Interacting particles in $d > 1$ and on comb-like structures

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Fluctuations in small complex systems VII

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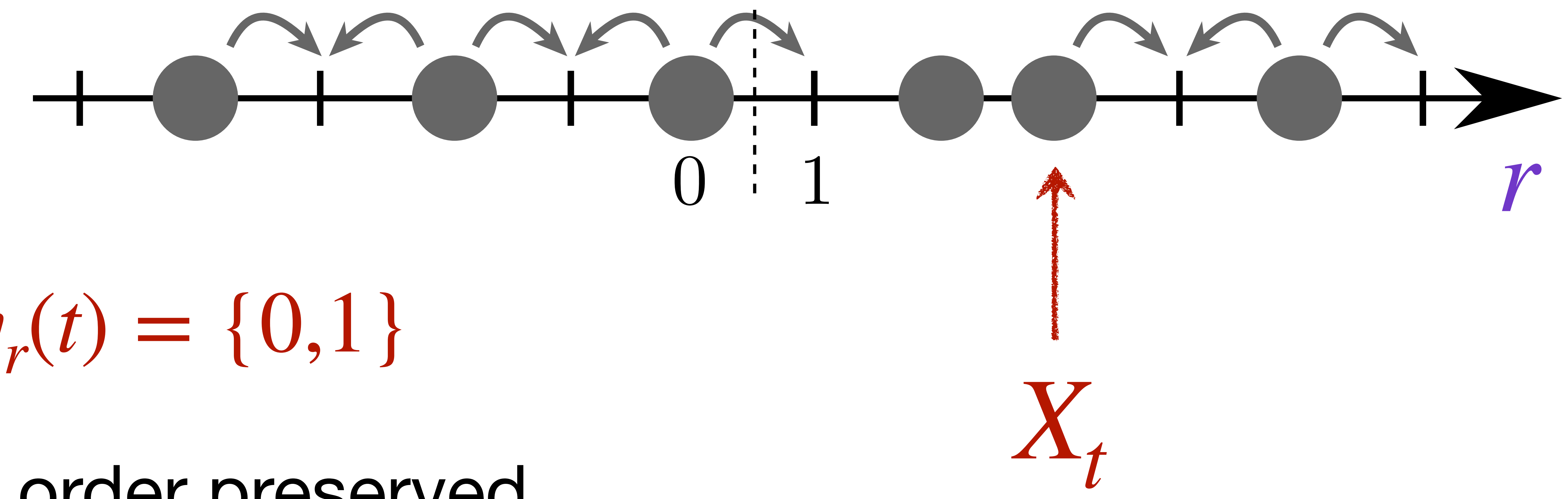
Work in collaboration with T. Berlioz, A. Grabsch, O. Bénichou

Symmetric Exclusion Process

as paradigmatic diffusive system

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



- **State of the system**: occupations $\eta_r(t) = \{0,1\}$

- 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)

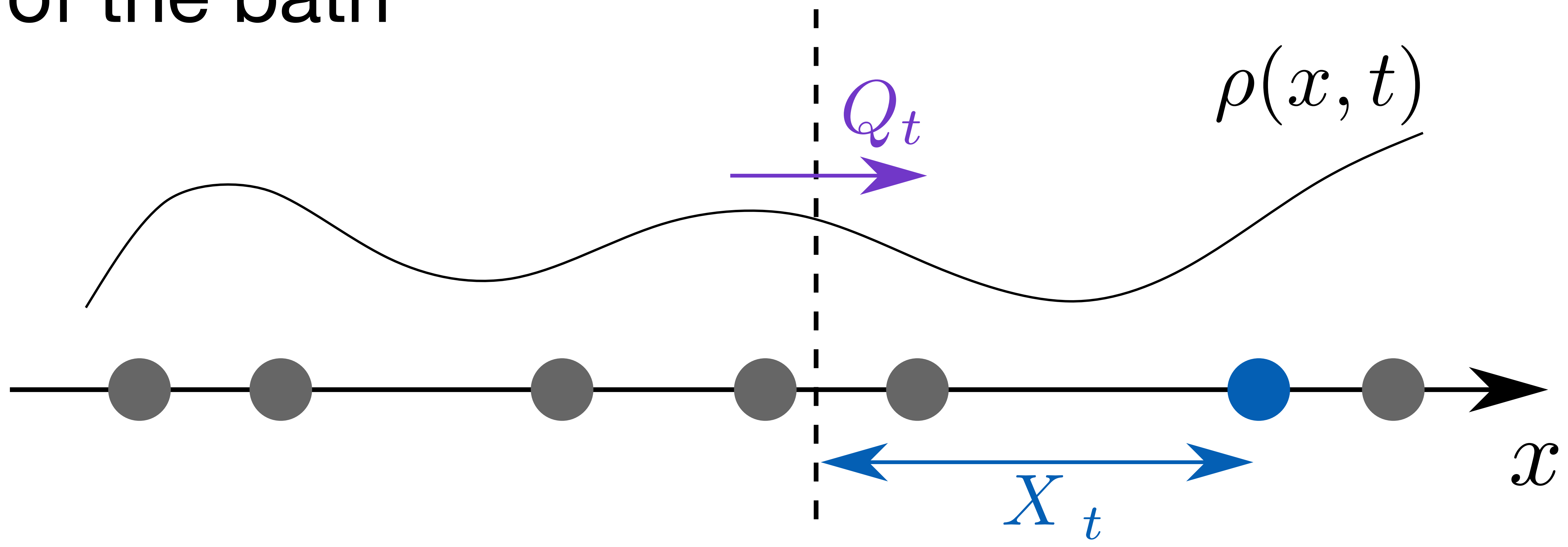
Hahn, Kärger, Kukla, Phys. Rev. Lett. **76** (15), 2762-2765 (1996)

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

Role of correlations

with surrounding bath

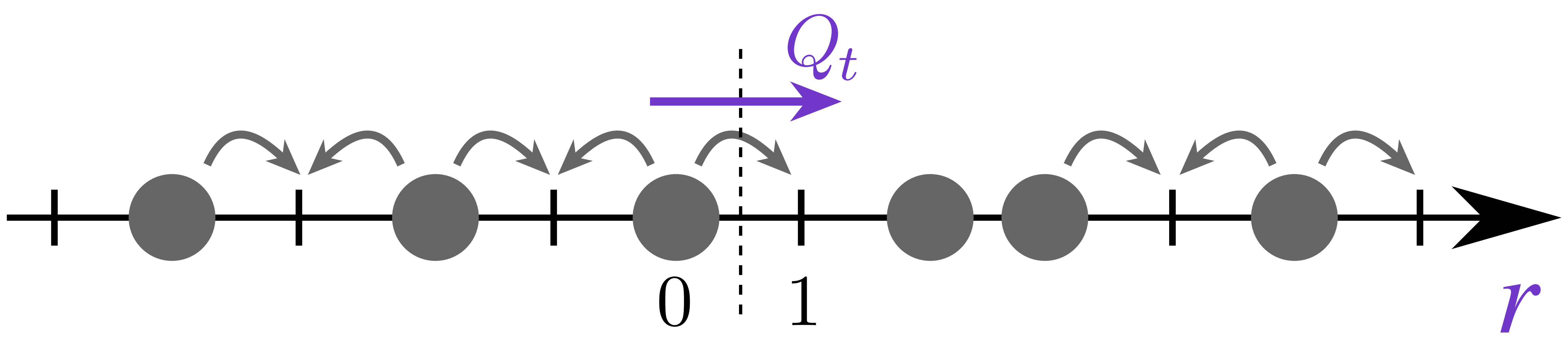
- Q_t = integrated current (net # of parts crossing 0—1), $\langle Q_t^2 \rangle \propto \sqrt{t}$
- A positive fluctuation of Q_t is correlated with an increase of $\eta_r(t)$ on its r.h.s.
  → correlations dictate the subdiffusive behavior of Q_t
- $\langle \eta_r(t)\, \mathrm{e}^{\lambda Q_t} \rangle$ encodes the response of the bath
- Fully understood in 1d SEP
- Open problem in $d > 1$



