

Fractional Feynman-Kac equation for anomalous diffusion functionals

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Section 1

Introduction

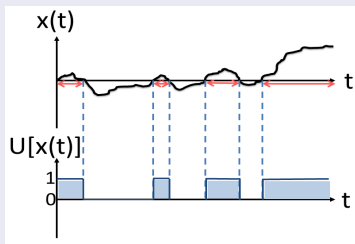


Brownian functionals

- $x(t)$ – the trajectory of a Brownian particle.
- The functional: $A \equiv \int_0^t U[x(\tau)]d\tau$.

Example

- $U(x) = \Theta(x) = \begin{cases} 1 & x > 0, \\ 0 & x < 0. \end{cases}$



- A – The occupation time in the positive half space.



The Feynman-Kac equation

- Denote $G(x, A, t)$ the joint PDF of x and A at time t .
- $G(x, p, t) = \int_0^\infty e^{-pA} G(x, A, t) dA$.
- The Feynman-Kac equation (M. Kac, 1949):

$$\frac{\partial}{\partial t} G(x, p, t) = D \frac{\partial^2 G(x, p, t)}{\partial x^2} - pU(x)G(x, p, t)$$

- D – the diffusion coefficient.
- $p = 0 \Rightarrow$ The diffusion equation $\frac{\partial}{\partial t} G(x, t) = D \frac{\partial^2 G(x, t)}{\partial x^2}$.
- Structurally similar to Schrödinger equation in imaginary time
 $i\hbar \frac{\partial}{\partial t} \Psi(x, t) = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x, t) + V(x)\Psi(x, t)$.

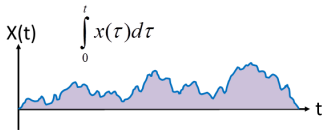


Examples of functionals and applications

$$U(x) = x$$

- The area under the random walk curve.
- The time-averaged position of the particle ($\bar{x} = \frac{1}{t} \int_0^t x(\tau) d\tau$).
- NMR (phase of each spin: $\varphi = \gamma \int_0^t B[x(\tau)] d\tau$, $B(x) = x$ is the magnetic field).

D.S. Grebenkov, *Rev. Mod. Phys.* **79**, 1077 (2007).



$$U(x) = \begin{cases} 1 & \text{in a certain domain} \\ 0 & \text{otherwise} \end{cases}$$

- The emitted light if fluorescent particles are excited only in the domain.
- The survival probability if the domain is absorbing.
- The distribution of the first passage time.
- The distribution of the maximal displacement.

G. Zumofen et al., *Phys. Rev. Lett.* **93**, 260601 (2004).



A few more applications

$$A = \int_0^t x(\tau) \Theta[x(\tau)] d\tau$$

- The integrated excess temperature up to time t .
- S.N. Majumdar et al., *Phys. Rev. E* **65**, 051112 (2002).

$$A = \int_0^t x^2(\tau) d\tau$$

- The fluctuations in the height of a KPZ surface.
- G. Foltin et al., *Phys. Rev. E* **50**, R639 (1994).

$$A = \int_0^t e^{-\beta x(\tau)} d\tau$$

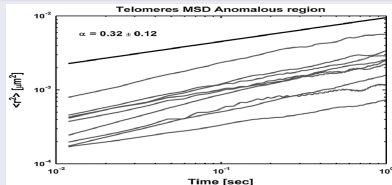
- The partition function of a particle in a random potential (Sinai model).
- Models of stock prices.
- Reviewed in S.N. Majumdar, *Curr. Sci.* **89**, 2076 (2005).



Non-Brownian motion

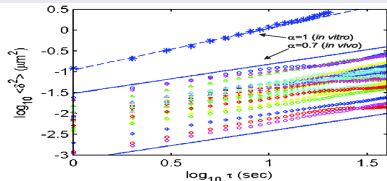
- In many physical and biological systems diffusion is anomalous.
- $\langle x^2 \rangle \sim t^\alpha$, $0 < \alpha < 1$.

DNA



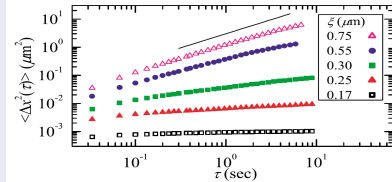
I. Bronstein et al., *Phys. Rev. Lett.* 103, 018102 (2009).

RNA



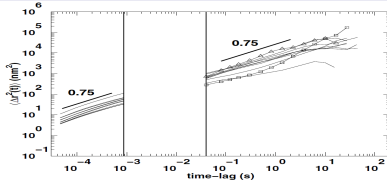
I. Golding et al., *Phys. Rev. Lett.* 96, 098102 (2006).

Beads in Actin



I.Y. Wong et al., *Phys. Rev. Lett.* 92, 178101 (2004).

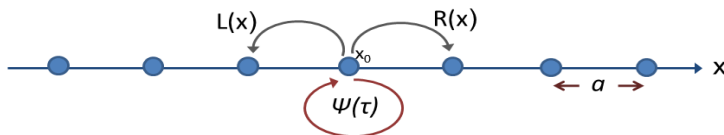
Lipid granules



I.M. Tulić-Nørrelykke et al., *Phys. Rev. Lett.* 93, 078102 (2004).

Continuous-time random walk (CTRW)- A model for anomalous diffusion

- An infinite 1D lattice with spacing a .
- Jumps to nearest neighbors.
 - For a free particle, $R(x) = L(x) = 1/2$.
 - For a bounded particle, $R(x)$ and $L(x)$ depend on the force at x .
- Start at x_0 . Wait time τ and jump. Wait and jump again, ...
- Waiting times are distributed according to $\psi(\tau) \sim \tau^{-(1+\alpha)}$.

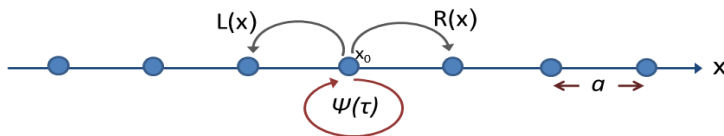


- $0 < \alpha < 1 \Rightarrow \langle \tau \rangle = \infty \Rightarrow \langle x^2 \rangle \sim t^\alpha \Rightarrow$ anomalous (sub-) diffusion.



