Anomalous Diffusion

Alberto Rosso

Laboratoire Physique Theorique et Modeles Statistiques

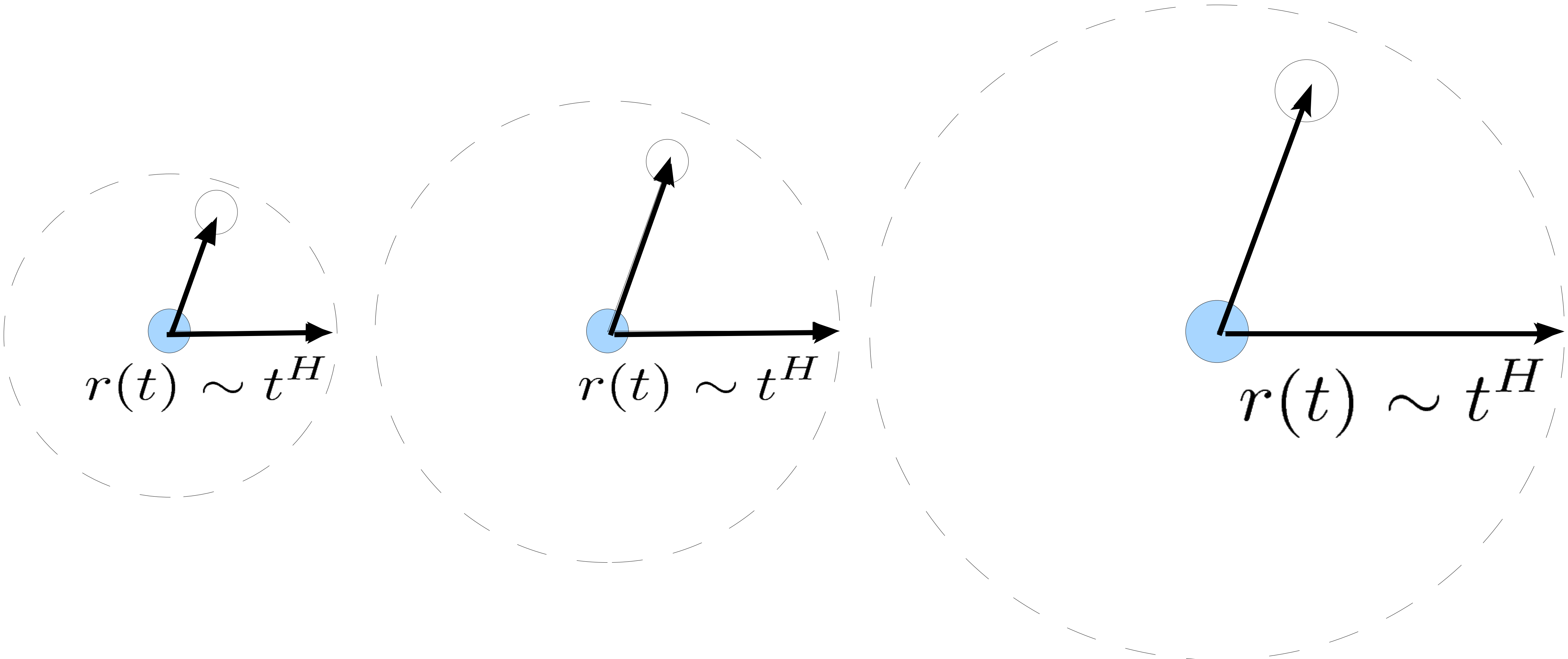
Orsay Paris-Sud

A. Zoia, S. Majumdar, A. R., PRL 102, 120602 (2009)

S. Majumdar, A. R., A. Zoia, PRL 104, 020602 (2010)

K. Wiese, S. Majumdar, A. R., PRE 83, 06114 (2011)

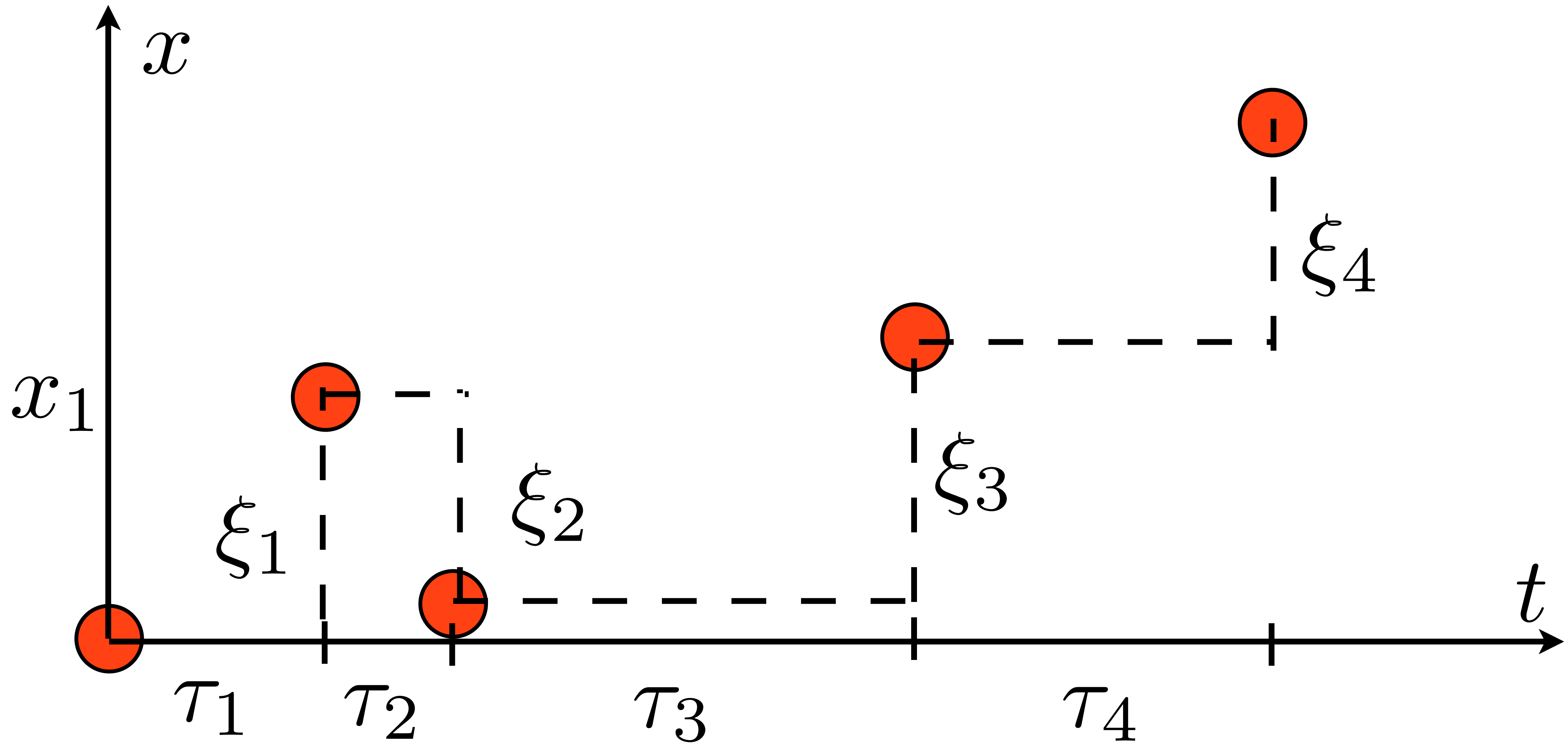
Anomalous Diffusion



$H < 1/2$ Subdiffusion

$H = 1/2$ Diffusion

$H > 1/2$ Super-diffusion



We suppose τ_i identically distributed

We suppose ξ_i identically distributed

Brownian motion

1. Local in time: $\langle \tau \rangle < \infty$
2. Local in space: $\langle \xi^2 \rangle < \infty$
3. Markovian: $\langle \xi_i \xi_j \rangle = \delta_{i,j}$

$$x(t) \sim \sqrt{t}$$

$$Z(x, x_0, t) = \frac{e^{-\frac{(x-x_0)^2}{2t}}}{\sqrt{2\pi t}}$$

Fractional Brownian Motion (fBm)

$$Z(x, x_0, t) = \frac{e^{-\frac{(x-x_0)^2}{2t^{2H}}}}{\sqrt{2\pi t^H}} \quad \text{with} \quad 0 < H < 1$$

