

# Dynamical tracer—bath correlations in interacting particle systems

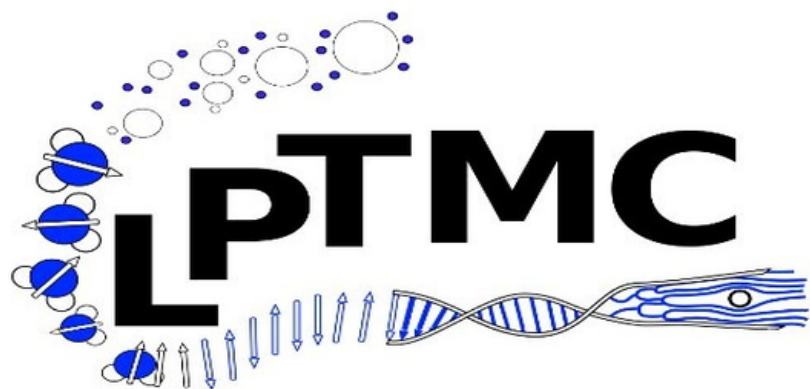
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*4èmes Journées du GDR IDE*

Sète, 9 September 2025

Work in collaboration with T. Berlioz, P. Illien, A. Grabsch, O. Bénichou



# Tracer particle

## in a thermal bath

$$m \ddot{X}(t) = -\gamma \dot{X}(t) + \zeta(t)$$

$$\langle \zeta(t) \zeta(t') \rangle = 2\gamma k_B T \delta(t - t')$$

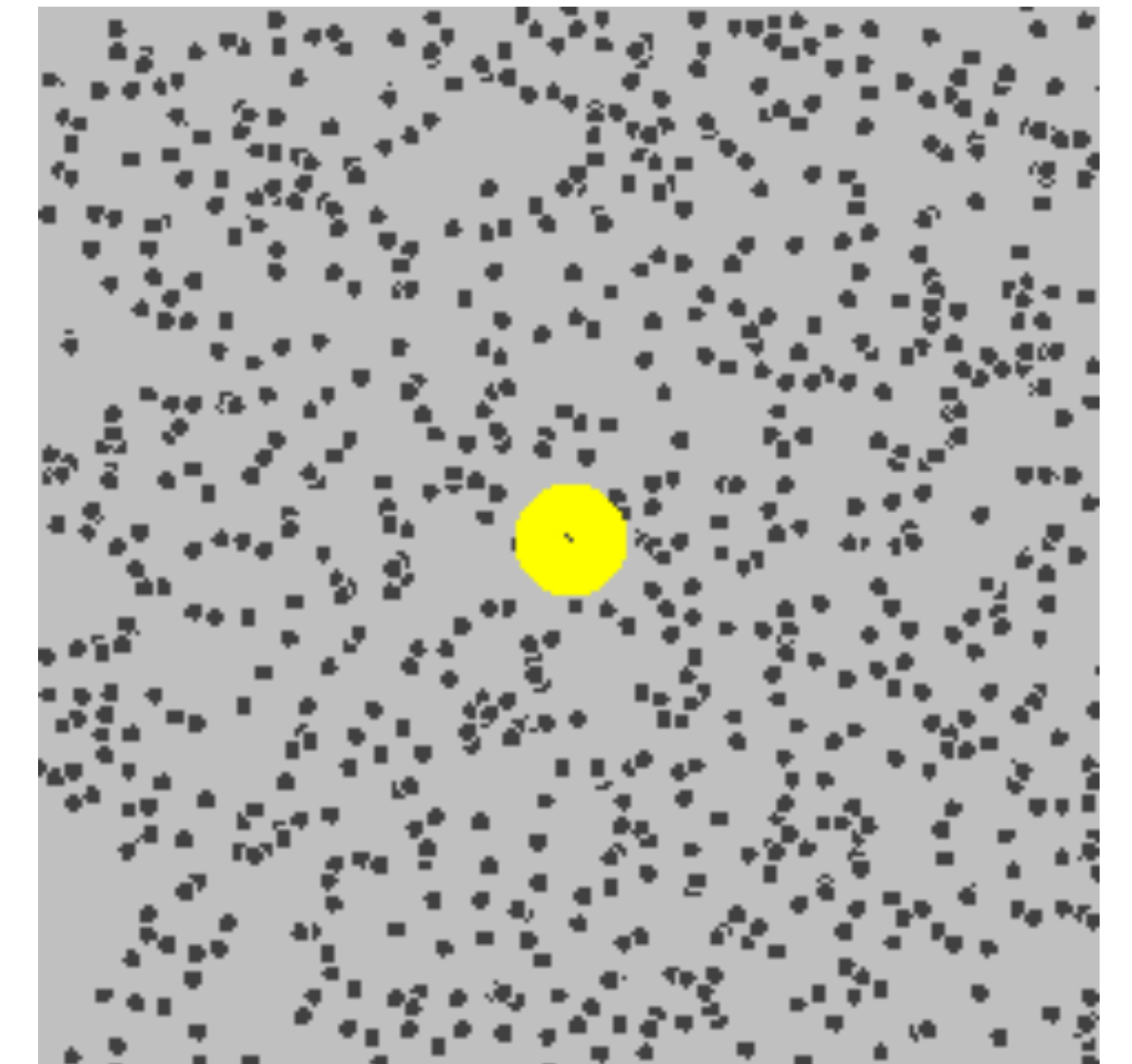
📌 **Brownian motion:** bath in **equilibrium**, **structureless**,

no **tracer-bath** correlations, **diffusive** behaviour

$$\langle X^n(t) \zeta(t) \rangle = 0, \quad \langle X^2(t) \rangle \propto t$$

📌 What if particles have similar sizes?

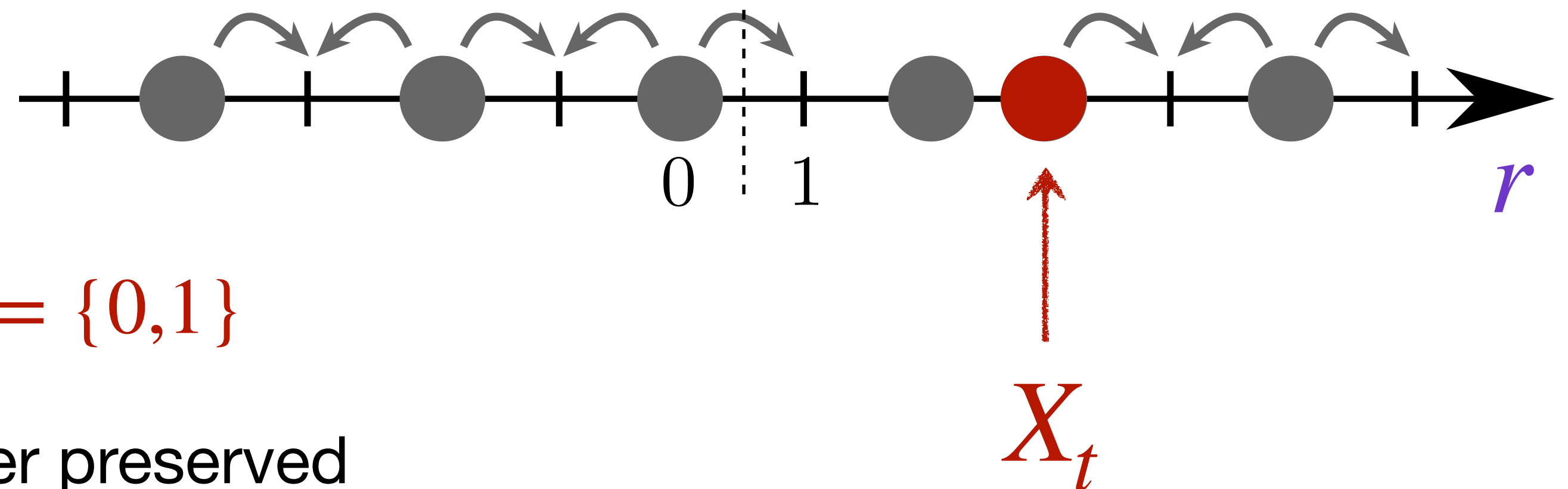
📌 **Interacting particle systems:** lattice gases, interacting Brownian particles, simple liquids...



# Symmetric Exclusion Process

## as paradigmatic interacting particle system

- Particles on a lattice  
+ random hoppings (equal rates),  
only if target site is empty



- **State of the system:** occupations  $\rho_r(t) = \{0,1\}$
- In  $1d$ , **single-file** geometry  $\rightarrow$  initial order preserved
- Subdiffusive behavior of tracer

$$\langle X_t^2 \rangle \propto \sqrt{t}$$

(zeolites, confined colloids, dipolar spheres...)

Lin, Meron, Cui, Rice, Diamant, Phys. Rev. Lett. **94** (21), 216001 (2005)

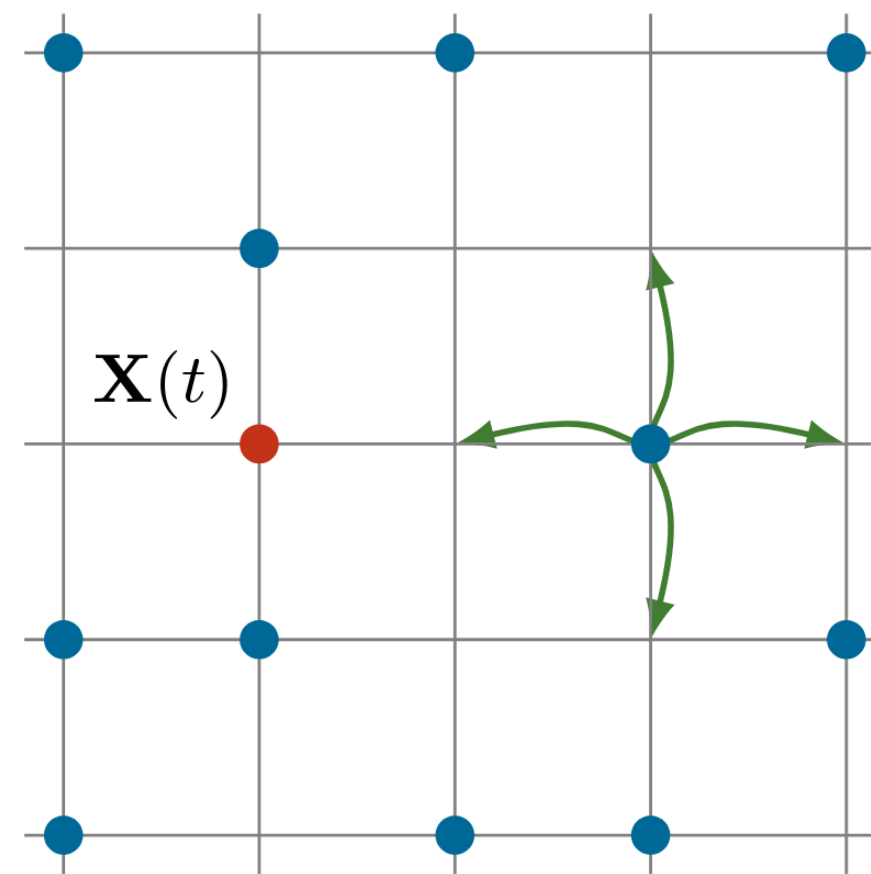
Wei, Bechinger, Leiderer, Science **287** (5453), 625-7 (2000)

Hahn, Kärger, Kukla, Phys. Rev. Lett. **76** (15), 2762-2765 (1996)

H. Spohn, *Large scale dynamics of interacting particles* (1991)

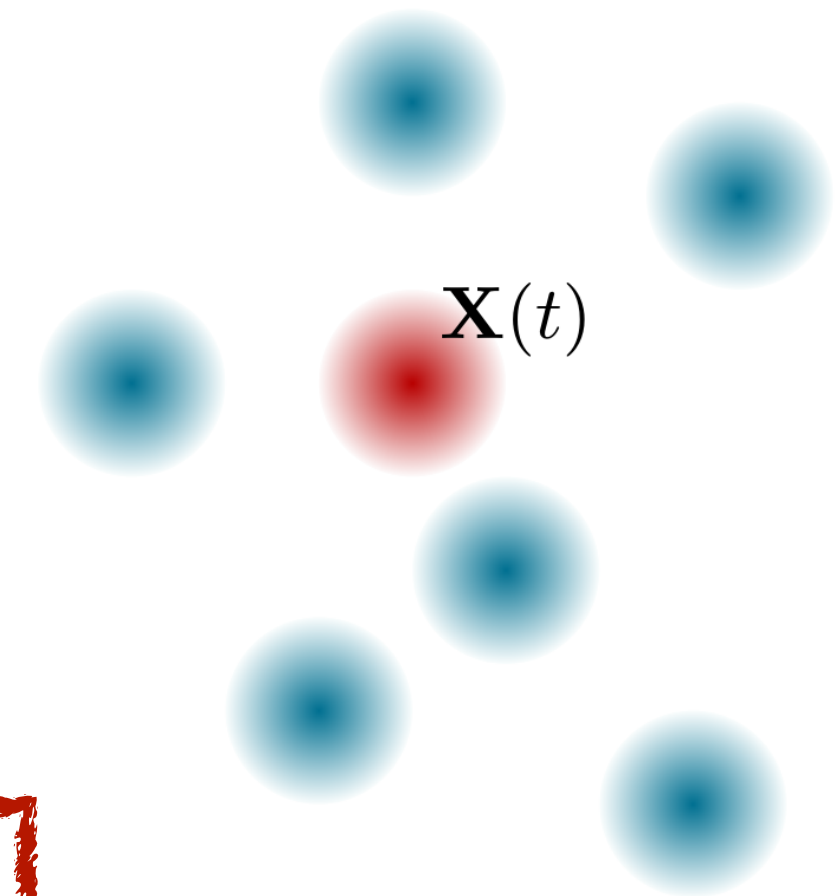


# Tracer-bath correlation profiles



Hard-core lattice gas  
(SEP)

Brownian particles  
+ two-body potential  $U(\vec{r}_i - \vec{r}_j)$



 **Key observable:** position  $X(t)$  of a tagged particle

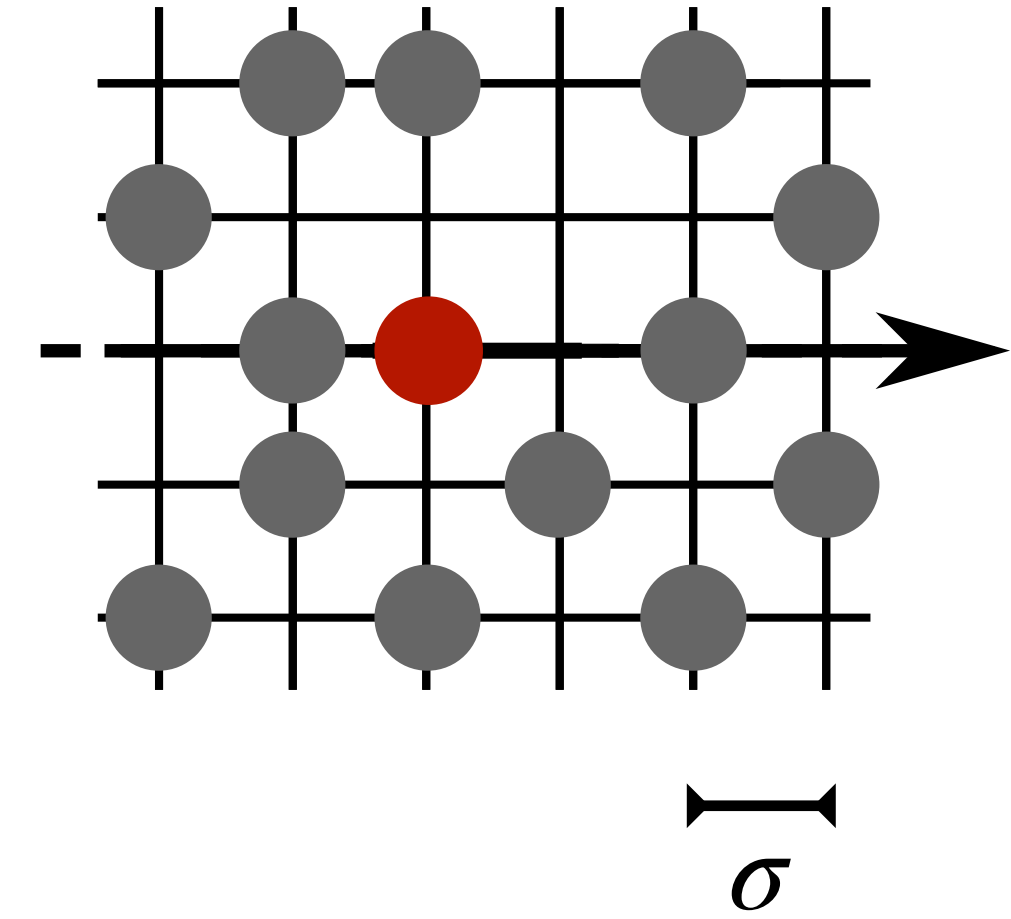
- how does the displacement of the **tracer** affect the **bath** (= other particles)?
- how does the **bath** affect the displacement of the **tracer**?

