“The Random Walk’s Guide to Anomalous Diffusion: A Fractional Dynamics Approach”

By Ralf Metzler and Joseph Klafter

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McKinley Group Summer Reading Club
“Fractional Derivatives and Fractional Calculus in Rheology”
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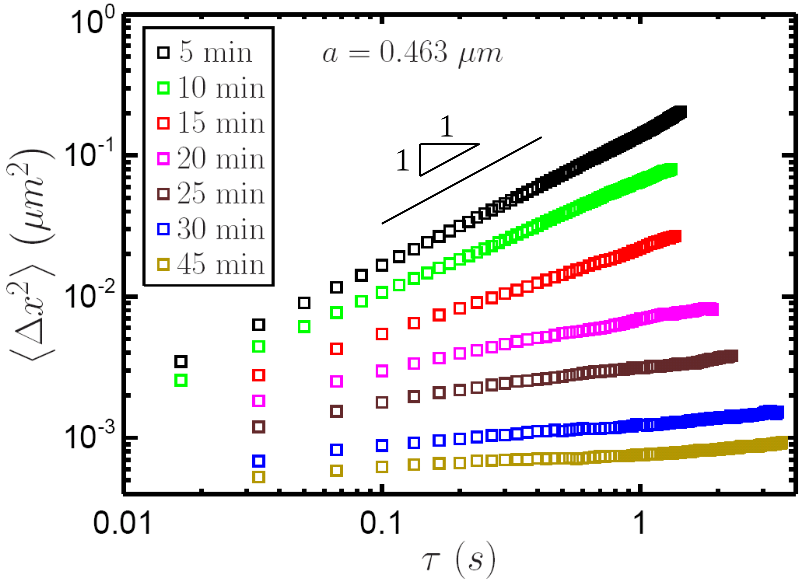
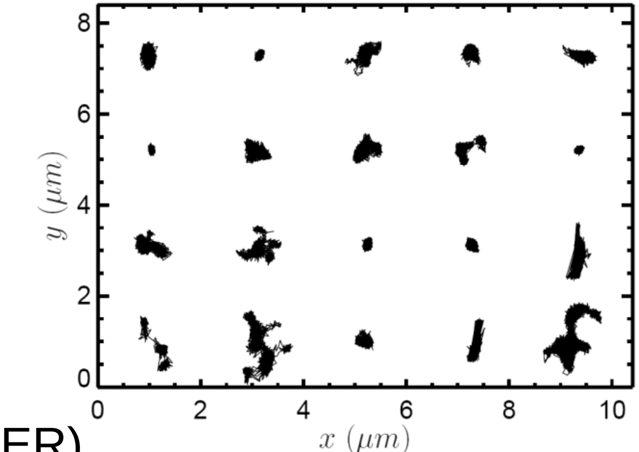
Anomalous Diffusion in Laponite

- Tracer particle diffusion in gelling systems like Laponite



$$\langle \Delta x^2 \rangle = 2D\tau^{\alpha}$$

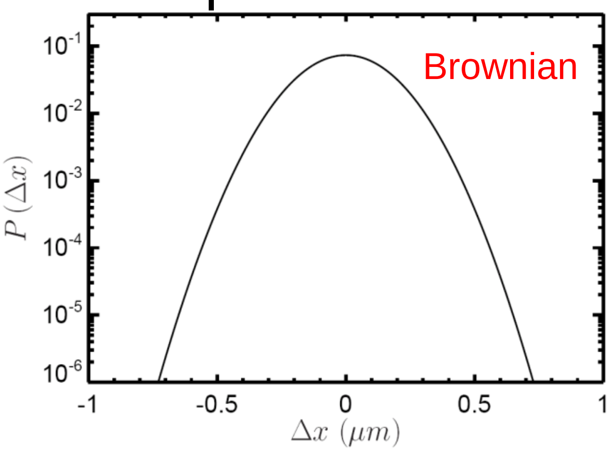
$\alpha(\tau)$ related to micro-scale viscoelasticity

