The 18th KIAS-APCTP Winter School on Statistical Physics

Mathematical models for anomalous diffusion

0. Characteristic functions & the CLT
1. α-stable distribution and the generalized CLT
2. Continuous time random walks (CTRWs)
   - 2.1 Subdiffusive CTRWs
   - 2.2 Levy flights
3. Space-time coupled CTRWs
   - 3.1 Levy walks
4. Fractional diffusion equations
5. Aging and time-averaging

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Reference

- An introduction to probability theory and its application Vol. II by W. Feller (Wiley, 3rd ed., 1968)
- First steps in random walks by J. Klafter and I. M. Sokolov (Oxford University Press, 2011)
- R. Metzler and J. Klafter, The random walk's guide to anomalous diffusion: a fractional dynamics approach, Phy Rep 339, 1 (2000).
- Anomalous diffusion and fractional transport equation by R. Metzler & J.-H. Jeon in Fractional dynamics recent advances (World Scientific, 2011)
- Stable non-Gaussian random process by G. Samorodnitsky and M. S. Taqque (Chapman & Hall/CRC, 1994)
- Lecture note (R. Metzler)

0. Characteristic functions & the CLT

Let us think of a (discrete time) random walk in a one-dimensional space.

The position after *n* steps: $$X_n = \underbrace{x_1 + \cdots + x_n}$$

- The steps are independent and identically distributed (i.i.d.) random variables from a probability density function (PDF) *p*(*x*).
- Alternatively, $x_1 \overset{d}{=} x_2 \overset{d}{=} \cdots \overset{d}{=} x_n$
- *p*(*x*) is a function defined in (-∞, ∞) and normalized.

We ask the probability density (that the position of the particle is at [x, x+dx])

$$P_n(x) = \langle \delta(x - X_n) \rangle$$

Characteristic function (Fourier transform of PDFs)

$$\lambda(k) = \int_{-\infty}^{\infty} dx \exp(ikx) p(x) = \langle \exp(ikx) \rangle$$

$$p(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \exp(-ikx) \lambda(k)$$ Inverse transform

Characteristic function is also called a generating function of moments:

$$\lambda(k) = \int_{-\infty}^{\infty} dx p(x) \left[1 + ikx - \frac{k^2 x^2}{2} + \cdots \right]$$

$$= \sum_{n=0}^{\infty} i^n \frac{M_n}{n!} k^n$$

where $M_n = \langle x^n \rangle = \int_{-\infty}^{\infty} dx x^n p(x) dx$ is *n*-th moment.

Thus, *n*-th moment of random variable *x* is obtained via:

$$\langle x^n \rangle = (-i)^n \partial_k^n \lambda(k)|_{k=0}$$

Characteristic function of $P_n(x)$

$$P_n(k) = \int_{-\infty}^{\infty} dx \exp(ikx) P_n(x)$$

Recursive relation for $P_n(x)$

$$P_n(x) = \int dy P_{n-1}(y) p(x-y)$$

$$P_n(x) = \int \Pi_{k=1}^{n-1} dx_k p(x - x_{k-1}) p(x_{k-1} - x_{k-2}) \cdots p(x_2 - x_1) p(x_1)$$

Characteristic function of $P_n(x)$

$$P_n(k) = P_{n-1}(k)\lambda(k) \; = \cdots = [\lambda(k)]^n$$

Simply the *n* times product of the characteristic function of single step.

$P_n(x)$ can be obtained by the inverse Fourier transform of $[\lambda(k)]^n$

$$P_n(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk \exp(-ikx)[\lambda(k)]^n$$

The Central Limit Theorem (CLT)

The distribution of a sum of *n* i.i.d random variables having a *finite* mean μ and a variance σ^2, for large *n*, converges to a Gaussian with the mean $n\mu$ and the variance $n\sigma^2$.

Example 1: Consider a Laplace PDF $p(x) = \frac{a}{2} e^{-|x|a}$

$$\lambda(k) = \frac{a^2}{a^2 + k^2} \approx 1 - \frac{k^2}{a^2} + \cdots$$ for small *k* (i.e., large *x*)

$$P_n(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \left[1 - \frac{k^2}{a^2} + \cdots \right]^n \exp(-ikx)$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \underbrace{\exp\left[n \ln\left(1 - \frac{k^2}{a^2} + \cdots \right) \right]}_{\approx e^{-\frac{nk^2}{a^2}}} \exp(-ikx)$$

for small *k* & large *n*

$$\simeq \frac{a}{\sqrt{4\pi n}} e^{-\frac{a^2 x^2}{4n}}$$ for small *k* & large *n*

$$\frac{1}{\sqrt{2\pi n \sigma^2}} e^{-\frac{x^2}{2n\sigma^2}}$$ NOTE: the variance of *p*(*x*) $\sigma^2 = 2/a^2$

Example 2: Consider a Gaussian PDF $p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{x^2}{2\sigma^2}}$

$$\lambda(k) = e^{-\frac{k^2\sigma^2}{2}} \longrightarrow P_n(k) = e^{-\frac{k^2\sigma^2}{2}n} \qquad P_n(x) = \frac{1}{\sqrt{2\pi n\sigma^2}} e^{-\frac{x^2}{2n\sigma^2}}$$

From the two examples we can infer the following property:

For a symmetric PDF *p*(*x*) that has a finite second moment, its characteristic function can be expanded in the form of

$$\lambda(k) = 1 - \frac{\sigma^2 k^2}{2} + \cancel{O(k^4)}$$ for small *k*-limit. $M_2 = \sigma^2$

Then, regardless of *p*(*x*), $P_n(x)$ tends to be a Gaussian shape for large-*n* limit:

$$P_n(x) = \frac{1}{\sqrt{2\pi n\sigma^2}} e^{-\frac{x^2}{2n\sigma^2}}$$

More generally, let us consider random variable *x* that has the mean μ and the variance σ^2.

Define a new variable $s = (x - \mu)/\sigma \longrightarrow \langle s \rangle = 0 \ \& \ \langle s^2 \rangle = 1$

A rescaled sum $Z_n = (s_1 + \cdots + s_n)/n^{1/2} \equiv z_1 + \cdots + z_n$

The rescaled variable *z*: $\lambda_z(k) = 1 - \frac{k^2}{2n} + \cdots \quad [\lambda_z(k)]^n = \left(1 - \frac{k^2}{2n} + \cdots\right)^n \underset{n \to \infty}{=} e^{-\frac{k^2}{2}}$

The CLT

$$P_n(z) = \frac{1}{2\pi} e^{-z^2/2} \longrightarrow P_n(x) = \frac{1}{\sqrt{2\pi n \sigma^2}} e^{-\frac{(x - n\mu)^2}{2n\sigma^2}}$$

Single random variable		Sum of i.i.d. random variables
Gaussian random variable	$\longrightarrow$	Gaussian PDF
non-Gaussian random variable with finite variance	$\longrightarrow$	Gaussian PDF

1. α-stable distribution and the generalized CLT

- Prologue: Consider a Cauchy distribution

$$p(x) = \frac{b}{\pi(b^2 + x^2)}$$

It is normalizable, but its second moment does not exist. $\langle x^2 \rangle = \infty$

$$\lambda(k) = \int_{-\infty}^{\infty} dx e^{ikx} \frac{b}{\pi(b^2 + x^2)} = e^{-b|k|}$$

no differentiable at *k*=0

(Moments do not exist!).

Sum of *n* i.i.d. Cauchy random variables

$$[\lambda(k)]^n = e^{-nb|k|} \longrightarrow P_n(x) = \frac{nb}{\pi(n^2 b^2 + x^2)}$$

⇨ Sum of Cauchy random variables is also Cauchy!

- Definition of stable random variable

The random variable x is stable if there exists real numbers b_n>0 and a_n satisfying the following relation.

$$X_n = \sum_{j=1}^{n} x_j \overset{d}{=} a_n + b_n x$$

x_i is i.i.d. x is strictly stable if a_n = 0.

Theorem (Feller 1971 VI.1.1)

$$b_n = n^{1/\alpha} \text{ with } 0 < \alpha \leq 2$$

Index of stability (or characteristic exponent)

(Recall that α=2 for Gaussian random variables)

Example: Cauchy distribution

$$p(x) = \frac{\sigma}{\pi(\sigma^2 + x^2)} \qquad \lambda(k) \equiv p(k) = e^{-\sigma|k|}$$

L.H.S. $\langle e^{ikX_n} \rangle = \langle e^{ikx} \rangle^n = e^{-n\sigma|k|}$

R.H.S. $\langle e^{ik(a_n + b_n x)} \rangle = e^{ika_n} \langle e^{ikb_n x} \rangle = e^{ika_n - \sigma b_n |k|}$

⇨ $a_n = 0 \ \& \ b_n = n^{1/1}$ strictly stable and the stability index α=1

- Alternative definition of strictly stable variable

x is strictly stable if for any positive numbers *a* and *b* there is a positive number *c* satisfying the relation

$$ax_1 + bx_2 \stackrel{d}{=} cx$$

Theorem: the scaling factor c is given by $c^\alpha = a^\alpha + b^\alpha$ with $0 < \alpha \leq 2$

- Strictly stable distribution (characteristic function) $L_\alpha(k)$

$$\langle e^{ikax_1} \rangle \langle e^{ikbx_2} \rangle = \langle e^{ikcx} \rangle$$

$$\Rightarrow \ L_\alpha(ak) L_\alpha(bk) = L_\alpha(ck)$$

The strictly stable distribution is inferred to be a form of

$$L_\alpha(k) = e^{-\sigma^\alpha |k|^\alpha}$$

scale parameter (positive)

Normalization of the PDF: $L_\alpha(k \to 0) = 1 \;\Rightarrow\; \alpha > 0$

The range of α: the second moment $M_2 = -\partial_k^2 L_\alpha(k)|_{k=0} = 0 \;\; \text{if } \alpha > 2$

⇨ $0 < \alpha \leq 2$ (α=2: the Gaussian limit)

⇨ $\alpha > 2$ (The distribution is no longer stable & the CLT is applied)

Levy α-stable distribution

- More generally, the stable distribution is given by its characteristic function of the following form:

$$L_{\alpha,\beta,\mu,\sigma}(k) = \exp\left[-\sigma^{\alpha}|k|^{\alpha}(1 - i\beta\mathrm{sign}(k)\omega(|k|,\alpha)) + i\mu k\right]$$

where

$$\omega(|k|,\alpha) = \begin{cases} \tan(\pi\alpha/2) & \text{if } \alpha \neq 1 \ (0 < \alpha < 2) \\ -(2/\pi)\ln|k| & \text{if } \alpha = 1 \end{cases}$$

Four parameters
(1) Levy index: $0 < \alpha \leq 2$, (2) Skewness parameter: $-1 \leq \beta \leq 1$, (3) Scale parameter: $\sigma > 0$,
(4) Shift parameter: μ is real.