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

- As **first step**, focus on

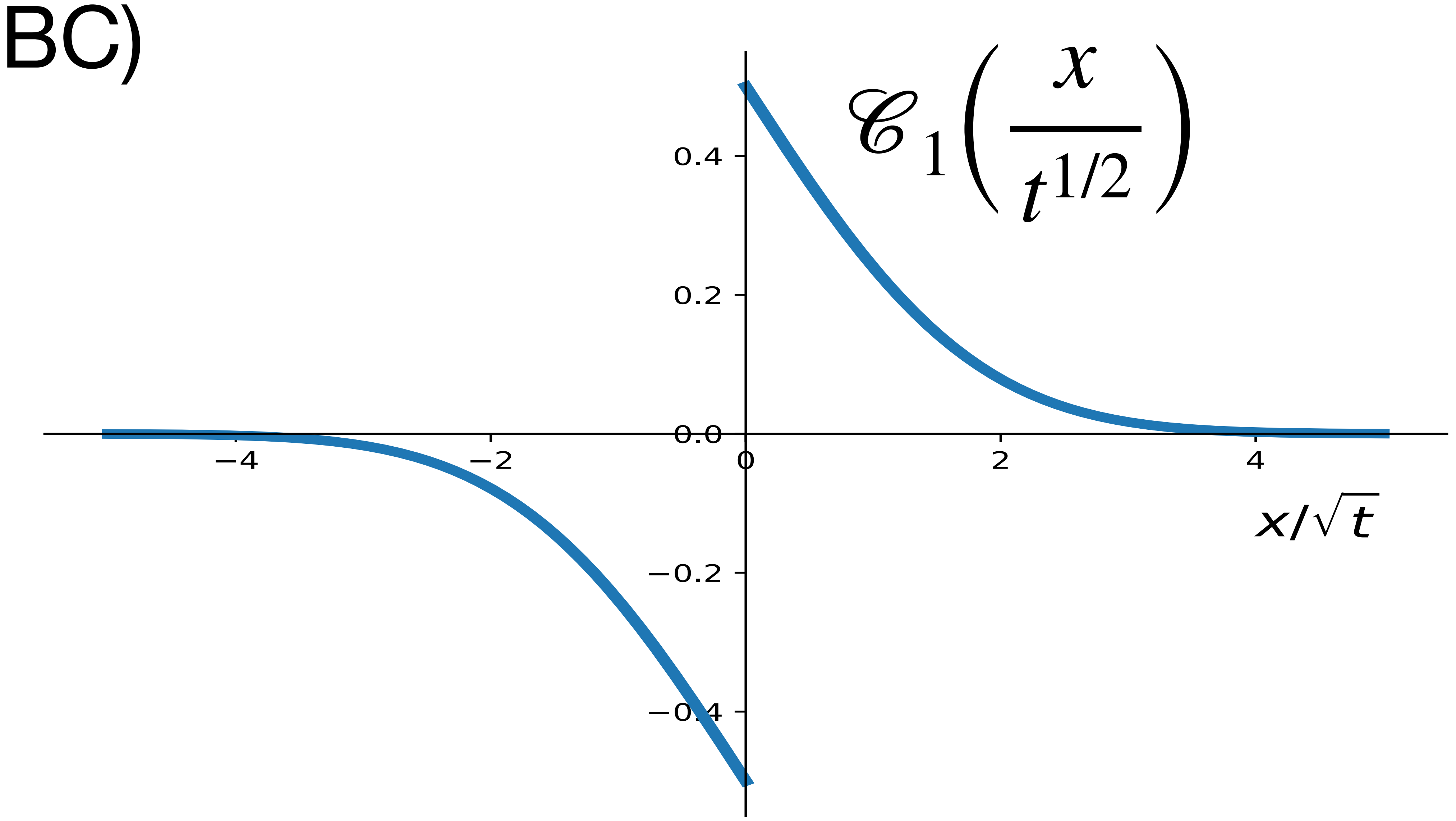
$$c_r(t) \equiv \langle Q_t \eta_r(t) \rangle$$



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

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

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



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

$$c_{\vec{r}}(t) \xrightarrow[t \to \infty]{} c_{\vec{r}}, \qquad \langle Q_t^2 \rangle \propto t$$

infinite lattices in $d > 1$?

