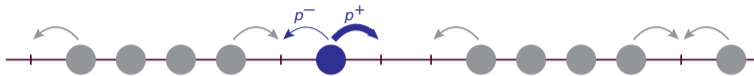
Probability law of a biased intruder



$$\langle X(t) \rangle_{t \rightarrow \infty} \sim A\sqrt{t} \quad [\text{Burlatsky 1996; Landim 1998}]$$

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Probability law of a biased intruder

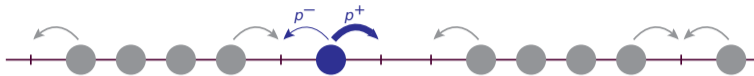


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Can we write the full probability law at all times?

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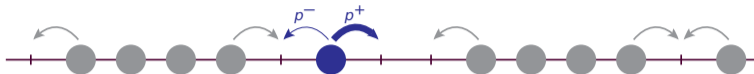


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Can we obtain the N-time statistics at large times?*

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Driving effect of a biased intruder



Only simpler models: RAP [Cividini 2016], pointlike particles [Ooshida 2018]

Can we obtain the 2-point statistics?

HIGH DENSITY LIMIT: VACANCY-BASED APPROACH

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High density ($\rho \rightarrow 1$): the vacancies are independent from one another



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[Brummelhuis & Hilorst 1989; Illien *et al.* 2013]

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High density ($\rho \rightarrow 1$): the vacancies are independent from one another



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[Brummelhuis & Hilorst 1989; Illien *et al.* 2013]

$$\lim_{\rho \rightarrow 1} \frac{\psi(k_1, k_2, t)}{1 - \rho} = \sum_Z [\tilde{\rho}_Z(k_1, k_2, t) - 1]$$

$$\psi(k_1, k_2, t) = \ln \langle e^{i(k_1 X_1 + k_2 X_2)} \rangle$$

Generating function giving $\langle X_1 \rangle$, $\langle X_2 \rangle$, $\langle X_1 X_2 \rangle$, etc.

$$\tilde{\rho}_Z(k_1, k_2, t)$$

Fourier-transform of the propagator of (X_1, X_2) with a *single vacancy* initially at Z .

BIASED PARTICLE: STATISTICS AT ALL TIMES



[Poncet, Grabsch, Bénichou & Illien, PRE 2022]

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$$\lim_{\rho \rightarrow 1} \frac{\langle X(t)^{2n+1} \rangle}{1-\rho} = s t e^{-t} [I_0(t) + I_1(t)]$$

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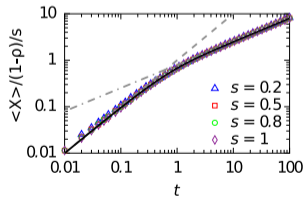
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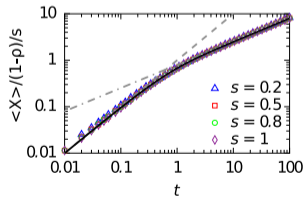


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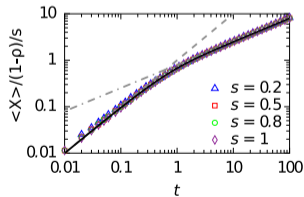
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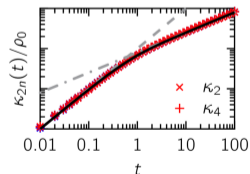
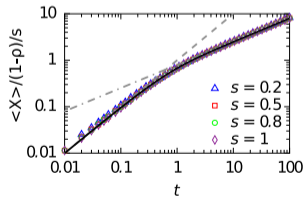
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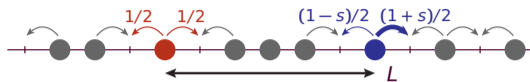
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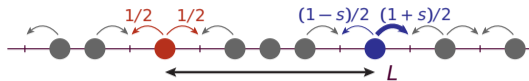
(also comb structure and 2D lattice)

BIASED PARTICLE: DRIVING OF ANOTHER PARTICLE



[Poncet, Bénichou, Démery & Oshanin, PRR 2019]