Easy check: (the above $L(k)$ satisfies the definition of stable distribution)

$$[L_{\alpha,\beta,\mu,\sigma}(k)]^n = e^{ika_n}\langle e^{ikn^{1/\alpha}x}\rangle$$

$\alpha \neq 1$

$$[L(k)]^n = \exp\left[-n\sigma^\alpha |k|^\alpha (1 - i\beta \mathrm{sign}(k)\omega(|k|, \alpha) + in\mu k\right]$$

$$= e^{ika_n} \exp\left[-n\sigma^\alpha |k|^\alpha (1 - i\beta \mathrm{sign}(k) \tan(\pi/2) + i\mu k n^{1/\alpha}\right]$$

$$a_n = \mu n - \mu n^{1/\alpha} \qquad\qquad b_n = n^{1/\alpha}$$

$\alpha = 1$

$$[L(k)]^n = \exp\left[-n\sigma |k| (1 + (2i/\pi)\beta \mathrm{sign}(k) \ln |k| + in\mu k\right]$$

$$= e^{ika_n} \exp\left[-n\sigma |k| (1 + (2i/\pi)\beta \mathrm{sign}(k) \ln(n|k|) + i\mu k n\right]$$

$$a_n = \frac{2}{\pi}\sigma\beta n \ln n \qquad\qquad b_n = n^{1/1}$$

- There are only a few cases that the closed form of α-stable densities is obtained.

$\alpha = 2$ (Gaussian distribution)

$$L_{2,0,\mu,\sigma}(k) = e^{-\sigma^2 k^2 + i\mu k}$$

↑

(actually, no dependency on β)

$$L_{2,0,\mu,\sigma}(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk e^{-ikx} e^{-\sigma^2 k^2 + i\mu k} = \frac{1}{4\pi\sigma^2} e^{-\frac{(\mu-x)^2}{4\sigma^2}} = N(\mu, 2\sigma^2)$$

$\alpha = 1$ & $\beta = 0$ (Cauchy distribution)

$$L_{1,0,\mu,\sigma}(k) = e^{-\sigma|k| + i\mu k}$$

$$L_{1,0,\mu,\sigma}(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk e^{-ikx} e^{-\sigma|k| + i\mu k} = \frac{1}{2\pi}\left[\frac{1}{\sigma + i(x-\mu)} + \frac{1}{\sigma - i(x-\mu)}\right]$$

$$= \frac{\sigma}{\pi[(x-\mu)^2 + \sigma^2]}$$

We do not consider the scale and shift parameters because of the property

Stable variable *x* $L_{\alpha,\beta,\mu,\sigma}(x)$ $\Leftrightarrow$ normalized variable $L_{\alpha,\beta,0,1}(\frac{x-\mu}{\sigma})$

$x = \sigma y + \mu$

From now on, we use the notation $L_{\alpha,\beta}(x) = L_{\alpha,\beta,0,1}(x)$

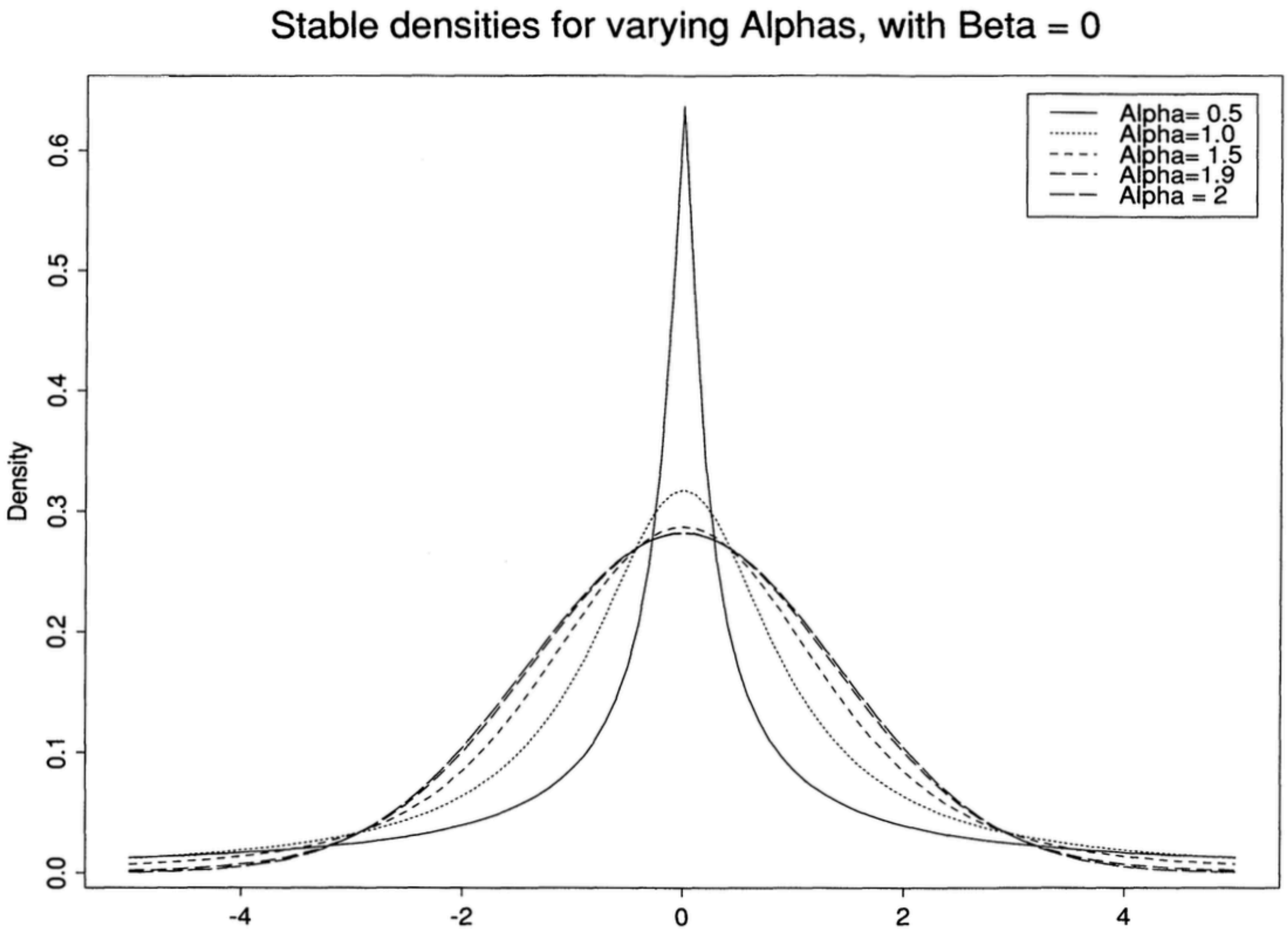
Symmetric α-stable distribution (β=0)

- Characteristic function

$$L_{\alpha,0}(k) = L_\alpha(k) = e^{-|k|^\alpha}$$

$$\simeq 1 - |k|^\alpha + \cdots \ (k \to 0)$$

NOTE: In the previous section, when the second moment exists, $\lambda(k) = 1 - \frac{\sigma^2 k^2}{2} + O(k^4)$



from Stable non-Gaussian random process (Samorodnitsky)

- Asymptotic form of $L_\alpha(x)$ at large *x*

$$L_\alpha(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk \exp(-ikx - |k|^\alpha) = \frac{1}{\pi}\mathrm{Re}\int_0^\infty dk \exp(-ikx - k^\alpha)$$

$$= \mathrm{Re}\left[-i\int_0^\infty dy e^{-y} \exp\left(-\frac{y^\alpha}{x^\alpha} e^{-\frac{i\pi\alpha}{2}}\right)\right]$$ using a complex integral

$$= -\frac{1}{\pi x}\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\sin\left(\frac{\pi n\alpha}{2}\right)\frac{1}{x^{n\alpha}}\int_0^\infty dy e^{-y} y^{n\alpha}$$

$$= \frac{\sin\left(\frac{\pi\alpha}{2}\right)\Gamma(1+\alpha)}{\pi x^{\alpha+1}} + O(1/x^{2\alpha+1})$$ for *x*>0