From $d = 1$ to generic d

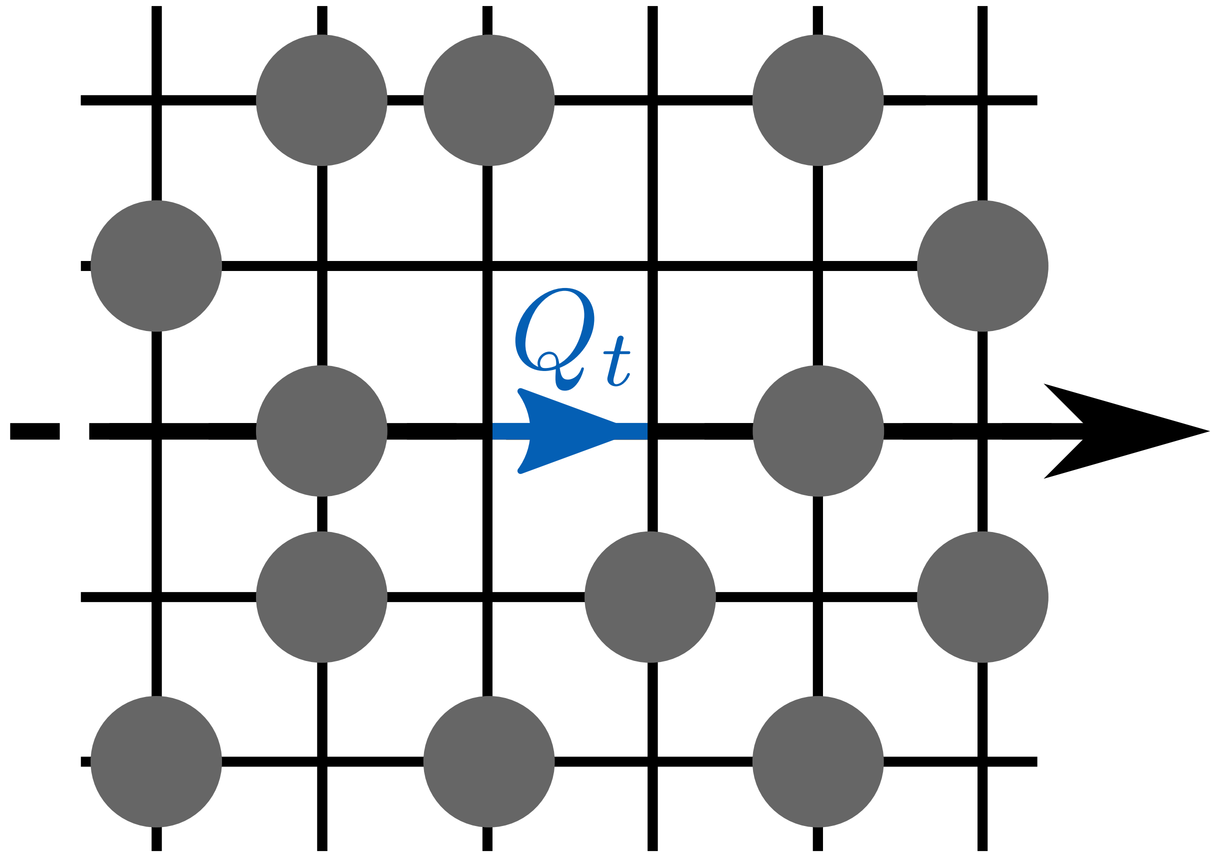
passing through the comb

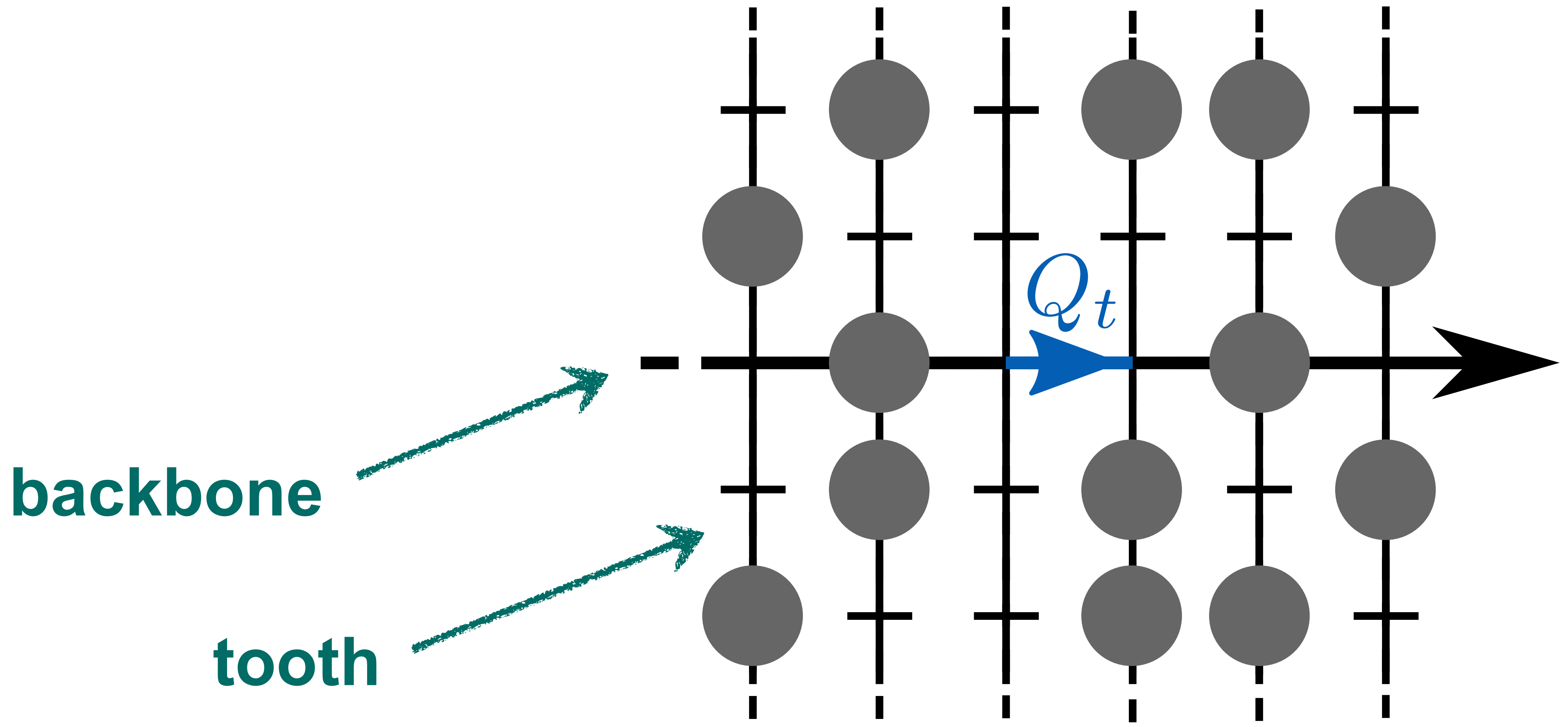
1. Order-preserving (single-file)
2. Tree-like (no loops!)

Need both to make $c_r(t)$ non-stationary?

- **Higher d** : ~~(1)~~ ~~(2)~~
- **Comb lattice** : ~~(1)~~ (2)

