Anomalous Diffusion

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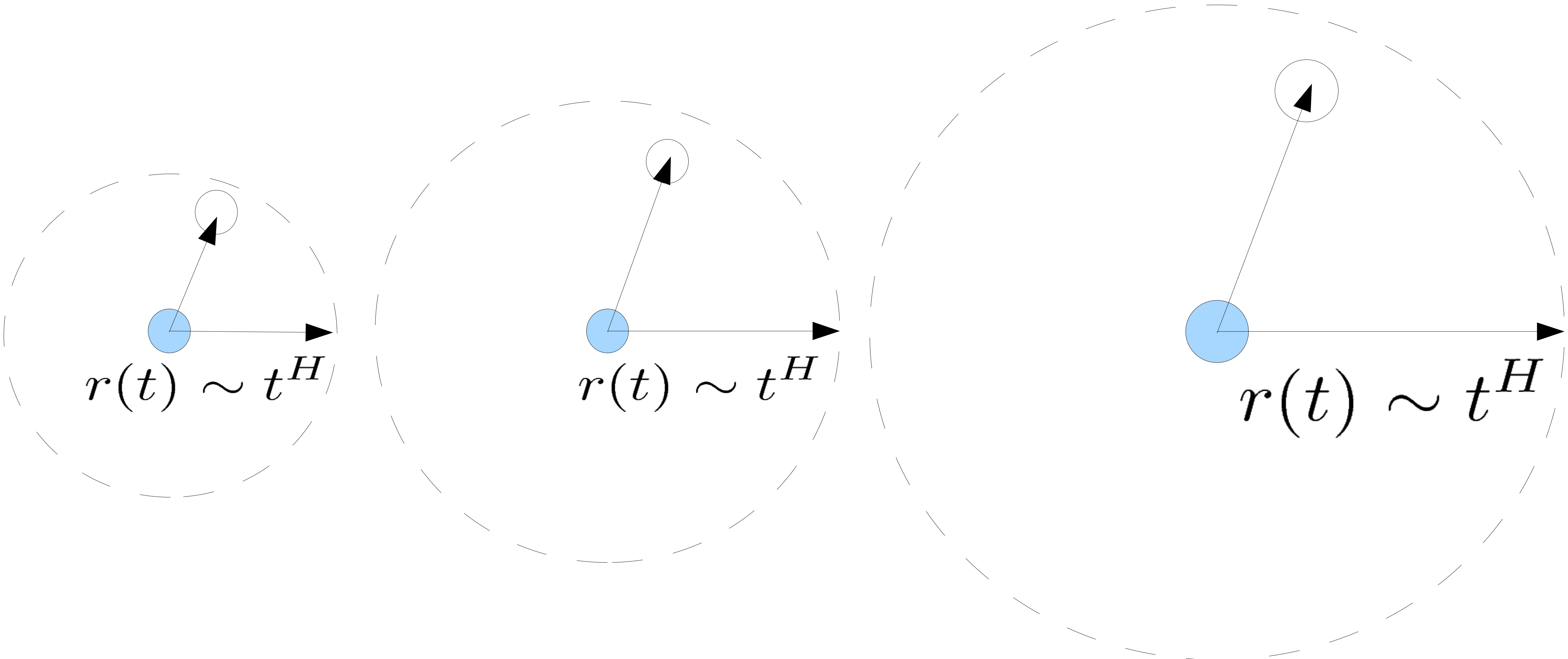
Polymer translocation: A. Zoia (Saclay) + S. Majumdar

Perturbation theory: K. J. Wiese (ENS) + S. Majumdar

Longest excursion: R. Garcia (Bariloche) + G. Schehr

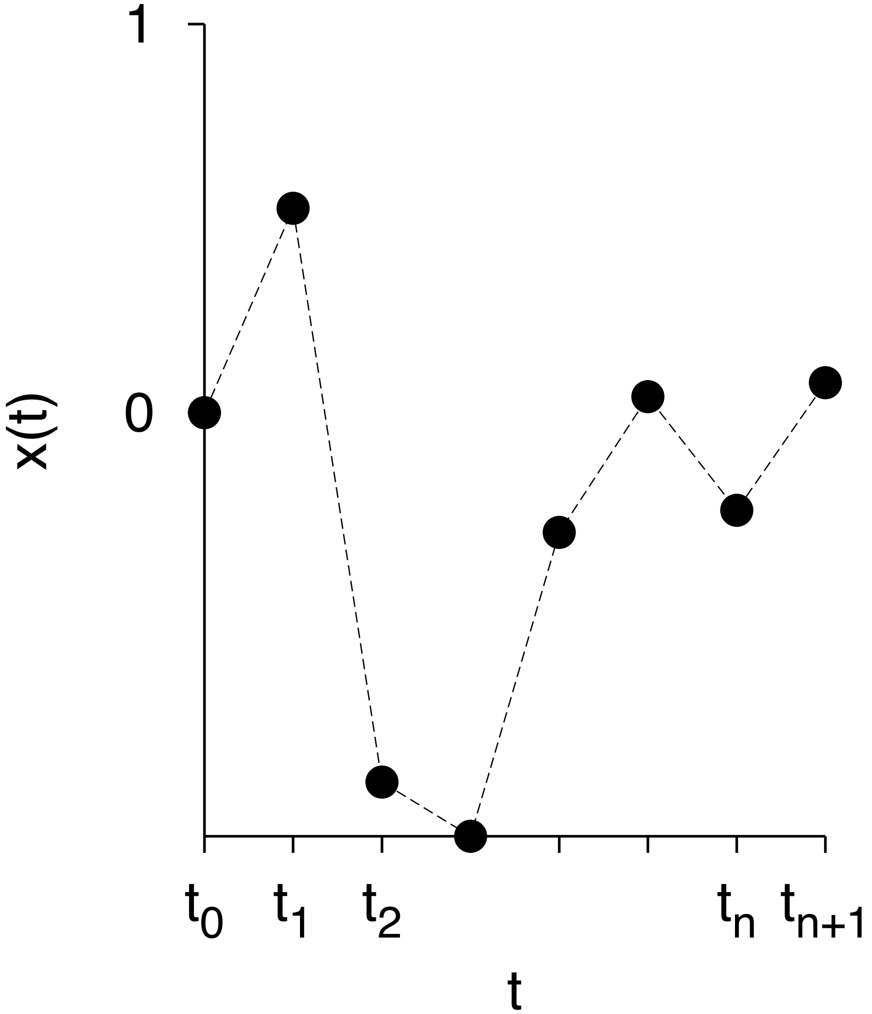
Anomalous Diffusion



$H < 1/2$	$H = 1/2$	$H > 1/2$
Subdiffusion	Diffusion	Super-diffusion

Central Limit Theorem

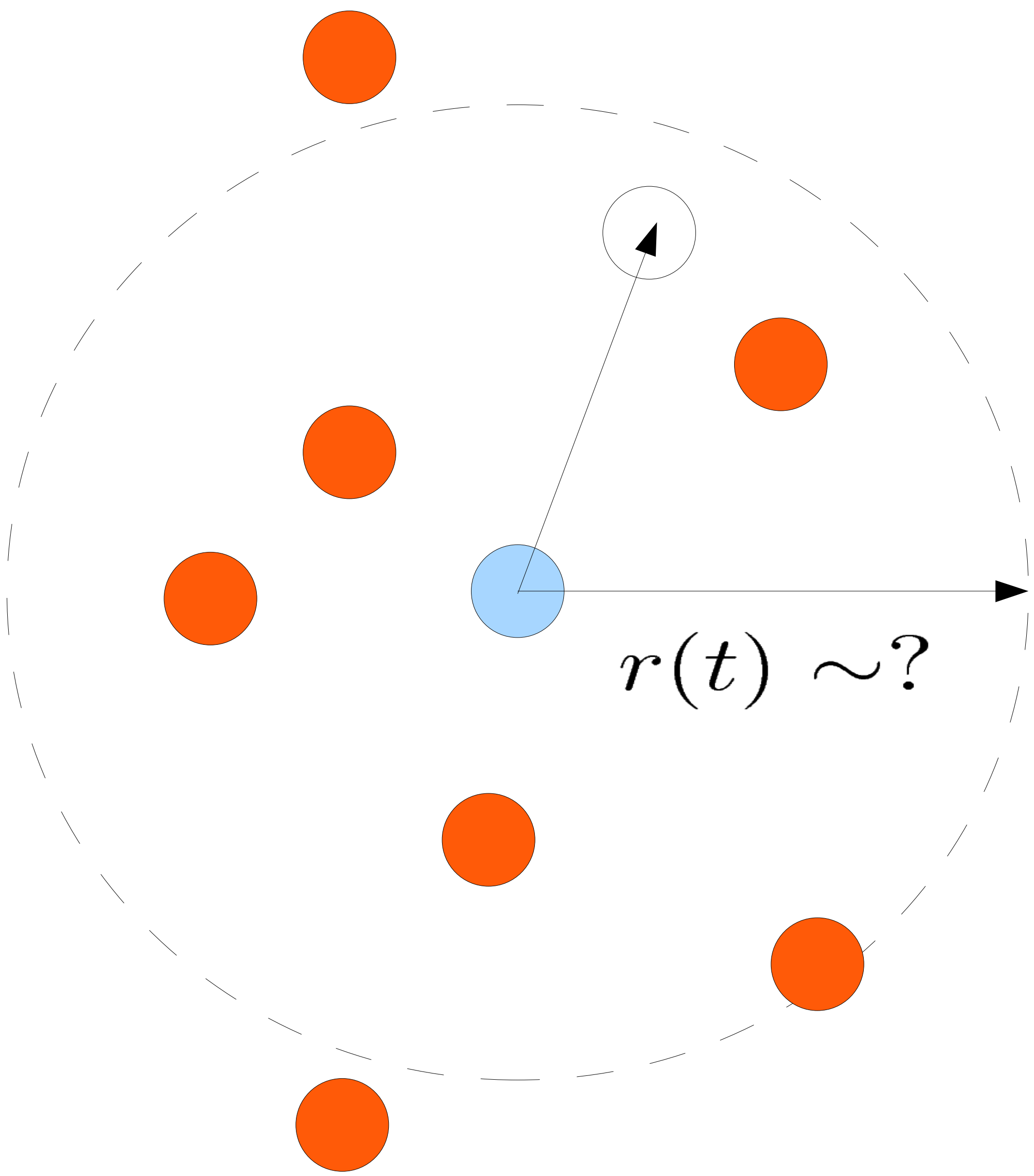
$$x(t) = \sum_{t'=1}^{t} \xi_{t'}$$



- *Identical*: $\pi_{t'}(\xi) = \pi(\xi)$. (Homogeneous)
- *Independent*: $\langle \xi_{t_0} \xi_{t_0+t} \rangle = 0$. (Markov)
- $\langle \xi^2 \rangle < \infty$: Continuous process.

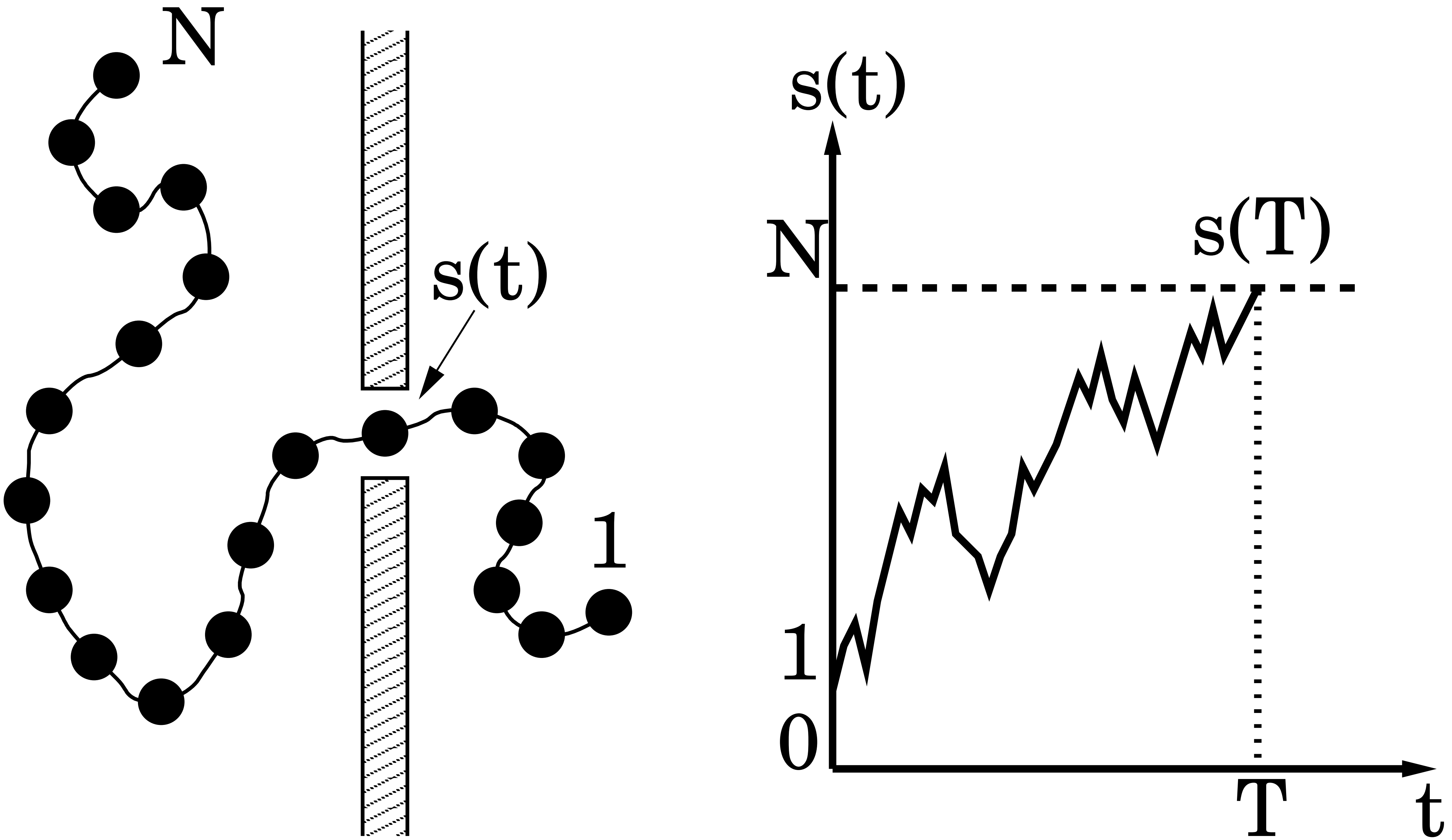
Conclusion: $x(t)$ **is Gaussian and** $x(t) \sim \sqrt{t}$

Correlations

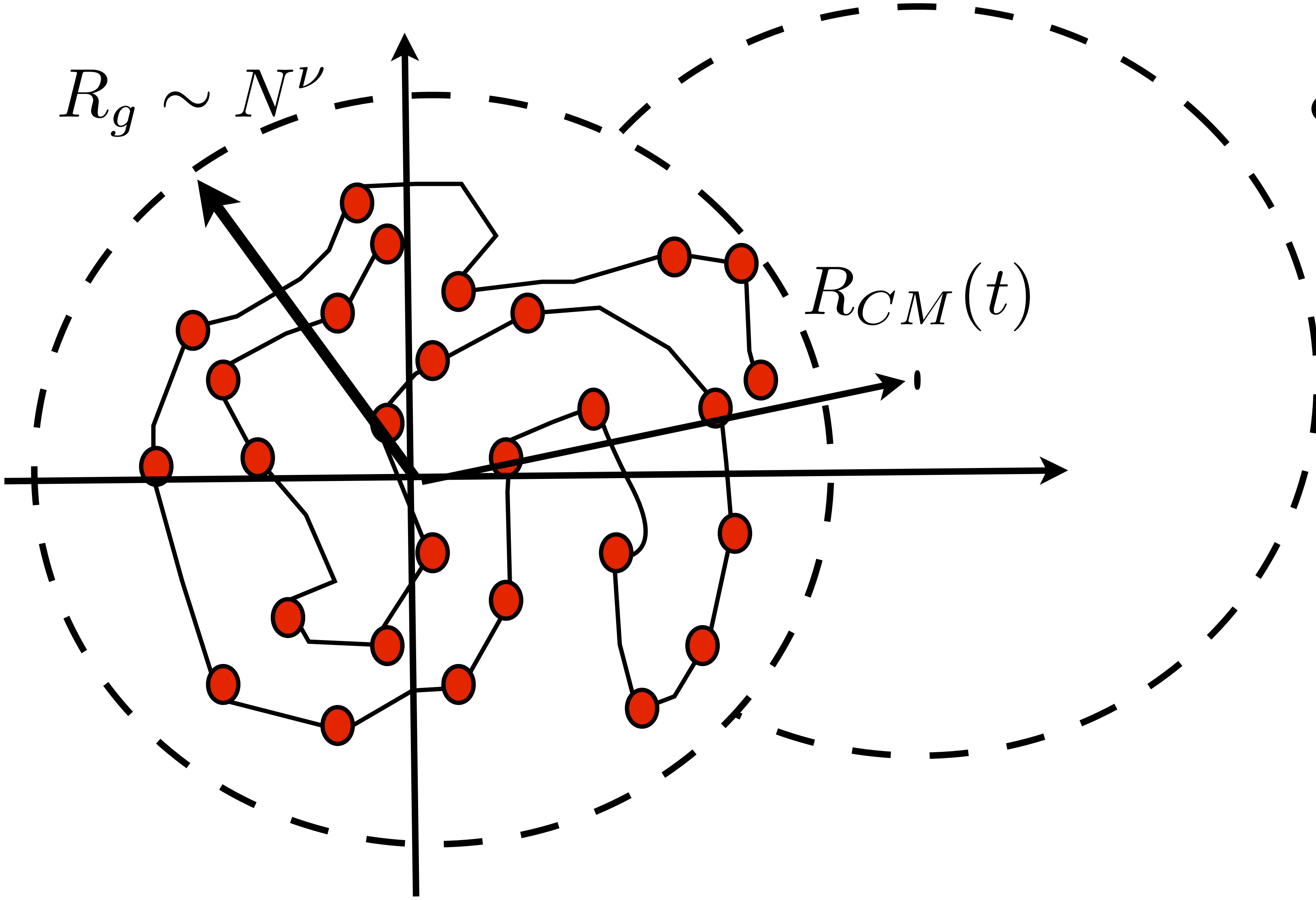


- jumps and waiting times are local
- colloids interact (strongly non-Markovian)

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 $\nu = 1/2$

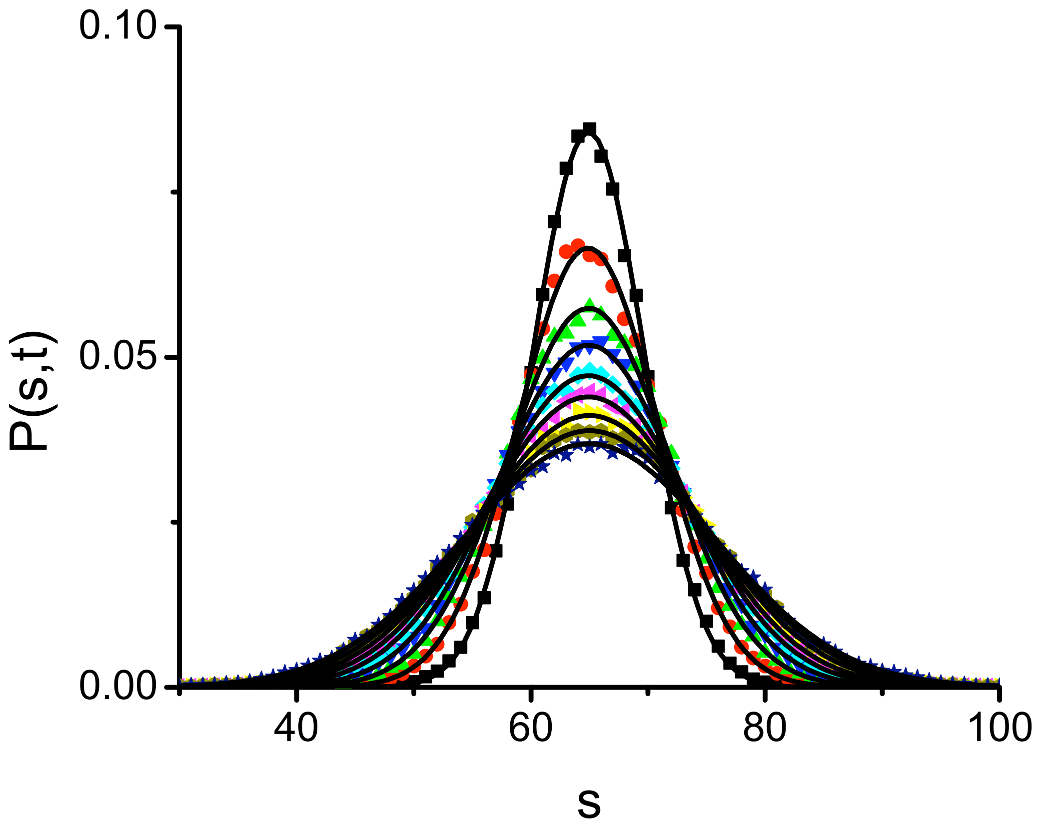
Excluded Volume $\nu > 1/2$

- $R_{CM}(t)$ Center of Mass

$$\langle R^2_{\mathrm{CM}}(t_{\mathrm{eq.}})\rangle = R_g^2 \quad \Rightarrow \quad \frac{D_1 t_{\mathrm{eq.}}}{N} \sim N^{2\nu} \quad \Rightarrow \quad t_{\mathrm{eq.}} \sim N^{2\nu+1}$$

$$T \gg t_{\mathrm{eq.}} \quad \Rightarrow \quad H \leq \frac{1}{1+2\nu} \quad \text{numerically} \quad H \approx \frac{1}{1+2\nu}$$

Fractional Brownian motion



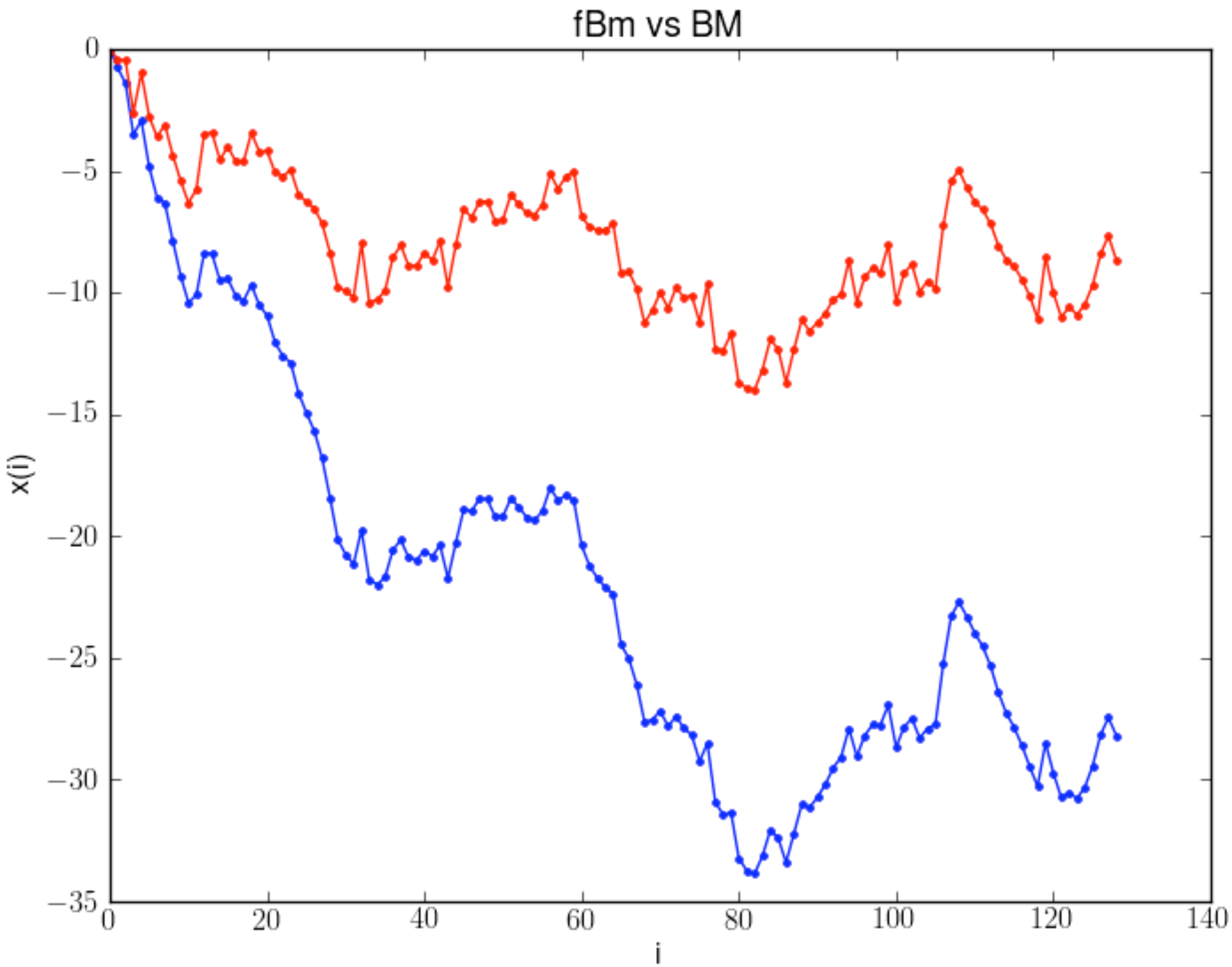
Monte Carlo simulation of polymer translocation in d=2,
Chatelain, Kantor, Kardar, PRE 78, 021129 (2008)

- Equilibrium with the solvent $\Rightarrow$ stationary increments
- is a Gaussian process $\Rightarrow$ local jumps
- $\Rightarrow$ non-Markov process

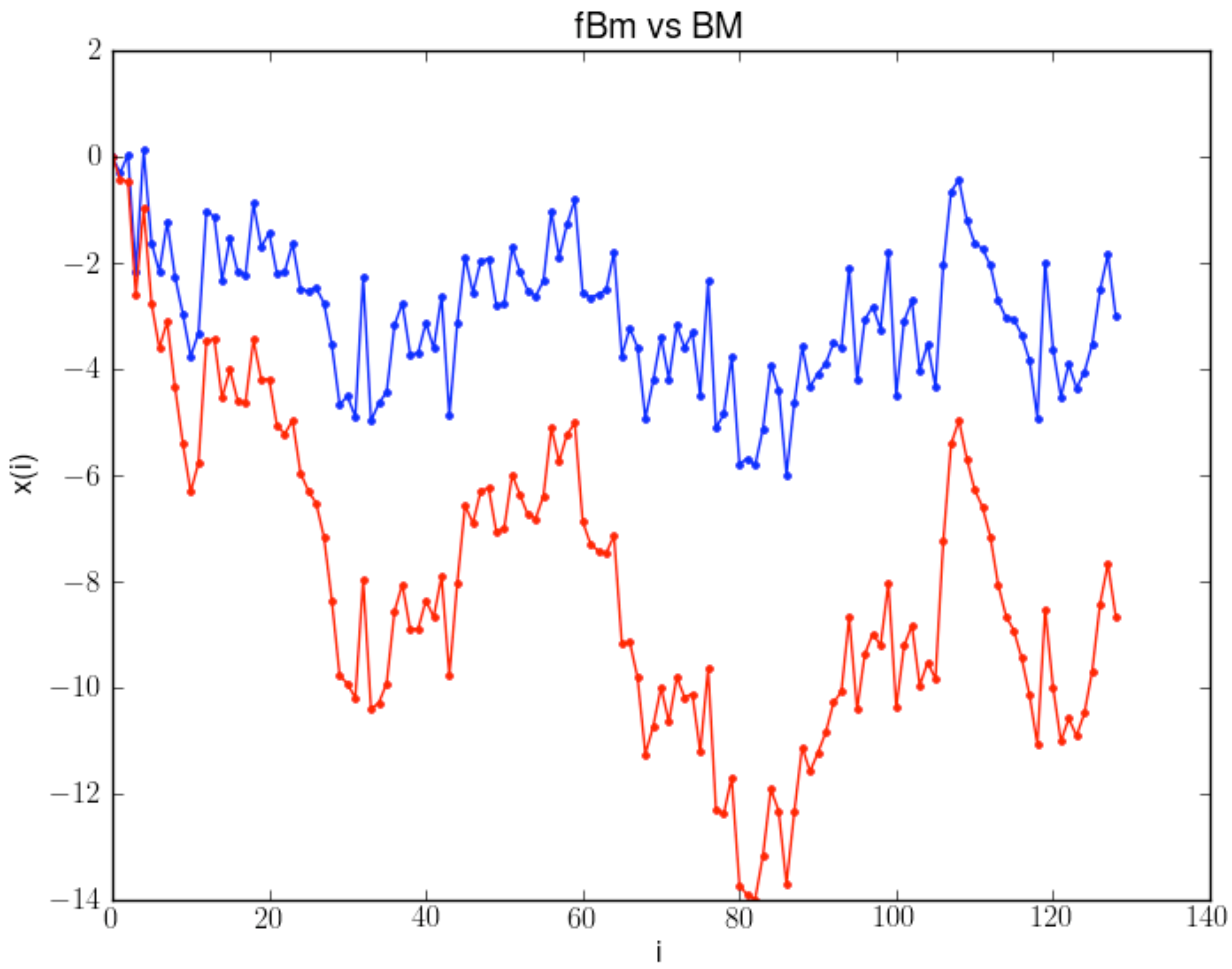
Gaussianity + self-affinity $H = \frac{1}{2\nu+1}$ + stationary increments
$\Rightarrow$ fractional Brownian motion:

$$\langle s(t_1)s(t_2)\rangle \propto \left(t_1^{2H} + t_2^{2H} - |t_1 - t_2|^{2H}\right),$$