For large-*x* limit (*x*→∞)

$$L_\alpha(x) \approx \frac{C_\alpha}{|x|^{1+\alpha}} \qquad 0 < \alpha < 2$$

$$C_\alpha = \frac{1}{\pi}\sin\left(\frac{\pi\alpha}{2}\right)\Gamma(1+\alpha)$$

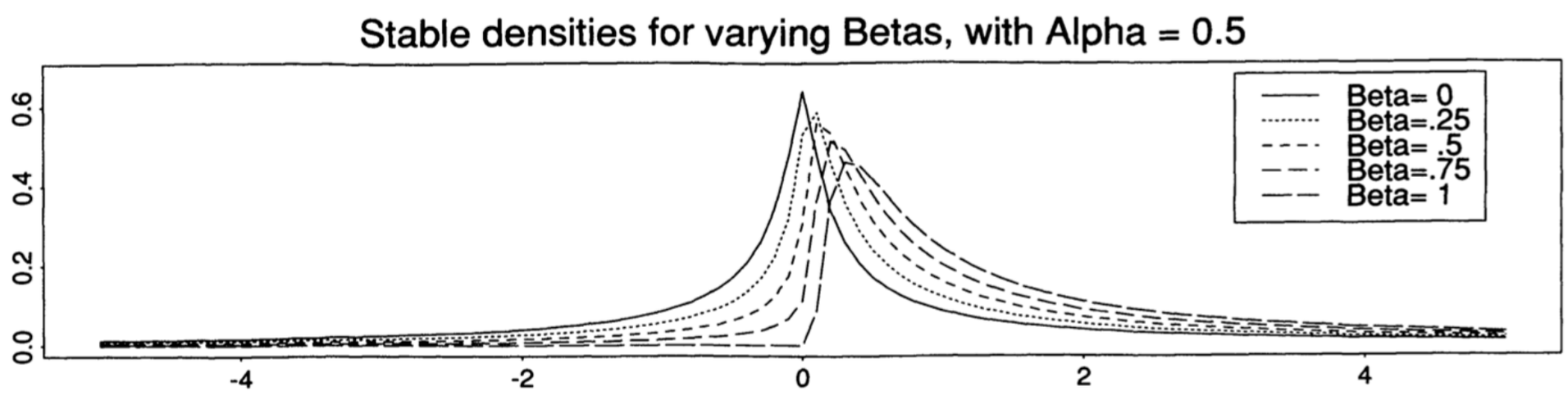
- Moments

$$\langle |x|^q \rangle = \int_{-\infty}^{\infty} |x|^q L_\alpha(x) dx \; = \begin{cases} < \infty, & q < \alpha \\ \infty, & q \geq \alpha \end{cases}$$

The second moment does not exist for α-stable random variables.

One-sided α-stable distribution (β=1 & 0<α<1)

- The PDF is defined on the positive half-line (x>0). (Later we use this PDF for the description of a heavy-tailed waiting time $\psi(t)$).



from Stable non-Gaussian random process (Samorodnitsky)

* When $\beta \neq 0$

$$L^{+}_{\alpha,\beta}(x) = \frac{1}{2\pi}\int_0^\infty dk \exp(-ikx - k^\alpha(1 - i\beta\tan(\pi\alpha/2))$$

$$\approx \frac{C^{+}_{\alpha}}{x^{1+\alpha}} \qquad C^{+}_{\alpha} = \frac{(1+\beta)}{\pi}\Gamma(1+\alpha)\sin(\pi\alpha/2)$$

$$L^{-}_{\alpha,\beta}(x) = \frac{1}{2\pi}\int_{-\infty}^0 dk \exp(-ikx - (-k)^\alpha(1 + i\beta\tan(\pi\alpha/2))$$

$$\approx \frac{C^{-}_{\alpha}}{(-x)^{1+\alpha}} \qquad C^{-}_{\alpha} = \frac{(1-\beta)}{\pi}\Gamma(1+\alpha)\sin(\pi\alpha/2)$$

skewness parameter $\quad \beta = \dfrac{C^{+}_{\alpha} - C^{-}_{\alpha}}{C^{+}_{\alpha} + C^{-}_{\alpha}}$

- Moments

$$\langle |x|^q \rangle = \int_{-\infty}^{\infty} |x|^q L_\alpha(x) dx \; = \begin{cases} < \infty, & q < \alpha \\ \infty, & q \geq \alpha \end{cases}$$

The second moment does not exist for α-stable random variables.

One-sided α-stable distribution (β=1 & 0<α<1)

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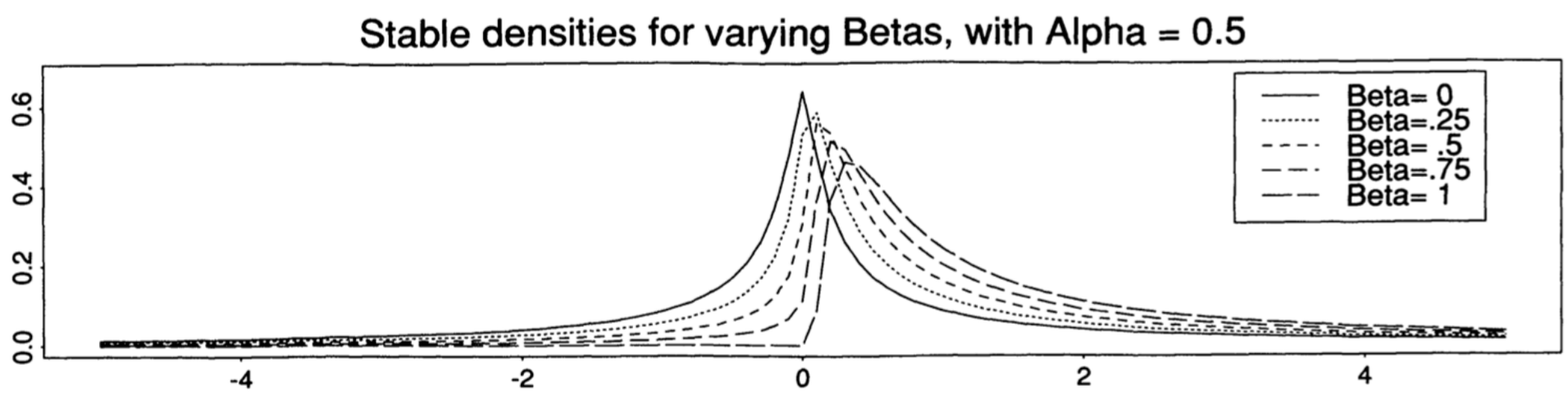


from Stable non-Gaussian random process (Samorodnitsky)

- Moments

$$\langle |x|^q \rangle = \int_{-\infty}^{\infty} |x|^q L_\alpha(x) dx \ = \begin{cases} < \infty, & q < \alpha \\ \infty, & q \geq \alpha \end{cases}$$

The second moment does not exist for α-stable random variables.

One-sided α-stable distribution (β=1 & 0<α<1)

- The PDF is defined on the positive half-line (x>0). (Later we use this PDF for the description of a heavy-tailed waiting time $\psi(t)$).

The one-sided density is defined by the form

$$L_{\alpha,\beta=1}(k) = \exp\left(-|k|^\alpha (1 - i \tan\left(\frac{\pi\alpha}{2}\right) \mathrm{sign}(k)\right)$$

- Laplace transformed form

$$\int_0^\infty e^{-ux} L_{\alpha,1}(x) dx = \exp\left(-\frac{u^\alpha}{\cos(\pi\alpha/2)}\right)$$

- Asymptotic forms of $L_{\alpha,1}(x)$

At large *x* (→∞) $$L_{\alpha,1}(x) \sim \frac{1}{x^{1+\alpha}}$$

At small *x* (→0) $$L_{\alpha,1}(x) \simeq C_1 x^{-1-\alpha/(2(1-\alpha))} \exp\left(-\frac{C_2}{x^{\alpha/(1-\alpha)}}\right)$$
$$\to 0 \ (x \to 0)$$

e.g. Levy-Smirnov density (the first-passage time density of returning random walk)

$$L_{1/2,1}(x) = \frac{1}{\sqrt{2\pi x^3}} \exp\left(-\frac{1}{2x}\right)$$

Generalized CLT

The distribution of a sum of i.i.d random variables whose probability densities have infinite variance and asymptotically decay with a power-law tail

$$p(x) \overset{|x| \to \infty}{\propto} \frac{A}{|x|^{1+\alpha}} \qquad 0 < \alpha < 2$$

tend to the corresponding symmetric Levy stable distribution.