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

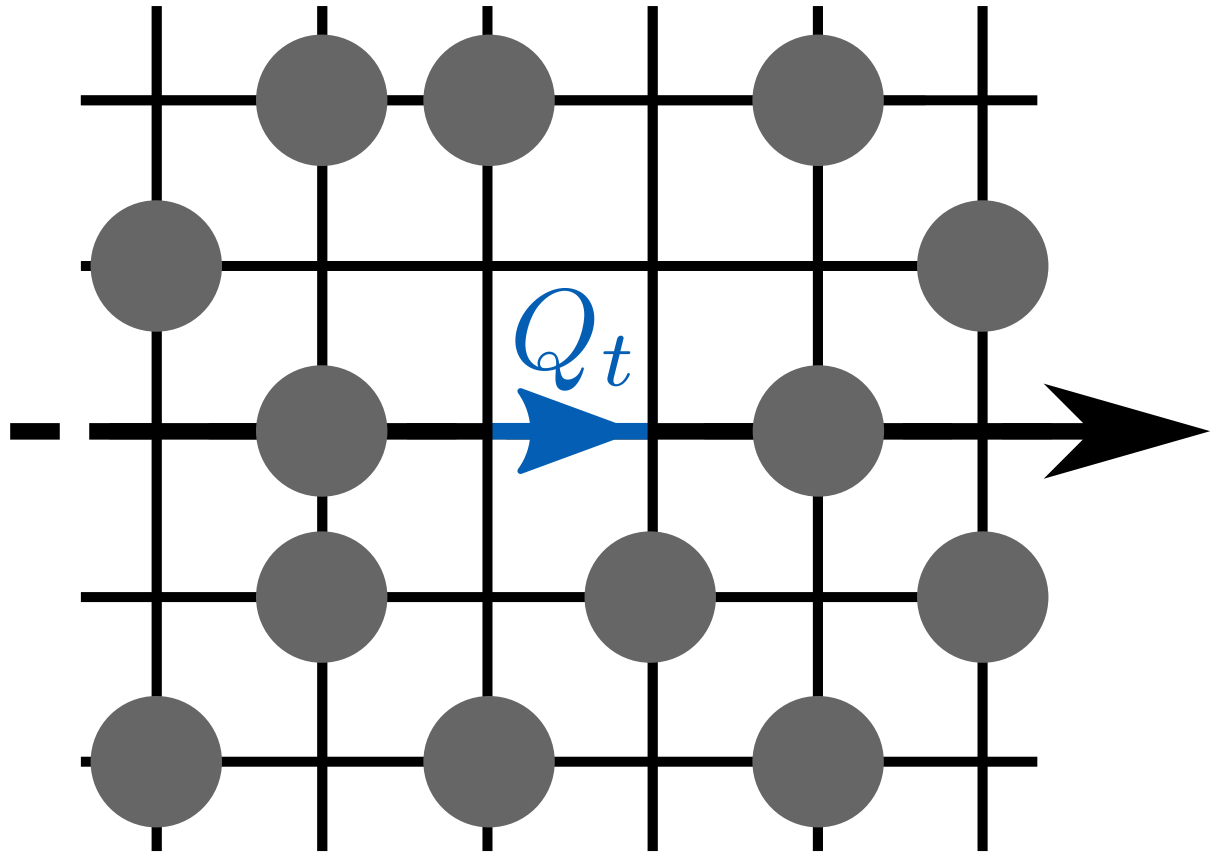




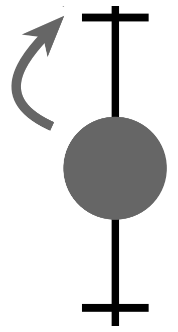
Bénichou, Illien, Oshanin, Sarracino, Voituriez, Phys. Rev. Lett. **115**, 220601 (2015)

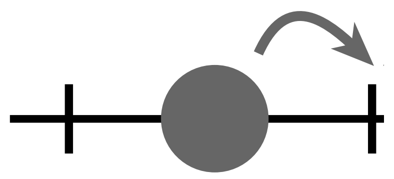
Ben-Avraham, Havlin, *Diffusion and reactions in fractals and disordered systems* (2000)

Microscopic calculation

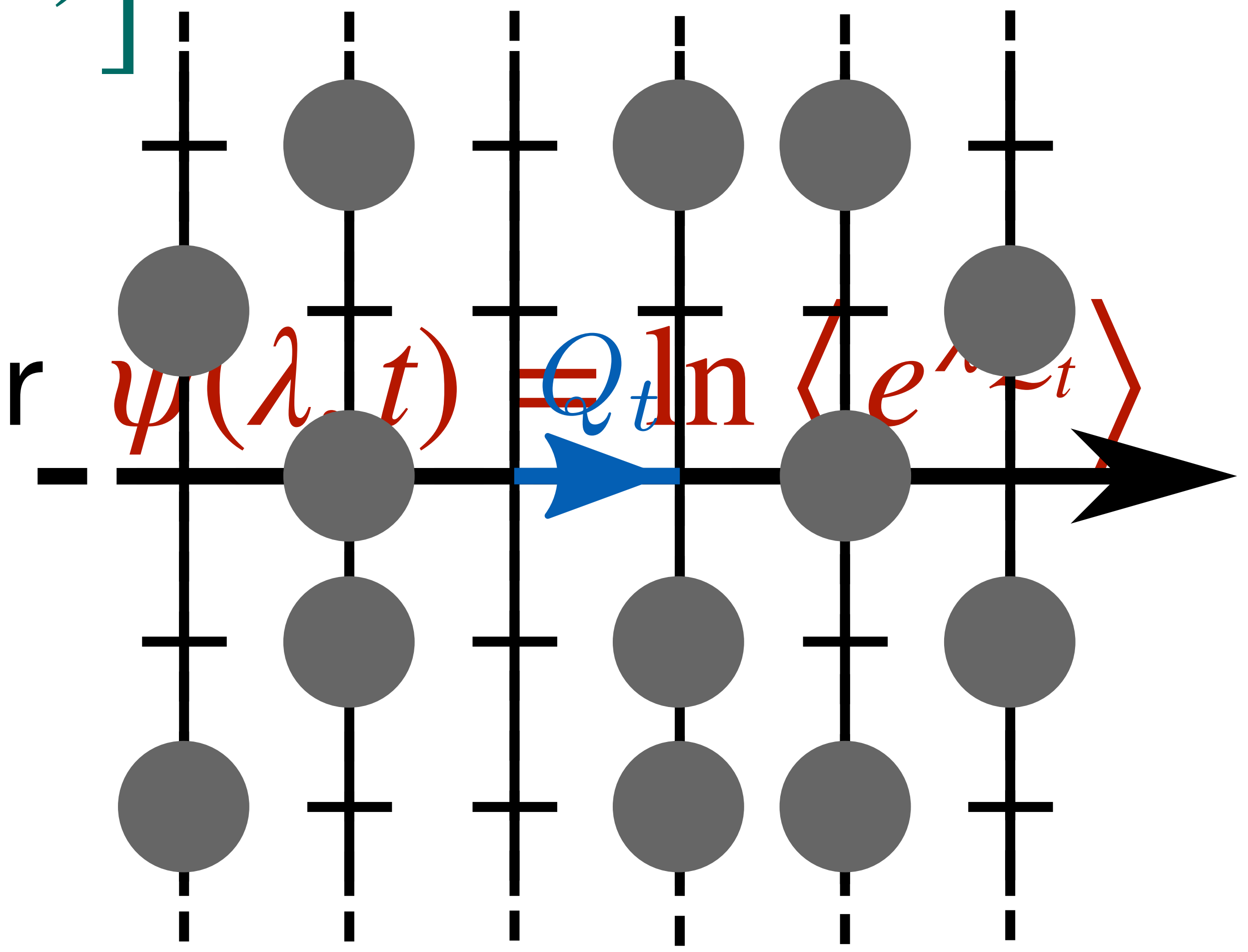


- Master equation





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



- Use it to write an equation for $c_{\vec{r}}(t) = \langle Q_t \eta_{\vec{r}}(t)\rangle$ and one for $\psi(\lambda,t) = \ln\langle e^{\lambda Q_t}\rangle$
- Find exact closed equations for $c_{\vec{r}}(t)$ (unlike for $\langle X_t \eta_{\vec{r}}(t)\rangle$)
- Solve them in Fourier-Laplace (self-consistently)

T. Berlioz, D. Venturelli, A. Grabsch, O. Bénichou, arXiv:2407.14317

Results

- $d = 1$

$$c_r(t) \xrightarrow[t\to\infty]{} \bar\rho(1-\bar\rho)\,\mathscr{C}_1\!\left(\frac{r}{t^{1/2}}\right)$$

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

- Comb

$$c_{\vec r}(t) \xrightarrow[t\to\infty]{} \bar\rho(1-\bar\rho)\,\mathscr{C}_c\!\left(\frac{x}{t^{1/4}},\frac{y}{t^{1/2}}\right)$$