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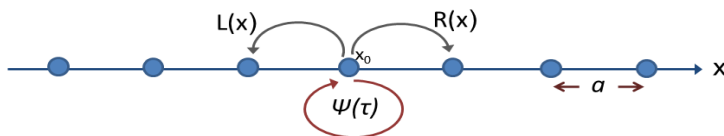


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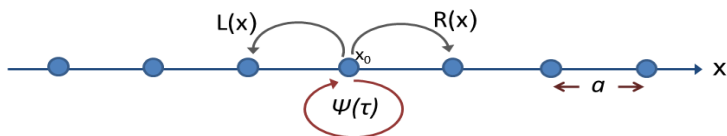


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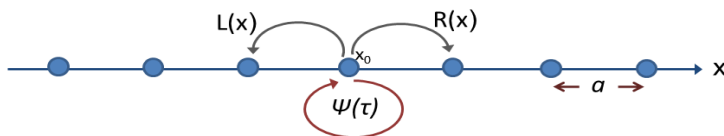


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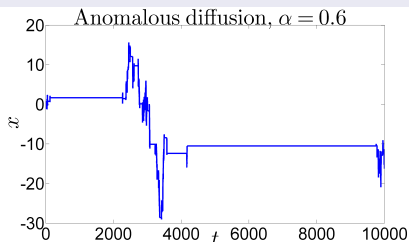
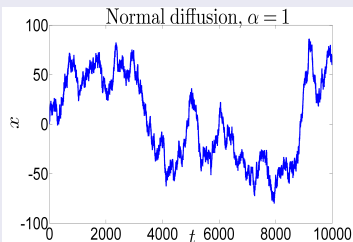
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CTRW example

CTRW is characterized by long periods of stagnation, whose lengths have no typical scale.

Sample trajectories



The fractional Fokker-Planck equation

- The continuum limit of CTRW is described by the fractional Fokker-Planck equation.
- Denote $G(x, t)$ the PDF of x at time t .

$$\frac{\partial}{\partial t} G(x, t) = K_{\alpha} \mathcal{D}_t^{1-\alpha} \mathcal{L}_{\text{FP}} G(x, t)$$

- $\mathcal{L}_{\text{FP}} = \frac{\partial^2}{\partial x^2} - \frac{\partial}{\partial x} \frac{F(x)}{k_B T}$ (Fokker-Planck operator).
- $F(x) = 0 \Rightarrow$ the fractional diffusion equation.
- K_{α} — The generalized diffusion coefficient (units $\text{m}^2/\text{sec}^{\alpha}$).
- $\mathcal{D}_t^{1-\alpha}$ is a fractional derivative.
- What is a fractional derivative???



Fractional derivatives

- $\mathcal{D}_t^\alpha f(t) \equiv \frac{1}{\Gamma(1-\alpha)} \frac{\partial}{\partial t} \int_0^t \frac{f(\tau)}{(t-\tau)^\alpha} d\tau \quad (0 < \alpha < 1).$
- In Laplace space:
 $\mathcal{D}_t^\alpha \tilde{f}(s) = s^\alpha \tilde{f}(s).$
- Example: $\mathcal{D}_t^\alpha t^n = \frac{\Gamma(n+1)}{\Gamma(n+1-\alpha)} t^{n-\alpha}.$
- Reduces to $\mathcal{D}_t^m t^n = \frac{n!}{(n-m)!} t^{n-m}$ for integer m , as expected.
- Composition of fractional derivatives makes sense (e.g.,
 $\mathcal{D}_t^{1/2} \mathcal{D}_t^{1/2} = \frac{d}{dt}).$
- Riemann, Liouville, Cauchy.



The problem

- Many functionals are interesting in systems exhibiting anomalous diffusion.
- How can we find the PDF of these functionals?

In the following:

- Find an equation for the PDF of functionals of CTRW.
- Solve the equation for interesting functionals.
- Study implications to ergodicity breaking.



Section 2

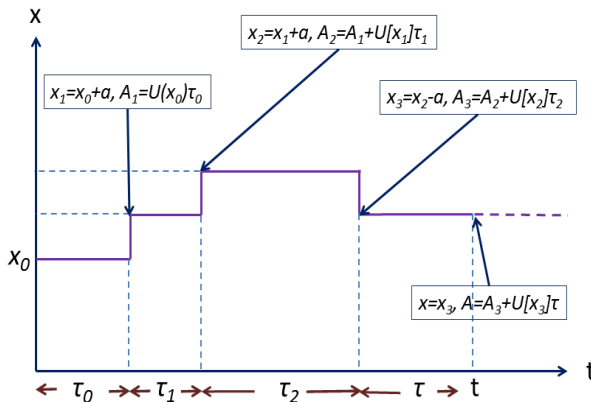
The fractional Feynman-Kac equation



Illustration of the derivation method

- $A = \int_0^t U[x(\tau)]d\tau = U(x_0)\tau_0 + U(x_1)\tau_1 + U(x_2)\tau_2 + \dots$

A trajectory and its corresponding functional



Outline of the derivation

- $W(\tau) = 1 - \int_0^\tau \psi(\tau') d\tau'$:

The probability not to jump until time τ .

- $\chi(x, A, t)dt$ – the probability to jump into (x, A) during $[t, t + dt]$.
- $G(x, A, t) = \int_0^t W(\tau) \chi[x, A - \tau U(x), t - \tau] d\tau$.
- $\chi(x, A, t) = \int_0^t \psi(\tau) L(x + a) \chi[x + a, A - \tau U(x + a), t - \tau] d\tau$
 $+ \int_0^t \psi(\tau) R(x - a) \chi[x - a, A - \tau U(x - a), t - \tau] d\tau$
 $+ \delta(x - x_0) \delta(A) \delta(t)$.
- Laplace-Fourier transform $A \rightarrow p, t \rightarrow s, x \rightarrow k$.
- $\chi(k, p, s) = e^{-ika} \int_{-\infty}^{\infty} e^{ikx} L(x) \hat{\psi}[s + pU(x)] \chi(x, p, s) dx$
 $+ e^{ika} \int_{-\infty}^{\infty} e^{ikx} R(x) \hat{\psi}[s + pU(x)] \chi(x, p, s) dx$
 $+ e^{ikx_0}$.
- Use detailed balance and assume thermal equilibrium to show:
$$R(x) \approx \frac{1}{2} \left[1 + \frac{aF(x)}{2k_B T} \right] = 1 - L(x).$$