- We here heuristically explain the GCLT. For the above *p*(*x*), its characteristic function behaves

$$\lambda(k) = A \int_{-\infty}^{\infty} e^{ikx} \frac{1}{|x|^{1+\alpha}} dx = 2A \int_{-\infty}^{\infty} \cos(kx) \frac{1}{|x|^{1+\alpha}} dx$$

$$= 1 - 2A \int_{0}^{\infty} (1 - \cos(kx)) \frac{1}{x^{1+\alpha}} dx = 1 - 2A|k|^{\alpha} \int_{0}^{\infty} \frac{1 - \cos(y)}{y^{1+\alpha}} dy$$

$$\approx 1 - \frac{A}{C_\alpha} |k|^{\alpha} \qquad C_\alpha = \frac{1}{\pi} \sin\left(\frac{\pi\alpha}{2}\right) \Gamma(1+\alpha)$$

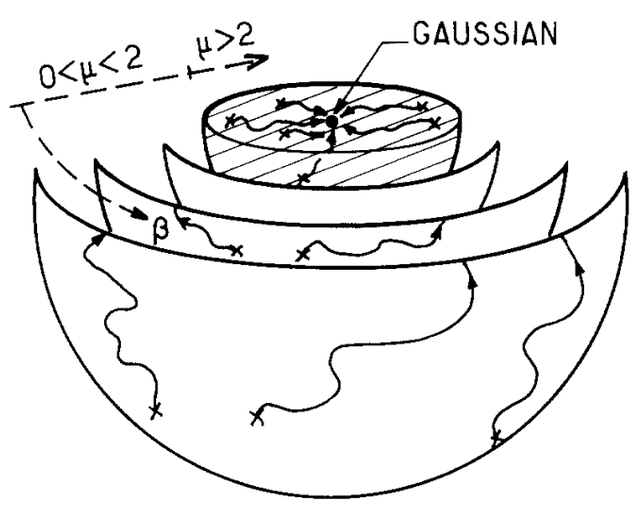
For the sum of *n* i.i.d such random variables,

$$P_n(k) = [\lambda(k)]^n = (1 - \frac{A}{C_\alpha}|k|^\alpha)^n = \exp\left(n \ln(1 - A|k|^\alpha / C_\alpha + \cdots)\right)$$

$$\approx e^{-(A/C_\alpha)n|k|^\alpha} = L_{\alpha,0,0,\sigma}(k) \quad \text{with} \quad \sigma = \left(\frac{An}{C_\alpha}\right)^{1/\alpha}$$

$$\downarrow$$

$$\boxed{P_n(x) \propto L_{\alpha,0,0,\sigma}(x) \simeq \frac{An}{|x|^{1+\alpha}} \qquad |x| \to \infty}$$



$$p(x) \overset{|x| \to \infty}{\propto} \frac{1}{|x|^{1+\mu}}$$

$0 < \mu < 2$ $\quad L_{\alpha=\mu}(x)$ (GCLT)

$\mu \geq 2$ $\quad$ Gaussian (CLT)

(also including any functions decay faster than $1/|x|^3$)

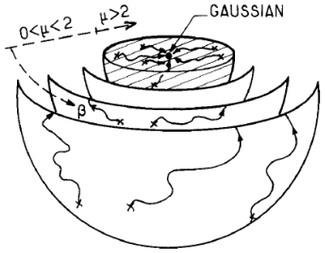
from Bouchaud & Georges, Phys Rep 195, 127 (1990)

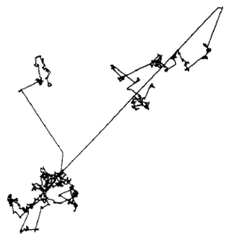
Why anomalous? *Breakdown of the central limit theorem*

$$\langle x^2(t) \rangle \propto t^\alpha \ (\alpha \neq 1)$$

The anomalous diffusion may have mechanism(s) invoking

(1) broad distributions in step lengths & times



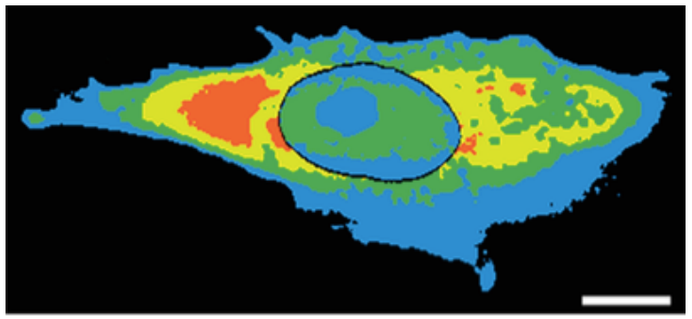


e.g. Continuous-time random walks, Levy flights, Levy walks

(2) long-range correlation

e.g. Fractional Brownian motion, fractional Langevin equation, Percolation

(3) inhomogeneity



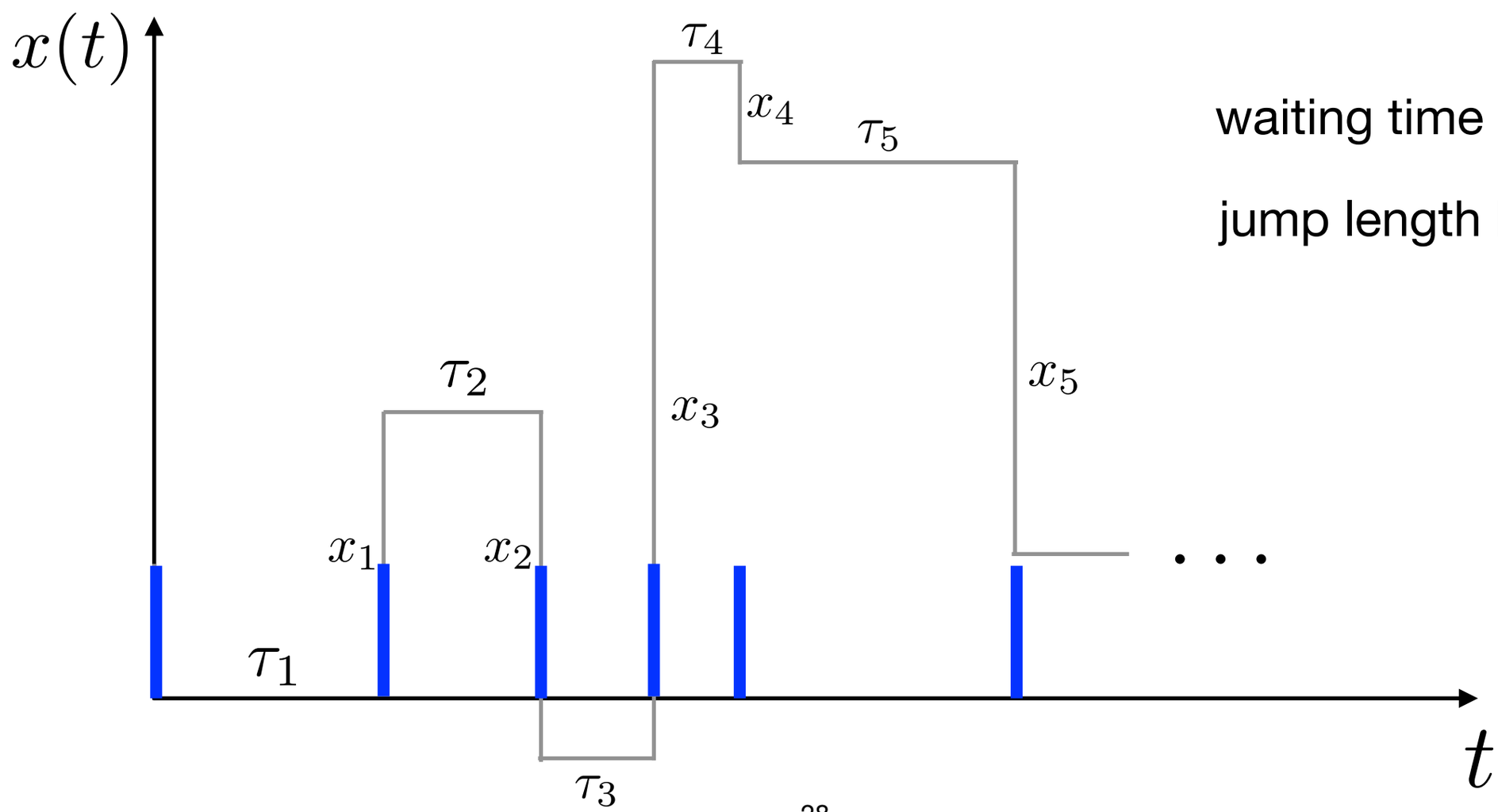
Fluctuating diffusivity model, grey Brownian motion, Sinai, etc

In nature, anomalous diffusion is commonly observed including the biological systems

2. Continuous time random walks

One can generalize random walk processes in the scheme of CTRW.

"A random walker jumps instantaneously from one site to another, following a waiting (sojourn) period on a site with sojourn time *t* drawn by a PDF of waiting times $\psi(t)$. At each jump, the jump length can be random (either finite or infinite variance) with the PDF of jump lengths $\lambda(x)$."



waiting time PDF $\psi(\tau)$

jump length PDF $\lambda(x)$

- Consider the PDF $\eta(x,t)$ that a random walker *just have arrived* at position x at time t. This PDF fulfills the following equation:

$$\eta(x,t) = \int_{-\infty}^{\infty} dx' \int_0^t dt' \eta(x',t')\lambda(x-x')\psi(t-t') + \delta(x)\delta(t)$$

initial condition

In the Fourier-Laplace space:

$$\eta(k,u) = \lambda(k)\psi(u)\eta(k,u) + 1$$

$$\eta(k,u) = \frac{1}{1-\lambda(k)\psi(u)}$$

- Now we consider the PDF $P(x,t)$ that the particle is found at position x at time t, which can be written as:

$$P(x,t) = \int_0^t dt' \eta(x,t')\Psi(t-t')$$

survival probability

The survival probability (of the waiting time PDF)

