Geometry-Induced Superdiffusion in Driven Crowded Systems

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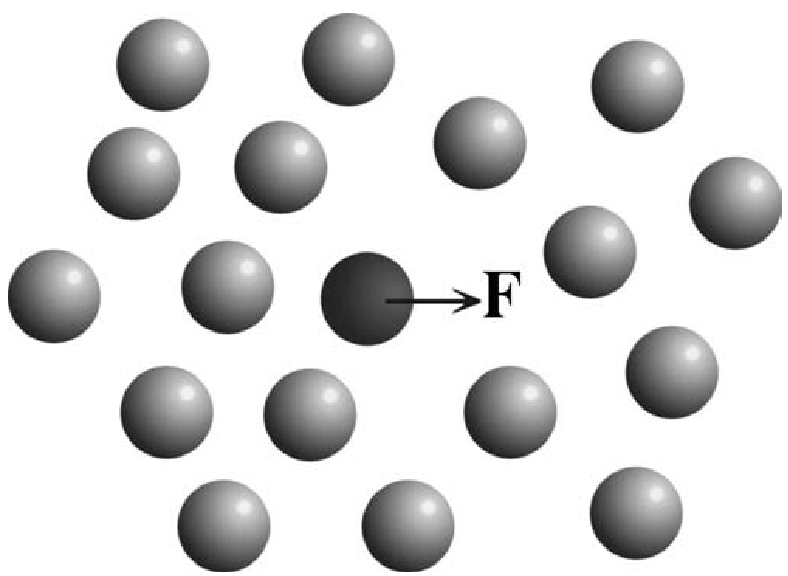
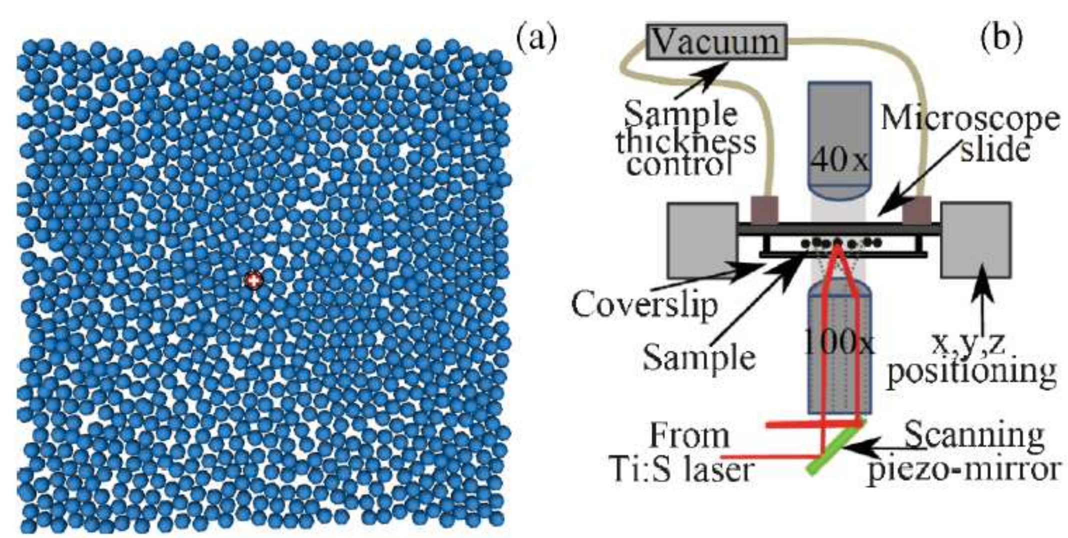
Galileo Galilei Institute, Arcetri Florence May 2014

Active micro-rheology

Active manipulation of small probe particles by external forces, using magnetic fields, electric fields, or micro-mechanical forces.



- Optical tweezers
- Magnetic manipulation
- Atomic force microscopy

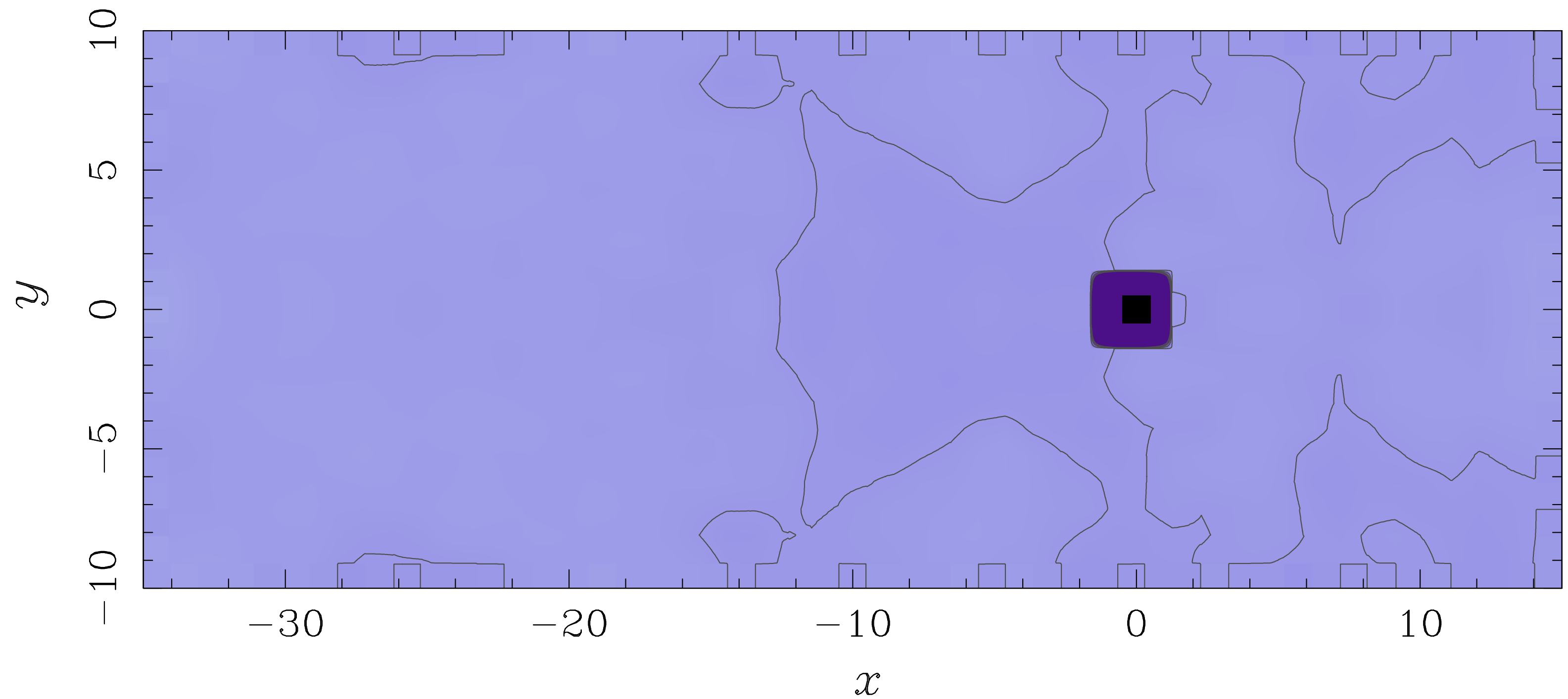


J Pesic, et al, PRE (2012) **86**, 031403

Nonequilibrium inhomogeneity

As the force increases ...

- a traffic jammed region in front of the intruder
- a wake region behind the it



C M-M, G Oshanin Soft Matter (2011), **7** 993

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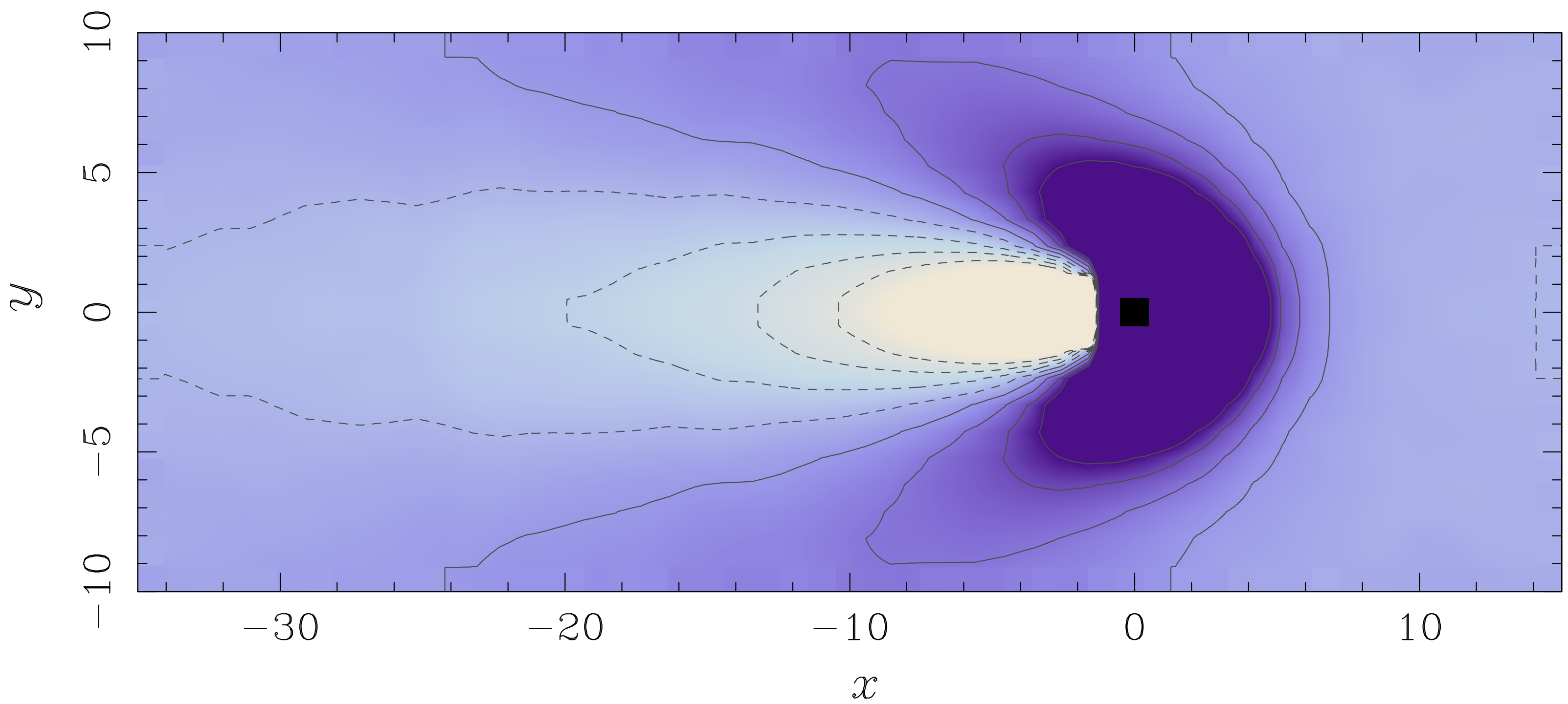
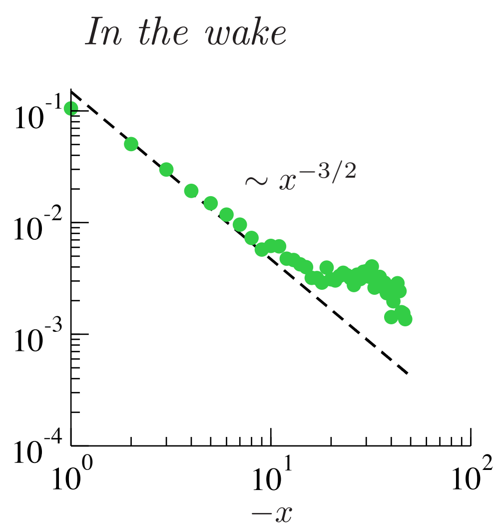
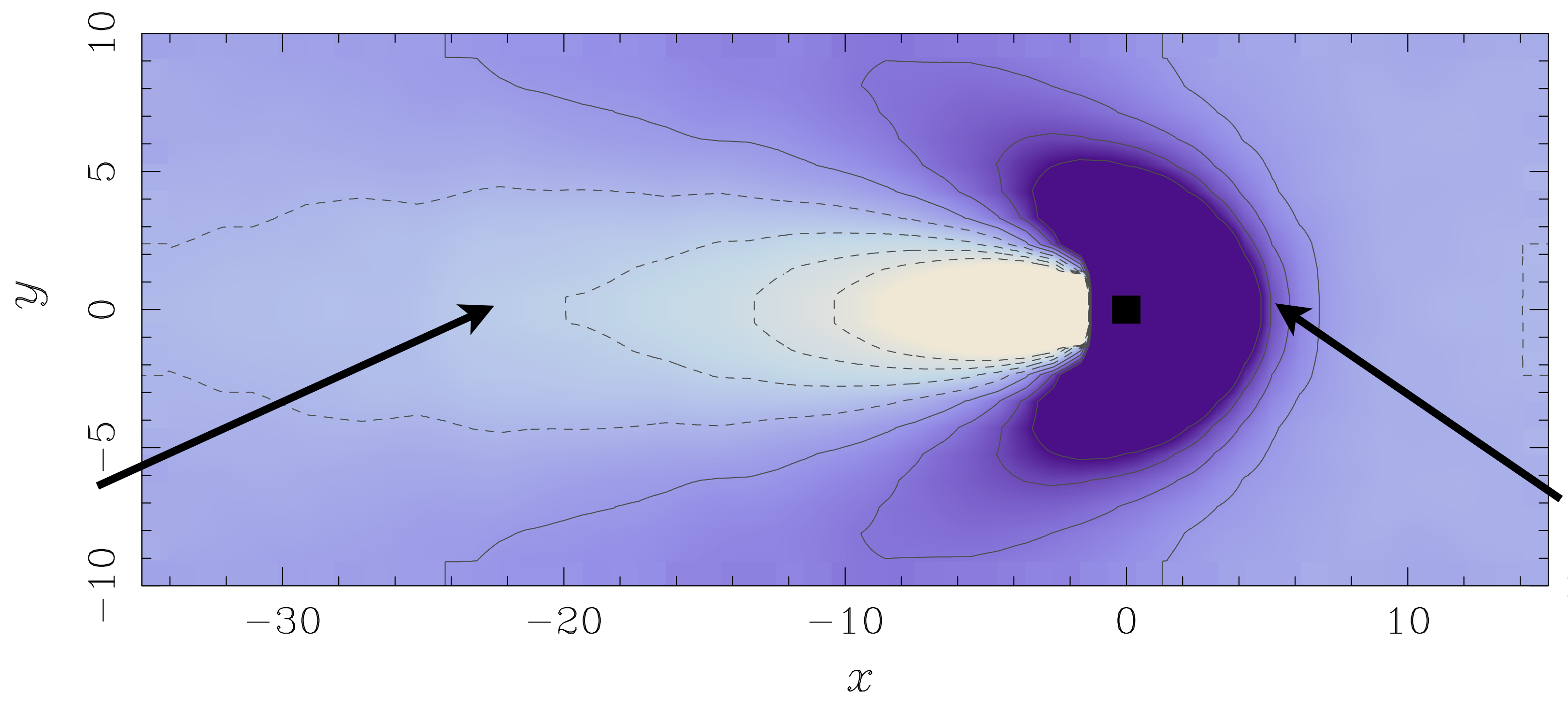
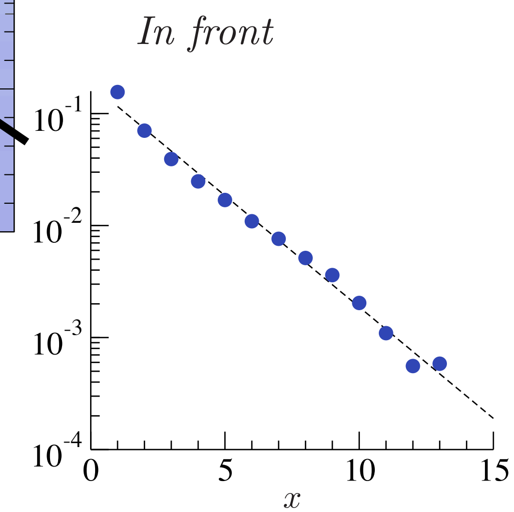


