

Large deviation in single-file diffusion

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A joint work with [P. L. Krapivsky](#) and [Kirone Mallick](#)

June 27, 2014



What is Single-file diffusion?



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 - Sliding of DNA-binding proteins along DNA. [Gene-Wei Li *et al.*, 2009]

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- **2390** published articles containing the word “single-file diffusion”;
69 published in this year

[Google scholar]

Tagged particle



- Motion of **individual** particles is **sub-diffusive**

$$\langle x_T^2 \rangle_{\text{single-file}} \simeq D\sqrt{T}$$

$$\langle x_T^2 \rangle_{\text{normal}} \simeq 2DT.$$

- **Observed in experiment:**

- Transport of large molecules in Zeolite

[Kukla et al, 1996]

- Colloids in 1d channels

[Wei et al, 2000][Lutz et al, 2004][Lin et al, 2005]

- Water molecules in carbon nanotube.

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theoretical studies

At large times the probability of tracer position is **asymptotically Gaussian** with variance $D\sqrt{T}$

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- **On lattice (SEP):** [Arratia, 1983]

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- Point particle: [Harris, 1965]
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- On lattice (SEP): [Arratia, 1983]
- Colloidal system: [Kollmann, 2003]
- Dependence on initial condition:[Leibovich et al, 2013]

$$\langle X^2 \rangle_{annealed} \neq \langle X^2 \rangle_{quenched}$$

Our work

What about higher cumulants? Any general framework?

Our work

- a general approach: macroscopic fluctuation theory.

[Bertini et al,2001]

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- at large time T , cumulants

$$\langle X_T^n \rangle_c \simeq k_n \sqrt{T}$$

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depends on system

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$$Prob_T(X) \asymp e^{-\sqrt{T} \phi\left(\frac{x}{\sqrt{T}}\right)}$$

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large deviation function

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- compute $\phi(\xi)$ for point particles
- An exact microscopic calculation for point particles.

A macroscopic approach

A macroscopic approach

- Continuous space: 
- On lattice (SEP): 



No bias

Infinite system size

At a hydrodynamic scale

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

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density

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mobility

white noise
 $\langle \eta(x, t) \eta(x', t') \rangle = \delta(x - x') \delta(t - t')$

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Microscopic details of system are in the function $D(\rho)$ and $\sigma(\rho)$

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- For point particles: $D(\rho) = 1$ and $\sigma(\rho) = 2\rho$

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Microscopic details of system are in the function $D(\rho)$ and $\sigma(\rho)$

- For point particles: $D(\rho) = 1$ and $\sigma(\rho) = 2\rho$
- For SEP: $D(\rho) = 1$ and $\sigma(\rho) = 2\rho(1 - \rho)$

tracer position

How is **tracer position** linked to density field $\rho(x, t)$?

No particle can cross each other \implies Number of particles on right of tracer is **unchanged**.

$$\int_{X_T}^{\infty} \rho(z, T) dz = \int_0^{\infty} \rho(z, 0) dz$$

X_T is a **functional** of the density profile $\rho(x, t)$.

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How to compute large deviation function?

step 1 cumulant generating function

$$\mu(\lambda, T) = \log \left[\langle e^{\lambda X_T} \rangle \right]$$

$$\mu(\lambda, T) = \langle X_T \rangle_c \lambda + \frac{1}{2} \langle X_T^2 \rangle_c \lambda^2 + \dots$$

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How to compute large deviation function?

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first cumulant $\mu(\lambda, T) = \log \left[\langle e^{\lambda X_T} \rangle \right]$

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second cumulant

tracer position

How is **tracer position** linked to density field $\rho(x, t)$?