$$\langle [x(t_1) - x(t_2)]^2 \rangle \sim |t_1 - t_2|^{2H}$$

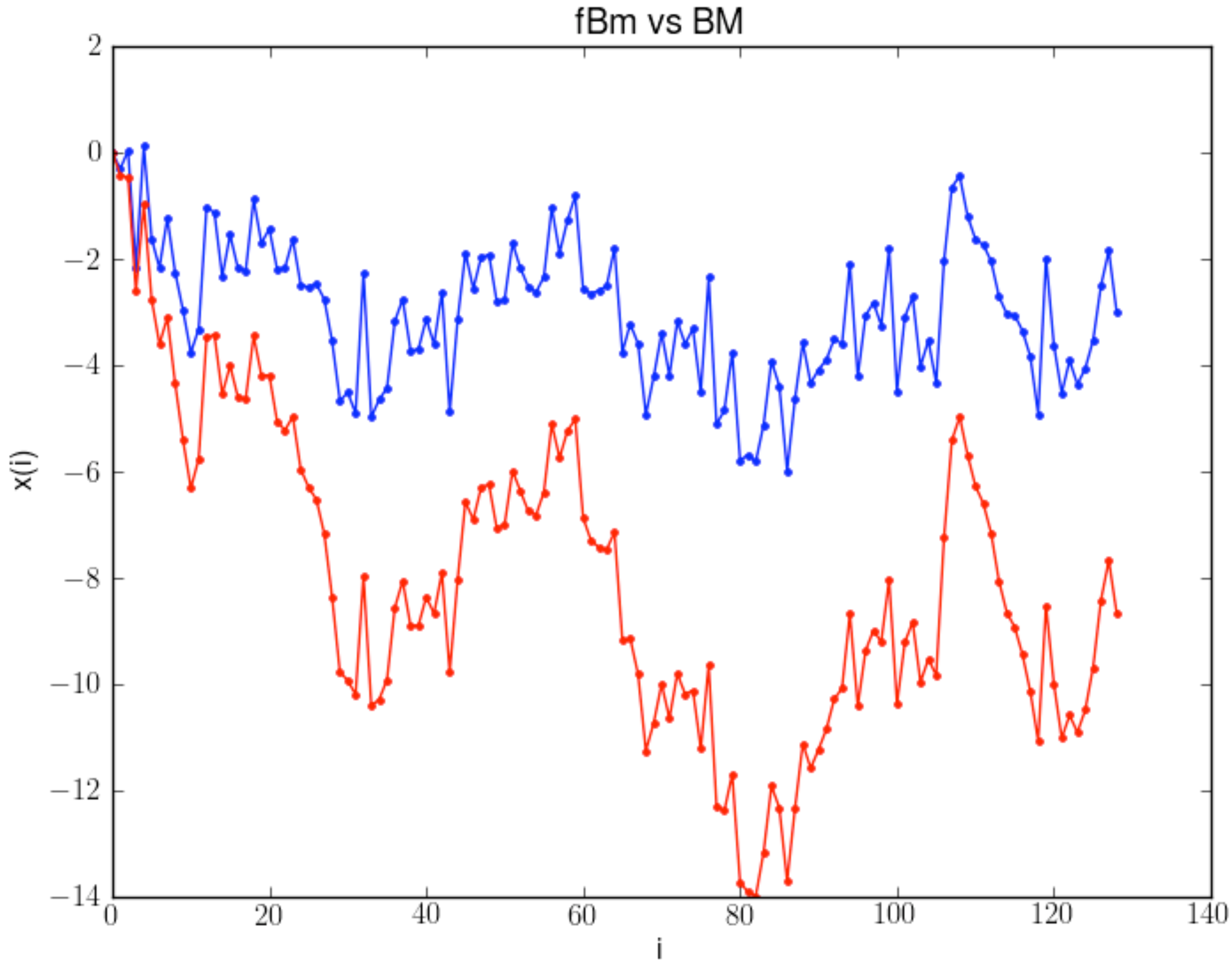
$$\xi_t = x(t+1) - x(t)$$

$$\langle \xi_0 \xi_t \rangle \sim f(t)$$

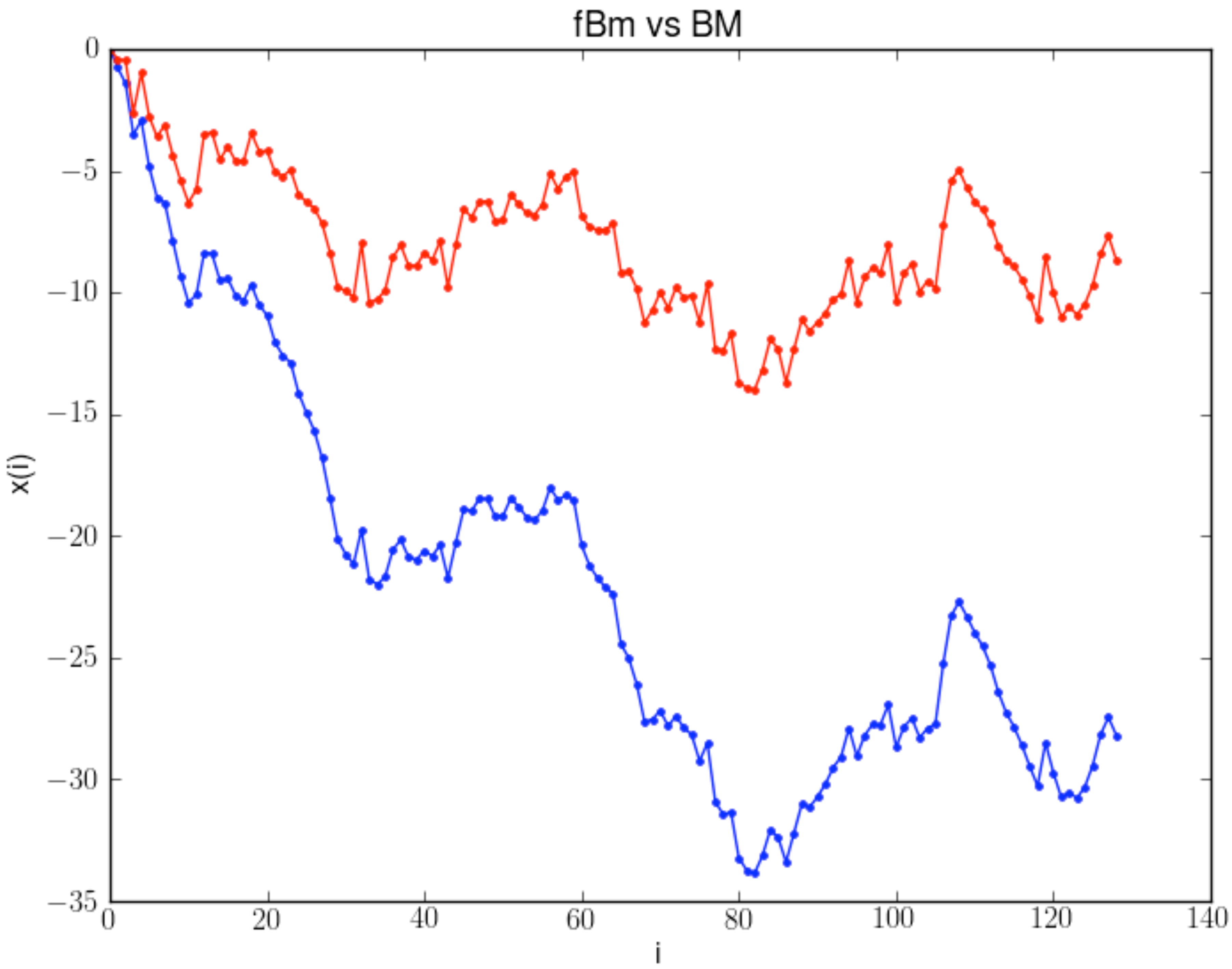
$$\rightarrow f(t) \sim -\frac{1}{t^{2-2H}} \quad H < 1/2$$

$$\rightarrow f(t) \sim +\frac{1}{t^{2-2H}} \quad H > 1/2$$

Subdiffusion: $H = 1/4$



Superdiffusion: $H = 3/4$



Continuous Time Random Walk (CTRW)

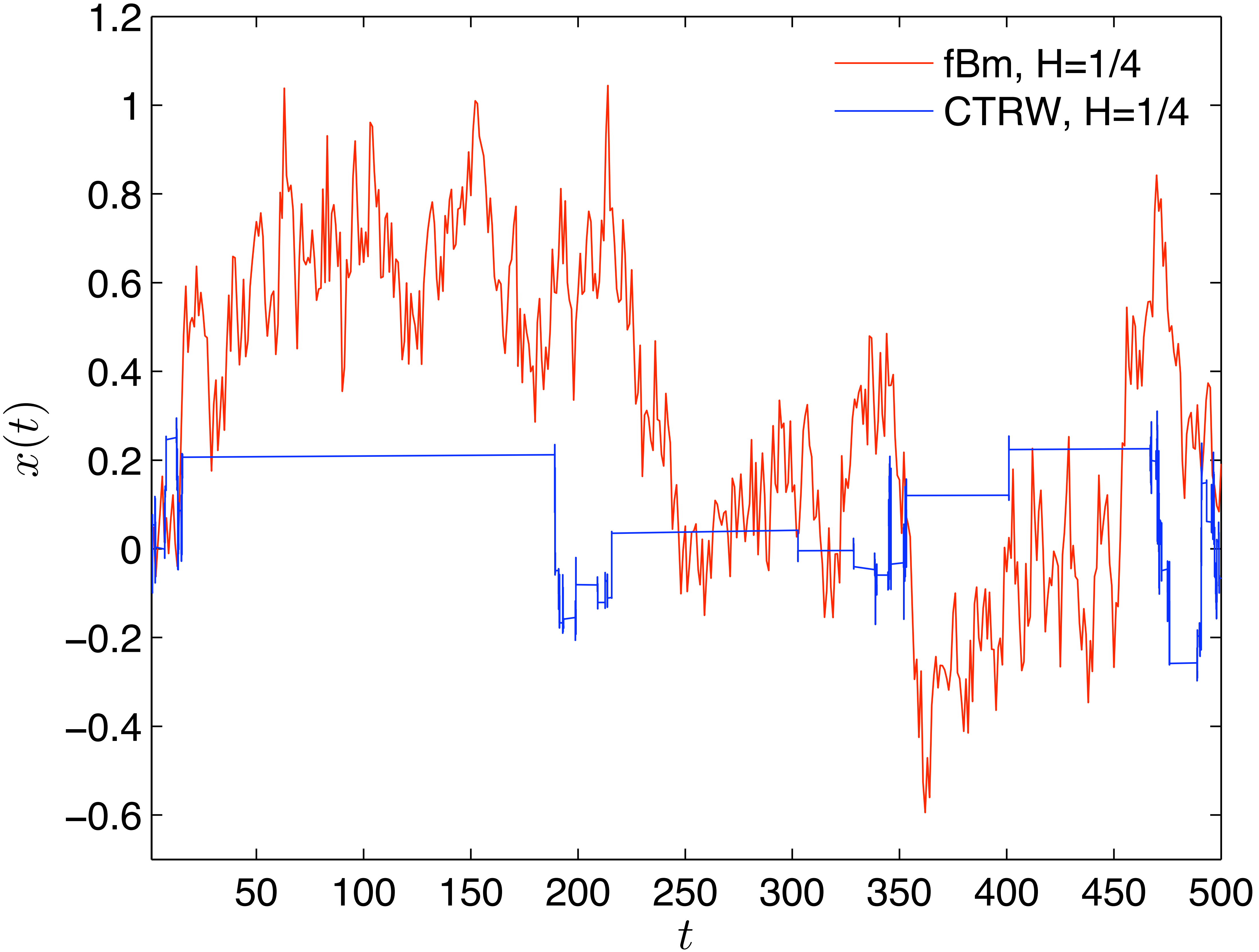
$$p(\tau) \xrightarrow{\tau \gg 1} \frac{1}{\tau^{\alpha+1}}$$

$$\text{For } 0 < \alpha < 1,\ x(t) \sim t^{\frac{\alpha}{2}}$$

$$Z(x, x_0, t) = \frac{1}{t^{\frac{\alpha}{2}}} F\left(\frac{x - x_0}{t^{\frac{\alpha}{2}}}\right)$$

Non Gaussian Process

CTRW vs fBm



fBm, H=1/4
CTRW, H=1/4
1.2
1
0.8
0.6
0.4
0.2
0
−0.2
−0.4
−0.6
$x(t)$
50
100
150
200
250
300
350
400
450
500
t

Lévy flights

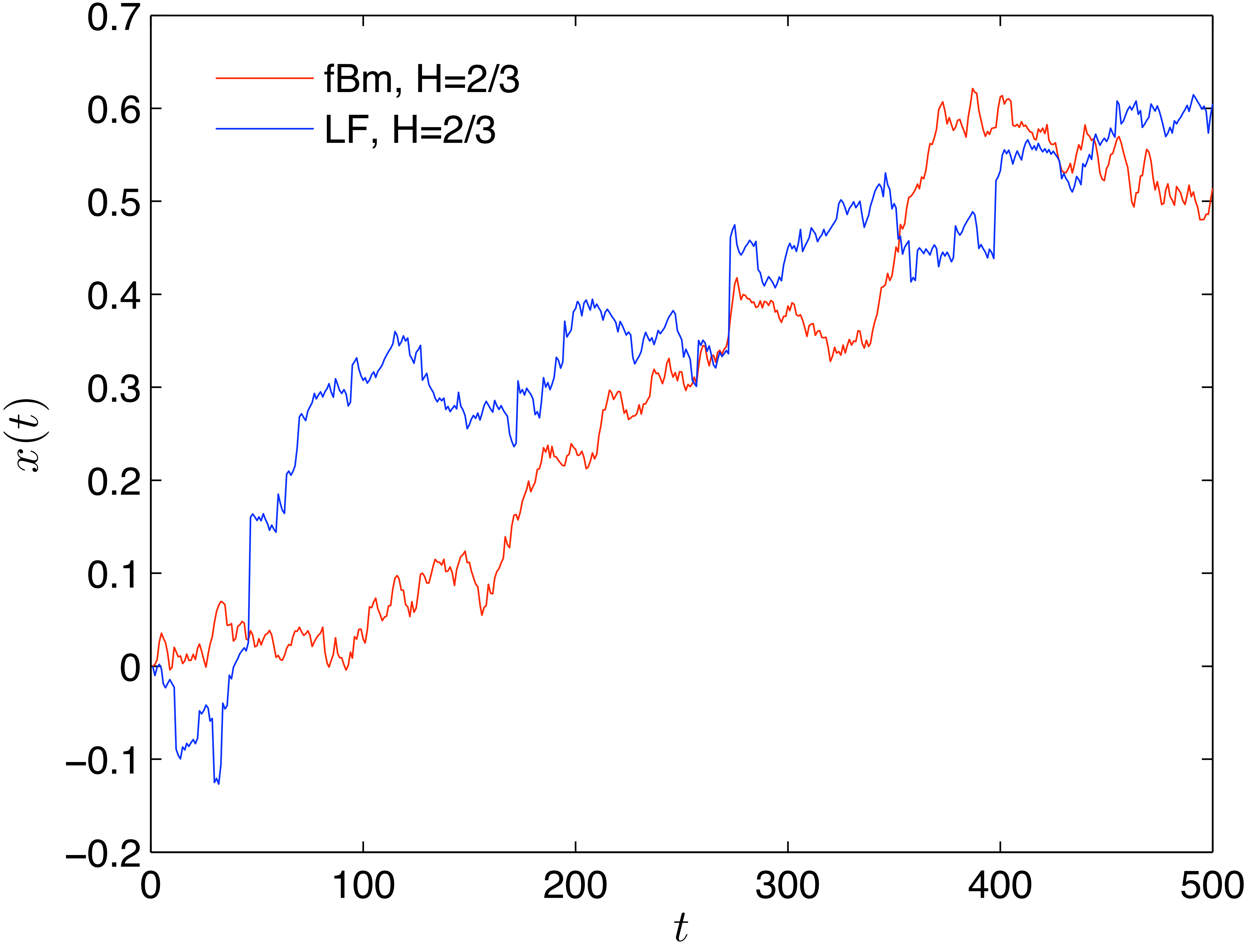
$$p(\xi) \xrightarrow{\xi \gg 1} \frac{1}{\xi^{\mu+1}}$$

