Fractional calculus and anomalous diffusion

Alfredo Fiorentino

Università di Trieste

Horizon seminars, 3-27-2019

Outline

- Introduction: physical phenomena and F. Calculus
- Anomalous diffusion
- Fractional Calculus
- Examples and applications

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What's the link?

Between physical phenomena like:

- **Anomalous diffusion**
- Fluid dynamics
- Nuclear physics

and this kind of differential operator of order $m-1<\alpha<m$:

$$D^{\alpha}f(t)=\frac{1}{\Gamma(m-\alpha)}\int_0^t \frac{f^{(m)}(\tau)}{(t-\tau)^{\alpha+1-m}}d\tau \qquad +\textit{initial conditions terms}. \tag{1}$$

On September 30^{th},1695, Guillaume del'Hopital wrote to Leibniz asking him about a particular notation he had used for the n-th derivative

$$\frac{d^n f}{dt^n}$$

His question was: "What would be the result if $n = 1/2$?"
Leibniz's response followed:**"An apparent paradox, from which one day useful consequence will be drawn."**

Brownian diffusion

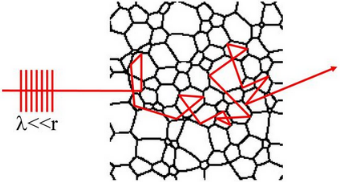


Figure: Left: a drop of ink in the water. Right: multiple scattering of light in the foam

Brownian diffusion

Diffusion is a process resulting from particle random motion, inducing a net flow of the diffusive substance from a region of high concentration to a region of low concentration.
Examples:

- perfume in a room
- neutrons triggering a nuclear reaction
- heat diffusion

Second Fick's law and consequences

$$\frac{\partial W(x,t)}{\partial t} = D \frac{\partial^2 W(x,t)}{\partial x^2} \tag{2}$$

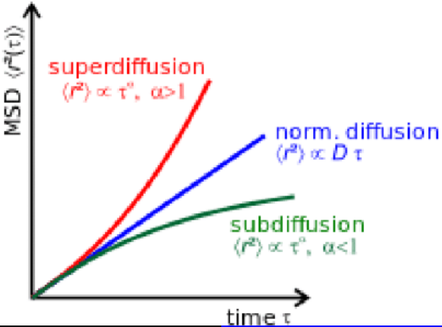
$$\langle x^2 \rangle = 2Dt \tag{3}$$

Anomalous diffusion

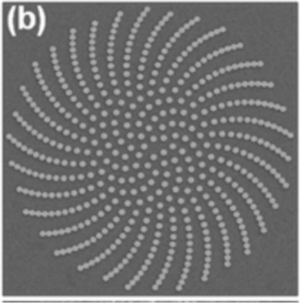
It has been observed in many phenomena, such as

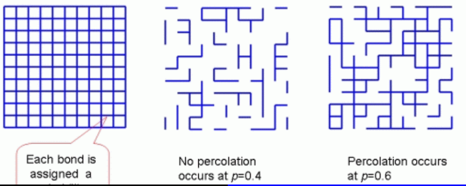
- diffusion through percolation and fractal media
- cellular transport
- electron transport in amorphous media