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$$\times \left\{ 1 - \left[\cos(ka) + i \sin(ka) \frac{aF \left(-i \frac{\partial}{\partial k} \right)}{2k_B T} \right] \hat{\psi} \left[s + pU \left(-i \frac{\partial}{\partial k} \right) \right] \right\}^{-1} e^{ikx_0}.$$
- Apply the continuum approximation $\hat{\psi}(s) \sim 1 - B_\alpha s^\alpha$, $\cos(ka) \sim 1 - \frac{1}{2}a^2 k^2$, and $K_\alpha = a^2/(2B_\alpha)$.
- $$sG(k, p, s) - e^{ikx_0} =$$

$$-K_\alpha \left[k^2 - ik \frac{F \left(-i \frac{\partial}{\partial k} \right)}{k_B T} \right] \left[s + pU \left(-i \frac{\partial}{\partial k} \right) \right]^{1-\alpha} G(k, p, s) -$$

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The fractional Feynman-Kac equation

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$$\frac{\partial}{\partial t} G(x, p, t) = K_{\alpha} \mathcal{L}_{\text{FP}} \mathcal{D}_t^{1-\alpha} G(x, p, t) - pU(x)G(x, p, t)$$

- $\mathcal{L}_{\text{FP}} = \frac{\partial^2}{\partial x^2} - \frac{\partial}{\partial x} \frac{F(x)}{k_B T}$.
- Here, $\mathcal{D}_t^{1-\alpha} G(x, p, t) = \frac{1}{\Gamma(\alpha)} \left[\frac{\partial}{\partial t} + pU(x) \right] \int_0^t \frac{e^{-(t-\tau)pU(x)}}{(t-\tau)^{1-\alpha}} G(x, p, \tau) d\tau$.
- $\mathcal{D}_t^{1-\alpha} G(x, p, s) = [s + pU(x)]^{1-\alpha} G(x, p, s)$.
- Substantial fractional derivative operator (Friedrich/Metzler).
- $\alpha = 1 \Rightarrow$ The Feynman-Kac equation.
- $p = 0 \Rightarrow$ The fractional Fokker-Planck equation.
- For a free particle, $\mathcal{L}_{\text{FP}} = \frac{\partial^2}{\partial x^2}$.



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$$\frac{\partial}{\partial t} G(x, p, t) = K_{\alpha} \mathcal{L}_{\text{FP}} \mathcal{D}_t^{1-\alpha} G(x, p, t) - pU(x)G(x, p, t)$$

- $\mathcal{L}_{\text{FP}} = \frac{\partial^2}{\partial x^2} - \frac{\partial}{\partial x} \frac{F(x)}{k_B T}$.
- Here, $\mathcal{D}_t^{1-\alpha} G(x, p, t) = \frac{1}{\Gamma(\alpha)} \left[\frac{\partial}{\partial t} + pU(x) \right] \int_0^t \frac{e^{-(t-\tau)pU(x)}}{(t-\tau)^{1-\alpha}} G(x, p, \tau) d\tau$.
- $\mathcal{D}_t^{1-\alpha} G(x, p, s) = [s + pU(x)]^{1-\alpha} G(x, p, s)$.
- Substantial fractional derivative operator (Friedrich/Metzler).
- $\alpha = 1 \Rightarrow$ The Feynman-Kac equation.
- $p = 0 \Rightarrow$ The fractional Fokker-Planck equation.
- For a free particle, $\mathcal{L}_{\text{FP}} = \frac{\partial^2}{\partial x^2}$.



General $U(x)$ (not necessarily positive)

- *Fourier transform* $A \rightarrow p$.
- $\frac{\partial}{\partial t} G(x, p, t) = K_{\alpha} \frac{\partial^2}{\partial x^2} \mathcal{D}_t^{1-\alpha} G(x, p, t) + ipU(x)G(x, p, t).$

Lévy flights

- Displacements Δ_x have PDF $f(\Delta_x) \sim |\Delta_x|^{-(1+\mu)}$ ($0 < \mu < 2$).
- $\frac{\partial}{\partial t} G(x, p, t) = K_{\alpha, \mu} \nabla_x^{\mu} \mathcal{D}_t^{1-\alpha} G(x, p, t) - pU(x)G(x, p, t).$
- $\nabla_x^{\mu} \rightarrow -|k|^{\mu}$ is the Riesz spatial fractional derivative operator.

Time dependent force

- $R(x)$ and $L(x)$ depend on the force at the time of the jump.
- $\frac{\partial}{\partial t} G(x, p, t) = K_{\alpha} \mathcal{L}_{\text{FP}} \mathcal{D}_t^{1-\alpha} G(x, p, t) - pU(x)G(x, p, t).$
- $\mathcal{L}_{\text{FP}} = \frac{\partial^2}{\partial x^2} - \frac{\partial}{\partial x} \frac{F(x, t)}{k_B T}.$



How to solve the equation

A recipe

- 1 Solve the fractional Feynman-Kac equation in (p, s) space.
$$sG(x, p, s) - \delta(x - x_0) = K_\alpha \mathcal{L}_{\text{FP}}[s + pU(x)]^{1-\alpha} G(x, p, s) - pU(x)G(x, p, s).$$
- 2 Integrate the solution over all x to eliminate the dependence on the final position of the particle.
- 3 Invert $(p, s) \rightarrow (A, t)$, to obtain $G(A, t)$, the PDF of A at time t .