$$\text{For } 0 < \mu < 2,\ x(t) \sim t^{\frac{1}{\mu}}$$

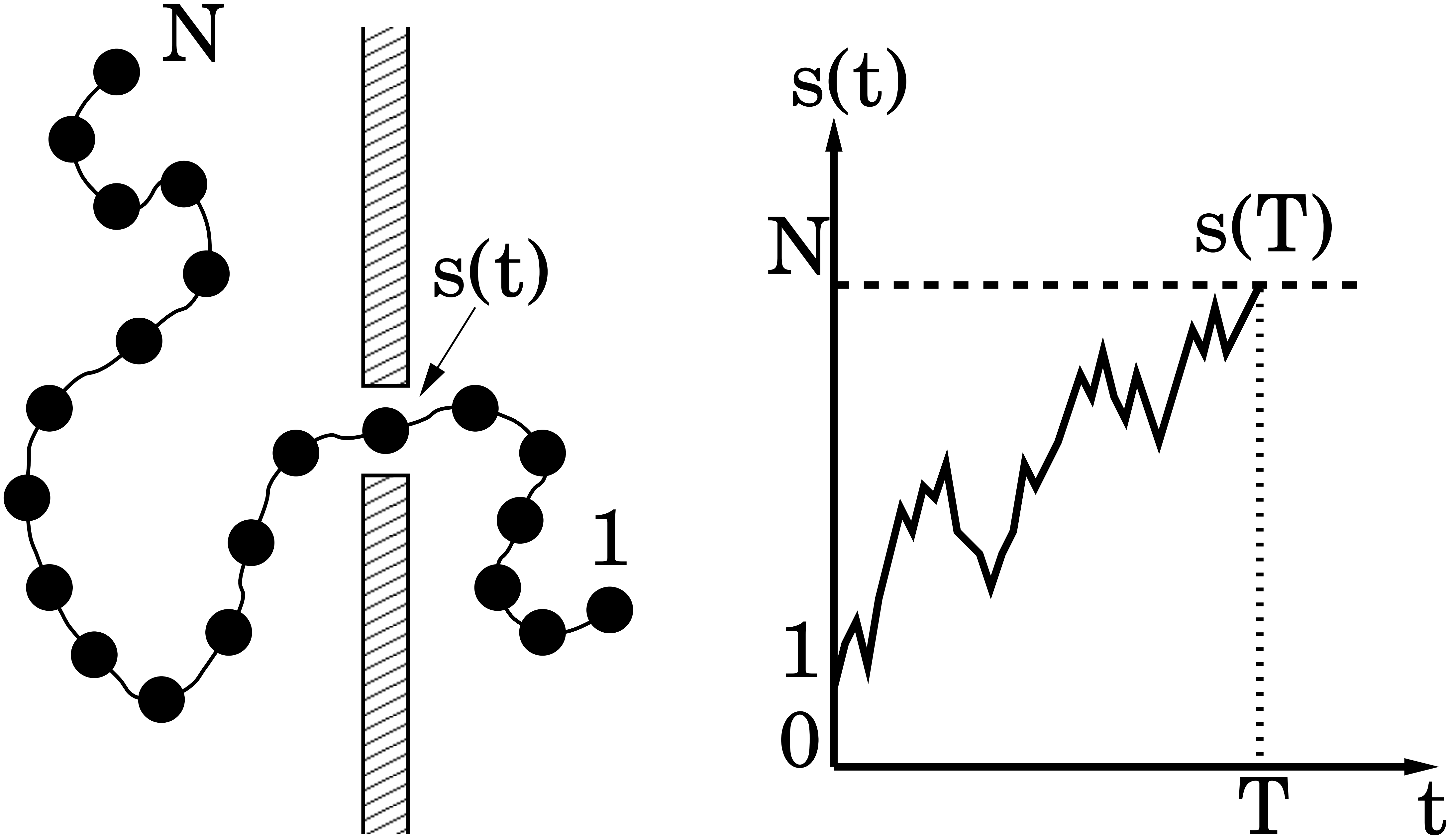
$$Z(x, x_0, t) = \frac{1}{t^{\frac{1}{\mu}}} F\left(\frac{x - x_0}{t^{\frac{1}{\mu}}}\right)$$

Non Gaussian Process

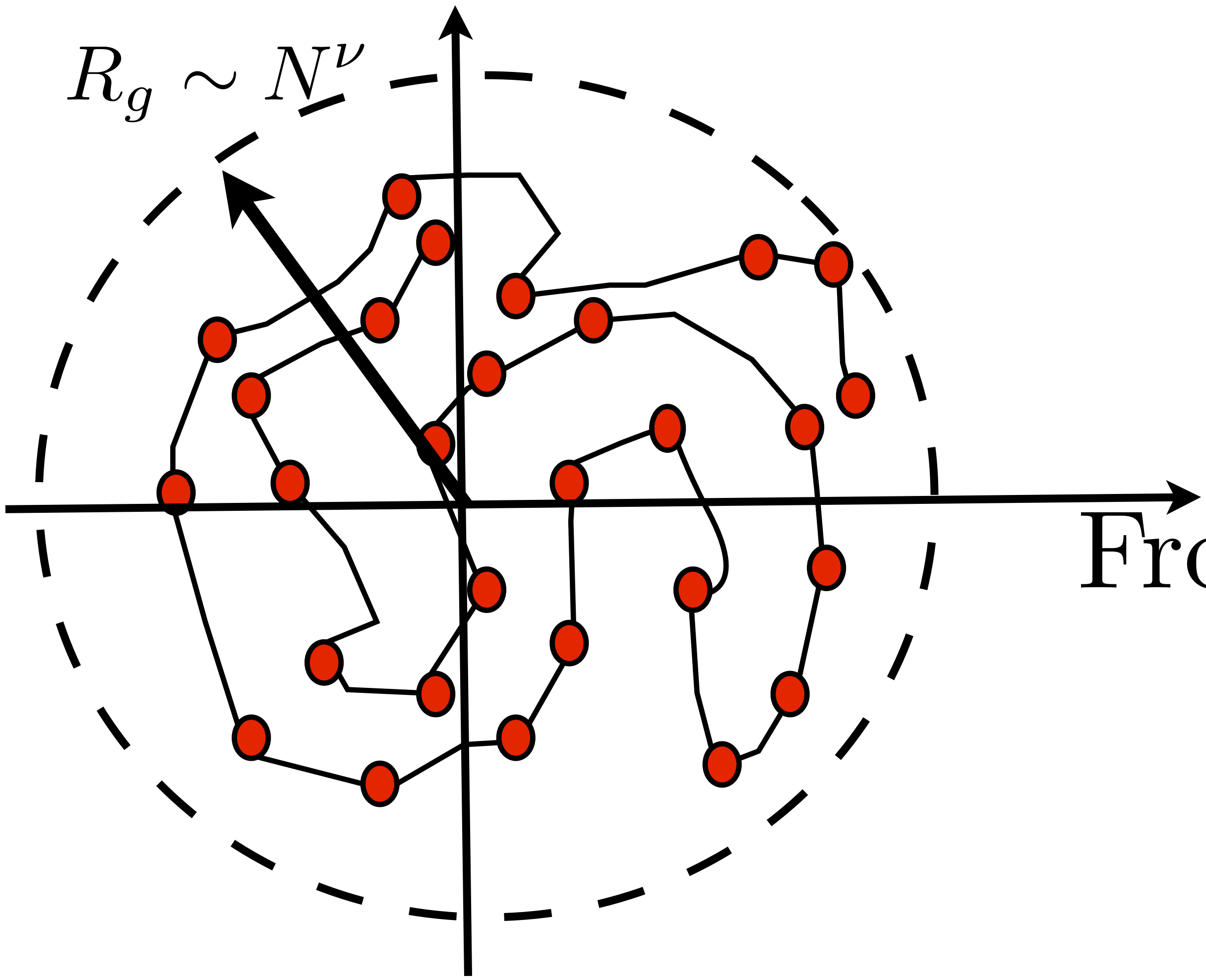
Lévy flights vs fBm



Polymer Translocation



$$s(T) = N, \text{ if } s(t) \sim t^H \text{ then } T \sim N^{1/H}$$



$R_g(N)$ gyration Radius

Phantom polymer $\nu = 1/2$

Excluded Volume $\nu > 1/2$

From polymer physics: $s(t) \sim t^H$

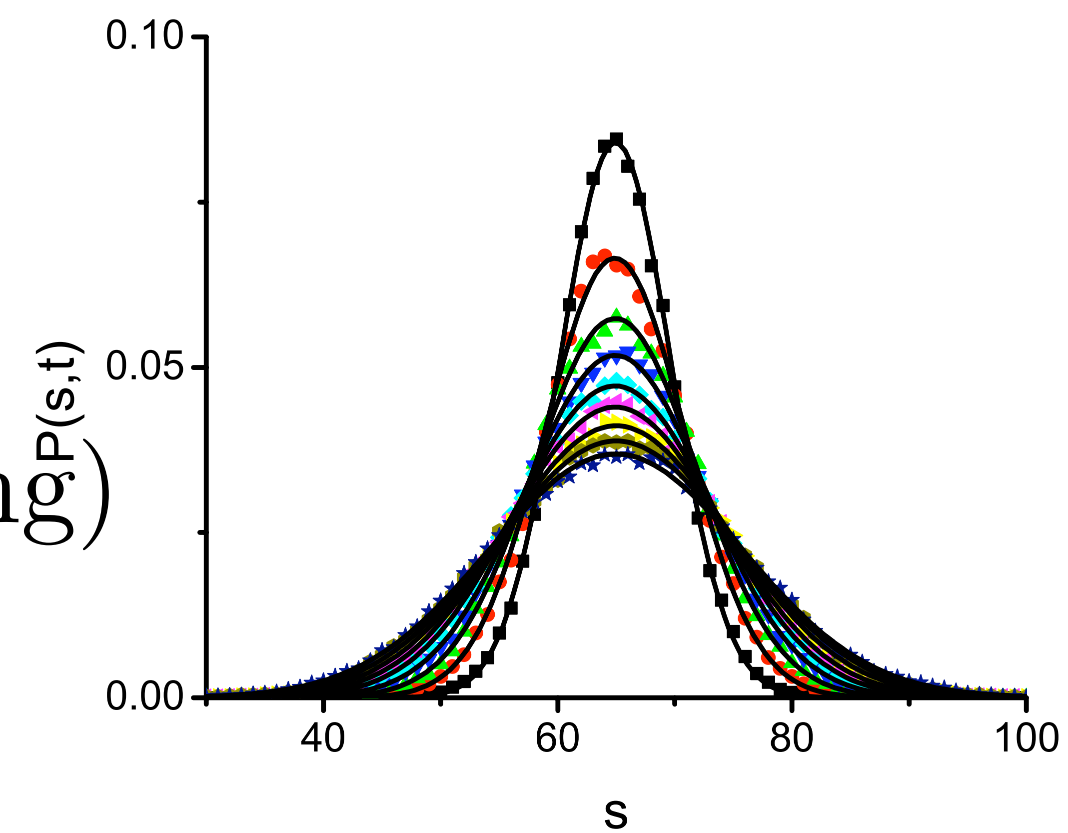
$$H = \frac{1}{2\nu+1}$$

Numerical Simulations

Gaussian process!