C M-M, G Oshanin Soft Matter (2011), **7** 993

Nonequilibrium inhomogeneity







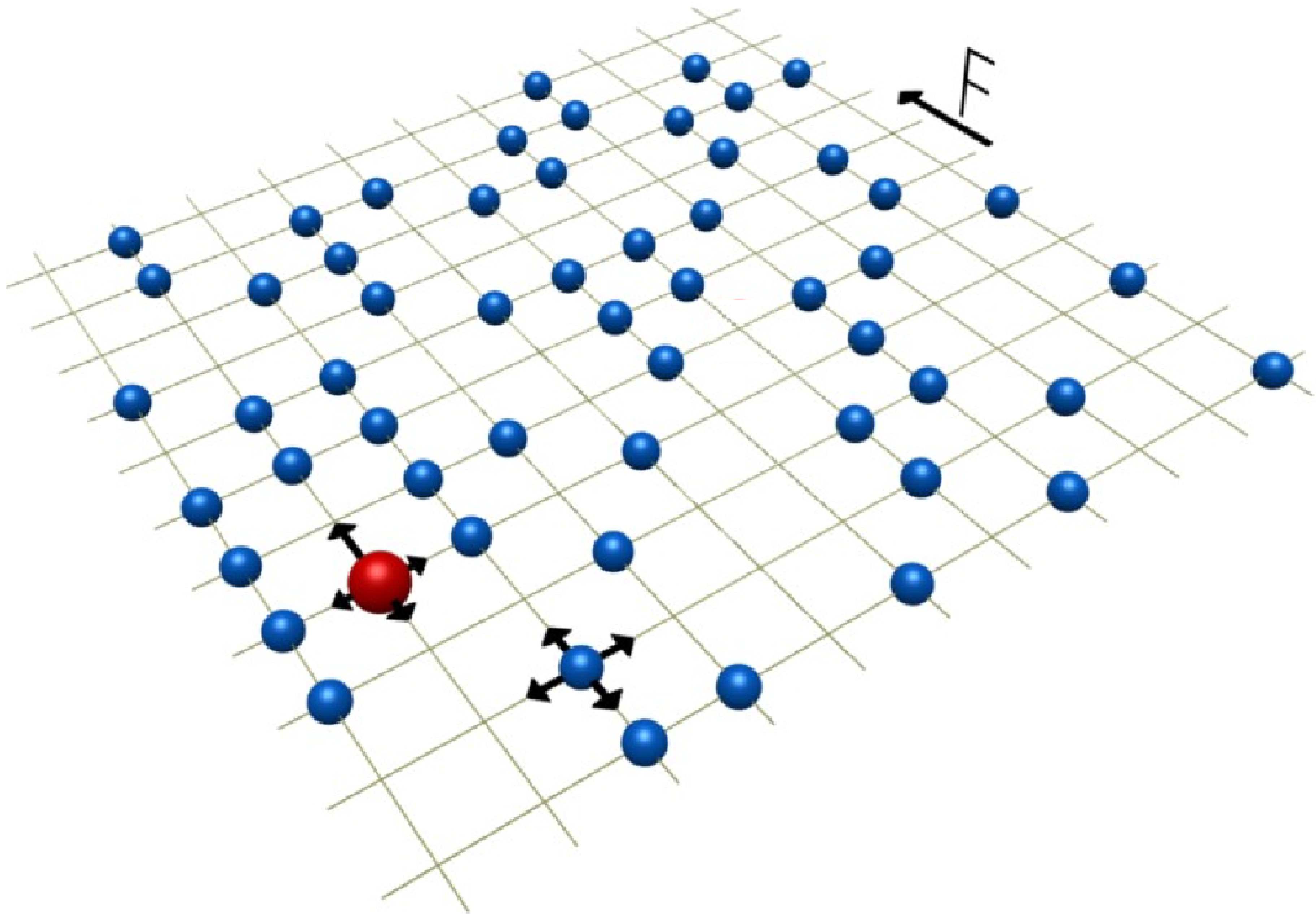
The medium remembers the passage of the intruder on large temporal and spatial scales

observed in colloidal suspensions, monolayers of vibrated grains and in glass systems.

C M-M, G Oshanin Soft Matter (2011), **7** 993

The model

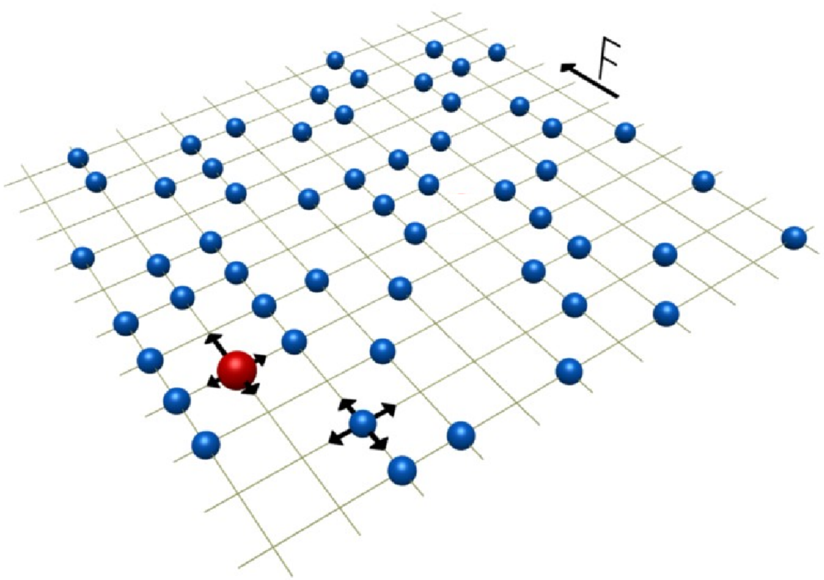
Simple Exclusion Process



The model

Simple Exclusion Process

- We consider a square lattice of $L_x \times L_y$ sites, of unit spacing, with P.B.C and populated with hard-core particles.
- Each site can be either empty or occupied by at most one particle.
- The system evolves in discrete time n and particles move randomly.
- One particle, *the intruder*, is subject to a constant force $\mathbf{F}$



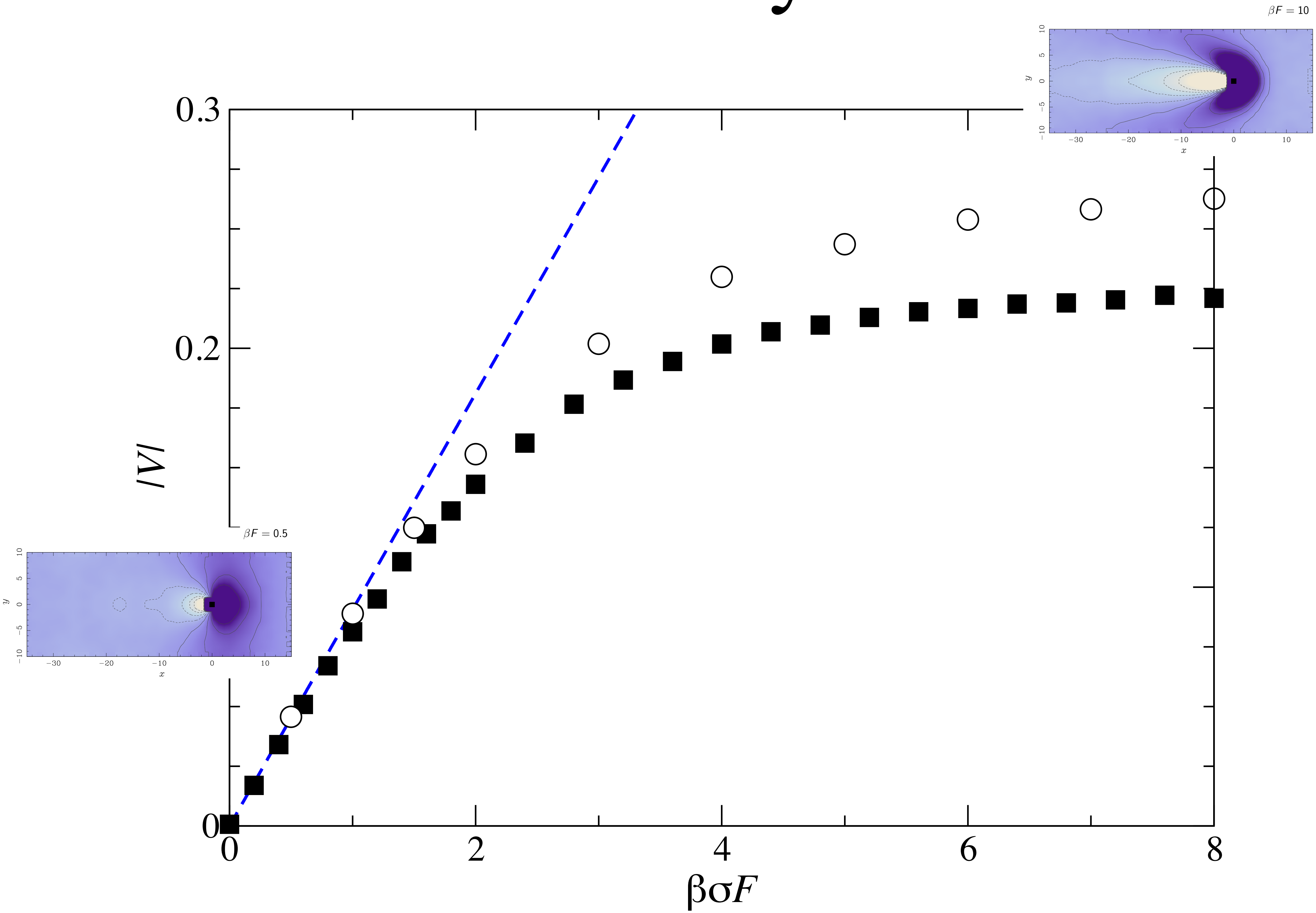
Simple Exclusion Process

• Bath particles move in either direction with equal jump probability $1/4$.
• The intruder moves in direction $\mathbf{e}_\nu$ with probability