BIASED PARTICLE: DRIVING OF ANOTHER PARTICLE

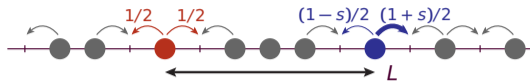


[Poncet, Bénichou, Démercy & Oshanin, PRR 2019]

$$\lim_{\rho \rightarrow 1} \frac{\langle X_1(t) \rangle}{1 - \rho} \underset{t \rightarrow \infty}{\sim} s \sqrt{\frac{2t}{\pi}} g\left(\frac{L}{\sqrt{2t}}\right)$$

$$\text{avec } g(u) = e^{-u^2} - \sqrt{\pi} u \operatorname{erfc} u$$

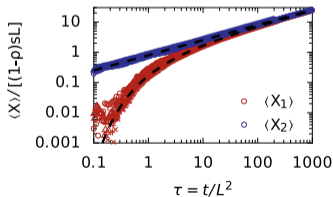
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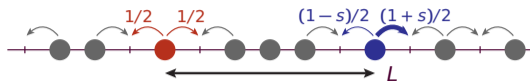
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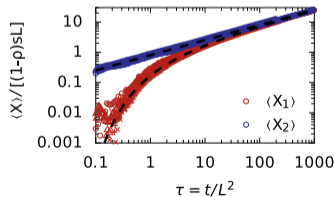


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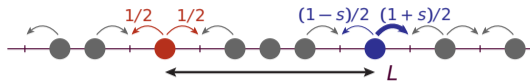
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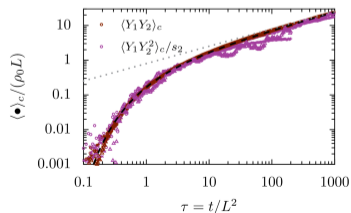
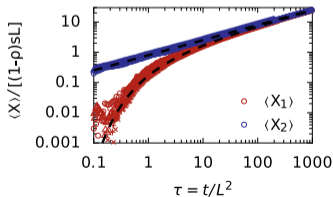


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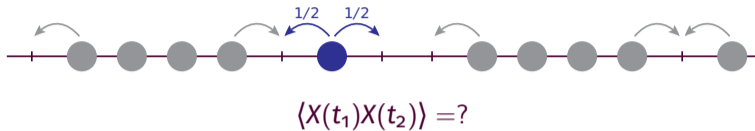
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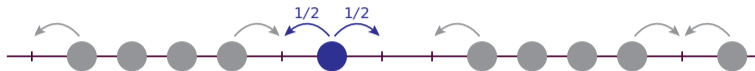
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TWO-TIME STATISTICS OF THE SEP



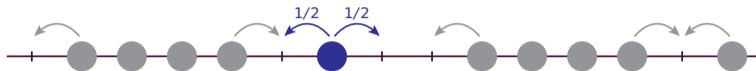
TWO-TIME STATISTICS OF THE SEP



$$\langle X(t_1)X(t_2) \rangle = ?$$

- ▶ Edwards-Wilkinson universality class [Majumdar & Barma 1991]
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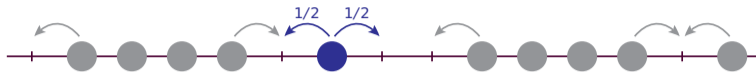


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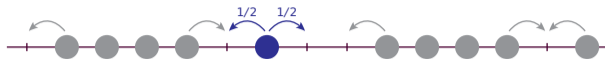
Can we also have such a result for a biased particle?

What about higher order, non-Gaussian, statistics?

(What about the dependence on initial conditions?)