The backward equation

- We would like to avoid the x -dependence.
- $$G_{x_0}(A, t) = \int_0^t \psi(\tau) R(x_0) G_{x_0+a}[A - \tau U(x_0), t - \tau] d\tau$$
$$+ \int_0^t \psi(\tau) L(x_0) G_{x_0-a}[A - \tau U(x_0), t - \tau] d\tau$$
$$+ W(t) \delta[A - tU(x_0)].$$
- $G_{x_0}(A, t)$ — the PDF of A when the process started at x_0 .
- The *backward* fractional Feynman-Kac equation:

$$\frac{\partial}{\partial t} G_{x_0}(p, t) = K_\alpha \mathcal{D}_t^{1-\alpha} \mathcal{L}_{\text{FP}}^{(\text{B})} G_{x_0}(p, t) - pU(x_0) G_{x_0}(p, t)$$

- $$\mathcal{L}_{\text{FP}}^{(\text{B})} = \frac{\partial^2}{\partial x_0^2} + \frac{F(x_0)}{k_B T} \frac{\partial}{\partial x_0}.$$



Section 3

Functionals of free particles



Functionals of free particles

Functional	Result
The PDF of the occupation fraction in $x > 0$	$G(\lambda) = \frac{\sin(\pi\alpha/2)}{\pi} \frac{\lambda^{\alpha/2-1}(1-\lambda)^{\alpha/2-1}}{\lambda^\alpha + (1-\lambda)^\alpha + 2\lambda^{\alpha/2}(1-\lambda)^{\alpha/2}\cos(\pi\alpha/2)}$
The first passage time from 0 to b	$f(t_f) = \frac{1}{\tau_f} l_{\alpha/2} \left(\frac{t_f}{\tau_f} \right); \quad \tau_f = (b^2/K_\alpha)^{1/\alpha}$
The maximal displacement	$P(x_m, t) = \frac{2}{\alpha\sqrt{K_\alpha}} \frac{t}{(x_m/\sqrt{K_\alpha})^{1+2/\alpha}} l_{\alpha/2} \left[\frac{t}{(x_m/\sqrt{K_\alpha})^{2/\alpha}} \right]$
The probability of hitting L before 0	$Q_L(x_0) = \frac{x_0}{L}$
The first two moments of the time in $[-b, b]$	$\langle T_i \rangle \sim \frac{b}{\sqrt{K_\alpha}\Gamma(2-\alpha/2)} t^{1-\alpha/2} \quad ; \quad \langle T_i^2 \rangle \sim \frac{2b(1-\alpha)}{\sqrt{K_\alpha}\Gamma(3-\alpha/2)} t^{2-\alpha/2}$
The survival probability when $[-b, b]$ absorbing with rate R	$\langle S \rangle \sim \left[\Gamma(1-\alpha/2) \sinh \left(\frac{bR^{\alpha/2}}{\sqrt{K_\alpha}} \right) \right]^{-1} (Rt)^{-\alpha/2}$
The fluctuations of the time-averaged position	$\langle (\Delta \bar{x})^2 \rangle = \frac{4K_\alpha}{\Gamma(3+\alpha)} t^\alpha$
A scaling form for the distribution of $U(x) = x^k$ functionals	$G(A_{x^k}, t) = \frac{1}{K_\alpha^{k/2} t^{1+\alpha k/2}} g_{\alpha,k} \left(\frac{A_{x^k}}{K_\alpha^{k/2} t^{1+\alpha k/2}} \right)$



The occupation time in the positive half-space

- $T_+ \equiv \int_0^t \Theta[x(\tau)]d\tau$, or $U(x) = \Theta(x)$.

- The backward equation is:

$$sG_{x_0}(p, s) - 1 = \begin{cases} K_\alpha s^{1-\alpha} \frac{\partial^2}{\partial x_0^2} G_{x_0}(p, s) & x_0 < 0, \\ K_\alpha (s+p)^{1-\alpha} \frac{\partial^2}{\partial x_0^2} G_{x_0}(p, s) - pG_{x_0}(p, s) & x_0 > 0. \end{cases}$$

- Solve in each half-space separately, and match G_{x_0} and its derivative. Substitute $x_0 = 0$.

- $G_0(p, s) = \frac{s^{\alpha/2-1} + (s+p)^{\alpha/2-1}}{s^{\alpha/2} + (s+p)^{\alpha/2}}$.

- The PDF of $\lambda \equiv T_+/t$ is the *Lamperti* PDF:

$$G(\lambda) = \frac{\sin(\pi\alpha/2)}{\pi} \frac{\lambda^{\alpha/2-1}(1-\lambda)^{\alpha/2-1}}{\lambda^\alpha + (1-\lambda)^\alpha + 2\lambda^{\alpha/2}(1-\lambda)^{\alpha/2} \cos(\pi\alpha/2)}.$$



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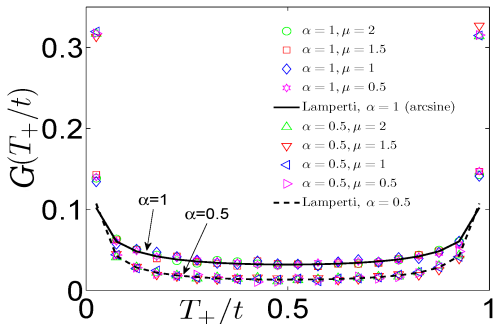
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The occupation time in the positive half-space

Lamperti's PDF



- The particle is almost all the time in one half!

- For $\alpha = 1$, reduces to the famous *Lévy's arcsine law*:

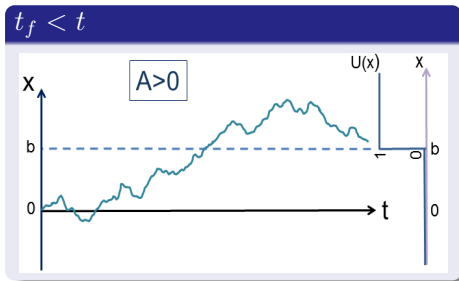
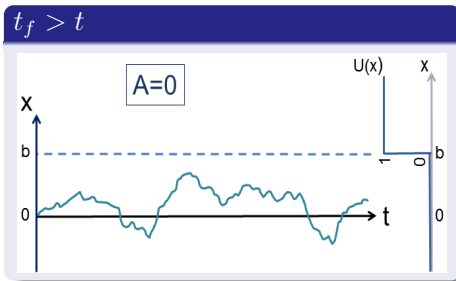
$$G(\lambda) = \frac{1}{\pi \sqrt{\lambda(1-\lambda)}}.$$

- Occupation time PDF is Lamperti's even for Lévy flights.