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step 2 Legendre transform $\mu(\lambda, T)$ to get **large deviation function**

Variational formulation

Macroscopic fluctuation theory:[Bertini et al,2001]

$$\langle e^{\lambda X_T} \rangle = \int \mathcal{D}[\rho, \hat{\rho}] \exp \left\{ \lambda X_T[\rho] - F[\rho(x, 0)] - \int_0^T dt \int_{-\infty}^{\infty} dx [\hat{\rho} \partial_t \rho - H] \right\}$$

Let $X_T[q] = Y$ (the tracer position for least action path)

Variational formulation

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Path integral
within time $[0, T]$

Let $X_T[q] = Y$ (the tracer position for least action path)

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$$\mathcal{P}[\rho(x, 0)] = e^{-F[\rho(x, 0)]}$$

for quench $F = 0$

for annealed $F = \text{free energy}$

Let $X_T[q] = Y$ (the tracer position for least action path)

Variational formulation

Macroscopic fluctuation theory: [Bertini et al, 2001]

prob of
each path

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$$H = \frac{\sigma(\rho)}{2} (\partial_x \hat{\rho})^2 - D(\rho) (\partial_x \rho) (\partial_x \hat{\rho})$$

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Action

$$\langle e^{\lambda X_T} \rangle = \int \mathcal{D}[\rho, \hat{\rho}] e^{-S[\rho, \hat{\rho}, \lambda, T]}$$

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Action

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At large time, contribution from paths of least action $(\rho, \hat{\rho}) \equiv (q, p)$.

$$\mu(\lambda, T) = \log \left[\langle e^{\lambda X_T} \rangle \right] = -S[q, p, \lambda, T].$$

Let $X_T[q] = Y$ (the tracer position for least action path)

Least action

Paths of least action

$$\begin{aligned}\partial_t q &= \partial_x [D(q)\partial_x q - \sigma(q)\partial_x p] \\ \partial_t p &= -D(q)\partial_{xx} p - \frac{\sigma'(q)}{2} (\partial_x p)^2\end{aligned}$$

Boundary condition

Least action

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Boundary condition

annealed (initial density fluctuating)

$$\begin{aligned}p(x, T) &= \frac{\lambda}{q(Y, T)} \theta(x - Y) \\ p(x, 0) &= \frac{\lambda}{q(Y, T)} \theta(x) + \frac{\delta F}{\delta q(x, 0)}\end{aligned}$$

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from $\frac{\delta X_T}{\delta q(x, T)}$

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quenched (initial density fixed)

$$\begin{aligned}p(x, T) &= \frac{\lambda}{q(Y, T)} \theta(x - Y) \\ q(x, 0) &= \rho\end{aligned}$$

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uniform initial density

- least action equations

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- cumulant generating function

$$\begin{aligned}\mu(\lambda, T) &= \lambda Y - \int_{-\infty}^{\infty} dx \int_{\rho}^{q(x,0)} dr \frac{2D(r)}{\sigma(r)} (q(x,0) - r) \\ &\quad - \int_0^T dt \int_{-\infty}^{\infty} dx \frac{\sigma(q)}{2} (\partial_x p)^2\end{aligned}$$

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- cumulant generating function

$$\mu(\lambda) = \lambda Y - \int_0^T dt \int_{-\infty}^{\infty} dx \frac{\sigma(q)}{2} (\partial_x p)^2$$

What can be extracted without solving?

- $\mu(\lambda, T)$ is even in λ .

$$\mu(\lambda, T) = \frac{\lambda^2}{2!} \langle X_T^2 \rangle_c + \frac{\lambda^4}{4!} \langle X_T^4 \rangle_c + \dots$$

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 - all cumulants scale as \sqrt{T} .

What can be extracted without solving?

- $\mu(\lambda, T)$ is even in λ .

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 - taking Legendre transformation

$$\text{Prob} \left(\frac{X}{\sqrt{T}} = \xi \right) \asymp \exp \left[-\sqrt{T} \phi(\xi) \right]$$

$\phi(\xi)$ is an even function.

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$$\text{Prob}\left(\frac{X}{\sqrt{T}} = \xi\right) \asymp \exp\left[-\sqrt{T}\phi(\xi)\right]$$

$\phi(\xi)$ is an even function.

- At large T , using Taylor expansion of $\phi(\xi)$,

$$\text{Prob}(X) \asymp \exp\left[-\frac{X^2}{D\sqrt{T}}\right]$$

An exact solution

Point particles with hard core repulsion

$$D(\rho) = 1 \quad \text{and} \quad \sigma(\rho) = 2\rho$$

least action equations

$$\begin{aligned}\partial_t p + \partial_{xx} p &= -(\partial_x p)^2 \\ \partial_t q - \partial_{xx} q &= -\partial_x (2q \partial_x p)\end{aligned}$$

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boundary condition (annealed)

$$\begin{aligned}p(x, T) &= B\theta(x - Y) \quad \text{where} \quad B = \frac{\lambda}{q(Y, T)} \\ q(x, 0) &= \rho \exp [p(x, 0) - B\theta(x)]\end{aligned}$$

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treat B as parameter and solve it self-consistently

An exact solution

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how to solve?