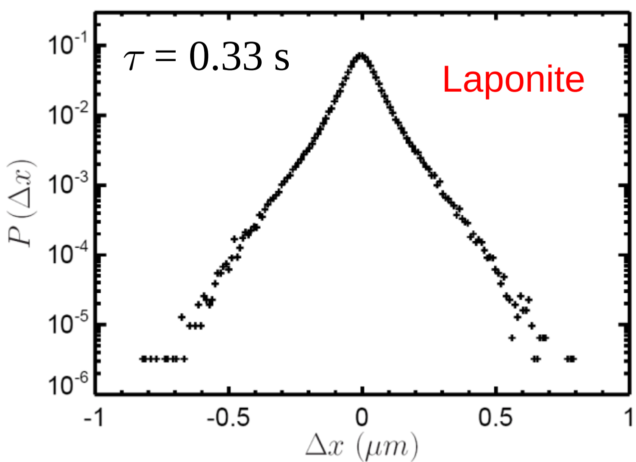


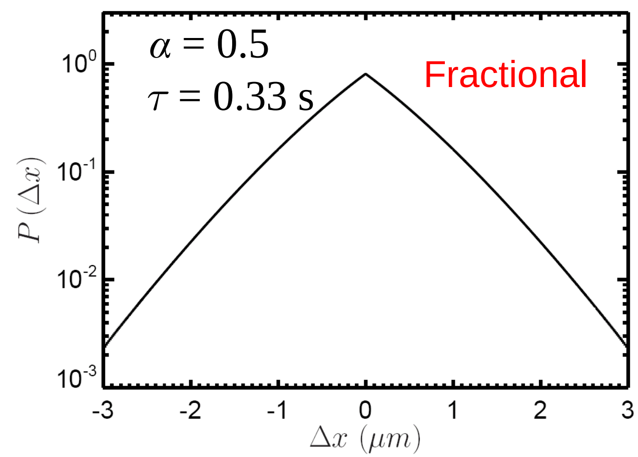
Generalized Stokes-Einstein Relation (GSER)

$$G^*(\omega = 1/\tau) = \left\{\frac{1}{a\langle \Delta x^2(\tau) \rangle}\right\} \frac{k_B T}{3\pi} \frac{\exp[i\pi\alpha(\tau)/2]}{\Gamma[1+\alpha(\tau)]}$$