$$\partial_t \langle X^{n+1} \rangle_c = F \left[ \dots \langle X^n \rho_{X+r} \rangle_c \dots \right]$$

density of bath particles  
at distance  $r$



# Hard-core lattice gas



Master equation  $\partial_t P(X, \underline{\rho}, t) = \left[ \mathcal{L}_{\text{tracer}} + \mathcal{L}_{\text{bath}} \right] P(X, \underline{\rho}, t)$

Multiply by  $e^{\lambda \cdot X}$  and average,

$$\partial_t \Psi(\lambda, t) = \frac{1}{2d\tau} \sum_{\mu=-d}^d \left( e^{\sigma \lambda \cdot \hat{e}_\mu} - 1 \right) \left[ 1 - w_{\mathbf{e}_\mu}(\lambda, t) \right]$$

tracer cumulants

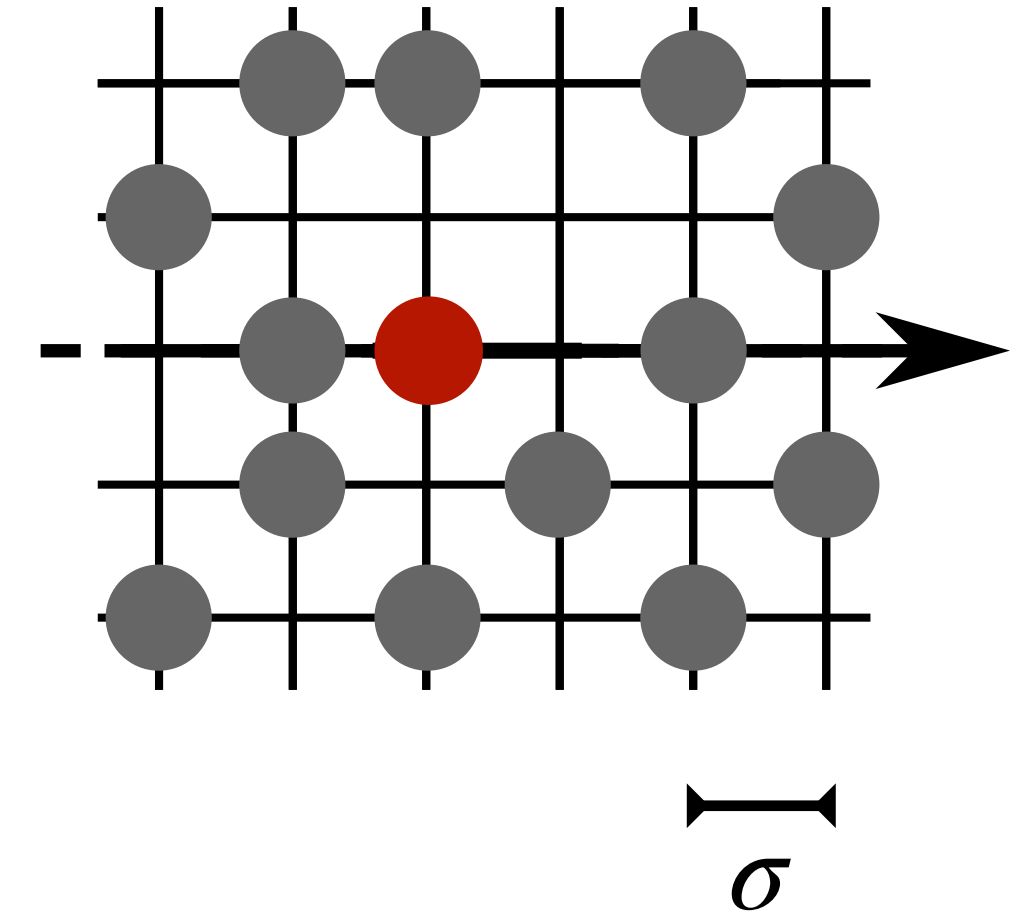
$$\Psi(\lambda, t) = \ln \langle e^{\lambda \cdot X} \rangle = \sum_{n=1}^{\infty} \frac{\lambda^n}{n!} \langle X^n \rangle_c,$$

tracer-bath profiles

$$w_r(\lambda, t) = \frac{\langle \rho_{X+r} e^{\lambda \cdot X} \rangle}{\langle e^{\lambda \cdot X} \rangle} = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} \langle \rho_{X+r} X^n \rangle_c$$

# Role of correlations

## with surrounding bath



$$\partial_t \Psi(\lambda, t) = \frac{1}{2d\tau} \sum_{\mu=-d}^d \left( e^{\sigma\lambda \cdot \hat{\mathbf{e}}_\mu} - 1 \right) \left[ 1 - w_{\mathbf{e}_\mu}(\lambda, t) \right]$$

📌 Knowing  $w_{\mathbf{e}_\mu}(\lambda, t)$  (= **response** of the bath) on neighbouring sites is enough to deduce  $\Psi(\lambda, t)$

📌  $\partial_t w_{\mathbf{e}_\mu}(\lambda, t) = \dots [w_{\mathbf{r}}(\lambda, t)] \dots$

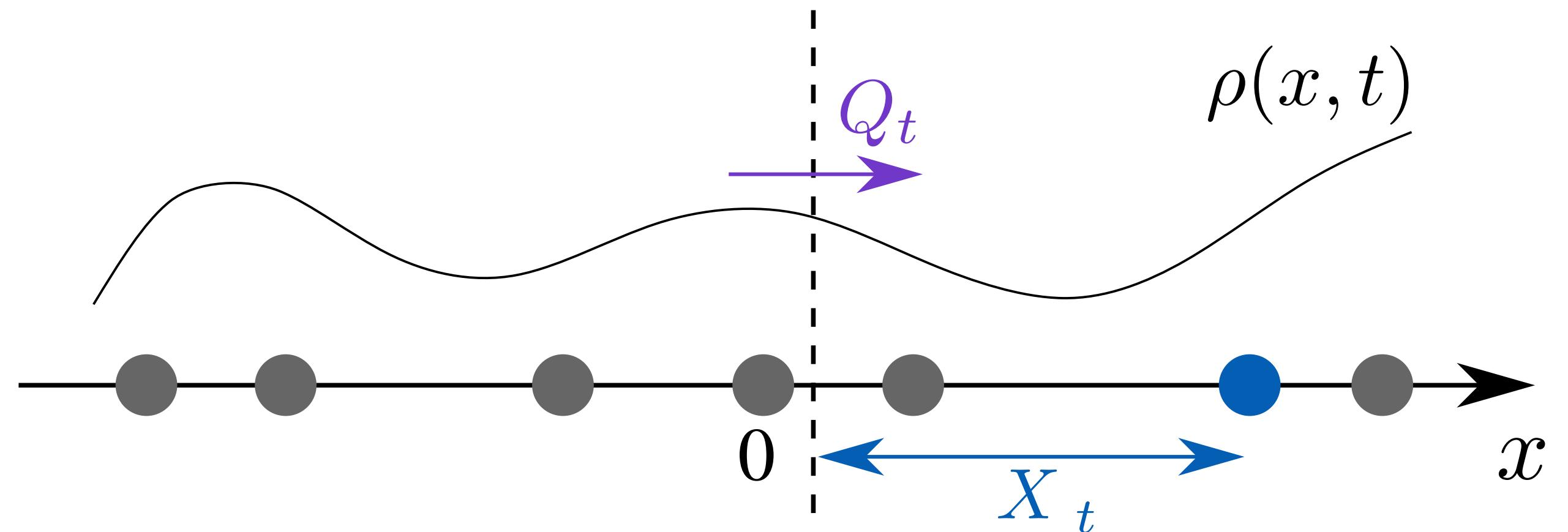
generically depends on  $w_{\mathbf{r}}(\lambda, t)$  even from far away  $\mathbf{r}$

**Context:**  $w_{\mathbf{r}}(\lambda, t)$  fully understood in 1d SEP  $\longrightarrow \langle e^{\lambda \cdot X} \rangle$  as a **byproduct**

**Aim:** characterize these profiles in  $d > 1$

# Integrated current $Q_t$

- $Q_t$  = net # of particles crossing (0—1)  
→ in  $d = 1$ ,  $\langle Q_t^2 \rangle \propto \sqrt{t}$
- A positive fluctuation of  $Q_t$  is correlated with an increase of  $\rho_r(t)$  on its r.h.s.  
→ **correlations dictate the subdiffusive behavior of  $Q_t$**
- $\langle \rho_r(t) Q_t^n \rangle$  encodes the **response** of the bath  
    ↑                      ↑  
bath structure      local observable
- Fully understood in  $1d$  SEP,  
open problem in  $d > 1$



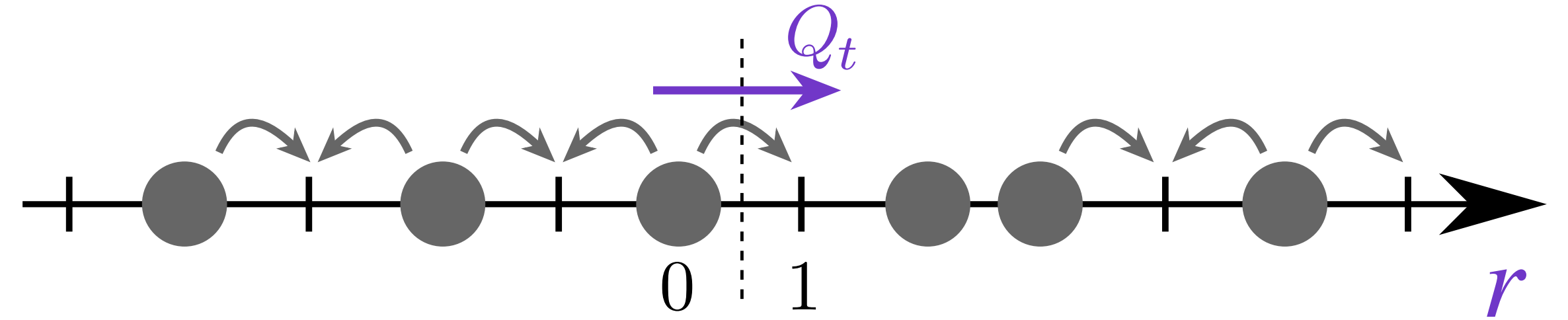
Grabsch, Poncet, Rizkallah, Illien, Bénichou, Sci. Adv. 8, eabm5043 (2022)



# **1. Current fluctuations in SEP**

📌 As **first step**, focus on

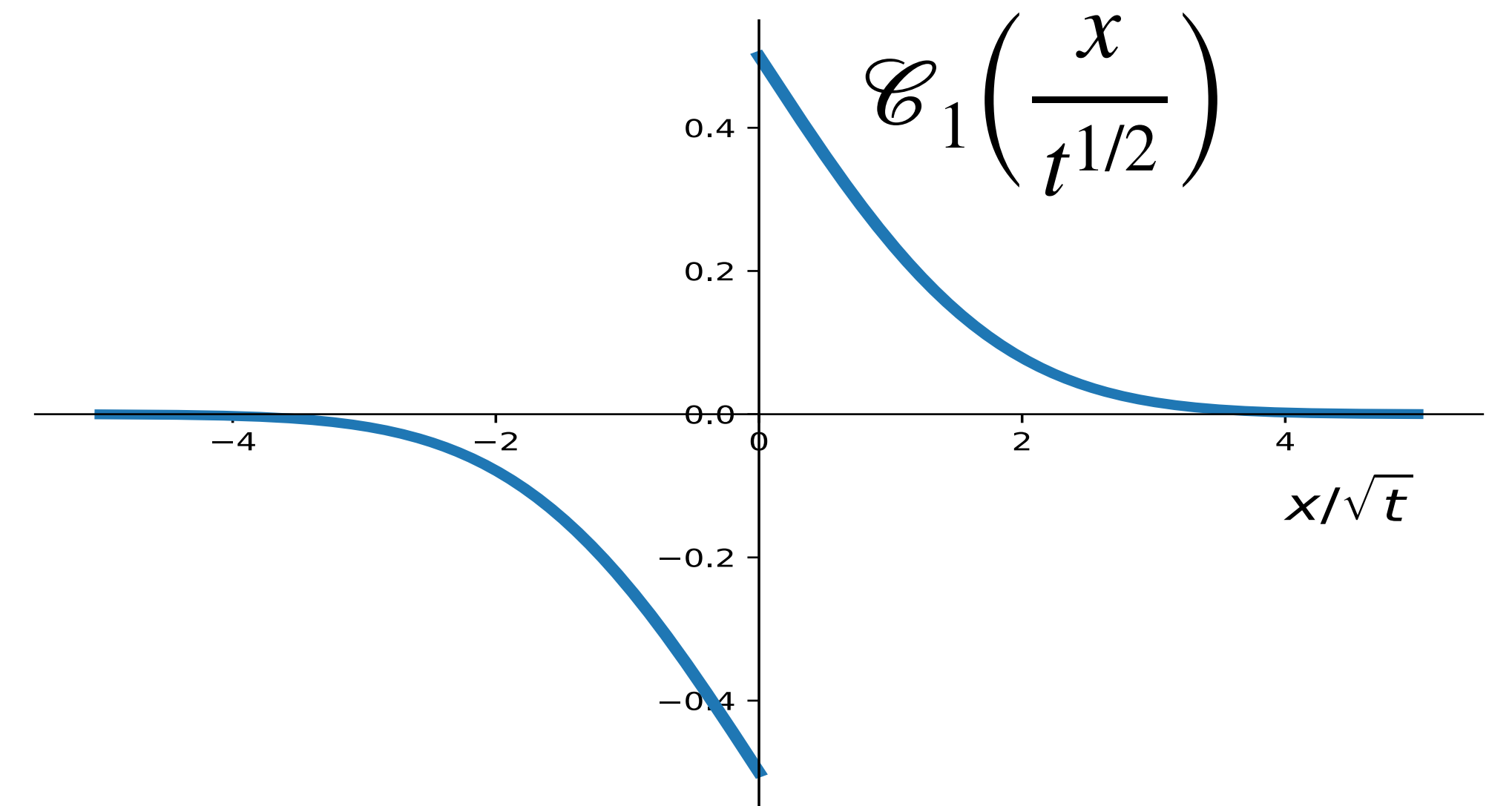
$$c_r(t) \equiv \langle Q_t \rho_r(t) \rangle$$



📌 **Fact 1:** infinite lattice  $d = 1$  (no reservoirs, no PBC)

$$c_r(t) \xrightarrow{t \rightarrow \infty} \bar{\rho}(1 - \bar{\rho}) \mathcal{C}_1\left(\frac{r}{t^{1/2}}\right),$$

$$\langle Q_t^2 \rangle \propto \bar{\rho}(1 - \bar{\rho}) t^{1/2}$$



📌 **Fact 2:** finite systems (any spatial dimension  $d$ )

$$c_{\vec{r}}(t) \xrightarrow{t \rightarrow \infty} c_{\vec{r}}, \quad \langle Q_t^2 \rangle \propto t$$

Recall  $\partial_t \langle Q_t^{n+1} \rangle = \dots F \left[ \langle Q_t^n \rho_{\vec{r}}(t) \rangle \right] \dots$   
 $\partial_t \langle Q_t^2 \rangle = \dots F \left[ c_{\vec{r}}(t) \right] \dots$

**infinite lattices in  $d > 1$  ?**



# From $d = 1$ to higher $d$ passing through the comb

1. Order-preserving (single-file)
2. Tree-like (no loops!)

Do we need both, to have  $\langle Q_t^2 \rangle \propto t^\alpha$  with  $\alpha < 1$ ?