Define $P = e^p$ and $Q = qe^{-p}$, then

$$\partial_t P + \partial_{xx} P = 0 \quad \text{and} \quad \partial_t Q - \partial_{xx} Q = 0$$

- Solution

$$p(x, t) = \log \left[1 + (e^B - 1) \frac{1}{2} \operatorname{erfc} \left(\frac{Y - x}{\sqrt{4D(T - t)}} \right) \right]$$
$$q(x, t) = \rho \left[1 + (e^{-B} - 1) \frac{1}{2} \operatorname{erfc} \left(\frac{x - Y}{\sqrt{4D(T - t)}} \right) \right]$$
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$$\left[1 + (e^B - 1) \frac{1}{2} \operatorname{erfc} \left(\frac{x}{\sqrt{4Dt}} \right) \right]$$

- What is Y?

$$\frac{Y/\sqrt{4DT}}{\frac{\exp[-Y^2/4DT]}{\sqrt{4\pi}} - \frac{Y}{\sqrt{4DT}} \frac{1}{2} \operatorname{erfc} \left(\frac{Y}{\sqrt{4DT}} \right)} = e^{2B} - 1$$

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$$\text{using } \int_Y^\infty dx q(x, T) = \int_0^\infty dx q(x, 0)$$

- Solution

$$p(x, t) = \log \left[1 + (e^B - 1) \frac{1}{2} \operatorname{erfc} \left(\frac{Y - x}{\sqrt{4D(T - t)}} \right) \right]$$

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- Cumulant generating function

$$\mu(\lambda) = \left[\lambda - \rho \frac{e^B - 1}{e^B + 1} \right] Y$$

determine B

Definition $B = \lambda/q(Y, T)$

$q(Y, T)$ can not be determined self-consistently

determine B

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$$q(x, t) = \rho \left[1 + (e^{-B} - 1) \frac{1}{2} \operatorname{erfc} \left(\frac{x - Y}{\sqrt{4D(T - t)}} \right) \right] \left[1 + (e^B - 1) \frac{1}{2} \operatorname{erfc} \left(\frac{x}{\sqrt{4Dt}} \right) \right]$$

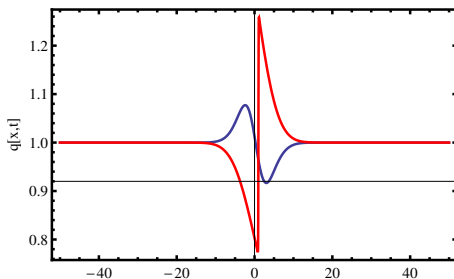
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$q(x, T)$ is non-analytic at (Y, T)



$q(Y, T)$ can not be determined self-consistently

determine B

Determine B by minimizing the action [Baruch Meerson]

$$\mu_B(\lambda) = \lambda Y(B) + \frac{1 - e^B}{1 + e^B} Y(B).$$

This yields

$$\lambda = \rho(1 - e^{-B}) \left[1 + (e^B - 1) \frac{1}{2} \operatorname{erfc} \left(\frac{x}{\sqrt{4DT}} \right) \right]$$

Annealed

Results (parametric form)

$$\mu(\lambda) = \sqrt{4DT} \rho \left[\lambda y + (e^B - 1) \alpha(y) + (e^{-B} - 1) \alpha(-y) \right]$$

$$y = (e^B - 1) \alpha(y) - (e^{-B} - 1) \alpha(-y)$$

$$\lambda = (1 - e^{-B}) \left[1 + (e^B - 1) \frac{1}{2} \operatorname{erfc}(y) \right]$$

Annealed

Results (parametric form)

$$\int_y^\infty \frac{1}{2} \operatorname{erfc}(z) dz$$

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$$\lambda = (1 - e^{-B}) \left[1 + (e^B - 1) \frac{1}{2} \operatorname{erfc}(y) \right]$$