$$p_\nu = Z^{-1} e^{\frac{\beta}{2}\mathbf{F}\cdot\mathbf{e}_\nu} ,$$

where $Z = 2(1 + \cosh(\beta\sigma F/2))$ and β is the inverse temperature.

Force-velocity relation



Force-velocity relation

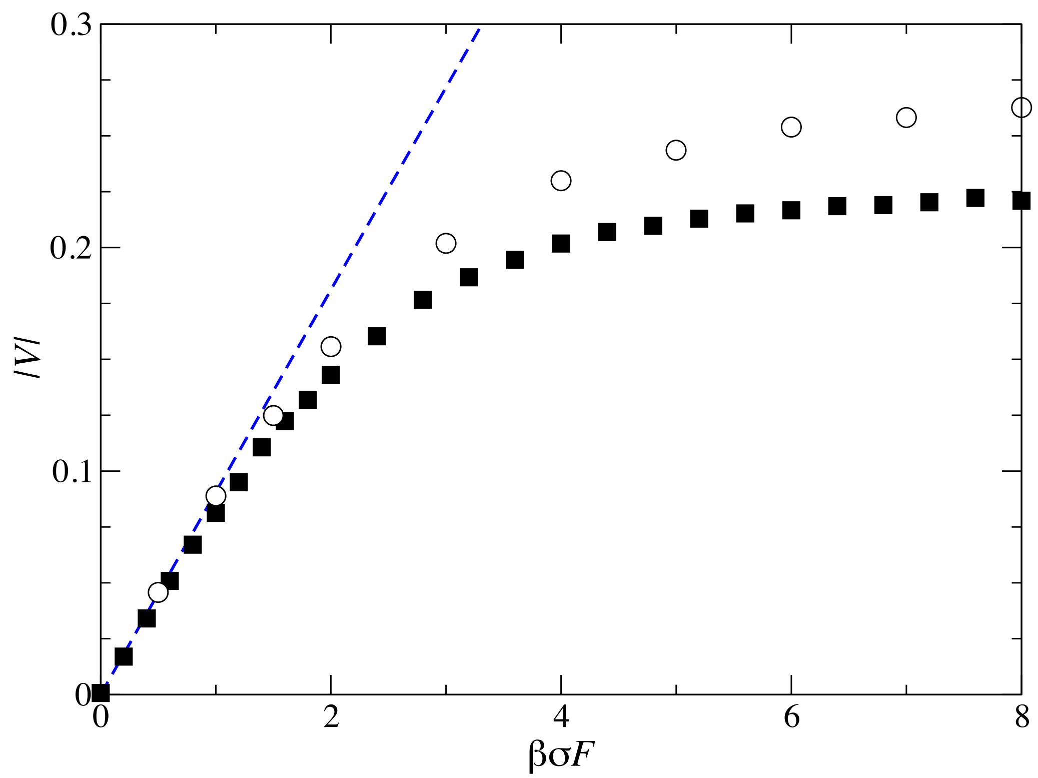
Stokesian regime

$$V = \frac{F}{\xi} \ ,$$

with friction coefficient

$$\xi = \xi_{\mathrm{mf}} + \xi_{\mathrm{coop}}$$

where



$$\xi_{\mathrm{mf}} = \frac{4\tau}{\beta\sigma^2(1-\rho)} \quad \text{and} \qquad \xi_{\mathrm{coop}} = \frac{4\tau}{\beta\sigma^2(1-\rho)} \frac{(\pi-2)\rho}{1+(1-\rho)}$$

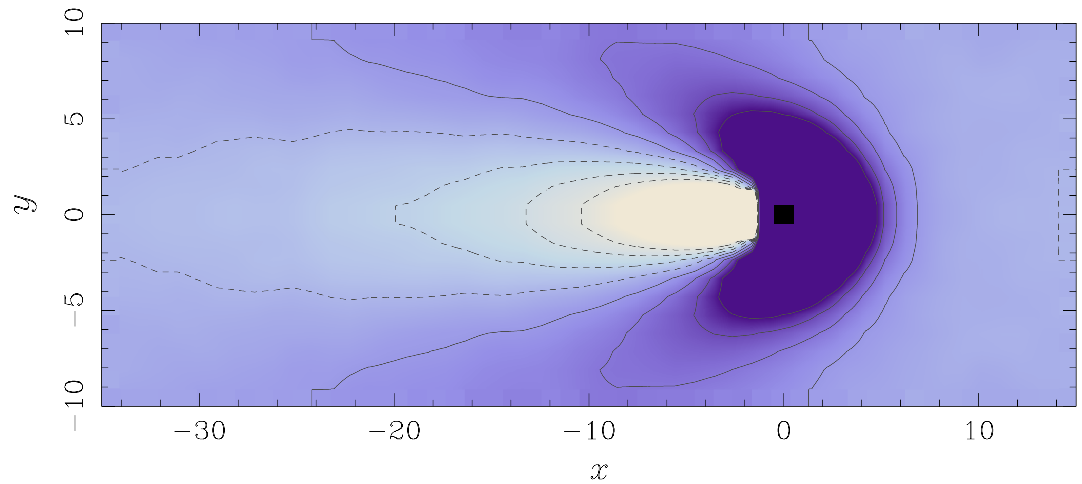
O Bénichou, et al, PRL (2000) **84**, 511; PRB (2001) **63**, 235413

C M-M, G Oshanin, Soft Matter (2011) **7**, 993

The problem

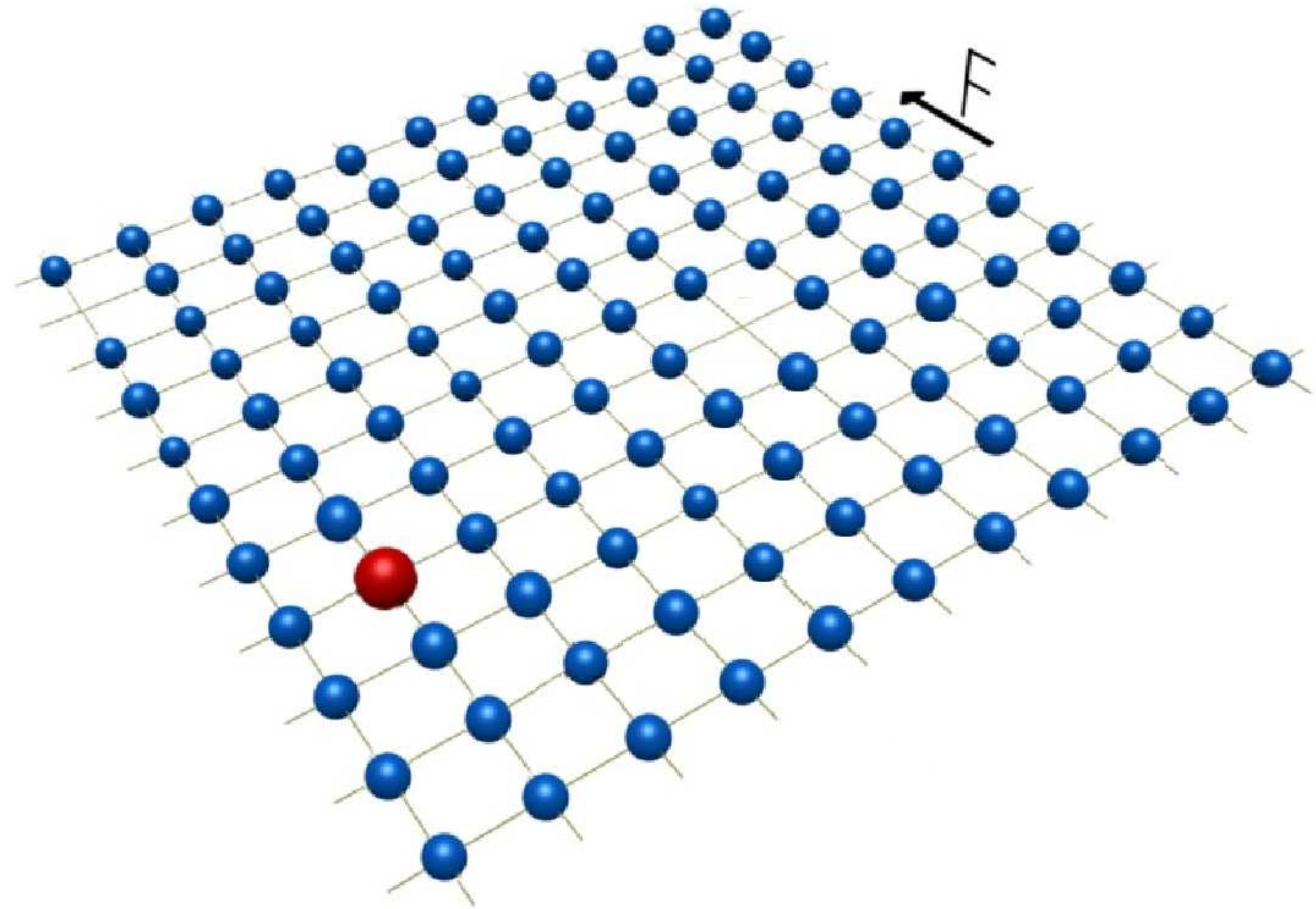
What is the probability distribution function of the intruder's displacement at time *n*?

$$P(\mathbf{R}_n)$$



We are interested in the limit of very dense lattices or very strong pulling forces.

The limit of high density 2D

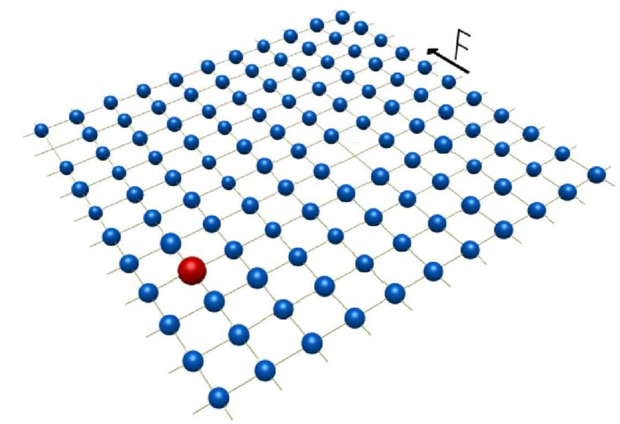


- Limit of small vacancy density $\rho_0 = M/(L_x \times L_y) \ll 1$
- Idea: trapping of the intruder by diffusive vacancies.

O Bénichou, G Oshanin, PRE (2001) **64**. 020103

MJAM Brummelhuis, HJ Hilhorst, Physica A (1989) **156**, 575

The limit of high density 2D



- many vacancies problem as many single vacancy problems.