Anomalous diffusion has a different behaviour of $\langle x^2(t) \rangle$



Anomalous diffusive medium





Microscopic explanation: Continuous Time Random Walk

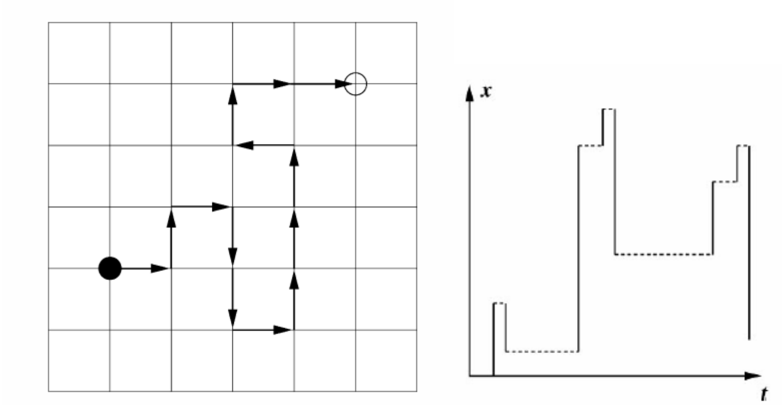


Figure: *Left:* 2D Brownian random walk; *Right:* 1D CTRW. (Sokolov *et al.*, 2012).

Brownian diffusion: a brief recap

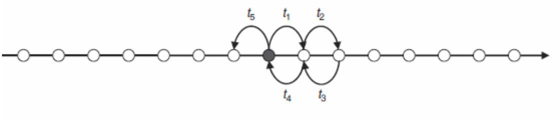


Figure: 1D brownian diffusion

Master equation:

$$W(x_i, t + \Delta t) = \frac{1}{2} W(x_{i+1}, t) + \frac{1}{2} W(x_{i-1}, t) \tag{4}$$

For $\Delta x, \ \Delta t \to 0$

$$\frac{\partial W(x,t)}{\partial t} = \frac{\Delta x^2}{2\Delta t} \frac{\partial^2 W(x,t)}{\partial x^2} \tag{5}$$

Brownian diffusion: a brief recap

By a Laplace-Fourier transform (time and space) with initial condition $W(x, 0) = \delta(x)$:

$$sW(k, s) - 1 = -k^2 DW(k, s) \tag{6}$$

Therefore:

$$W(x, t) = \frac{1}{\sqrt{4\pi Dt}} exp\left(-\frac{x^2}{2Dt}\right) \tag{7}$$

Microscopic explanation: Continuous time random model

Brownian case 1D

$$W_j(t+\Delta t) = \frac{1}{2} W_{j-1}(t) + \frac{1}{2} W_{j+1}(t) \qquad (8)$$

Anomalous case 1D. Fixed length and time step $\rightarrow$ jump probability density function $\psi(x,t) = \lambda(x) w(t)$

$$W(k,s) = \frac{1 - w(s)}{s} \frac{W_0(k)}{1 - \psi(k,s)} \qquad (9)$$

Fractal time sub-diffusion

Jump length fixed. $w(t) \sim A_\alpha(\tau/t)^{\alpha+1}$ for long times. $0 < \alpha \leq 1$.
By inverse Fourier-Laplace transform and Eq. 9,

$$\frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{1}{(t-\tau)^\alpha} \frac{\partial W}{\partial \tau} d\tau = \tag{10}$$

$$D_t^\alpha W = K_\alpha \frac{\partial^2 W}{\partial x^2}.$$

A straightforward consequence:

$$\langle x^2(t) \rangle = \frac{2K_\alpha t^\alpha}{\Gamma(\alpha+1)} \tag{11}$$

Fractional Calculus: origins and remarkable features

Cauchy's integral formula:

$$J^n f(t) = \frac{1}{(n-1)!} \int_0^t (t-\tau)^{n-1} f(\tau) d\tau, \quad f(t) = 0 \tag{12}$$

becomes:

$$J^\alpha f(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t-\tau)^{\alpha-1} f(\tau) d\tau. \tag{13}$$