The first passage time

- The time t_f when a particle starting at $x_0 = 0$ first hits $x = b > 0$ is called the first passage time.
- A trick due to Kac, 1951:
- $\Pr \{t_f > t\} = \Pr \left\{ \max_{0 \leq \tau \leq t} x(\tau) < b \right\} = \lim_{p \rightarrow \infty} G_{x_0}(p, t)$
- $U(x) = \begin{cases} 0 & x < b, \\ 1 & x > b. \end{cases}$
- Works because $G_{x_0}(p, t) = \int_0^\infty e^{-pA} G_{x_0}(A, t) dA$.



The first passage time

- $sG_{x_0}(p, s) - 1 = \begin{cases} K_\alpha s^{1-\alpha} \frac{\partial^2}{\partial x_0^2} G_{x_0}(p, s) & x_0 < b, \\ K_\alpha (s+p)^{1-\alpha} \frac{\partial^2}{\partial x_0^2} G_{x_0}(p, s) - pG_{x_0}(p, s) & x_0 > b. \end{cases}$
- Solve, take the limit $p \rightarrow \infty$, and invert:
- $\lim_{p \rightarrow \infty} G_0(p, t) = \Pr\{t_f > t\} = 1 - \int_0^t \frac{1}{\tau_f} l_{\alpha/2} \left(\frac{\tau}{\tau_f} \right) d\tau.$
 - $\tau_f = (b^2/K_\alpha)^{1/\alpha}.$
 - $l_{\alpha/2}(t)$ is the one-sided Lévy distribution of order $\alpha/2$.
 - $\tilde{l}_{\alpha/2}(s) = e^{-s^{\alpha/2}}.$
- The first passage time PDF: $f(t_f) = \frac{1}{\tau_f} l_{\alpha/2} \left(\frac{t_f}{\tau_f} \right).$
- For long times, $f(t_f) \sim t_f^{-(1+\alpha/2)}$ (famous $t_f^{-3/2}$ for $\alpha = 1$).



The first passage time

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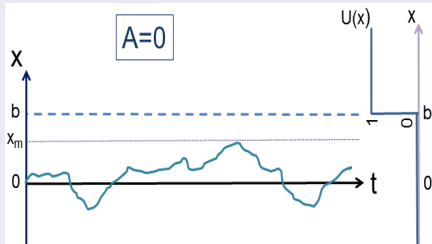
The maximal displacement

- Use exactly the same trick:

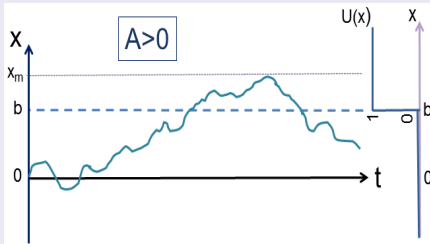
$$\Pr \left\{ x_m \equiv \max_{0 \leq \tau \leq t} x(\tau) < b \right\} = \lim_{p \rightarrow \infty} G_{x_0}(p, t).$$

- $P(x_m, t) = \frac{2}{\alpha \sqrt{K_\alpha}} \frac{t}{(x_m / \sqrt{K_\alpha})^{1+2/\alpha}} l_{\alpha/2} \left[\frac{t}{(x_m / \sqrt{K_\alpha})^{2/\alpha}} \right].$
- Exactly twice the PDF of x (for $x > 0$).

$x_m < b$

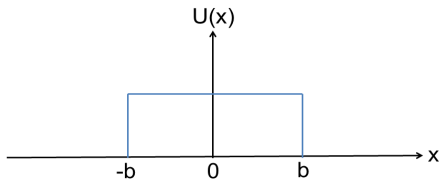


$x_m > b$



The time in $[-b, b]$

- $T_i \equiv \int_0^t U[x(\tau)] d\tau$.
- $U(x) = \begin{cases} 1 & -b < x < b, \\ 0 & \text{Otherwise.} \end{cases}$



- Solve backward equation in (p, s) space for $x_0 = 0$.

$$G_0(p, s) = \frac{p+s \left\{ \cosh \left[\frac{(s+p)^{\alpha/2}}{\sqrt{K_\alpha}} b \right] + \frac{(s+p)^{\alpha/2}}{s^{\alpha/2}} \sinh \left[\frac{(s+p)^{\alpha/2}}{\sqrt{K_\alpha}} b \right] \right\}}{s(s+p) \left\{ \cosh \left[\frac{(s+p)^{\alpha/2}}{\sqrt{K_\alpha}} b \right] + \frac{(s+p)^{\alpha/2}}{s^{\alpha/2}} \sinh \left[\frac{(s+p)^{\alpha/2}}{\sqrt{K_\alpha}} b \right] \right\}}.$$

$$\langle T_i \rangle(s) = -\frac{\partial}{\partial p} G_0(p, s) \Big|_{p=0}; \quad \langle T_i^2 \rangle(s) = \frac{\partial^2}{\partial p^2} G_0(p, s) \Big|_{p=0}.$$

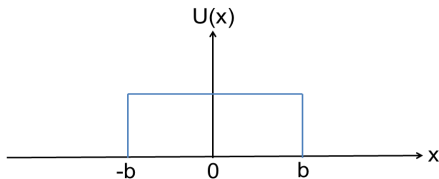
$$\langle T_i \rangle \sim t^{1-\alpha/2} \frac{b}{\sqrt{K_\alpha} \Gamma(2-\alpha/2)}.$$

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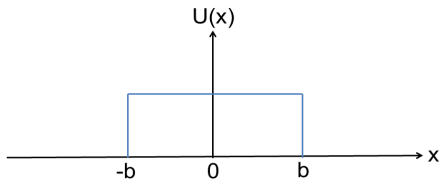
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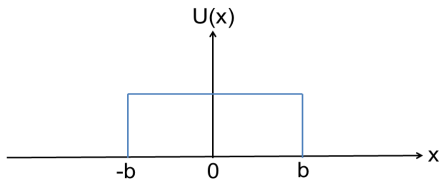


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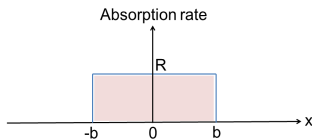


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- $\langle T_i \rangle \sim t^{1-\alpha/2} \frac{b}{\sqrt{K_\alpha} \Gamma(2-\alpha/2)}.$
- $\langle T_i^2 \rangle \sim t^{2-\alpha/2} \frac{2b(1-\alpha)}{\sqrt{K_\alpha} \Gamma(3-\alpha/2)} + t^{2-\alpha} \frac{b^2(3\alpha-1)}{K_\alpha \Gamma(3-\alpha)}.$



The average survival probability when the domain $[-b, b]$ is absorbing

- The survival probability is $S = e^{-RT_i}$.
- $\langle S \rangle = \int_0^\infty e^{-RT_i} G_{x_0}(T_i, t) dT_i = G_{x_0}(R, t)$.