Large deviation function

$$\phi(y) = \rho \left[\sqrt{\alpha(y)} - \sqrt{\alpha(-y)} \right]$$

probability of tracer position

$$P \left[\frac{X_T}{\sqrt{4DT}} = y \right] \asymp e^{-\sqrt{4DT} \phi(y)}$$

Results (parametric form)

$$\frac{\mu(\lambda)}{\rho\sqrt{4DT}} = \lambda y + \int_{-\infty}^{\infty} dz \left[\log \left\{ 1 + (e^B - 1) \frac{1}{2} \operatorname{erfc}(-z) \right\} - B e^B \frac{\frac{1}{2} \operatorname{erfc}(-z)}{1 + (e^B - 1) \frac{1}{2} \operatorname{erfc}(-z)} \right]$$

$$y = (e^B - 1) \int_{-\infty}^{\infty} dz \frac{\frac{1}{2} \operatorname{erfc}(z) \frac{1}{2} \operatorname{erfc}(-z)}{1 + (e^B - 1) \frac{1}{2} \operatorname{erfc}(-z)}$$

$$\lambda = \lambda(B, Y)$$

Annealed vs Quenched

- annealed

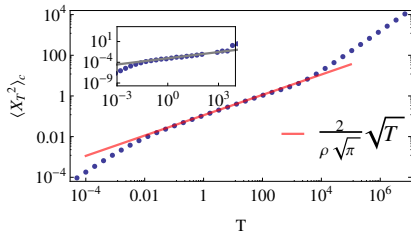
$$\langle X_T^2 \rangle_c = \frac{2}{\rho\sqrt{\pi}}\sqrt{T}$$

$$\langle X_T^4 \rangle_c = \frac{6(4-\pi)}{(\rho\sqrt{\pi})^3}\sqrt{T}$$

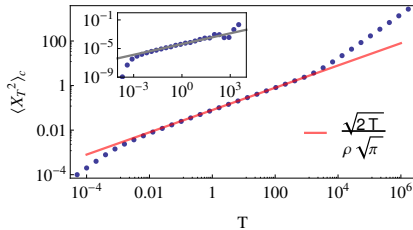
- quenched

$$\langle X_T^2 \rangle_c = \frac{\sqrt{2}}{\rho\sqrt{\pi}}\sqrt{T}$$

$$\langle X_T^4 \rangle_c = \frac{2\sqrt{2}}{\rho^3\sqrt{\pi}} \left[\frac{9}{\pi} \arctan\left(\frac{1}{2\sqrt{2}}\right) - 1 \right] \sqrt{T}$$



annealed



quenched

what about more general systems ?

Perturbative expansion

$$q(x, t) = q_0(x, t) + \lambda q_1(x, t) + \lambda^2 q_2(x, t) + \dots$$

$$p(x, t) = p_0(x, t) + \lambda p_1(x, t) + \lambda^2 p_2(x, t) + \dots$$

$$\mu(\lambda) = \frac{1}{2!} \langle X_T^2 \rangle_c \lambda^2 + \frac{1}{4!} \langle X_T^4 \rangle_c \lambda^4 + \dots$$

Quenched case

- zeroth order

$$q_0(x, t) = \rho \quad \text{and} \quad p_0(x, t) = 0$$

- first order

$$\partial_t p_1 = -D(\rho) \partial_{xx} p_1 \quad \text{with} \quad p_1(x, T) = \frac{1}{\rho} \theta(x)$$

$$\partial_t q_1 = D(\rho) \partial_{xx} q_1 - \sigma(\rho) \partial_{xx} p_1 \quad \text{with} \quad q_1(x, 0) = 0$$

- cumulants

$$\frac{1}{2} \langle X_T^2 \rangle = \frac{1}{\rho} \int_{-\infty}^{\infty} dx [q_1(x, T) - q_1(x, 0)] - \frac{\sigma(\rho)}{2} \int_0^T dt \int_{-\infty}^{\infty} dx (\partial_x p_1)^2$$

- Quenched

$$\langle X_T^2 \rangle = \frac{\sigma(\rho)}{\rho^2} \frac{\sqrt{T}}{\sqrt{2\pi D(\rho)}}$$