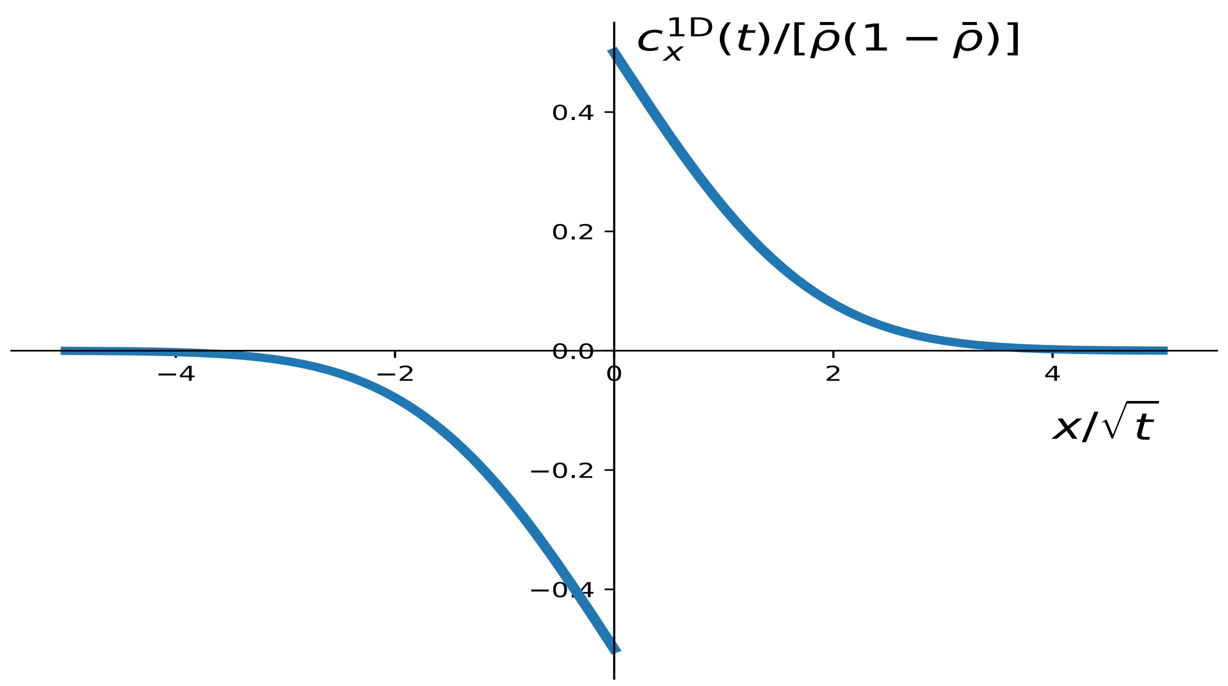
$$\langle Q_t^2 \rangle = n_c\,\bar\rho(1-\bar\rho)\;t^{3/4}$$

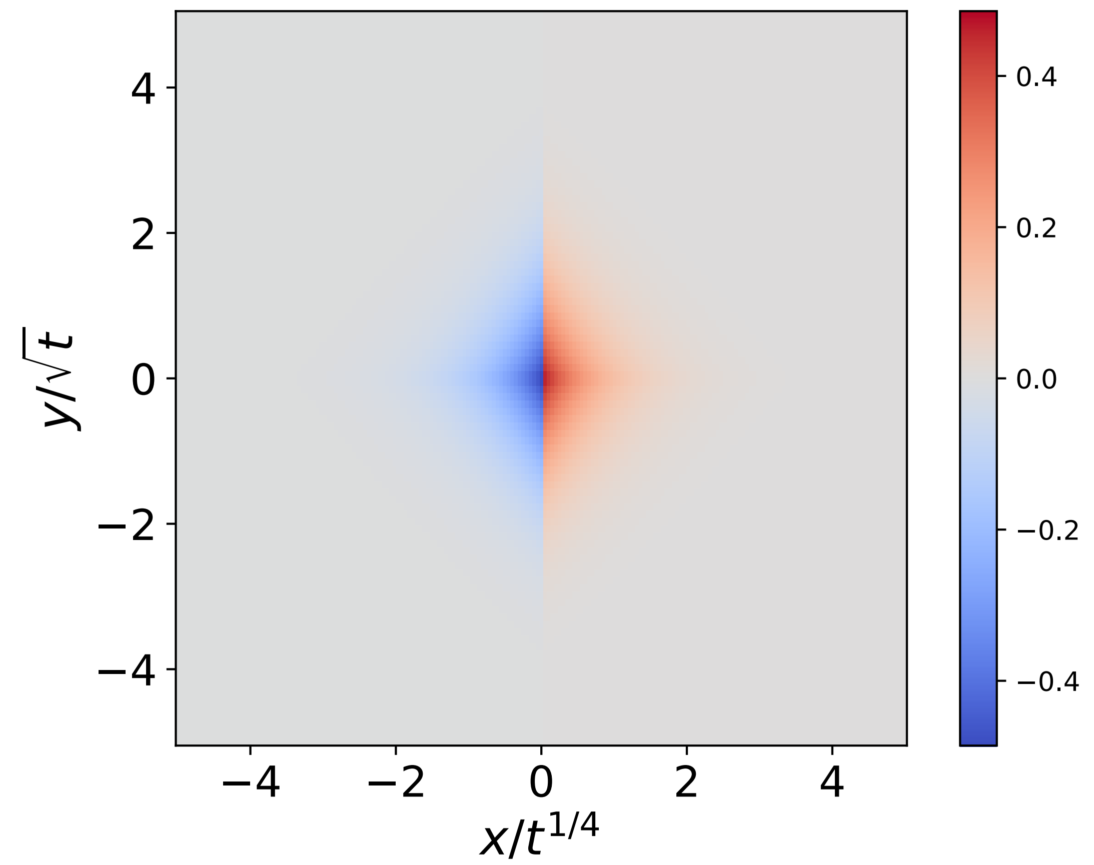
- $d = 2$

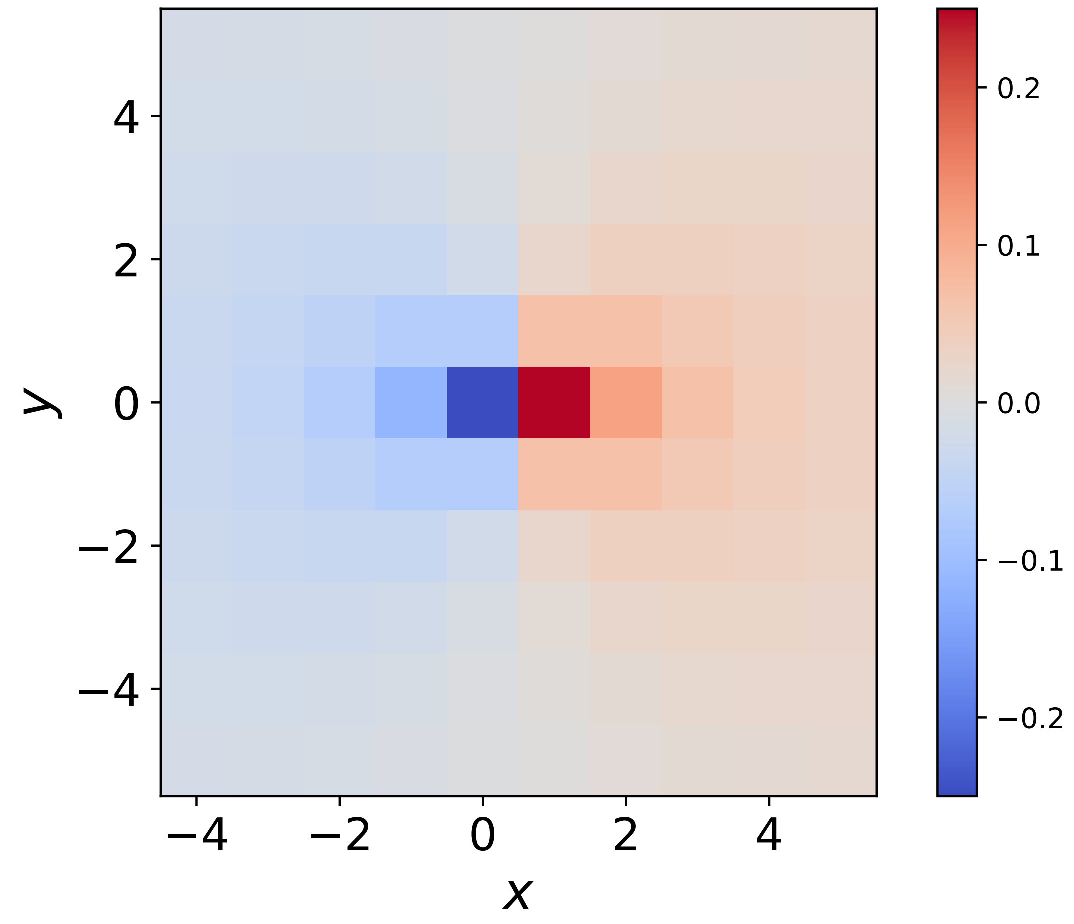
$$c_{\vec r}(t) \xrightarrow[t\to\infty]{} \bar\rho(1-\bar\rho)\,\mathscr{C}_2(\vec r)$$

