IX. Fractional Brownian motion & fractional Langevin equation motion.

(Kolmogorov 1940, Mandelbrot 1968)

$$\frac{dx(t)}{dt} = \xi(t) \quad \text{FBM}$$

The noise $\xi(t)$ is Gaussian distributed, $p(\xi) = \frac{1}{4\pi} \exp\left(-\frac{\xi^2}{4}\right)$

Its correlations decay in power-law fashion, $\langle \xi(t_1)\, \xi(t_2) \rangle \sim \alpha K_\alpha (\alpha-1) |t_1 - t_2|^{\alpha-2}$

Here $x(t) = \int_0^t \xi(t')\,dt'$ is the position of the particle (formal solution).

To calculate the position autocorrelation function we use the autocorrelation of the noise & assume that $t_1 > t_2$:

$$\langle x(t_1) x(t_2) \rangle = \int_0^{t_1} dt' \int_0^{t_2} dt'' \,\langle \xi(t')\, \xi(t'') \rangle$$

$$= \alpha K_\alpha (\alpha - 1) \int_0^{t_1} dt' \int_0^{t_2} dt'' \, |t' - t''|^{\alpha-2}$$

$$= \alpha K_\alpha (\alpha-1) \int_0^{t_1} dt' \left\{ \int_0^{t'} (t'-t'')^{\alpha-2} dt'' + \int_{t'} (t''-t')^{\alpha-2} dt'' \right\}$$

$$= \alpha K_\alpha (\alpha-1) \int_0^{t_1} dt' \left\{ \left[-\frac{(t'-t'')^{\alpha-1}}{\alpha-1} \right]_0^{t'} + \left[\frac{(t''-t')^{\alpha-1}}{\alpha-1} \right]_{t'}^{t_2} \right\}$$

$$= \alpha K_\alpha (\alpha-1) \int_0^{t_1} dt' \left\{ \frac{(t')^{\alpha-1}}{\alpha-1} + \frac{|t_2 - t'|^{\alpha-1}}{\alpha-1} \right\}$$

$$= \alpha K_\alpha (\alpha-1) \left\{ \int_0^{t_1} \frac{(t')^{\alpha-1}}{\alpha-1} dt' + \int_0^{t_2} \frac{(t_2-t')^{\alpha-1}}{\alpha-1} dt' + \int_{t_2}^{t_1} \frac{(t'-t_2)^{\alpha-1}}{\alpha-1} dt' \right\}$$

$$= K_\alpha \; t_1^\alpha + t_2^\alpha + |t_1 - t_2|^\alpha$$

MSD: $\langle x^2(t)\rangle = 2K_\alpha t^\alpha$.

The noise is Gaussian $\Rightarrow$ the process has a Gaussian PDF:

$$P_{FBM}(x,t) = \frac{1}{\sqrt{4\pi K_\alpha t^\alpha}} \exp\left(-\frac{x^2}{4K_\alpha t^\alpha}\right)$$

This fulfills the generalised diffusion ~~constant~~ equation

$$\frac{\partial}{\partial t} P_{FBM}(x,t) = \alpha K_\alpha t^{\alpha-1} \frac{\partial^2}{\partial x^2} P_{FBM}(x,t) \qquad (*)$$

which is local in time. In contrast, the CTRW process produced the fractional diffusion equation

$$\frac{\partial}{\partial t} P_{CTRW}(x,t) = {}_0D_t^{1-\alpha} K_\alpha \frac{\partial^2}{\partial x^2} P_{CTRW} = K_\alpha \frac{1}{\Gamma(\alpha)} \frac{\partial}{\partial t} \int_0^t \frac{dt'}{(t-t')^{1-\alpha}} \frac{\partial^2}{\partial x^2} P_{CTRW}(x,t')$$

which is non-local in time (memory integral).

The Gaussian form for $P_{FBM}(x,t)$ and the FBM-diffusion equation is <u>only</u> valid for motion in an <u>unbounded</u> domain (natural boundary conditions). Otherwise the solution P_{FBM} and the associated dynamic equation are ~~n~~ not known to date. In an external potential, we can use the Langevin equation formulation to deduce the correlation functions.