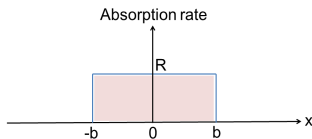
- We know $G_{x_0}(R, s)$ from the previous slide.
- We can invert for long times:

$$\langle S \rangle \sim \left[\Gamma(1 - \alpha/2) \sinh \left(\frac{bR^{\alpha/2}}{\sqrt{K_\alpha}} \right) \right]^{-1} (Rt)^{-\alpha/2} + \mathcal{O}[(Rt)^{-\alpha}].$$



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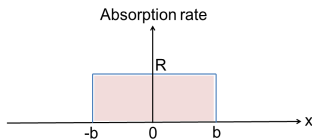
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The functionals $U(x) = x^k$

- $sG(x, p, s) - \delta(x) = K_\alpha \frac{\partial^2}{\partial x^2} (s + px^k)^{1-\alpha} G(x, p, s) - px^k G(x, p, s).$
- Operate on each term with $(-1)^n \frac{\partial^n}{\partial p^n}$, substitute $p = 0$, multiply each term by x^m , and integrate over all x .
- $\langle A_{x^k}^n x^m \rangle (s) = c_{n,m}(k) K_\alpha^{\frac{m+nk}{2}} s^{-(1+n+\frac{m+nk}{2}\alpha)}.$
- Substitute $m = 0$ and invert $s \rightarrow t$:
- $\langle A_{x^k}^n \rangle (t) = c_{n,0}(k) \frac{K_\alpha^{\frac{nk}{2}}}{\Gamma(1+n+\frac{n\alpha k}{2})} t^{n(1+\frac{\alpha k}{2})}.$
- Leads to the scaling form:

$$G(A_{x^k}, t) = \frac{1}{K_\alpha^{k/2} t^{1+\alpha k/2}} g_{\alpha,k} \left(\frac{A_{x^k}}{K_\alpha^{k/2} t^{1+\alpha k/2}} \right).$$



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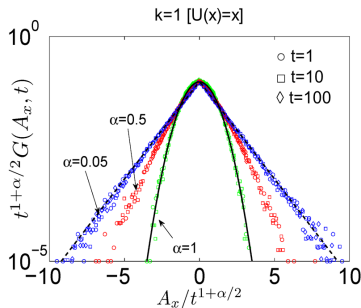
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Section 4

Functionals of bounded particles: weak ergodicity breaking



Ensemble and time averages

What is the average of $U(x)$ at time t in a closed system?

Ensemble average

$$\langle U(x) \rangle_t = \int_{-\infty}^{\infty} G(x, t) U(x) dx.$$

Time average

$$\overline{U(x)}_t = \frac{1}{t} \int_0^t U[x(\tau)] d\tau.$$

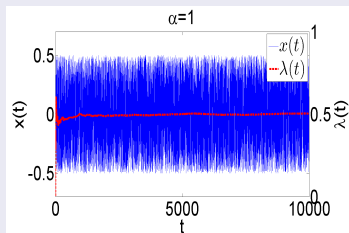
- In ergodic systems, for $t \rightarrow \infty$, $\langle U(x) \rangle = \overline{U(x)} = \int_{-\infty}^{\infty} G_{\text{eq}}(x) U(x) dx$.
- When ergodicity is broken, $\overline{U(x)}$ is a random variable even for $t \rightarrow \infty$.
- Two examples...



Weak ergodicity breaking of the occupation time

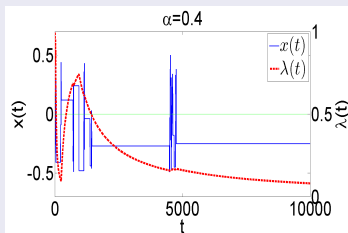
Consider the occupation fraction $\lambda = \frac{1}{t} \int_0^t \Theta[x(\tau)] d\tau$ for a particle in a box.

Normal diffusion



- Ergodic.
- For $t \rightarrow \infty$, $\lambda \rightarrow 1/2$.
- $\langle (\Delta\lambda)^2 \rangle = 0$.

Anomalous diffusion



- Non-ergodic.
- Even for $t \rightarrow \infty$, λ is a random variable or $\langle (\Delta\lambda)^2 \rangle > 0$.

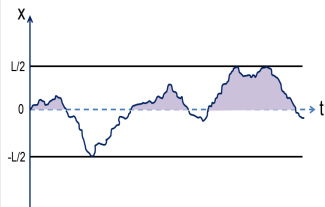


The occupation time in half box

- The fluctuations of $\lambda = T_+/t$:
$$\langle (\Delta\lambda)^2 \rangle \sim \frac{1-\alpha}{4} + \frac{\alpha L^2}{24K_\alpha\Gamma(3+\alpha)} t^{-\alpha}.$$
- For $t \rightarrow \infty$ and $\alpha = 1$, $\langle (\Delta\lambda)^2 \rangle = 0$
and $G(\lambda) = \delta(\lambda - 1/2)$.
- For $t \rightarrow \infty$ and $\alpha < 1$,
$$\langle (\Delta\lambda)^2 \rangle = \frac{1-\alpha}{4} > 0.$$

 $\Rightarrow$ weak ergodicity breaking!