📌 Higher  $d$  :

~~(1)~~

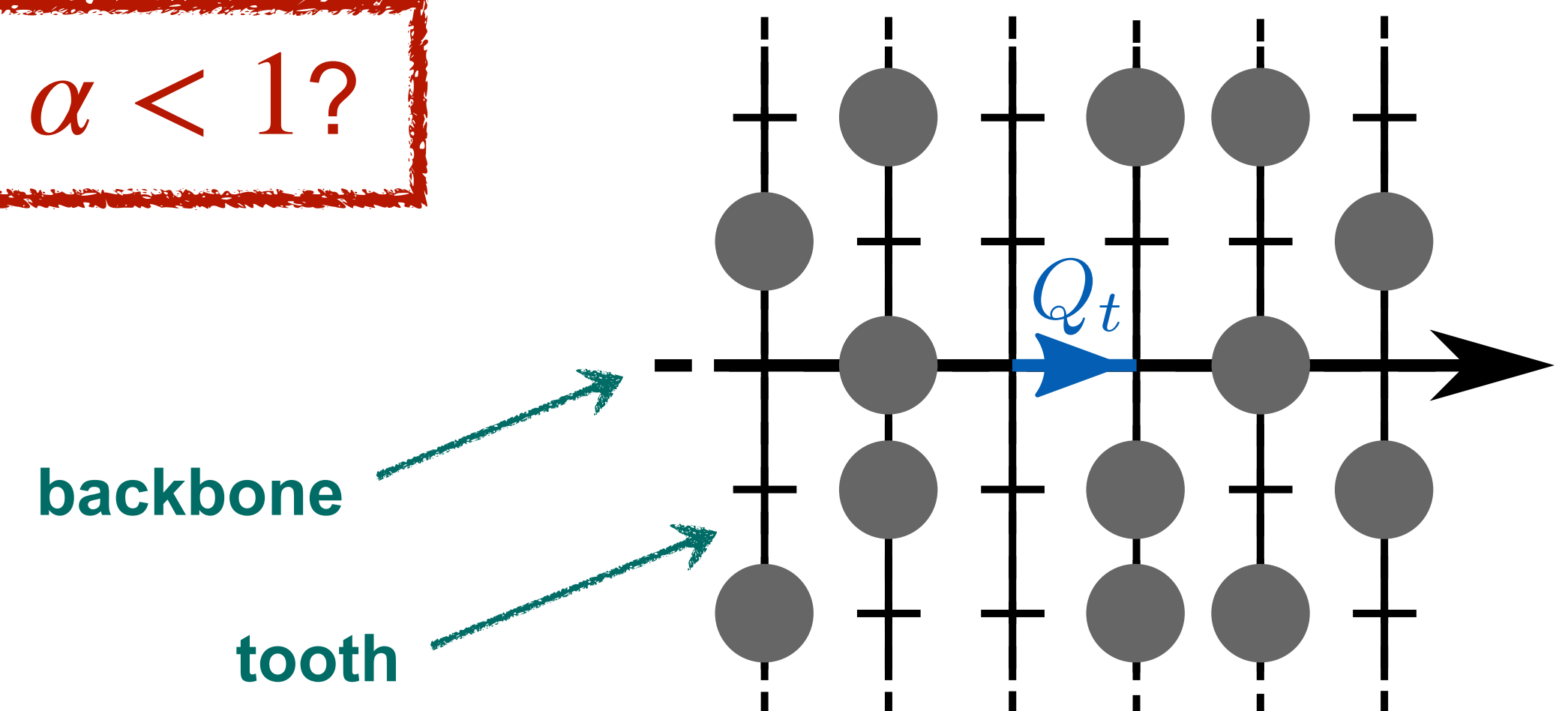
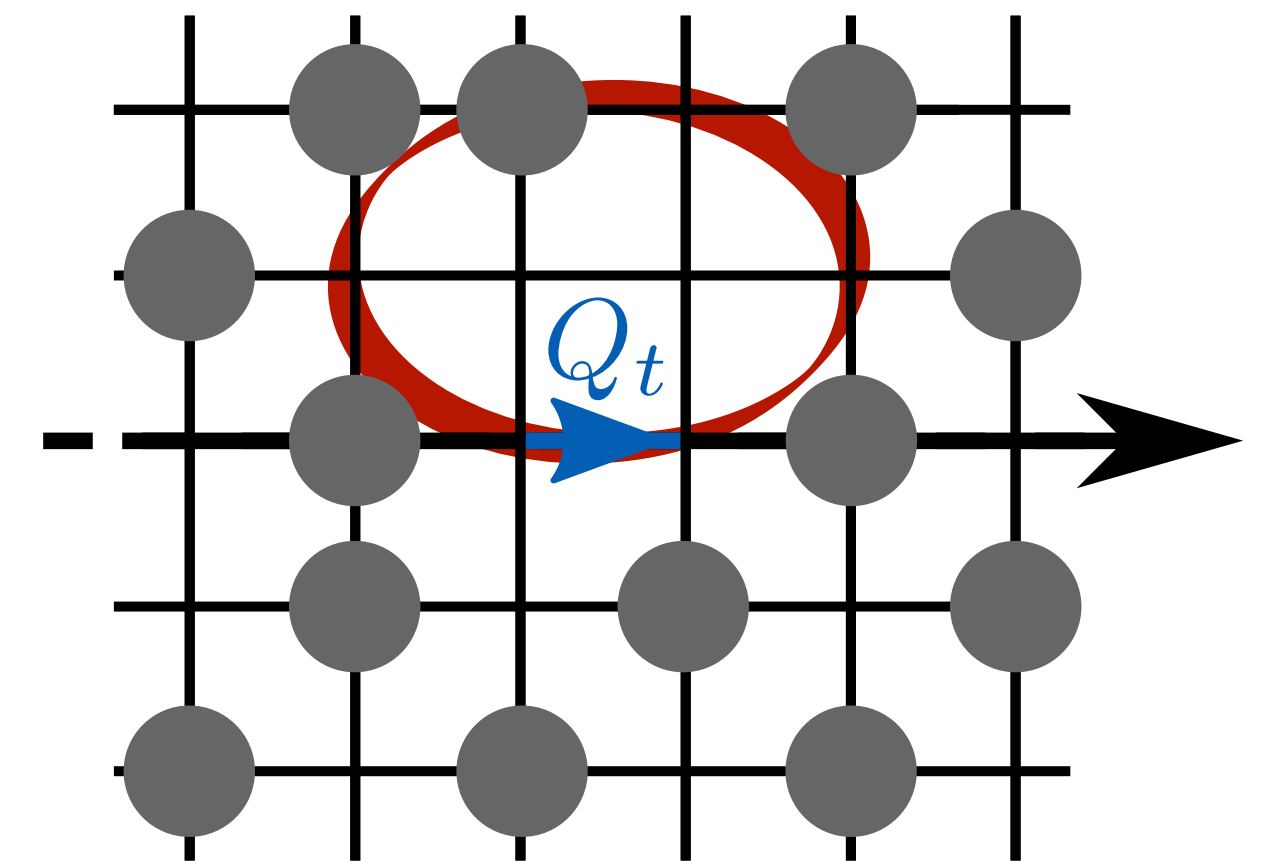
~~(2)~~

📌 Comb lattice :

~~(1)~~

(2)

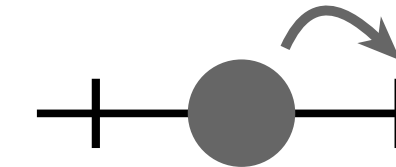
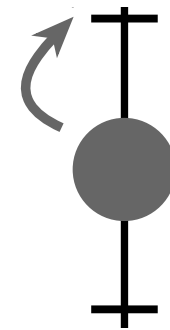
Transport in porous media,  
subdiffusion (even single particle!)



Bénichou, Illien, Oshanin, Sarracino, Voituriez, Phys. Rev. Lett. **115**, 220601 (2015)  
Ben-Avraham, Havlin, *Diffusion and reactions in fractals and disordered systems* (2000)

# Microscopic calculation

- Master equation

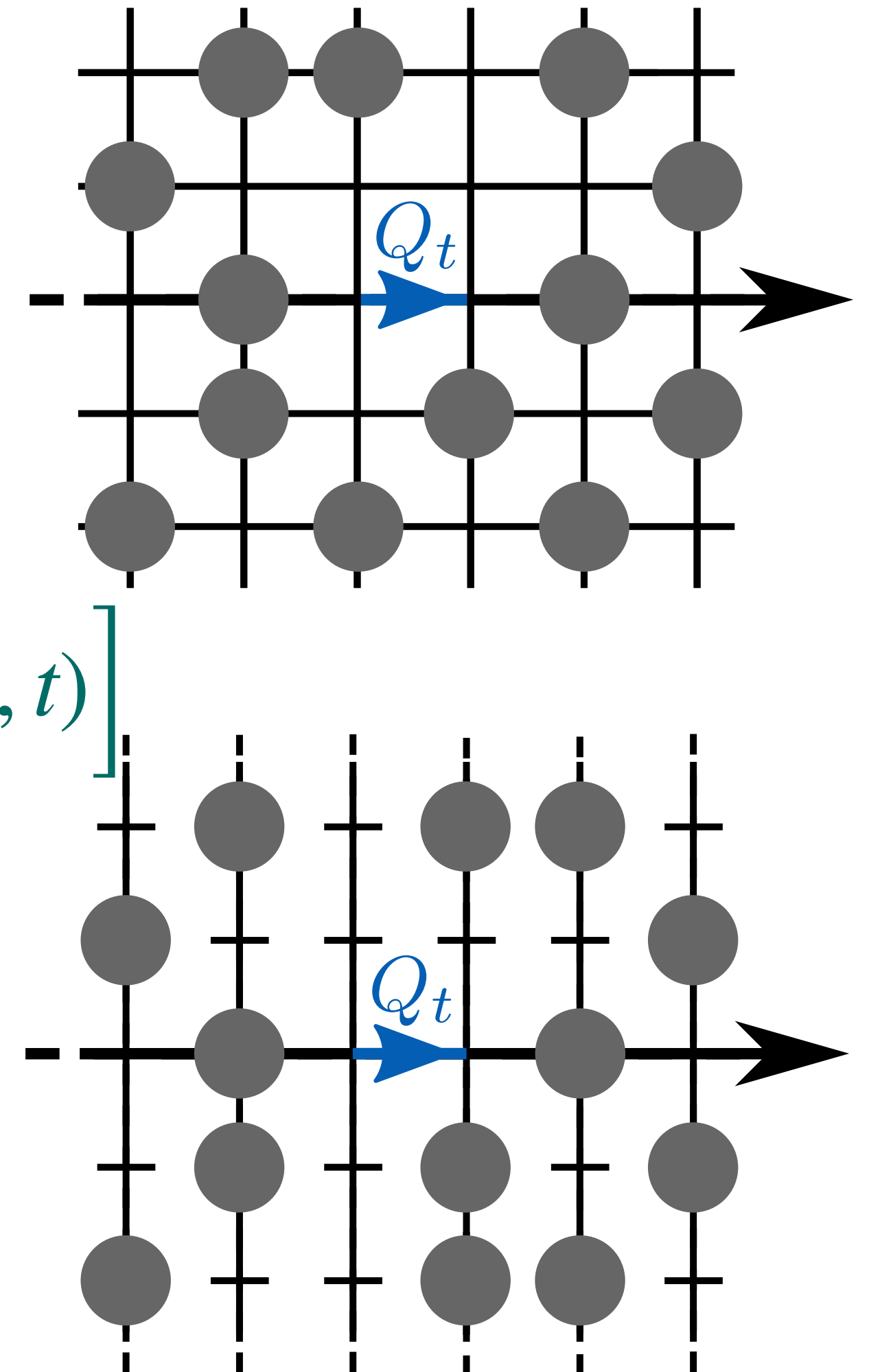


$$\partial_t P_t(\underline{\rho}) = \sum_{x,y} \left[ P(\underline{\rho}^{x,y+}, t) - P(\underline{\rho}, t) \right] + \sum_{x,y} \left[ P(\underline{\rho}^{x+,y}, t) - P(\underline{\rho}, t) \right]$$

- Look for moments, e.g.  $\partial_t \langle Q_t^2 \rangle = \dots [c_{\vec{r}}(t)] \dots$

- Find **exact closed** equations  $\partial_t c_{\vec{r}}(t)$  for  $c_{\vec{r}}(t) = \langle Q_t \rho_{\vec{r}}(t) \rangle$

- Solve them in Fourier-Laplace (**self-consistently**)



# Results

📌  $d = 1$       $c_r(t) \xrightarrow{t \rightarrow \infty} \bar{\rho}(1 - \bar{\rho}) \mathcal{C}_1\left(\frac{r}{t^{1/2}}\right)$