- Annealed

$$\langle X_T^2 \rangle = \sqrt{2} \frac{\sigma(\rho)}{\rho^2} \frac{\sqrt{T}}{\sqrt{2\pi D(\rho)}}$$

Point particles

$$\frac{\langle X_T^2 \rangle_{ann}}{\sqrt{T}} = \frac{2}{\rho} \frac{1}{\sqrt{\pi}}$$

[Harris, 1965]

SEP

$$\frac{\langle X_T^2 \rangle_{ann}}{\sqrt{T}} = \frac{2(1-\rho)}{\rho} \frac{1}{\sqrt{\pi}}$$

colloidal system

$$\frac{\langle X_T^2 \rangle_{ann}}{\sqrt{T}} = \frac{2S}{\rho^2} \sqrt{\frac{D}{\pi}}$$

- Quenched

$$\langle X_T^2 \rangle = \frac{\sigma(\rho)}{\rho^2} \frac{\sqrt{T}}{\sqrt{2\pi D(\rho)}}$$

- Annealed

$$\langle X_T^2 \rangle = \sqrt{2} \frac{\sigma(\rho)}{\rho^2} \frac{\sqrt{T}}{\sqrt{2\pi D(\rho)}}$$

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[Arratia, 1983]

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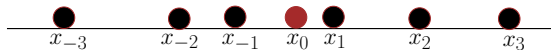
$$\frac{\langle X_T^2 \rangle_{ann}}{\sqrt{T}} = \frac{2S}{\rho^2} \sqrt{\frac{D}{\pi}}$$

[Kollman, 2003]

Microscopic calculation

Point particles

Point particles



Diffusion in the sector $x_j < x_{j+1}$

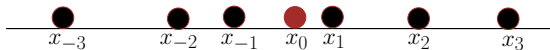
$$\partial_t P_t(\mathbf{X}|\mathbf{Y}) = D \sum_{i=-n}^n \partial_{x_i}^2 P_t(\mathbf{X}|\mathbf{Y})$$

reflecting boundary

$$\partial_{x_j} P_t(\mathbf{X}|\mathbf{Y}) = \partial_{x_{j+1}} P_t(\mathbf{X}|\mathbf{Y})$$

along $x_j = x_{j+1}$

Point particles



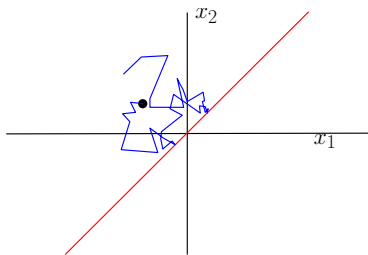
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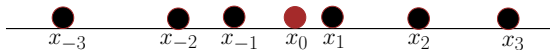
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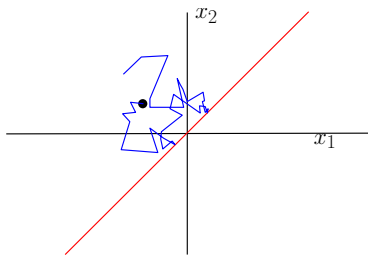
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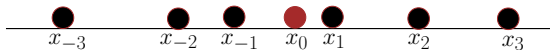
along $x_j = x_{j+1}$

solution

$$\begin{aligned} P_t(\mathbf{X}|\mathbf{Y}) &= \sum_{\sigma} \prod_j g_t(x_j | y_{\sigma(j)}) \\ &= g_t(x_{-n} | y_{-n}) g_t(x_{-n+1} | y_{-n+1}) \cdots g_t(x_n | y_n) \\ &\quad + g_t(x_{-n} | y_{-n+1}) g_t(x_{-n+1} | y_{-n}) \cdots g_t(x_n | y_n) + \dots \end{aligned}$$



Point particles

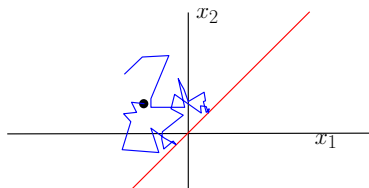


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reflecting boundary

$$\partial_{x_j} P_t(\mathbf{X}|\mathbf{Y}) = \partial_{x_{j+1}} P_t(\mathbf{X}|\mathbf{Y})$$



$$\frac{1}{\sqrt{4\pi Dt}} \exp \left[\frac{-(x_j - y_{\sigma(j)})^2}{4Dt} \right]$$

along $x_i = x_{i+1}$

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tracer position

Let central particle is the tracer.