Illustration

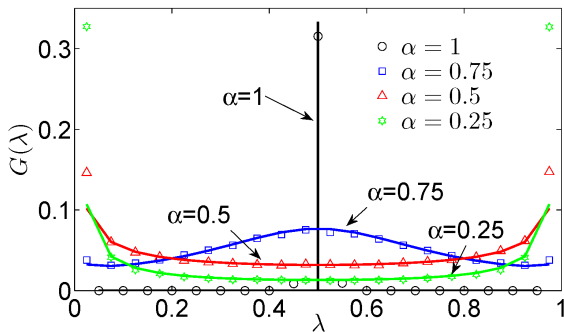


- The PDF for long times is again Lamperti:
$$G_\alpha(\lambda) = \frac{\sin(\pi\alpha)}{\pi} \frac{\lambda^{\alpha-1}(1-\lambda)^{\alpha-1}}{\lambda^{2\alpha} + (1-\lambda)^{2\alpha} + 2\lambda^\alpha(1-\lambda)^\alpha \cos(\pi\alpha)}.$$
- Here the exponent is α , compared to $\alpha/2$ for the free particle.



The occupation time in half box

Lamperti PDF



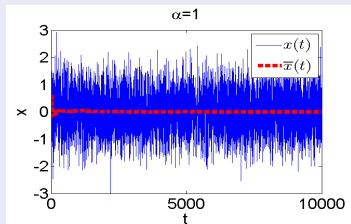
- For $\alpha = 1$, the particle uniformly covers the box in each trajectory.
- For small α , the particle remains in one side almost the entire time.



Weak ergodicity breaking of the time-averaged position

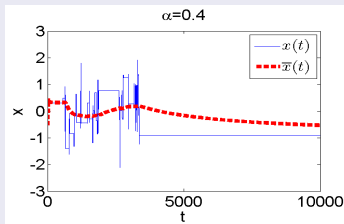
Consider the time-averaged position $\bar{x} = \frac{1}{t} \int_0^t x(\tau) d\tau$ in a harmonic field.

Normal diffusion



- Ergodic.
- For $t \rightarrow \infty$, $\bar{x} \rightarrow \langle x \rangle = 0$.
- $\langle (\Delta \bar{x})^2 \rangle = 0$.

Anomalous diffusion



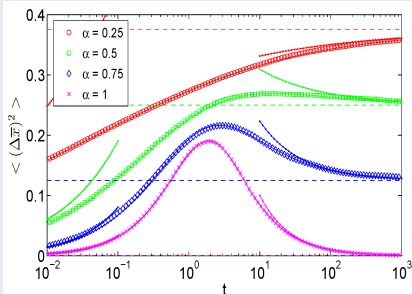
- Non-ergodic.
- Even for $t \rightarrow \infty$, $\bar{x}$ is a random variable or $\langle (\Delta \bar{x})^2 \rangle > 0$.

The fluctuations of the time-averaged position in a harmonic potential

- $\langle (\Delta \bar{x})^2 \rangle = \langle x^2 \rangle \{ (1 - \alpha) + 4\alpha E_{\alpha,3} [-(t/\tau)^\alpha] - 2(1 + \alpha) E_{\alpha,3} [-2(t/\tau)^\alpha] \}.$
 - $E_{\alpha,3}(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(3+\alpha n)}$ is the Mittag-Leffler function.
 - $\langle x^2 \rangle \equiv K_\alpha \tau^\alpha = k_B T / (m\omega^2).$

- For long times $\langle (\Delta \bar{x})^2 \rangle \sim (1 - \alpha) \langle x^2 \rangle + \frac{(3\alpha-1)\langle x^2 \rangle}{\Gamma(3-\alpha)} (t/\tau)^{-\alpha}.$
- For $t \rightarrow \infty$ and $\alpha = 1$, $\langle (\Delta \bar{x})^2 \rangle = 0$ and $G(\bar{x}) = \delta(\bar{x}).$
- For $t \rightarrow \infty$ and $\alpha < 1$, $\langle (\Delta \bar{x})^2 \rangle = (1 - \alpha) \langle x^2 \rangle > 0.$
 $\Rightarrow$ weak ergodicity breaking!

Simulations and theory



Section 5

Summary



Summary

- We developed a **fractional Feynman-Kac equation** for functionals of **anomalous diffusion** in the **CTRW** model.
- Using our equation, we could calculate several properties of anomalous diffusion such as the **occupation time**, the **first passage time**, the **maximal displacement**, and others.
- Our equation uncovers the kinetics of **weak ergodicity breaking**.



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Thank you for your attention

 Lior Turgeman, Shai Carmi, and Eli Barkai.

Fractional Feynman-Kac equation for non-Brownian functionals.
Phys. Rev. Lett. **103**, 190201 (2009).

 Shai Carmi, Lior Turgeman, and Eli Barkai.

On distributions of functionals of anomalous diffusion paths.
J. Stat. Phys. **141**, 1071 (2010).

 Shai Carmi and Eli Barkai.

A fractional Feynman-Kac equation for weak ergodicity breaking.
In preparation (2011).



Fractional Schrödinger equation

- We have seen that the Schrödinger equation in imaginary time is structurally similar to the Feynman-Kac equation.
- Is there a fractional Schrödinger equation?
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- The particle experiences a constant force F .

Functional	Result
The first moment of the occupation time in $x > 0$	$\langle T_+ \rangle = t \left\{ 1 - \frac{1}{4\Gamma(2-\alpha)} (t/\tau)^{-\alpha} + \mathcal{O}[(t/\tau)^{-2\alpha}] \right\}$
The second moment of the occupation time in $x > 0$	$\langle T_+^2 \rangle = t^2 \left\{ 1 - \frac{1}{2\Gamma(3-\alpha)} (t/\tau)^{-\alpha} + \mathcal{O}[(t/\tau)^{-2\alpha}] \right\}$
The first moment of the time-averaged position	$\langle \bar{x} \rangle = \frac{\mu}{\Gamma(2+\alpha)} t^\alpha$
The second moment of the time-averaged position	$\langle \bar{x}^2 \rangle = \frac{4K_\alpha}{\Gamma(3+\alpha)} t^\alpha + \frac{2\mu^2(2+\alpha)}{\Gamma(3+2\alpha)} t^{2\alpha}$

- $\tau^\alpha = \frac{4(k_B T)^2}{K_\alpha F^2}$; $\mu = \frac{K_\alpha F}{k_B T}$.

The long times PDF $G_{\text{eq}}(\bar{U})$

- Consider a functional $A = \int_0^t U[x(\tau)]d\tau$, and $\bar{U} = A/t$.