- Displacement PDF

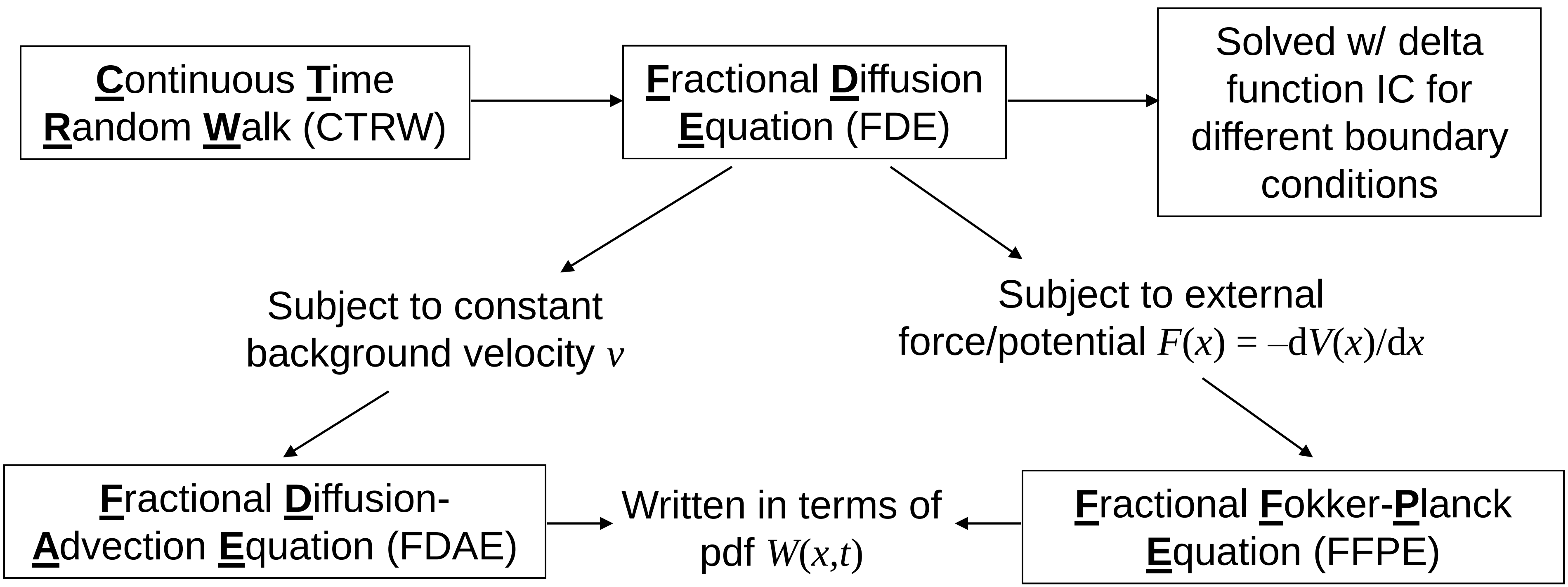






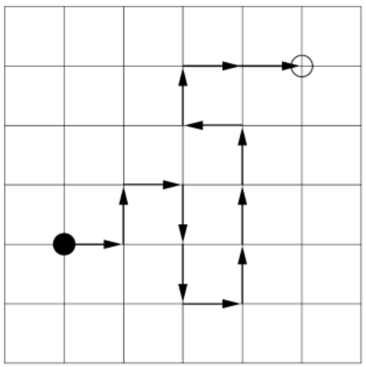
Overview of Metzler and Klafter

- In "Normal" diffusion, connection between random walks and diffusion eqn
  - Random walks provide microscopic description of stochastic events
  - Diffusion eqn is deterministic and useful for solving BVP's w/ ext. forces
- Same for anomalous diffusion and fractional dynamics

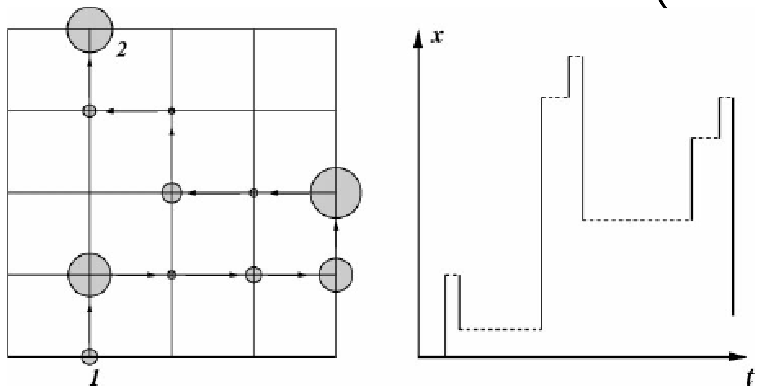


Continuous Time Random Walks

Brownian random walk on a lattice



Continuous Time Random Walks (CTRWs)



$\lambda(x)$ = jump length pdf

$w(t)$ = waiting time pdf

Assumed to be independent

$T = \int_0^{\infty} \mathrm{d}t\, w(t) t$ = mean waiting time

$\Sigma^2 = \int_{-\infty}^{\infty} \mathrm{d}x\, \lambda(x) x^2$ = jump length variance

- If T and Σ^2 are finite, Brownian motion is recovered at long times
  - Diverging $T \rightarrow$ Sub-diffusion, Diverging $\Sigma^2 \rightarrow$ Superdiffusion
- pdf for position and time $W(x,t)$ for CTRW

$\eta(x,t) = \int_{-\infty}^{\infty} dx' \int_0^{\infty} dt' \eta(x',t') \lambda(x-x') w(t-t') + \delta(x)\delta(t)$ = pdf of just having arrived at position x at time t

$\delta(x)\delta(t)$ → Initial Condition

$W(x,t) = \int_0^t \mathrm{d}t\, \eta(x,t') \Psi(t-t')$ = pdf of arrival at position x at time t' and not having moved since

$\Psi(t) = 1 - \int_0^t \mathrm{d}t'\, w(t')$

Taking Laplace (^) and Fourier (~) transforms of $W(x,t)$ gives

$$\hat{\tilde{W}}(k,u) = \frac{1-\hat{w}(u)}{u} \frac{\tilde{W}_0(k)}{1-\hat{w}(u)\tilde{\lambda}(k)}$$

$\tilde{W}_0(k)$ = Fourier transform of initial condition

Fractional Diffusion Eqn from CTRW

- pdf for position and time $W(x,t)$ for CTRW…(Aside: why proceed?)

$$\hat{\tilde{W}}(k,u) = \frac{1-\hat{w}(u)}{u}\frac{\tilde{W}_0(k)}{1-\hat{w}(u)\tilde{\lambda}(k)}$$