H=3/4 Superdiffusion

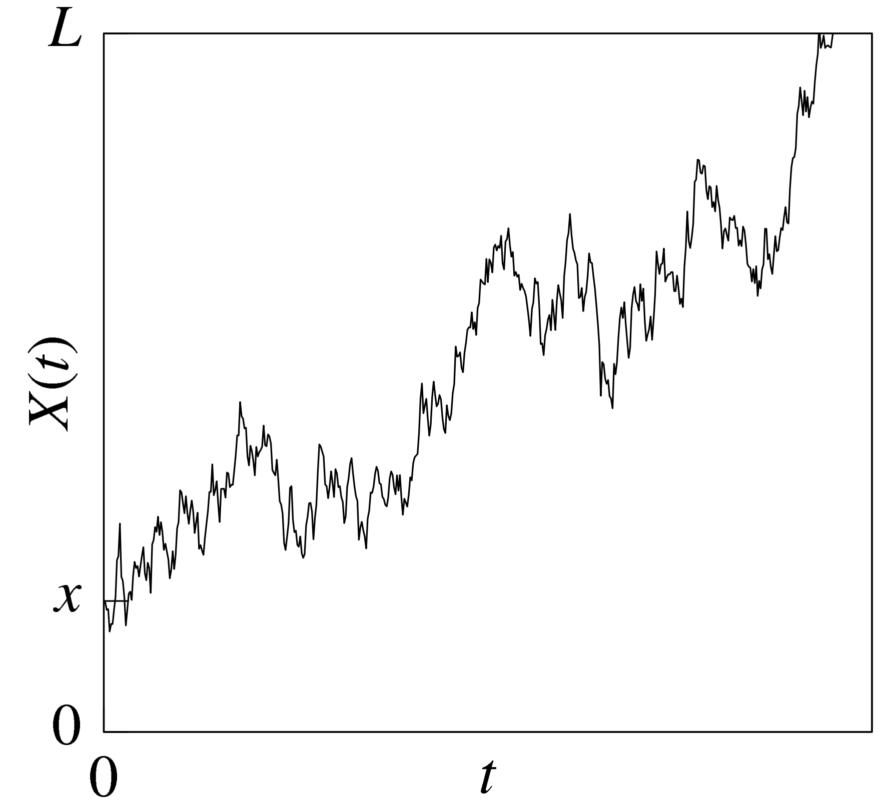


H=1/4 Subdiffusion



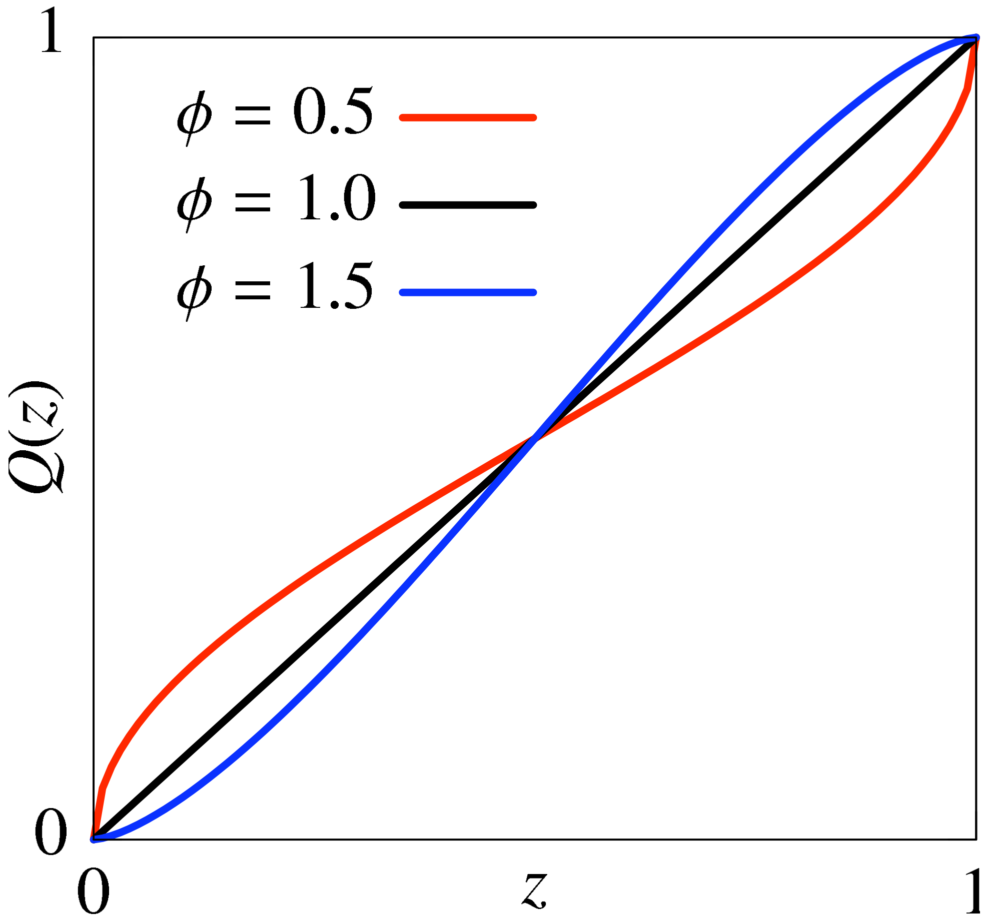
Question I: A polymer chain will ultimately succeed in translocating through a pore ?

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



For **self affine** processes:

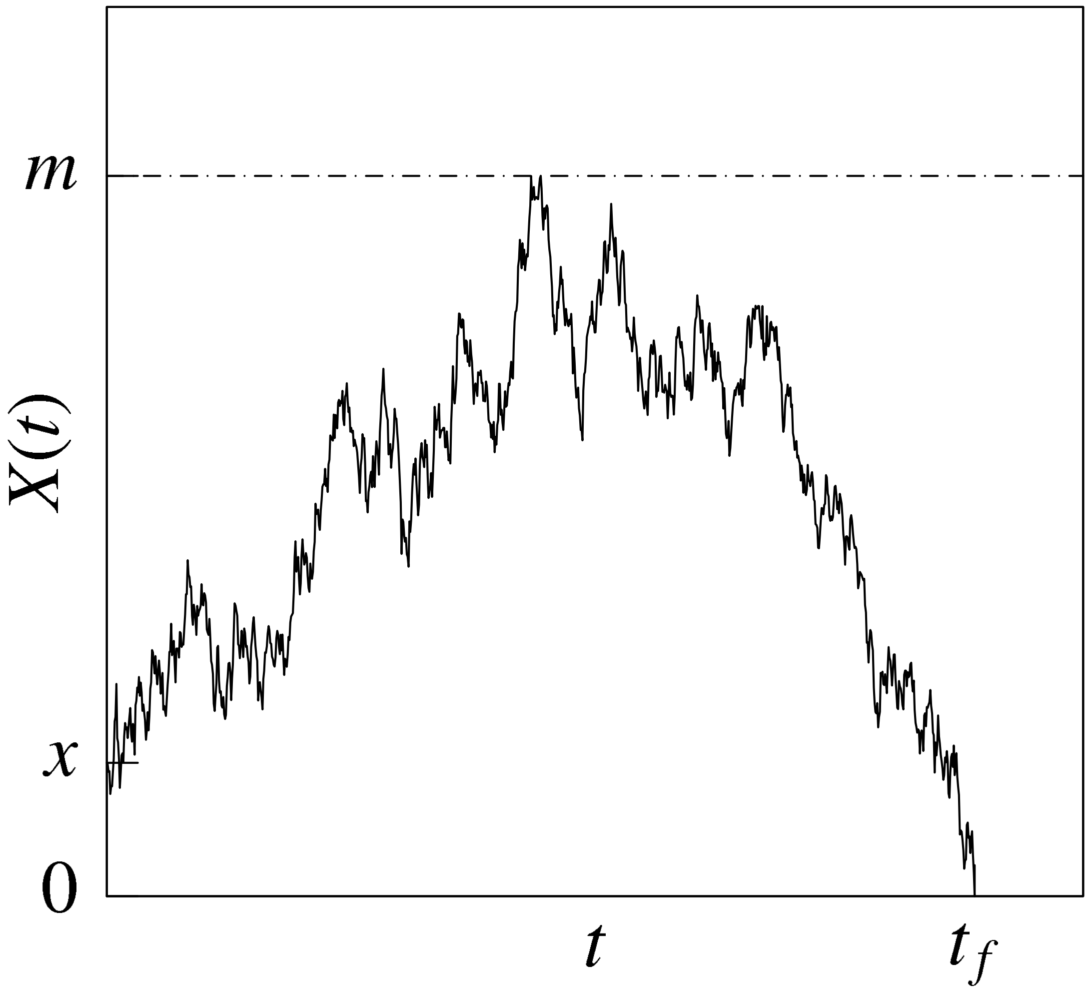
$$Q(x, L) = Q\left(z = \frac{x}{L}\right)$$



- Basic: $Q(z) = 1 - Q(1 - z)$; $Q(1/2) = 1/2$; $Q(z) = 0$
- $H = 1/2$: $Q(z) = z$
- Expansion: $Q(z) \sim c_1 z^{\phi} + \dots$

Translocation is enhanced or suppressed by excluded volume effects?

A scaling argument: $\phi = \frac{\theta}{H}$



- $Q(x, L) = \text{Prob}[m > L]$
- Self-affinity I: $m \sim t_f^H$

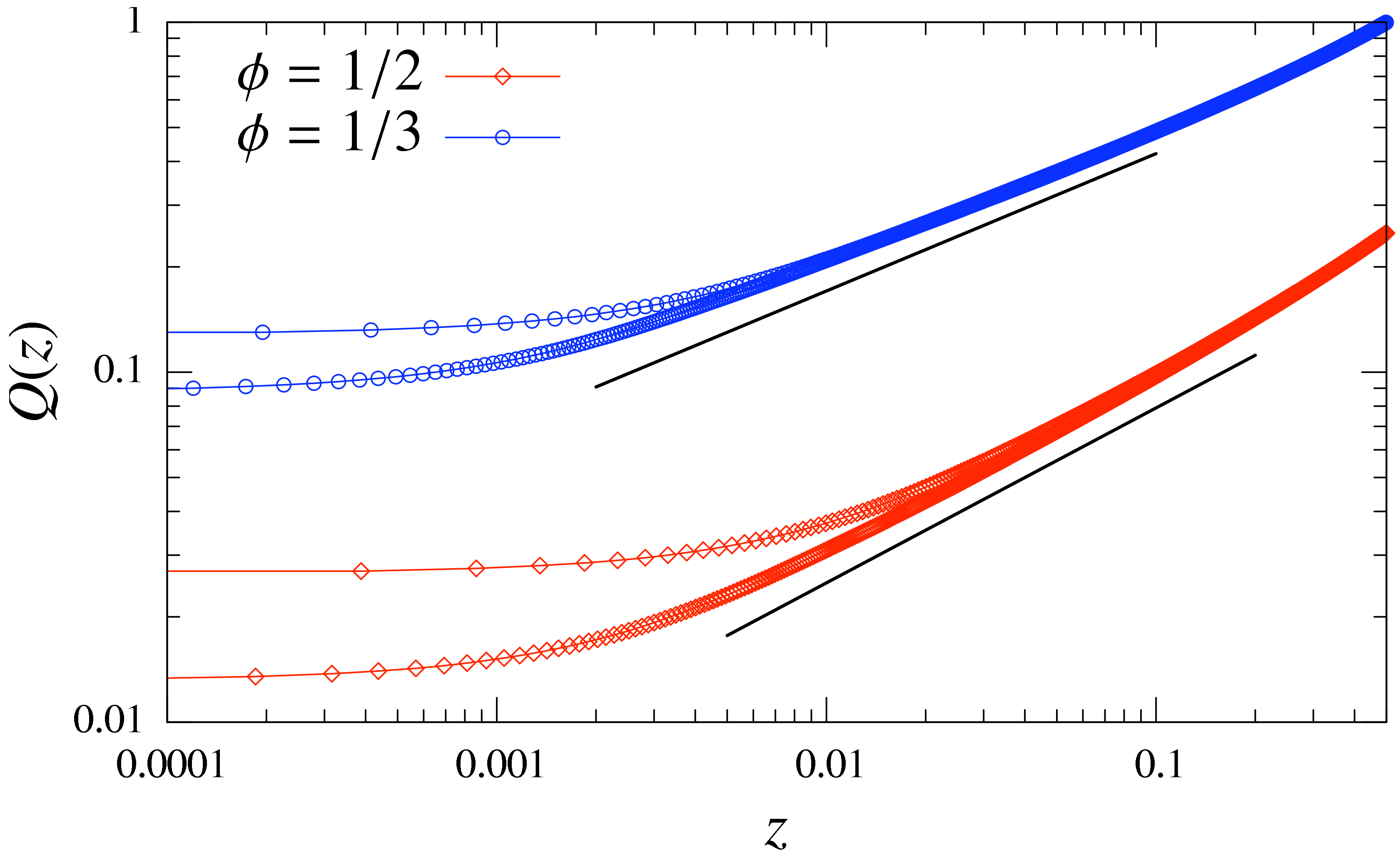
$$\Longrightarrow Q(x, L) \simeq \text{Prob}[t_f^H > L]$$
$$Q(x, L) \sim \text{Prob}[t_f > L^{\frac{1}{H}}]$$

- Survival probability: $\text{Prob}[t_f > T] = S(x, T) =\sim \frac{f(x)}{T^\theta}$
  θ persistence exponent

- Self-affinity II: $S(x, T) \sim \left(\frac{x}{T^H}\right)^{\frac{\theta}{H}}$

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

Hitting probability: numerical test



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

Previous results... recast using ϕ

(i) Random acceleration process: $\ddot{x} = \eta(t),\ x(0) = x,\ \dot{x}(0) = 0$

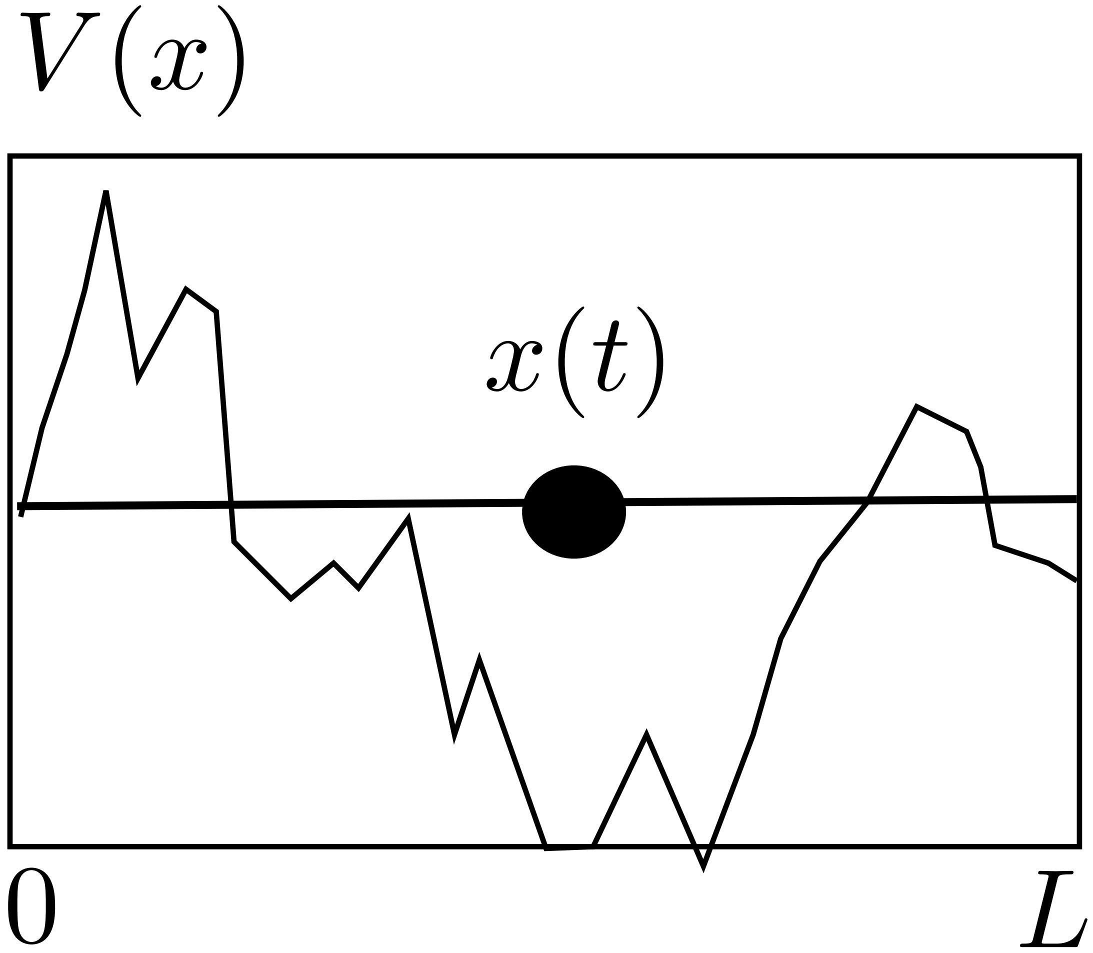
Burkhardt: $H = \frac{3}{2}$ and $\theta = \frac{1}{4} \implies \phi = \frac{1}{6}$

$Q(z = \frac{x}{L}) = I_z[\frac{1}{6}, \frac{1}{6}]$. Where $I_z(\phi, \phi) = \frac{\Gamma(2\,\phi)}{\Gamma^2(\phi)} \int_0^z \frac{du}{[u(1-u)]^{1-\phi}}$

(ii) Lévy fligths: $x_{t+1} = x_t + \xi_t$ with $\pi(\xi) \sim \xi^{-(\mu+1)}$

Sparre Andersen: $H = \frac{1}{\mu}$ and $\theta = \frac{1}{2} \implies \phi = \frac{\mu}{2}$

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



Sinai model

$$t \sim e^{V(x)} \sim e^{\sqrt{x}} \Rightarrow x(t) \sim [\log(t)]^2$$

$$S(x_0, t) \sim [\log(t)]^{-1}$$

Using $\tau = \log(t) \Longrightarrow H = 2$ and $\theta = 1$

From Backward Fokker Planck: $Q(x, L) = \frac{\int_0^x e^{\beta V(x')} dx'}{\int_0^L e^{\beta V(x')} dx'}$

$$\overline{Q(z)} = \int_0^z dz' \, \overline{p_{eq}(z')}; \quad \text{From } \overline{p_{eq}(z)} = \frac{1}{\pi} \frac{1}{\sqrt{z(1-z)}}$$

We deduce $\overline{Q(z)} = I_z(1/2, 1/2) = \frac{2}{\pi} \arcsin(\sqrt{z}) \sim \sqrt{z}$

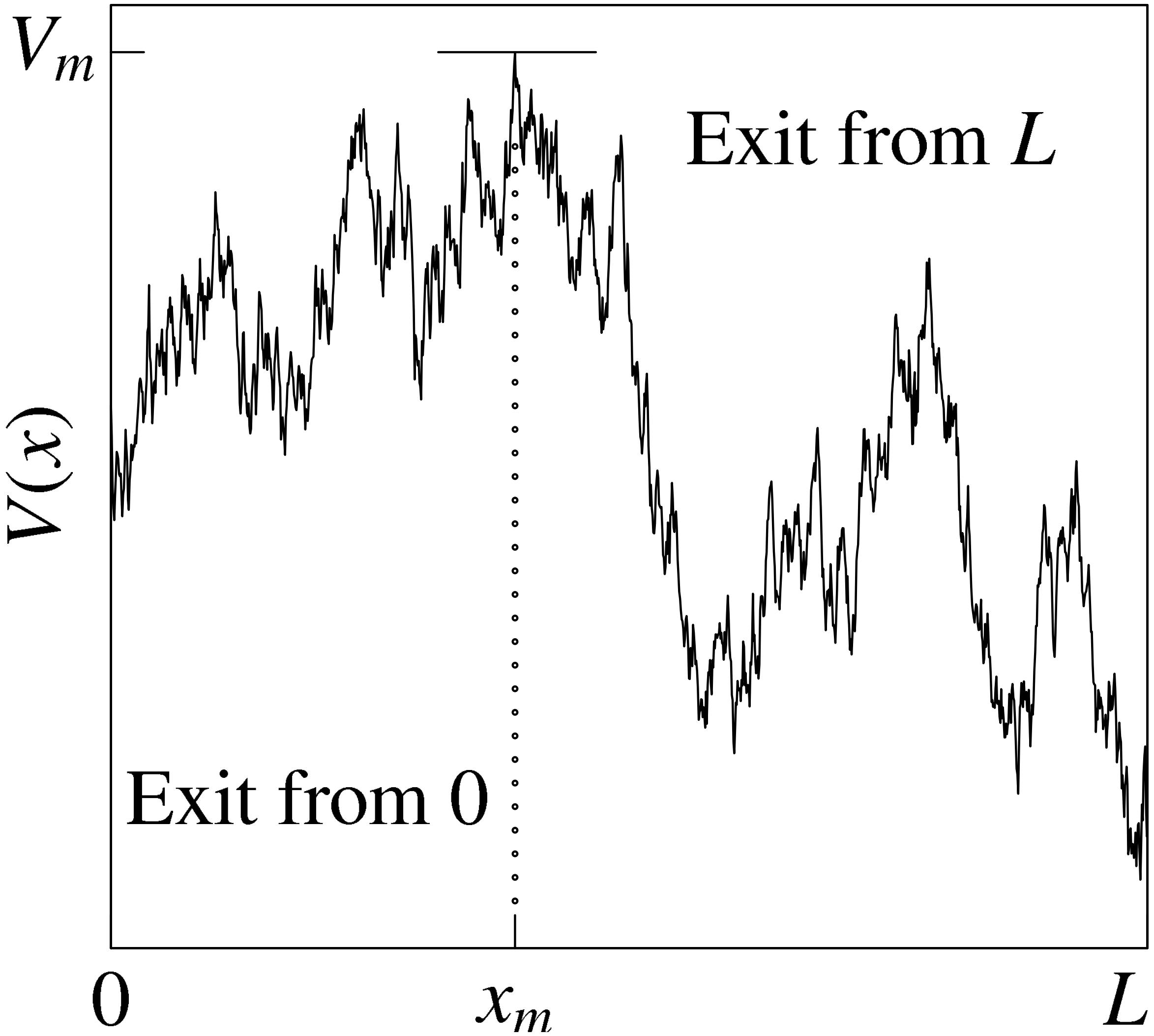
So that $\phi = \theta / H = 1/2$

See Oshanin, Redner, Comtet, Monthus, Texier...