- propagator of the intruder in the presence of a single vacancy is given in terms of First-Passage Time distributions of the vacancy to the site ocupied by the intruder.

- results in the long time limit

Intruder's displacement

- Let Z_n^j denote the position of the j-th vacancy at time n, $j = 1, 2, \ldots, M$.

- We want to compute the probability of finding the intruder at position $\mathbf{r}_n$ at time n conditioned to $\{\mathbf{Z}_n^j\}$

$$P(\mathbf{r}_n|\{\mathbf{Z}_n^j\}) = \sum_{\mathbf{r}_n^1} \cdots \sum_{\mathbf{r}_n^M} \delta(\mathbf{r}_n, \mathbf{r}_n^1 + \cdots + \mathbf{r}_n^M) P(\mathbf{r}_n^1, \ldots, \mathbf{r}_n^M|\{\mathbf{Z}_n^j\})$$

- $P(\mathbf{r}_n^1, \ldots, \mathbf{r}_n^M|\{\mathbf{Z}_n^j\})$ is the conditional probability that within the time interval n the intruder moved to $\mathbf{r}_n^1$ due to its interaction with vacancy 1, to $\mathbf{r}_n^2$ due to its interaction with vacancy 2, etc.

- In the lowest order in ρ_0 the vacancies contributions are independent and

$$P(\mathbf{r}_n^1, \ldots, \mathbf{r}_n^M|\{\mathbf{Z}_n^j\}) \simeq \prod_{j=1}^{M} P(\mathbf{r}_n|Z_n^j)$$

The problem reduces to M single vacancies, correct to $\mathcal{O}(\rho_0)$.

Intruder's displacement

- Averaging $P(\mathbf{r}_n|Z_n^j)$ over the initial distribution of vacancies

$$P(\mathbf{r}_n) \simeq \sum_{\mathbf{r}_n^1} \cdots \sum_{\mathbf{r}_n^M} \delta(\mathbf{r}_n, \mathbf{r}_n^1 + \cdots + \mathbf{r}_n^M) \prod_{j=1}^{M} \langle P(\mathbf{r}_n|Z_n^j)\rangle$$

- Defining the Fourier transformed distribution

$$P_n(\mathbf{k}) = \sum_{\mathbf{r}_n} exp\,(-i\mathbf{k}\cdot\mathbf{r}_n)\,\langle P(\mathbf{r}_n|\{Z_n^j\})\rangle$$

and summing over $\mathbf{r}_n$ one obtains that it factorizes into

$$P_n(\mathbf{k}) = \left(\sum_{\mathbf{r}_n} exp\,(-i\mathbf{k}\cdot\mathbf{r}_n)\,\langle P(\mathbf{r}_n|Z_n^j)\rangle\right)^M$$

Intruder's displacement

Taking the thermodynamic limit $L_x,\ L_y \to \infty$ with ρ_0 fixed we obtain for the characteristic function

$$P_n(k) \simeq \exp(-\rho_0 \Omega_n(\mathbf{k}))$$

$\Omega_n(\mathbf{k})$ is implicitly defined by

$$\Omega_n(\mathbf{k}) = \sum_{l=0}^{n} \sum_{\nu} \Delta_{n-l}(\mathbf{k}|\mathbf{e}_\nu) \sum_{\mathbf{Z}\neq 0} F_l^*(\mathbf{0}|\mathbf{e}_\nu|\mathbf{Z}),$$

$F_l^*(\mathbf{0}|\mathbf{e}_\nu|\mathbf{Z})$ is the FPT conditional probability for a RW starting at $\mathbf{Z}$ to be at $\mathbf{0}$ at time l, given that it is at site $\mathbf{0}+\mathbf{e}_\nu$ at time $l-1$ and

$$\Delta_l(\mathbf{k}|\mathbf{e}_\nu) = 1 - p_l(\mathbf{k}) \exp\left(i(\mathbf{k}\cdot\mathbf{e}_\nu)\right)$$

$$\boxed{P(\mathbf{R}_n) \simeq \frac{1}{4\pi^2} \int_{-\pi}^{\pi} \mathrm{d}\mathbf{k} \, \exp\left(-\mathrm{i}\left(\mathbf{k}\cdot\mathbf{R}_n\right) - \rho_0 \, \Omega_n(\mathbf{k})\right)}$$

Intruder's displacement

$\Omega_n(\mathbf{k})$ can be solved explicitly in terms of its generating function

$$\Omega_z(\mathbf{k}) = \sum_{n=0}^{\infty} \Omega_n(\mathbf{k})\, z^n$$

In the large n (and $\rho_0 \ll 1$) limit $z \to 1^-$

$$\Omega_z(\mathbf{k}) \sim \frac{1}{(1-z)} \frac{\Phi(\mathbf{k})}{1 - z + \Phi(\mathbf{k})/\chi_{\mathbf{z}}}$$

with

$$\chi_z \sim -\frac{\pi}{(1-z)\ln(1-z)}$$

the leading asymptotic term of the generating function of the *mean* number of "new" (virgin) sites visited on the n-th step

BD Hughes, (2005) *Random walks in random environments*

Intruder's displacement

Then

$$\Omega_z(\mathbf{k}) \sim \frac{\Phi(\mathbf{k})}{(1-z)^2}\left(1 - \frac{\ln(1-z)}{\pi}\Phi(\mathbf{k})\right)^{-1} ,$$

with

$$\Phi(\mathbf{k}) = -ia_0 k_x + a_1 k_x^2/2 + a_2 k_y^2/2$$

$$a_0 = \frac{\sinh(\beta F/2)}{(2\pi - 3)\cosh(\beta F/2) + 1} ,$$

$$a_1 = \frac{\cosh(\beta F/2)}{(2\pi - 3)\cosh(\beta F/2) + 1} ,$$

$$a_2 = \frac{1}{\cosh(\beta F/2) + 2\pi - 3} .$$

Intruder's displacement

In the large n (and $\rho_0 \ll 1$)

$$\boxed{P(\mathbf{R}_n) \simeq \frac{1}{4\pi^2} \int_{-\pi}^{\pi} \mathrm{d}\mathbf{k} \, \exp\left(-\mathrm{i}\left(\mathbf{k} \cdot \mathbf{R}_n\right) - \rho_0 \, \Omega_n(\mathbf{k})\right)}$$

$$\Phi(\mathbf{k}) = -ia_0 k_x + a_1 k_x^2/2 + a_2 k_y^2/2$$

$$\Omega_z(\mathbf{k}) = \sum_{n=0}^{\infty} \Omega_n(\mathbf{k}) \, z^n$$

$$\sim \frac{1}{(1-z)} \frac{\Phi(\mathbf{k})}{1 - z + \Phi(\mathbf{k})/\chi_z}$$

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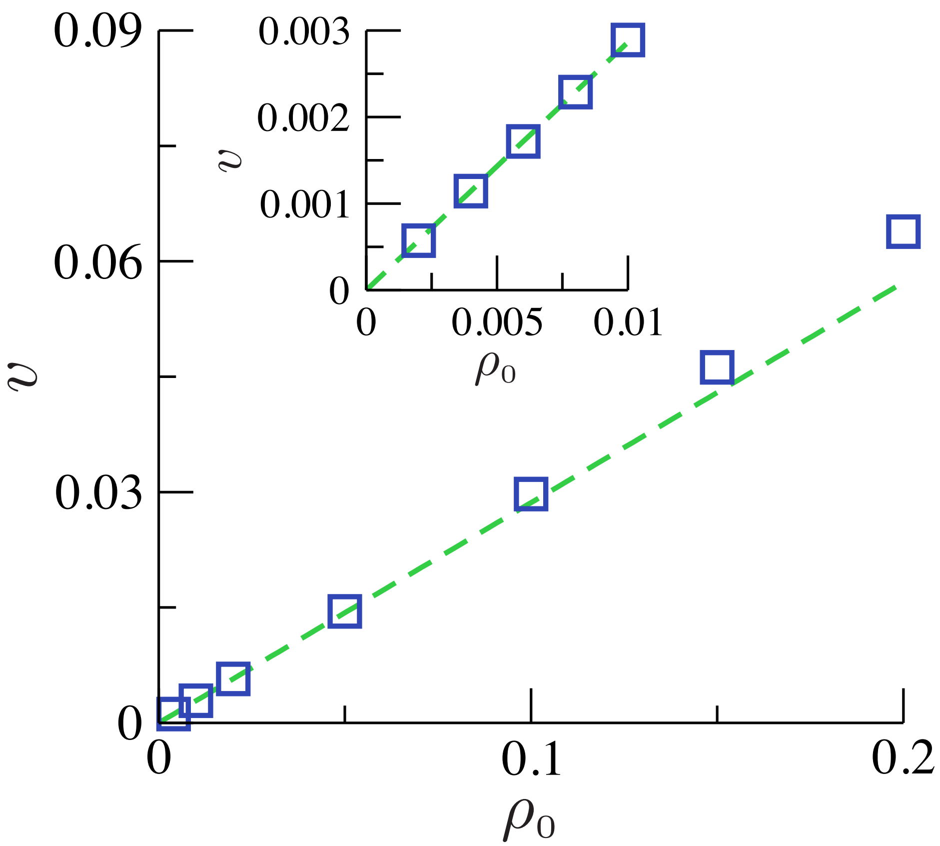
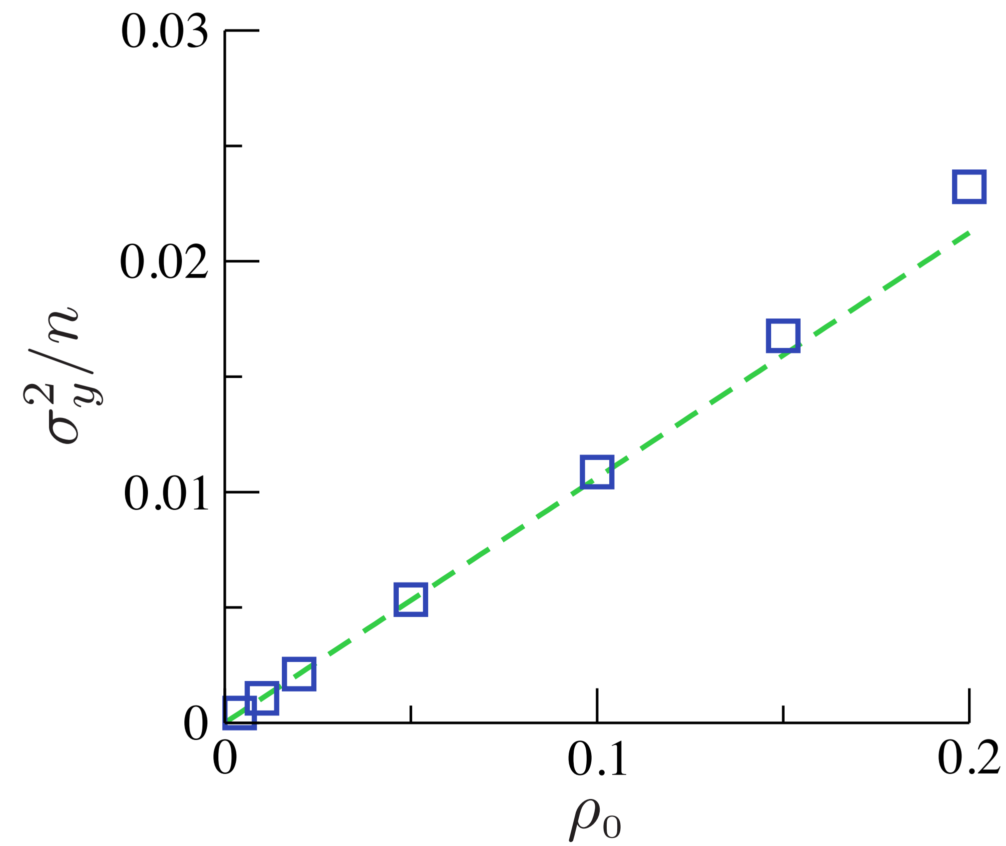
BD Hughes, (2005) *Random walks in random environments*