$\tilde{W}_0(k)$ = Fourier transform of initial condition

- Now must pick $\lambda(x)$ and $w(t)$: Sub-diffusion

$$\lambda(x) = (4\pi\sigma^2)^{-1/2}\exp(-x^2/(4\sigma^2))$$ (Gaussian) $\Sigma^2 = 2\sigma^2 =$ finite

Fourier Transform $\longrightarrow$ $\tilde{\lambda}(k) \sim 1 - \sigma^2 k^2 + O(k^4)$

$w(t) \sim A_\alpha(\tau/t)^{1+\alpha}$ $\{0 < \alpha < 1\}$ T diverges Laplace Transform $\longrightarrow$ $\hat{w}(u) \sim 1 - (u\tau)^\alpha$

- Plugging into the equation above gives $$\hat{\tilde{W}}(k,u) = \frac{\left[\tilde{W}_0(k)/u\right]}{1+K_\alpha u^{-\alpha}k^2}$$
- Laplace transform rule for fractional derivatives $$\mathcal{L}\{{}_0D_t^{-p}W(x,t)\} = u^{-p}\hat{W}(x,u)$$
- Fractional Diffusion Eqn (FDE)

$$\frac{\partial W}{\partial t} = {}_0D_t^{1-\alpha}K_\alpha\frac{\partial^2}{\partial x^2}W(x,t)$$

Solution and Diffusion Profiles

- Closed form solution to FDE: $$W(x,t) = \frac{1}{\sqrt{4\pi K_\alpha t^\alpha}} H^{2,0}_{1,2}\left[\frac{x^2}{4K_\alpha t^\alpha}\middle| \begin{matrix}(1-\alpha/2,\alpha)\\(0,1),(\frac{1}{2},1)\end{matrix}\right]$$

$$H^{mn}_{pq}(z) = H^{mn}_{pq}\left[z\middle|\begin{matrix}(a_p,A_p)\\(b_q,B_q)\end{matrix}\right] = \frac{1}{2\pi i}\int_L ds\,\chi(s) z^s$$ = "Fox function"

$$\chi(s) = \frac{\prod_1^m \Gamma(b_j - B_j s)\prod_1^n \Gamma(1-a_j+A_j s)}{\prod_{m+1}^q \Gamma(1-b_j+B_j s)\prod_{n+1}^p \Gamma(a_j - A_j s)}$$

- Fox functions in anomalous diffusion
  - Very general functions, generalizations of hypergeometric functions
  - Important property $${}_0D_z^\nu\left(z^\alpha H^{m,n}_{p,q}\left[(az)^\beta\middle|\begin{matrix}(a_p,A_p)\\(b_q,B_q)\end{matrix}\right]\right) = z^{\alpha-\nu} H^{m,n+1}_{p+1,q+1}\left[(az)^\beta\middle|\begin{matrix}(-\alpha,\beta),(a_p,A_p)\\(b_q,B_q),(\nu-\alpha,\beta)\end{matrix}\right]$$
- Diffusion Profiles for delta-function I.C. ($\alpha = 1/2$)

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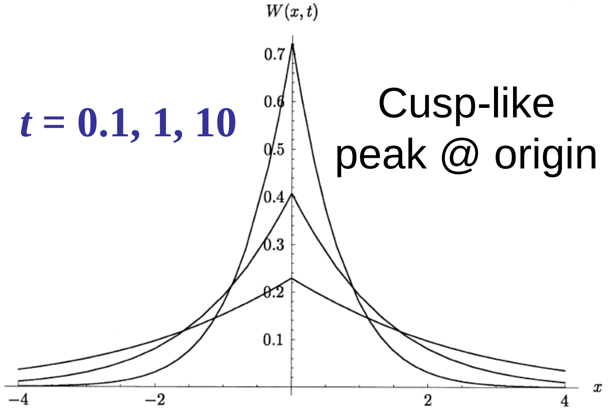
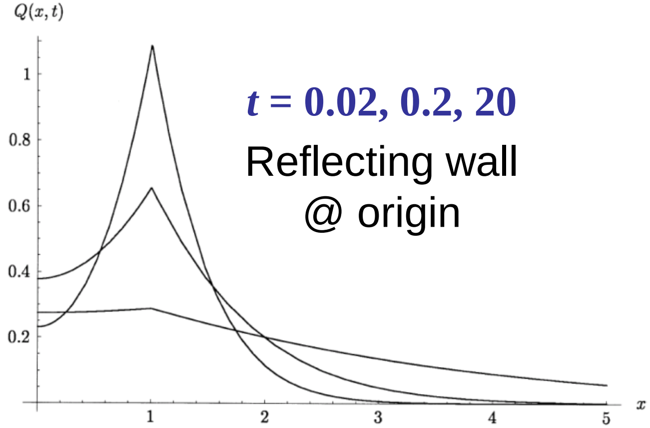
Mathematician
McGill U.