Extreme statistics: maximum location in $V(x) \sim x^{H_V}$

$$p_{eq}(x,L) = \frac{e^{\beta V(x)}}{\int_0^L e^{\beta V(x')} dx'} \propto \left\{ \int_0^1 dz' \, \exp\left[\beta L^{H_V} \cdot (V(z') - V(z))\right] \right\}^{-1}$$

$$p_{eq}(x,L) \sim \delta(x - x_m) \Longrightarrow \overline{p_{eq}(x,L)} \sim p_V(x_m, L) \quad \text{[Sinai: arcsine law]}$$



Fixed realization: $Q(x,L) = \theta(x - x_m)$

Average $\overline{Q(z = \frac{x}{L})} = \text{Prob}[z_m < z]$

If $V(x) \sim x^{H_V}$, using Arrhenius $H = 1/H_V$

$$\text{Prob}[x_m < x \to 0] \sim \text{Prob}[V < 0 \text{ up to } L] \sim \frac{1}{L^{\theta_V}}$$

$$\text{So that } Q(x, L) \to \left(\tfrac{x}{L}\right)^{\theta_V}$$

We Conclude $\phi = \theta_V$ **and** $\theta = H \cdot \phi = \theta_V / H_V$

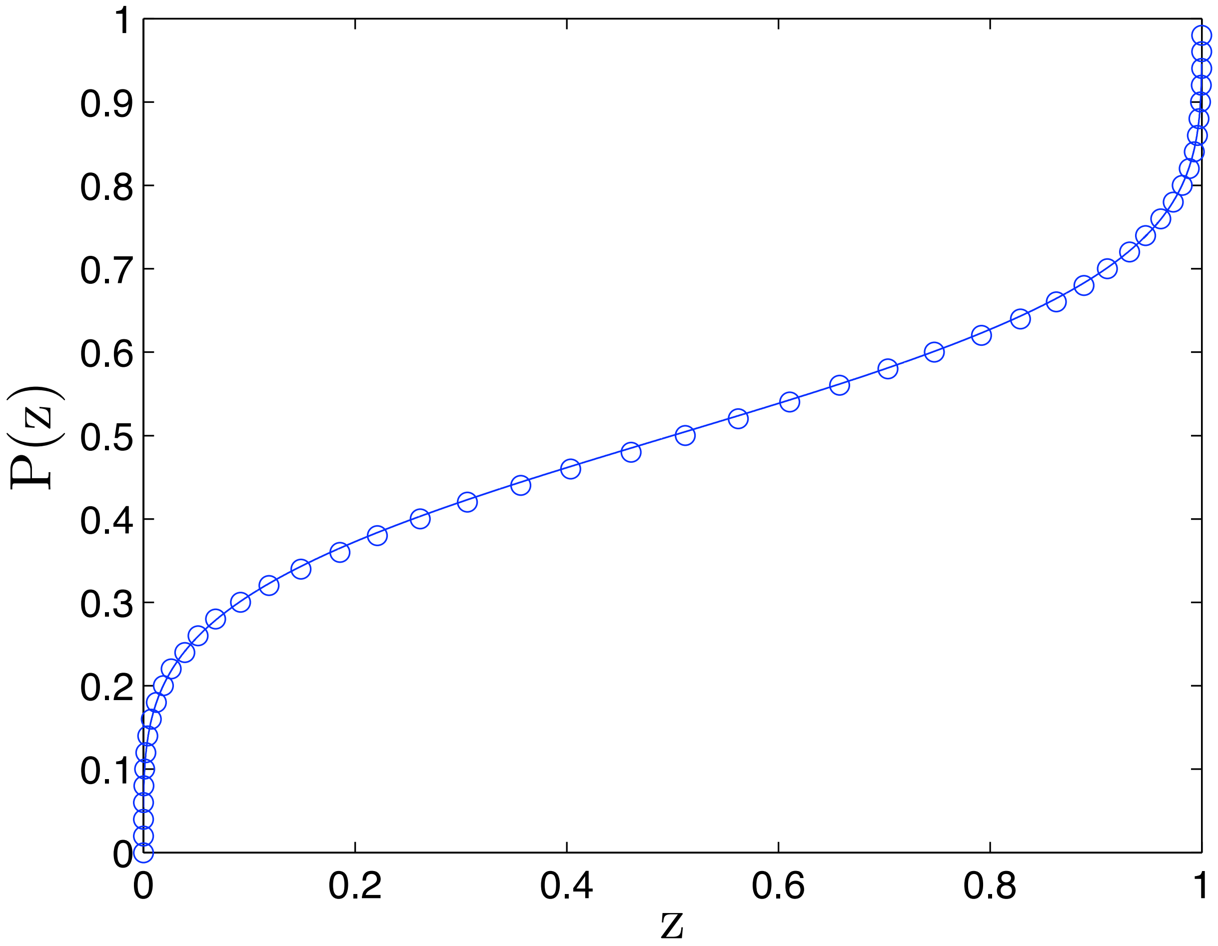
$V(x)$ is a random acceleration process: $H_V = 3/2$, $\theta_V = 1/4$

$$\text{Bridge case } (V'(L) = 0)\text{:}\quad p(z_m) = \tfrac{\Gamma(1/2)}{\Gamma^2(1/4)} \tfrac{1}{(z_m(1-z_m))^{3/4}}$$

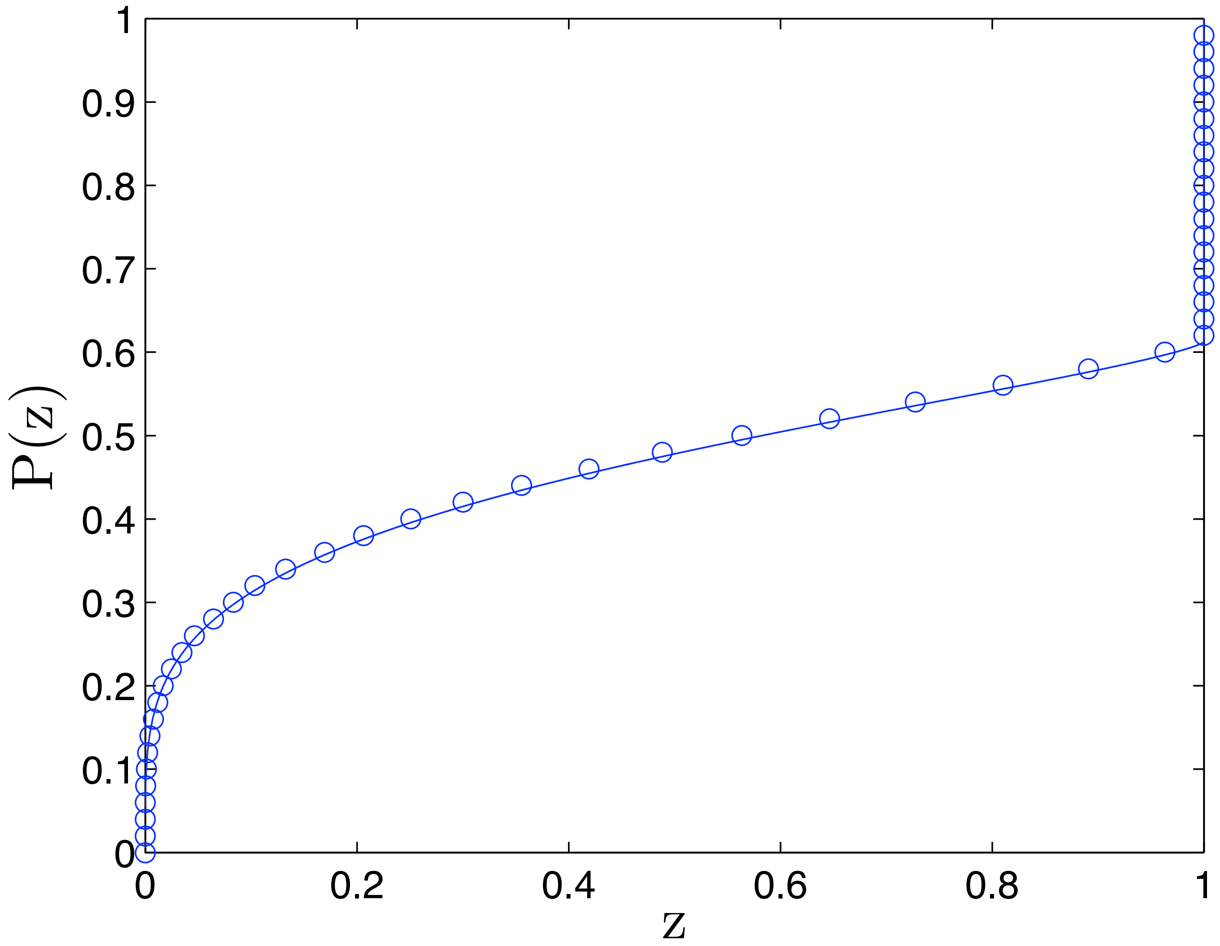
$$\text{Free case:}\quad p(z_m) = (1 - \sqrt{\tfrac{3}{8}})\delta(z_m - 1) + \tfrac{\sqrt{3}}{4\pi z_m^{3/4}(1-z_m)^{1/4}}$$

(See also Maximum location, for CTRW : Le Doussal and Schehr)

Hitting Bridge

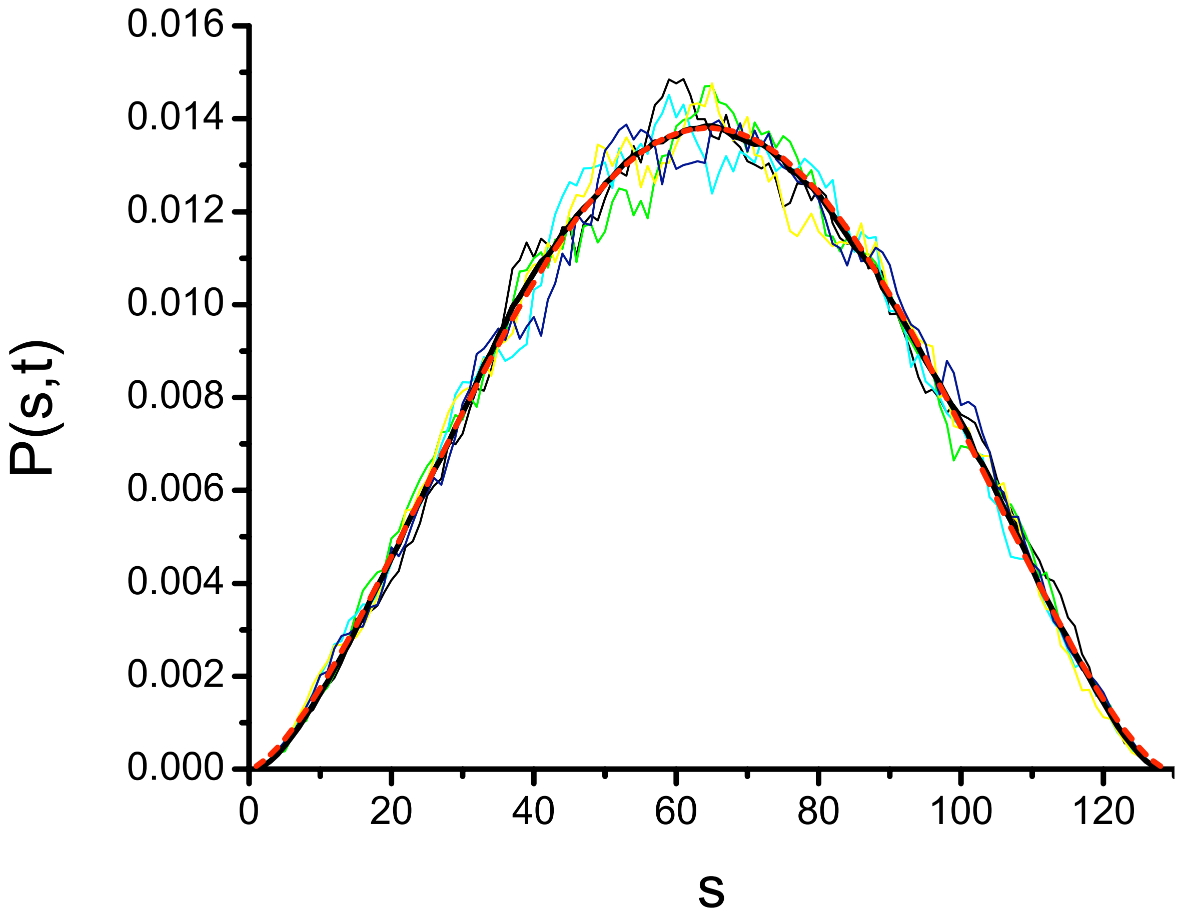


Hitting Free

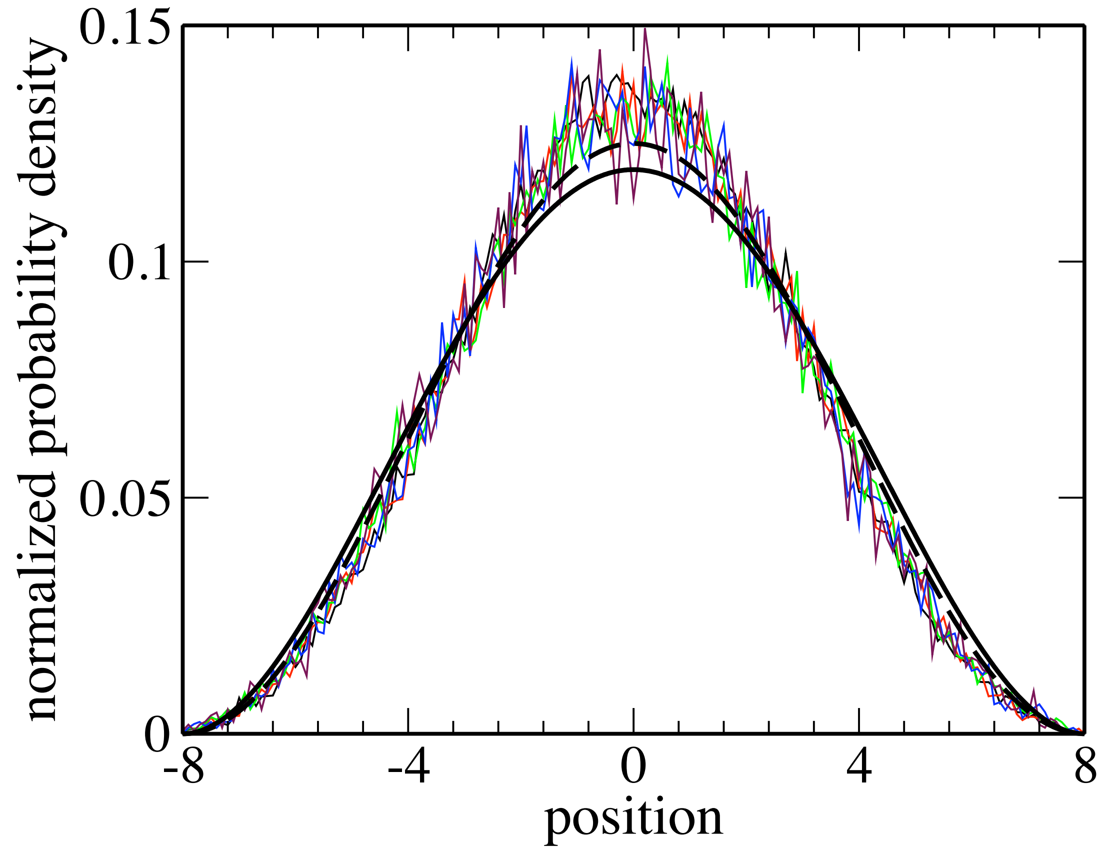


...and the persistence $S(x_0, t) \sim \frac{1}{\log(t)^{\frac{1}{6}}}$

“Anomalies” of anomalous diffusion



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)

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

At large t, $P(s,t) \sim s^{1.44}$

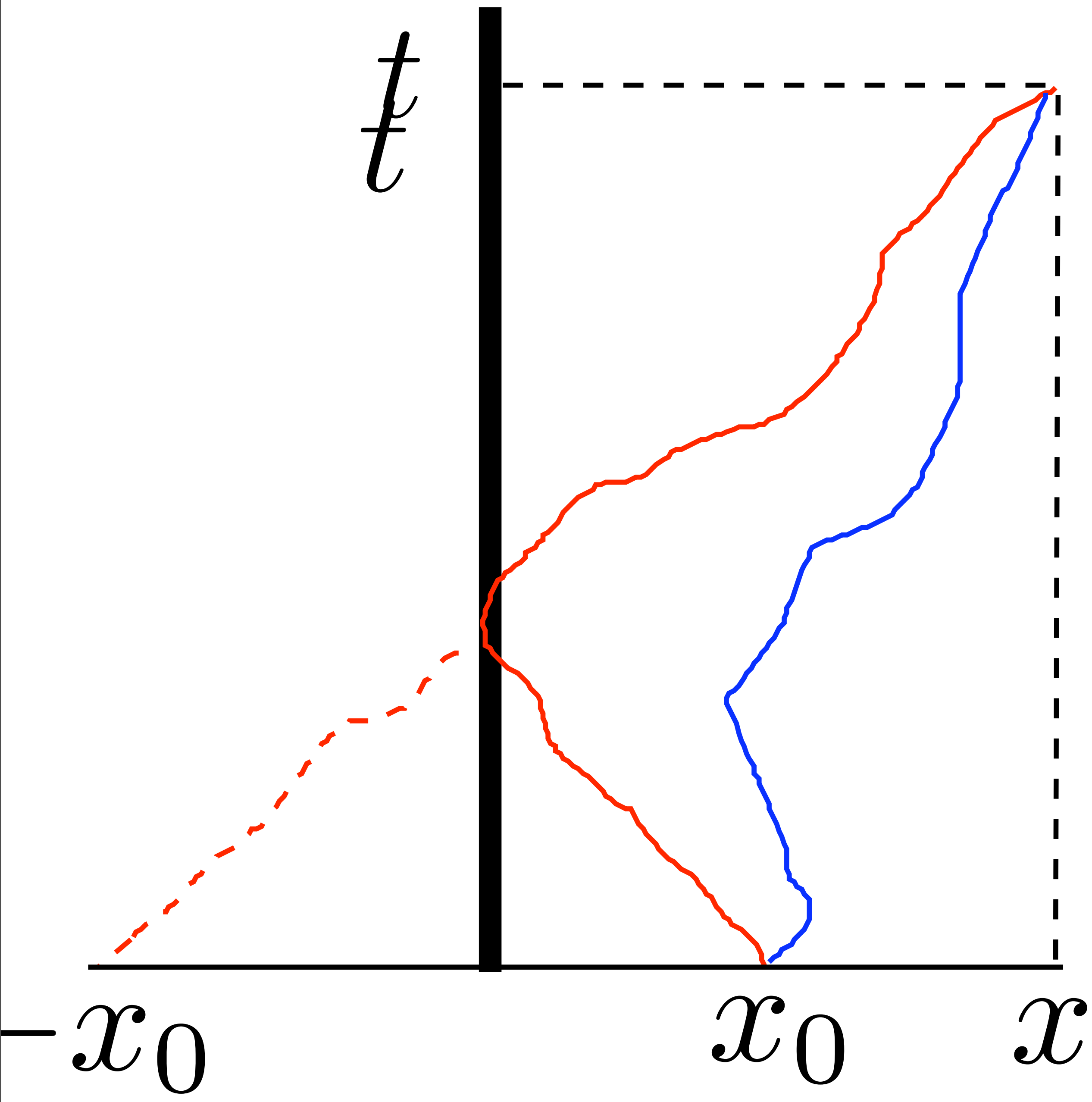
We predict $\phi = \frac{1-H}{H} = 1.5$

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

At large t, $P(s,t) \sim s^{\alpha}$, with $\alpha > 2$

We predict $\phi = \frac{1-H}{H} = 3$

Single Boundary: Images method



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

After normalization

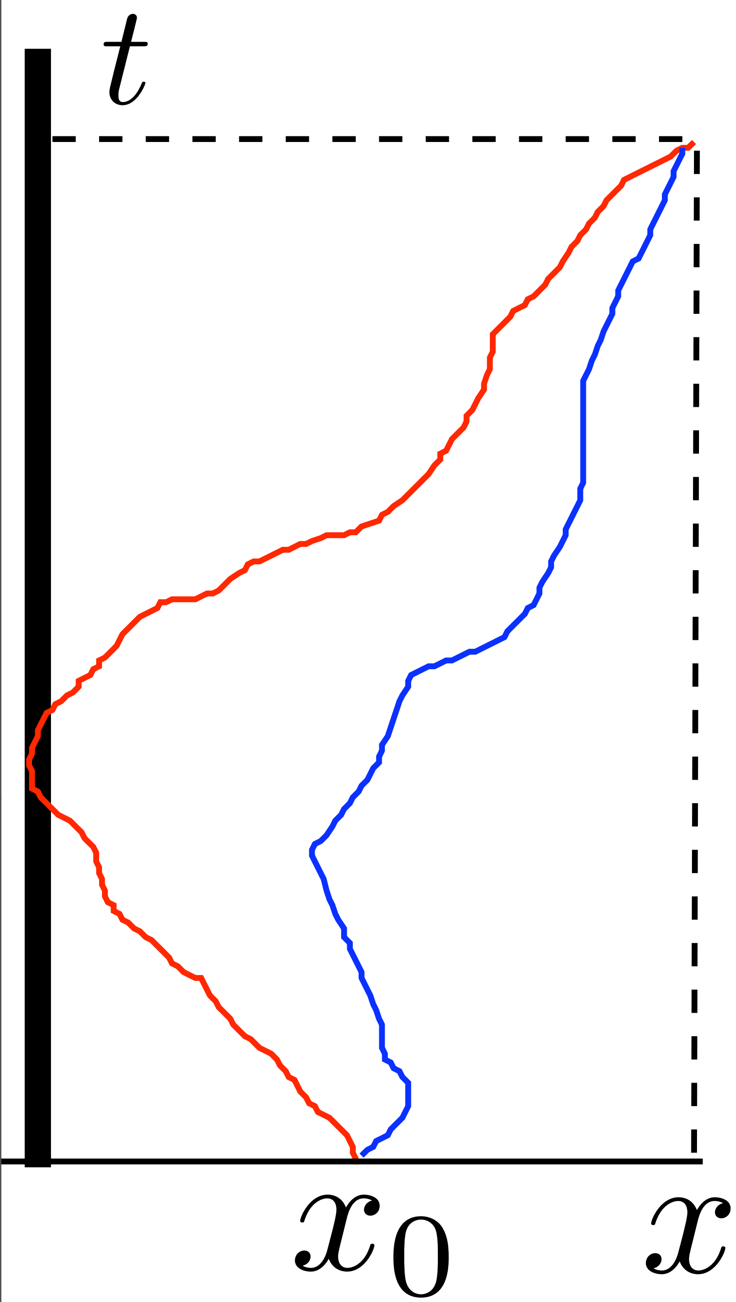
$$P_+(x, x_0, t) \xrightarrow{t \to \infty \textbf{ or } x_0 \to 0} P_+(x, t)$$

Self-Affinity III: $y = \frac{x}{\sqrt{2Dt}}$

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

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

Perturbation Theory



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

$$P_+(x,t) = \lim_{x_0 \to 0} \frac{Z_+(x_0, x, t)}{\int_0^\infty dx Z_+(x_0, x, t)}$$

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

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

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

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

Perturbation

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

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

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

$$G = G^{(0)} - \epsilon G^{(0)} K G^{(0)}$$

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

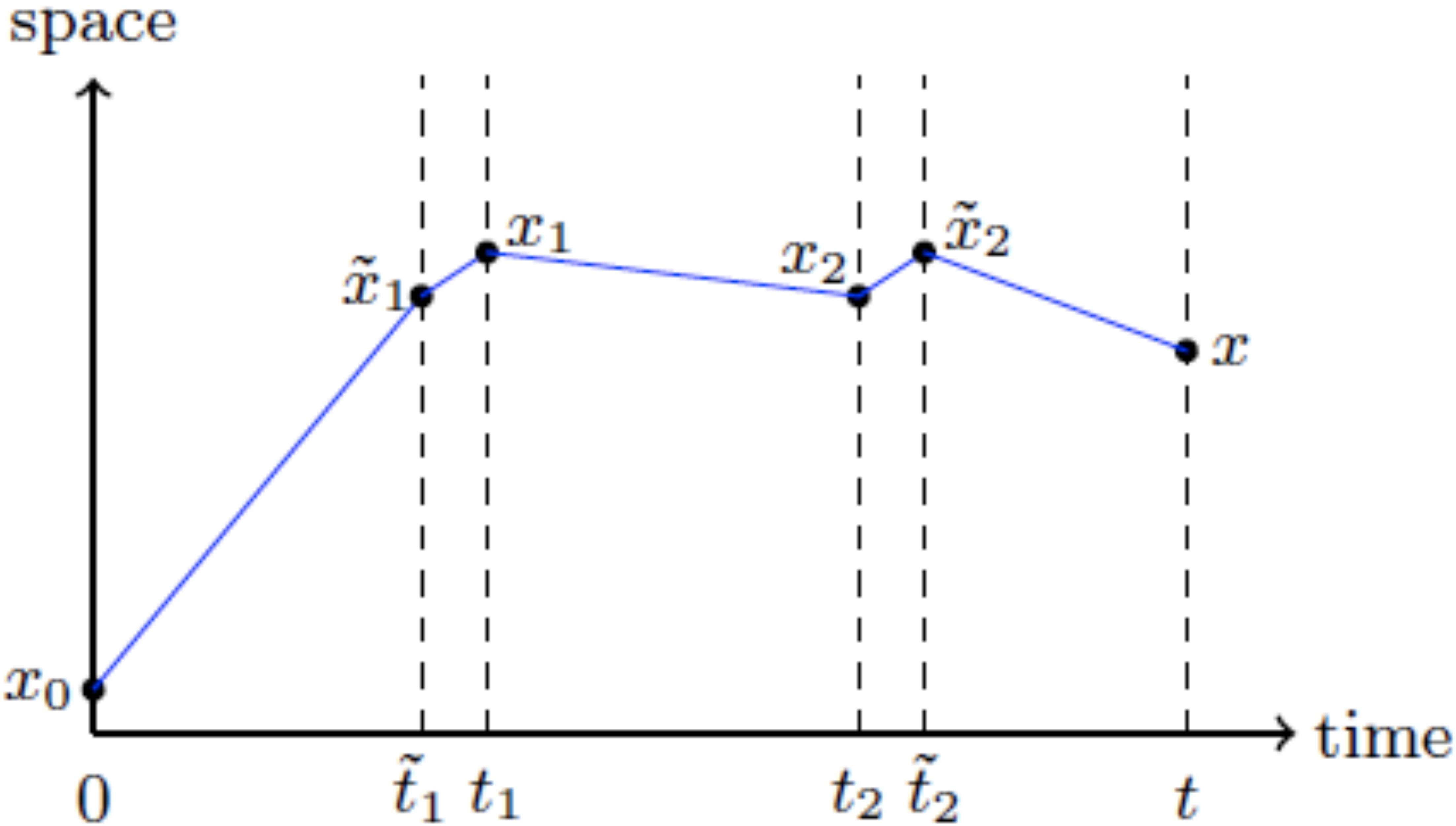
$$\mathcal{S}^{(1)}[x] \quad \propto \quad -\frac{1}{2} \int_0^t dt_1 \int_{t_1}^t dt_2\, \frac{\partial_{t_1} x(t_1) \partial_{t_2} x(t_2)}{|t_1 - t_2|}$$

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

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

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

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



Brownian 2-points correlation function

Final Result I

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

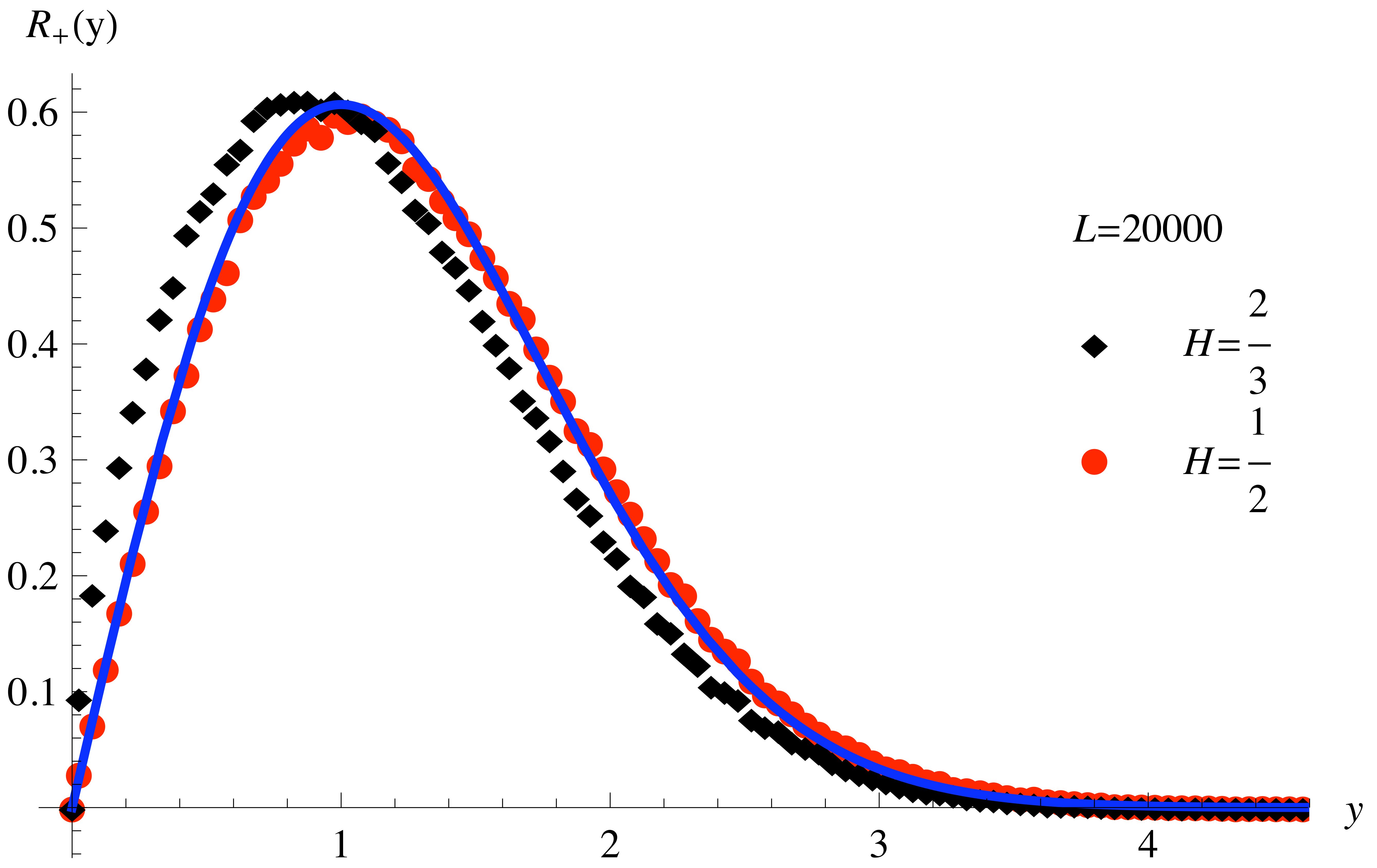
Final Result II

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

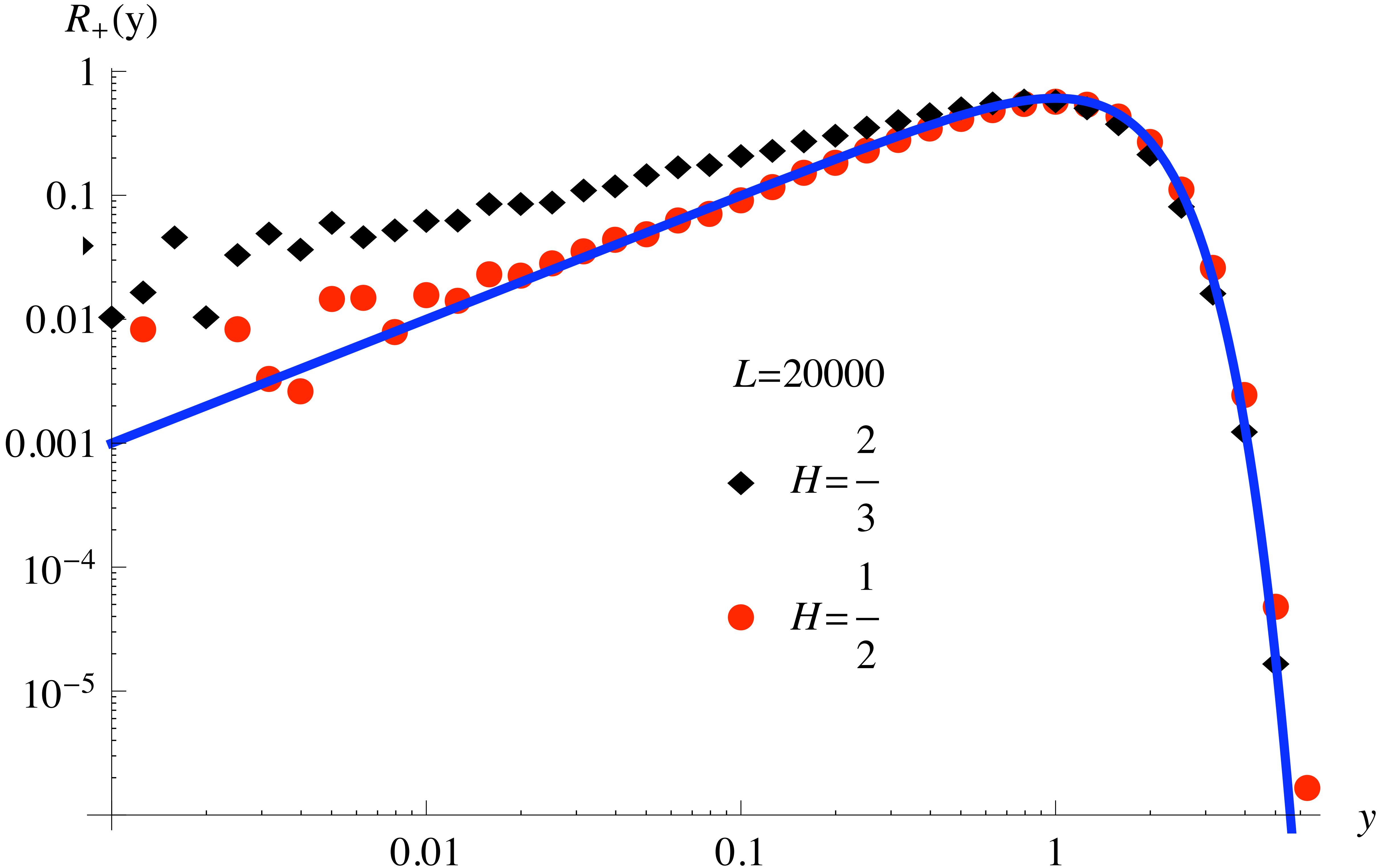
$$R_+(y) \xrightarrow{y \to \infty} y^{\gamma} e^{-\frac{y^2}{2}}$$