$$\Psi(t) = \int_t^\infty dt' \psi(t') = 1 - \int_0^t dt' \psi(t')$$

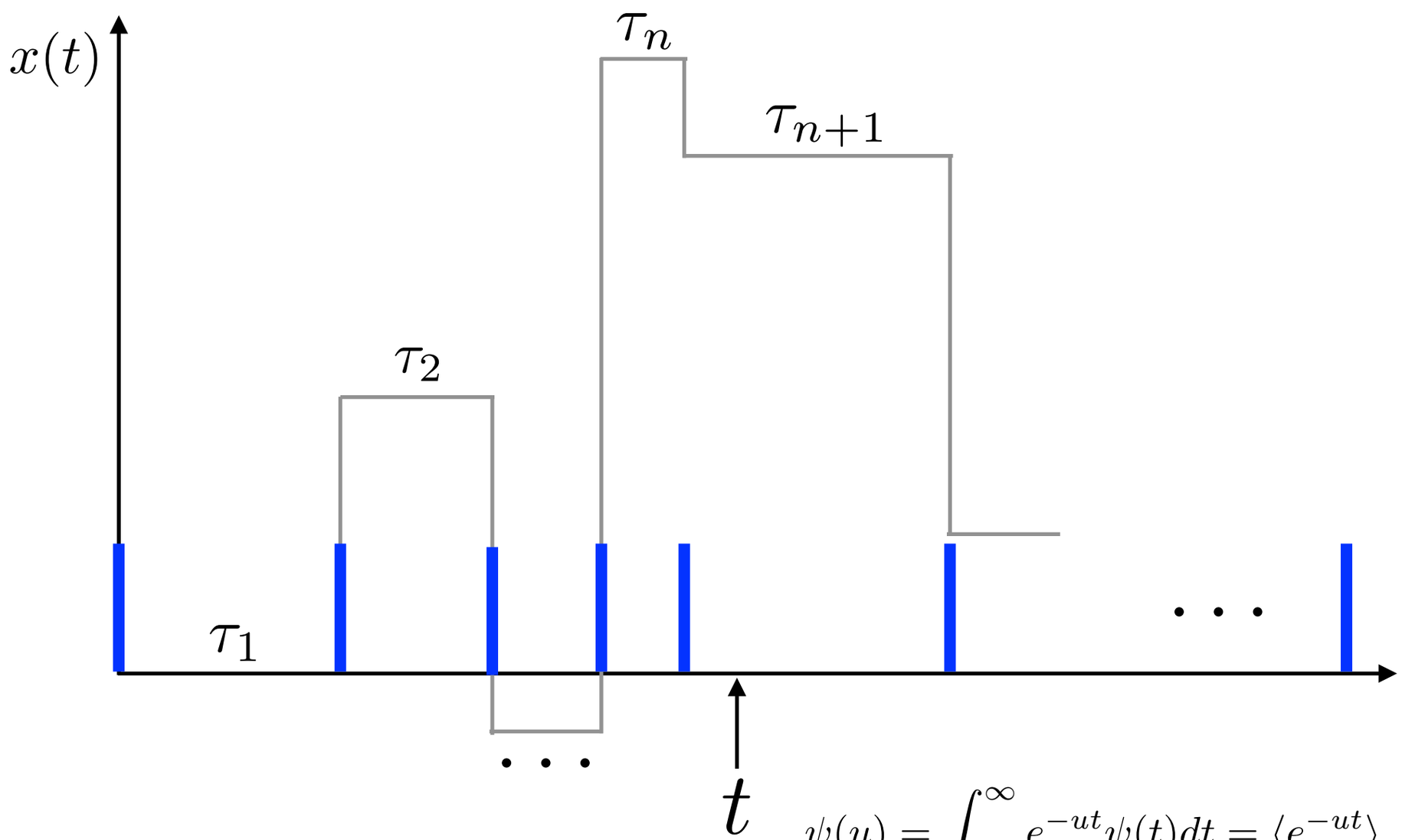
In the Laplace space:

$$\Psi(u) = \frac{1}{u} - \frac{\psi(u)}{u}$$

Combining the two, we obtain the general expression of the PDF *P*(*x*,*t*) in the framework of CTRW. In the Fourier-Laplace space:

$$\boxed{\begin{aligned} P(k,u) &= \eta(k,u)\Psi(u) \\ &= \frac{\overset{P_0(k)}{1}}{1-\lambda(k)\psi(u)} \frac{1-\psi(u)}{u} \end{aligned}}$$

Renewal approach



$$\psi(u) = \int_0^\infty e^{-ut}\psi(t)dt = \langle e^{-ut}\rangle$$

$\psi_n(t)$: prob. density that *n*th jumps occur exactly at $t = \tau_1 + \cdots \tau_n$

$$\psi_n(u) = \langle e^{-u\tau_1}\rangle \cdots \langle e^{-u\tau_n}\rangle = [\psi(u)]^n$$

$Q_n(t)$: probability that there are *n*th jumps until time *t*

$$Q_n(t) = \int_0^t \psi_n(t')\Psi(t-t')dt' \;\Rightarrow\; Q_n(u) = \psi_n(u)\frac{1-\psi(u)}{u} = [\psi(u)]^n \frac{1-\psi(u)}{u}$$

Idea of subordination

$$\boxed{P(x,t) = \sum_{n=0}^{\infty} P_n(x) Q_n(t)}$$

$$P(x,u) = \sum_{n=0}^{\infty} P_n(x)[\psi(u)]^n \frac{1-\psi(u)}{u}$$

$$P(k,u) = \sum_{n=0}^{\infty} P_n(k)[\psi(u)]^n \frac{1-\psi(u)}{u}$$

$$P(k,u) = \frac{1-\psi(u)}{u}\sum_{n=0}^{\infty}[\lambda(k)]^n[\psi(u)]^n$$

$$= \frac{1}{1-\lambda(k)\psi(u)}\frac{1-\psi(u)}{u}$$

- Mean squared displacement

$$\langle x^2(t)\rangle = \sum_{n=0}^{\infty} Q_n(t)\int x^2 P_n(x)dx$$

$$= \sum_{n=0}^{\infty}\langle \delta x^2\rangle n Q_n(t) \; = \langle \delta x^2\rangle \underbrace{\langle n(t)\rangle}_{\sim\sim\sim\sim\sim\sim\sim}$$

The mean number of jumps until time *t*

2.0 Normal diffusion

- Condition: the mean waiting time exists and the variance of step lengths is finite (the CLT is applied).

- When the mean waiting time exists: $\langle \tau \rangle = \int_0^\infty t\psi(t)dt < \infty$

$$\psi(u) = \int_0^\infty dt\psi(t)[1 - ut + \cdots] = 1 - \langle \tau \rangle u + O(u^2)$$

$$\approx 1 - \langle \tau \rangle u$$ at large times $(t \to \infty \leftrightarrow u \to 0)$

e.g. $\psi(t) = \delta(t - \tau) \to \psi(u) = \exp(-u\tau)$

$$\psi(t) = \exp(-t/\tau)/\tau \to \psi(u) = 1/[1 + u\tau]$$

- When the variance of step lengths is finite: $\langle \delta x^2 \rangle = \int_{-\infty}^\infty x^2 \lambda(x)dx < \infty$

$$\lambda(k) = \int_{-\infty}^\infty dx\lambda(x)[1 + ikx - \frac{k^2}{2}x^2 + \cdots] = 1 - \frac{k^2}{2}\langle \delta x^2 \rangle + O(k^3)$$

$(x \to \infty \leftrightarrow k \to 0)$ $\approx 1 - \frac{k^2}{2}\langle \delta x^2 \rangle$ at large *x*

e.g. $\lambda(x) = \frac{1}{2}[\delta(x-a) + \delta(x+a)] \to \lambda(k) = \cos(ka)$

Also short-ranged PDFs such as Gaussian, exponential…

- At large times and lengths (*u* and *k* are small), we obtain

$$P(k,u) \approx \frac{1}{u + k^2 \frac{\langle \delta x^2 \rangle}{2\langle \tau \rangle}}.$$

D: diffusivity

The inverse Laplace transform: $P(k,t) = \exp(-Dk^2 t)$

- After the inverse Fourier transform, we obtain the Gaussian propagator for an ordinary diffusion equation [CLT]

$$P(x,t) = \frac{1}{\sqrt{2\pi D t}} \exp(-x^2/[2Dt])$$

2.1 Subdiffusive CTRWs

- Condition: the mean waiting time diverges while the variance of step lengths is finite.

- In terms of the Levy α-stable distribution, we now consider waiting time PDFs belonging to the one-sided Levy distribution

$$\psi(t) = L_{\alpha,1}(t) \text{ and } \psi(u) = \exp(-\sigma^\alpha u^\alpha) \quad 0 < \alpha < 1$$

- More generally, we think of (asymptotically) power-law PDFs of the form

$$\psi(t) \sim \frac{\alpha}{\Gamma(1-\alpha)} \frac{\tau^\alpha}{t^{1+\alpha}} \qquad 0 < \alpha < 1$$

In this range of α, $\langle \tau \rangle = \int_0^\infty t\psi(t)dt \to \infty$

To find the PDF in the Laplace domain, we consider $\Psi(t) = \frac{\tau^\alpha}{\Gamma(1-\alpha)} t^{-\alpha}$

- The Laplace transform of $\boldsymbol{\Psi}$ is doable by making use of the Tauberian theorem.

Tauberian theorem

For a function *F*(*t*) which behaves as $F(t) \simeq t^{\rho-1}L(t),\ 0 < \rho < \infty$
with *L*(*t*) being a slowly varying function of *t*, for *t*→∞. Its Laplace transformed counterpart is given by $F(u) \simeq \Gamma(\rho)u^{-\rho}L(1/u)$

Using the Tauberian theorem, we have

$$\Psi(u) = \tau^{\alpha}u^{-1+\alpha} = \frac{1-\psi(u)}{u}$$

$$\psi(u) = 1 - \tau^{\alpha}u^{\alpha}$$ for small *u*.