$$\langle Q_t^2 \rangle = n_1 \bar{\rho}(1 - \bar{\rho}) t^{1/2}$$

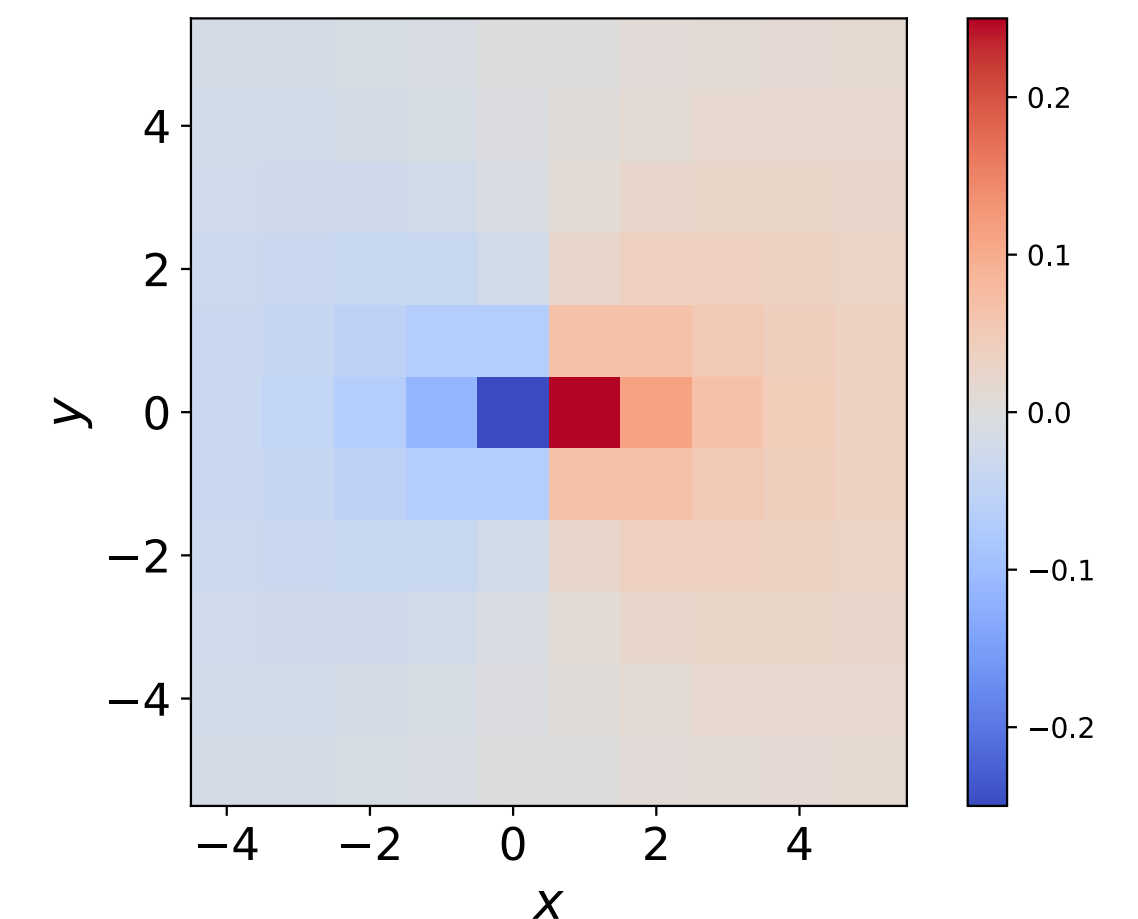
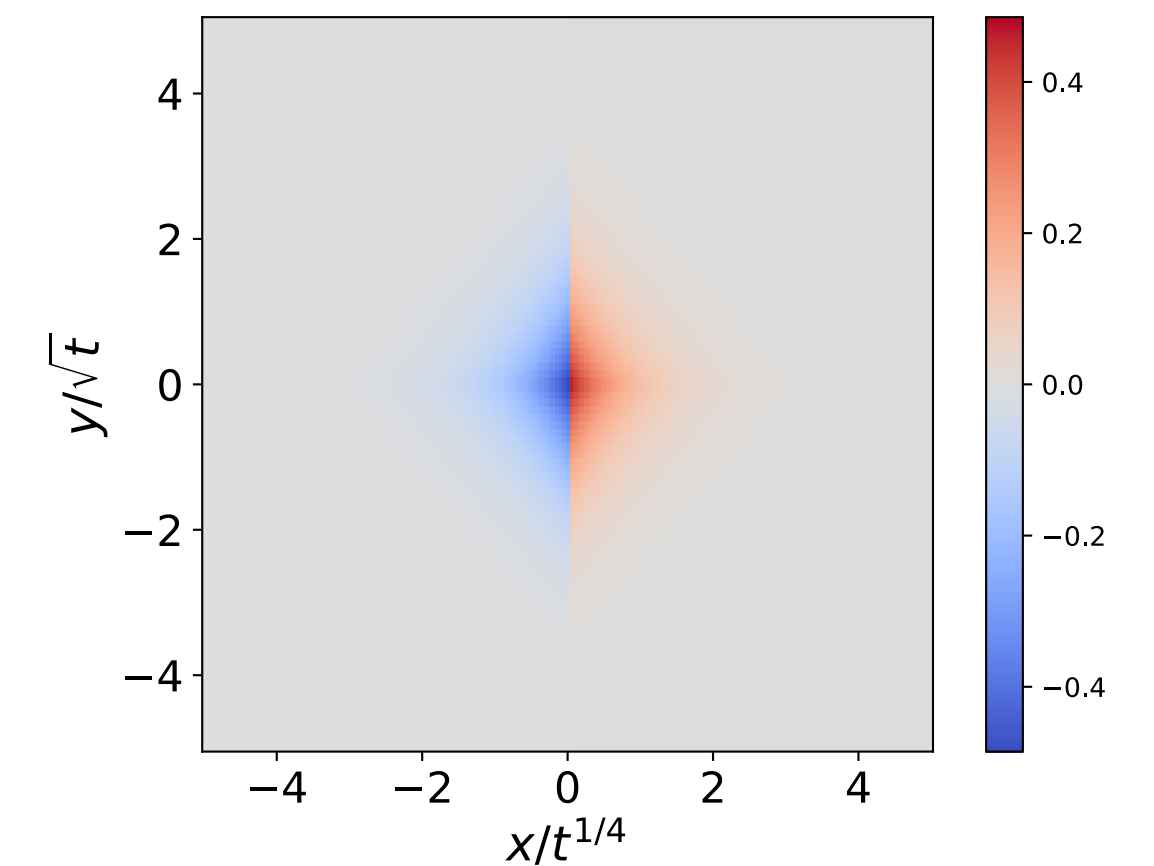
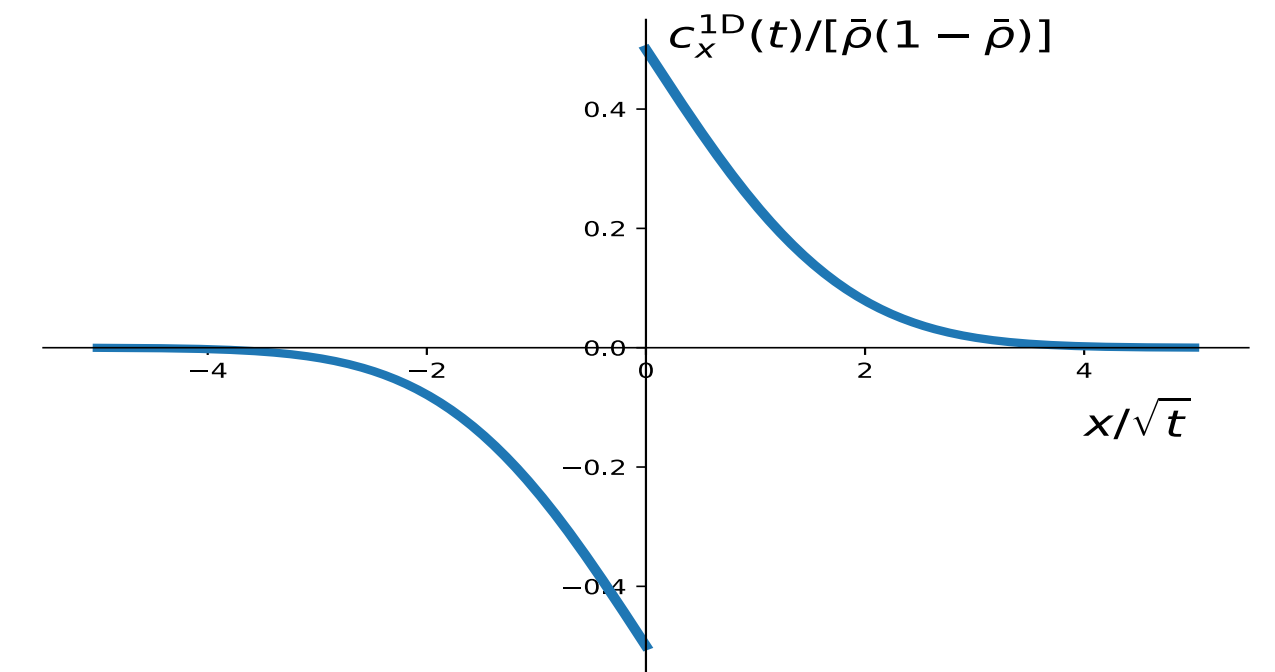
📌 Comb      $c_{\vec{r}}(t) \xrightarrow{t \rightarrow \infty} \bar{\rho}(1 - \bar{\rho}) \mathcal{C}_c\left(\frac{x}{t^{1/4}}, \frac{y}{t^{1/2}}\right)$

$$\langle Q_t^2 \rangle = n_c \bar{\rho}(1 - \bar{\rho}) t^{3/4}$$

📌  $d = 2$       $c_{\vec{r}}(t) \xrightarrow{t \rightarrow \infty} \bar{\rho}(1 - \bar{\rho}) \mathcal{C}_2(\vec{r})$

$$\langle Q_t^2 \rangle = n_2 \bar{\rho}(1 - \bar{\rho}) t$$

$\langle Q_t^2 \rangle \propto t$  requires loops!

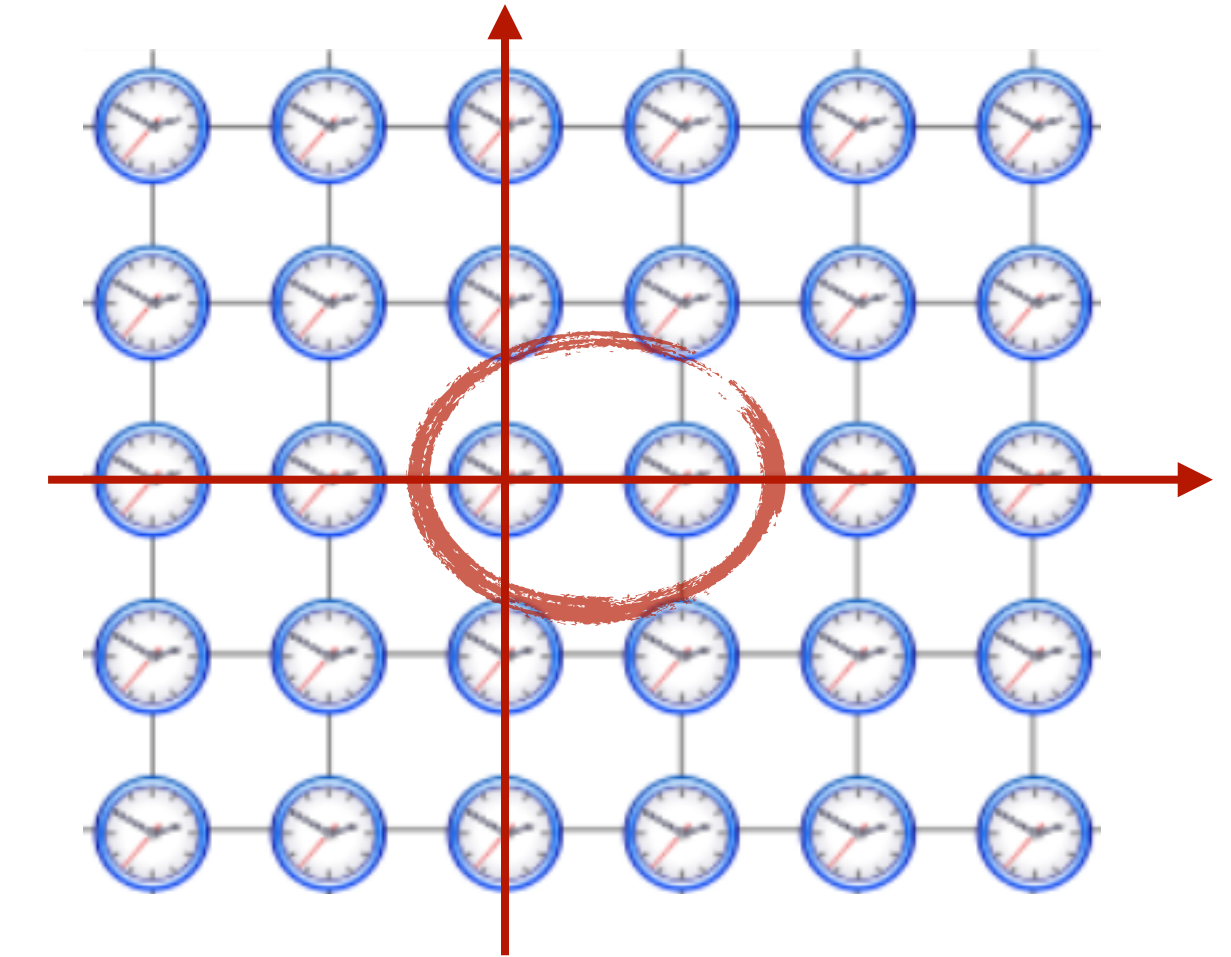




# Microscopic path-integral representation

$$\rho_{\vec{r}}(t + dt) - \rho_{\vec{r}}(t) = dt \sum_{\vec{\nu}} \left( \vec{j}_{\vec{r}-\vec{\nu}}(t) - \vec{j}_{\vec{r}}(t) \right) \cdot \vec{\nu},$$

$$\vec{j}_{\vec{r}}(t) dt = \sum_{\vec{\nu}} \left[ \rho_{\vec{r}}(1 - \rho_{\vec{r}+\vec{\nu}}) \xi_{\vec{r},\vec{\nu}}(t) - \rho_{\vec{r}+\vec{\nu}}(1 - \rho_{\vec{r}}) \xi_{\vec{r}+\vec{\nu},-\vec{\nu}}(t) \right] \vec{\nu},$$



equivalent to the M.E. if Poissonian noise is  $\xi_{\vec{r},\vec{\mu}}(t) = \begin{cases} 1 & \text{prob. } \gamma dt, \\ 0 & \text{prob. } 1 - \gamma dt. \end{cases}$

Usual **MSR** machinery gives

$$\langle e^{\lambda Q_T} \rangle = \int \mathcal{D}\theta_{\vec{r}} \mathcal{D}\vec{\varphi}_{\vec{r}} e^{-S[\rho_{\vec{r}}, \vec{j}_{\vec{r}}, \theta_{\vec{r}}, \vec{\varphi}_{\vec{r}}] + \lambda Q_T} \longrightarrow Q_T = \int_0^T dt \left( \vec{j}_{\vec{r}=\vec{0}}(t) \right)_1$$

# Microscopic path-integral representation

- Saddle-point eqs are **difference equations** for  $\rho_{\vec{r}}, \vec{j}_{\vec{r}}, \theta_{\vec{r}}, \vec{\varphi}_{\vec{r}}$ , to be solved order by order, e.g.

$$\vec{j}_{\vec{r}} = \vec{j}_{\vec{r}}^{(0)} + \lambda \vec{j}_{\vec{r}}^{(1)} + \dots \qquad \langle e^{\lambda Q_T} \rangle = \int \mathcal{D}\theta_{\vec{r}} \mathcal{D}\vec{\varphi}_{\vec{r}} e^{-S[\rho_{\vec{r}}, \vec{j}_{\vec{r}}, \theta_{\vec{r}}, \vec{\varphi}_{\vec{r}}] + \lambda Q_T}$$

- Turn out to relax to a **stationary** limit,

$$\mathcal{S} = \int_0^T dt \mathcal{L}[\{\rho, \vec{j}, \theta, \vec{\varphi}\}] \simeq T \mathcal{L}[\{\rho^*, \vec{j}^*, \theta^*, \vec{\varphi}^*\}]$$