In an external harmonic potential $V(x) = k x^2/2$:

$$\frac{dx(t)}{dt} = -k x(t) + \xi(t)$$

Formal solution: $x(t) = \int_0^t e^{-k(t-t')} \xi(t') dt'$

Evaluating such integrals with the noise correlator $\langle \xi(t_1)\xi(t_2)\rangle$ we obtain the ensemble-averaged MSD:

$$\langle x^2(t)\rangle = \frac{K_\alpha}{k^\alpha}\,\gamma(\alpha+1, kt) + 2K_\alpha t^\alpha e^{-kt}$$
$$- \frac{k K_\alpha}{\alpha+1} t^{\alpha+1} e^{-2kt}\, M(\alpha+1; \alpha+2; kt)$$

with the incomplete γ-function:

$$\gamma(z,x) = \int_0^x e^{-t} t^{z-1}\, dt$$

and the Kummer function:

$$M(a;b;z) = \frac{\Gamma(b)}{\Gamma(b-a)\Gamma(a)} \int_0^1 e^{zt}\, t^{a-1} (1-t)^{b-a-1} dt$$

(see, e.g., Abramowitz/Stegun, or Mathematica).

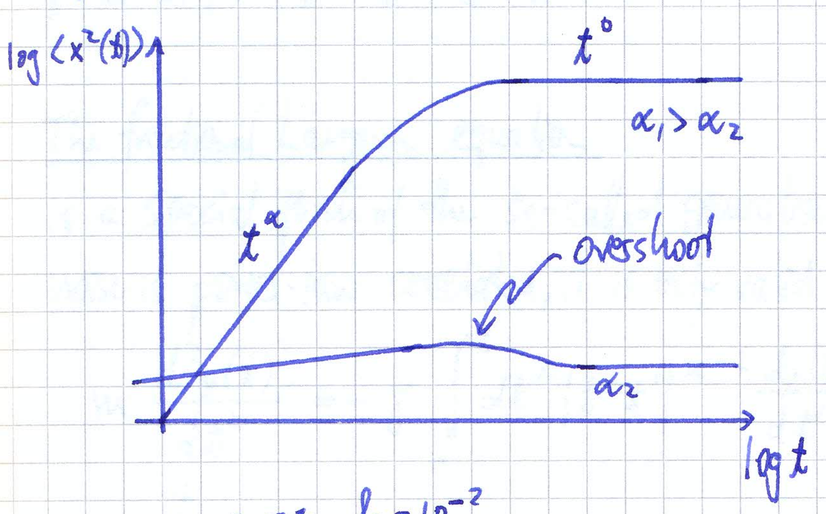
We find the asymptotic behaviour

$$\langle x^2(t)\rangle \sim \begin{cases} 2K_\alpha t^\alpha, & t \ll k^{-1} \\ \langle x^2\rangle_{th} - \frac{2}{k^2}\alpha(\alpha-1)K_\alpha t^{\alpha-2} e^{-kt}, & t \gg k^{-1} \end{cases}$$

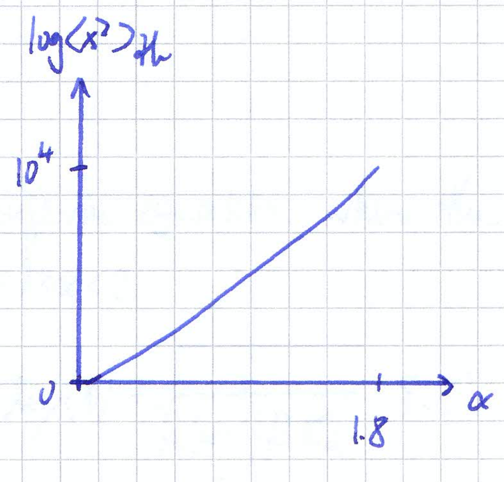
Here the plateau value is

$$\langle x^2\rangle_{th} = \lim_{t\to\infty} \langle x^2(t)\rangle = \frac{K_\alpha}{k^\alpha}\Gamma(\alpha+1),$$ which depends on α!

Physically, the noise $\xi(t)$ in FBM is external, and no temperature is defined.