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

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

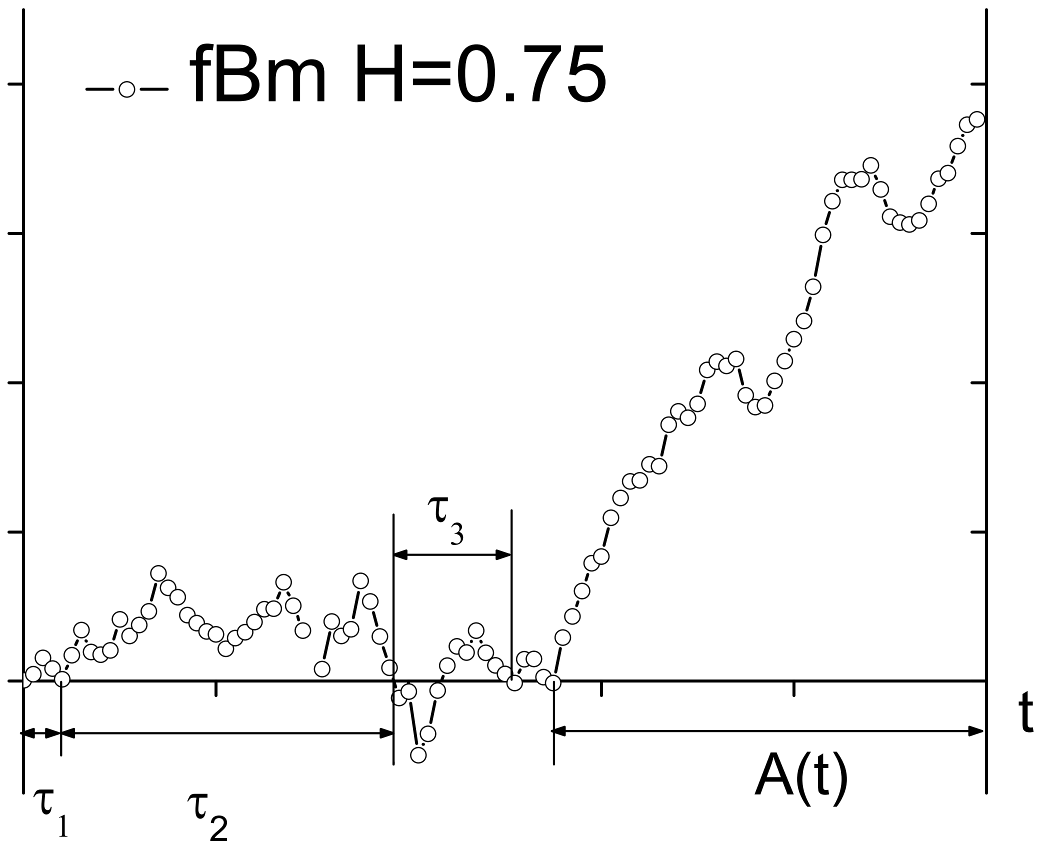


$R_+(y)$
0.6
0.5
0.4
0.3
0.2
0.1
1
2
3
4
y
$L=20000$
$H=\frac{2}{3}$
$H=\frac{1}{2}$

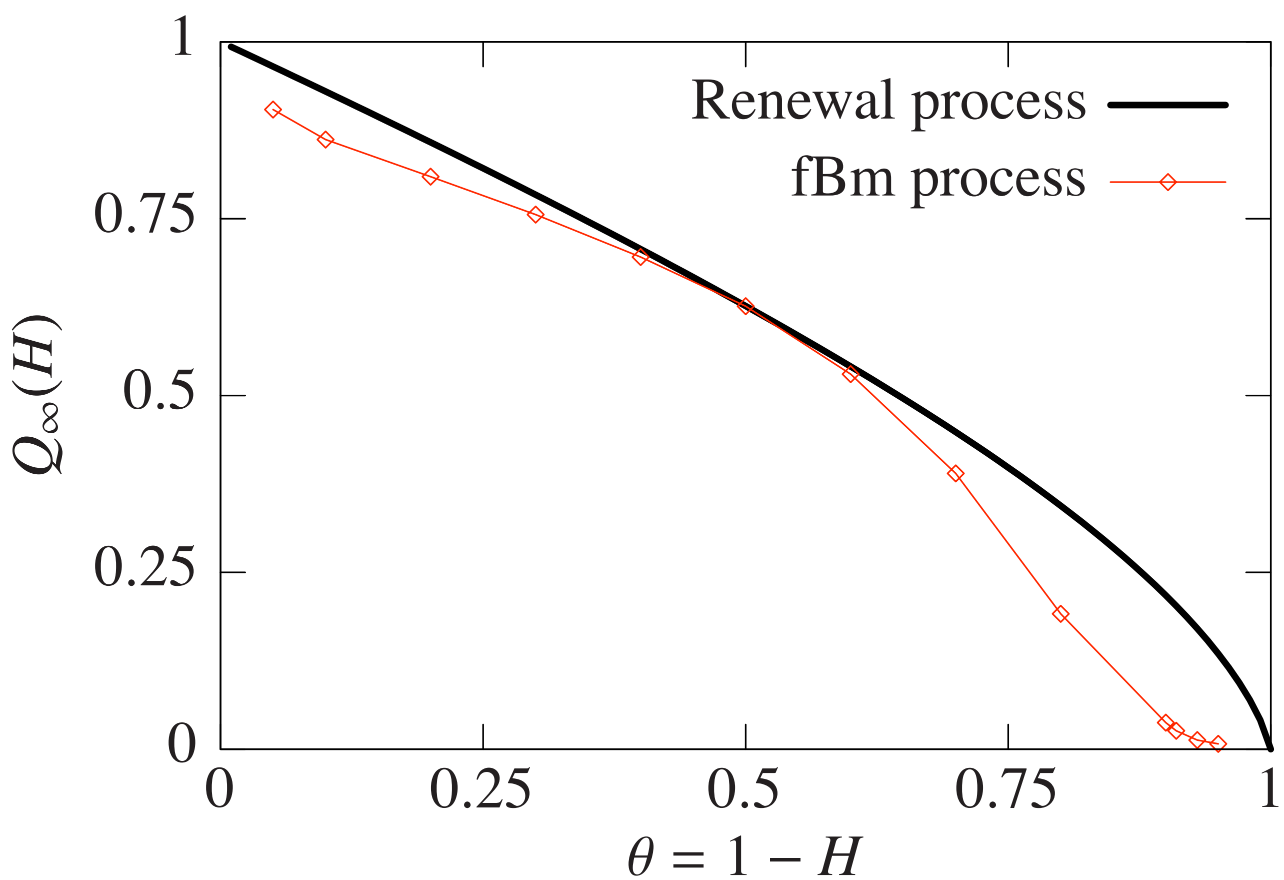

$R_+(y)$
1
0.1
0.01
0.001
10^{-4}
10^{-5}
0.01
0.1
1
y
L=20000
$H=\frac{2}{3}$
$H=\frac{1}{2}$

Non Markovianity and extremes...

The probability $Q(t)$ that $A(t)$ is the *longest excursion*?

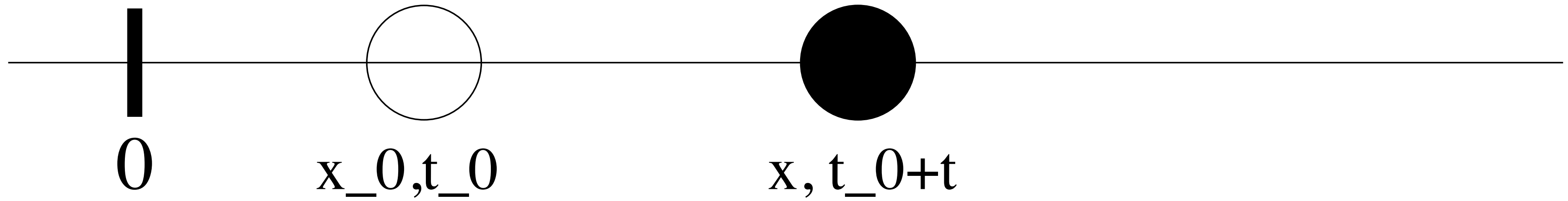


Exact solution for RENEWAL process
[Godrèche, Majumdar, Schehr]

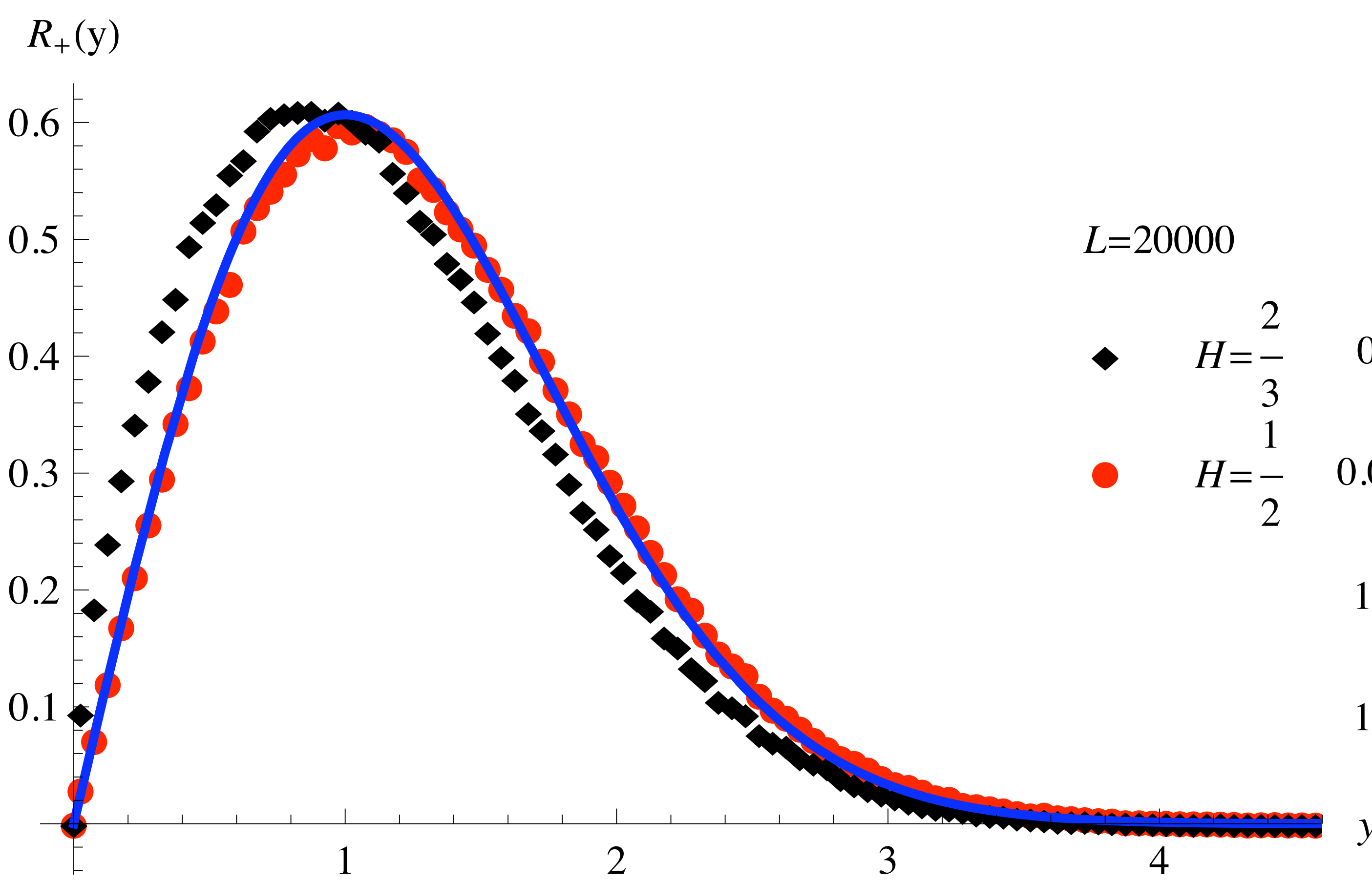


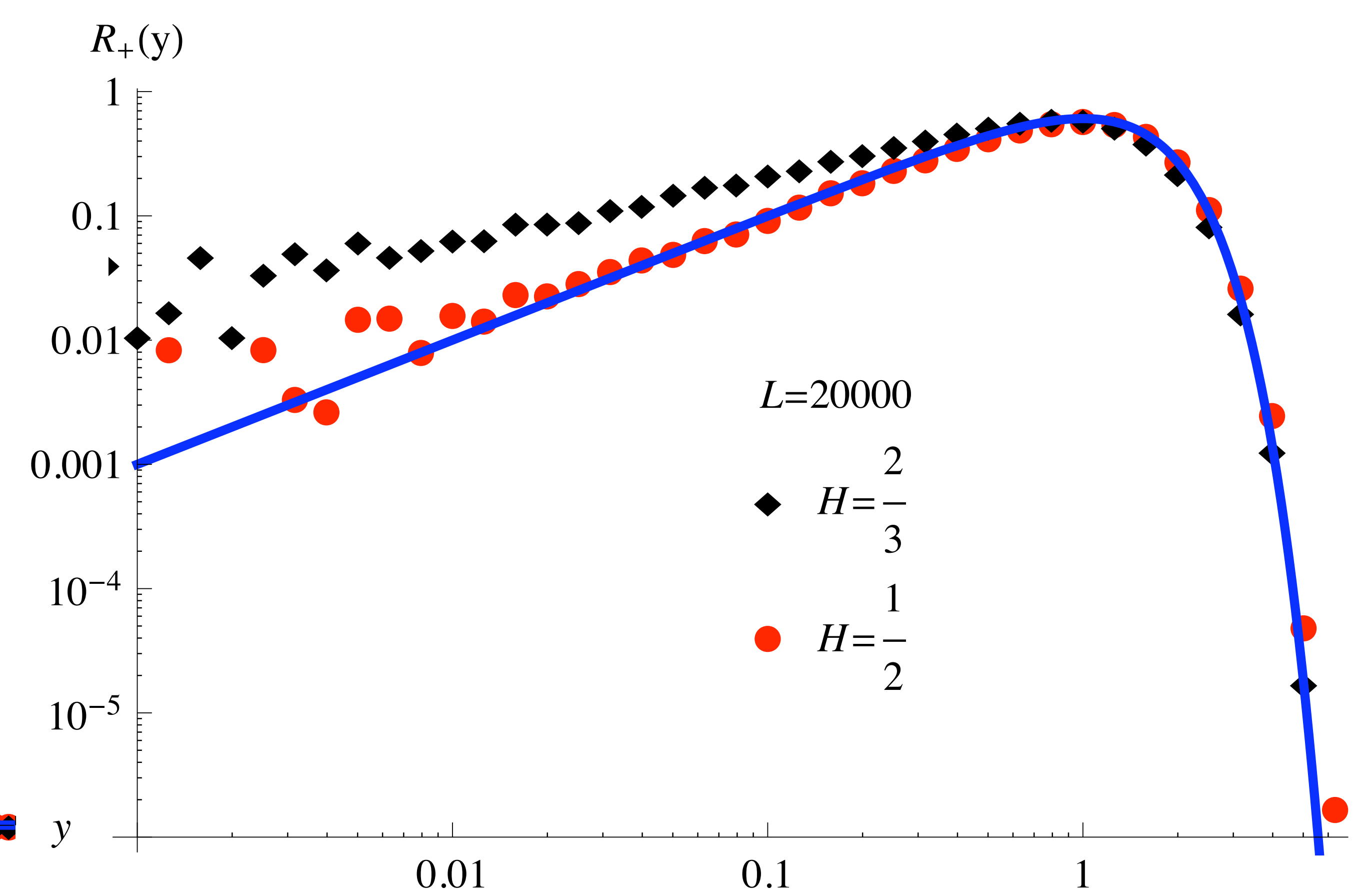
with Schehr and Garcia

Single Boundary



- Large time: $P_+(x, t; x_0, t_0) \xrightarrow{t \to \infty} P_+(x, t)$
- Self Affinity III: $P_+(x, t) = R_+(y)$ with $y = \frac{x}{\sqrt{\langle x^2(t) \rangle}} \sim \frac{x}{t^H}$
- Brownian $H = 1/2$: $R_+(y) = y e^{-\frac{y^2}{2}} \sim y + \dots$





How to generate a correlated path:

- time discretization: $x(t) \longrightarrow x_t = x_0 + \sum_{t'=1}^{t} \xi_{t'}$
- $\vec{\xi} = \{\xi_1, \xi_2, \ldots, \xi_T\}$ is a vector of Gaussian numbers with a given covariance matrix $\langle \xi_{t_1} \xi_{t_2} \rangle = C(|t_1 - t_2|)$
- we compute $A = \sqrt{C}$ $[T^3$ operations$]$ and generate uncorrelated Gaussian numbers $\vec{\epsilon} = \{\epsilon_1, \ldots, \epsilon_T\}$
- Then the vector $\vec{\xi}$ can be generated $[T^2$ operations$]$:

$$\vec{\xi} = A\vec{\epsilon}$$

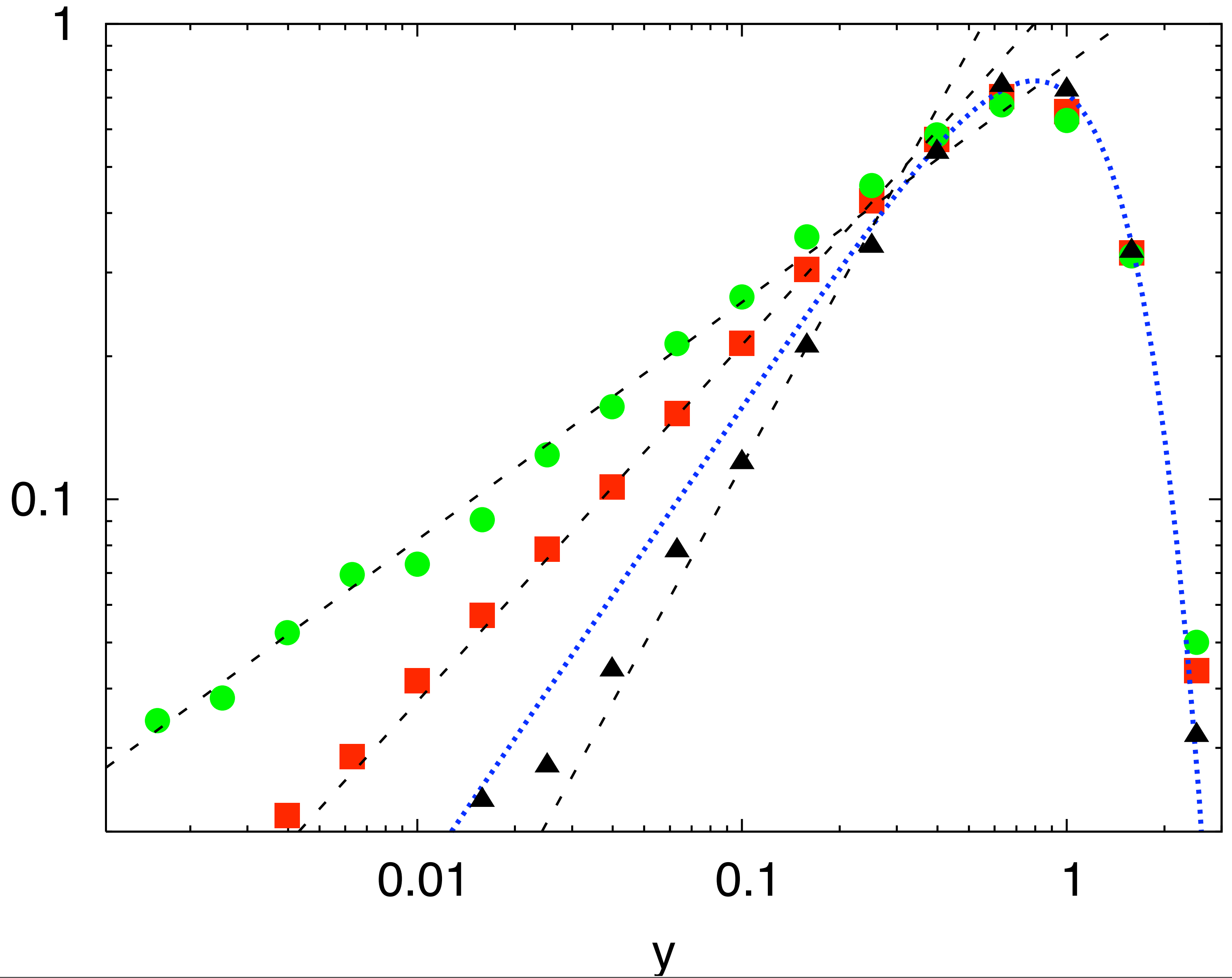
Proof:

$$\langle \xi_i \xi_j \rangle = \langle \sum_{i'} A_{i,i'} \epsilon_{i'} \sum_{j'} A_{j,j'} \epsilon_{j'} \rangle = \sum_{i',j'} A_{i,i'} A_{j,j'} \delta_{i',j'} = (A^2)_{i,j} = C_{i,j}$$

- Special algorithms if Covariance is Toeplitz matrix: $C_{i,j} = C(|i-j|)$.

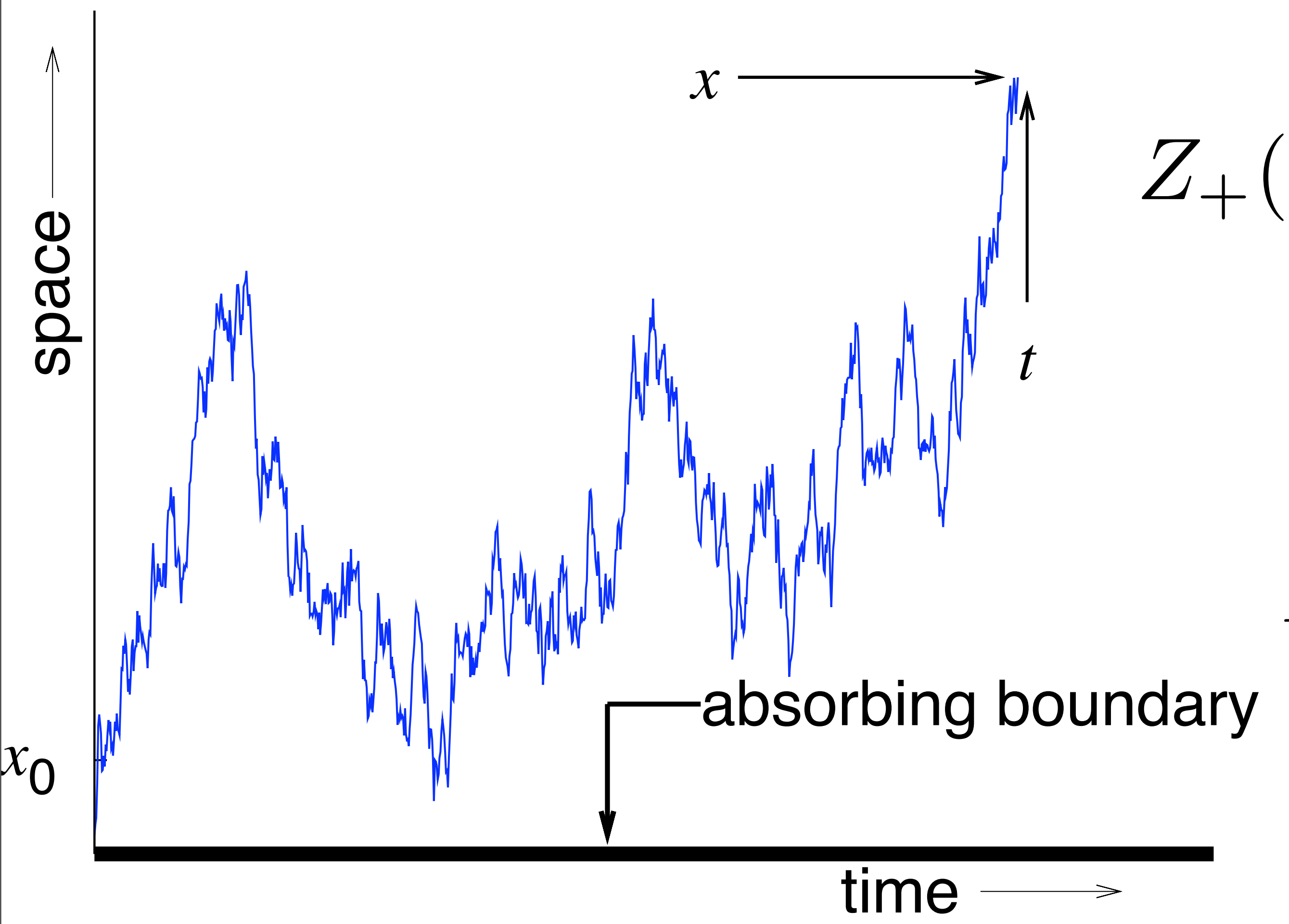
Single Boundary

- In general we expect $R_+(y) \sim y^\phi$
- For stationary increments, a scaling argument gives $\phi = \frac{\theta}{H}$
- numerical simulations agrees



- Circle $H = \frac{2}{3}$, $\phi = \frac{1}{2}$
- Square $H = \frac{4}{7}$, $\phi = \frac{3}{4}$
- Line $R_+(y) = ye^{-y^2/2}$
- Triangle $H = \frac{4}{9}$, $\phi = \frac{5}{4}$

Perturbation Theory



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

$$P_+(x,t) = \lim_{x_0 \to 0} \frac{Z_+(x_0, x, t)}{\int_0^\infty dx Z_+(x_0, x, t)}$$

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

where $G^{-1}(t_1, t_2) = \langle x(t_1) x(t_2) \rangle$ it is known

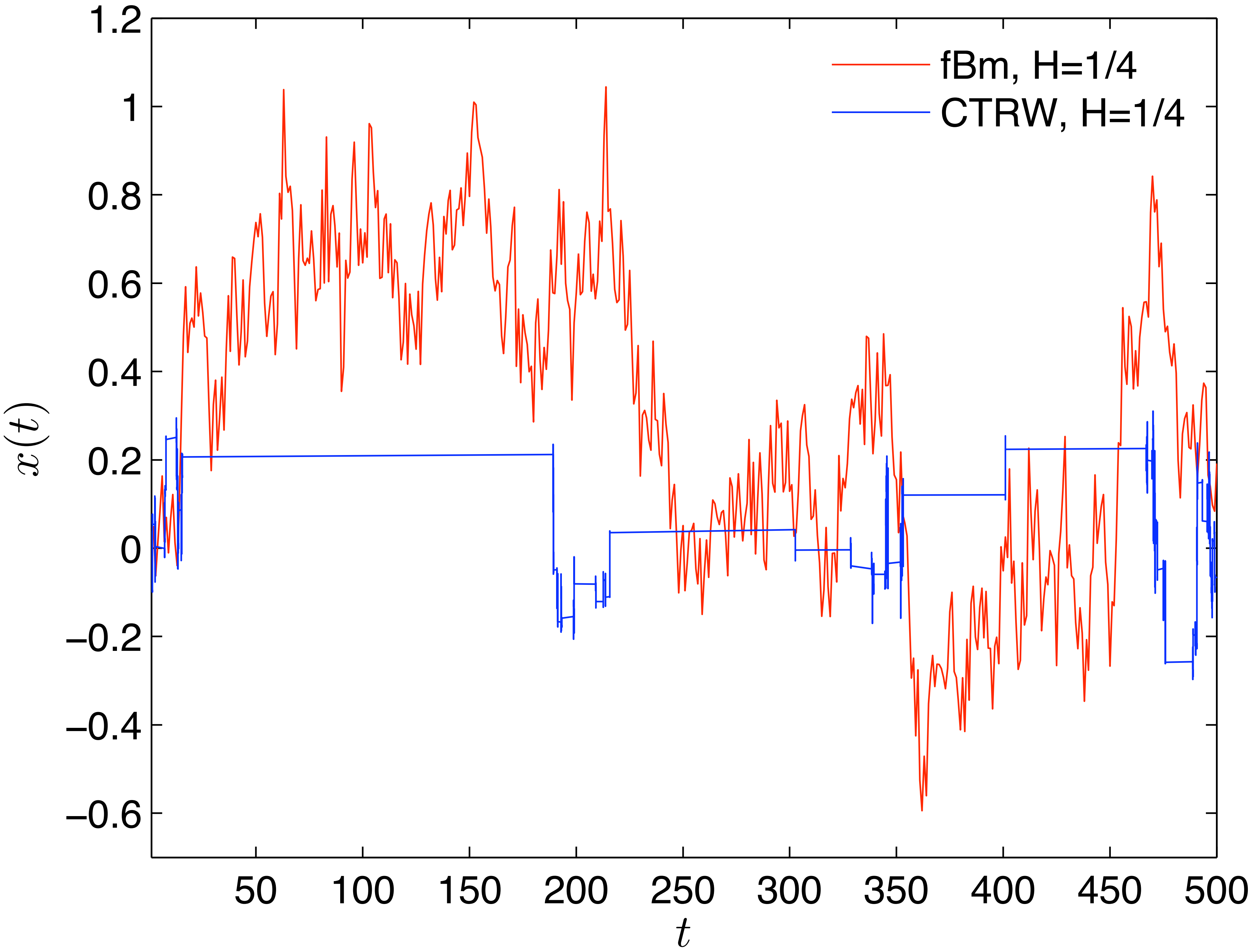
Diffusion and Central Limit Theorem

- $\left\langle x^2(t) \right\rangle = 2Dt \propto t$ and D is diffusion constant

- $x(t)$ (for large t) is a **Gaussian** process

- Propagator from x_0 to x: $P(x_0, x, t) = \frac{e^{-\frac{(x(t)-x_0)^2}{4Dt}}}{\sqrt{4\pi Dt}}$

And the Fractional Fokker Planck Equation (CTRW)?