- Can be used to recover

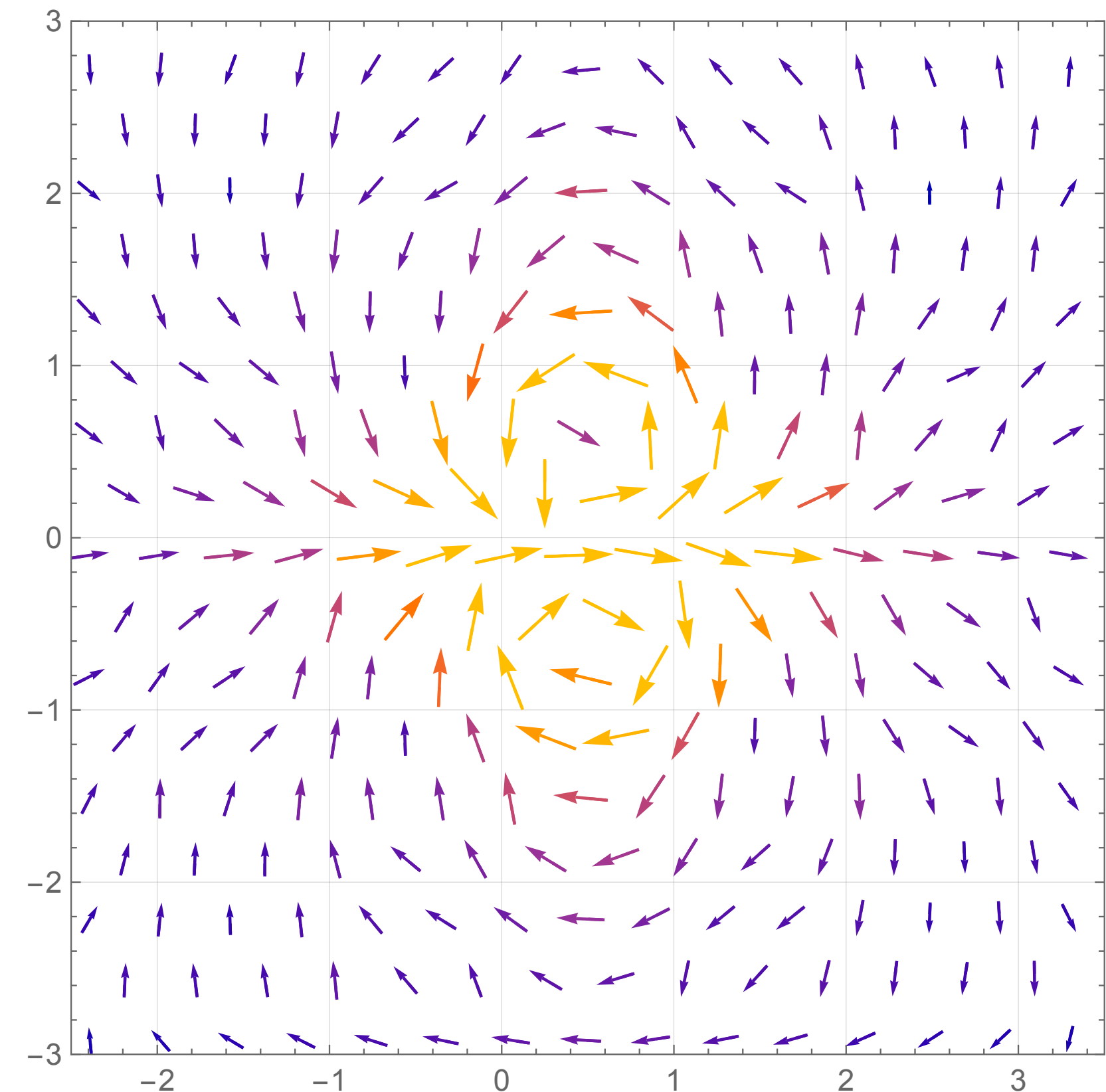
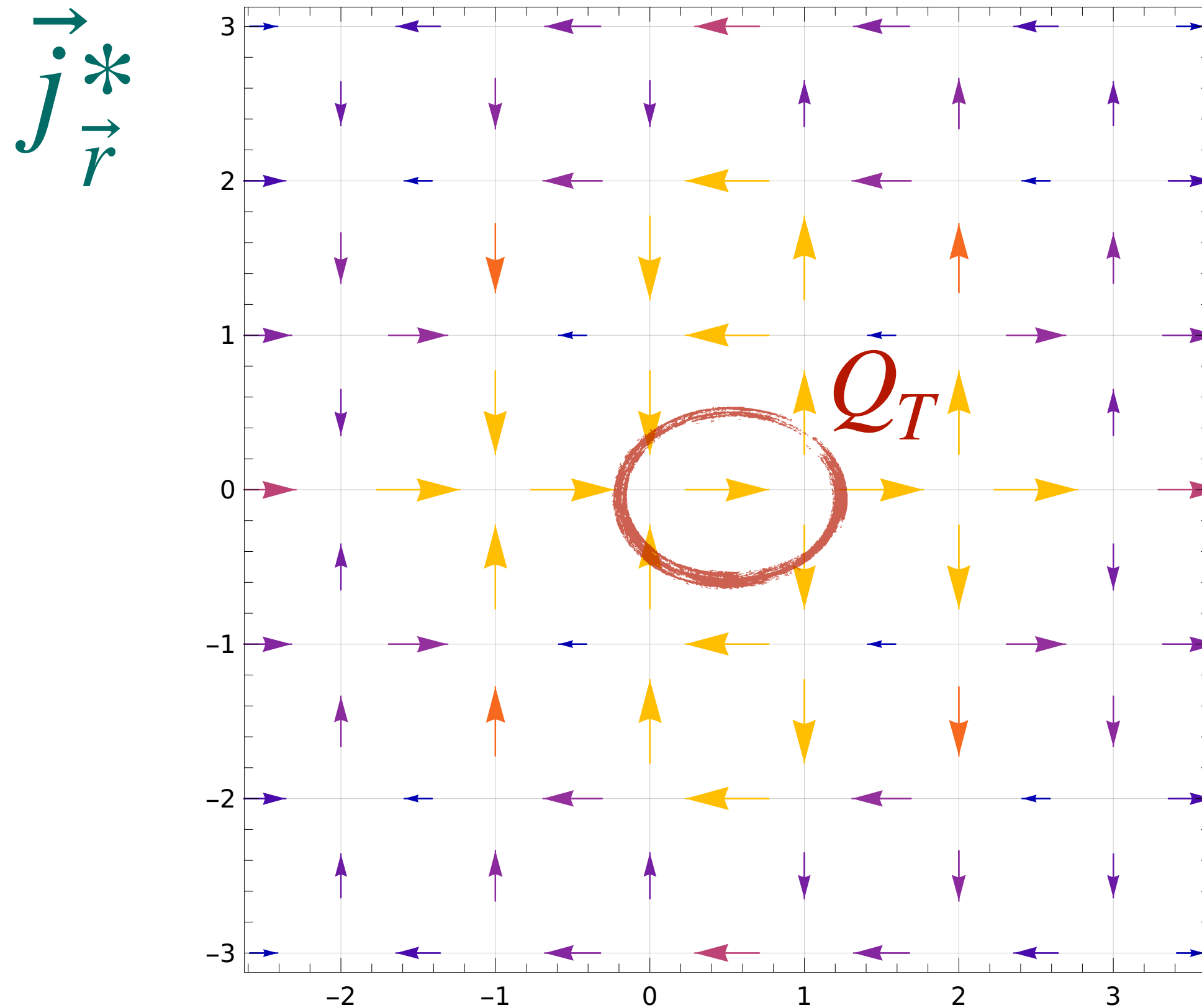
$$\langle e^{\lambda Q_T} \rangle \simeq \exp\{-T[\mathcal{L}^* - \lambda(\vec{j}_{\vec{r}=\vec{0}}^*)_1]\} \quad \longrightarrow \quad \langle Q_t^2 \rangle = 2\gamma \left(1 - \frac{1}{d}\right) \bar{\rho}(1 - \bar{\rho}) t$$

$$\text{correlation profile} \longrightarrow \langle \rho_{\vec{r}}(t) e^{\lambda Q_T} \rangle / \langle e^{\lambda Q_T} \rangle \simeq \rho_{\vec{r}}^*(t) \longleftarrow \text{optimal profile}$$



# Role of loops

$$\frac{\langle \vec{j}_{\vec{r}}(t) e^{\lambda Q_T} \rangle}{\langle e^{\lambda Q_T} \rangle} \simeq \vec{j}_{\vec{r}}^*(t) \longrightarrow \langle \vec{j}_{\vec{r}}(t) Q_T \rangle$$



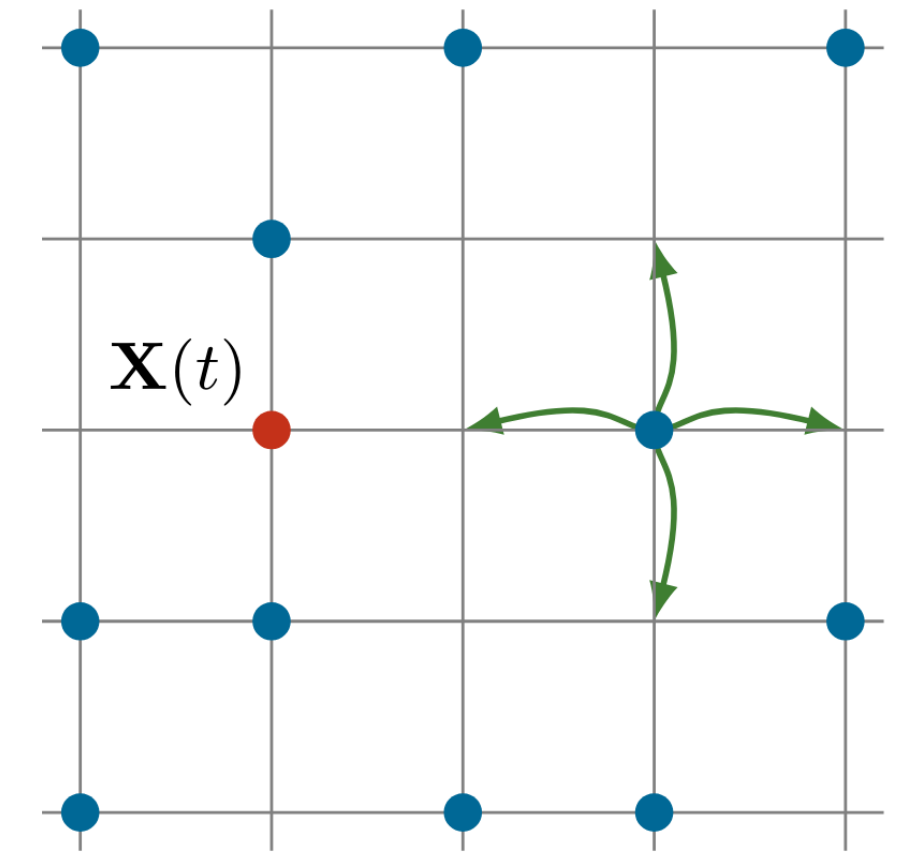
**looped** structure of the lattice allows for **vortex** configurations, and thus for  $\langle Q_t^2 \rangle \propto t$



## **2. Tracer-bath correlations**

# Hard-core lattice gas

in  $d$  dimensions:  $\langle X_t \rho_{X+r}(t) \rangle$



Using the ME, write an equation for  $g_r(t) = \langle X_t \rho_{X+r}(t) \rangle \rightarrow$  **not closed!**

$\partial_t g_r(t) = (\dots)$  can be closed upon **decoupling** (exact for large/small  $\bar{\rho}$ )

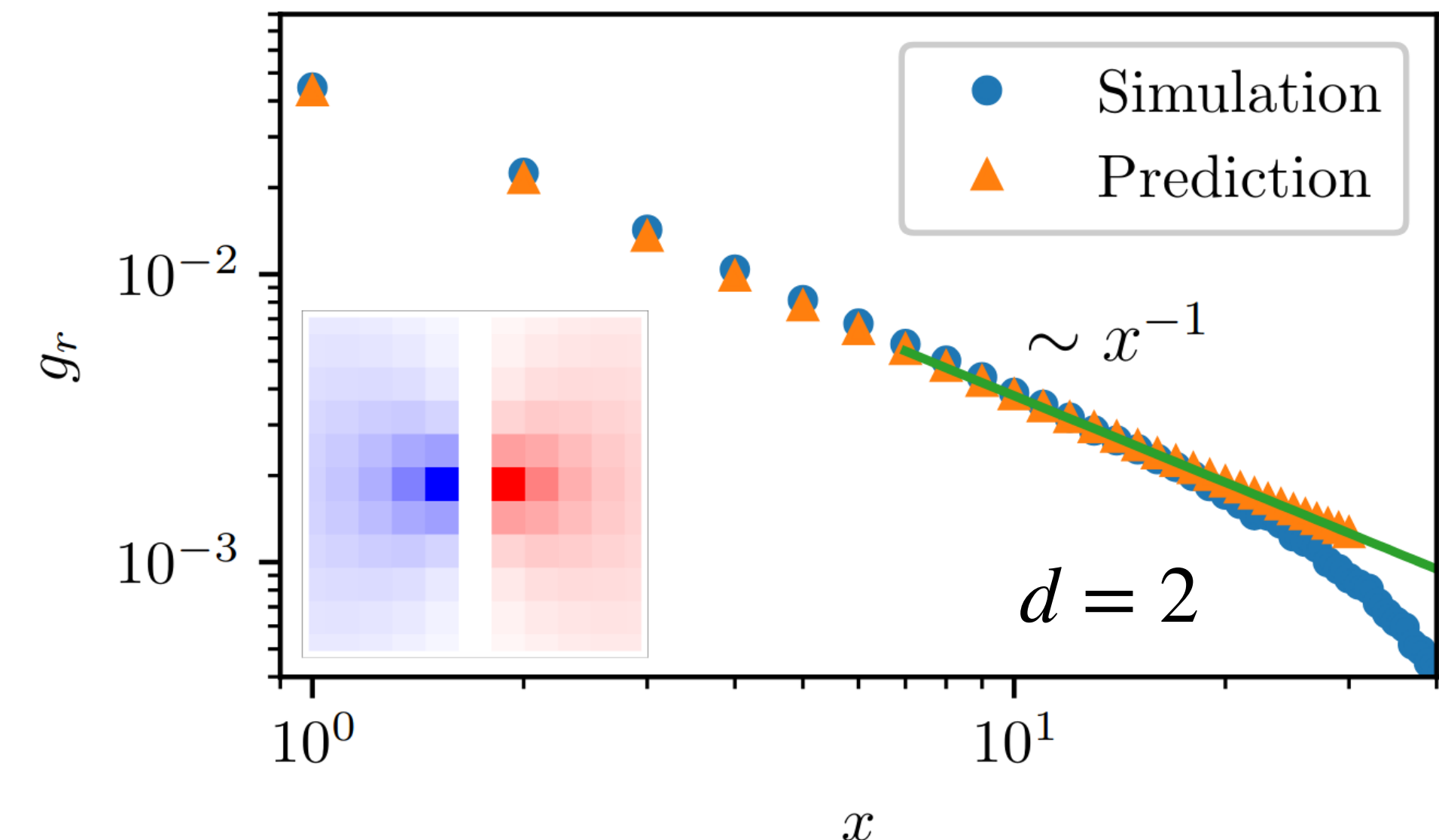
$$\langle \rho_{X+r} \rho_{X+r'} \rangle \simeq \langle \rho_{X+r} \rangle \langle \rho_{X+r'} \rangle$$

$$\langle X_t \rho_{X+r} \rho_{X+r'} \rangle \simeq \langle X_t \rho_{X+r} \rangle \langle \rho_{X+r'} \rangle + \langle X_t \rho_{X+r'} \rangle \langle \rho_{X+r} \rangle$$

Solve for  $g_r(t) \rightarrow g_r$  at long  $t$ . For large  $x = \mathbf{r} \cdot \hat{\mathbf{e}}_1$ ,

$$g_x \sim x^{1-d}$$

**Q:** is this specific to SEP?



Bénichou, Illien, Oshanin, Sarracino, Voituriez, Phys. Rev. Lett. **115**, 220601 (2015)

D. Venturelli, P. Illien, A. Grabsch, O. Bénichou, arXiv:2411.09326 (to appear in Phys. Rev. Lett.)

# Interacting Brownian particles

$$\dot{\mathbf{X}}_i(t) = -\mu \sum_{j \neq i} \nabla_i U(\mathbf{X}_i(t) - \mathbf{X}_j(t)) + \boldsymbol{\eta}_i(t),$$

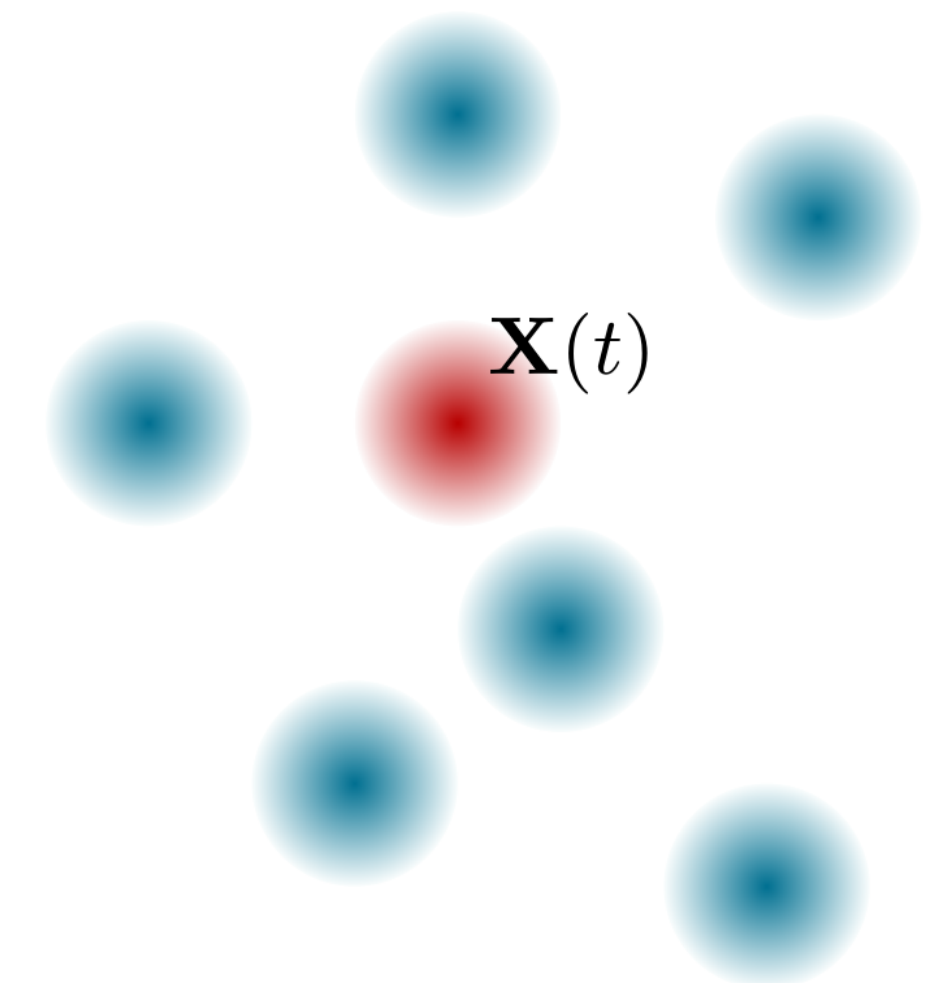
$$\langle \boldsymbol{\eta}_i(t)^T \boldsymbol{\eta}_j(t') \rangle = 2\mu T \delta_{ij} \delta(t - t') I_d$$

📌 **Tracer**  $i = 0$  (omitted)