$$J^\alpha J^\beta = J^\beta J^\alpha = J^{\alpha+\beta} \tag{14}$$

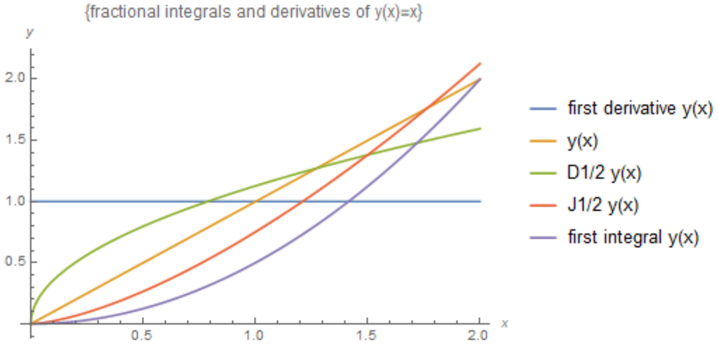
Under Laplace Transform

$$D^\alpha f(t) \div s^\alpha \tilde{f}(s) - \sum_{k=0}^{m-1} f^{(k)}(0^+) s^{\alpha-1-k} \tag{15}$$

Fractional Calculus

The Mittag-Leffler function

$$E_\alpha(z) := \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(\alpha n + 1)}, \qquad \alpha > 0, \qquad z \in \mathbb{C}. \qquad (16)$$



Basset's Problem

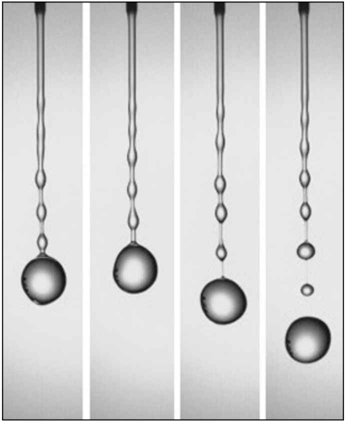


Figure: A sphere falling in a fluid

$$F = F_A - \eta(V - u) + F_B$$

$$F_B \propto D^{\frac{1}{2}}(V - u)$$

Photonic transport

Let us consider a multilayer generated by inflation rules that act on two consituent layers, say A and B, with different refractive indices. In the Fibonacci case: $A \to AB$ and $B \to A$.

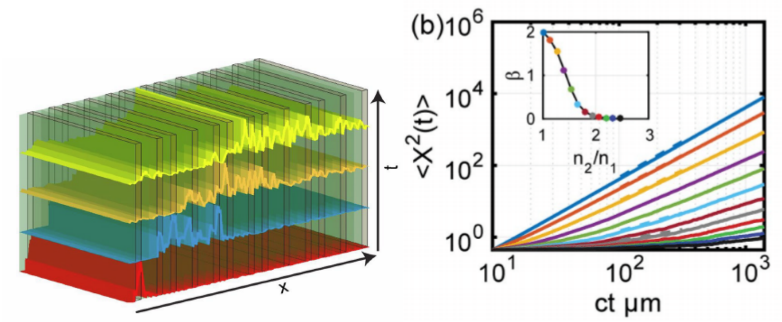


Figure: Photonic transport in aperiodic multilayer (Dal Negro, 2017).

Half-thickness of beta decay

For the article here.

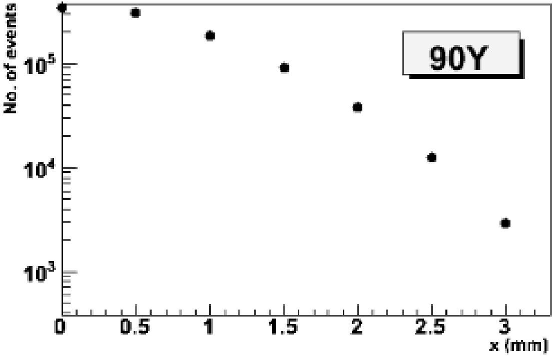


Figure: Geant simulations give result different from $\frac{dI}{dx} = -\mu I$ (Prof.Riggi UniCt.)