Anomalous Diffusion

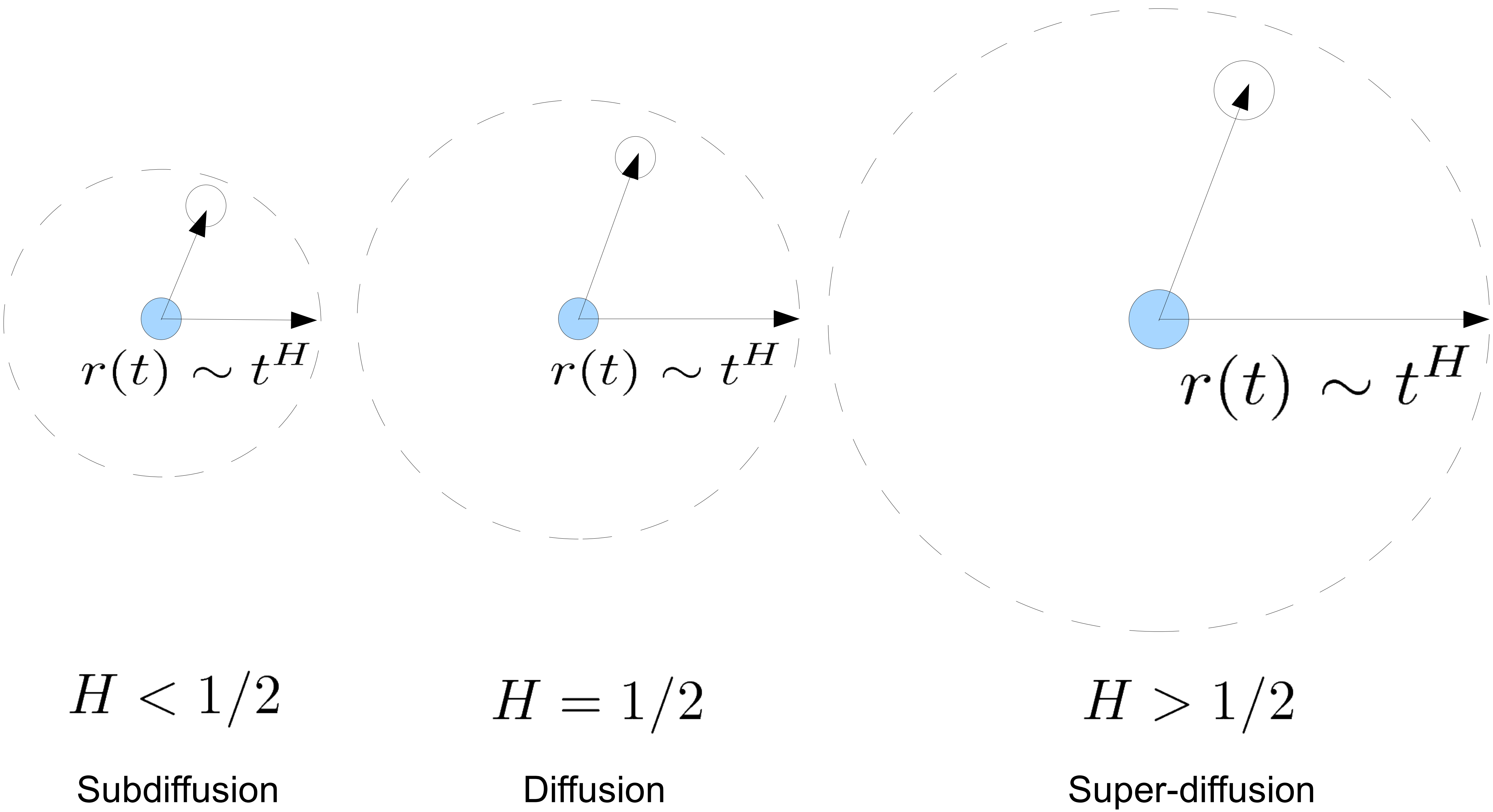
Alberto Rosso (LPTMS-Orsay)

Polymer translocation: A. Zoia (Saclay) + S. Majumdar

Perturbation theory: K. J. Wiese (ENS) + S. Majumdar

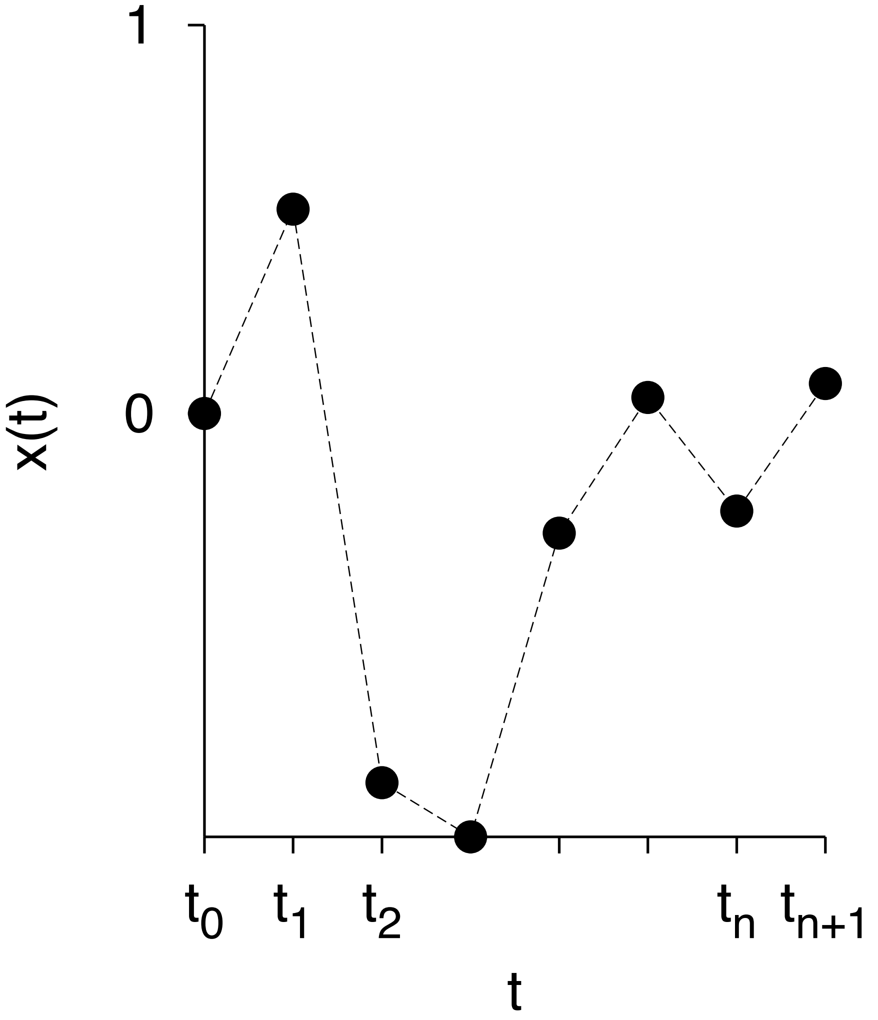
Longest excursion: R. Garcia (Bariloche) + G. Schehr

Anomalous Diffusion



Central Limit Theorem

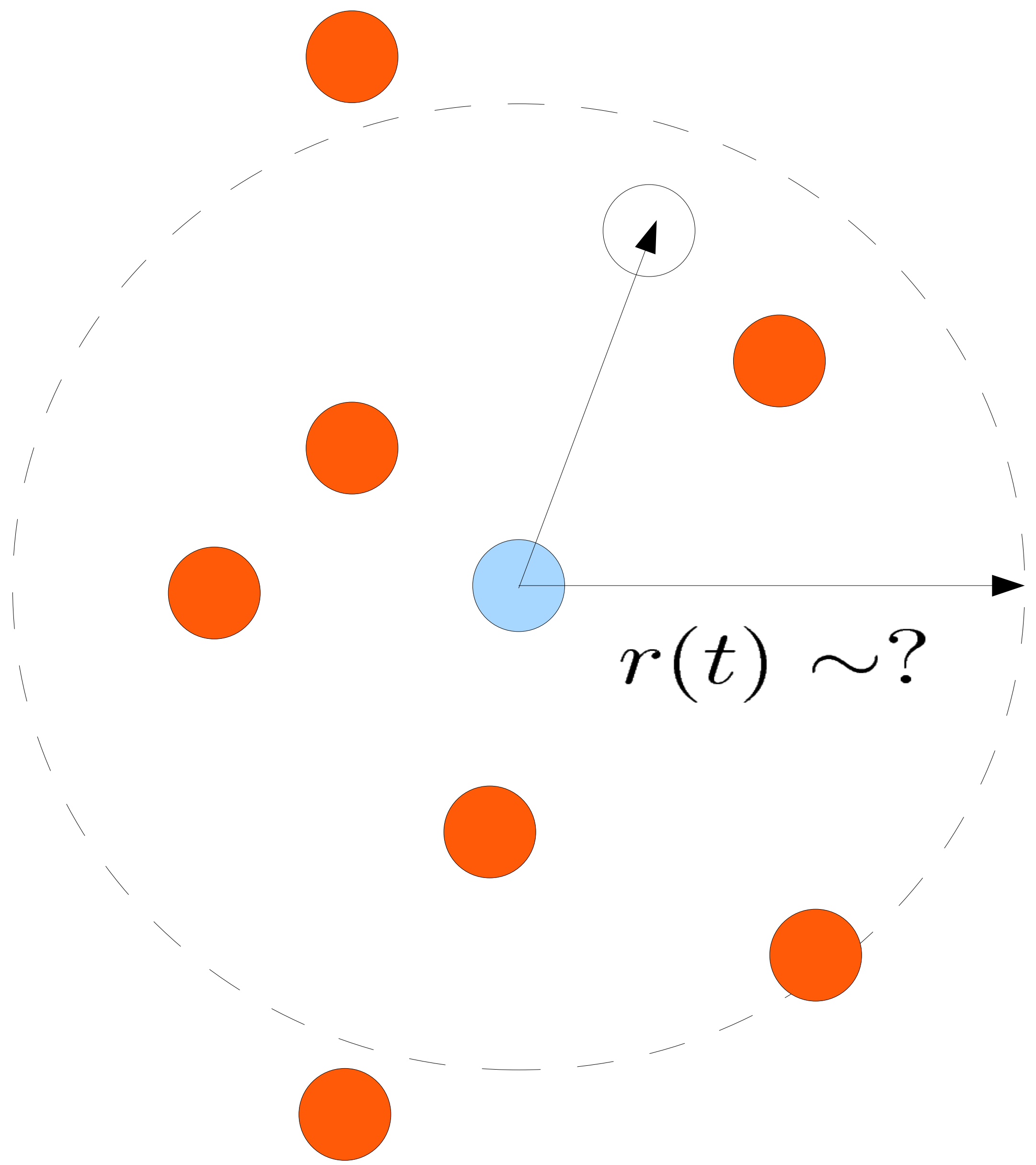
$$x(t) = \sum_{t'=1}^{t} \xi_{t'}$$



- *Identical*: $\pi_{t'}(\xi) = \pi(\xi)$. (Homogeneous)
- *Independent*: $\langle \xi_{t_0} \xi_{t_0+t} \rangle = 0$. (Markov)
- $\langle \xi^2 \rangle < \infty$: Continuous process.

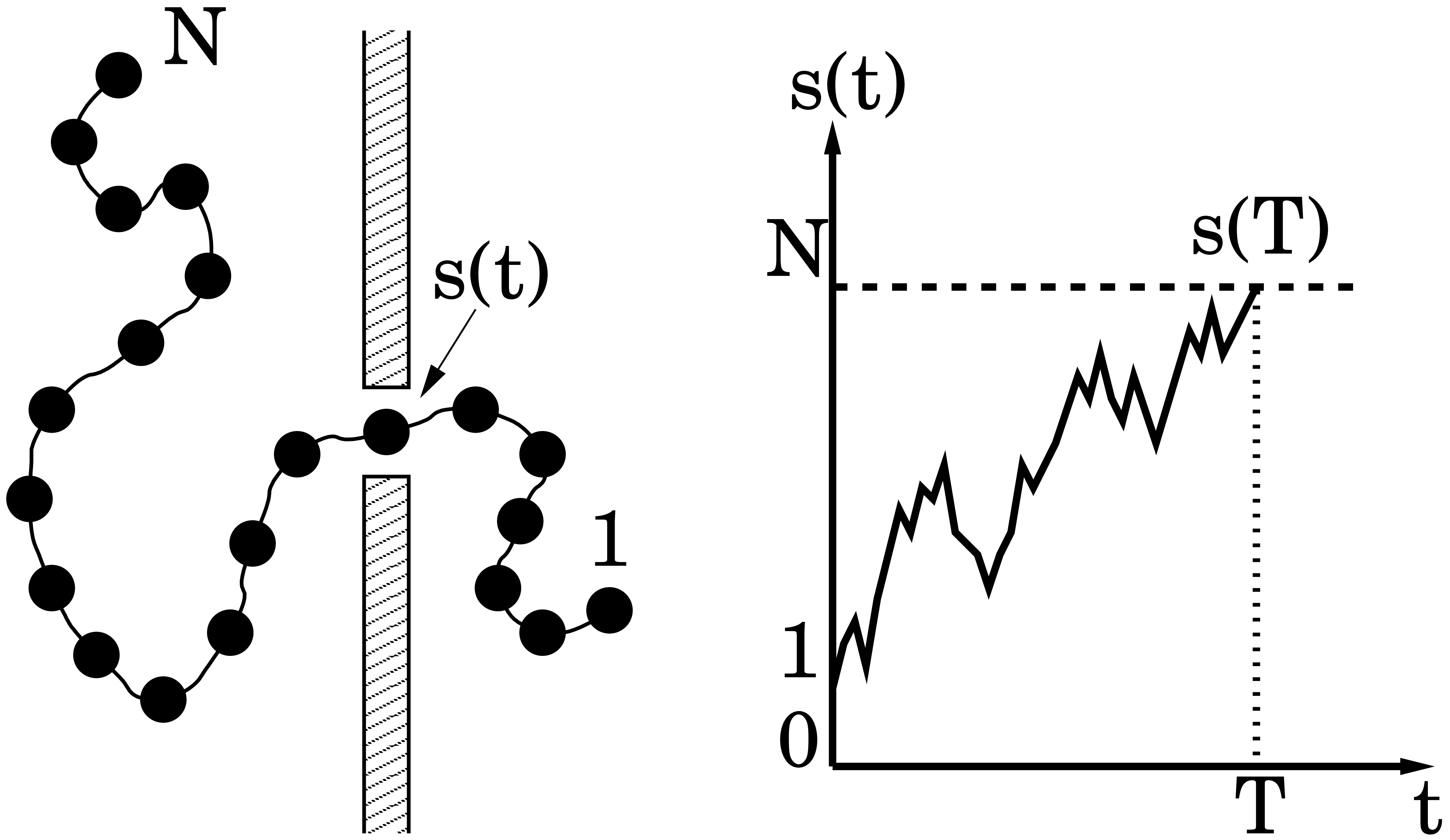
Conclusion: $x(t)$ **is Gaussian and** $x(t) \sim \sqrt{t}$

Correlations

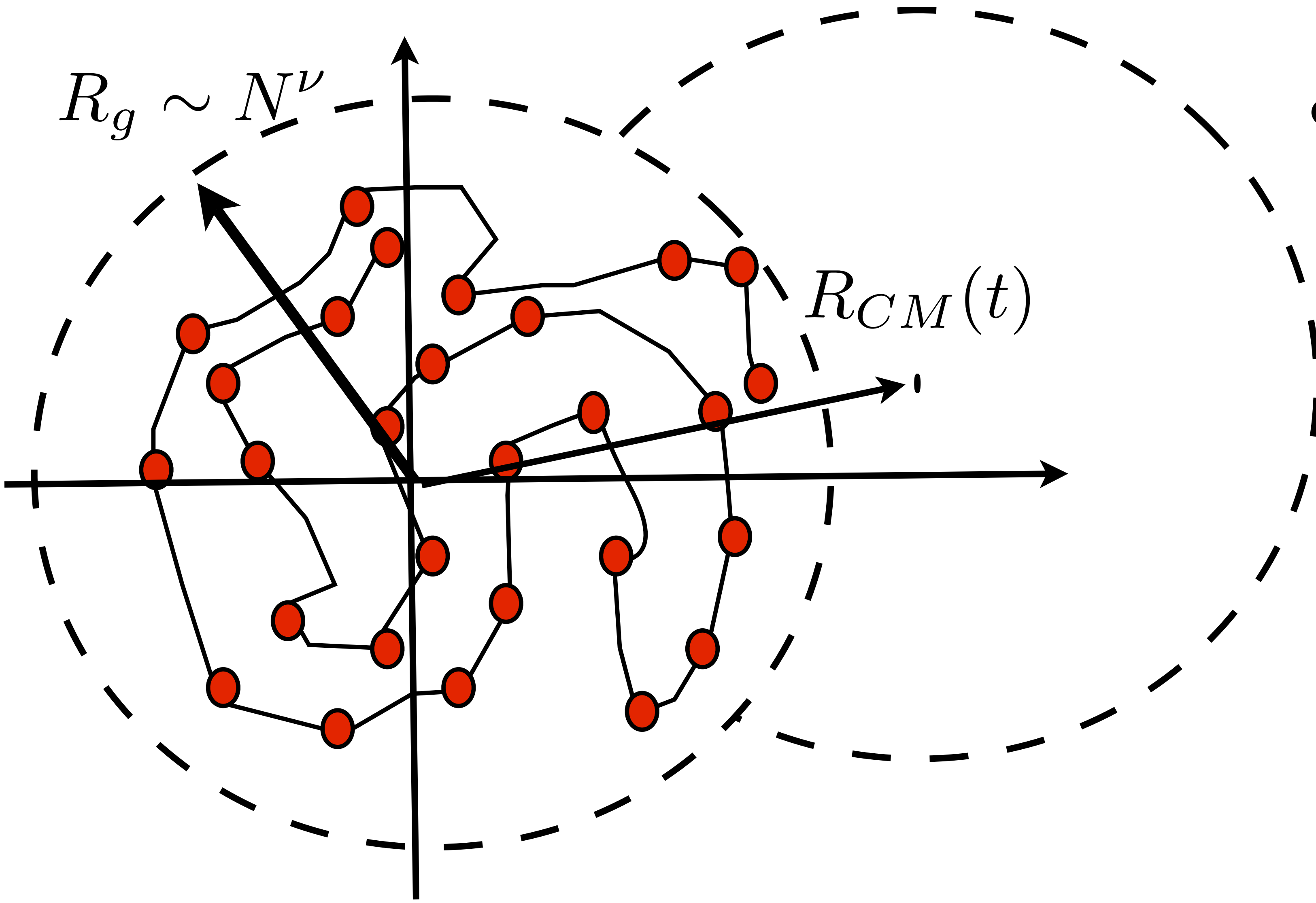


- jumps and waiting times are local
- colloids interact (strongly non-Markovian)

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 $\nu = 1/2$

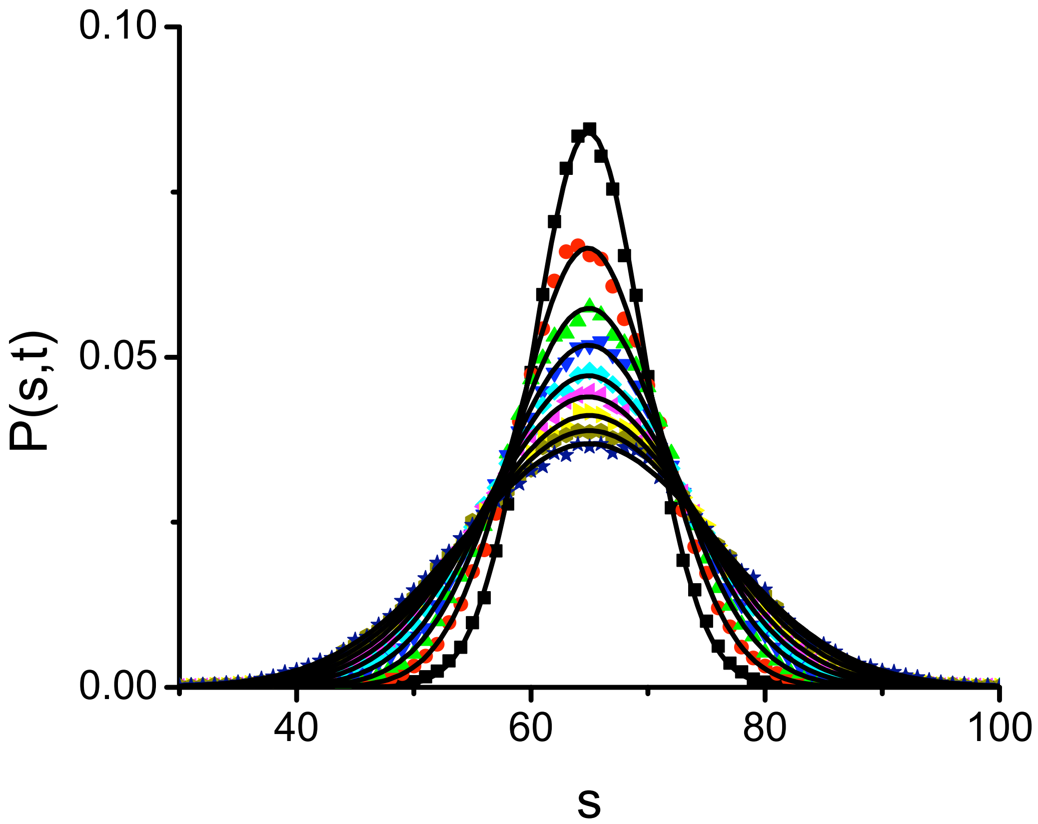
Excluded Volume $\nu > 1/2$

- $R_{CM}(t)$ Center of Mass

$$\langle R^2_{\mathrm{CM}}(t_{\mathrm{eq.}})\rangle = R_g^2 \quad \Rightarrow \quad \frac{D_1 t_{\mathrm{eq.}}}{N} \sim N^{2\nu} \quad \Rightarrow \quad t_{\mathrm{eq.}} \sim N^{2\nu+1}$$

$$T \gg t_{\mathrm{eq.}} \quad \Rightarrow \quad H \leq \frac{1}{1+2\nu} \quad \text{numerically} \quad H \approx \frac{1}{1+2\nu}$$

Fractional Brownian motion



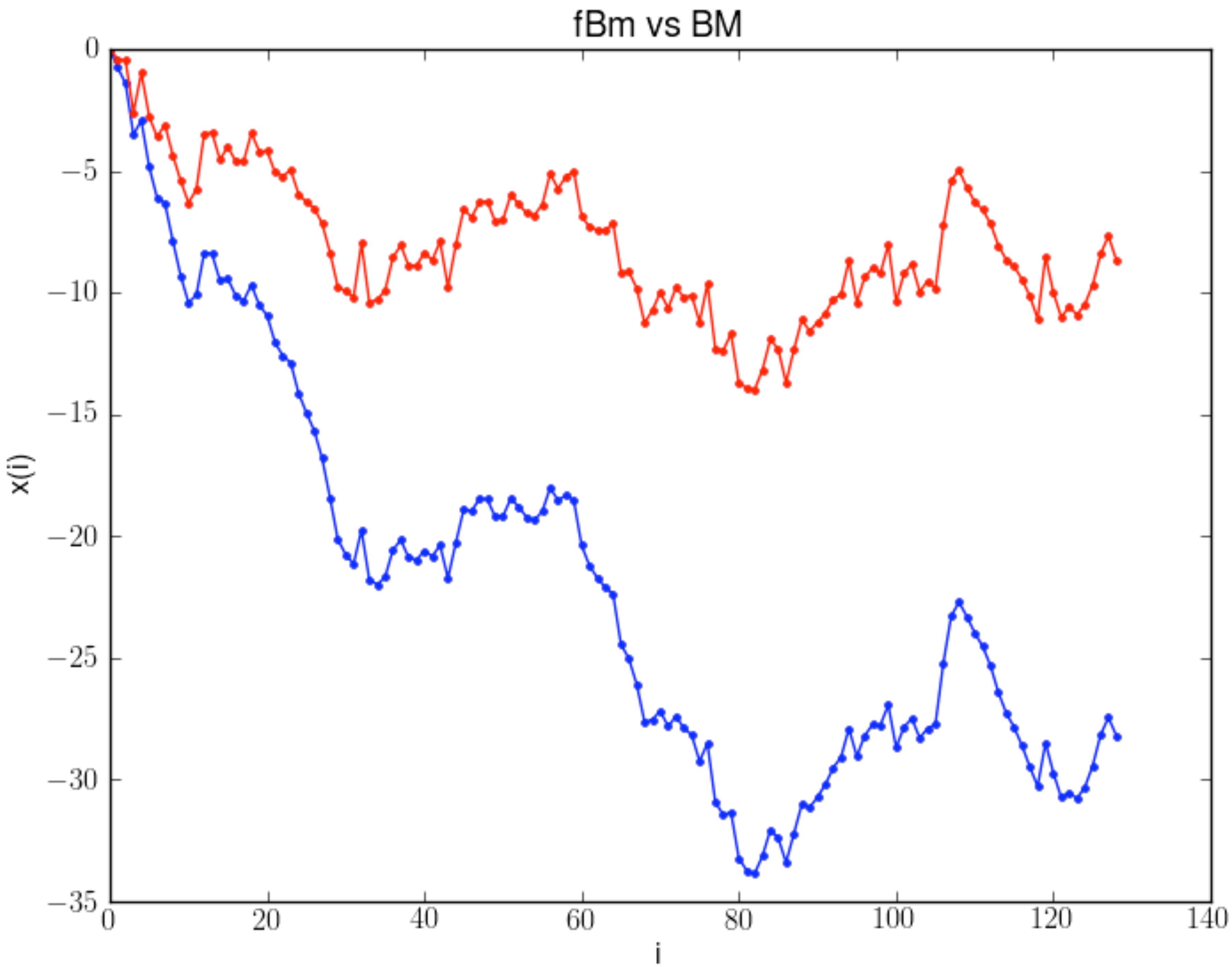
Monte Carlo simulation of polymer translocation in d=2,
Chatelain, Kantor, Kardar, PRE 78, 021129 (2008)