System is equilibrated (no aging)

fBm

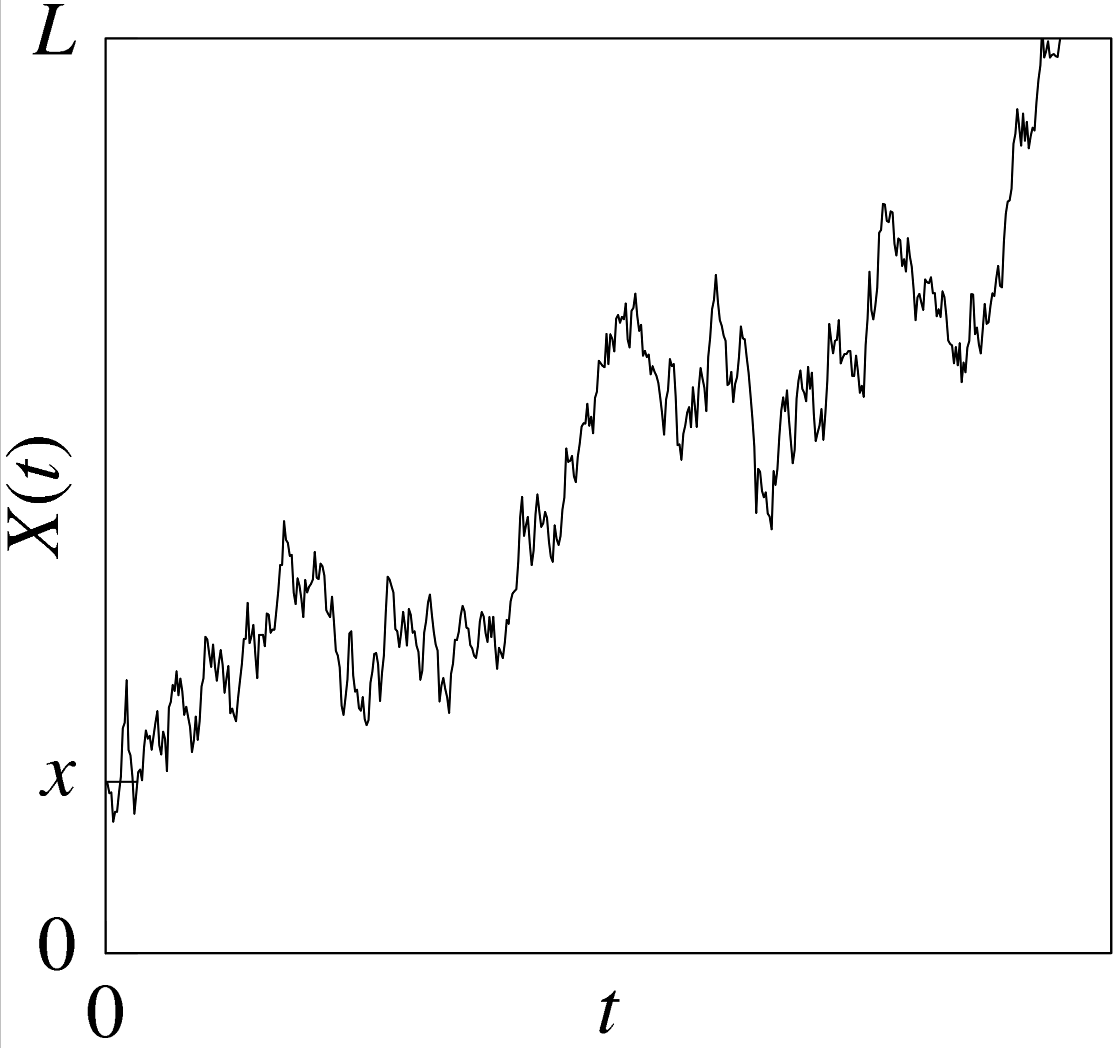


Monte Carlo simulation of polymer translocation in d=2, Chatelain, Kantor, Kardar, PRE 78, 021129 (2008)

Question I: A polymer chain will ultimately succeed in translocating through a pore ?

Question II: Which portion of the polymer has translocated at time t?

Hitting probability $Q(x,L)$: probability of exiting through L



Markov process:

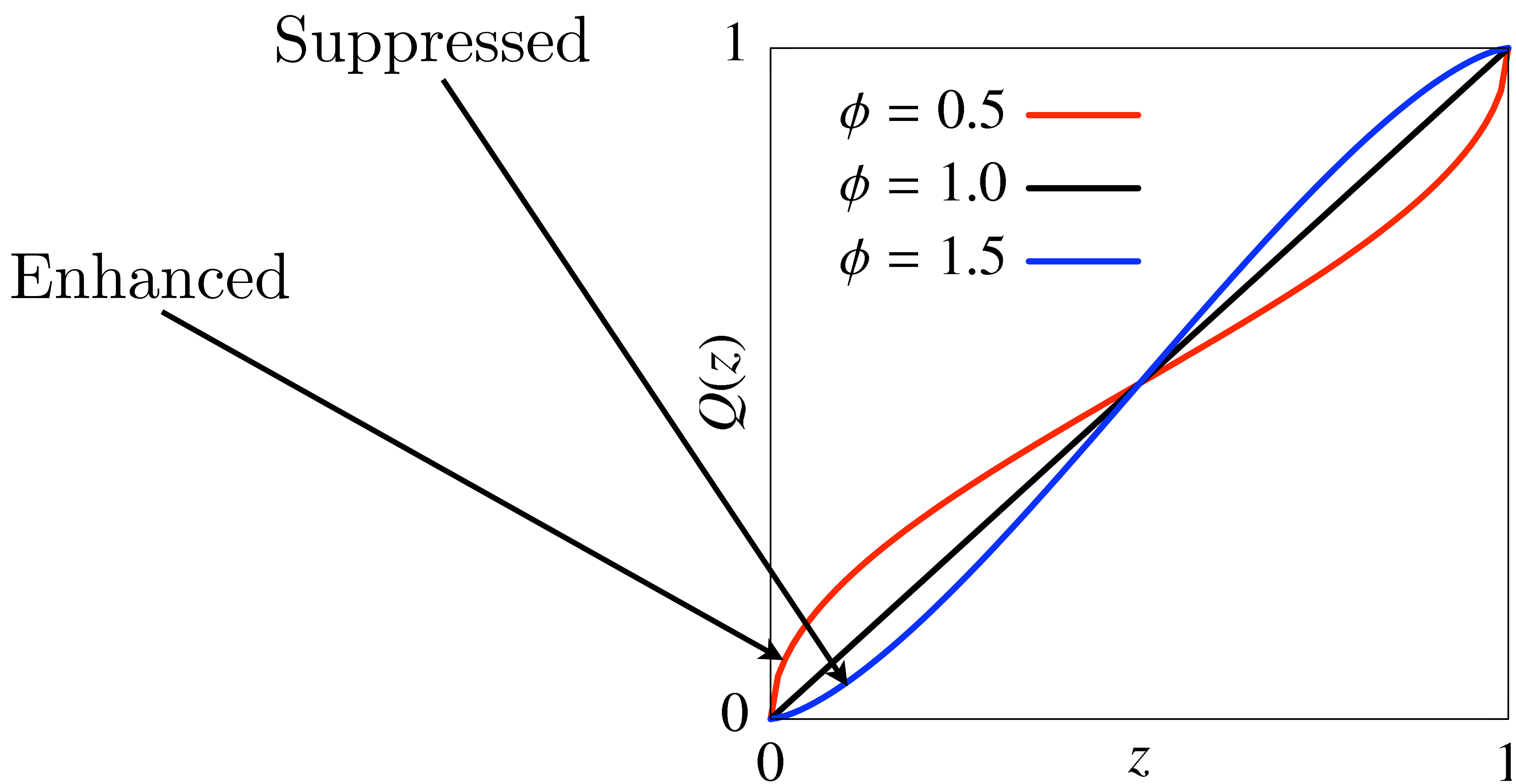
$$Q(x,L) = \langle Q(x+\xi_1, L)\rangle$$

For BM $\langle \xi_1 \rangle = 0$, $\langle \xi_1^2 \rangle = \delta$

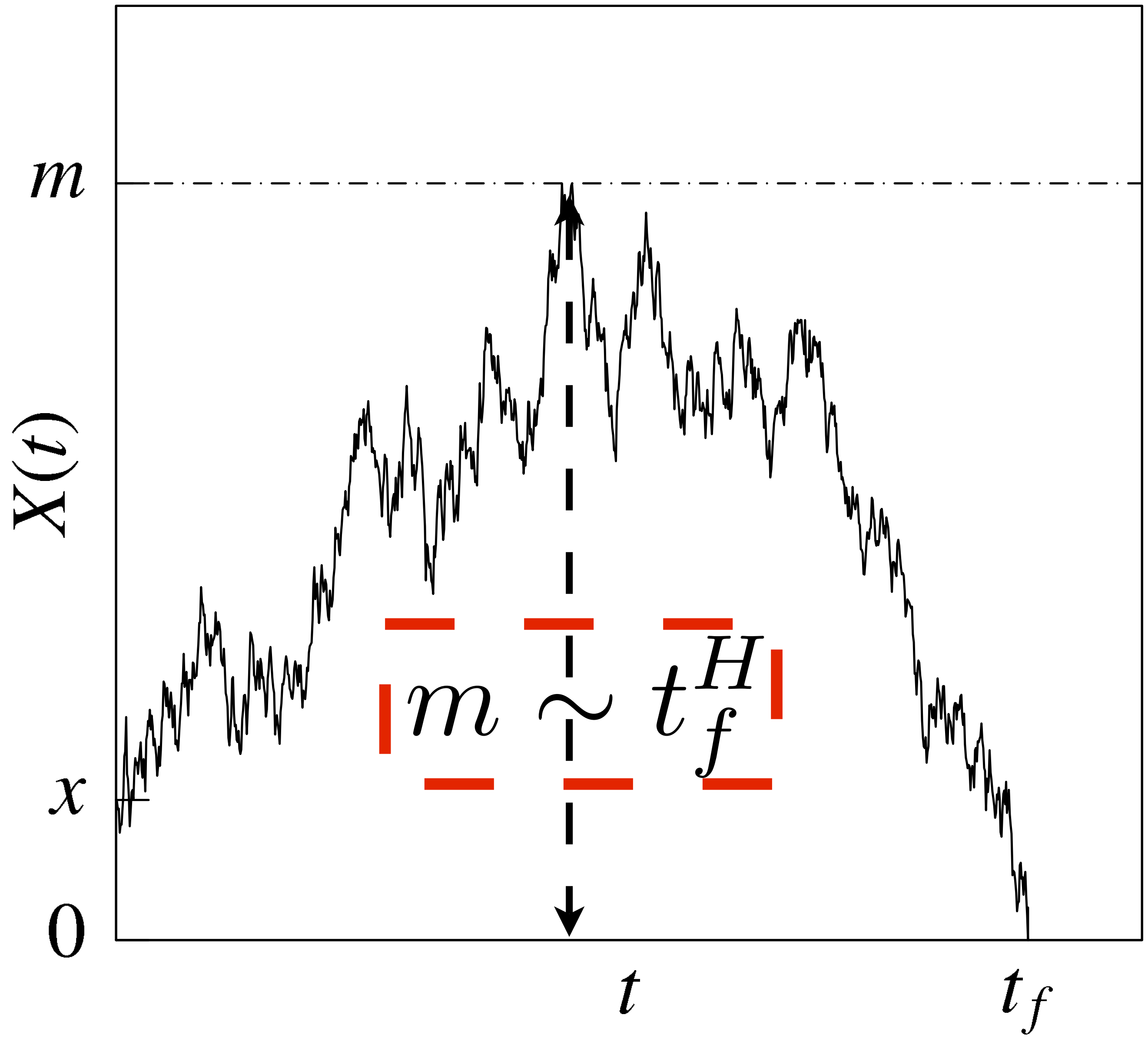
$$\frac{\partial^2 Q}{\partial x^2} = 0 \quad Q(0,L)=0,\ Q(L,L)=1$$

$$Q(x,L) = \frac{x}{L}$$

- Self affine process: $Q(x, L) = Q(z = \frac{x}{L})$
- Symmetric process: $Q(1/2) = 1/2$; $Q(z) = 1 - Q(1 - z)$
- Close to the origin: $Q(z) \sim c_1 z^{\phi} + \dots$



Translocation is enhanced or suppressed by excluded volume effects?