- Plugging this result into *P*(*k*,*u*), we find

$$P(k,u) = \frac{1}{u + \frac{k^2\langle\delta x^2\rangle}{2\tau^{\alpha}}u^{1-\alpha}} = \frac{1}{u + k^2 D_{\alpha}u^{1-\alpha}}$$

Generalized diffusivity ~ [length]^2/[time]^$\boldsymbol{\alpha}$

- The inverse-Laplace transform of *P* is obtained using the so-called Mittag-Leffler function.

$$P(k,t) = E_\alpha[-D_\alpha k^2 t^\alpha] = \sum_{n=0}^{\infty} \frac{(-D_\alpha k^2 t^\alpha)^n}{\Gamma(1+n\alpha)}$$

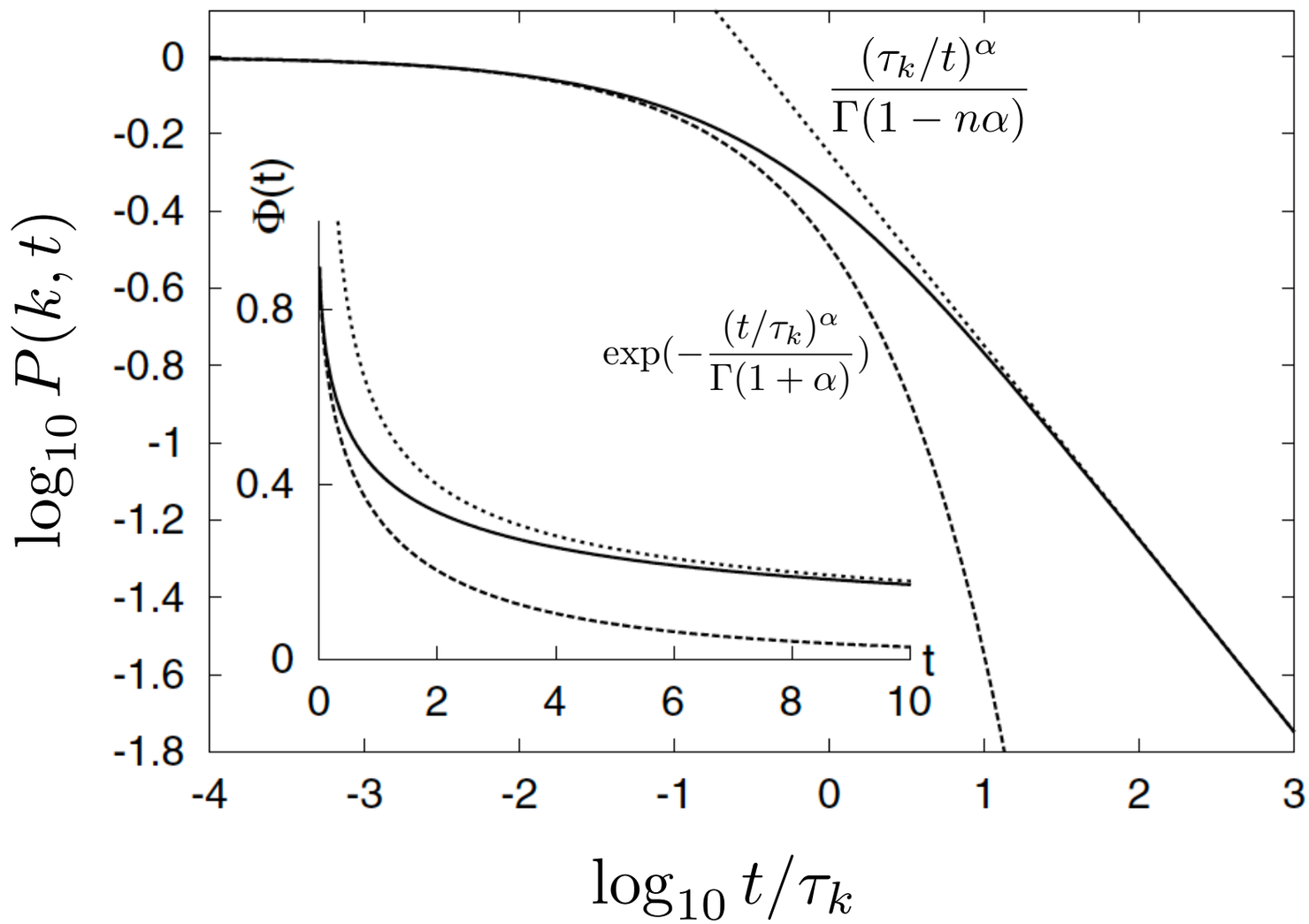
Mittag-Leffler function $E_\alpha(x) = \sum_{n=0}^{\infty} \frac{x^n}{\Gamma(1+n\alpha)}$ $\quad E_\alpha(-(t/\tau)^\alpha) = \mathcal{L}^{-1}\left\{\frac{1}{u+\tau^{-\alpha}u^{1-\alpha}}\right\}$

(a generalized exponential function. $\boldsymbol{\alpha}$=1: $E_1(x) = e^x$)

<u>Limiting behaviors</u>

With the definition of *k*-mode char. time τ_k

$$\begin{cases} P(k,t) \approx 1 - \frac{(t/\tau_k)^\alpha}{\Gamma(1+\alpha)} \approx \exp(-\frac{(t/\tau_k)^\alpha}{\Gamma(1+\alpha)}) & \text{stretched exponential} \quad (t \ll \tau_k) \\ P(k,t) = \sum_{n=1}^{\infty} \frac{(-1)^{n-1}(\tau_k/t)^{\alpha n}}{\Gamma(1-n\alpha)} \approx \frac{(\tau_k/t)^\alpha}{\Gamma(1-n\alpha)} & \text{power-law} \quad (t \gg \tau_k) \end{cases}$$



- The scaling structure of *P*(*x*,*t*)

$$P(k,t) = E_\alpha[-D_\alpha k^2 t^\alpha] = \tilde{\mathcal{P}}_\alpha(kt^{\alpha/2}) \quad \Rightarrow \quad P(x,t) = \frac{1}{t^{\alpha/2}}\mathcal{P}_\alpha(\frac{x}{t^{\alpha/2}})$$

scaling function

The inverse Fourier transform of *P*(*k*,*t*) requires the expression using the so-called Fox functions. Via the series expansion we find

$$P(x,t) = \frac{1}{\sqrt{4D_\alpha t^\alpha}} \sum_{n=0}^{\infty} \frac{(-1)^n}{n!\Gamma(1-\alpha[n+1]/2)} \left(\frac{x^2}{D_\alpha t^\alpha}\right)^{n/2}$$

- Ensemble-averaged MSD

$$\langle x^2(u)\rangle = -\partial_k^2 P(k,u)|_{k=0} = 2D_\alpha u^{-1-\alpha}$$

Using the Tauberian theorem

Subdiffusion $$\langle x^2(t)\rangle = \frac{2D_\alpha}{\Gamma(1+\alpha)} t^\alpha$$

anomalous exponent

$$0 < \alpha < 1$$

NOTE: Anomalous exponent is the index of α in the waiting time PDF. $\psi(t) \sim \frac{\alpha}{\Gamma(1-\alpha)} \frac{\tau^\alpha}{t^{1+\alpha}}$

- The mean number of jumps

$$\langle n(t)\rangle = \sum_{n=0}^{\infty} nQ_n(t)$$

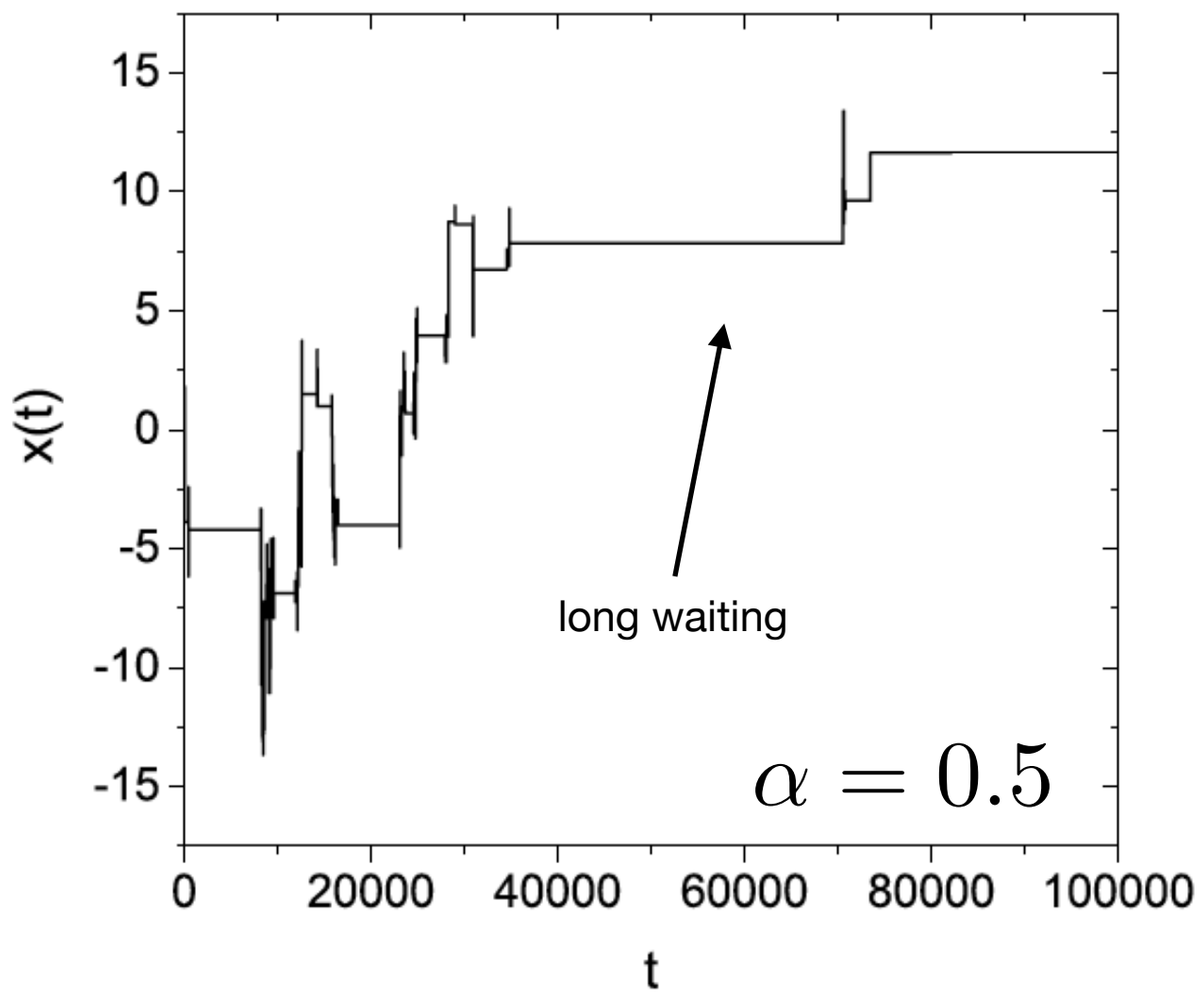
$$\langle n(u)\rangle = \sum_{n=0}^{\infty} nQ_n(u) = \frac{1-\psi(u)}{u}\sum_{n=0}^{\infty} n[\psi(u)]^n$$