📌 Dean-Kawasaki equation for  $\rho(\mathbf{r}, t) = \sum_{i=1}^N \delta(\mathbf{r} - \mathbf{X}_i(t))$ ,

$$\begin{aligned} \partial_t \mathbf{X}(t) &= -\mu \nabla_{\mathbf{X}} \mathcal{F}[\rho, \mathbf{X}] + \boldsymbol{\eta}_0(t), \\ \partial_t \rho(\mathbf{r}, t) &= \mu \nabla \cdot \left[ \rho(\mathbf{r}, t) \nabla \frac{\delta \mathcal{F}}{\delta \rho(\mathbf{r}, t)} \right] + \nabla \cdot \left[ \rho^{\frac{1}{2}}(\mathbf{r}, t) \boldsymbol{\xi}(\mathbf{r}, t) \right], \end{aligned}$$

$$\mathcal{F}[\rho, \mathbf{X}] = T \int d\mathbf{x} \rho(\mathbf{x}) \log\left(\frac{\rho(\mathbf{x})}{\rho_0}\right) + \frac{1}{2} \int d\mathbf{x} d\mathbf{y} \rho(\mathbf{x}) U(\mathbf{x} - \mathbf{y}) \rho(\mathbf{y}) + \int d\mathbf{y} \rho(\mathbf{y}) U(\mathbf{y} - \mathbf{X})$$





# Tracer statistics

## from tracer-bath profiles

hard-core lattice gas

$$\partial_t \Psi(\lambda, t) = \frac{1}{2d\tau} \sum_{\mu=-d}^d \left( e^{\sigma \lambda \cdot \hat{\mathbf{e}}_\mu} - 1 \right) \left[ 1 - w_{\mathbf{e}_\mu}(\lambda, t) \right]$$

How does  $\Psi(\lambda, t) = \ln \langle e^{\lambda \cdot \mathbf{X}(t)} \rangle$  evolve?

$$\partial_t \Psi(\lambda, t) = \lambda^2 \mu T + \mu \lambda \cdot \int d^d r U(\mathbf{r}) \nabla_{\mathbf{r}} w(\mathbf{r}, \lambda, t),$$

with the profile

$$w(\mathbf{r}, \lambda, t) = \frac{\langle \rho(\mathbf{r} + \mathbf{X}(t), t) e^{\lambda \cdot \mathbf{X}(t)} \rangle}{\langle e^{\lambda \cdot \mathbf{X}(t)} \rangle} = \langle \rho(\mathbf{r} + \mathbf{X}(t), t) \rangle + \lambda \cdot \langle \mathbf{X}(t) \rho(\mathbf{r} + \mathbf{X}(t), t) \rangle + \mathcal{O}(\lambda^2)$$

average bath density profile

tracer-bath correlation profile

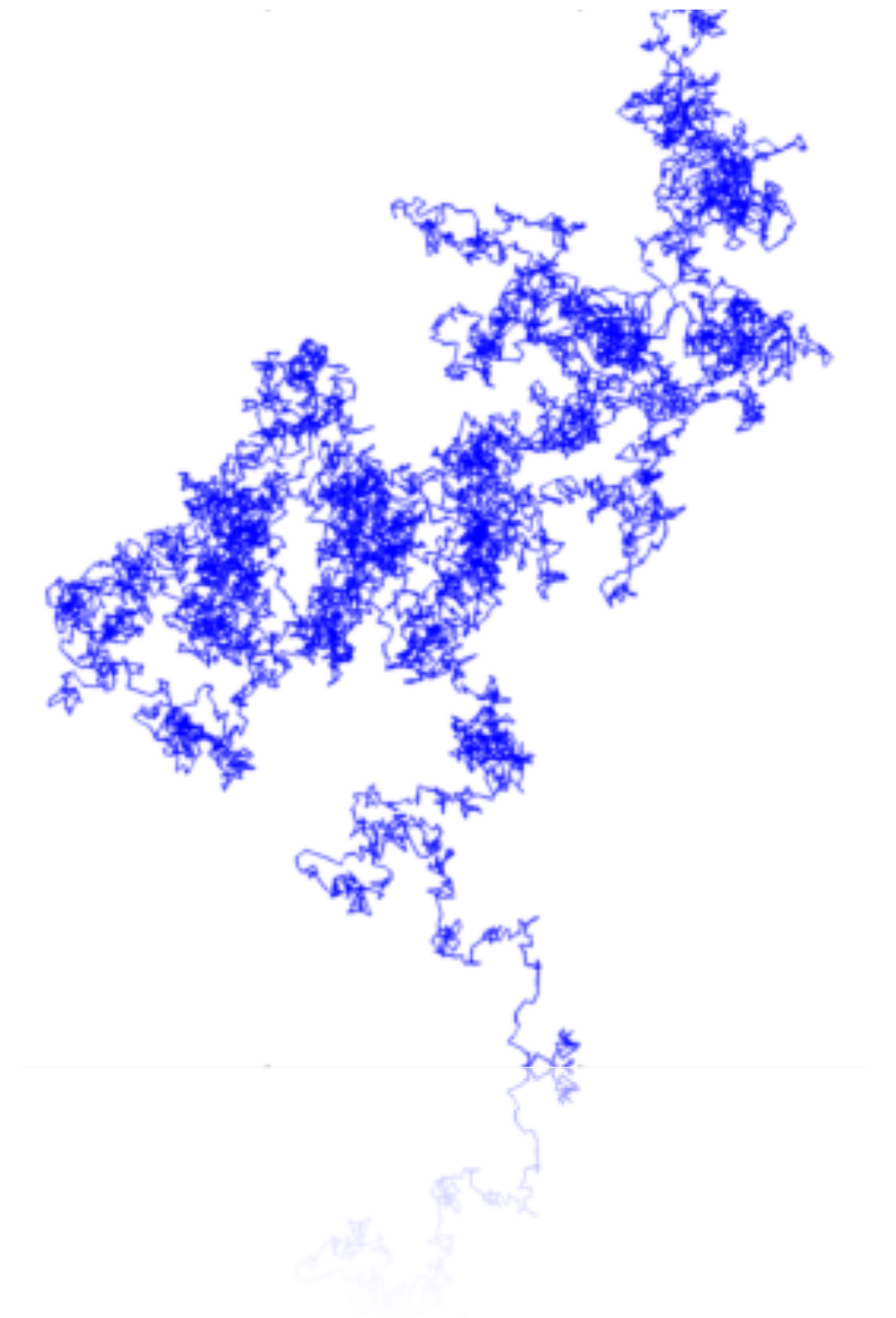
# Beware of zero modes

- For simple liquids, stationary quantities are computed as

$$\langle \mathbf{X} \rho(\mathbf{x} + \mathbf{X}) \rangle \propto \int \mathcal{D}\rho \int d\mathbf{X} e^{-\frac{1}{T} \mathcal{F}[\rho, \mathbf{X}]} [\mathbf{X} \rho(\mathbf{x} + \mathbf{X})] = 0$$

upon defining  $\rho'(\mathbf{x}) = \rho(\mathbf{x} + \mathbf{X})$ .

- Thermodynamic quantities only depend on  $|\mathbf{X}_i - \mathbf{X}_j|$ ,  
whereas  $[\mathbf{X} \rho(\mathbf{x} + \mathbf{X})]$  depends also on **COM**
- Trivial zero! → Need to use EOM to predict stationary profiles.





# Stationary tracer-bath profile $\langle X \rho_{X+r} \rangle$

📌  $\rho(\mathbf{r}, t) = \rho_0 + \sqrt{\rho_0} \phi(\mathbf{r}, t) \rightarrow$  linearize the DK eqs assuming  $\phi/\sqrt{\rho_0} \ll 1$

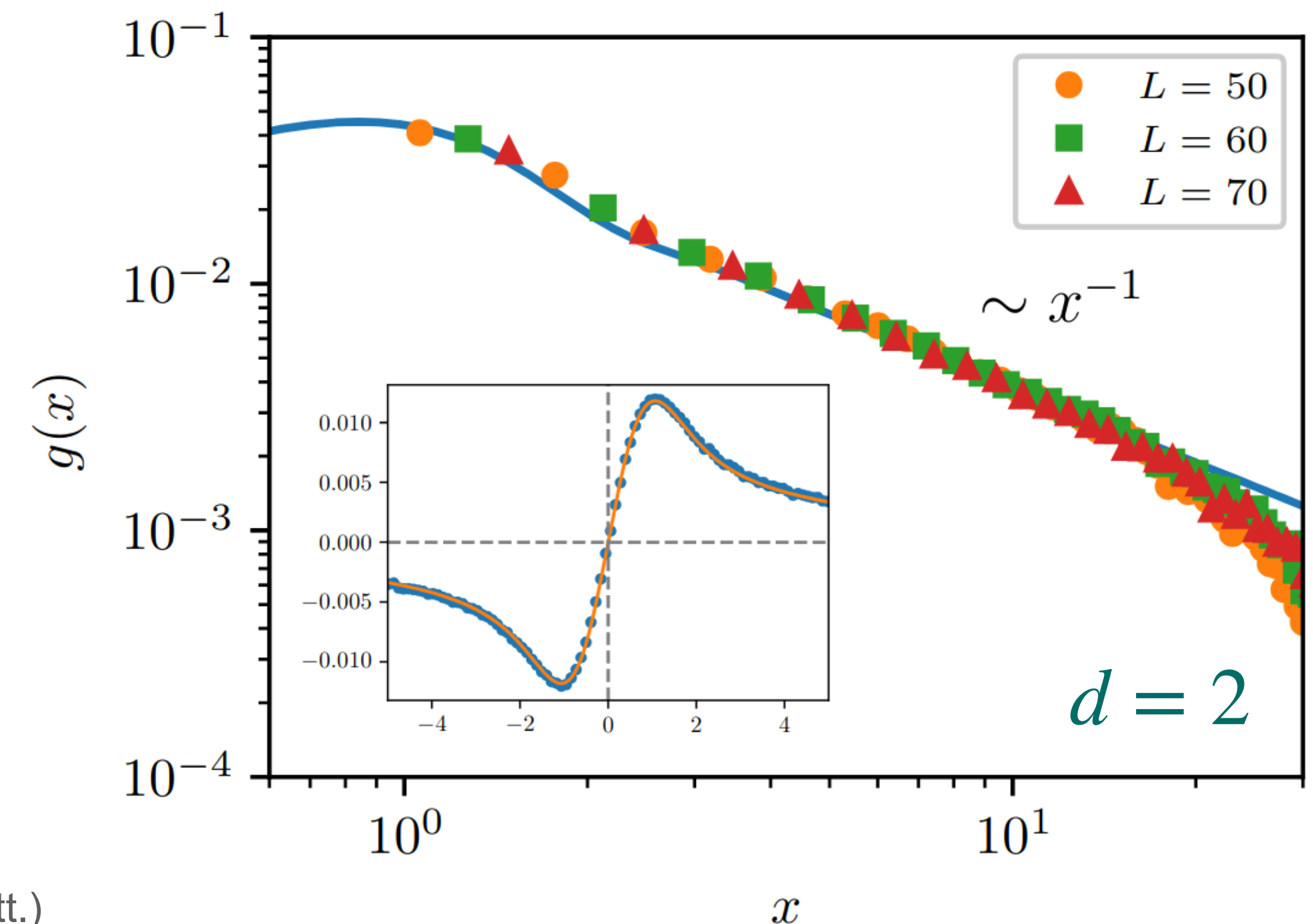
📌 From coupled eqs for  $\partial_t \mathbf{X}(t)$  and  $\partial_t \phi(\mathbf{r}, t)$ , write one for

$$g(\mathbf{r}, t) = \hat{\mathbf{e}}_1 \cdot \langle \mathbf{X}(t) \rho(\mathbf{r} + \mathbf{X}(t), t) \rangle$$