$$Q(x,L) = \text{Prob}[m > L]$$

means

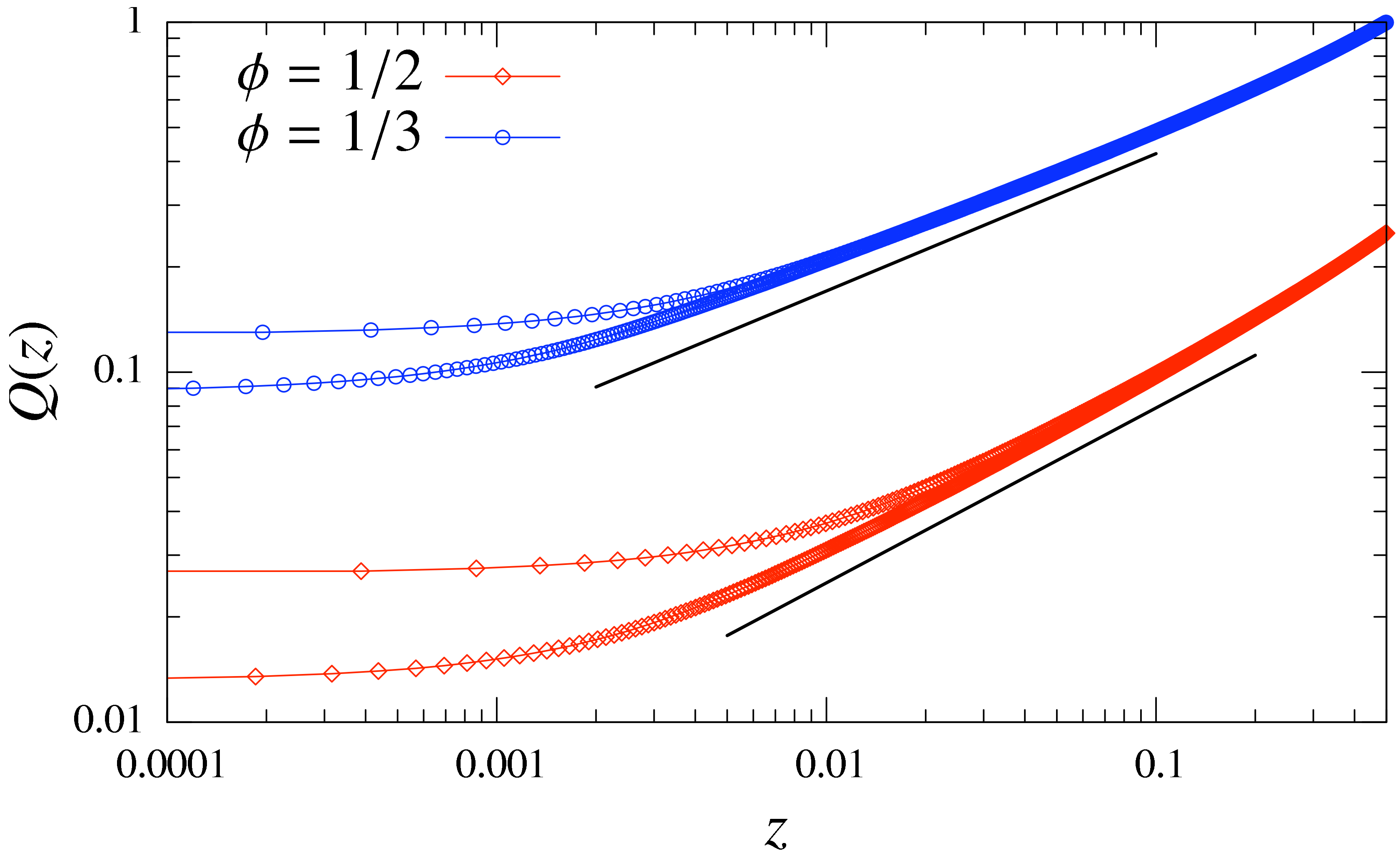
$$\text{Prob}[t_f > L^{1/H}]$$

Survival probability: $\text{Prob}[t_f > t] \sim \left(\frac{x^{1/H}}{t}\right)^{\theta}$

θ persistence exponent

$$Q(x,L) \sim \text{Prob}[t_f > L^{\frac{1}{H}}] \sim \left(\frac{x}{L}\right)^{\frac{\theta}{H}}, \qquad \phi = \frac{\theta}{H}$$

Numerical test $\phi = \theta/H$



Persistence of fBm in known $\theta = 1 - H$ (see Krug et al.)

Prediction: $\phi = \frac{\theta}{H} = \frac{1-H}{H}$

- Blue: $H = 3/4 \longrightarrow \phi = 1/3$
- Red: $H = 2/3 \longrightarrow \phi = 1/2$

Conclusion: volume effects "suppress" Translocation

Other models $\phi = \theta/H$:

CTRW: $H = \alpha/2,\ \theta = 2/\alpha$

$$\frac{\partial^2 Q}{\partial x^2} = 0 \quad Q(0,L) = 0,\ Q(L,L) = 1$$

$$\phi = 1$$

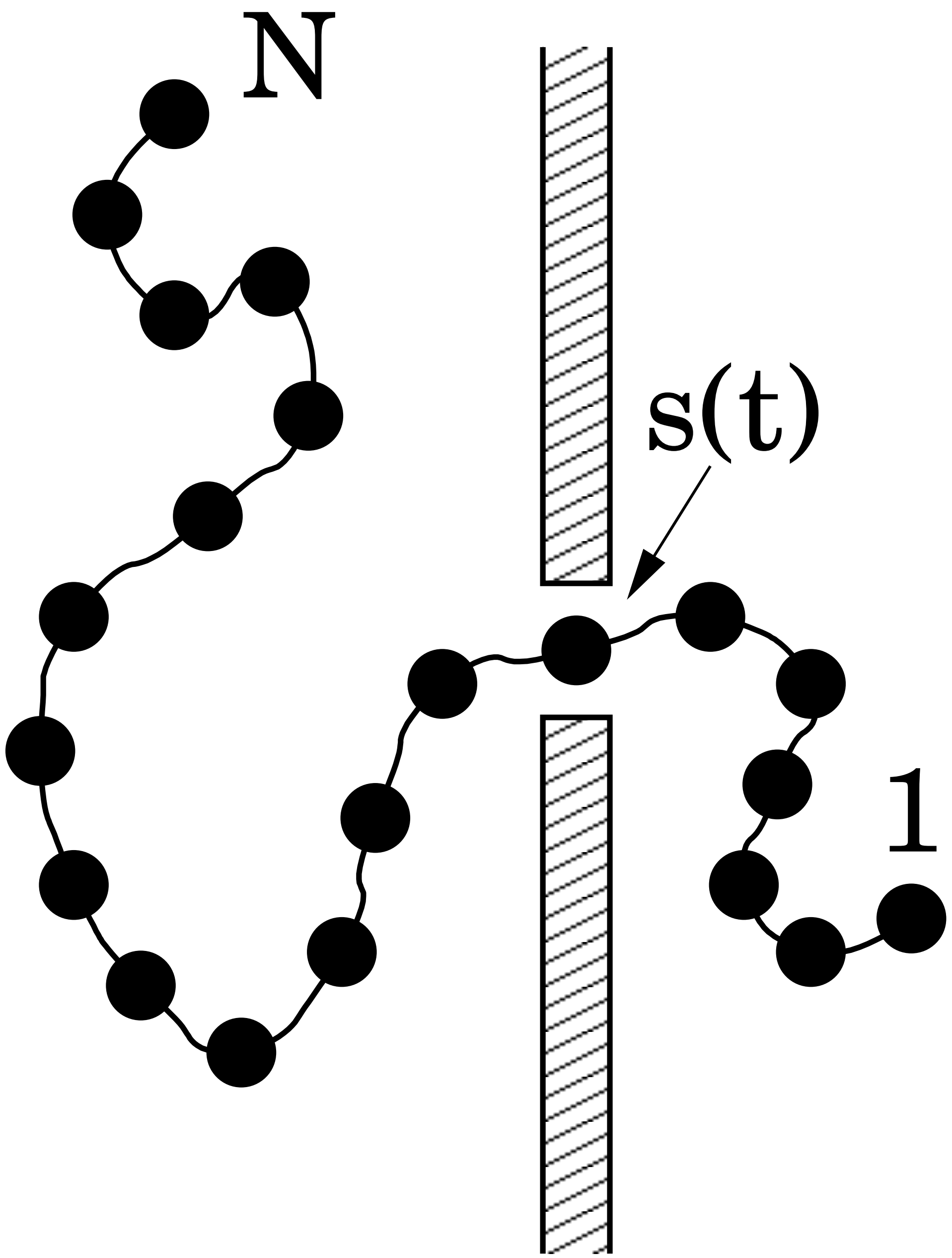
$$Q(x,L) = \frac{x}{L}$$

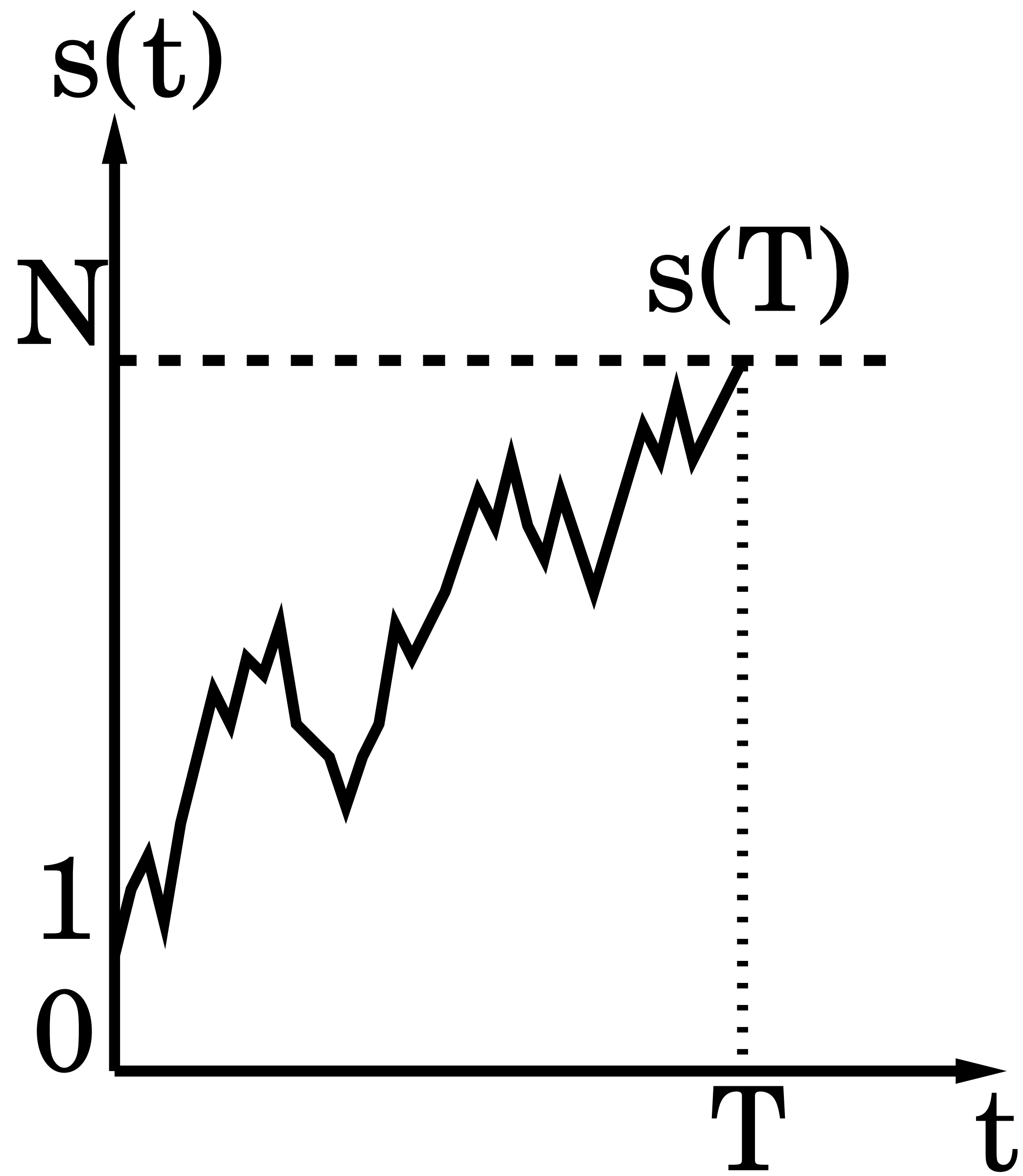
Lévy flights: $H = 1/\mu,\ \theta = 1/2$ (Sparre Andersen)