- Probability of tracer position

$$Prob_t(x_0|\mathbf{Y}) = \int_{-\infty}^{x_{-n+1}} dx_{-n} \cdots \int_{-\infty}^{x_0} dx_{-1} \int_{x_0}^{\infty} dx_1 \cdots \int_{x_{n-1}}^{\infty} dx_n P_t(\mathbf{X}|\mathbf{Y})$$

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- using combinatorial identities

$$Prob_t(x_0|\mathbf{Y}) = \sum_{k=-n}^n A_k[x_0, \mathbf{Y}, t] g_t(x_0|y_k)$$

$$A_k[x_0, \mathbf{Y}, t] = \sum_{s_{-n}=\pm 1} \cdots \sum_{s_{k-1}=\pm 1} \sum_{s_{k+1}=\pm 1} \cdots \sum_{s_n=\pm 1} \delta_{\sum_{q \neq k} s_q, 0} \prod_{j \neq k} \frac{1}{2} \operatorname{erfc} \left[s_j \frac{(x_0 - y_j)}{\sqrt{4Dt}} \right]$$

Averaging over initial positions

- **annealed**: Initially particles are distributed randomly in $[-L, L]$.

$$P(x_0) = \frac{n!n!}{L^{2n}} \int_{-L}^{y_{-n+1}} dy_{-n} \dots \int_{-L}^0 dy_{-1} \int_0^L dy_1 \dots \int_{y_{n-1}}^L$$
$$\sum_{k=-n}^n A_k[x_0, \mathbf{Y}, t] g_t(x_0 | y_k)$$

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$$\sum_{k=-n}^n A_k[x_0, \mathbf{Y}, t] g_t(x_0|y_k)$$

- at large n and L , with $n/L = \rho$

$$P_t(x_0) = \exp[-\rho R_t(x_0) - \rho R_t(-x_0)] I_0(2\rho\sqrt{R_t(x_0)R_t(-x_0)})$$
$$\left[g(x_0|0) + 2\rho H_t(x_0)H_t(-x_0) \right]$$
$$+ \rho \left\{ H_t(x_0)^2 \sqrt{\frac{R_t(x_0)}{R_t(-x_0)}} + H_t(-x_0)^2 \sqrt{\frac{R_t(-x_0)}{R_t(x_0)}} \right\} \frac{I_2(2\rho\sqrt{R_t(x_0)R_t(-x_0)})}{I_1(2\rho\sqrt{R_t(x_0)R_t(-x_0)})}$$

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$$\int_{x_0}^{\infty} dz \frac{1}{2} \operatorname{erfc} \left(\frac{z}{\sqrt{4Dt}} \right)$$

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$$\frac{1}{2} \operatorname{erfc} \left(\frac{x_0}{\sqrt{4Dt}} \right)$$

$$P_t(x_0) = \exp[-\rho R_t(x_0) - \rho R_t(-x_0)] I_0(2\rho\sqrt{R_t(x_0)R_t(-x_0)})$$

$$\left[g(x_0|0) + 2\rho H_t(x_0)H_t(-x_0) \right]$$

$$+ \rho \left\{ H_t(x_0)^2 \sqrt{\frac{R_t(x_0)}{R_t(-x_0)}} + H_t(-x_0)^2 \sqrt{\frac{R_t(-x_0)}{R_t(x_0)}} \right\} \frac{I_2(2\rho\sqrt{R_t(x_0)R_t(-x_0)})}{I_1(2\rho\sqrt{R_t(x_0)R_t(-x_0)})}$$

$$\int_y^\infty dz \frac{1}{2} \operatorname{erfc}(z)$$

at large times

$$P\left(\frac{x_0}{\sqrt{4Dt}} = y\right) \asymp \exp\left[-\sqrt{4Dt} \rho \left\{\sqrt{\alpha(y)} - \sqrt{\alpha(-y)}\right\}^2\right]$$

Same as obtained by macroscopic approach

- Take home message

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Thank you