- Equilibrium with the solvent $\Rightarrow$ stationary increments
- is a Gaussian process $\Rightarrow$ local jumps
- $\Rightarrow$ non-Markov process

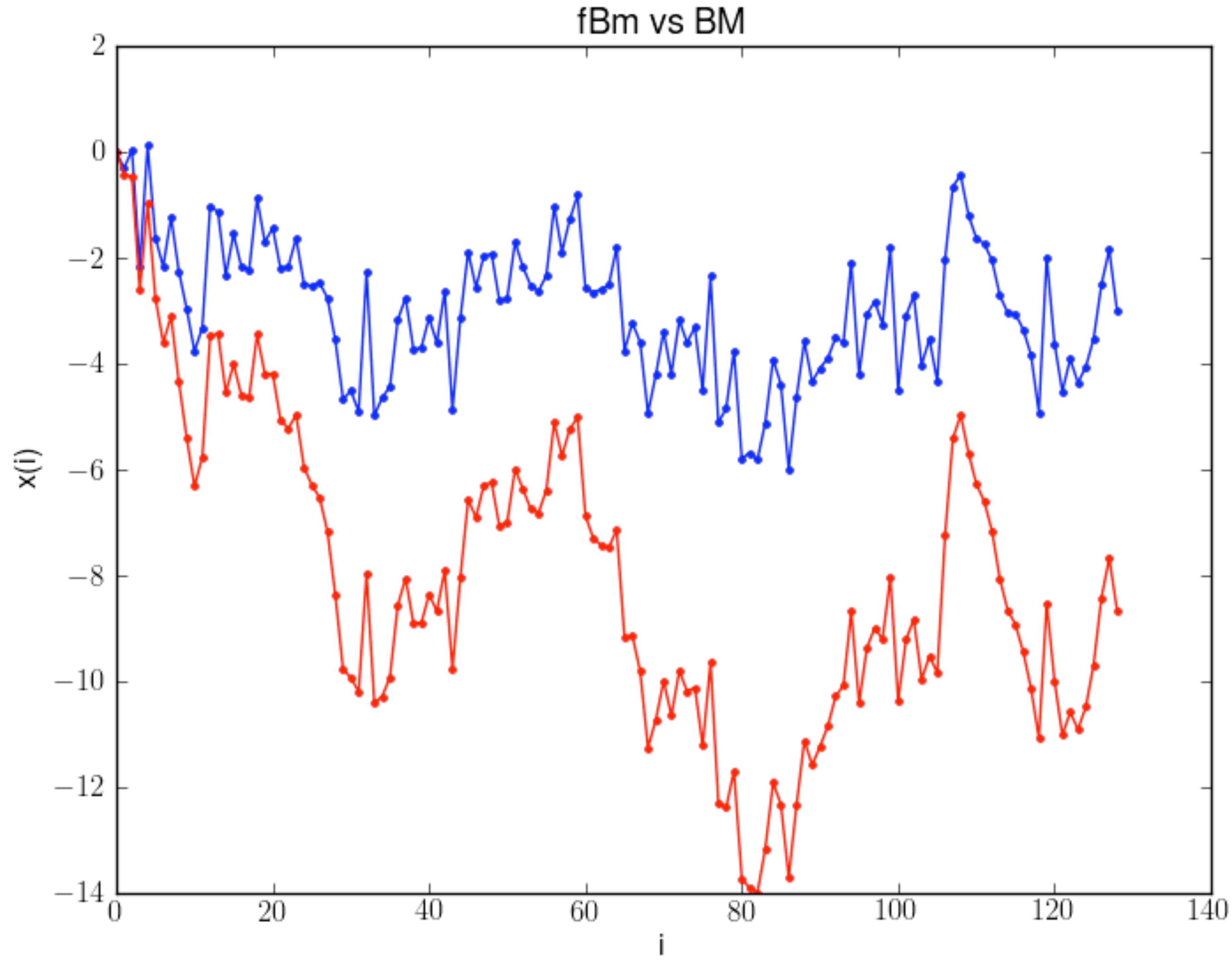
Gaussianity + self-affinity $H = \frac{1}{2\nu+1}$ + stationary increments
$\Rightarrow$ fractional Brownian motion:

$$\langle s(t_1)s(t_2)\rangle \propto \left(t_1^{2H} + t_2^{2H} - |t_1 - t_2|^{2H}\right),$$

H=3/4 Superdiffusion

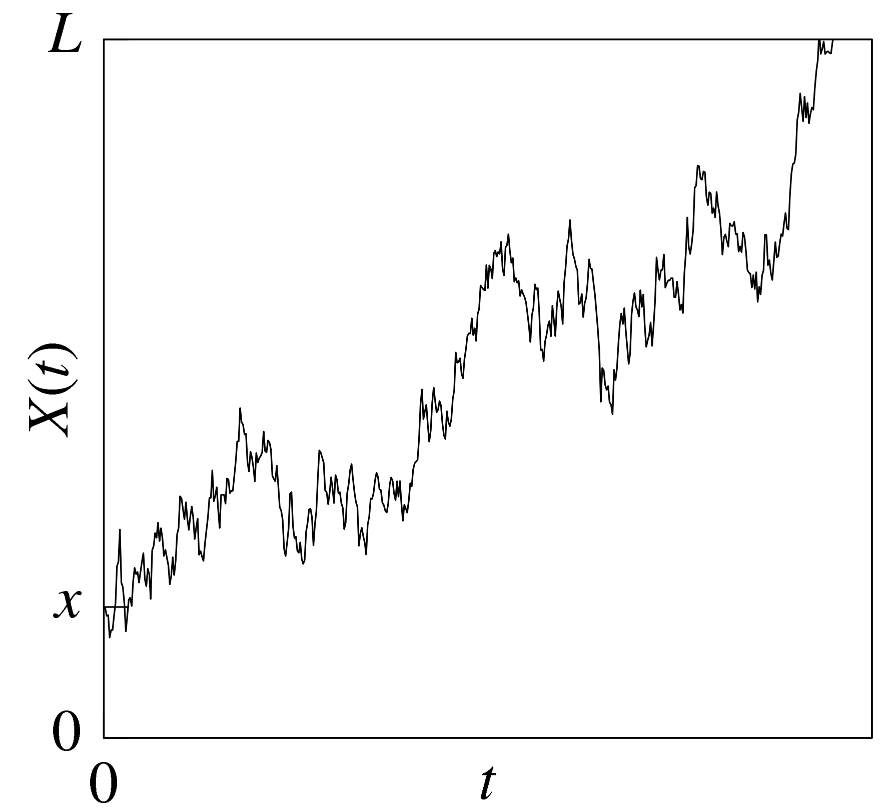


H=1/4 Subdiffusion



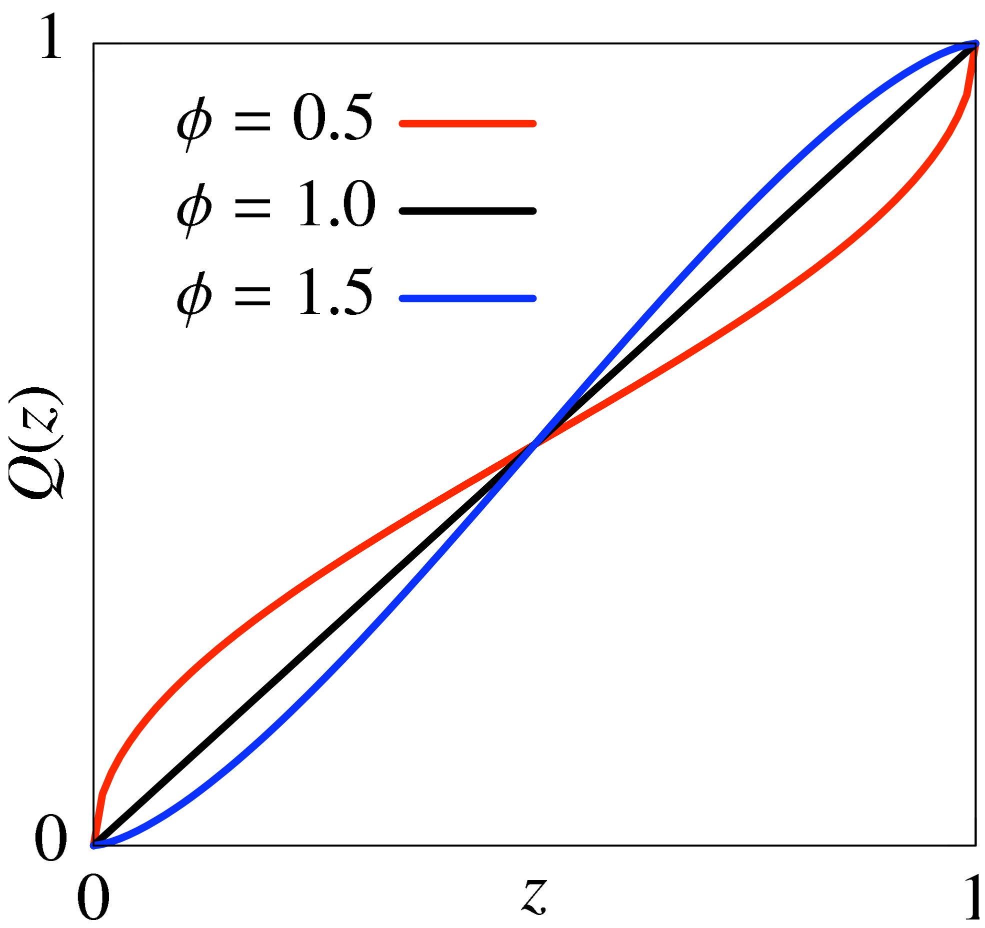
Question I: A polymer chain will ultimately succeed in translocating through a pore ?

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



For **self affine** processes:

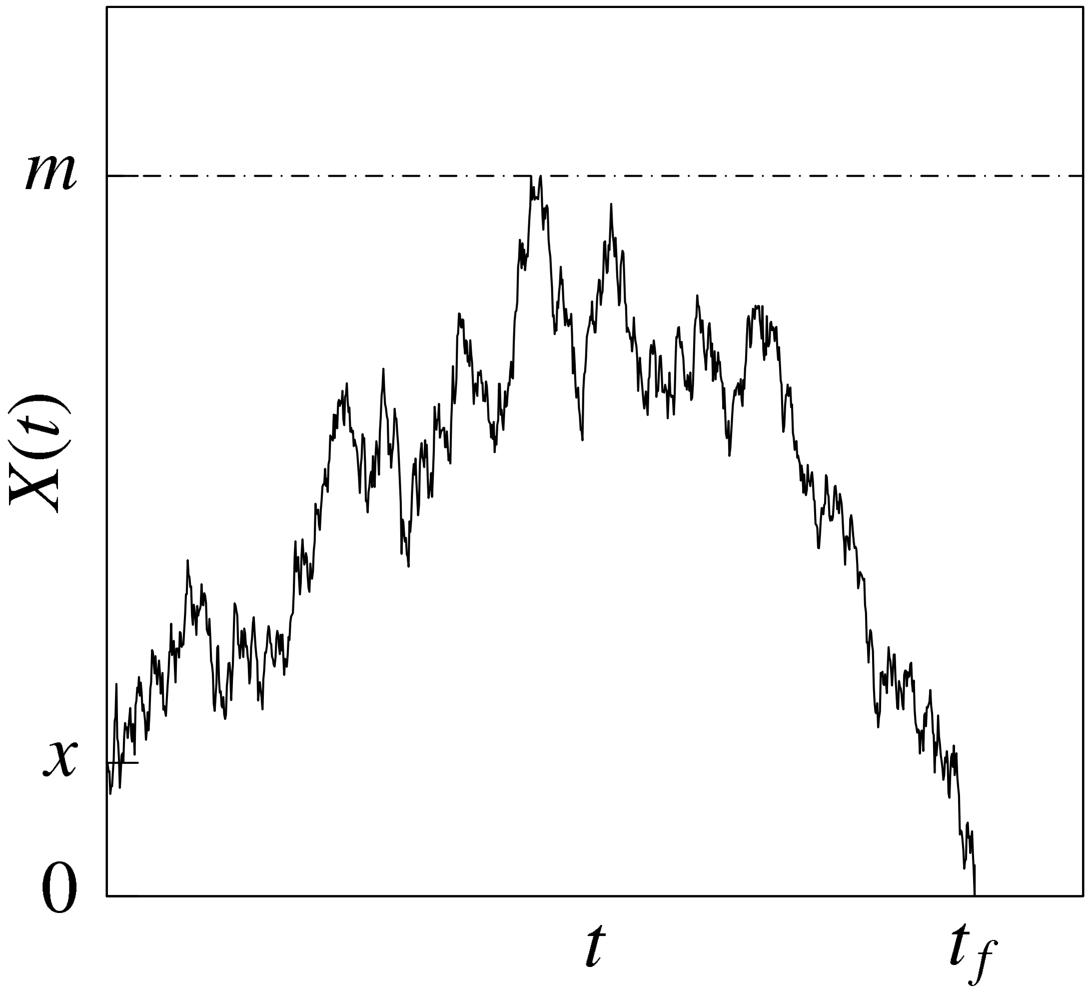
$$Q(x, L) = Q\left(z = \frac{x}{L}\right)$$



- Basic: $Q(z) = 1 - Q(1 - z)$; $Q(1/2) = 1/2$; $Q(z) = 0$
- $H = 1/2$: $Q(z) = z$
- Expansion: $Q(z) \sim c_1 z^{\phi} + \ldots$

Translocation is enhanced or suppressed by excluded volume effects?

A scaling argument: $\phi = \frac{\theta}{H}$



- $Q(x, L) = \mathrm{Prob}[m > L]$
- Self-affinity I: $m \sim t_f^H$

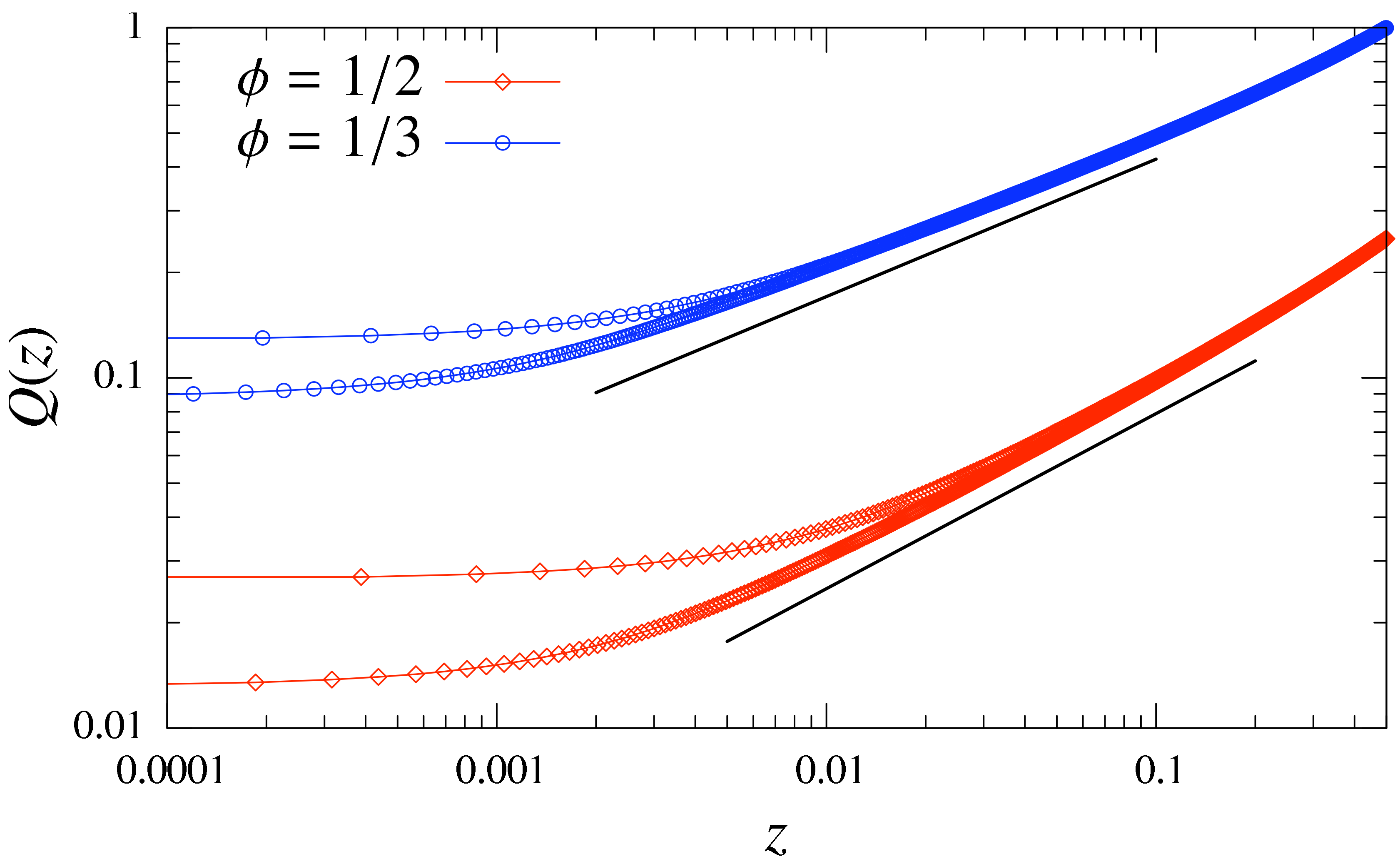
$\Longrightarrow Q(x, L) \simeq \mathrm{Prob}[t_f^H > L]$
$Q(x, L) \sim \mathrm{Prob}[t_f > L^{\frac{1}{H}}]$

- Survival probability: $\mathrm{Prob}[t_f > T] = S(x, T) =\sim \frac{f(x)}{T^\theta}$
  θ persistence exponent

- Self-affinity II: $S(x, T) \sim \left(\frac{x}{T^H}\right)^{\frac{\theta}{H}}$

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

Hitting probability: numerical test



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

Previous results... recast using ϕ

(i) Random acceleration process: $\ddot{x} = \eta(t),\ x(0) = x,\ \dot{x}(0) = 0$

Burkhardt: $H = \frac{3}{2}$ and $\theta = \frac{1}{4} \implies \phi = \frac{1}{6}$

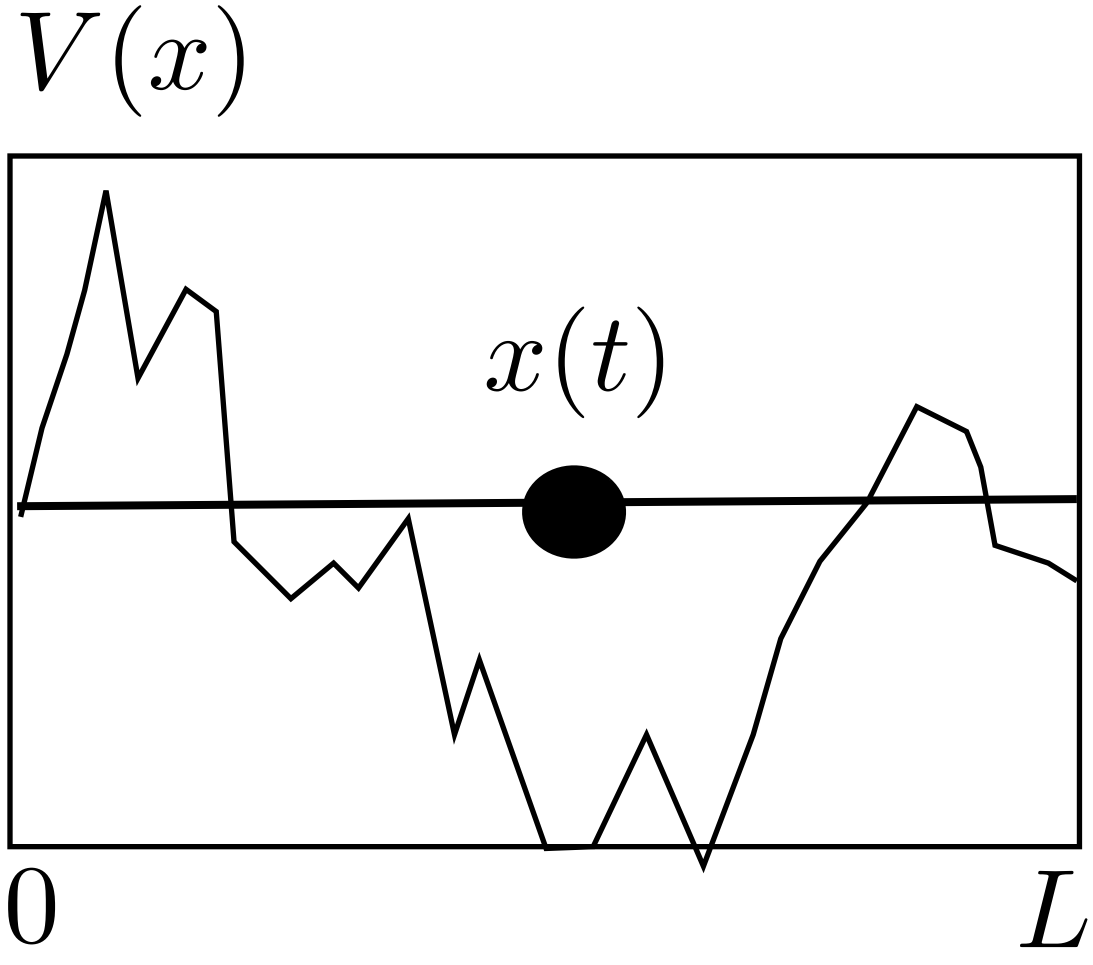
$Q(z = \frac{x}{L}) = I_z[\frac{1}{6}, \frac{1}{6}]$. Where $I_z(\phi,\phi) = \frac{\Gamma(2\,\phi)}{\Gamma^2(\phi)} \int_0^z \frac{du}{[u(1-u)]^{1-\phi}}$

(ii) Lévy fligths: $x_{t+1} = x_t + \xi_t$ with $\pi(\xi) \sim \xi^{-(\mu+1)}$

Sparre Andersen: $H = \frac{1}{\mu}$ and $\theta = \frac{1}{2} \implies \phi = \frac{\mu}{2}$

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

Sinai model



$$t \sim e^{V(x)} \sim e^{\sqrt{x}} \Rightarrow x(t) \sim [\log(t)]^2$$

$$S(x_0, t) \sim [\log(t)]^{-1}$$

Using $\tau = \log(t) \implies H = 2$ and $\theta = 1$

From Backward Fokker Planck: $Q(x, L) = \frac{\int_0^x e^{\beta V(x')} dx'}{\int_0^L e^{\beta V(x')} dx'}$

$$\overline{Q(z)} = \int_0^z dz' \, \overline{p_{eq}(z')}; \quad \text{From } \overline{p_{eq}(z)} = \frac{1}{\pi} \frac{1}{\sqrt{z(1-z)}}$$

We deduce $\overline{Q(z)} = I_z(1/2, 1/2) = \frac{2}{\pi} \arcsin(\sqrt{z}) \sim \sqrt{z}$

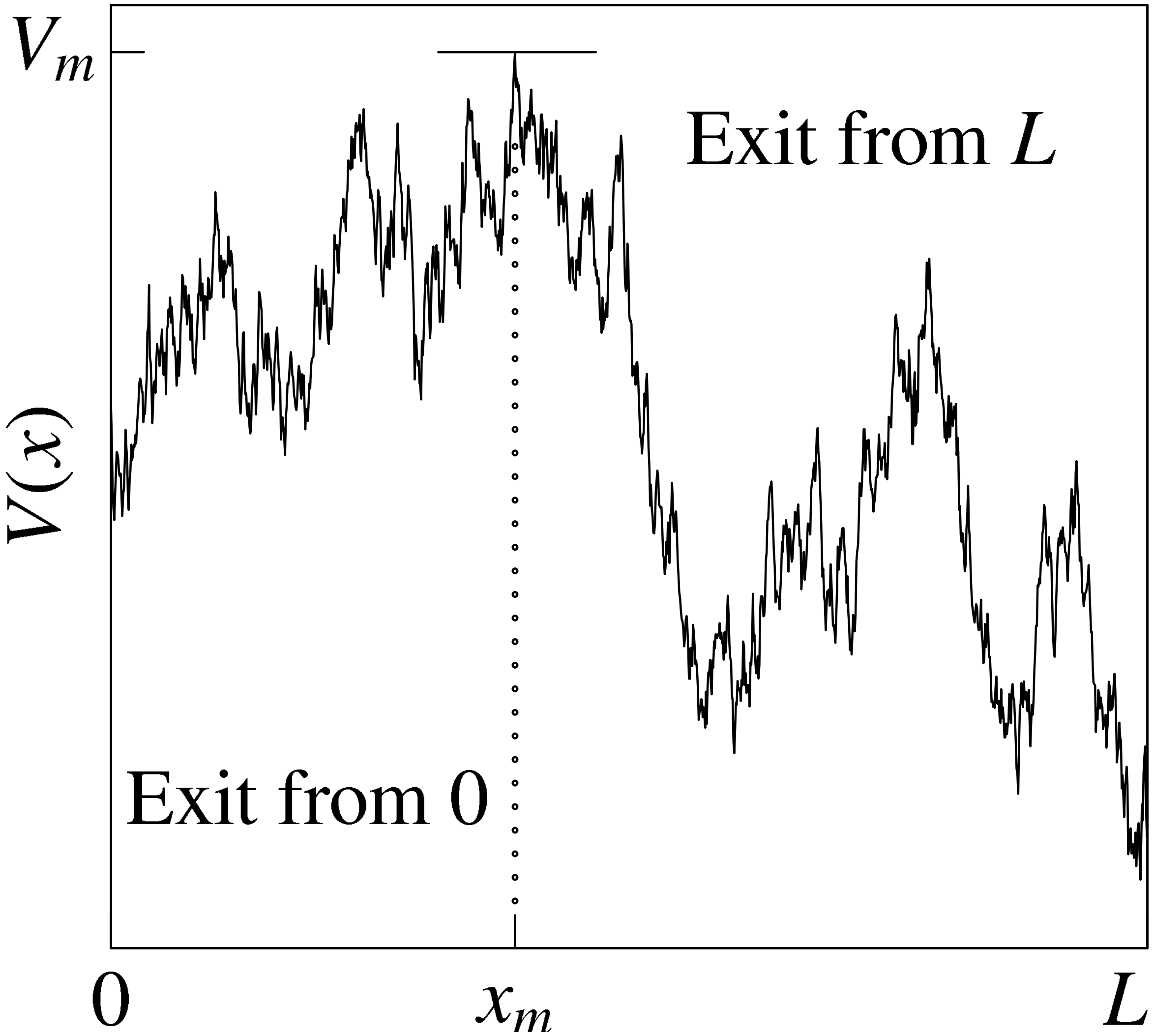
So that $\phi = \theta / H = 1/2$

See Oshanin, Redner, Comtet, Monthus, Texier...