📌 Solve for  $g(\mathbf{r})$  perturbatively, in the stationary limit

📌 At large distance  $x = \mathbf{r} \cdot \hat{\mathbf{e}}_1$ ,

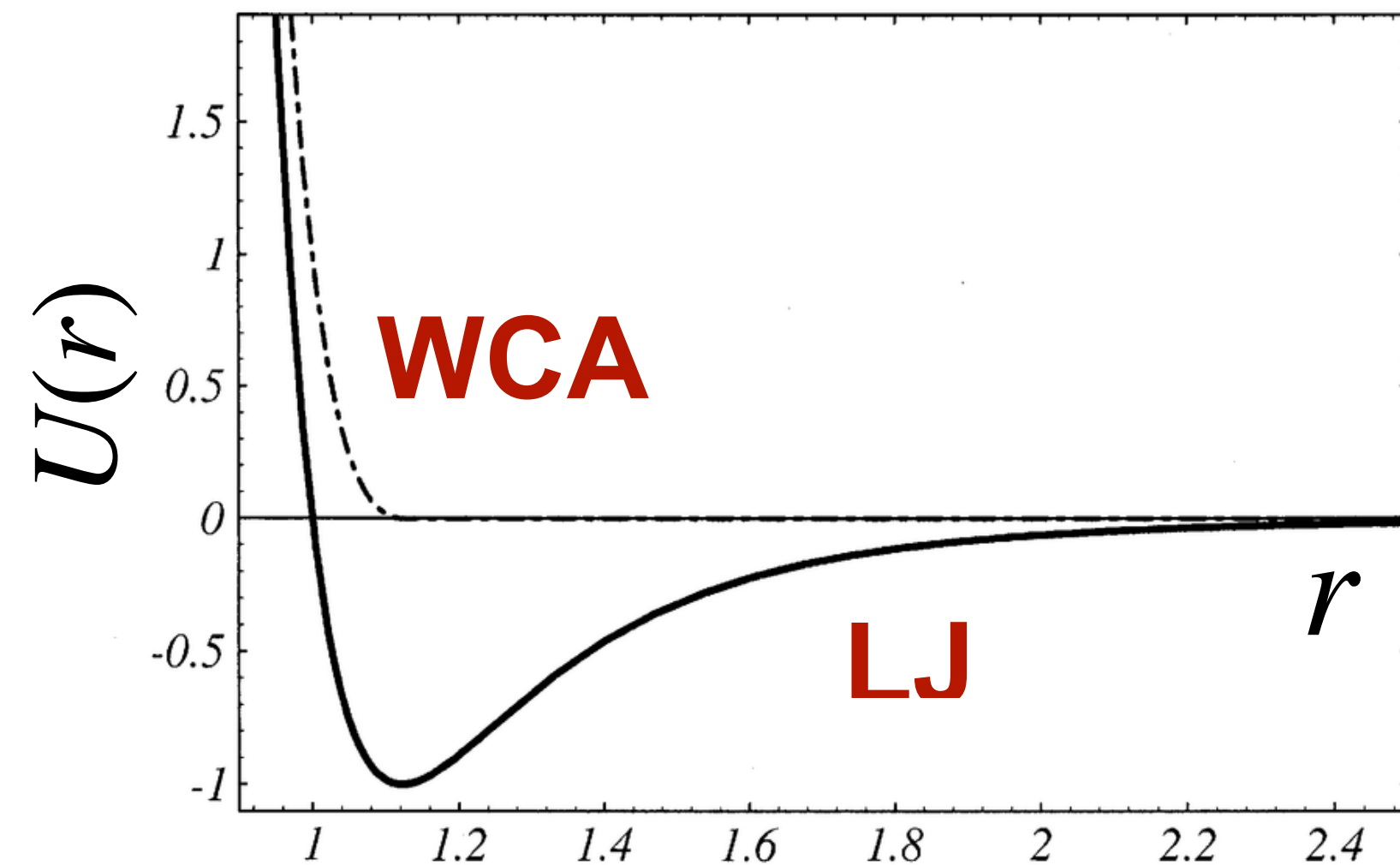
$$\underline{g(x) \sim x^{1-d}}$$



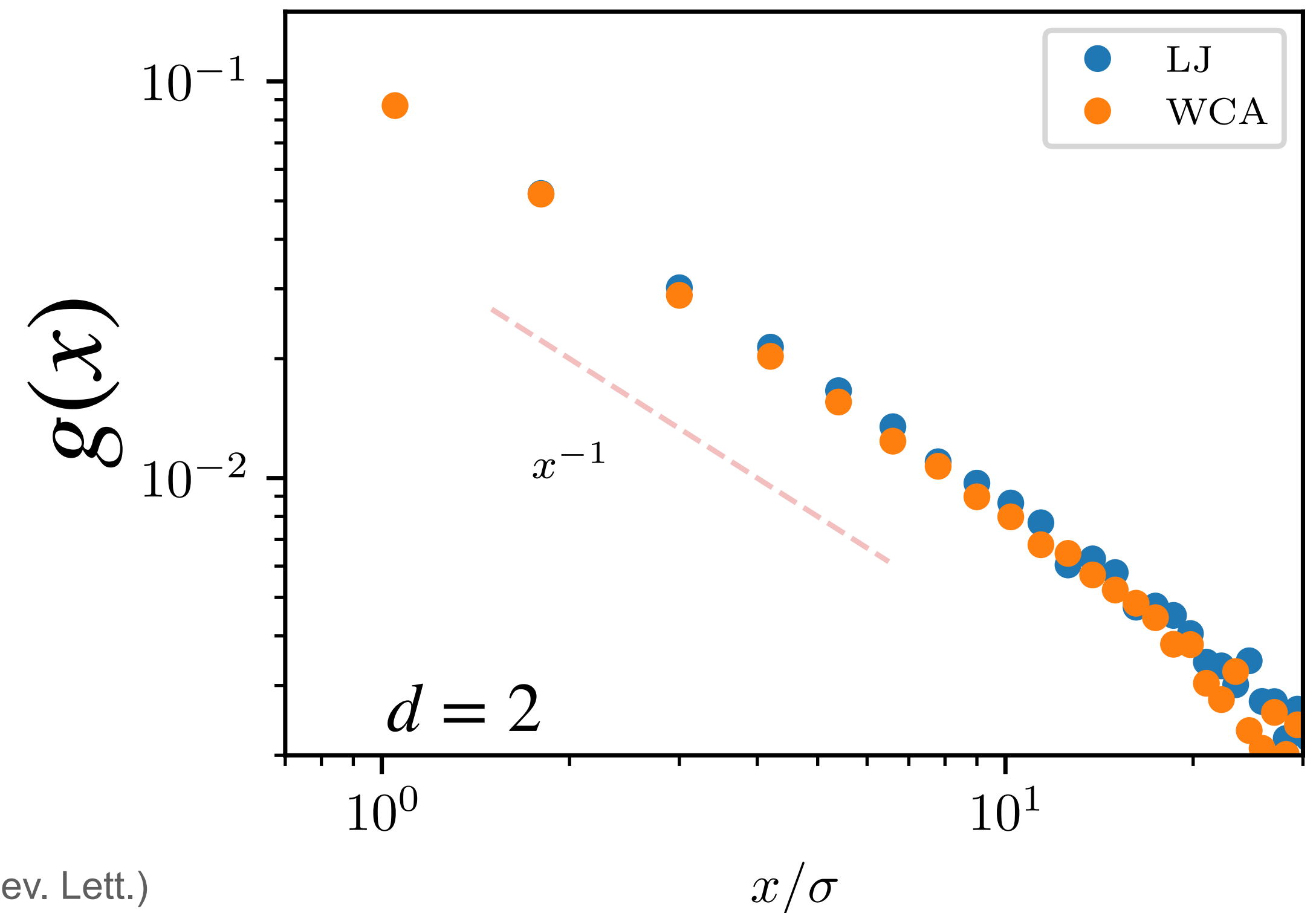
# Lennard-Jones fluids

## stationary tracer-bath profile

- Strong **repulsion** beyond linearised D-K theory
- Simulate** LJ and WCA suspensions



*Short-distance details of interactions irrelevant for large-distance behaviour of the bath response?*



# Average density profile under steady driving

📌 Stationary density profile in the frame of the tracer,

$$\varphi(\mathbf{x}, t) = \langle \rho(\mathbf{x} + \mathbf{X}(t), t) \rangle$$

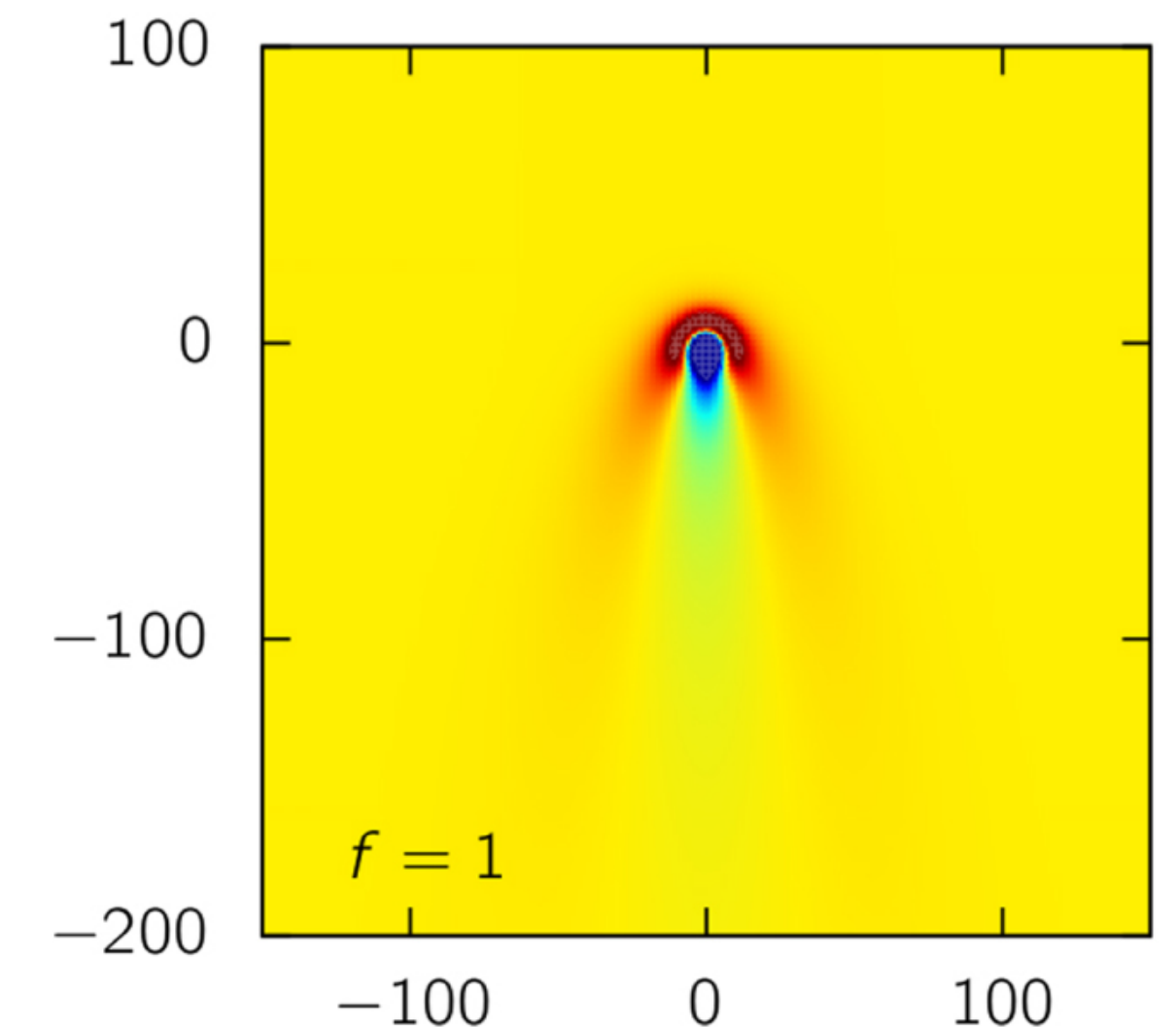
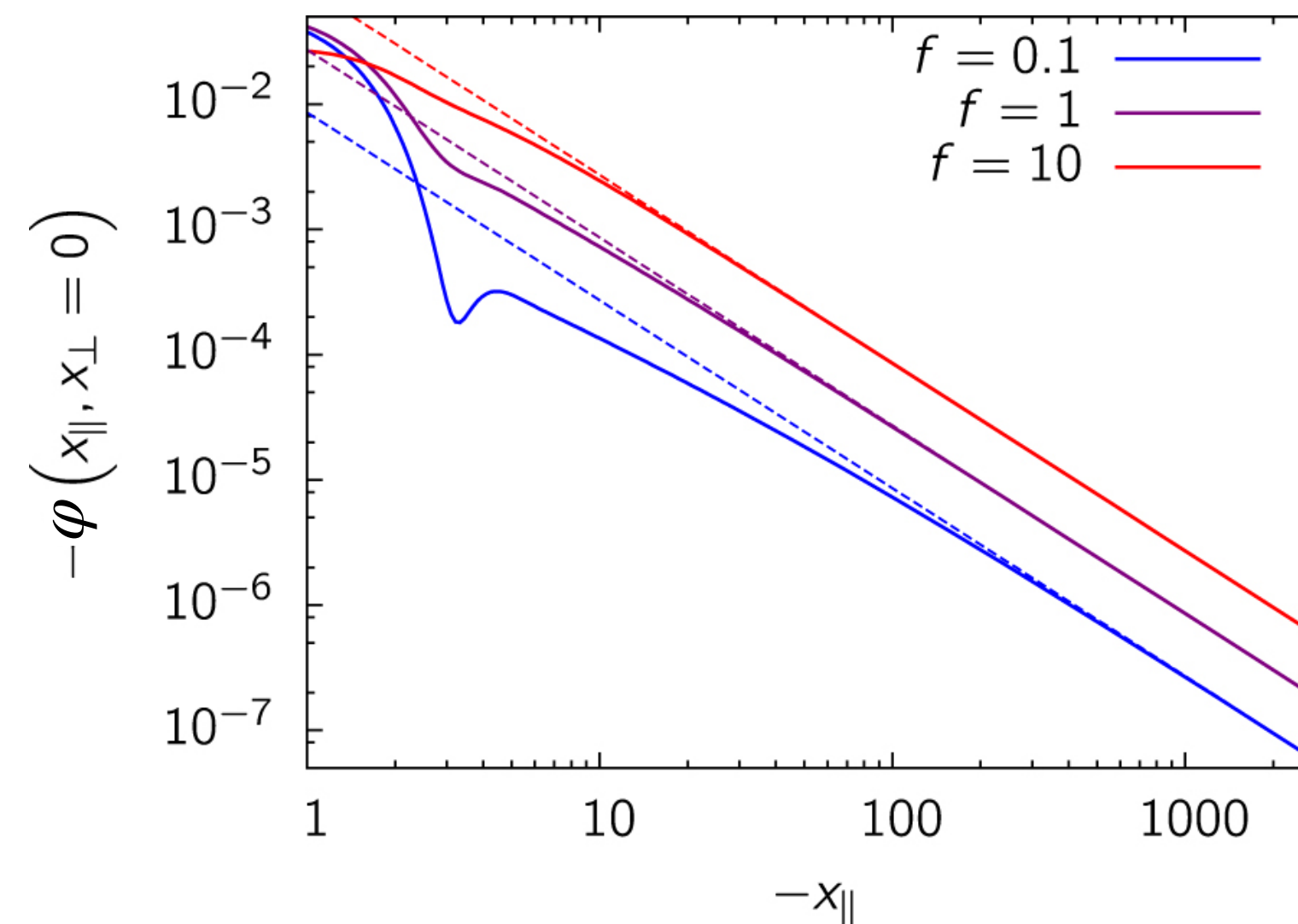
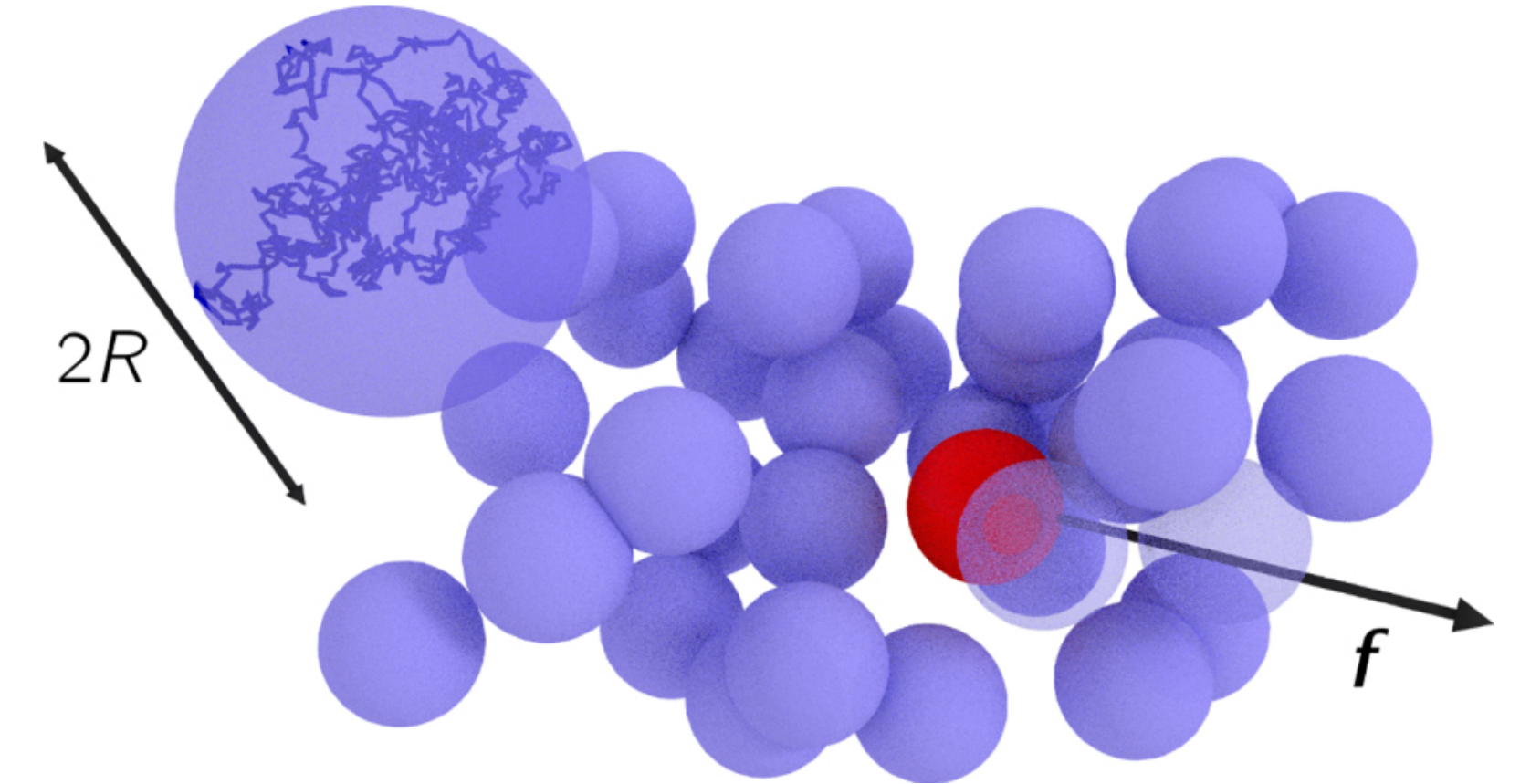
📌 For  $x_{||} \rightarrow -\infty$ ,

$$\varphi(x_{||}, \mathbf{x}_{\perp} = \mathbf{0}) \sim -|x_{||}|^{-\frac{1+d}{2}}$$

both for discrete and continuum

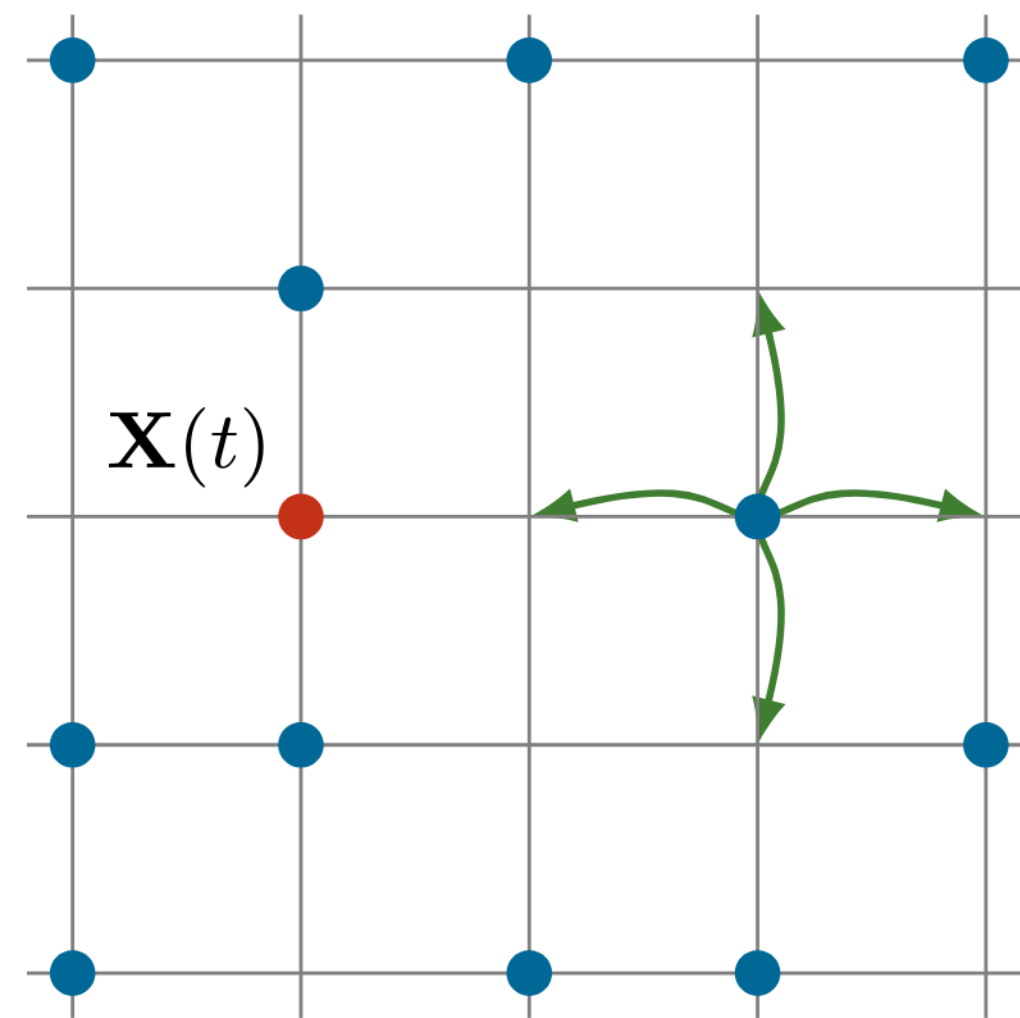
V. Démery et al., New J. Phys. **16** (2014) 053032