Velocity and variance



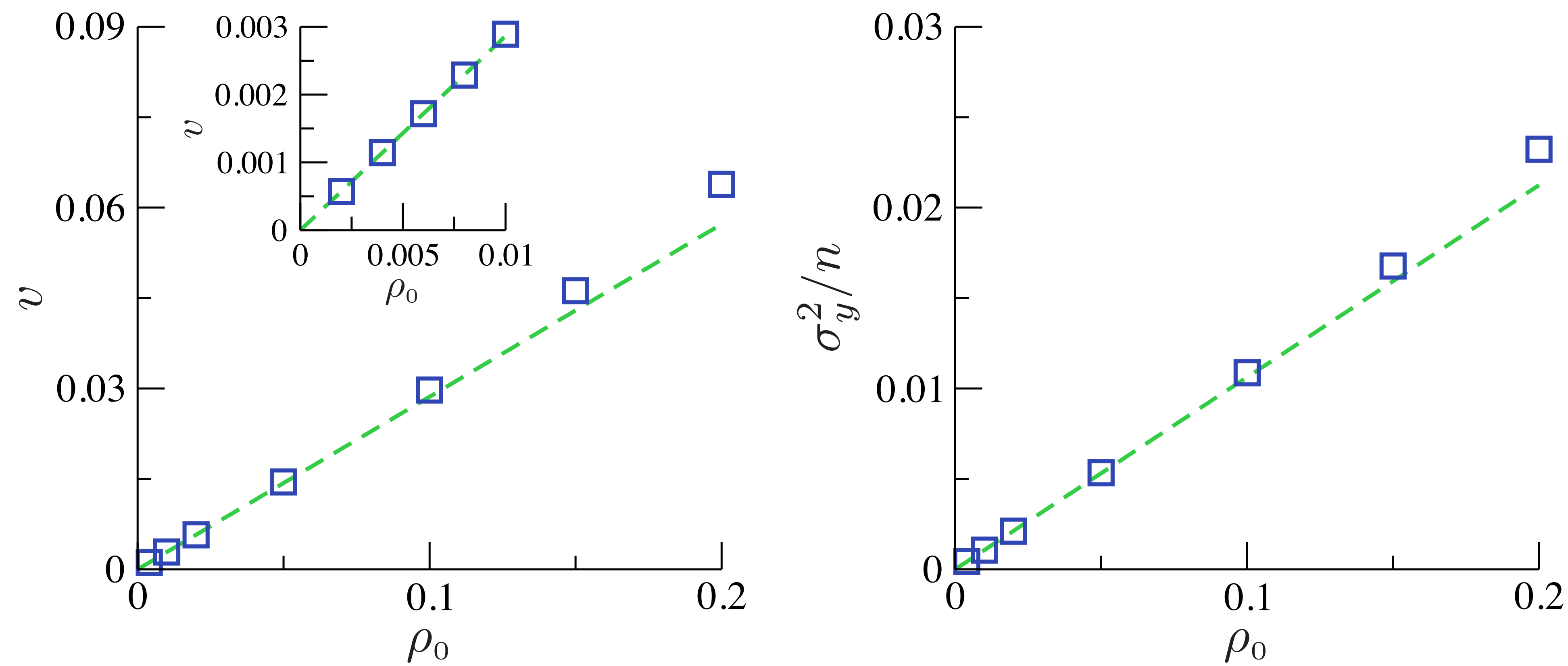


$$v \sim \frac{\rho_0 \sinh(\beta F/2)}{(2\pi - 3)\cosh(\beta F/2) + 1} \qquad \sigma_y^2 \sim \frac{\rho_0 n}{\cosh(\beta F/2) + 2\pi - 3}$$

The intruder moves at constant velocity along the field direction and diffuses along the transversal direction

O Bénichou, C M-M, G Oshanin, PRE **87** 020103 (2013)

Velocity and variance

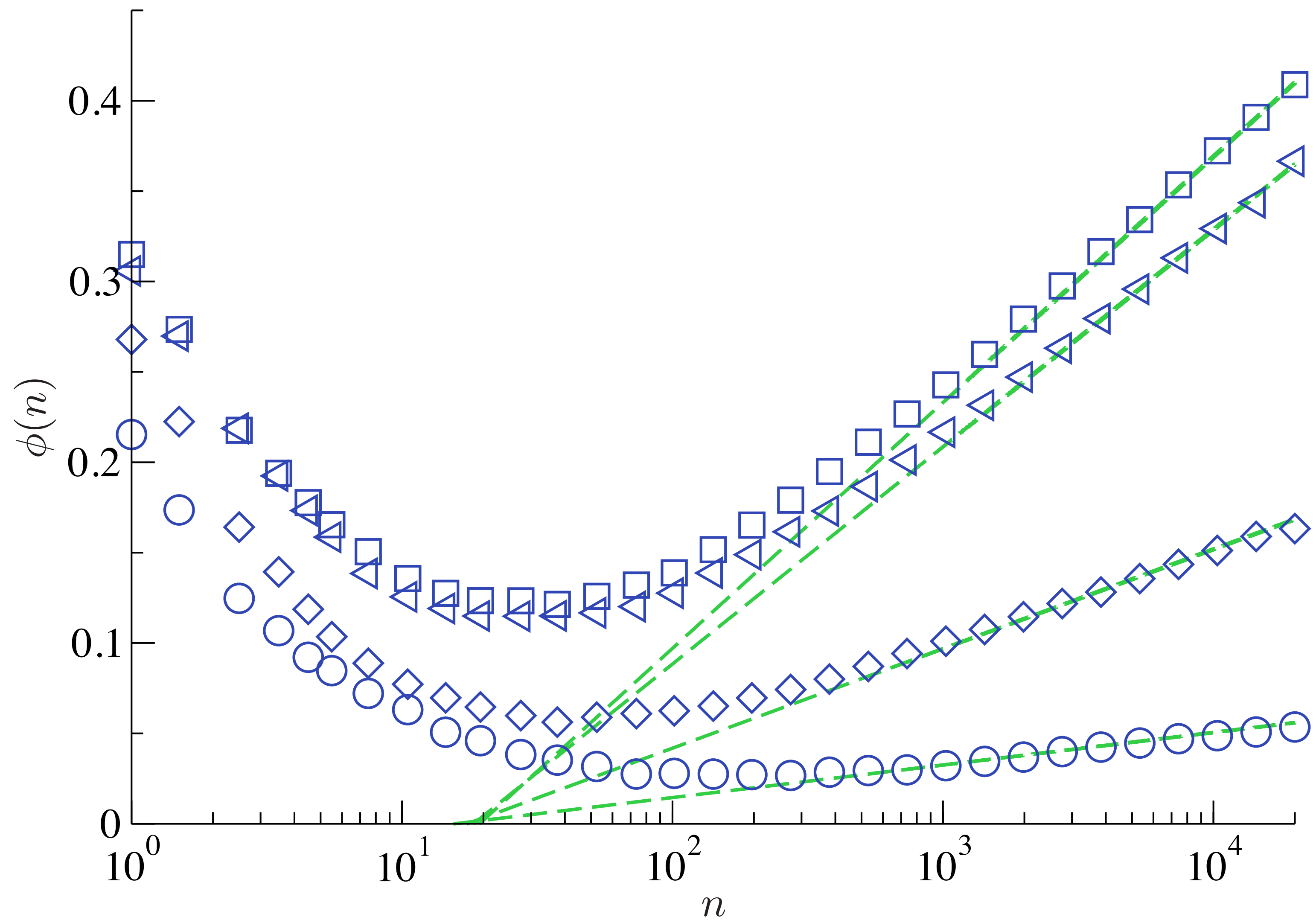


$$v \sim \frac{\rho_0 \sinh(\beta F/2)}{(2\pi - 3)\cosh(\beta F/2) + 1} = \begin{cases} \frac{\beta \rho_0}{4(\pi - 1)} F \,, & \beta F \ll 1 \\ v_\infty = \frac{\rho_0}{2\pi - 3} \,, & \beta F \gg 1 \end{cases}$$

O Bénichou, et al, PRL (2000) **84**, 511; PRB (2001) **63**, 235413

O Bénichou, C M-M, G Oshanin, PRE **87** 020103 (2013)

Weak superdiffusion

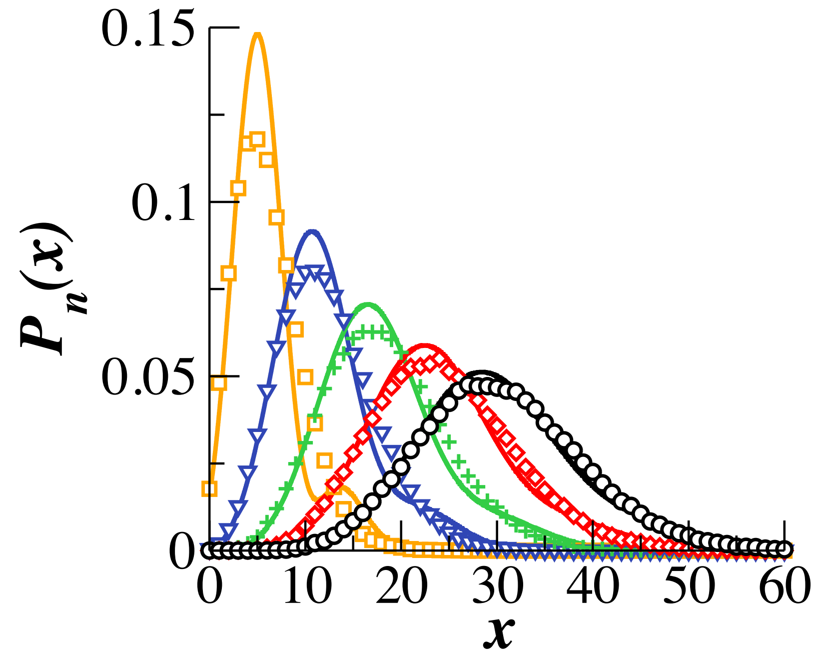


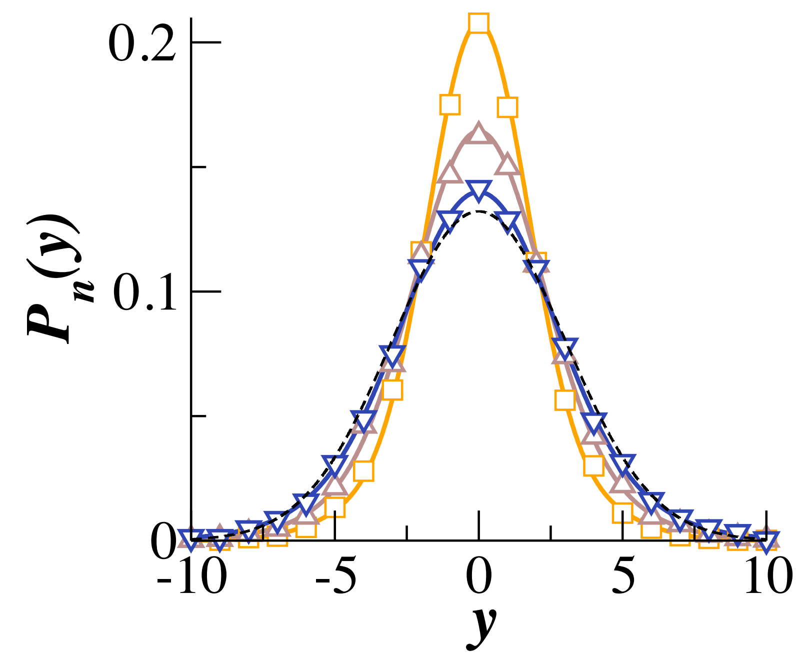
$$\sigma_x^2 \sim \rho_0 \left(a_1 + \frac{2a_0^2}{\pi}(\gamma - 1) + \frac{2a_0^2}{\pi} \ln(n) \right) n$$

$\lim_{n\to\infty} H_{n+1} = \ln(n) + \gamma + \mathcal{O}\left(\frac{1}{n}\right)$ with $\gamma \approx 0.577$

O Bénichou, C M-M, G Oshanin, PRE **87** 020103 (2013)

Anomalous fluctuations broadening





In the limit $\rho_0 \to 0$

$$P_n(x) = (2\pi\sigma_x^2)^{-1/2} \mathrm{e}^{-\frac{(x-vn)^2}{2\sigma_x^2}} \,(1 + A/n + \ldots) \ ,$$