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

loops!







Macroscopic Fluctuation Theory

towards higher moments and general diffusive processes

- Hydrodynamic description for $\eta_{\vec{r}}(t) \quad \rightarrow \quad \partial_t \rho(\vec{r}, t) = \vec{\nabla} \cdot [\mathbf{D}\, \vec{\nabla} \rho + \vec{\nu}]$
- Path-integral $\int \mathscr{D}\rho\, \mathscr{D}H\, e^{-T^{\alpha} S[\rho,H]}$ + saddle point for total time $T \gg 1 \rightarrow \left\langle e^{\lambda Q_T} \right\rangle$
- First application of MFT to an inhomogeneous system (**comb**)

T. Berlioz, D. Venturelli, A. Grabsch, O. Bénichou, arXiv:2407.14317

What about higher d ?

- In 1d & comb, correlations spread with t and vary slowly at the lattice scale
- In higher d correlations become stationary, no scaling limit!

Microscopic path-integral representation

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

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

equivalent to the M.E. if

$$\xi_{\vec r,\vec\mu}(t)=\begin{cases}1 & \textbf{with prob. } \gamma\,dt\,,\\ 0 & \textbf{with prob. } 1-\gamma\,dt\,.\end{cases}$$

Usual MSR machinery gives

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

A. Lefèvre, G. Biroli, J. Stat. Mech. (2007) P07024

Microscopic path-integral representation

- Saddle-point eqs are difference equations for $\eta_{\vec{r}}, \vec{j}_{\vec{r}}, \theta_{\vec{r}}, \vec{\varphi}_{\vec{r}}$
- Turn out to relax to a stationary limit,