- For long times, we can show that

$$K_\alpha \left[\frac{\partial^2}{\partial x^2} - \frac{\partial}{\partial x} \frac{F(x)}{k_B T} \right] [s + pU(x)]^{1-\alpha} G(x, p, s) = 0.$$

- Integrate the forward equation over all x to obtain:

$$\int_{-\infty}^{\infty} [s + pU(x)] G(x, p, s) dx = 1.$$

- This gives: $G(x, p, s) = \frac{[s+pU(x)]^{\alpha-1} e^{-V(x)/(k_B T)}}{\int_{-\infty}^{\infty} [s+pU(x)]^{\alpha} e^{-V(x)/(k_B T)} dx}.$

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- Invert: $G_{\text{eq}}(\bar{U}) = \frac{\sin(\pi\alpha)}{\pi} \frac{I_{\alpha-1}^<(\bar{U}) I_{\alpha}^>(\bar{U}) + I_{\alpha-1}^>(\bar{U}) I_{\alpha}^<(\bar{U})}{[I_{\alpha}^<(\bar{U})]^2 + [I_{\alpha}^>(\bar{U})]^2 + 2 \cos(\pi\alpha) I_{\alpha}^<(\bar{U}) I_{\alpha}^>(\bar{U})},$

- where

$$I_{\alpha}^<(\bar{U}) = \int_{\bar{U} < U(x)} e^{-V(x)/(k_B T)} [U(x) - \bar{U}]^{\alpha} dx,$$

$$I_{\alpha}^>(\bar{U}) = \int_{\bar{U} > U(x)} e^{-V(x)/(k_B T)} [\bar{U} - U(x)]^{\alpha} dx.$$



The long times PDF $G_{\text{eq}}(\bar{U})$

- Consider a functional $A = \int_0^t U[x(\tau)]d\tau$, and $\bar{U} = A/t$.
- For long times, we can show that

$$K_\alpha \left[\frac{\partial^2}{\partial x^2} - \frac{\partial}{\partial x} \frac{F(x)}{k_B T} \right] [s + pU(x)]^{1-\alpha} G(x, p, s) = 0.$$
- Integrate the forward equation over all x to obtain:

$$\int_{-\infty}^{\infty} [s + pU(x)] G(x, p, s) dx = 1.$$
- This gives: $G(x, p, s) = \frac{[s+pU(x)]^{\alpha-1} e^{-V(x)/(k_B T)}}{\int_{-\infty}^{\infty} [s+pU(x)]^{\alpha} e^{-V(x)/(k_B T)} dx}.$
- Invert: $G_{\text{eq}}(\bar{U}) = \frac{\sin(\pi\alpha)}{\pi} \frac{I_{\alpha-1}^<(\bar{U})I_{\alpha}^>(\bar{U}) + I_{\alpha-1}^>(\bar{U})I_{\alpha}^<(\bar{U})}{[I_{\alpha}^>(\bar{U})]^2 + [I_{\alpha}^<(\bar{U})]^2 + 2 \cos(\pi\alpha) I_{\alpha}^>(\bar{U}) I_{\alpha}^<(\bar{U})},$
- where

$$I_{\alpha}^<(\bar{U}) = \int_{\bar{U} < U(x)} e^{-V(x)/(k_B T)} [U(x) - \bar{U}]^{\alpha} dx,$$

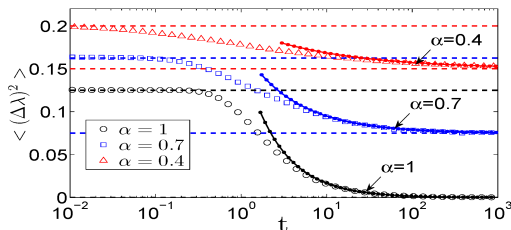
$$I_{\alpha}^>(\bar{U}) = \int_{\bar{U} > U(x)} e^{-V(x)/(k_B T)} [\bar{U} - U(x)]^{\alpha} dx.$$



The dynamics of the occupation time in a box

- For long times, the PDF is Lamperti with index α .
- $\langle (\Delta\lambda)^2 \rangle \rightarrow \frac{\alpha L^2}{24K_\alpha \Gamma(3+\alpha)} t^{-\alpha} + \frac{1-\alpha}{4}$.
- For short times, the PDF is Lamperti with index $\alpha/2$ (free particle).
- $\langle (\Delta\lambda)^2 \rangle \rightarrow \frac{1-\alpha/2}{4}$.

Simulations and theory



The first passage time in a box

- The time t_f when a particle starting at $x_0 = -b$ ($0 < b < L/2$) first hits $x = 0$ is the first passage time in a box.
- Use Kac's trick again:
- $\Pr \{t_f > t\} = \Pr \left\{ \max_{0 \leq \tau \leq t} x(\tau) < 0 \right\} = \lim_{p \rightarrow \infty} G_{x_0}(p, t)$
- Here, $U(x) = \Theta(x)$.

- The solution of the backward equation gives

$$\lim_{p \rightarrow \infty} G_{-b}(p, s) = \frac{1}{s} \left\{ 1 - \frac{\cosh \left[\left(\frac{L}{2} - b \right) \frac{s^{\alpha/2}}{\sqrt{K_\alpha}} \right]}{\cosh \left(\frac{L s^{\alpha/2}}{2\sqrt{K_\alpha}} \right)} \right\}.$$

- The first passage time PDF is $f(t_f) = \frac{b(L-b)}{2K_\alpha |\Gamma(-\alpha)|} t_f^{-(1+\alpha)}$.
- Here, $f(t_f) \sim t_f^{-(1+\alpha)}$ compared to $f(t_f) \sim t_f^{-(1+\alpha/2)}$ for a free particle.
- For $\alpha < 1$, $\langle t_f \rangle = \infty$.



The PDF of the time-averaged position

- We know the PDF for long times (long expression).
- For short times the PDF is equivalent to that of free particles.
- For $0 < \alpha < 1/3$ the PDF becomes wider in time.
- For $1/3 < \alpha < 1$ the PDF is first narrow (initial condition), then wide, then narrow again (but with finite width for $\alpha < 1$).

Simulations and theory