$x_0 = 0,\ k = 10^{-2}$

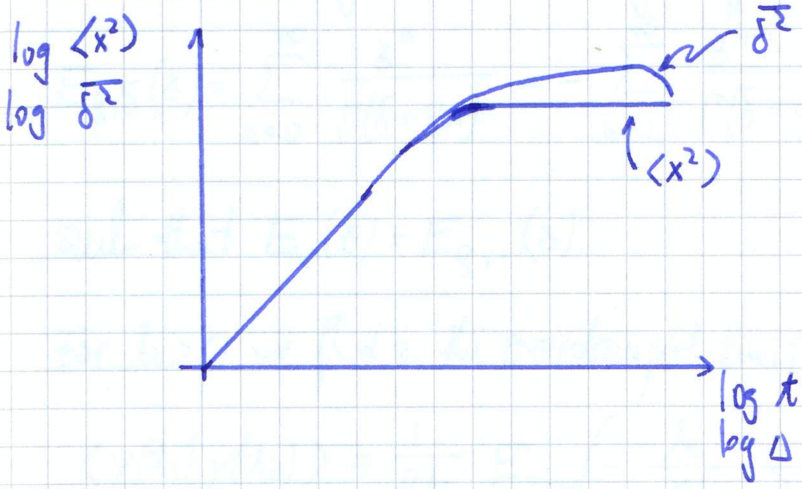


The time-averaged MSD is no longer ergodic @ intermediate times:

$$\overline{\delta^2(\Delta)} \sim 2\langle x^2\rangle_{th} - \underbrace{\frac{K_\alpha \Gamma(1+\alpha)}{k^2} e^{-k\Delta}}_{\text{dominant for } \alpha=1} - \frac{2\alpha(\alpha-1)K_\alpha}{k^2\,\Delta^{2-\alpha}}$$

$$\overset{\alpha<1}{\sim} 2\langle x^2\rangle_{th} - \frac{2\alpha(\alpha-1)K_\alpha}{k^2}\Delta^{\alpha-2}$$

While the EA MSD shows exponential relaxation towards the thermal value, the TA MSD relaxes in power-law form. This form has a diverging characteristic relaxation time when $1<\alpha<2$ ⇝ superdiffusive FBM leads to TA MSD, in which the inherent relaxation time k^{-1} cannot be read off from graphs.



The ergodic behaviour for free FBM is destroyed in the presence of a confining potential, i.e., when a new time scale is introduced.

<u>The fractional Langevin equation</u>

is a special form of the so-called generalised Langevin equation, when the noise is power-law correlated; it is only valid for $1<\alpha<2$

$$\underbrace{m\frac{d^2y(t)}{dt^2}}_{\text{inertia term}} = -\gamma\int_0^t dt'\,|t-t'|^{\alpha-2}\frac{dy(t')}{dt'} - k y(t) + \underbrace{\sqrt{\frac{\gamma}{\alpha(\alpha-1)\beta K_\alpha}}}_{\text{fluctuation - dissipation relation}}\,\xi(t)$$

Noise and kernel of the friction term are coupled by the fluctuation-dissipation relation (Kubo). This way a temperature is introduced in terms of the Boltzmann factor $\beta = (k_B T)^{-1}$.

In absence of a force ($k=0$) the EA MSD becomes

$$\langle x^2(t)\rangle = \frac{2t^2}{\beta m} E_{\alpha,3}\left(-\Gamma(\alpha-1)\frac{\gamma}{m}t^\alpha\right) \sim \begin{cases} t^2 & \text{inertial motion} \\ t^{2-\alpha} \end{cases}$$

turning over from ballistic motion to subdiffusion $\langle x^2(t)\rangle \sim t^\beta$: $\beta = 2-\alpha$.
The process is ergodic!

$$\langle x^2(t)\rangle = \overline{\delta^2(t)}$$

& we used the generalised Mittag-Leffler function

$$E_{\varrho,\delta}(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(\delta+\varrho n)} = -\sum_{n=1}^{\infty} \frac{z^{-n}}{\Gamma(\delta-\varrho n)}$$

such that $E_\alpha(z) = E_{\varrho,1}(z)$.

For $k>0$ we find in the overdamped limit (neglect inertia term):

$$\langle y(t_1)\,y(t_2)\rangle = \frac{1}{\beta k} E_{2-\alpha}\left(-\frac{k}{\gamma\Gamma(\alpha-1)}|t_2-t_1|^{2-\alpha}\right)$$

such that $\langle y^2\rangle_{th} = \frac{1}{\beta k}$ independent of α, as it should be.

The TA MSD becomes

$$\overline{\delta^2(\Delta)} = 2\langle y^2\rangle_{th}\left[1 - E_{2-\alpha}\left(-\frac{k}{\gamma\Gamma(\alpha-1)}\Delta^{2-\alpha}\right)\right]$$

$$\sim 2\langle y^2\rangle_{th}\left(1 - \frac{\gamma}{k\Delta^{2-\alpha}}\right)$$

Again, ergodicity is violated. Further reading: Jeon & RM, PRE (2012)
Deng & Barkai, PRE (2009).