BVP w/ method of images (folding)



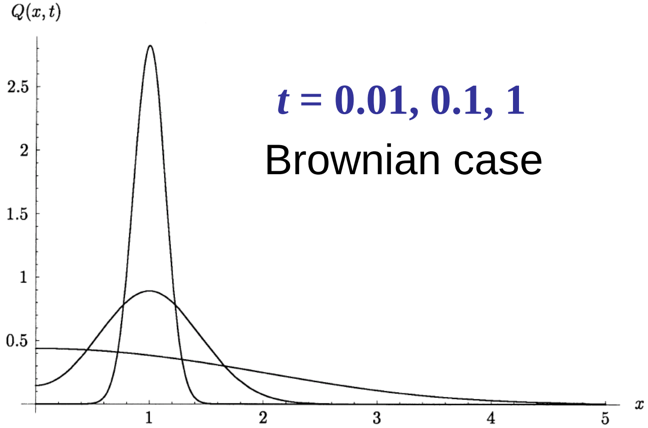
$t = 0.1, 1, 10$

Cusp-like peak @ origin



$t = 0.02, 0.2, 20$

Reflecting wall @ origin



$t = 0.01, 0.1, 1$

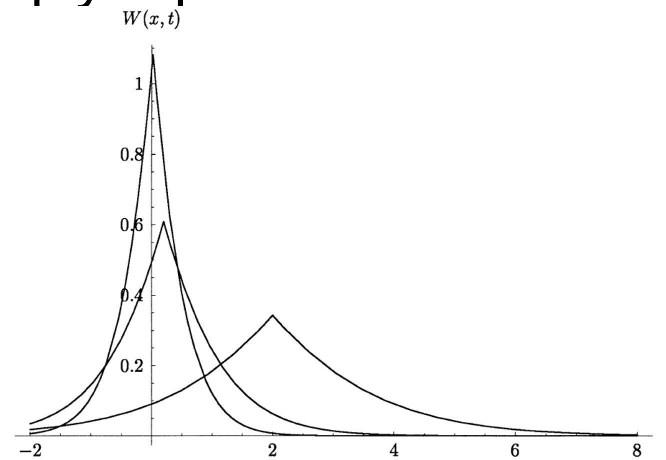
Brownian case

Diffusion-Advection

- Homogeneous background velocity v
- For Galilei invariant eqn, same strategy: simply replace x with $x - vt$

$$\frac{\partial W}{\partial t} + v\frac{\partial W}{\partial x} = {}_0D_t^{1-\alpha}K_\alpha\frac{\partial^2}{\partial x^2}W(x,t) \qquad \text{(FDAE)}$$

$$\langle x(t)\rangle = vt \qquad \langle x^2(t)\rangle = \frac{2K_\alpha}{\Gamma(1+\alpha)}t^\alpha + v^2t^2$$

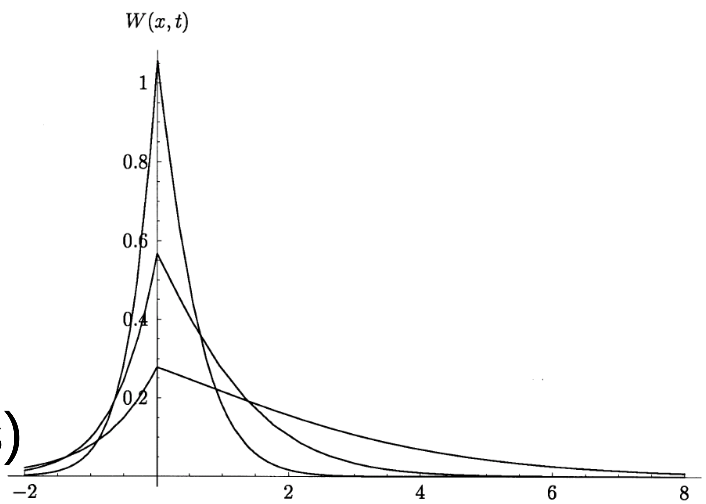


- Small particle in flowing polymer solution
- For $v = v(x)$ (inhomogeneous), jump length pdf depends on the starting point x_0
- In that case:

$$\frac{\partial W}{\partial t} = {}_0D_t^{1-\alpha}\left[-A_\alpha\frac{\partial}{\partial x}v(x) + K_\alpha\frac{\partial^2}{\partial x^2}\right]W(x,t)$$

$$\langle x(t)\rangle = \frac{A_\alpha vt^\alpha}{\Gamma(1+\alpha)} \qquad \langle x^2(t)\rangle = \frac{2A_\alpha^2v^2t^{2\alpha}}{\Gamma(1+2\alpha)} + \frac{2K_\alpha t^\alpha}{\Gamma(1+\alpha)}$$

- Advection-diffusion in porous media (traps)



Diffusion with an External Force

- Fokker-Planck Eqn for Brownian diffusion w/ an external force $F(x)$

$$\frac{\partial W}{\partial t} = \left[\frac{\partial}{\partial x} \frac{V'(x)}{m\eta_1} + K_1 \frac{\partial^2}{\partial x^2} \right] W(x,t)$$ (FPE) $F(x) = -V'(x)$ $V(x)$ = Potential

- Fractional Generalization: $$\frac{\partial W}{\partial t} = {}_0D_t^{1-\alpha} \left[\frac{\partial}{\partial x} \frac{V'(x)}{m\eta_\alpha} + K_\alpha \frac{\partial^2}{\partial x^2} \right] W(x,t)$$
- Solution: separation of variables $W_n(x,t) = T_n(t)\varphi_n(x)$

$$\frac{\mathrm{d}T_n(t)}{\mathrm{d}t} = -\lambda_{n,\alpha}\ {}_0D_t^{1-\alpha} T_n(t)$$ (familiar?) ⟶ $$T_n(t) = E_\alpha(-\lambda_{n,\alpha} t^\alpha) \equiv \sum_{j=0}^{\infty} \frac{(-\lambda_{n,\alpha} t^\alpha)^j}{\Gamma(1+\alpha j)}$$

Mittag-Leffler function

$$\frac{\partial}{\partial x} \frac{V'(x)}{m\eta_\alpha} + K_\alpha \frac{\partial^2 \varphi_n}{\partial x^2} = -\lambda_{n,\alpha} \varphi_n(x)$$ ⟶ Same as normal FPE, so equilibrium properties same as non-fractional case

- Solution properties

1.) $\langle x^2(t) \rangle_0 = \frac{2K_\alpha}{\Gamma(1+\alpha)} t^\alpha$ in the force-free limit

4.) $\langle x(t) \rangle_F = \frac{1}{2} \frac{F \langle x^2(t) \rangle_0}{k_B T}$

2.) $W_{st}(x) \equiv \lim_{t \to \infty} W(x,t) = N \exp\left(-\frac{V(x)}{m\eta_\alpha K_\alpha} \right)$ "Gibbs-Boltzmann distribution"

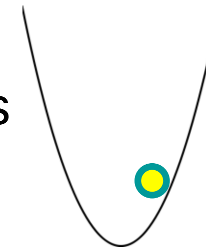
3.) $K_\alpha = k_B T / m\eta_\alpha$ A generalized Stokes-Einstein relation

Diffusion in a Potential Well

Leonard Ornstein
University of Utrecht

George Uhlenbeck
MIT and others

- Fractional *Ornstein-Uhlenbeck process* with $V(x) = ½m\omega^2x^2$
  - Essentially a noisy relaxation process
- Relaxation of moments of pdf $W(x,t)$ with I.C. $W_0(x) = \delta(x - x_0)$