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

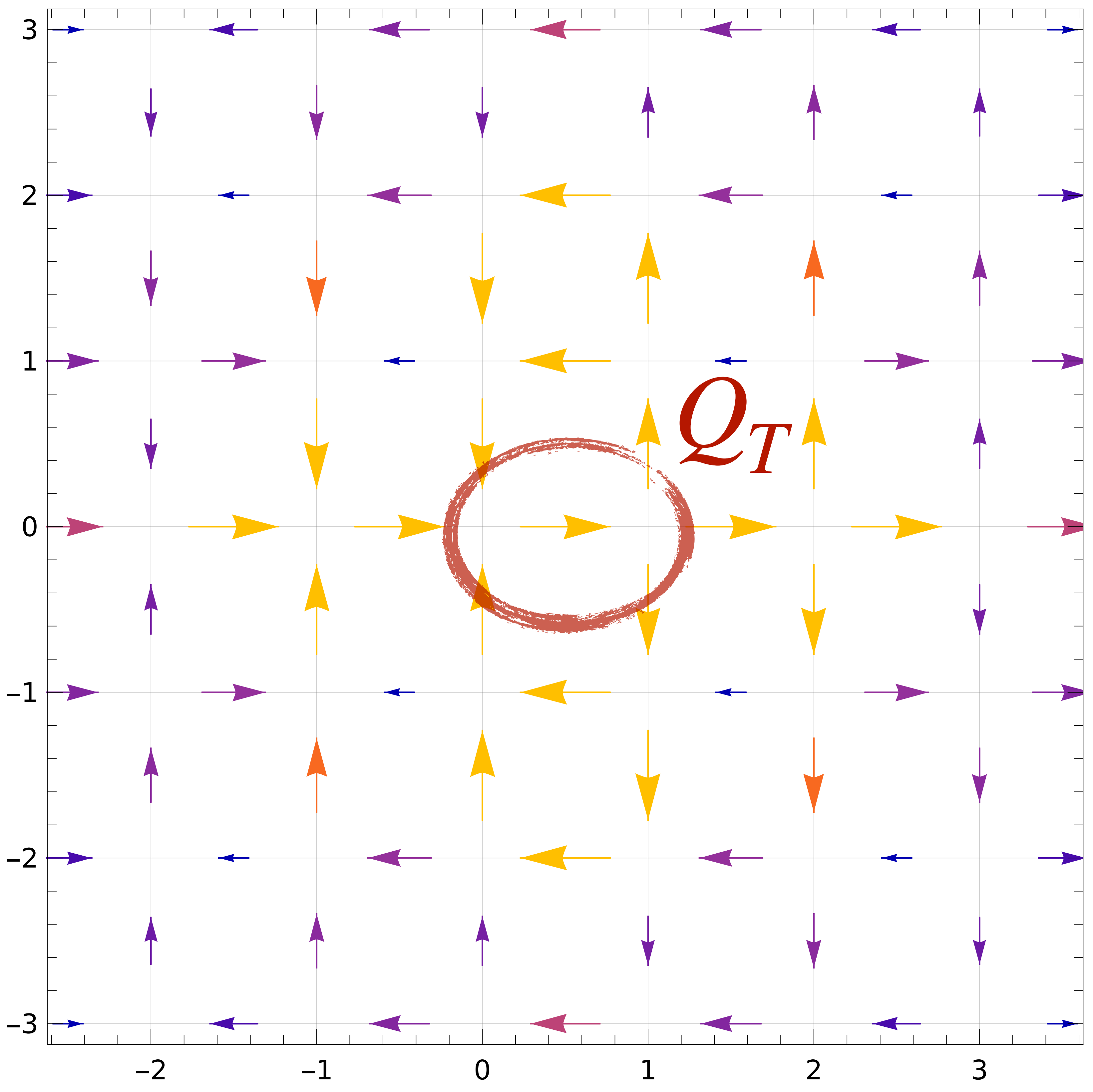
- Can be used to recover

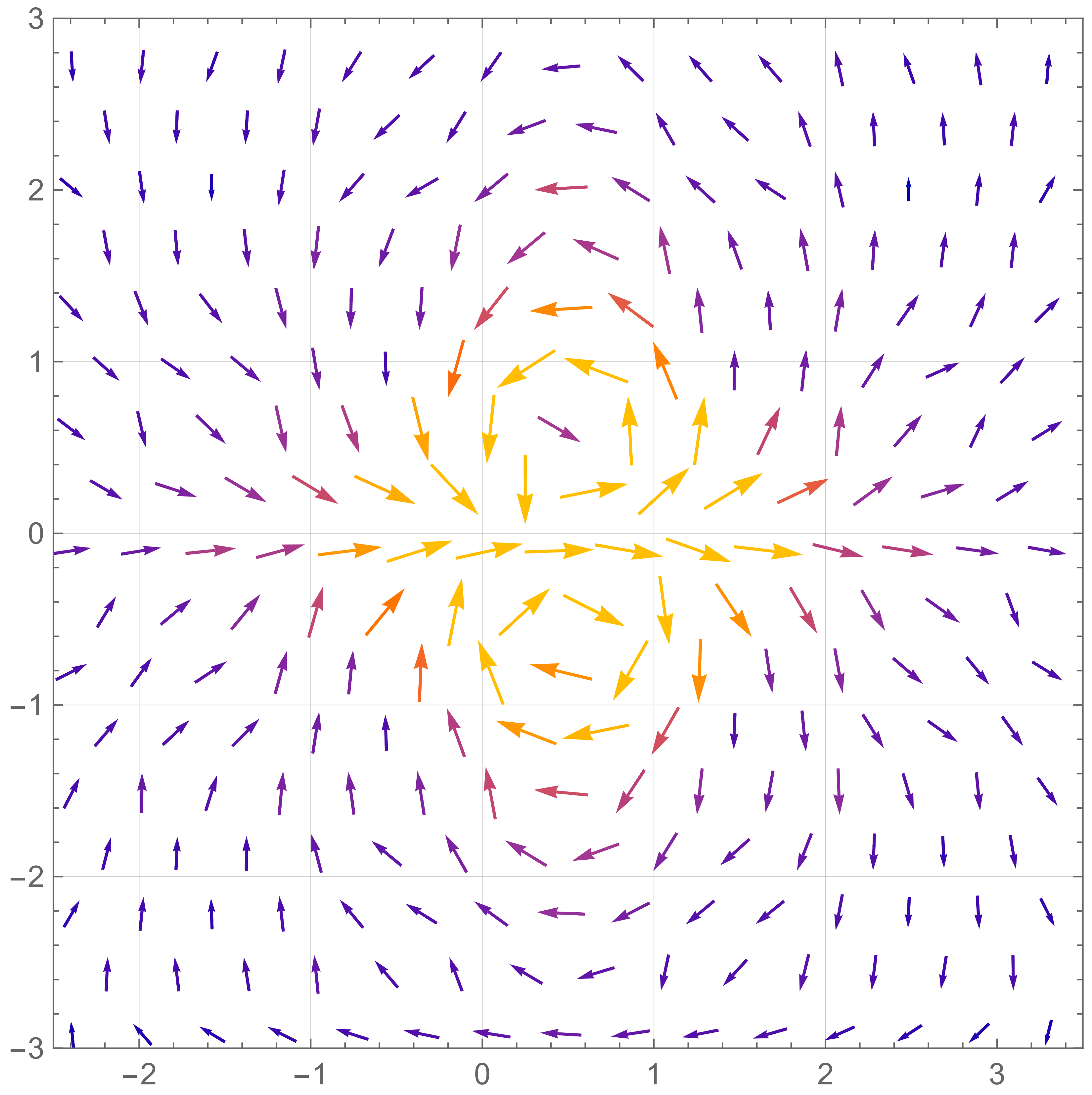
$$\left\langle e^{\lambda Q_T} \right\rangle \simeq \exp\{-T[\mathscr{L}^* - \lambda (\vec{j}^*_{\vec{r}=\vec{0}})_1]\} \longrightarrow \left\langle Q_t^2 \right\rangle = 2\gamma \left(1 - \frac{1}{d}\right) \bar{\rho}(1-\bar{\rho})\, t$$

Role of loops

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

$\vec{j}^{\,*}_{\vec{r}}$





looped structure of the lattice allows for **vortex** configurations, and thus for stationary $c_{\vec{r}}$

Summing up

- ☑ $\langle Q_t^2 \rangle$ through a bond in SEP on **infinite** lattices, **beyond** $1d$
- ☑ $\langle Q_t\, \eta_r(t) \rangle$ gives info on response of the bath
- ☑ Role of the **loops** in restoring normal diffusion
- ☐ Use **MFT** on comb to compute $\langle \exp(\lambda\, Q_t) \rangle$, beyond SEP
- ☐ Same in higher d via microscopic path-integral formalism
- ☐ Statistics of displacement X_t of a **tracer**

Thanks!