Widom ('61): $Q(z = \frac{x}{L}) = I_z[\frac{\mu}{2}, \frac{\mu}{2}]$

$$\phi = \mu/2$$

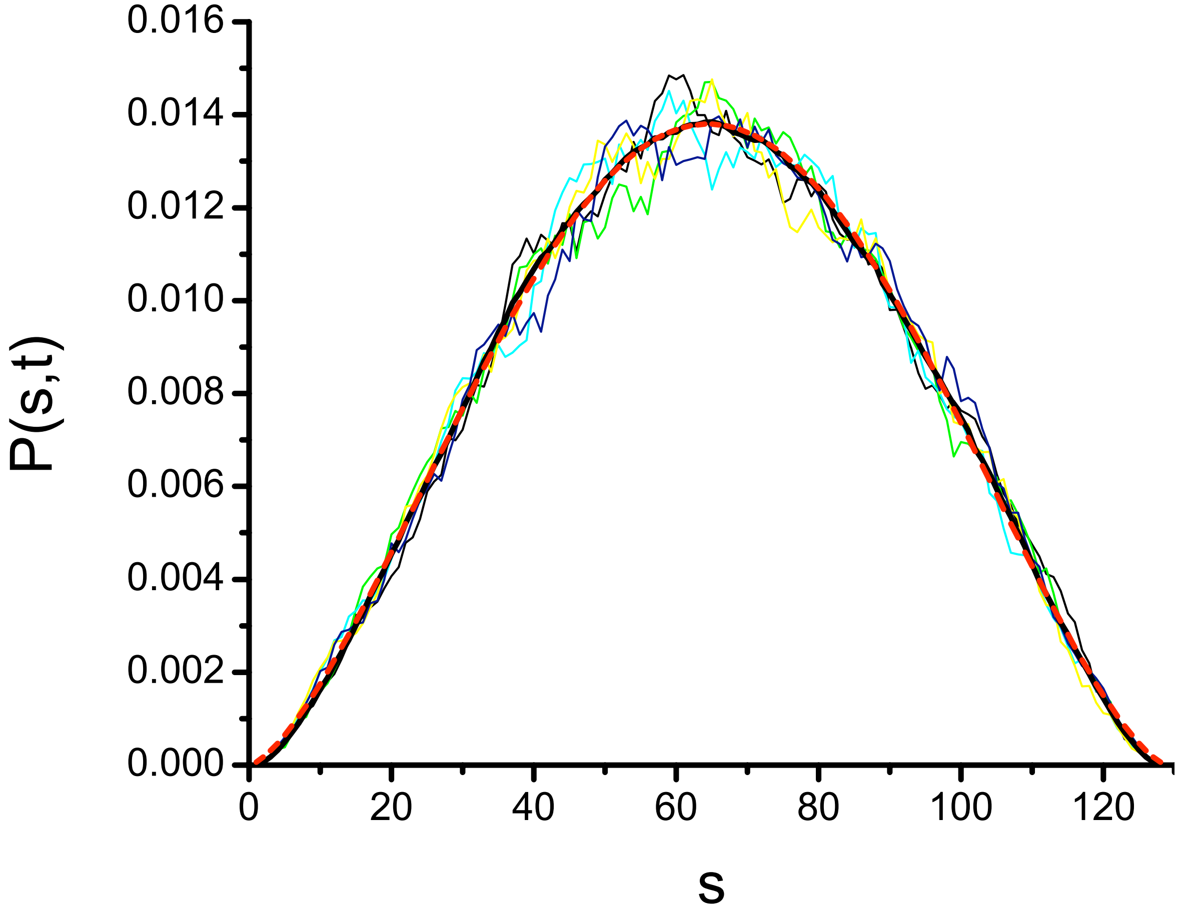
Polymer Translocation



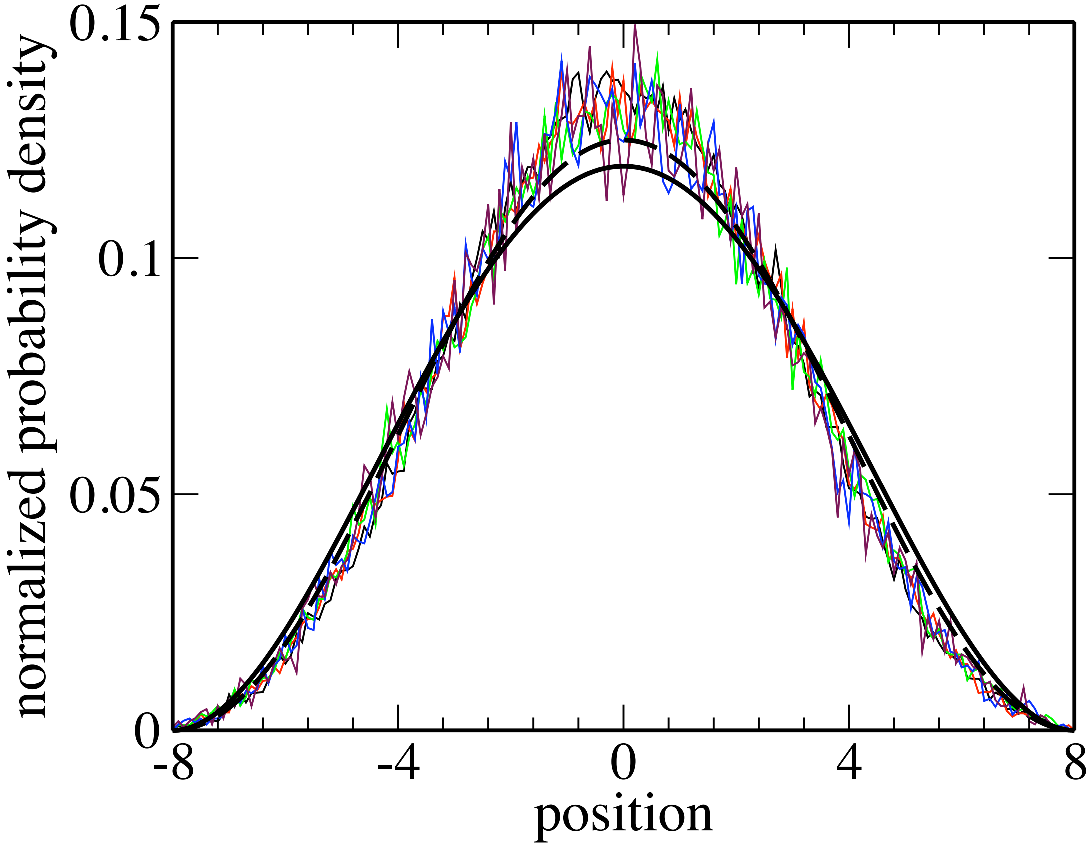


$$s(T) = N, \text{ if } s(t) \sim t^H \text{ then } T \sim N^{1/H}$$

Numerical Simulations:



Monte Carlo simulation of polymer translocation in d=2,
Chatelain, Kantor, Kardar, PRE 78, 021129 (2008)

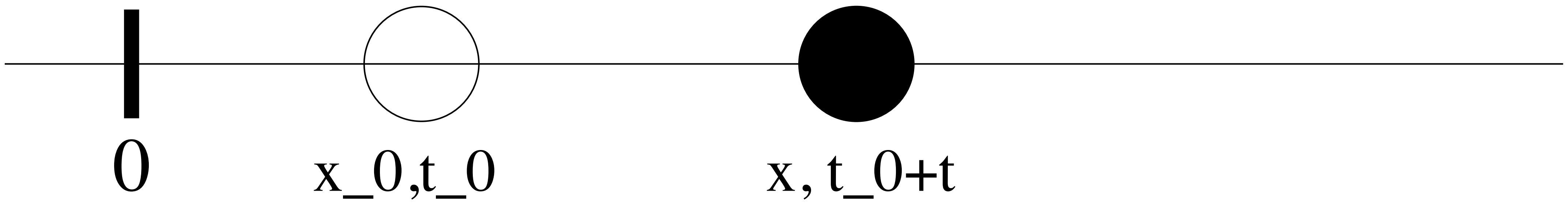


Monte Carlo simulation tagged monomer in a box (d=1)
Kantor, Kardar, PRE 76, 061121 (2007)