Extreme statistics: maximum location in $V(x) \sim x^{H_V}$

$$p_{eq}(x,L) = \frac{e^{\beta V(x)}}{\int_0^L e^{\beta V(x')} dx'} \propto \left\{ \int_0^1 dz' \, \exp\left[\beta L^{H_V} \cdot (V(z') - V(z))\right] \right\}^{-1}$$

$$p_{eq}(x,L) \sim \delta(x - x_m) \Longrightarrow \overline{p_{eq}(x,L)} \sim p_V(x_m, L) \quad \text{[Sinai: arcsine law]}$$



Fixed realization: $Q(x,L) = \theta(x - x_m)$

Average $\overline{Q(z = \frac{x}{L})} = \text{Prob}[z_m < z]$

If $V(x) \sim x^{H_V}$, using Arrhenius $H = 1/H_V$

$$\mathrm{Prob}[x_m < x \to 0] \sim \mathrm{Prob}[V < 0 \text{ up to } L] \sim \frac{1}{L^{\theta_V}}$$

So that $Q(x,L) \to \left(\frac{x}{L}\right)^{\theta_V}$

We Conclude $\phi = \theta_V$ **and** $\theta = H \cdot \phi = \theta_V / H_V$

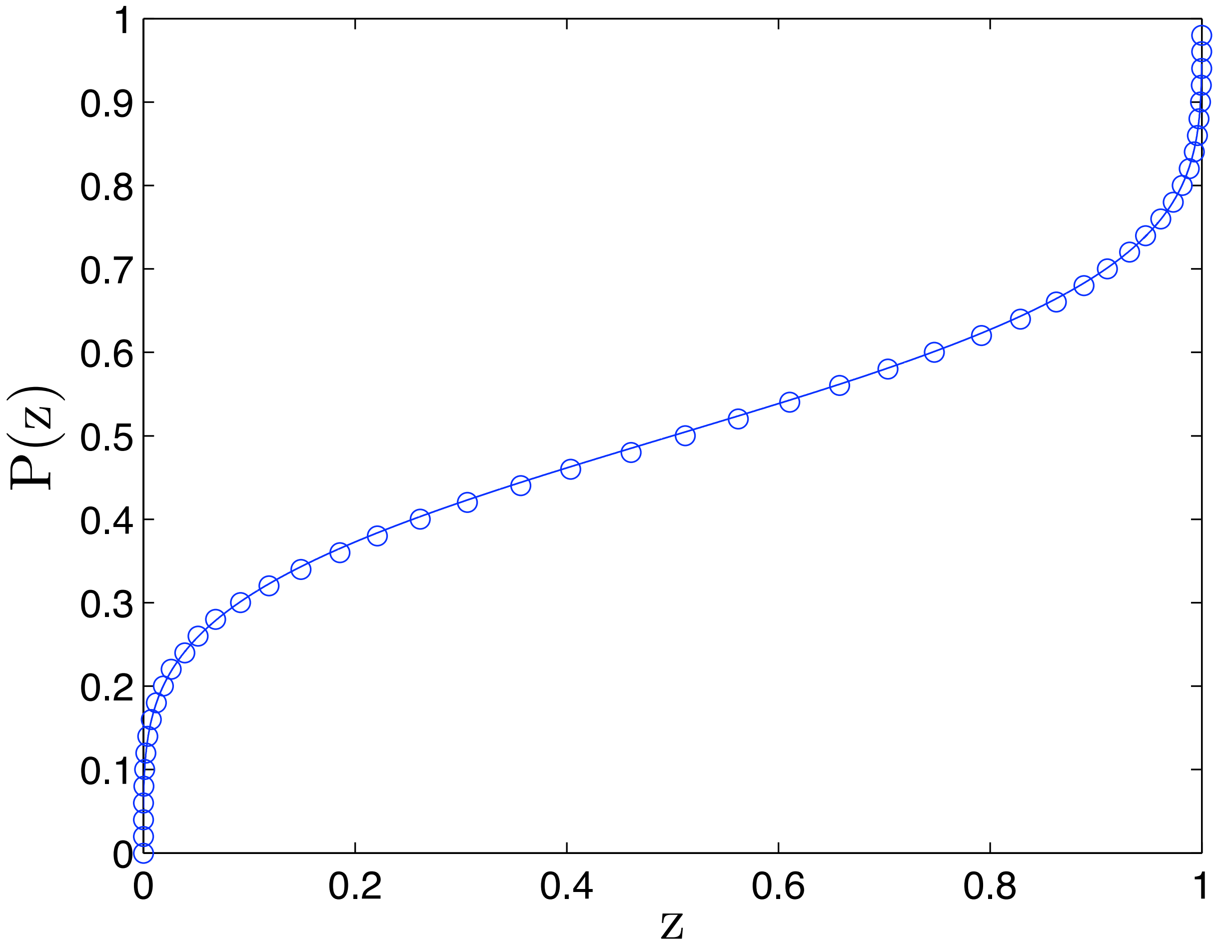
$V(x)$ is a random acceleration process: $H_V = 3/2$, $\theta_V = 1/4$

Bridge case ($V'(L) = 0$): $p(z_m) = \frac{\Gamma(1/2)}{\Gamma^2(1/4)} \frac{1}{(z_m(1-z_m))^{3/4}}$

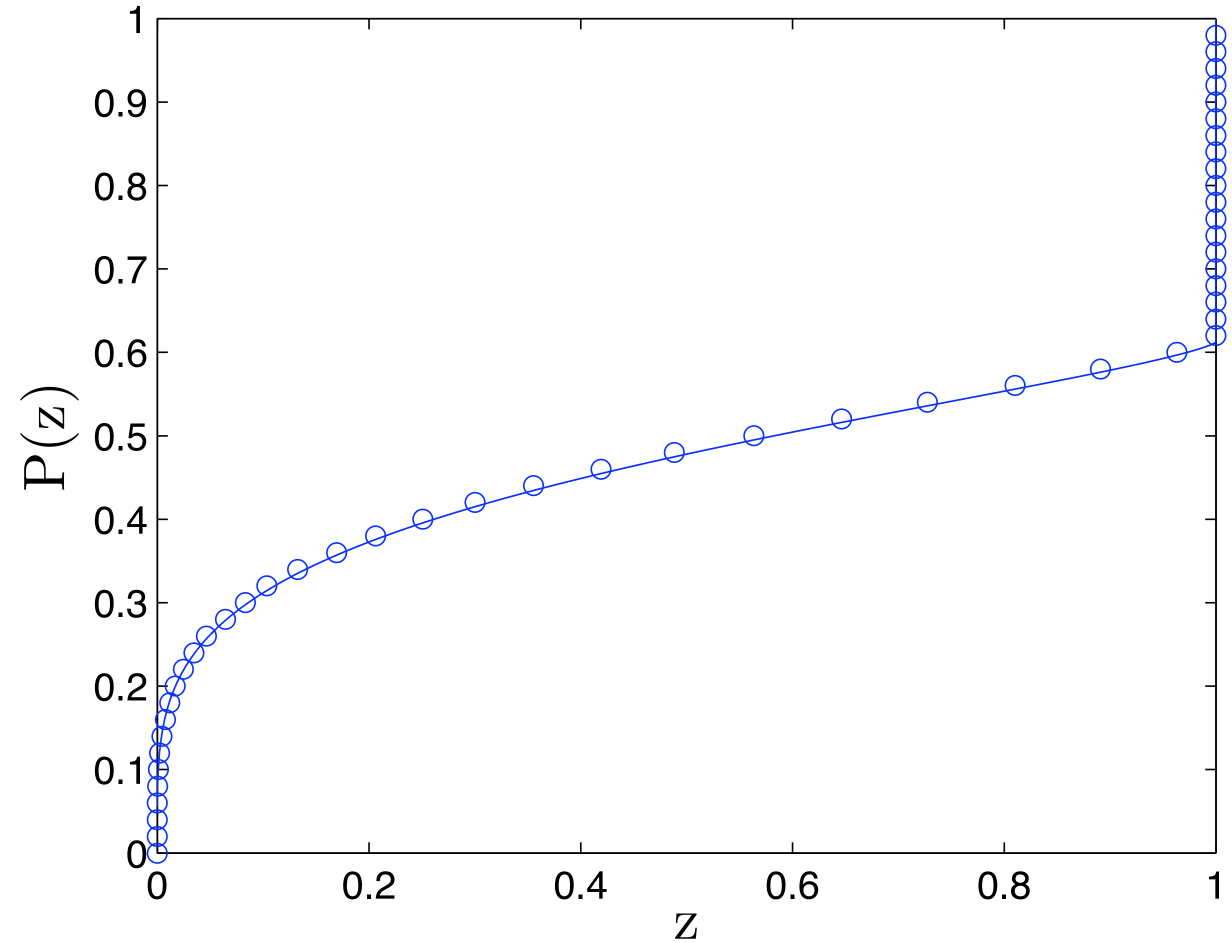
Free case: $p(z_m) = (1 - \sqrt{\frac{3}{8}})\delta(z_m - 1) + \frac{\sqrt{3}}{4\pi z_m^{3/4}(1-z_m)^{1/4}}$

(See also Maximum location, for CTRW : Le Doussal and Schehr)

Hitting Bridge

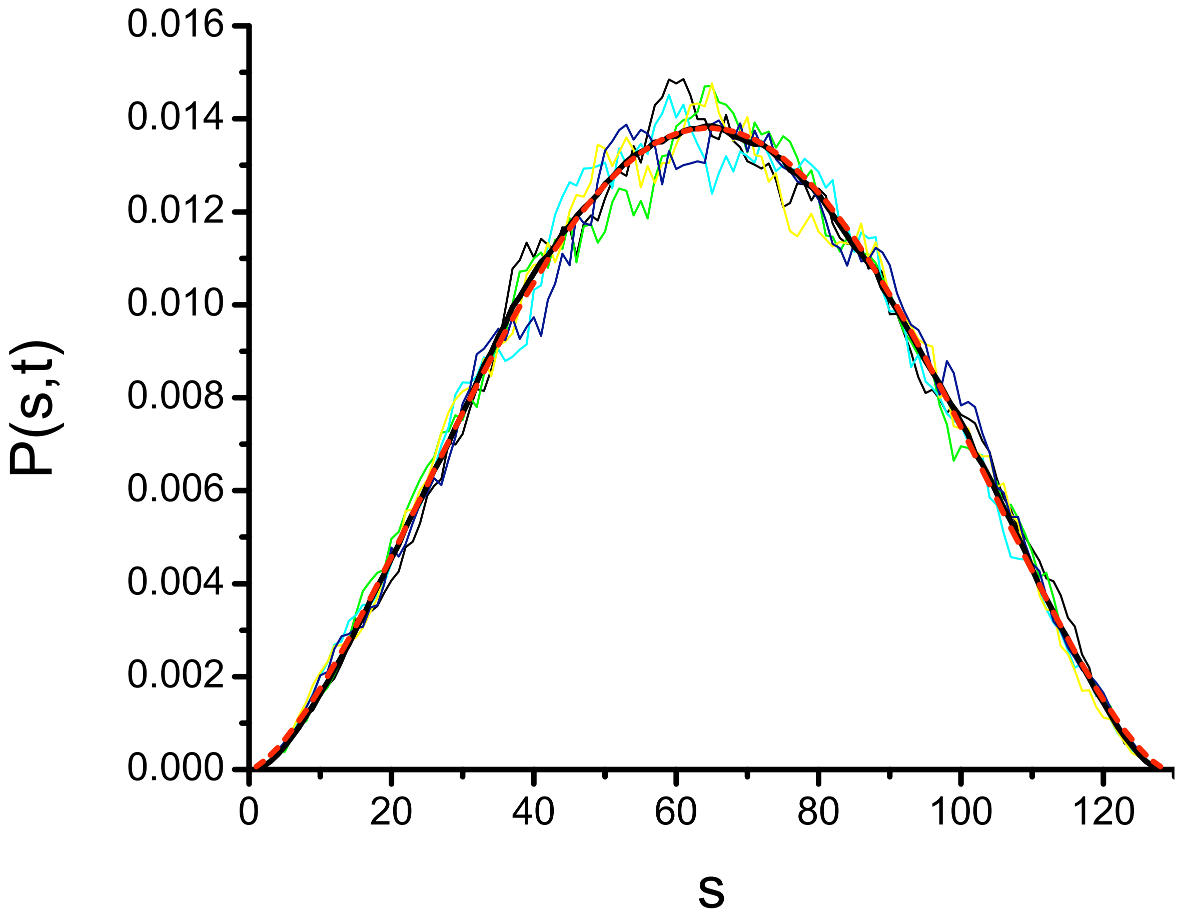


Hitting Free

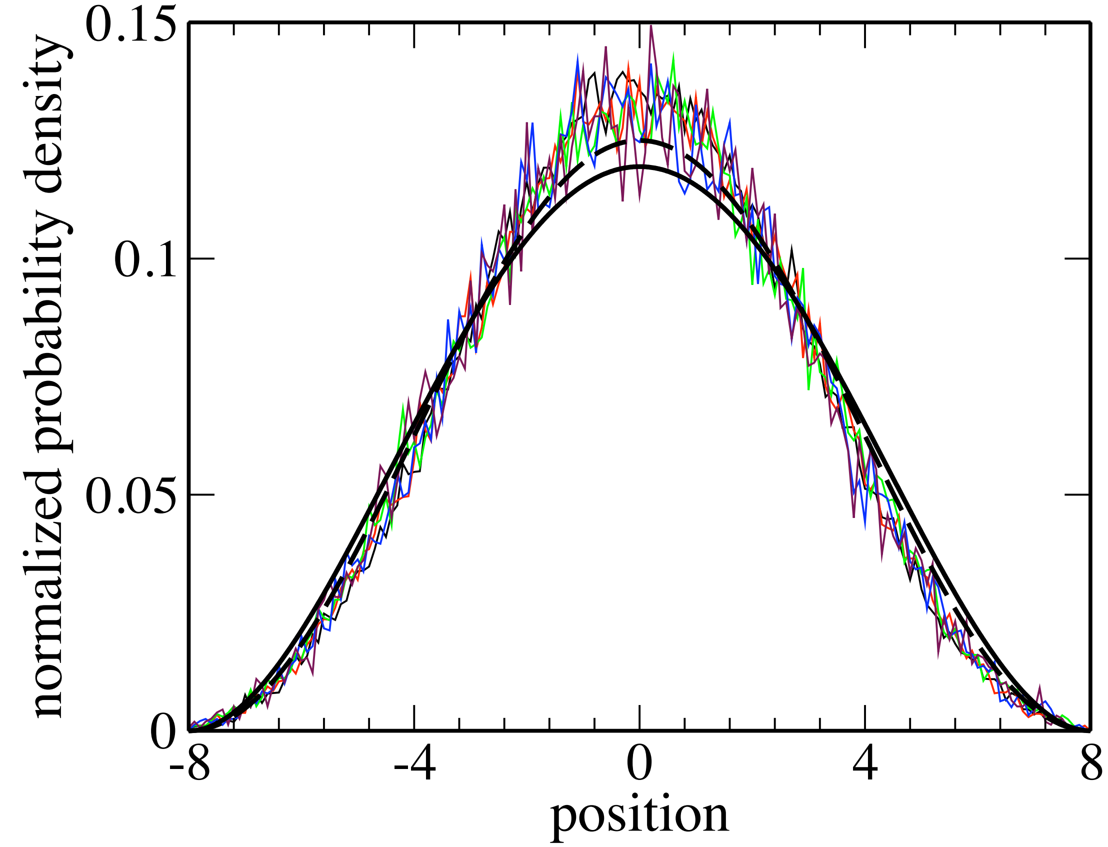


...and the persistence $S(x_0, t) \sim \frac{1}{\log(t)^{\frac{1}{6}}}$

“Anomalies” of anomalous diffusion



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)

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

At large t, $P(s,t) \sim s^{1.44}$

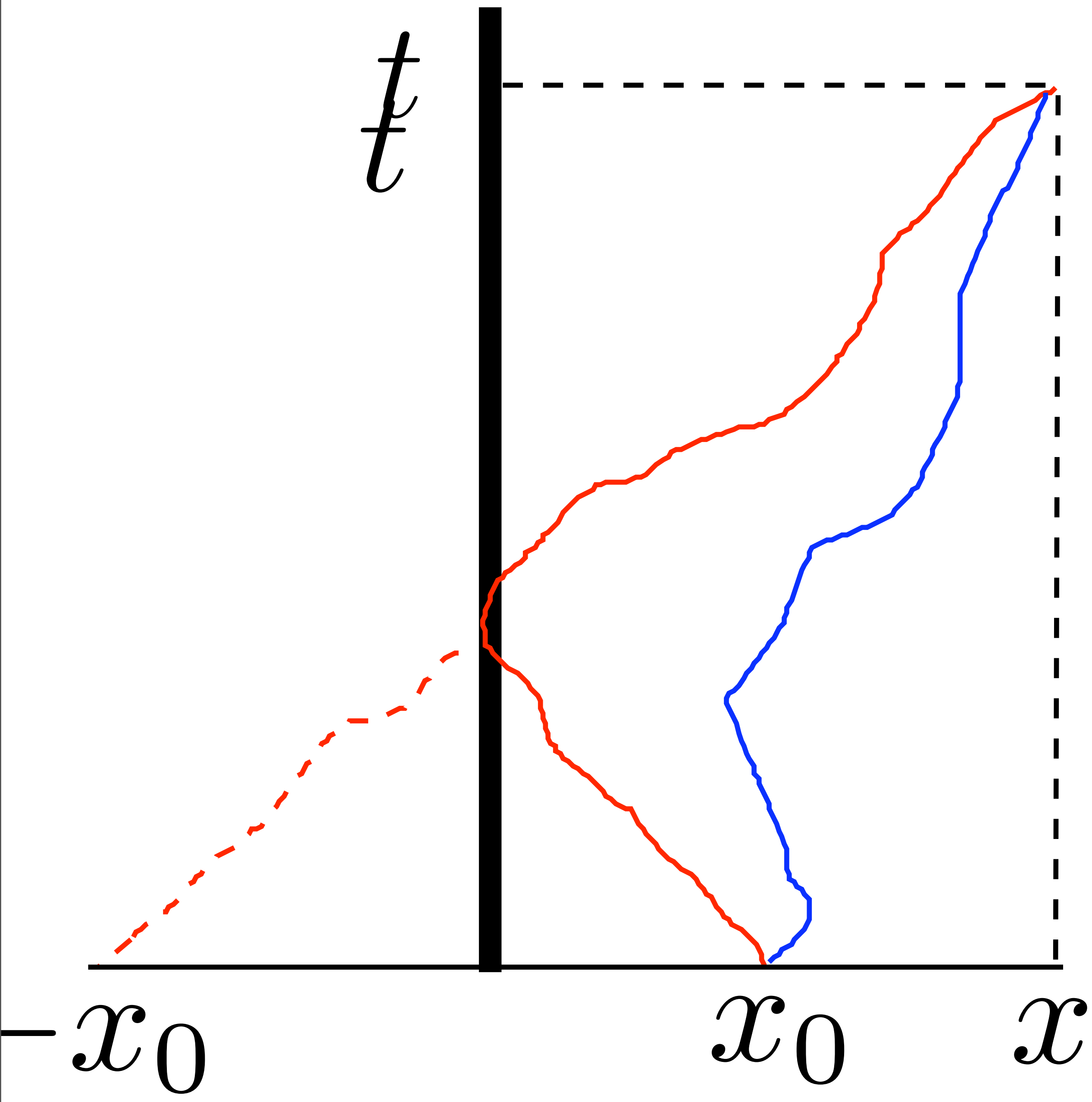
We predict $\phi = \frac{1-H}{H} = 1.5$

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

At large t, $P(s,t) \sim s^{\alpha}$, with $\alpha > 2$

We predict $\phi = \frac{1-H}{H} = 3$

Single Boundary: Images method



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

After normalization

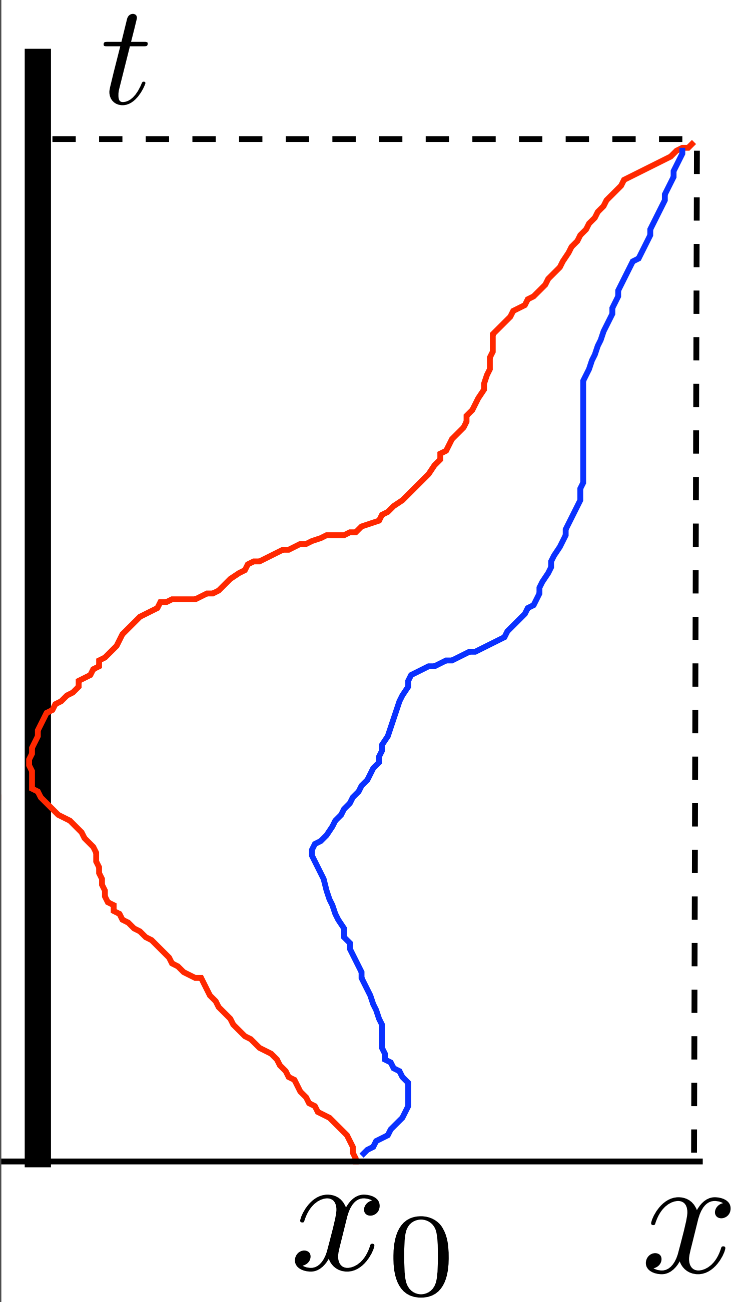
$$P_+(x, x_0, t) \xrightarrow{t \to \infty \textbf{ or } x_0 \to 0} P_+(x, t)$$

Self-Affinity III: $y = \frac{x}{\sqrt{2Dt}}$

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

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

Perturbation Theory



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

$$P_+(x,t) = \lim_{x_0 \to 0} \frac{Z_+(x_0, x, t)}{\int_0^\infty dx Z_+(x_0, x, t)}$$

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

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

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

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

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

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

$$G = G^{(0)} - \epsilon G^{(0)} K G^{(0)}$$

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

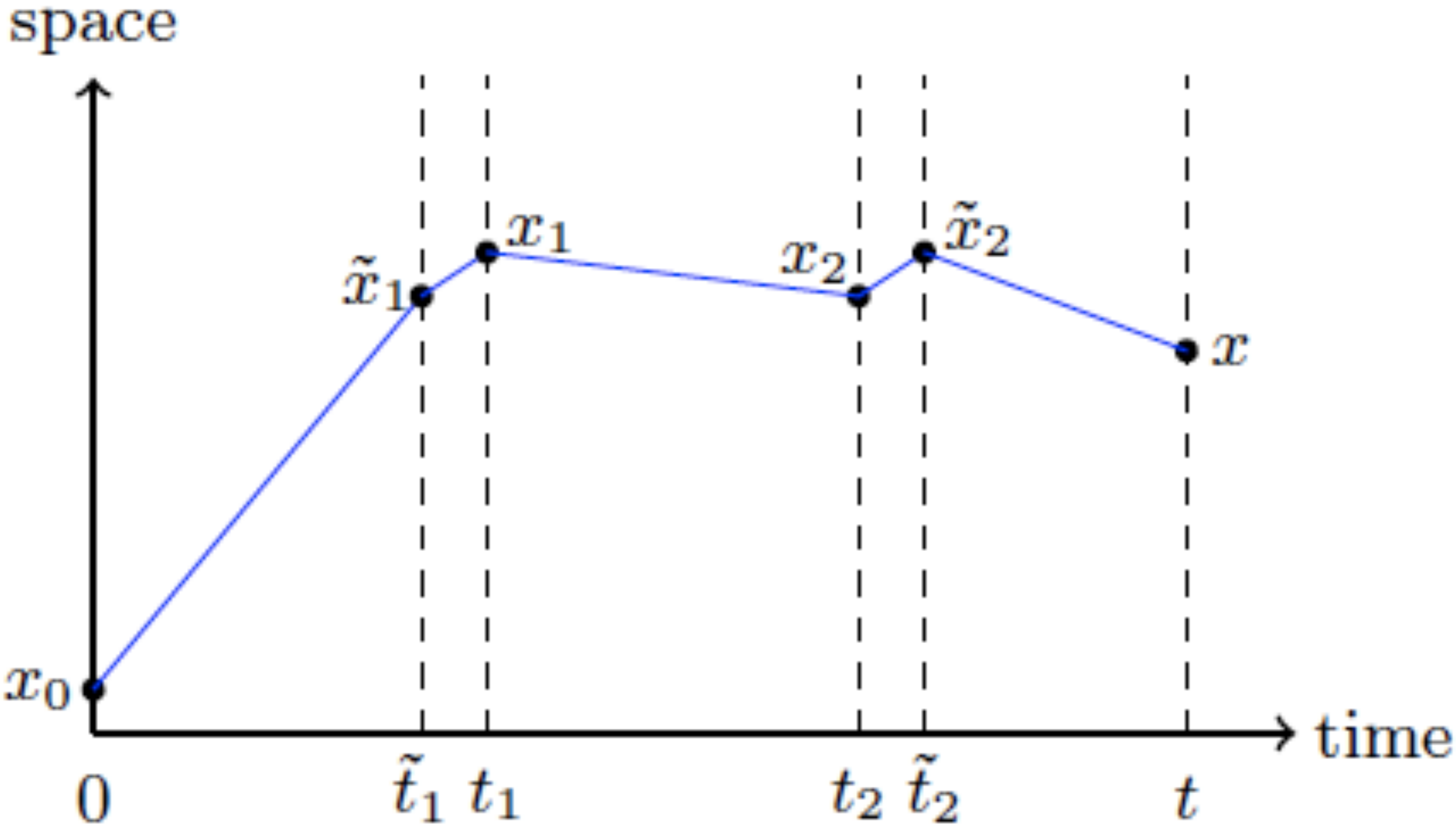
$$\mathcal{S}^{(1)}[x] \quad \propto \quad -\frac{1}{2} \int_0^t dt_1 \int_{t_1}^t dt_2 \, \frac{\partial_{t_1} x(t_1) \partial_{t_2} x(t_2)}{|t_1 - t_2|}$$