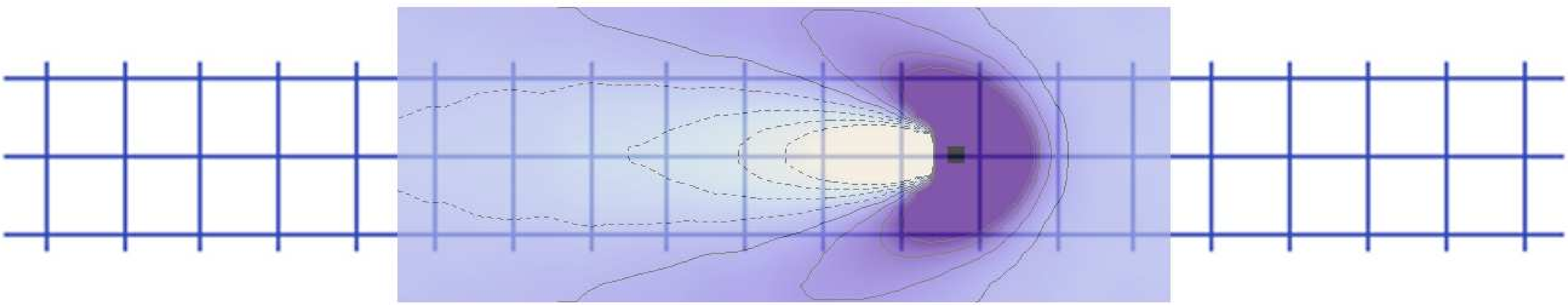
$$P_n(y) = (2\pi\sigma_y^2)^{-1/2} \mathrm{e}^{-\frac{y^2}{2\sigma_y^2}} \,(1 + B \ln n/n + \ldots) \ ,$$

$$v \sim \rho_0 \, a_0 \ ,$$

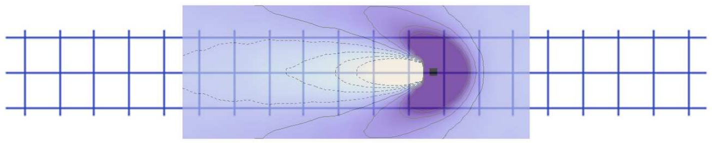
$$\sigma_x^2 \sim \rho_0 \left(a_1 + \frac{2a_0^2}{\pi} (\gamma - 1) + \frac{2a_0^2}{\pi} \ln(n) \right) n \ ,$$

$$\sigma_y^2 \sim \rho_0 \, a_2 n \ , \qquad a_i \equiv a_i(\beta F)$$

Confined geometries



Confined geometries



The variance of the intruder's displacement can be represented as

$$\sigma_x^2 \sim \rho_0 a_1 n + \rho_0 a_0^2 \frac{n}{\chi_n} \,,$$

χ_n: mean # of new sites visited on the n-th step by any vacancy.
In terms of S_n, the mean # of distinct lattice sites visited by any of the vacancies up to time n

$$\chi_n = S_n - S_{n-1}$$

S_n is a fundamental characteristic property of a *lattice discrete-time RW*.

O Bénichou, P Illien, C M-M, G Oshanin (2013)

Confined geometries

In general, for infinite systems (at least in one direction)

$$S_n \sim n^{\alpha}$$

α is and indicator of the *mixing* of the lattice gas and depends on the *effective* dimensionality of the lattice.

- for larger α, a vacancy mostly moves to new sites
- for smaller α, a vacancy predominantly revisits already visited sites

In general $\alpha < 1$ for systems in which the RW is *recurrent*, while $\alpha = 1$ for non-recurrent RW's.

Confined geometries

We have

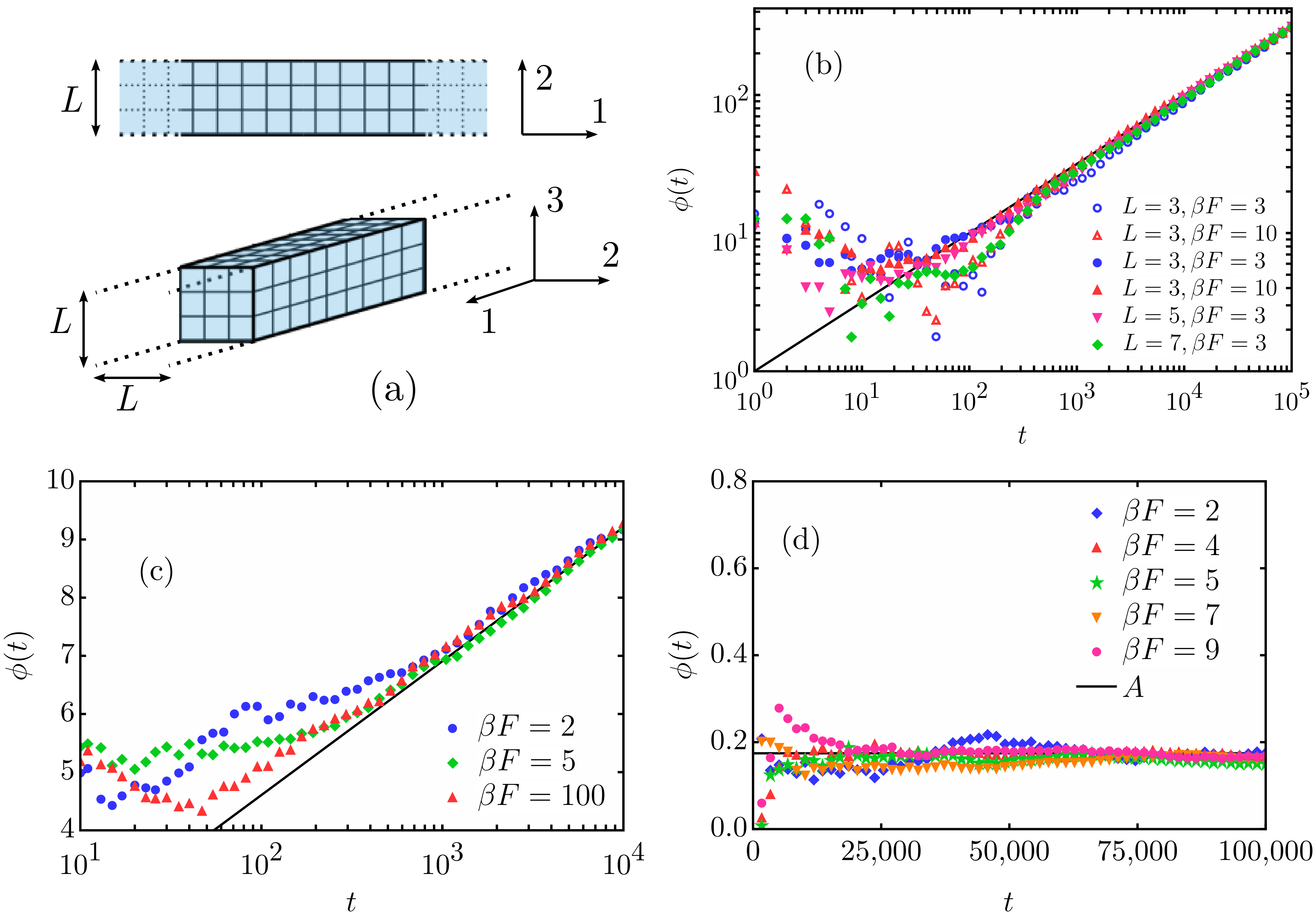
$$\chi_n \sim n^{\alpha-1} \qquad \Rightarrow \qquad \sigma_x^2 \sim \rho_0 a_1 n + \rho_0 a_0^2 n^{2-\alpha}$$

- For non-recurrent random walk ($\alpha = 1$), the behaviour is diffusive
- For recurrent random walks ($\alpha < 1$)

$$\sigma_x^2 \sim \rho_0 a_0^2 n^{2-\alpha}$$

The less efficient the mixing of the lattice gas is the faster the variance of the intruder's displacement grows

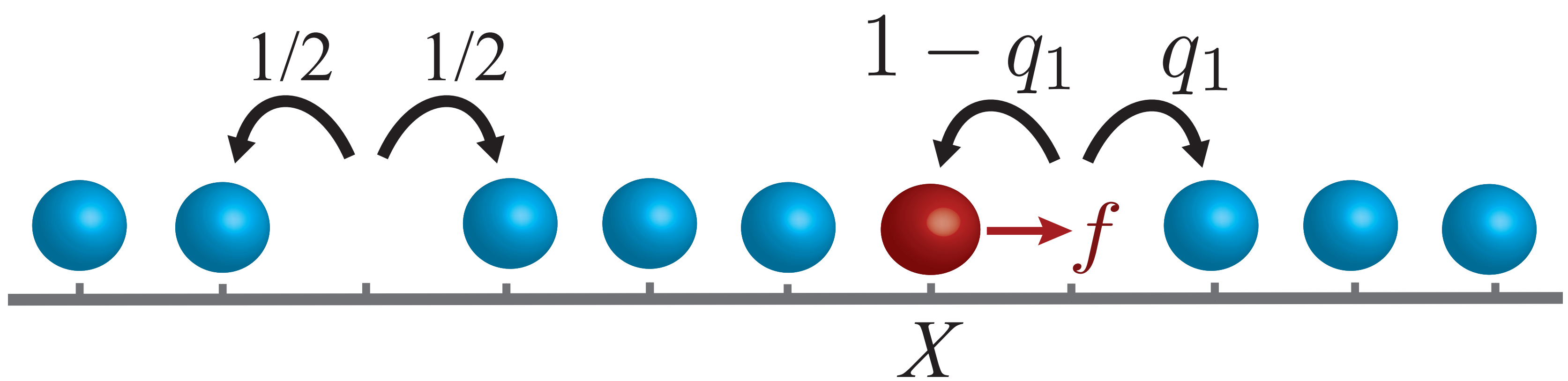
Stripes and Capillaries



capillaries: $\phi(t) = \sqrt{3\pi/2}L^2/(4a_0^2\rho_0 t)\sigma_x^2(t)$

stripes: $\phi(t) = 3\sqrt{\pi}L/(8a_0^2\rho_0 t)\sigma_x^2(t)$

Single-File dynamics



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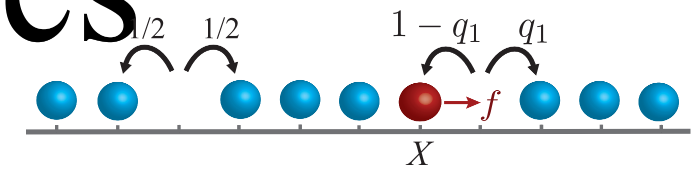
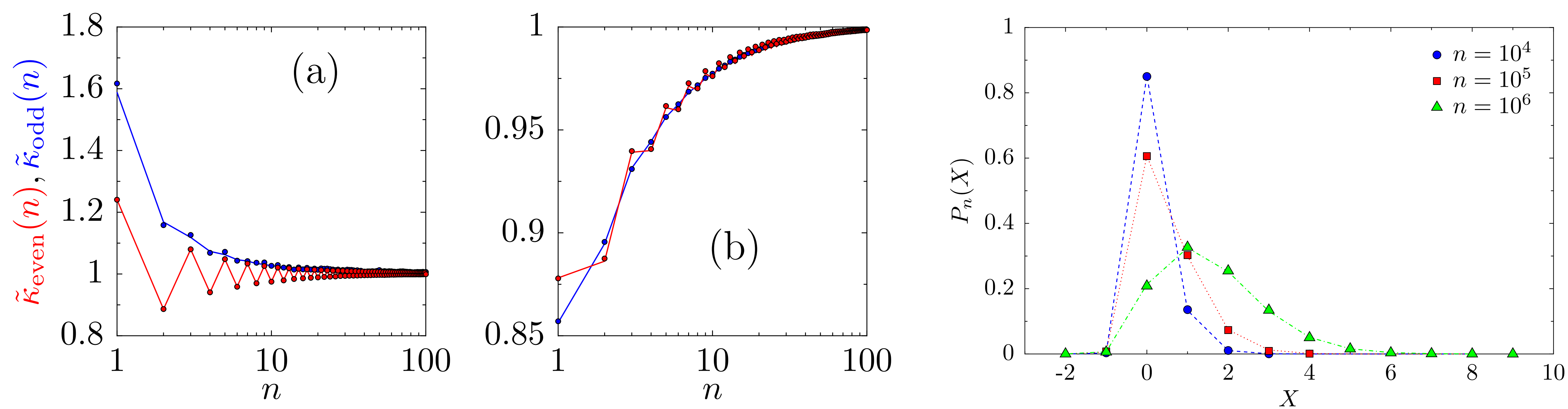


Skellman-type distribution

$$P_n(X) \underset{\rho_0\to 0}{\simeq} \exp\left(-\kappa_{\text{even}}(n)\right)\left(\frac{\kappa_{\text{even}}(n)+\kappa_{\text{odd}}(n)}{\kappa_{\text{even}}(n)-\kappa_{\text{odd}}(n)}\right)^{X/2} I_X\left(\sqrt{\kappa_{\text{even}}^2(n)-\kappa_{\text{odd}}^2(n)}\right)$$

$$\lim_{\rho_0\to 0}\frac{\kappa^n_{(2j+1)}}{\rho_0} = (p_1-p_{-1})\sqrt{\frac{2n}{\pi}} - 2p_1p_{-1}(p_1-p_{-1}) + o(1)$$

$$\lim_{\rho_0\to 0}\frac{\kappa^n_{(2j)}}{\rho_0} = \sqrt{\frac{2n}{\pi}} + o(1)\,, \quad j=0,1,2,\ldots.$$



Is superdiffusion transient?