$$d = 2, \quad \nu = \frac{3}{4}, \quad H = \frac{1}{2\nu + 1} = \frac{2}{5}$$

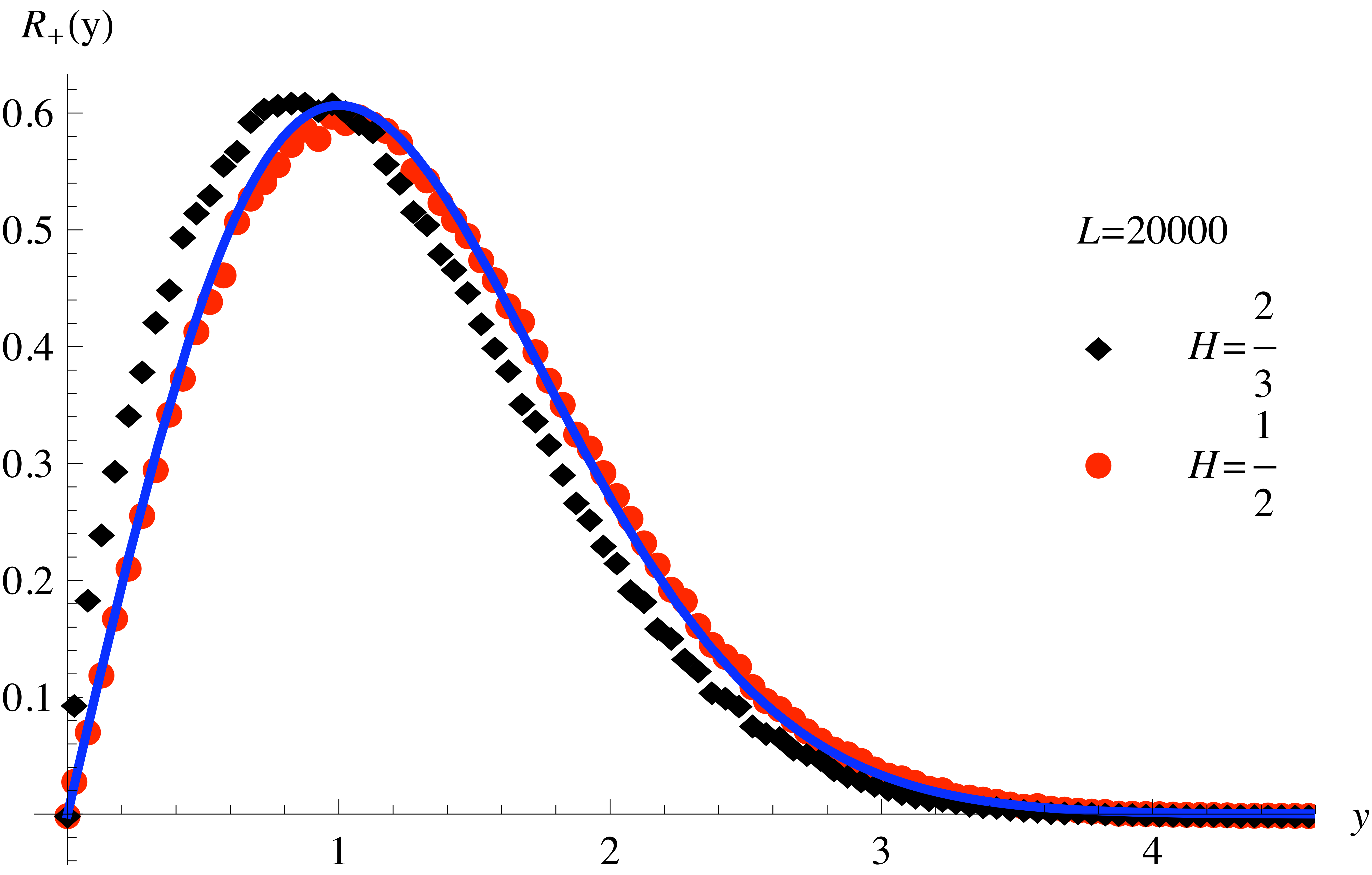
$$d = 1, \quad H = \frac{1}{4}$$

Single Boundary

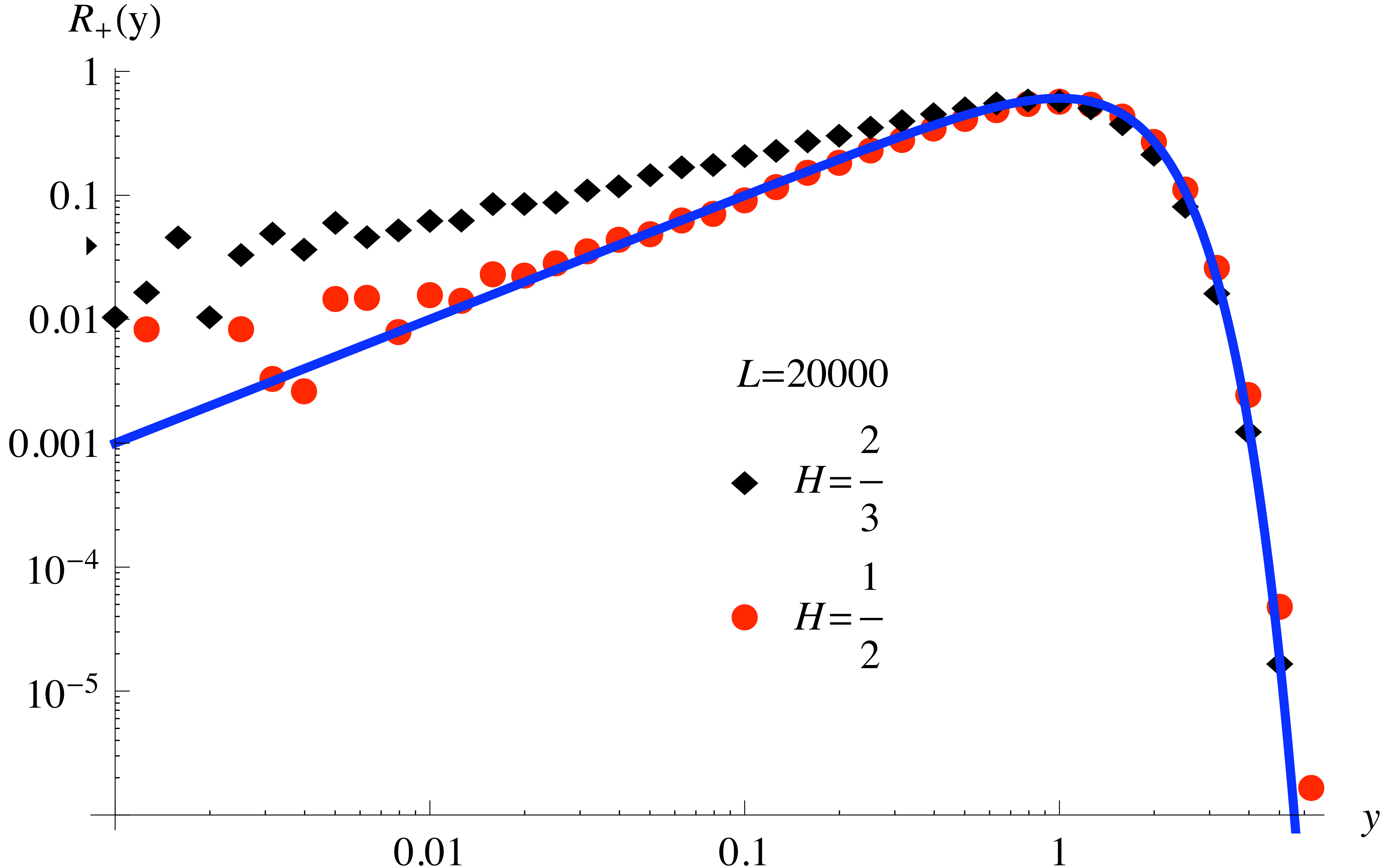


For homogeneous processes, we predict $\sim x^{\phi}$ with $\phi = \frac{\theta}{H}$

- 2d translocation: simulations give $\phi \sim 1.44$ we predict $\phi = 1.5$
- Tagged monomer: Simulations give $\phi > 2$ we predict $\phi = 3$
- Direct simulations on fBm agree with scaling argument

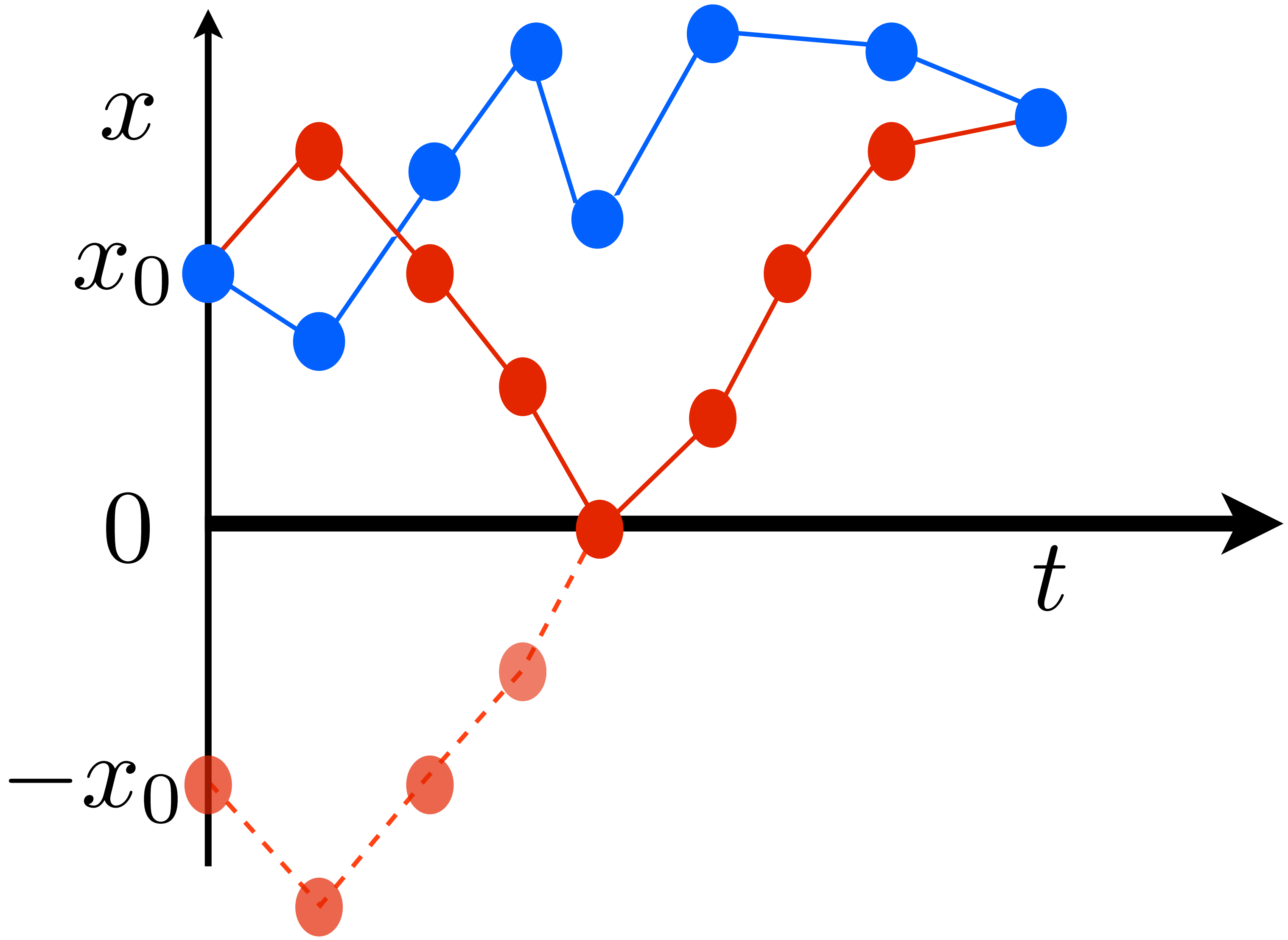


$R_+(y)$
0.6
0.5
0.4
0.3
0.2
0.1
1
2
3
4
y
$L=20000$
$H=\frac{2}{3}$
$H=\frac{1}{2}$



$R_+(y)$
1
0.1
0.01
0.001
10^{-4}
10^{-5}
0.01
0.1
1
y
L=20000
$H=\frac{2}{3}$
$H=\frac{1}{2}$

Images method: Brownian motion



$$Z(x, x_0, t) = \frac{e^{-\frac{(x-x_0)^2}{2t}}}{\sqrt{2\pi t}}$$

$$Z_+(x, x_0, t) = ?$$

$$Z_+(x, x_0, t) = Z(x, x_0, t) - Z(x, -x_0, t)$$

Images method: Brownian motion

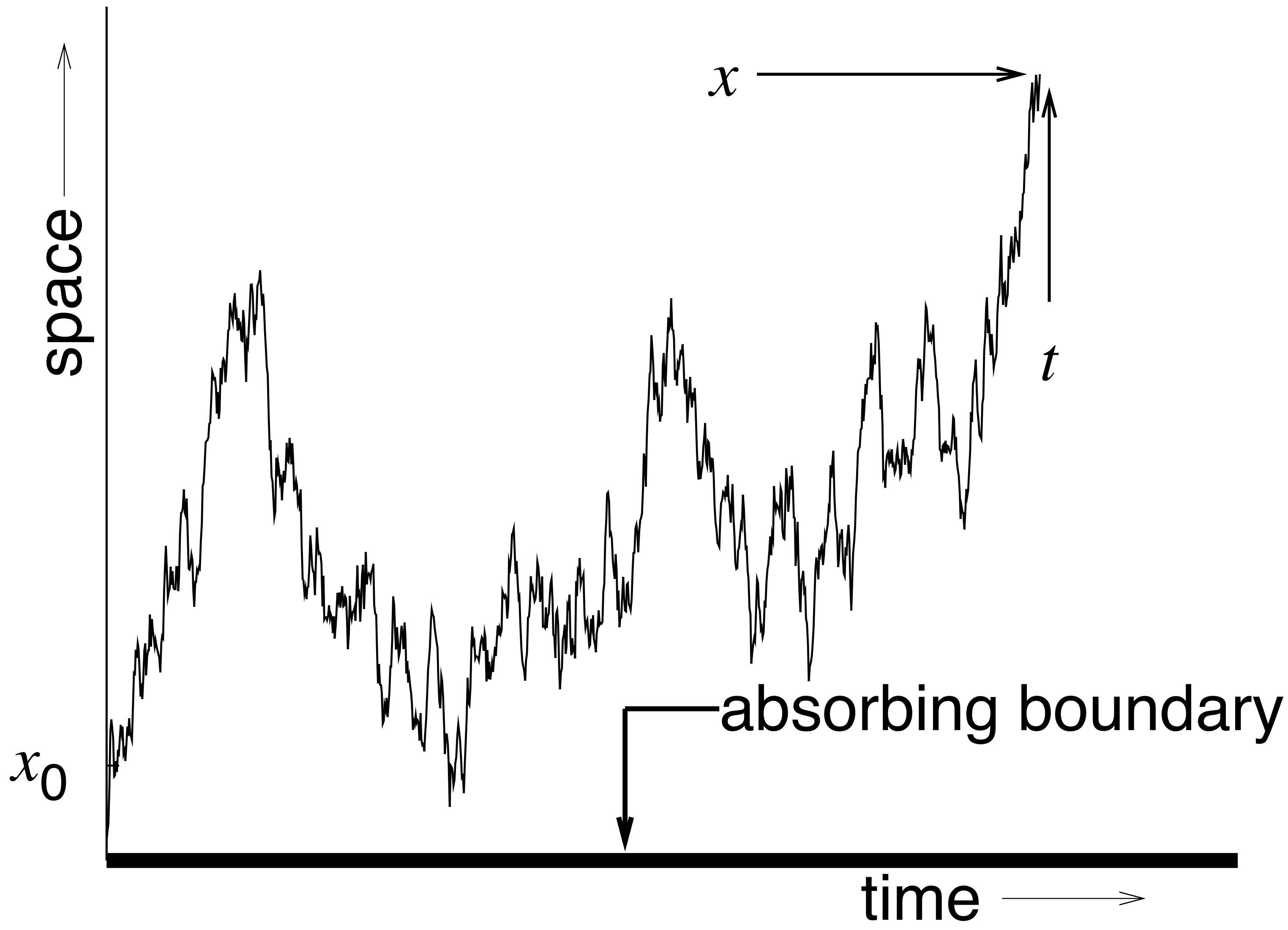
$$P_+(x,x_0,t) = \frac{Z_+(x,x_0,t)}{\int_0^\infty dx\, Z_+(x,x_0,t)} \xrightarrow{t\to\infty} P_+(x,t)$$

Using $y = \frac{x}{\sqrt{t}}$ $\qquad P_+(x,t)\,dx = R_+(y)\,dy = y\,e^{-\frac{y^2}{2}}\,dy$

$$\boxed{R_+(y) = y\,e^{-\frac{y^2}{2}}}$$

For images method $\phi = 1$ always.