Théotim Berlioz

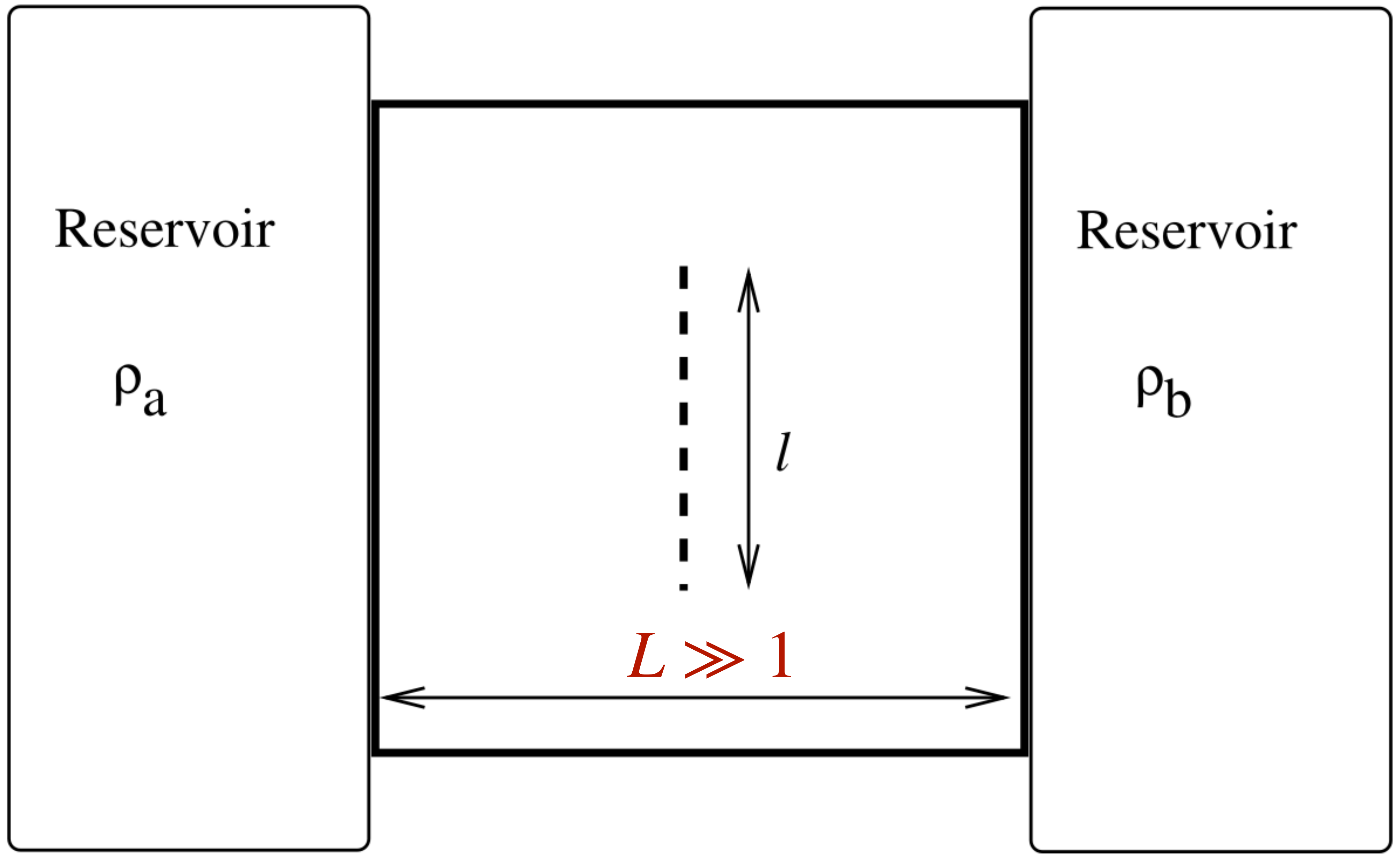
Aurélien Grabsch

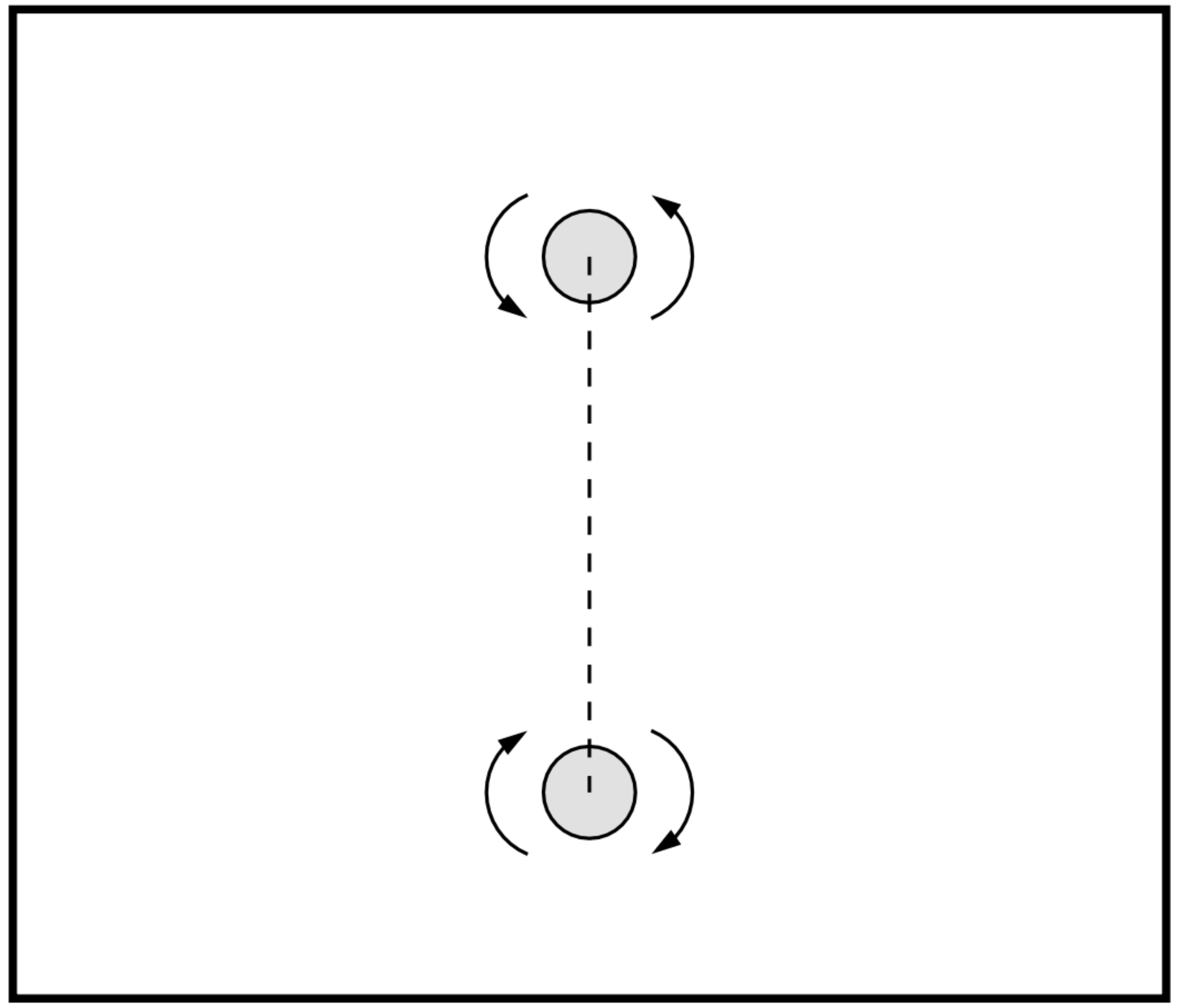
Olivier Bénichou

Backup slides

:)

Loops & vortices





… vortices as singularities in MFT

T. Bodineau, B. Derrida, J. L. Lebowitz, J. Stat. Phys. (2008) 131: 821–841

Macroscopic Fluctuation Theory on the comb

$$\partial_t \left\langle \eta_{\vec r}(t) \right\rangle = \delta_{y,0}\, \Delta_x \left\langle \eta_{\vec r}(t) \right\rangle + \Delta_y \left\langle \eta_{\vec r}(t) \right\rangle$$

$$\left\langle \eta_{\vec r}(t) \right\rangle \simeq \rho \left(\frac{x}{T^{1/4}}, \frac{y}{T^{1/2}}, \frac{t}{T} \right)$$

$\longrightarrow$

$$\partial_t \rho + \vec\nabla \cdot \vec j = 0$$

$$\vec j = -\mathbf{D}\,\vec\nabla \rho \; + \vec\nu$$

$$\mathbf{D} = \begin{pmatrix} \delta(y) & 0 \\ 0 & 1 \end{pmatrix}$$

Add noise:

$$\left\langle \nu_i(x,y,t)\nu_j(x',y',t') \right\rangle = \mathbf{\Sigma}_{i,j}(\rho(x,y,t))\, \delta(x-x')\delta(y-y')\delta(t-t')$$

$$\mathbf{\Sigma}(\rho) = 2\rho(1-\rho)\begin{pmatrix} \delta(y) & 0 \\ 0 & 1 \end{pmatrix}$$

T. Berlioz, D. Venturelli, A. Grabsch, O. Bénichou, arXiv:2407.14317

Macroscopic Fluctuation Theory

- Response field formalism

$$P[\rho] = \int \mathscr{D}H \, e^{-T^{3/4} S[\rho,H]}$$

- Integrated current fluctuations

$$Q_T \simeq T^{3/4} \int_0^\infty dx \int_{-\infty}^\infty dy \, [\rho(x,y,1) - \rho(x,y,0)]$$

$$\left\langle e^{\lambda Q_T} \right\rangle = \int \mathscr{D}\rho \, \mathscr{D}H \, e^{-T^{3/4} S[\rho,H] + \lambda Q_T}$$

- Saddle point for large T gives moments of Q_T and

$$\frac{\left\langle \eta_{\vec{r}=(x,y)}(T) \, e^{\lambda Q_T} \right\rangle}{\left\langle e^{\lambda Q_T} \right\rangle} \simeq \rho^*(x,y,1)$$

T. Berlioz, D. Venturelli, A. Grabsch, O. Bénichou, arXiv:2407.14317