$$= \frac{\psi(u)}{u[1-\psi(u)]} \xrightarrow[\psi(u)=1-\tau^\alpha u^\alpha]{} \langle n(u)\rangle \approx \frac{1}{u(\tau u)^\alpha}$$

⇨ $\langle n(t)\rangle = \frac{1}{\Gamma(1+\alpha)}\frac{t^\alpha}{\tau^\alpha}$ # of average jumps sublinearly increases with time *t*

⇨ $\langle x^2(t)\rangle = \langle \delta x^2\rangle\langle n(t)\rangle = \frac{\langle \delta x^2\rangle}{\Gamma(1+\alpha)}\frac{t^\alpha}{\tau^\alpha} = \frac{2D_\alpha}{\Gamma(1+\alpha)}t^\alpha$

- Typical pattern of a trajectory looks like this:



- The origin of the subdiffusion

As time goes on, there is a chance that a rare event occurs such that the magnitude of a waiting time is comparable to the total observation time!

Because there is no characteristic waiting time ($<\tau>=\infty$), the occurrence of such rare events is scale-free. No matter how long your observation time is, you have a chance to meet a waiting event comparable to your observation time.

- Weak ergodicity breaking (WEB)

Think about a subdiffusive CTRW process in a bounded domain. Because of the mean-free waiting times, on average it will take infinite time to explore the whole space. This means that “ensemble-averaging” ≠ “time-averaging” → *Ergodicity* is not fulfilled for this model. It is referred to as *“weak” ergodicity breaking* in the sense that ergodicity breaking is weak (requiring infinite time to explore the phase space).

⇨ The subdiffusive CTRW process is a non-equilibrium dynamic model (e.g. traps).

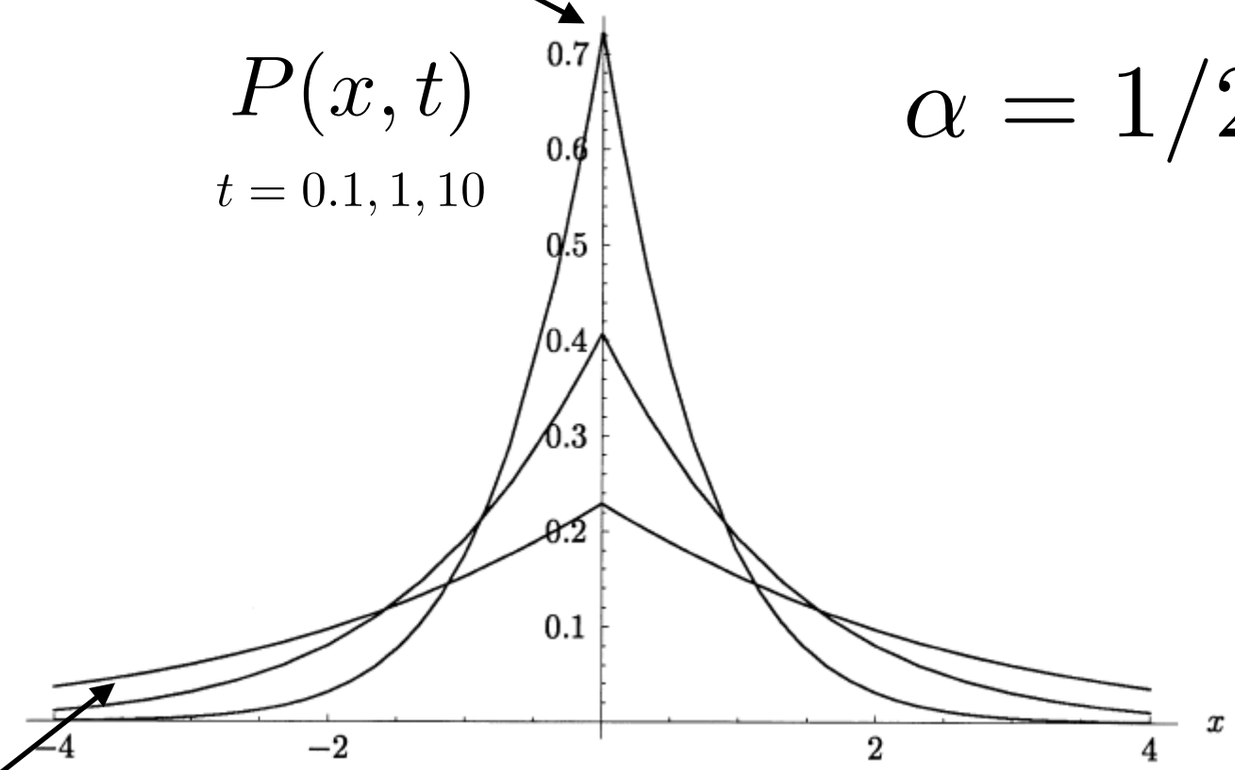
Comment: One can construct a CTRW process with $\alpha>1$. Then there is no extreme behavior w.r.t. time. As shown, this process becomes an ordinary random walk.

- Typical profile of $P(x,t)$

A cusp at x=0: distinct from a Gaussian PDF of ordinary random walks. The cusp is due to the diverging long waiting events.

$$P(x,t)$$

$$t = 0.1, 1, 10$$



$$\alpha = 1/2$$

from Metzler & Klafter, Phys Rep 339, 1 (2000)

For $|x| \gg \sqrt{D_\alpha t^\alpha}$, the profile has a stretched exponential form.

$$P(x,t) \sim \frac{1}{t^{\alpha/2}} \exp\left[-\frac{1}{2}\left(\frac{x}{t^{\alpha/2}}\right)^{2/(2-\alpha)}\right]$$

2.2 Levy flights

- Condition: the variance of step lengths diverges while the mean waiting time exists.

- Consider the case that the step length PDF is the symmetric α-stable density.

$$\lambda(k) = L_{\mu,0}(k) = \exp\left(-\frac{\sigma^\mu}{2}|k|^\mu\right) \approx 1 - \frac{\sigma^\mu}{2}|k|^\mu \quad (k \to 0) \qquad 0 < \mu < 2$$

see lecture note on the symmetric α-stable density

$$\lambda(x) \simeq \frac{\sigma^\mu}{2|x|^{1+\mu}} \quad 0 < \mu < 2 \quad (x \to \infty) \qquad \Rightarrow \qquad \langle \delta x^2 \rangle = \infty$$

- *P*(*x*,*t*)

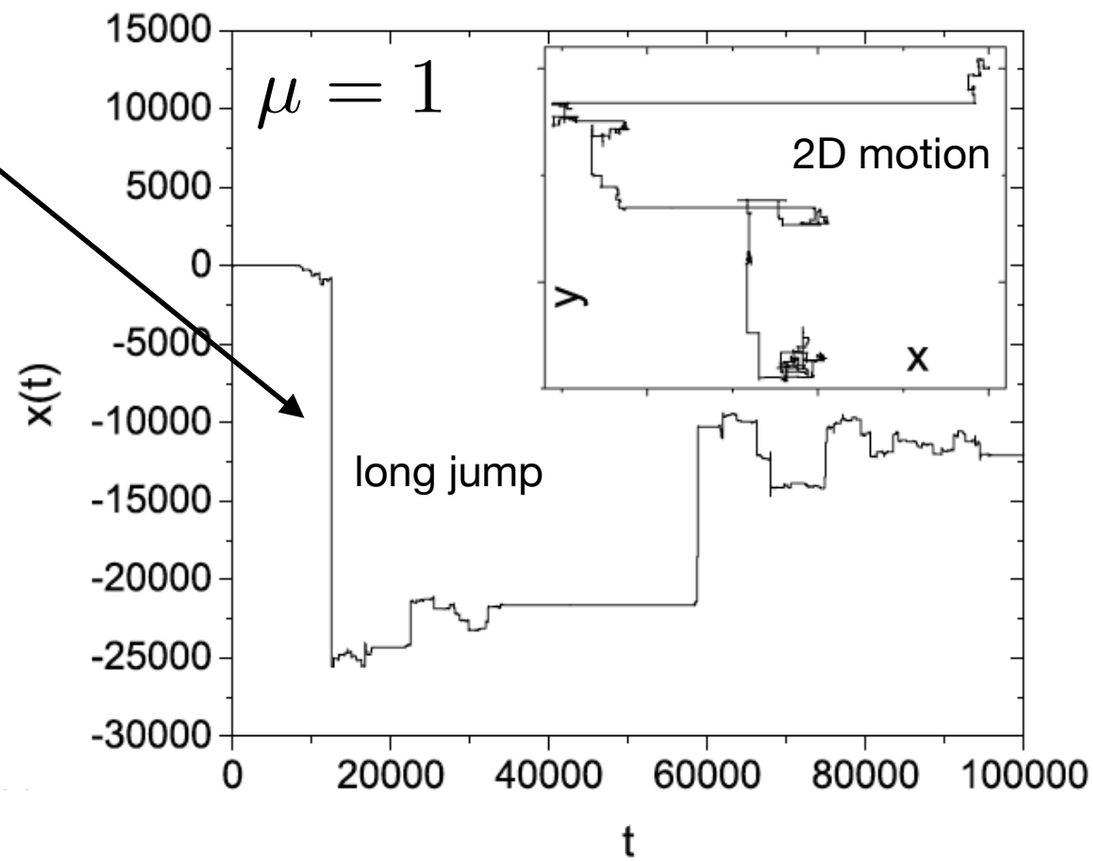
$$P(k,u) = \frac{1}{u + \frac{\sigma^\mu}{2\tau}|k|^\mu} = \frac{1}{u + D^\mu |k|^\mu} \quad \Rightarrow \quad P(k,t) = \exp(-D^\mu |k|^\mu t)$$