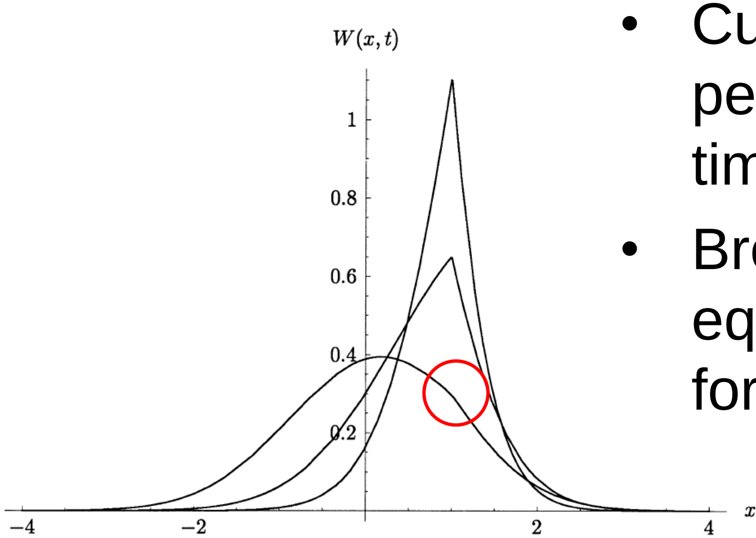
$$\langle x(t)\rangle = x_0 E_\alpha(-(t/\tau)^\alpha)$$

$$\langle x^2(t)\rangle = x_{th}^2 + [x_0^2 - x_{th}^2]E_\alpha(-2(t/\tau)^\alpha)$$

where $x_{th}^2 = k_B T/[m\omega^2]$

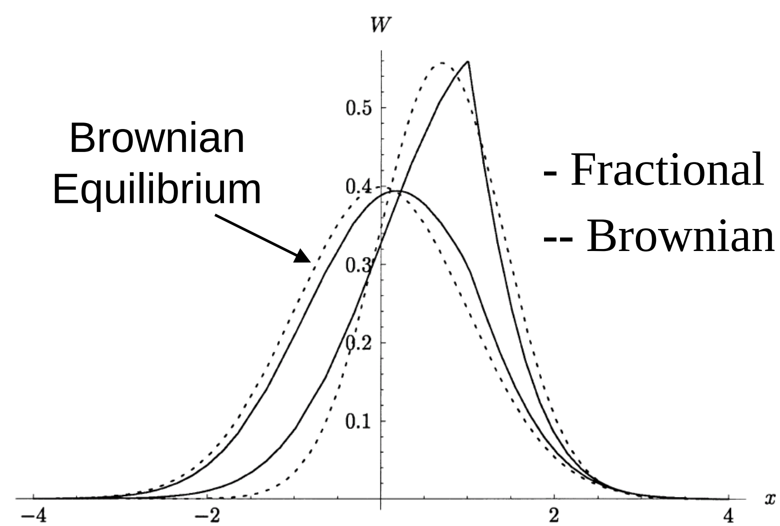
For $x_0 = 1$

Fractional Relaxation



- Cusp from I.C. persists for long times
- Brownian equilibrium pdf for $t \to \infty$

Comparing Brownian and Fractional Relaxation



Relating Brownian and Fractional

- A relatively convenient way to calculate pdf's for the FFPE

$$\hat{W}_{\alpha}(x,s) = \frac{\eta_{\alpha}}{\eta_{\alpha=1}} s^{\alpha-1} \hat{W}_{\alpha=1}\left(x, \frac{\eta_{\alpha}}{\eta_{\alpha=1}} s^{\alpha}\right)$$

In Laplace space

- Equivalently:

$$W_{\alpha}(x,t) = \int_0^{\infty} A(s,t) \hat{W}_{\alpha=1}(x,s)\, ds$$

where

$$A(s,t) = \frac{1}{\alpha s} H^{1,0}_{1,1}\left[\frac{s^{1/\alpha}}{t} \middle| \begin{matrix}(1,1) \\ (1,1/\alpha)\end{matrix}\right]$$

or the series representation

$$A(s,t) = \frac{1}{s}\sum_{n=0}^{\infty} \frac{(-1)^n}{\Gamma(1-\alpha-\alpha n)\Gamma(1+n)}\left(\frac{s}{t^{\alpha}}\right)^{1+n}$$

Thank you for your attention!

Markov Processes

- A process for which the probability of future states only depends on the current state
  - Not the past history
- Eg. Brownian motion and the probability a particle will be at a certain position at a certain time
- Diffusion in a viscoelastic fluid with *memory* can violate this
  - Future state probability may depend on both the current state and history