We need to determine the *long time limit* of the variance at fixed vacancy density

For confined geometries

$$\lim_{t\to\infty}\lim_{\rho_0\to 0}\sigma_x^2 \neq \lim_{\rho_0\to 0}\lim_{t\to\infty}\sigma_x^2$$

between two consecutive visits to the intruder, a given vacancy experiences an effective bias due to the motion of the intruder resulting from its interaction with the rest of the vacancies

O Bénichou, et al, PRL **111**, 260601 (2013)

Is superdiffusion transient?

The long time behaviour is always diffusive

$$\lim_{t\to\infty}\frac{\sigma_x^2}{t}\underset{\rho_0\to 0}{\sim}\begin{cases} B & \text{quasi-1D,}\\ 4a_0^2\pi^{-1}\rho_0\ln(\rho_0^{-1}) & \text{2D lattice,}\\ 2a_0^2[A+\coth(f/2)/(2a_0)]\rho_0 & \text{3D lattice,}\end{cases}$$

In quasi-1D the longitudinal diffusivity is enhanced $\quad \frac{D_\parallel}{D_\perp}\sim\frac{1}{\rho_0}$

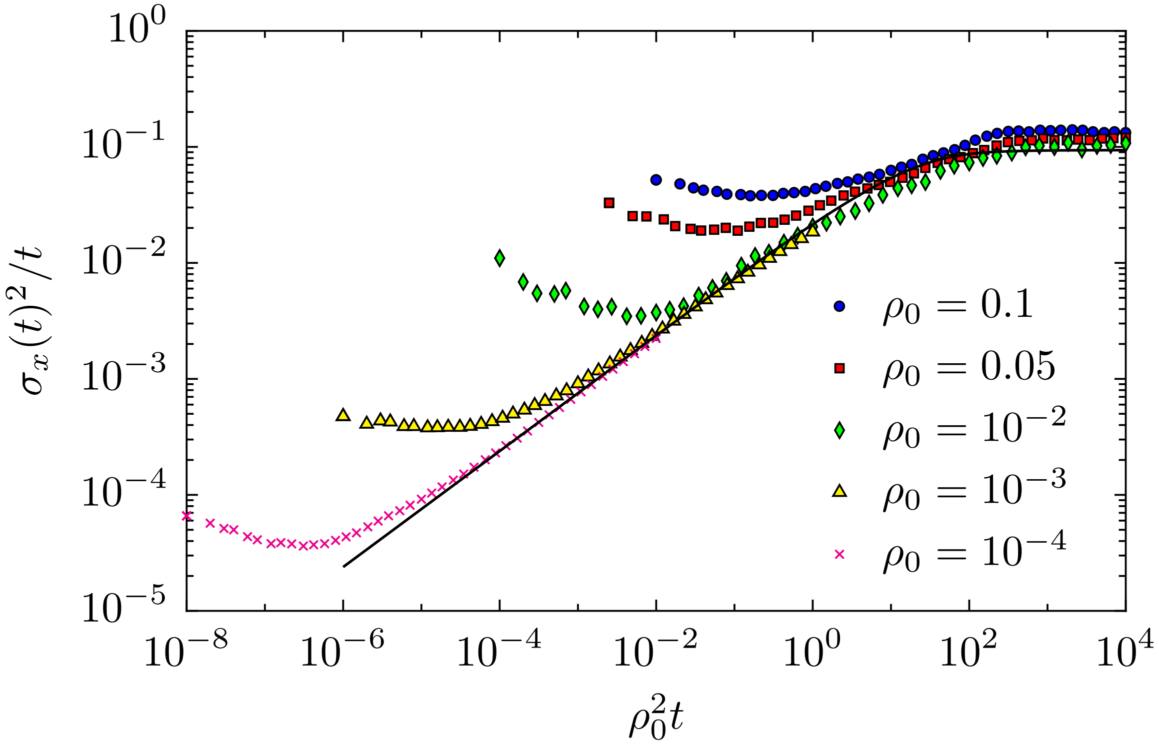
In 2D $\quad \frac{D_\parallel}{D_\perp}\sim\ln(\rho_0^{-1})$

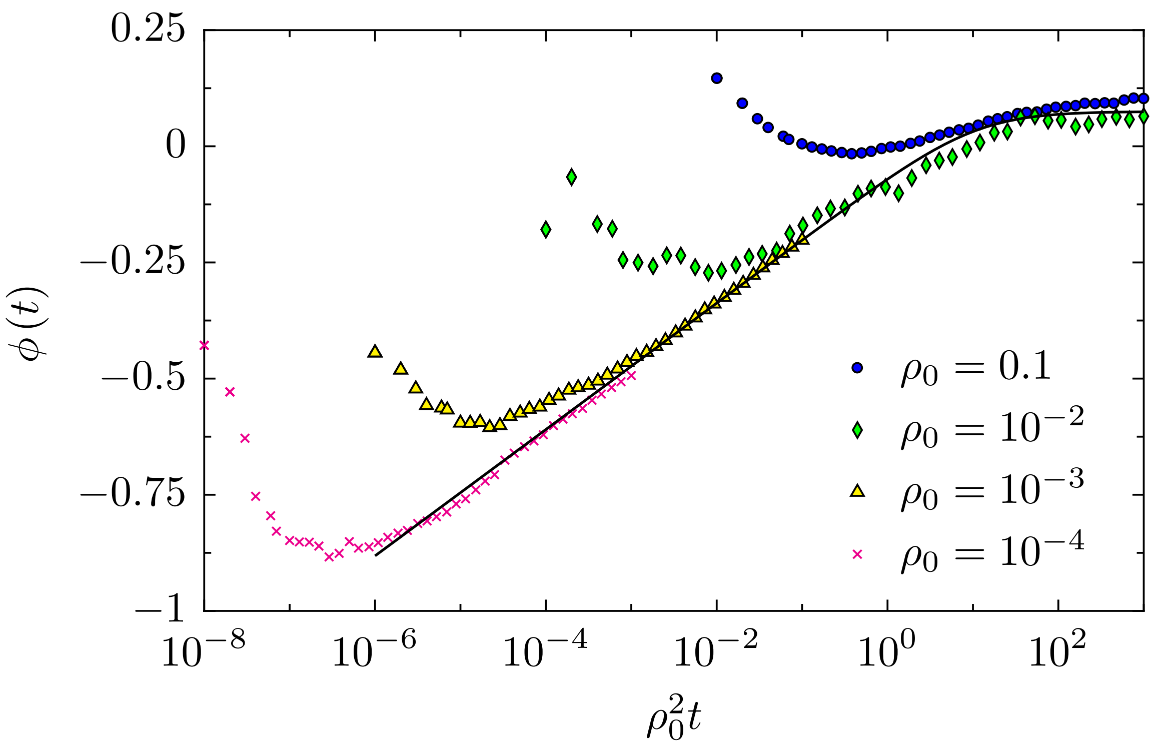
No enhancement is observed in 3D

O Bénichou, et al, PRL **111**, 260601 (2013)

Is superdiffusion transient?

In the intermediate regime we find





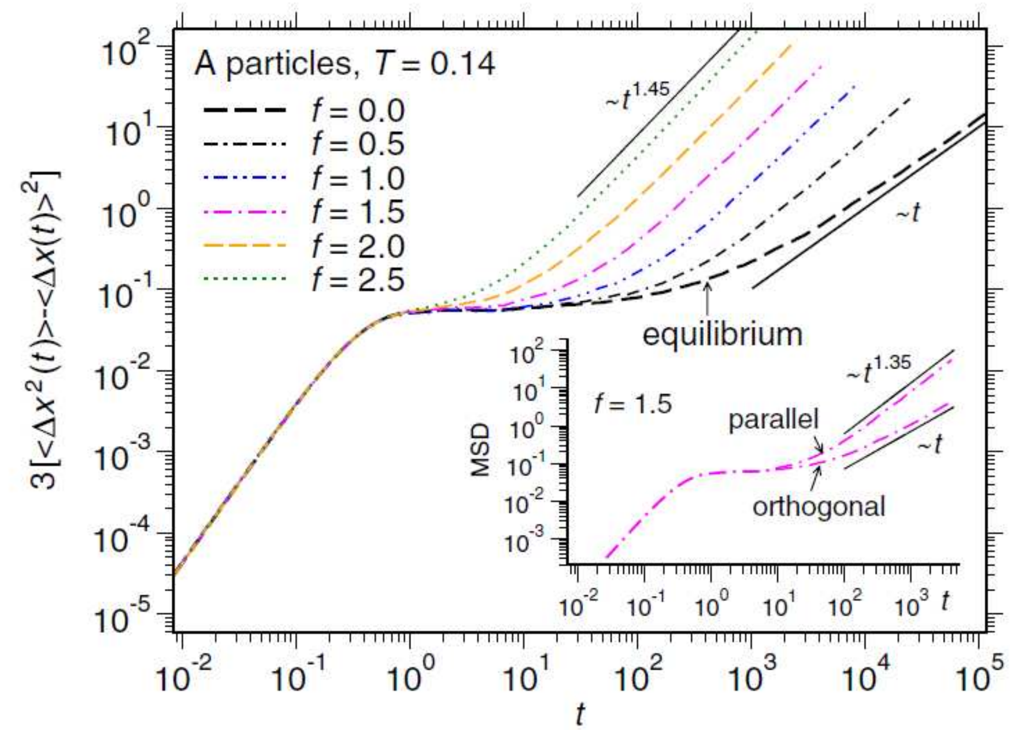
$$\sigma_x^2 \sim \begin{cases} t g(\rho_0^2 t) & \text{quasi-1D,} \\ -\frac{2a_0^2}{\pi}\rho_0 t \ln((\rho_0 a_0)^2 + 1/t) & \text{2D lattice,} \\ 2a_0^2[A + \coth(f/2)/(2a_0)]\rho_0 t & \text{3D lattice,} \end{cases}$$

O Bénichou, et al, PRL **111**, 260601 (2013)