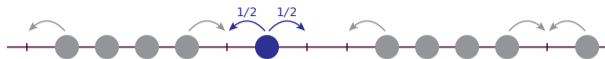
[Leibovich & Barkai 2013; Sadhu & Derrida 2015]

DENSE LIMIT: SIMPLE BROWNIAN MOTION

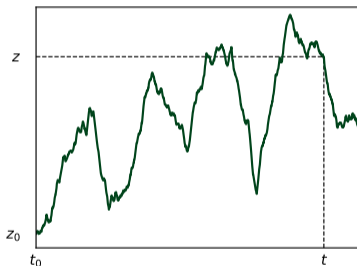


[Poncet, Grabsch & Bénichou, in preparation]

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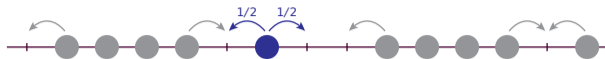


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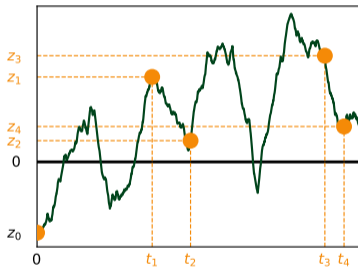


$$P(z, t|z_0, t_0) = \frac{e^{-\frac{(z-z_0)^2}{2(t-t_0)}}}{\sqrt{2\pi(t-t_0)}}$$

DENSE LIMIT: SIMPLE BROWNIAN MOTION



[Poncet, Grabsch & Bénichou, in preparation]



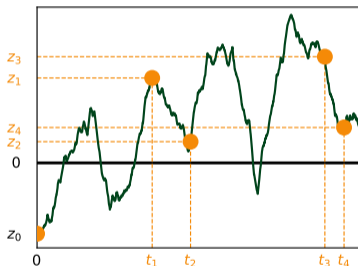
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$$\lim_{\rho \rightarrow 1} \frac{\langle X(t_1) \dots X(t_n) \rangle_c}{1-\rho} \sim 2\sqrt{2} \int_{-\infty}^0 dz_0 \mathbb{P}(Z(t_1) > 0, \dots, Z(t_n) > 0 | Z(0) = z_0)$$

DENSE LIMIT: SIMPLE BROWNIAN MOTION



[Poncet, Grabsch & Bénichou, in preparation]

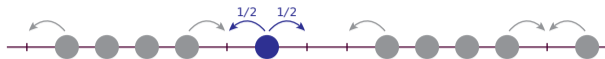


$$P(z, t|z_0, t_0) = \frac{e^{-\frac{(z-z_0)^2}{2(t-t_0)}}}{\sqrt{2\pi(t-t_0)}}$$

$$\lim_{\rho \rightarrow 1} \frac{\langle X(t_1) \dots X(t_n) \rangle_c}{1-\rho} \sim 2\sqrt{2} \int_{-\infty}^0 dz_0 \mathbb{P}(Z(t_1) > 0, \dots, Z(t_n) > 0 | Z(0) = z_0)$$

If biased, we need to consider the 2^n possibilities, $Z(t_1) \geq 0, \dots, Z(t_n) \geq 0$

DENSE LIMIT: RESULTS FOR TIME CORRELATIONS (NO BIAS)



[Poncet, Grabsch & Bénichou, in preparation]

$$\begin{aligned}\lim_{\rho \rightarrow 1} \frac{\langle X(t_1) \rangle}{1-\rho} &\sim 0 \\ \lim_{\rho \rightarrow 1} \frac{\langle X(t_1)X(t_2) \rangle_c}{1-\rho} &\sim \frac{1}{\sqrt{2\pi}} \left[\sqrt{t_1} + \sqrt{t_2} - \sqrt{t_2 - t_1} \right] \\ \lim_{\rho \rightarrow 1} \frac{\langle X(t_1)X(t_2)X(t_3) \rangle_c}{1-\rho} &\sim 0 \\ \lim_{\rho \rightarrow 1} \frac{\langle X(t_1)X(t_2)X(t_3)X(t_4) \rangle_c}{1-\rho} &\sim \sum_{0 \leq i < j \leq 4} C_{ij} \sqrt{t_j - t_i}\end{aligned}$$

DENSE LIMIT: RESULTS FOR TIME CORRELATIONS (BIASED)