O. Bénichou et al., Phys. Rev. Lett. **84**, 511 (2000)





# A common language for diffusive systems?

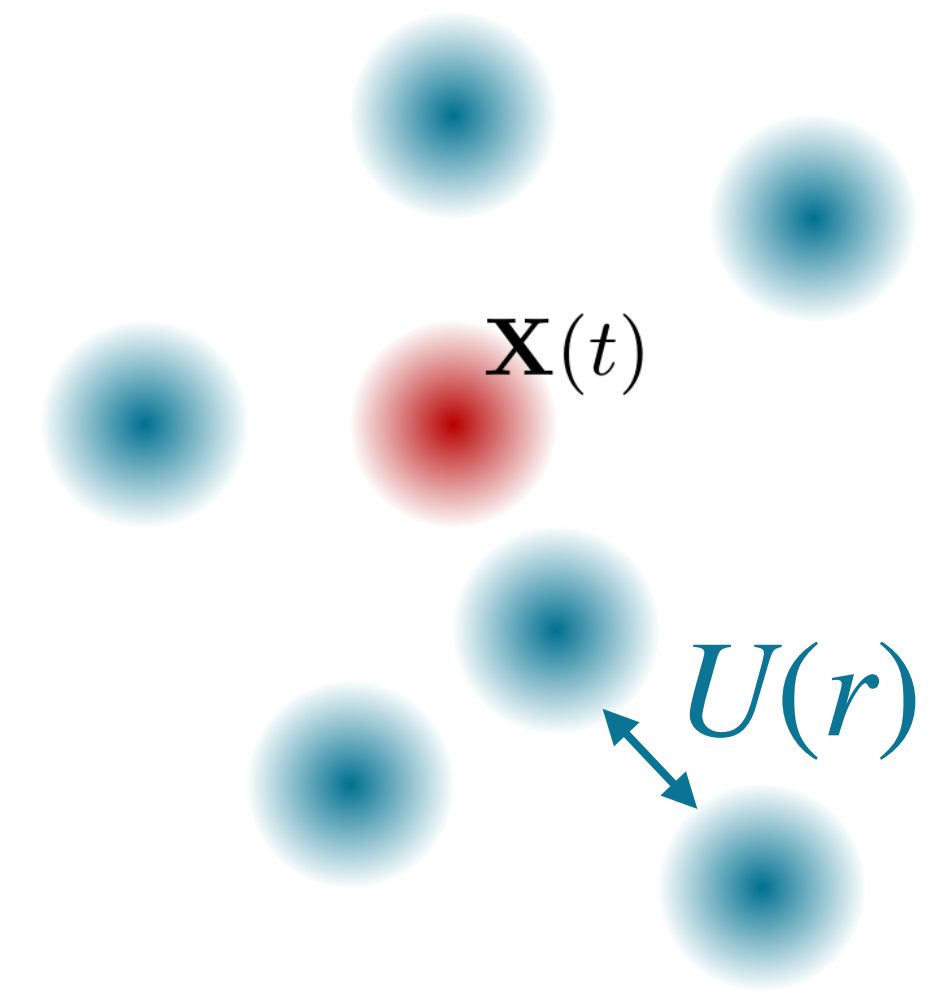


master equation

large-distance behaviour  
of tracer-bath correlations

$$\langle X \rho_{X+r} \rangle_c$$

??



Dean-Kawasaki theory

# Macroscopic fluctuation theory for interacting Brownian particles

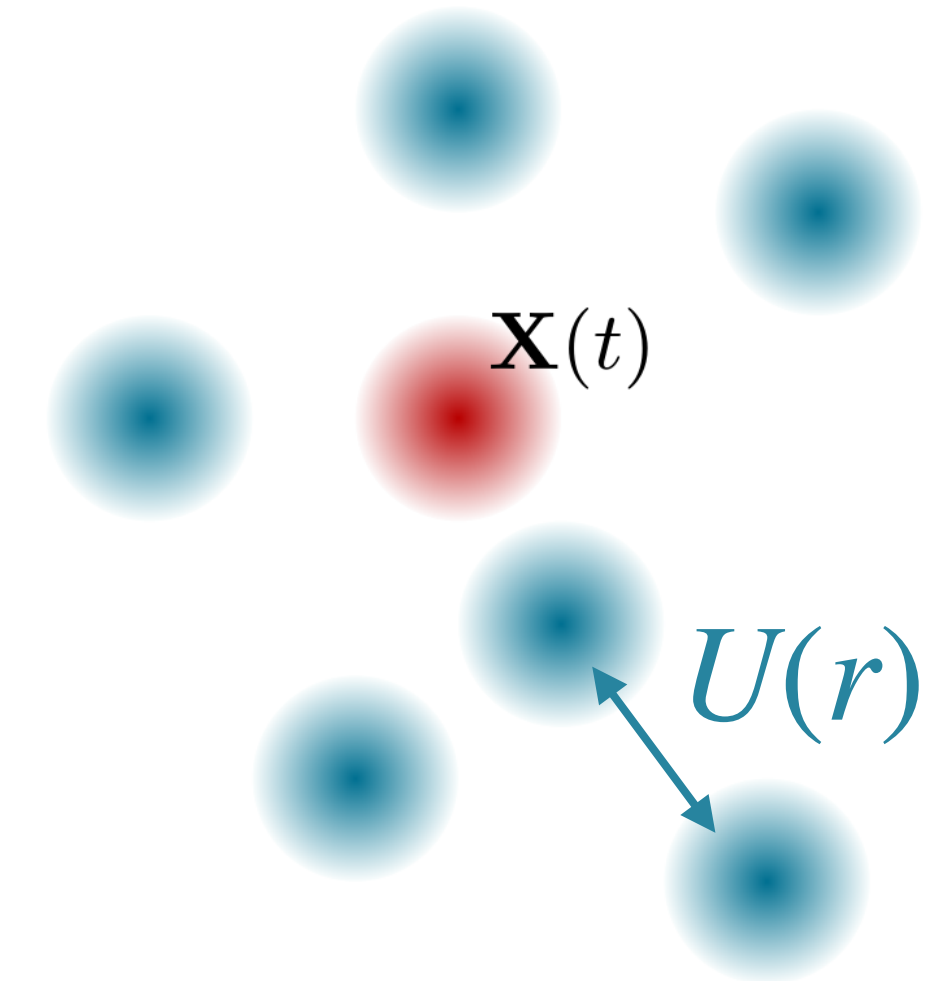
$$\partial_t \rho(x, t) = \partial_x [ \underset{\substack{\uparrow \\ \text{diffusion}}}{D(\rho)} \partial_x \rho + \underset{\substack{\uparrow \\ \text{mobility}}}{\sqrt{\sigma(\rho)}} \underset{\substack{\uparrow \\ \text{white Gaussian noise}}}{\eta(x, t)} ]$$

- 📌 Large-scale properties of **diffusive** systems
- 📌 **Example:**  $D(\rho) = 1$  and  $\sigma(\rho) = 2\rho(1 - \rho)$  for SEP

(1) Who are  $D(\rho)$  and  $\sigma(\rho)$  for generic  $U(r)$ ?

$$\sigma(\rho) = 2\mu k_B T \rho, \quad D(\rho) = \mu \partial_\rho P(\rho)$$

equilibrium pressure,  
conceptually solved problem  
(e.g. virial expansion)

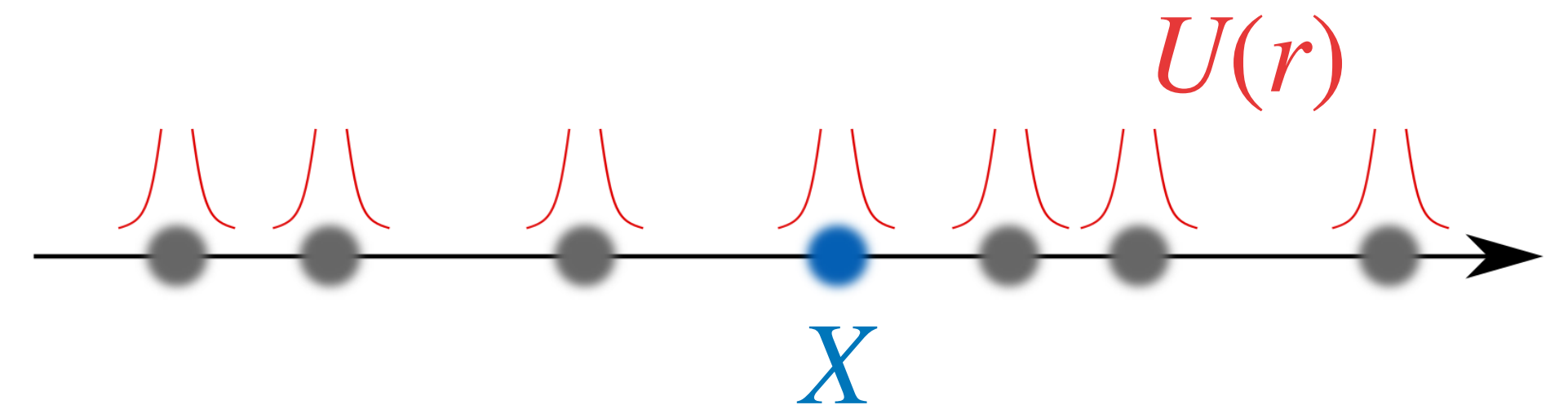




# Macroscopic fluctuation theory

## for interacting Brownian particles

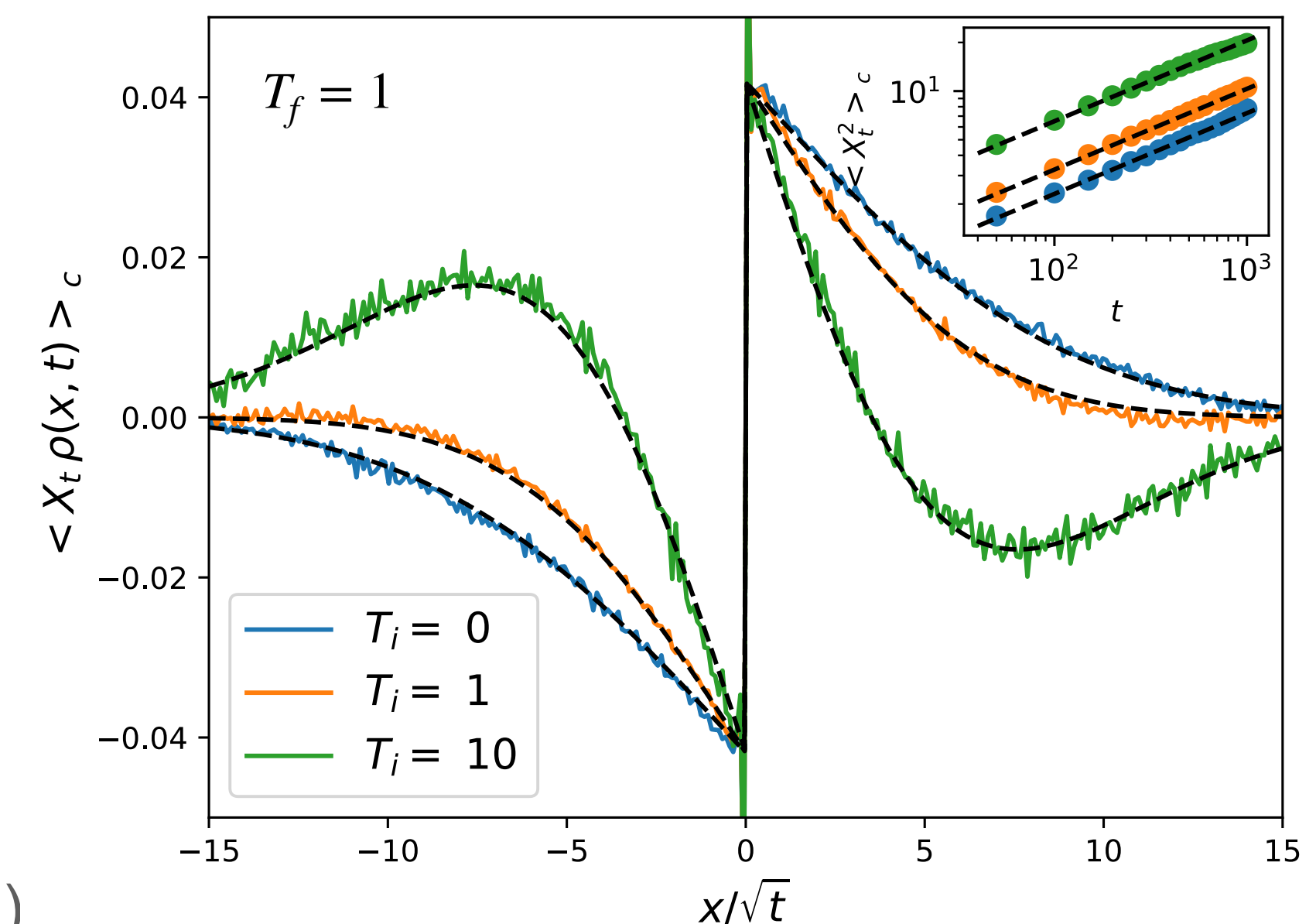
$$\partial_t \rho(x, t) = \partial_x [D(\rho) \partial_x \rho + \sqrt{\sigma(\rho)} \eta(x, t)]$$



### (2) Tracer-bath correlation profiles?

- In **single-file** systems,  $X = X[\rho]$  (conservation # of particles)
- $\langle X \rho(X + x) \rangle$  from large-deviations approach
- Even after a temperature quench

**Open problem:** how do we couple  $X$  and  $\rho$  in  $d > 1$  ?



# To sum up

## Spatial correlation profiles are worth checking out!

- ☒  $\langle Q_t^n \rho_r(t) \rangle$  give info on **response** of the bath in interacting particle systems (e.g. role of **loops**),
- ☒ and give access to **moments** of the current  $Q_t$ , e.g.  $\langle Q_t^2 \rangle$  on infinite lattices in  $d > 1$ .
- ☒ Tracer-bath profiles  $\langle X_t^n \rho_{X+r}(t) \rangle$  encode the **response** of the bath and control tracer statistics
- ☒  $\langle X_t \rho_{X+r}(t) \rangle \sim r^{1-d}$  **universal** wrt short-range 2-body interaction type
- ☐ Captured by **macroscopic fluctuation theory**?

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arXiv:2411.09326 (to appear in Phys. Rev. Lett.)

arXiv:2504.08560 (to appear in Phys. Rev. Lett.)

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# ***Thanks!***



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