Path integral method: Perturbation Theory



$$Z_+(x_0, x, t) = \int_{x(0)=x_0}^{x(t)=x} \mathcal{D}[x]\, e^{-\mathcal{S}[x]}\, \Theta[x]$$

$$Z_+(x_0, x, t) = \int_{x(0)=x_0}^{x(t)=x} \mathcal{D}[x]\, e^{-\mathcal{S}[x]}\, \Theta[x]$$

$$e^{-\mathcal{S}[x]} \sim e^{-\mathcal{S}^{(0)}[x]} \left(1 + \epsilon\, \mathcal{S}^{(1)}[x]\right)$$

$$Z_+(x_0, x, t) \sim Z_+^{(0)}(x_0, x, t) + \epsilon\, Z_+^{(1)}(x_0, x, t)$$

$$Z_+^{(1)}(x_0, x, t) = \int_{x(0)=x_0}^{x(t)=x} \mathcal{D}[x]\, \mathcal{S}^{(1)}[x]\, e^{-\mathcal{S}^{(0)}[x]}\, \Theta[x]$$

For Brownian Motion $$\mathcal{S}[x] = \frac{1}{2}\int_0^t dt\, \left(\frac{dx}{dt}\right)^2$$

For Gaussian process

$$\mathcal{S}[x] = \frac{1}{2}\int_0^t dt_1 \int_0^t dt_2\, x(t_1)G(t_1, t_2)x(t_2)$$

$$\boxed{\langle x(t_1)x(t_2)\rangle = G^{-1}(t_1, t_2)}$$

Brownian motion

$$H = \frac{1}{2} \quad \Rightarrow \quad \langle x(t_1)x(t_2)\rangle = 2\min(t_1, t_2) \quad \Rightarrow \quad \mathcal{S}^{(0)}[x] = \frac{1}{4}\int_0^t dt' \,(\partial_{t'} x)^2$$

Fractional Brownian motion

$$H-\mathrm{fBm} \quad \Rightarrow \quad \langle x(t_1)x(t_2)\rangle = t_1^{2H} + t_2^{2H} - |t_1 - t_2|^{2H} \quad \Rightarrow \quad \mathcal{S}[x]\ ??$$

Perturbation

$$H = \frac{1}{2} + \epsilon \quad \Rightarrow \quad \langle x(t_1)x(t_2)\rangle = 2\,\min(t_1, t_2) - \epsilon\,\Sigma(t_1, t_2) + O(\epsilon^2)$$

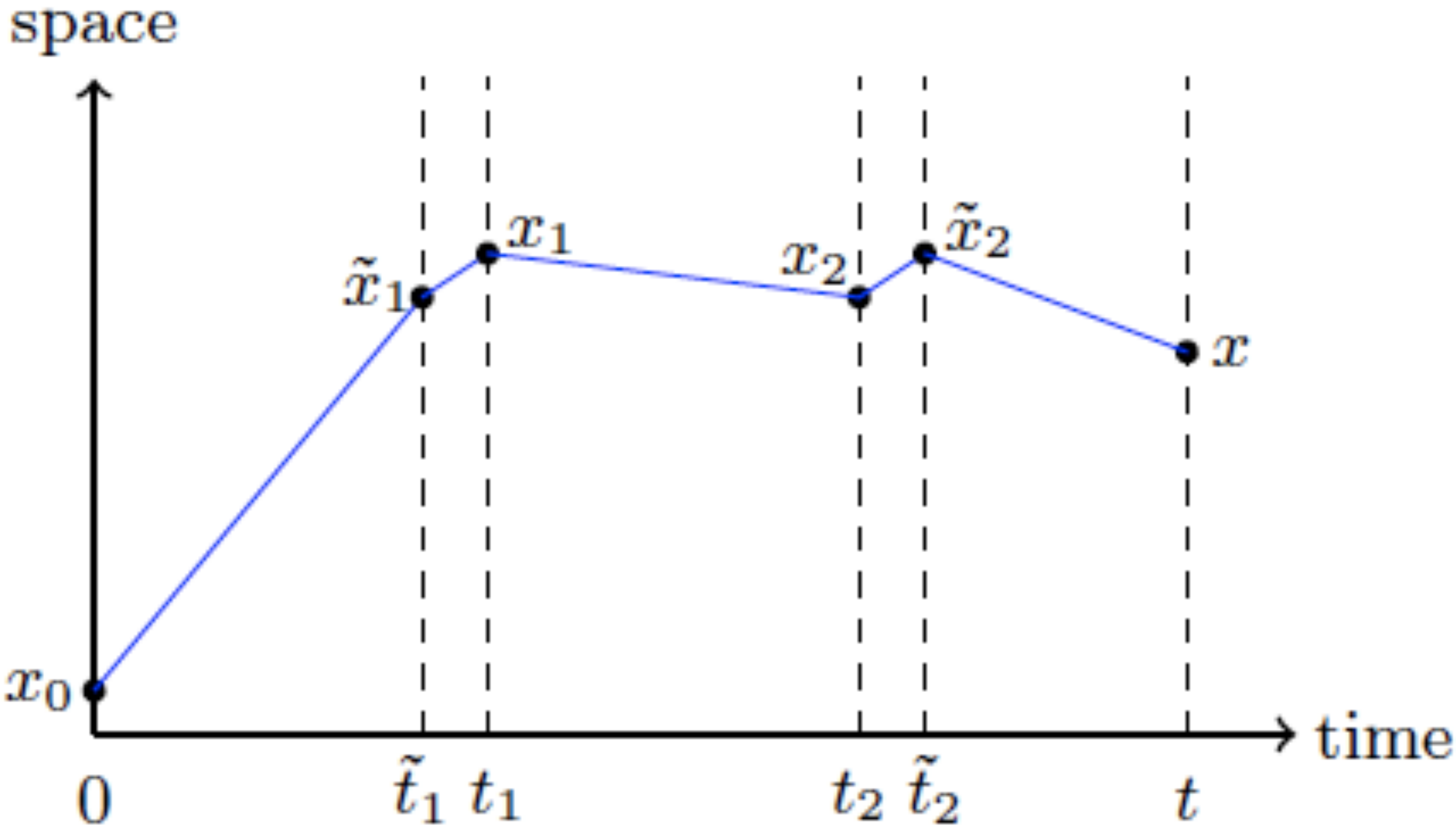
$$\Sigma(t_1, t_2) = -2\left[t_1 \ln t_1 + t_2 \ln t_2 - |t_1 - t_2| \ln |t_1 - t_2|\right]$$

$$G^{-1}(t_1,t_2) = [G^{(0)}]^{-1}(t_1,t_2) - \epsilon\Sigma(t_1,t_2) \implies \epsilon\Sigma = [\, G^{(0)}]^{-1} - G^{-1}$$

$$G = G^{(0)} + \epsilon G^{(0)}\Sigma G \implies G = G^{(0)} + \epsilon G^{(0)}\Sigma G^{(0)}$$

$$\mathcal{S}[x] = \mathcal{S}^{(0)}[x] + \epsilon\,\mathcal{S}^{(1)}[x]$$

$$\mathcal{S}^{(1)}[x] \quad \propto \quad -\frac{1}{2}\int_0^t dt_1 \int_{t_1}^t dt_2\, \frac{\partial_{t_1}x(t_1)\partial_{t_2}x(t_2)}{|t_1 - t_2|}$$



Brownian 2-points correlation function

Final Result I

$$
\begin{aligned}
R_+(y) &= R_+^{(0)}(y)\left[1+\epsilon W(y)+O(\epsilon^2)\right] \\
W(y) &= \frac{1}{6}y^4\,{}_2F_2\left(1,1;\frac{5}{2},3;\frac{y^2}{2}\right) \\
&\quad +\pi(1-y^2)\,\mathrm{erfi}\left(\frac{y}{\sqrt{2}}\right)+\sqrt{2\pi}e^{\frac{y^2}{2}}y \\
&\quad +\left(y^2-2\right)\left[\log\left(2y^2\right)+\gamma_{\mathrm{E}}\right]-3y^2
\end{aligned}
$$

Final Result II

$$R_+(y) \xrightarrow{y \to 0} y^{\phi}$$

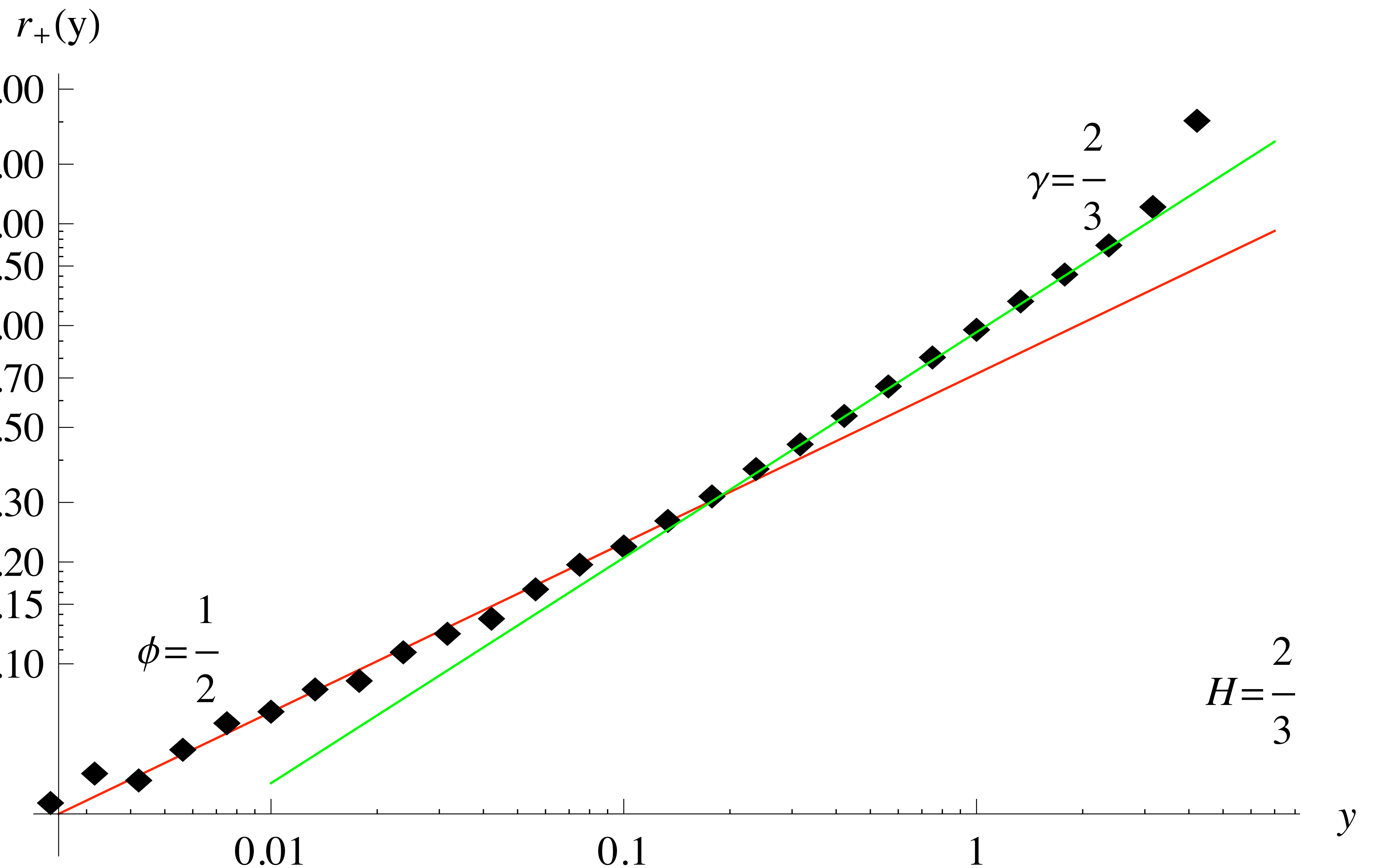
$$R_+(y) \xrightarrow{y \to \infty} y^{\gamma} e^{-\frac{y^2}{2}}$$

$$\phi = 1 - 4\epsilon + O(\epsilon^2)\ , \quad \gamma = 1 - 2\epsilon + O(\epsilon^2)\ .$$

- ϵ expansion in agreement with the conjecutre $\phi = \frac{1-H}{H}$
- At large y, Free Gaussian Propagator
- $+$ a New Exponent $\gamma \neq \phi$

The exponent γ

$$r_+(y) = e^{\frac{y^2}{2}} R_+(y)$$



Conclusions

- We have introduced different models displaying anomalous diffusion
- H is not enough to identify the universal behavior of the process
- $\phi = \theta/H$ characterizes the spatial properties of these processes
- Perturbation approach are possible around the Brownian results
- A new exponent γ has been found for the fBm