[Poncet, Grabsch & Bénichou, in preparation]

$$\lim_{\rho \rightarrow 1} \frac{\langle X(t_1) \rangle}{1-\rho} \sim s \sqrt{\frac{2t}{\pi}}$$

$$\lim_{\rho \rightarrow 1} \frac{\langle X(t_1)X(t_2) \rangle_c}{1-\rho} \sim \frac{1}{\sqrt{2\pi}} \left[(1+s^2)\sqrt{t_1} + (1-s^2)(\sqrt{t_2} - \sqrt{|t_2-t_1|}) \right]$$

$$\lim_{\rho \rightarrow 1} \frac{\langle X(t_1)X(t_2)X(t_3) \rangle_c}{1-\rho} \sim \frac{s}{2\sqrt{2\pi}} \left\{ \left[4 + (1-s^2)(a_{123} - 1) \right] \sqrt{t_1} \right. \\ \left. + (1-s^2) \left[\sqrt{t_2} + (b_{0123} - 1)\sqrt{t_3} - \sqrt{t_2-t_1} + \sqrt{t_3-t_1} - a_{012} \sqrt{t_3-t_2} \right] \right\}$$

$$\lim_{\rho \rightarrow 1} \frac{\langle X(t_1)X(t_2)X(t_3)X(t_4) \rangle_c}{1-\rho} \sim \sum_{0 \leq i < j \leq 4} C_{ij} \sqrt{t_j - t_i}$$

$$a_{ijk} = A\left(\frac{t_j - t_i}{t_k - t_j}\right), \quad b_{ijkl} = A\left(\frac{(t_j - t_i)(t_l - t_k)}{(t_l - t_j)(t_k - t_j)}\right), \quad A(u) = \arctan \sqrt{u}$$

At high density,
the **complex behavior of a driven intruder** in a single-file
is encoded in the **simple dynamics of a diffusive vacancy!**

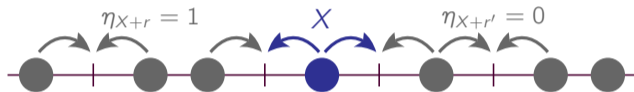
At high density,
the **complex behavior of a driven intruder** in a single-file
is encoded in the **simple dynamics of a diffusive vacancy!**

- ▶ One-time statistics at arbitrary time
- ▶ Driving effect on other particles
- ▶ Non-Gaussian N -time statistics

SINGLE-FILE SYSTEMS CAN BE STUDIED

1. At equilibrium

using generalized density profiles



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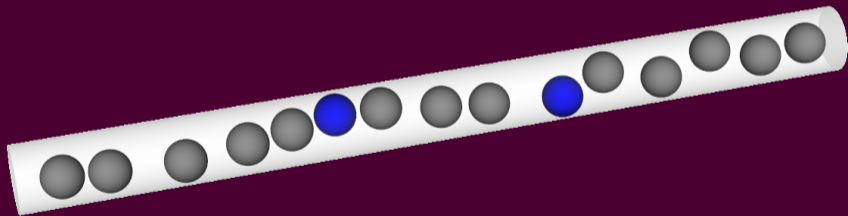


2. Out-of-equilibrium at high density

by looking at the dynamics of a single vacancy



THANK YOU FOR YOUR ATTENTION!



FOURTH ANNEALED CUMULANT (NO BIAS)

$$\lim_{\rho \rightarrow 1} \frac{\langle X(t_1)X(t_2)X(t_3)X(t_4) \rangle_C^A}{1 - \rho} \sim \frac{1}{4\sqrt{2\pi}} \sum_{0 \leq i < j \leq 4} C_{ij}^{(4)} \sqrt{t_j - t_i}$$

$$C_{01}^{(4)} = 1 + a_{123} + a_{124} + a_{234} \quad C_{02}^{(3)} = 1 + a_{234} \quad C_{03}^{(4)} = 1 + b_{0123} \quad C_{04}^{(4)} = 1 + b_{0124} + b_{0134} + b_{0234}$$

$$C_{12}^{(4)} = -1 - a_{234} \quad C_{13}^{(4)} = -1 \quad C_{14}^{(4)} = -1 - b_{1234}$$

$$C_{23}^{(4)} = -a_{012} \quad C_{24}^{(4)} = -a_{012} \quad C_{34}^{(4)} = -a_{013} - a_{023} + a_{123}$$

$$a_{ijk} = A\left(\frac{t_j - t_i}{t_k - t_j}\right), \quad b_{ijkl} = A\left(\frac{(t_j - t_i)(t_l - t_k)}{(t_l - t_i)(t_k - t_j)}\right), \quad A(u) = \arctan \sqrt{u}$$