Active nonlinear microrheology

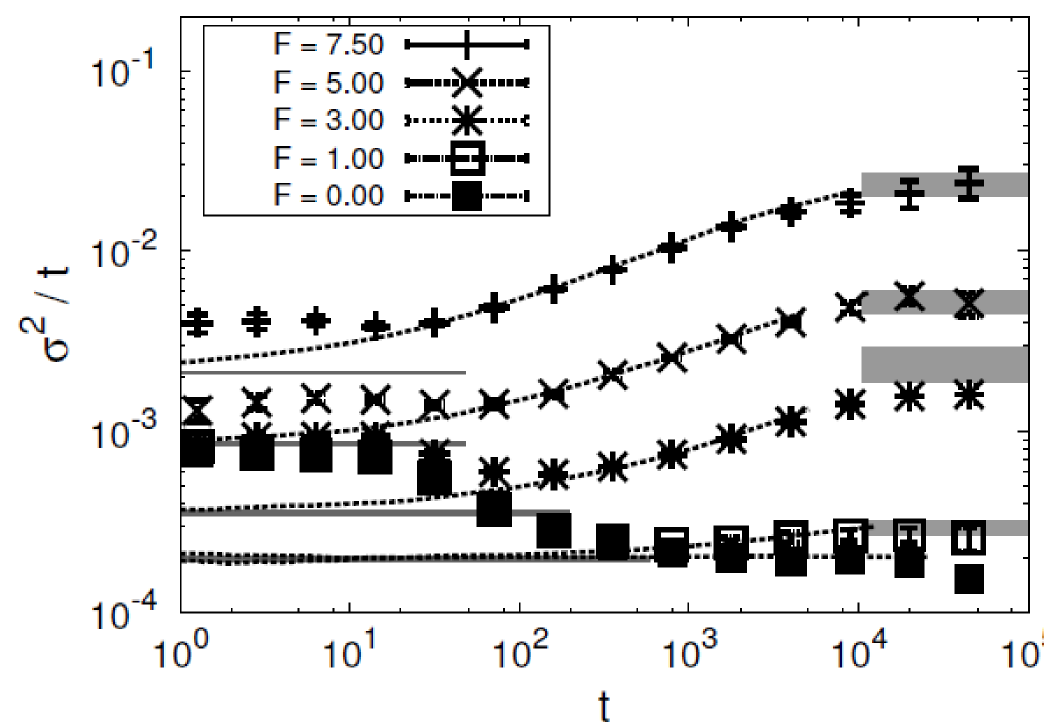
Glass-forming Yukawa fluid

Winter, et al., PRL **108**, 028303 (2012)

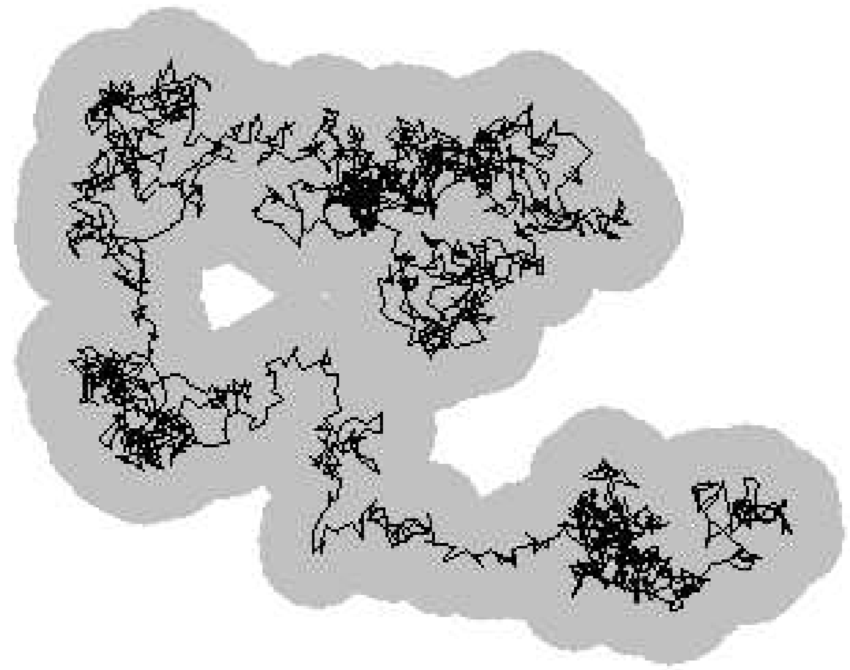


Binary mixture of Lennard-Jones particles

Schroer, Heuer, PRL **110**, 067801 (2013)



Off-lattice continuous systems



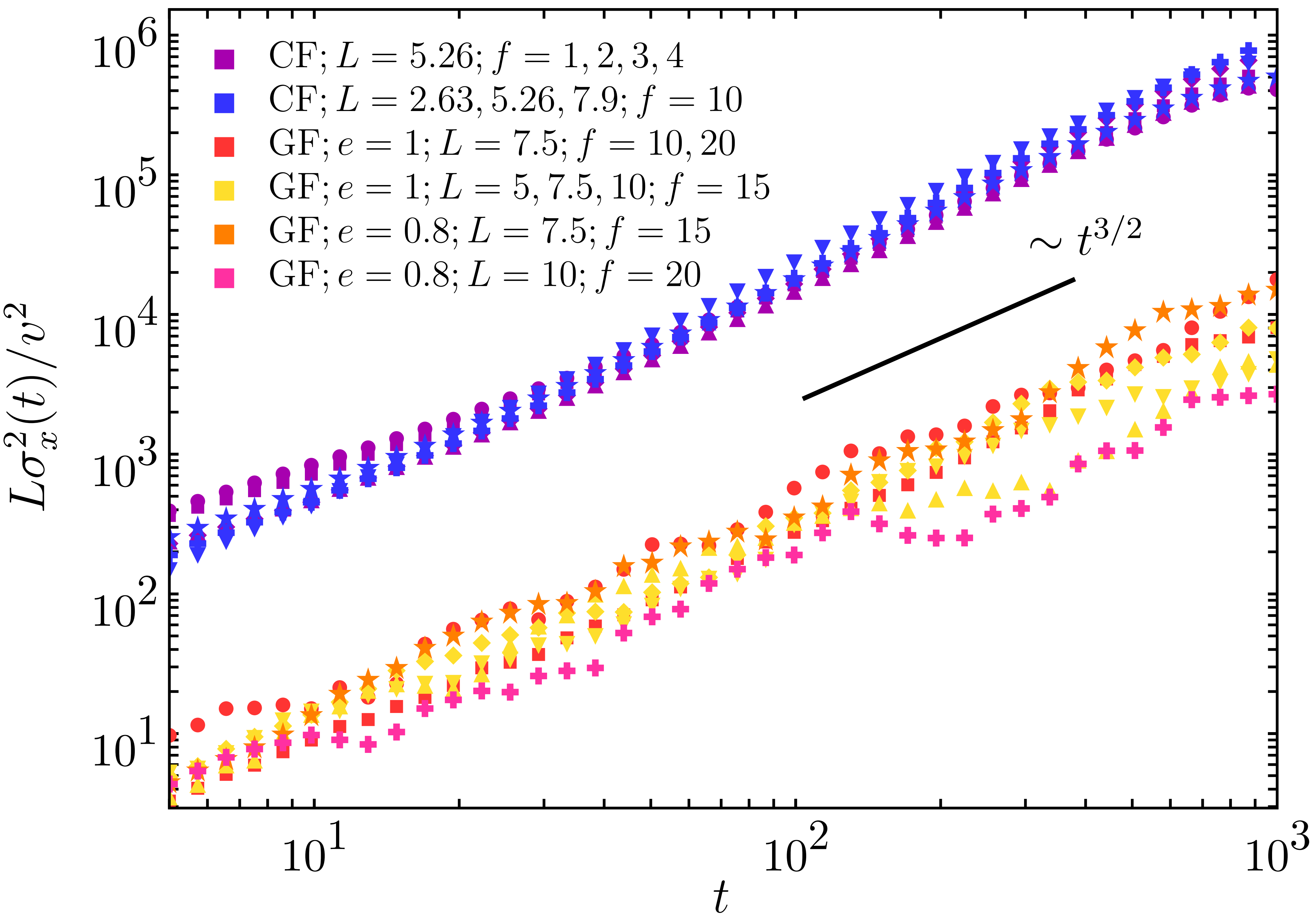
Mean volume of the Wiener saussage

The same power-law behaviour:

compact exploration $\alpha = 1$

non-compact exploration $\alpha < 1$

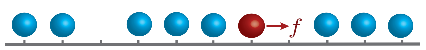
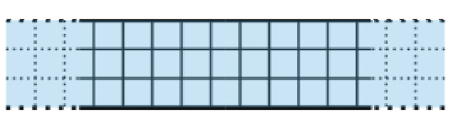
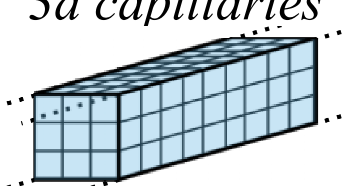
Off-lattice systems



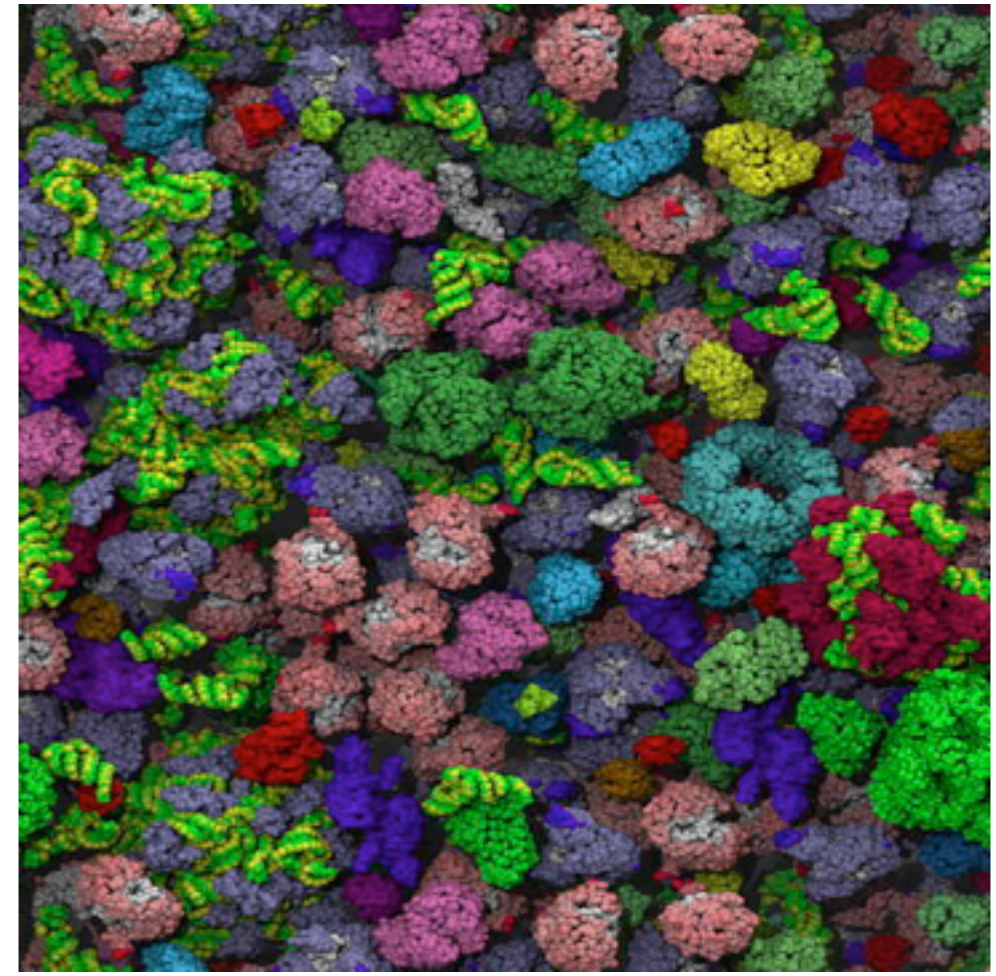
O Bénichou, et al, PRL **111**, 260601 (2013)

New phenomena

field-induced broadening of fluctuations in overcrowded environments

	L_x	L_y	L_z	S_n	χ_n	σ_x^2
1d single-file 	∞					$\sim n^{1/2}$
2d	∞	∞		$\frac{\pi n}{\ln(n)}$	$\frac{\pi}{\ln(n)}$	$\frac{\rho_0 a_0^2}{\pi} n \ln(n)$
3d	∞	∞	∞			$\sim n$
2d stripes 	∞	l	l	$l n^{1/2}$	$\frac{l}{n^{1/2}}$	$\frac{\rho_0 a_0^2}{l} n^{3/2}$
2d slit pores	∞	∞	l	$\frac{l n}{\ln(n)}$	$\frac{l}{\ln(n)}$	$\frac{\rho_0 a_0^2}{l} n \ln(n)$
3d capillaries 	l	l	∞	$l^2 n^{1/2}$	$\frac{l^2}{n^{1/2}}$	$\frac{\rho_0 a_0^2}{l^2} n^{3/2}$

Molecular overcrowding



McGuffee and Elcock, PLoS Computational Biology (2010)

In confined geometries, transport is passively subdiffusive but actively superdiffusive

Perspectives

- Glass and jamming transitions.
- Dynamical arrest and the broadening of the fluctuations.
- Extensions to non-Brownian dynamics.
- Stochastic entropy.
- Transitions between steady-states.

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