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

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

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

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



Brownian 2-points correlation function

Final Result I

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

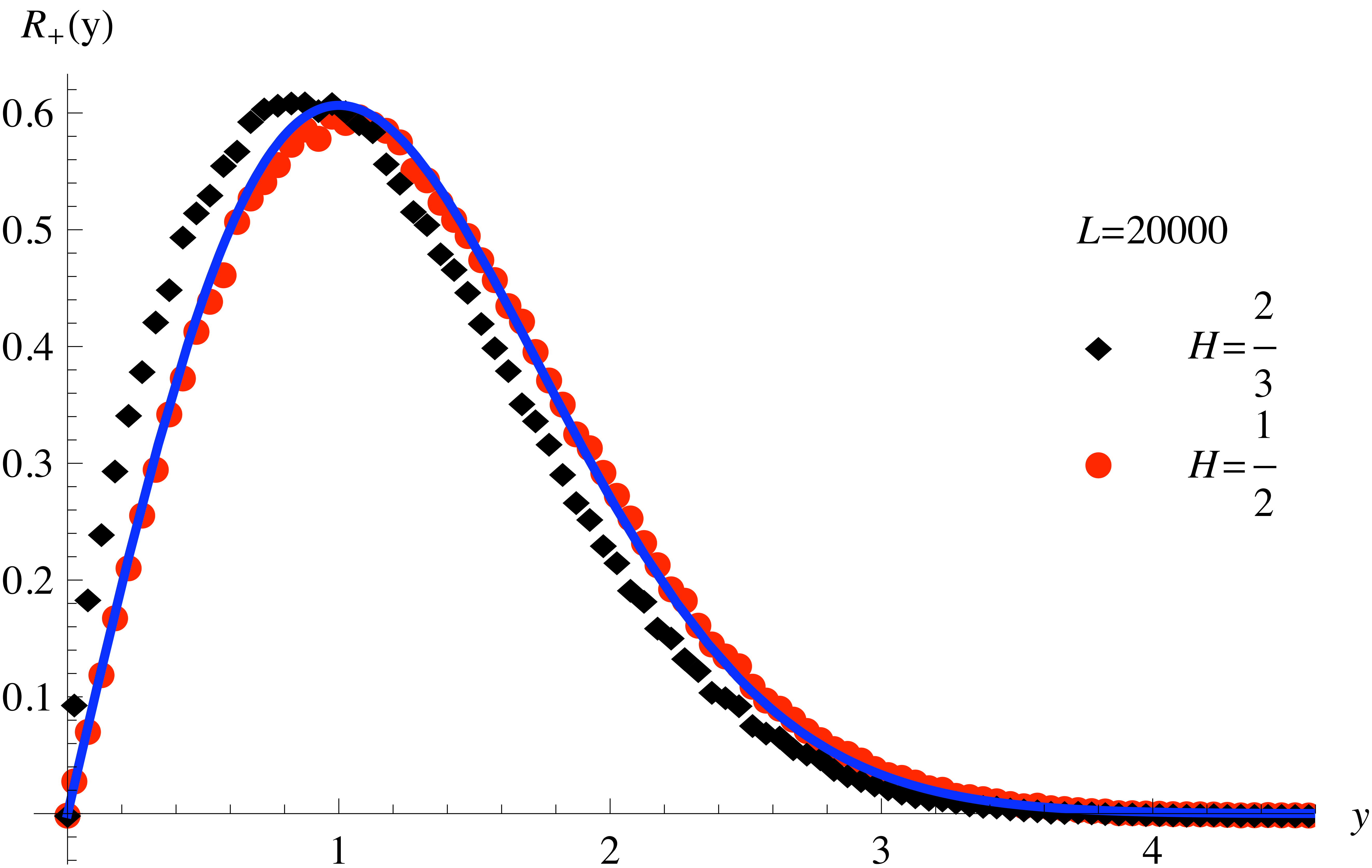
Final Result II

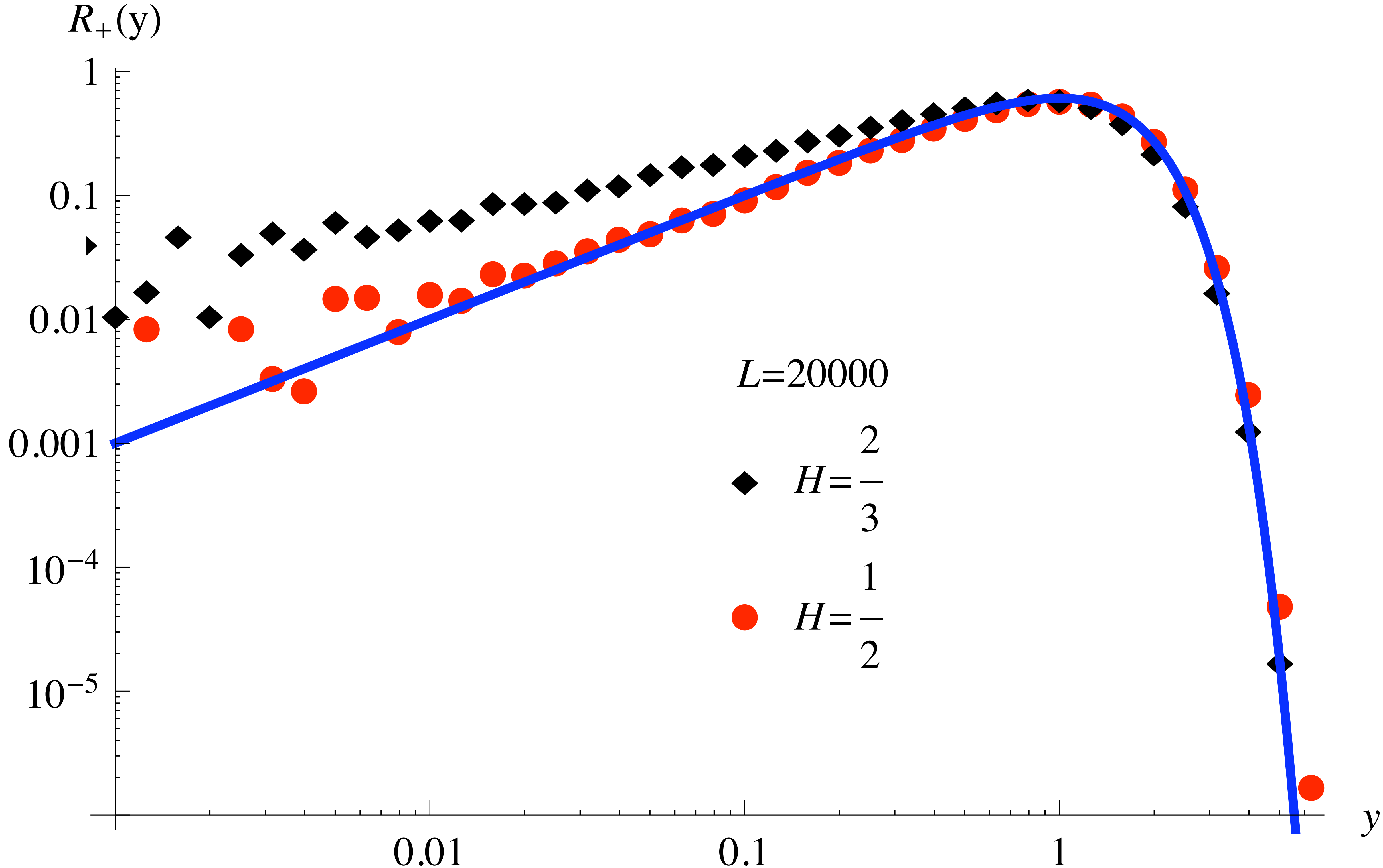
$$R_+(y) \xrightarrow{y \to 0} y^{\phi}$$

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

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

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

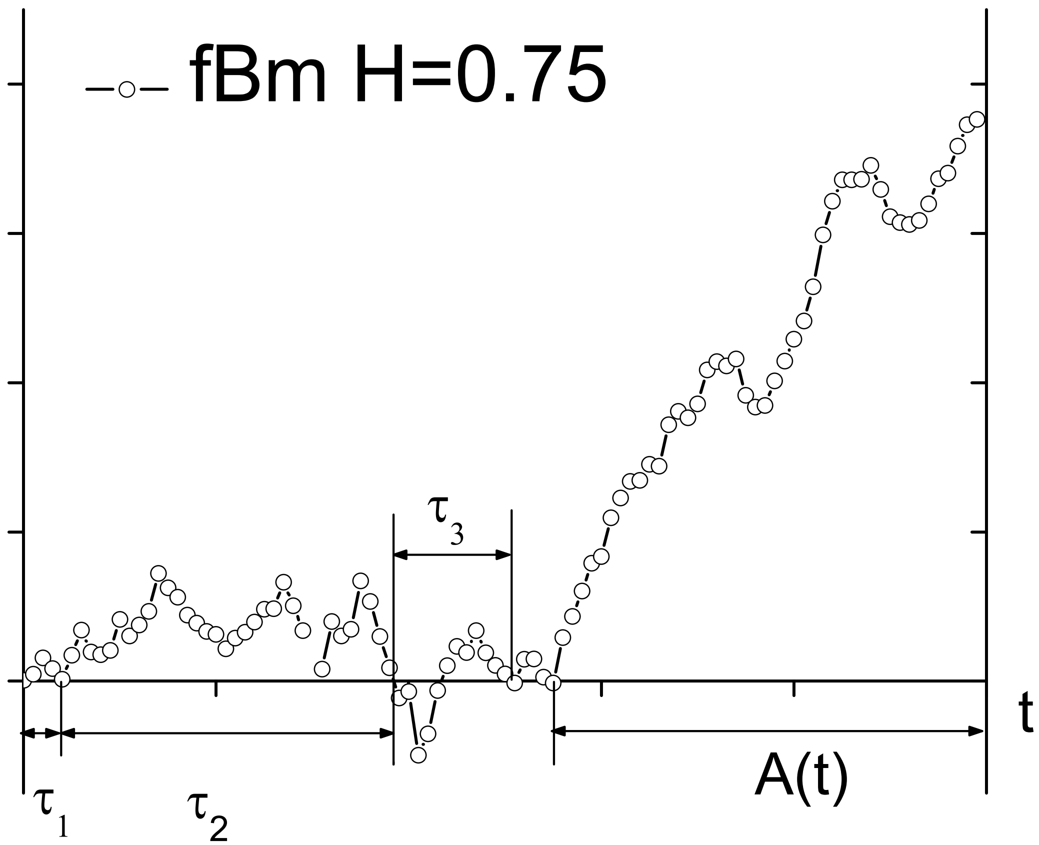

$R_+(y)$
0.6
0.5
0.4
0.3
0.2
0.1
1
2
3
4
y
$L=20000$
$H=\frac{2}{3}$
$H=\frac{1}{2}$



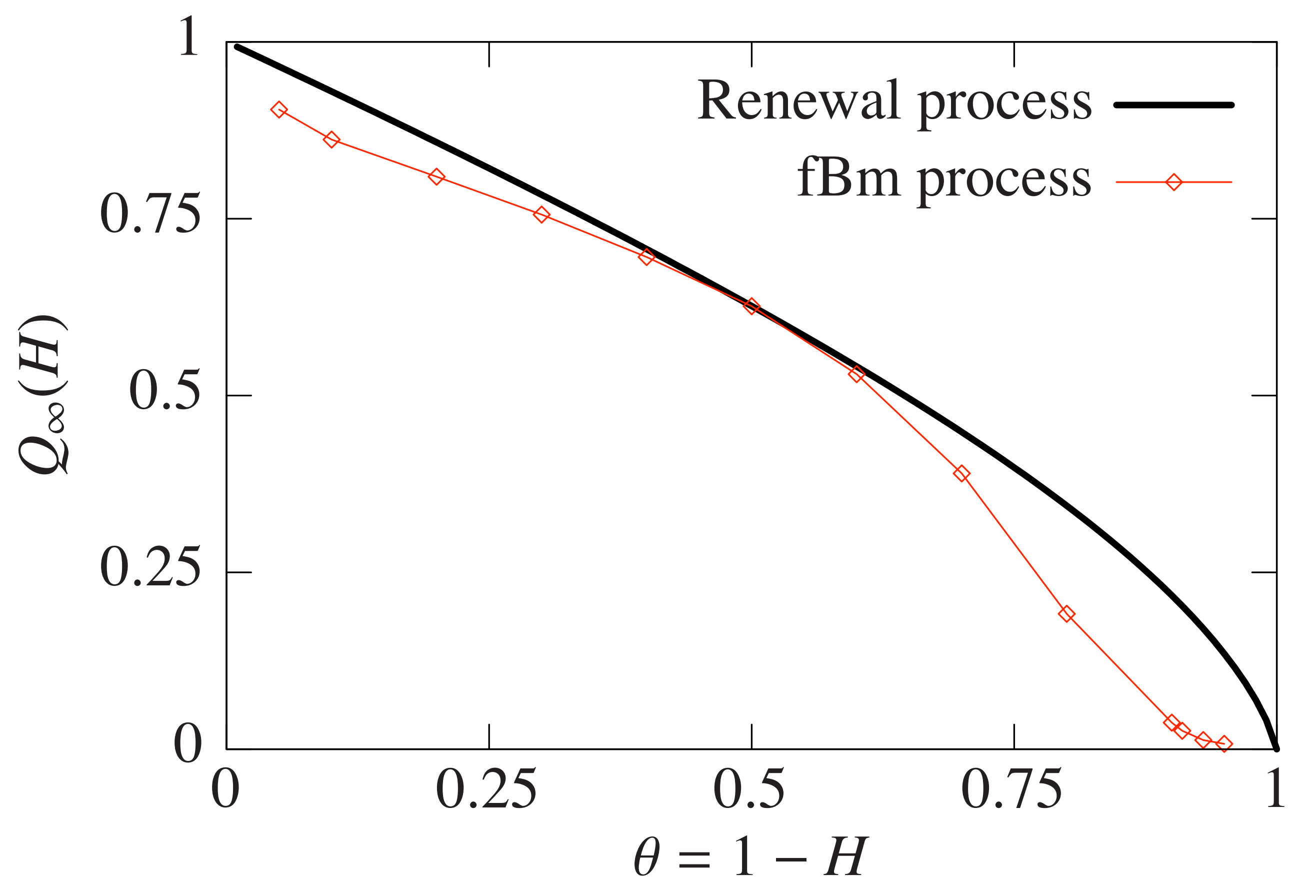
$R_+(y)$
1
0.1
0.01
0.001
10^{-4}
10^{-5}
0.01
0.1
1
y
L=20000
$H=\frac{2}{3}$
$H=\frac{1}{2}$

Non Markovianity and extremes...

The probability $Q(t)$ that $A(t)$ is the *longest excursion*?

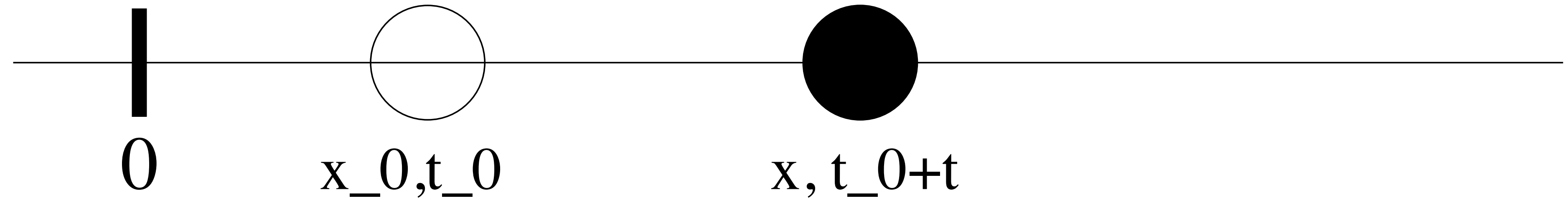


Exact solution for RENEWAL process [Godrèche, Majumdar, Schehr]

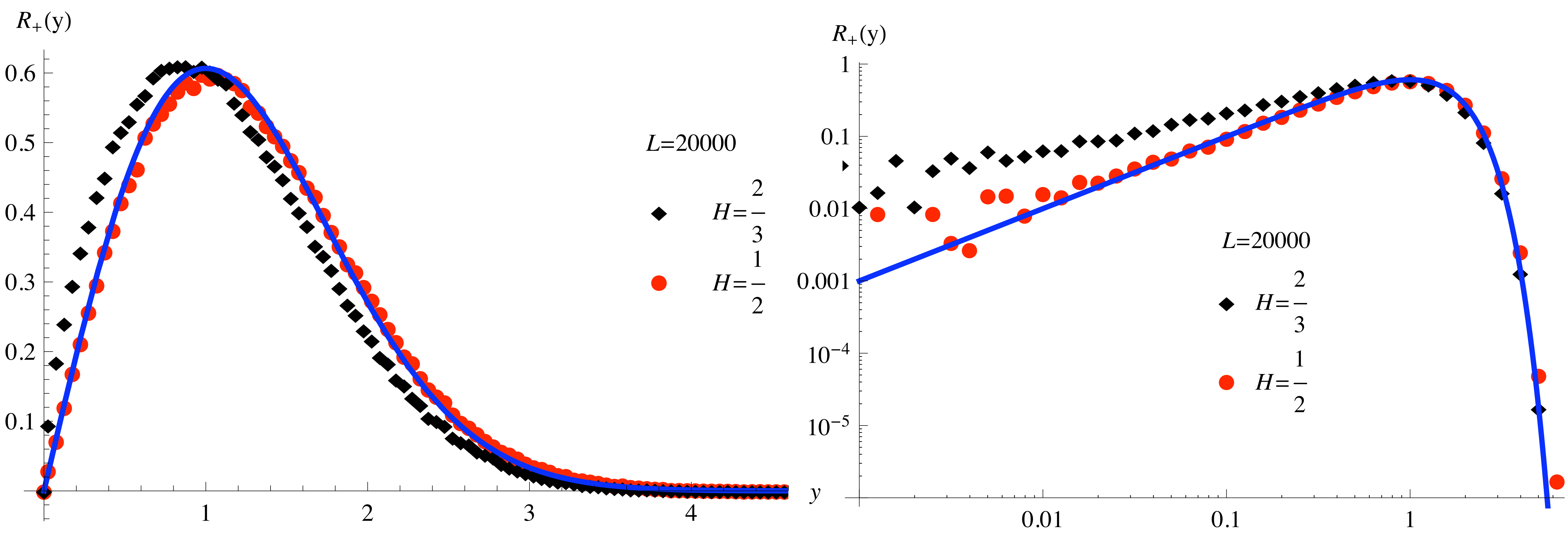


with Schehr and Garcia

Single Boundary



- Large time: $P_+(x,t;x_0,t_0) \xrightarrow{t\to\infty} P_+(x,t)$
- Self Affinity III: $P_+(x,t) = R_+(y)$ with $y = \frac{x}{\sqrt{\langle x^2(t)\rangle}} \sim \frac{x}{t^H}$
- Brownian $H = 1/2$: $R_+(y) = ye^{-\frac{y^2}{2}} \sim y + \dots$



How to generate a correlated path:

- time discretization: $x(t) \longrightarrow x_t = x_0 + \sum_{t'=1}^{t} \xi_{t'}$
- $\vec{\xi} = \{\xi_1, \xi_2, \ldots, \xi_T\}$ is a vector of Gaussian numbers
with a given covariance matrix $\langle \xi_{t_1} \xi_{t_2} \rangle = C(|t_1 - t_2|)$
- we compute $A = \sqrt{C}$ $[T^3$ operations]
and generate uncorrelated Gaussian numbers $\vec{\epsilon} = \{\epsilon_1, \ldots, \epsilon_T\}$
- Then the vector $\vec{\xi}$ can be generated $[T^2$ operations]:

$$\vec{\xi} = A\vec{\epsilon}$$

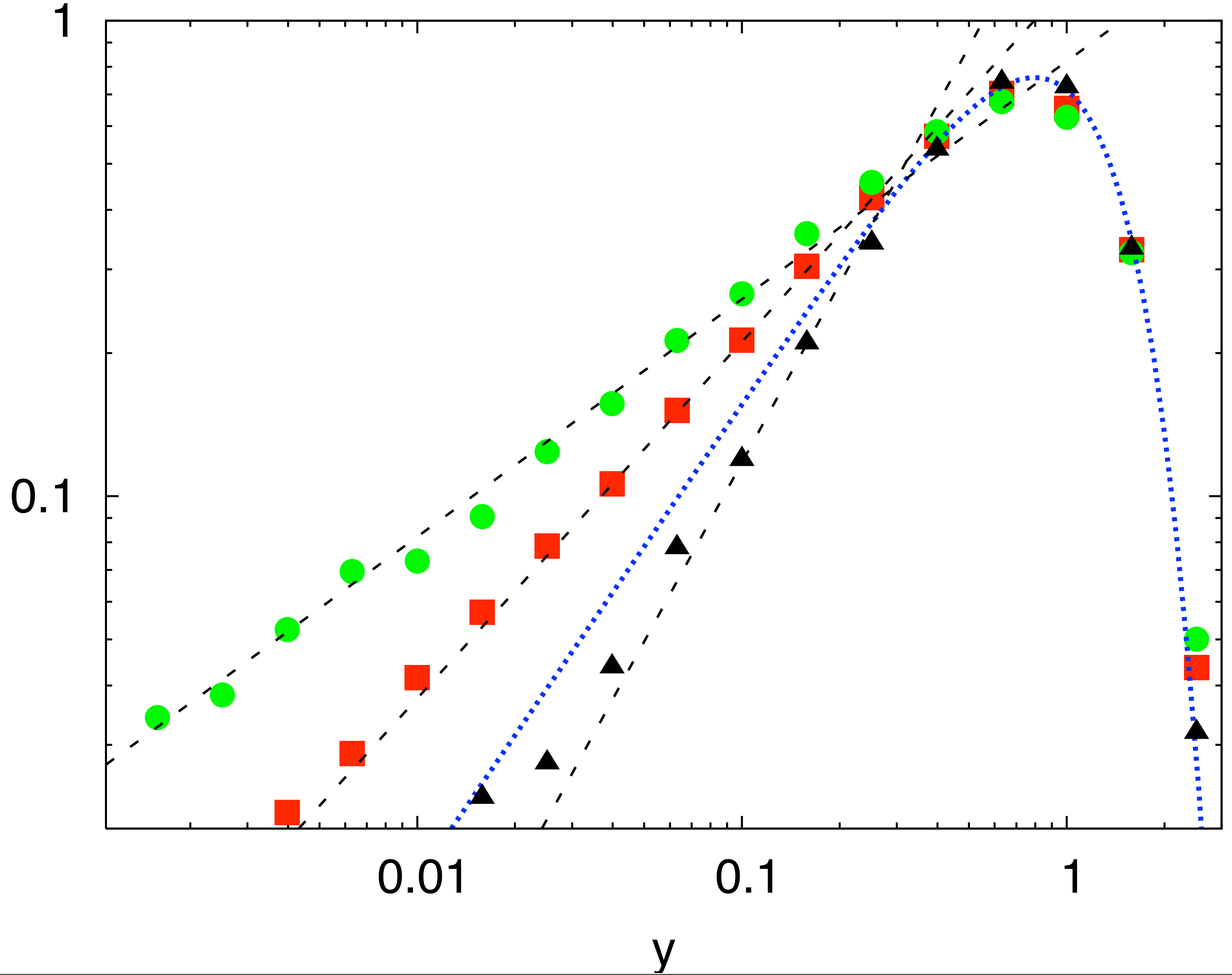
Proof:

$$\langle \xi_i \xi_j \rangle = \langle \sum_{i'} A_{i,i'} \epsilon_{i'} \sum_{j'} A_{j,j'} \epsilon_{j'} \rangle = \sum_{i',j'} A_{i,i'} A_{j,j'} \delta_{i',j'} = (A^2)_{i,j} = C_{i,j}$$

- Special algorithms if Covariance is Toeplitz matrix: $C_{i,j} = C(|i - j|)$.

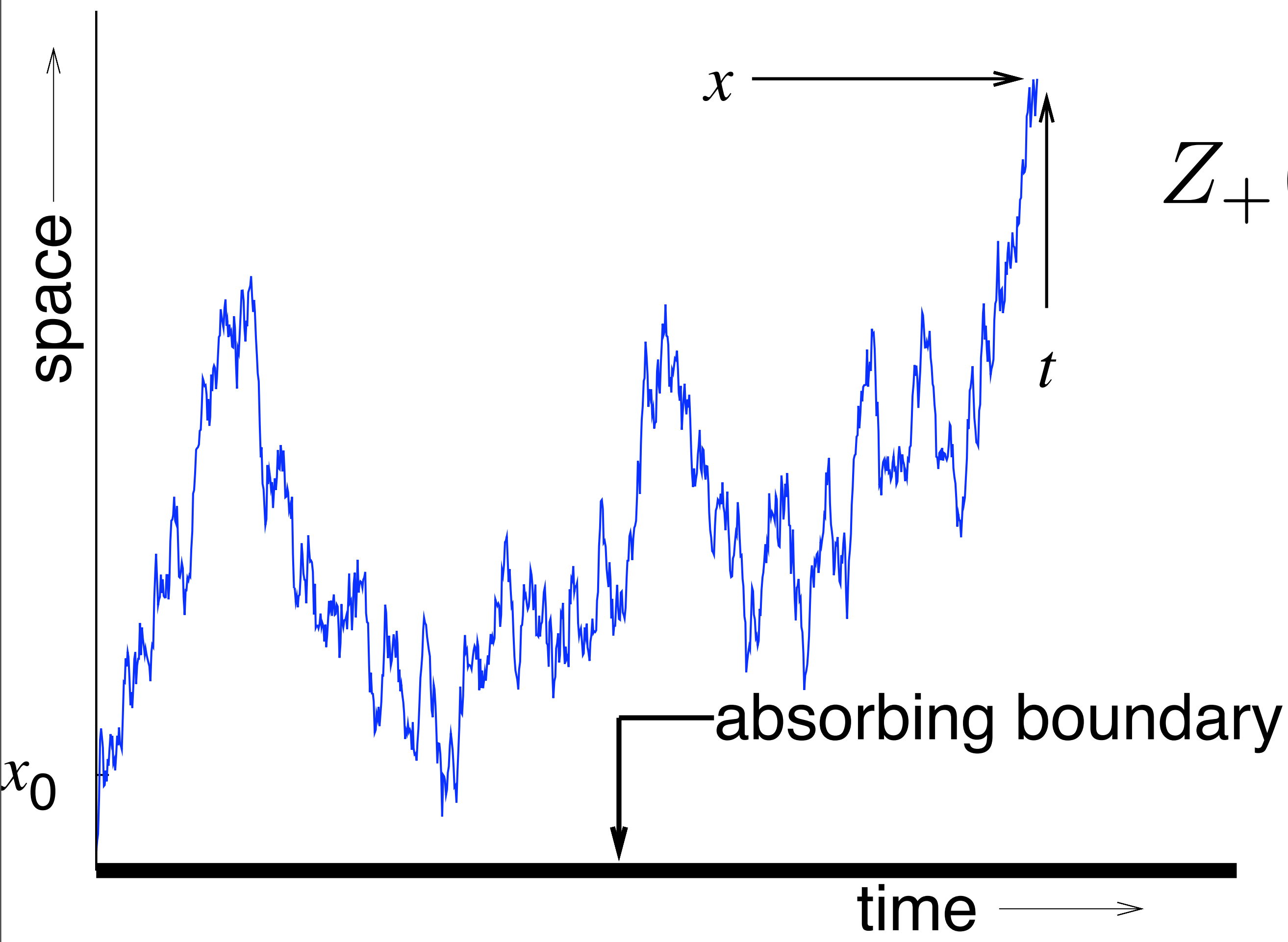
Single Boundary

- In general we expect $R_+(y) \sim y^\phi$
- For stationary increments, a scaling argument gives $\phi = \frac{\theta}{H}$
- numerical simulations agrees



- Circle $H = \frac{2}{3}$, $\phi = \frac{1}{2}$
- Square $H = \frac{4}{7}$, $\phi = \frac{3}{4}$
- Line $R_+(y) = ye^{-y^2/2}$
- Triangle $H = \frac{4}{9}$, $\phi = \frac{5}{4}$

Perturbation Theory



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

$$P_+(x, t) = \lim_{x_0 \to 0} \frac{Z_+(x_0, x, t)}{\int_0^\infty dx Z_+(x_0, x, t)}$$

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

where $G^{-1}(t_1, t_2) = \langle x(t_1) x(t_2) \rangle$ it is known

Diffusion and Central Limit Theorem

- $\langle x^2(t) \rangle = 2Dt \propto t$ and D is diffusion constant

- $x(t)$ (for large t) is a **Gaussian** process

- Propagator from x_0 to x: $P(x_0, x, t) = \frac{e^{-\frac{(x(t)-x_0)^2}{4Dt}}}{\sqrt{4\pi Dt}}$

And the Fractional Fokker Planck Equation (CTRW)?