FOURTH QUENCHED CUMULANT (NO BIAS)

$$\lim_{\rho \rightarrow 1} \frac{\langle X(t_1)X(t_2)X(t_3)X(t_4) \rangle_C^Q}{1-\rho} \sim \frac{1}{4\sqrt{2\pi}} \sum_{1 \leq i < j \leq 4} \left(D_{ij}^{(4)} \sqrt{t_j - t_i} + E_{ij}^{(4)} \sqrt{t_i + t_j} \right)$$

$$D_{ij}^{(4)} = a'_{ikl} - 2c_{ikl} + \tilde{D}_{ij}^{(4)}, \quad E_{ij}^{(4)} = -2d_{ijkl} + 6h_{ijkl} + \tilde{E}_{ij}^{(4)},$$

where k, l are the two indices in $\{1, 2, 3, 4\}$ that are different from i, j and such that $k < l$

$$\tilde{D}_{12}^{(4)} = -a_{234},$$

$$\tilde{D}_{13}^{(4)} = 0,$$

$$\tilde{D}_{14}^{(4)} = -b_{1234},$$

$$\tilde{D}_{23}^{(4)} = 1 - a'_{421},$$

$$\tilde{D}_{24}^{(4)} = 1 - a'_{312},$$

$$\tilde{D}_{34}^{(4)} = 1 + a_{123} - a'_{123} - a'_{213},$$

$$\tilde{E}_{12}^{(4)} = a_{134} + a_{234},$$

$$\tilde{E}_{13}^{(4)} = a_{124} - 2g_{1324},$$

$$\tilde{E}_{14}^{(4)} = a_{123} + e'_{1423},$$

$$\tilde{E}_{23}^{(4)} = -2g_{2314} - 2g_{3214},$$

$$\tilde{E}_{24}^{(4)} = e''_{2413} - 2g_{4213},$$

$$\tilde{E}_{34}^{(4)} = e''_{3412} + e''_{4312}.$$

$$a_{ijk} = A \left(\frac{t_j - t_i}{t_k - t_j} \right)$$

$$a'_{ijk} = A \left(\frac{t_i + t_j}{t_k - t_j} \right)$$

$$b_{ijkl} = A \left(\frac{(t_j - t_i)(t_l - t_k)}{(t_k - t_j)(t_l - t_i)} \right)$$

$$c_{ijk} = A \left(\frac{t_i^2}{t_i t_j + t_i t_k + t_j t_k} \right)$$

$$d_{ijkl} = A \left(\frac{t_i t_j + t_i t_k + t_j t_k}{(t_i + t_j)(t_l - t_k)} \right)$$

$$e_{ijkl} = A \left(\frac{(t_j - t_l)(t_i + t_k)}{(t_l - t_k)(t_i + t_j)} \right)$$

$$e'_{ijkl} = e_{ijkl} - 2g_{ijkl} - 2g_{ijlk}$$

$$e''_{ijkl} = e'_{ijkl} + f_{ijkl}$$

$$f_{ijkl} = A \left(\frac{(t_k - t_j)(t_l - t_j)}{(t_i + t_j)(t_k + t_l)} \right)$$

$$g_{ijkl} = A \left(\frac{t_i^2 (t_j - t_k)}{(t_i + t_j)(t_i t_k + t_i t_l + t_k t_l)} \right)$$

$$h_{ijkl} = A \left(\frac{t_i^2 t_j^2}{(t_i + t_j)[t_i t_j (t_k + t_l) + t_k t_l (t_i + t_j)]} \right)$$