Conclusions

- time-space correlations (es. aperiodicity) can lead to unexpected physics
- Processes concerning diffusion can be improved inducing anomalous diffusion
- A new old trick: to describe this kind of interactions we may require a change in the (order of) operators

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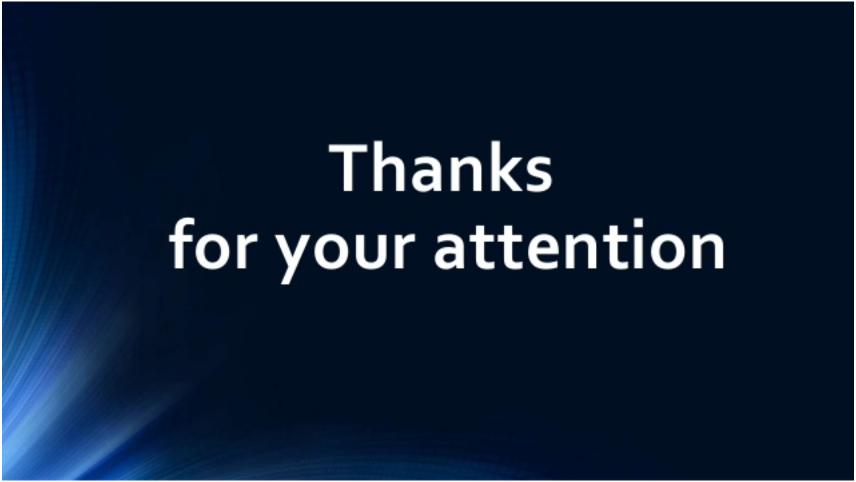
References

- *The Random's walk guide to anomalous diffusion: a fractional dynamics approach* Ralf Metzler, Joseph Klafter
- *Fractional calculus: integral and differential equations of fractional order*. Gorenflo, R., Mainardi, F.
- *Fractional calculus: some basic problems in continuum and statistical mechanics*. Mainardi, F.


Thanks
for your attention

Electron waves: quantum dynamics in aperiodic 1D systems

PHYSICAL REVIEW LETTERS

VOLUME 79 15 SEPTEMBER 1997 NUMBER 11

What Determines the Spreading of a Wave Packet?

R. Ketzmerick,[1,2] K. Kruse,[2,3] S. Kraut,[3] and T. Geisel[1,2]
[1]*Institute for Theoretical Physics, University of California, Santa Barbara, California 93106*
[2]*Max-Planck-Institut für Strömungsforschung und Institut für Nichtlineare Dynamik der Universität Göttingen, Bunsenstraße 10, D-37073 Göttingen, Germany**
[3]*Institut für Theoretische Physik und SFB Nichtlineare Dynamik, Universität Frankfurt, D-60054 Frankfurt/Main, Germany*

$$k - moment\ of\ wavepacket \propto t^{k\alpha}$$

$$\alpha = \frac{D_2^{\mu}}{D_2^{\psi}}$$

→ Fractality of both spectra and eigenmodes determine pulse spreading

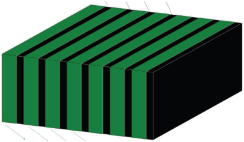
D_2^{μ} – *Correlation Dimension of Local Density of States*

D_2^{ψ} – *Correlation Dimension of Eigenstates of the System*

Connection with fractal kernels and processes

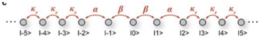
Classical wave transport in correlated disorder

Transfer Matrix based systems

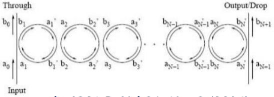


Planar Multi-Layers- Photonic multilayers

Tight Binding model of electrons

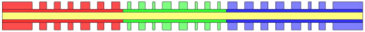


CROW



Poon et.al, *JOSA B*, Vol 21, No. 9 (2004)

Single Mode corrugated Waveguides



$$\begin{pmatrix} a_{j+1}^{-} \\ a_{j+1}^{+} \end{pmatrix} = \begin{bmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{bmatrix} \begin{pmatrix} a_j^{-} \\ a_j^{+} \end{pmatrix}$$