Generalized diffusivity
[length]^μ/[time]

$$\psi(u) = 1 - \tau u, \ (\langle \tau \rangle \equiv \tau)$$

$$\Rightarrow \quad P(x,t) \simeq \frac{D^{\mu} t}{|x|^{1+\mu}} \qquad 0 < \mu < 2$$

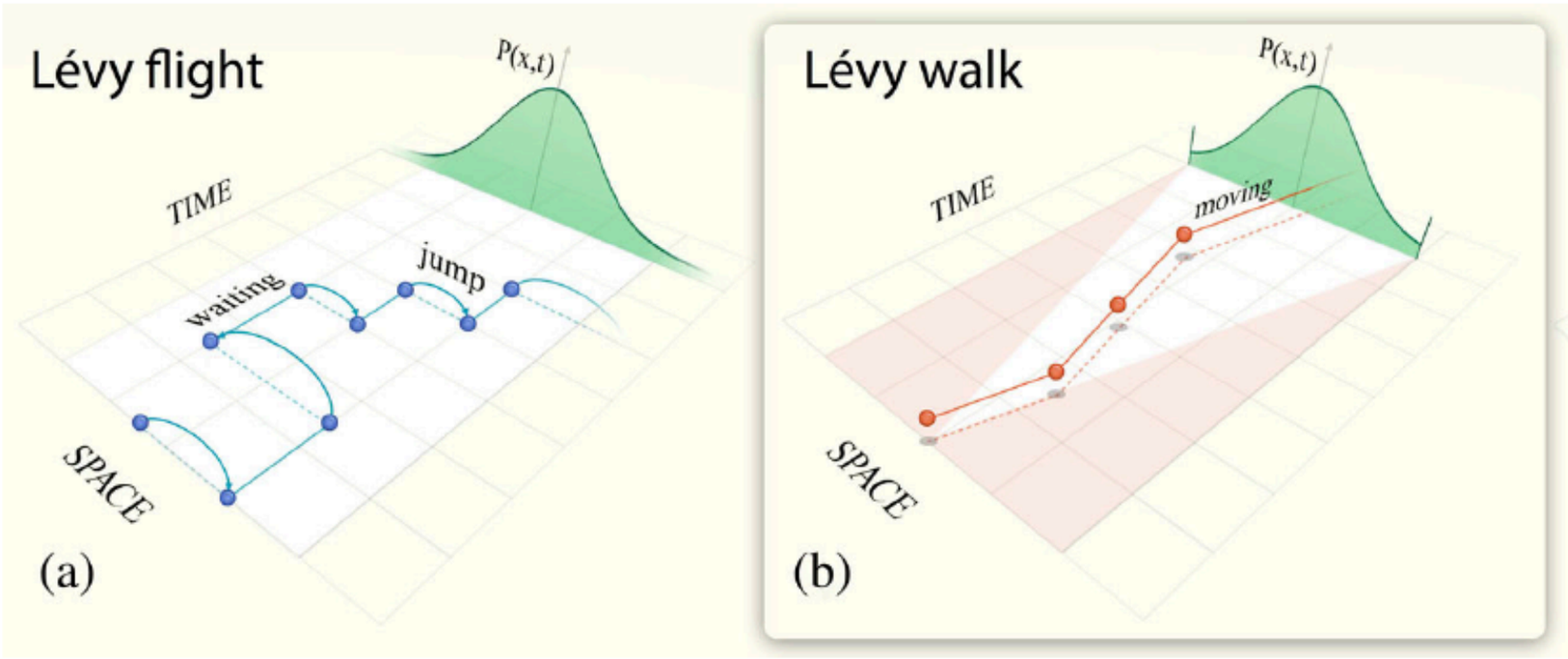
Long jumps sometime occur during the process, which makes $\langle x^2(t) \rangle = \infty$



Such moment-free jumps make this process called Levy *flight*. It is not a walk but a flight. Caution: In the scheme of CTRW, the jump is instantaneous, so such long jumps may be unphysical (faster than the speed of light). This is the reason why Levy *walk* model is introduced.

3. Space-time coupled CTRWs

3.1 Levy walks



from Zaburdaev, Denisov, & Klafter, Phys Mod Phy 87, 483 (2015)

- Now consider a joint probability that the jump and wait events are coupled.

$$\psi(t)\lambda(x) \longrightarrow \psi(x,t) = \psi(t)\phi(x|t)$$

conventional

space-time
coupled PDF

- We repeat the same procedure developed in the conventional CTRW process. The PDF η(x) that a random walker *just have arrived* at position *x* at time *t*.

$$\eta(x,t) = \int_{-\infty}^{\infty} dx' \int_0^t dt' \eta(x',t')\psi(x-x',t-t') + \delta(x)\delta(t)$$

$$\eta(k,u) = \frac{1}{1-\psi(k,u)}$$

- Now we consider the PDF *P*(*x*,*t*) such that the particle is found at position *x* at time *t*, which can be written as:

$$P(x,t) = \int dx' \int_0^t dt' \eta(x',t')\Psi(x-x',t-t')$$

survival time

$$\boxed{P(k,u) = \frac{\Psi(k,u)}{1-\psi(k,u)}}$$

- For the Levy walk, we consider the following the joint probability:

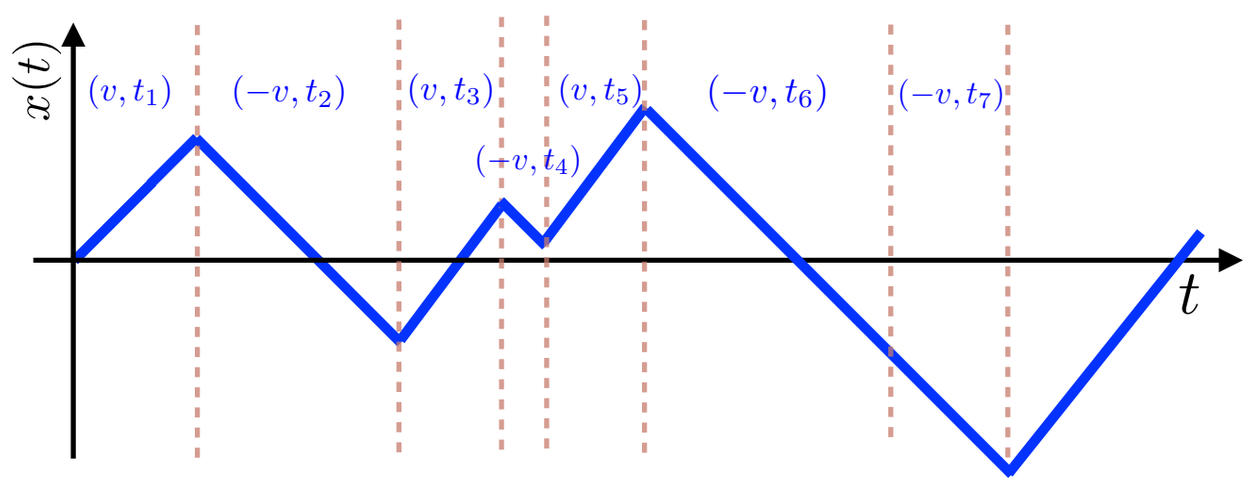
$$\psi(x,t) = \psi(t)\phi(x|t) = \frac{1}{2}\delta(|x| - vt)\psi(t)$$

particle's displacement for given *t* is |*v*|*t*

flight time PDF

$$\boxed{\psi(t) \propto \frac{1}{t^{1+\alpha}} \quad 0 < \alpha < 2 \quad \Rightarrow \quad \lambda(x) \propto \frac{1}{|x|^{1+\alpha}} \quad \text{with a constraint } x = \pm vt}$$

A particle performs a random walk with a constant velocity ±*v* & the waiting times *t* with their PDF $\psi(t)$.



- The survival joint probability

$$\Psi(x,t) = \frac{1}{2}\delta(|x| - vt)\int_t^\infty \psi(t')dt'$$

$$\Psi(k,u) = \frac{1}{2}\int\int e^{-ut+ikx}[\delta(x-vt) + \delta(-x-vt)]\tilde{\Psi}(t)dxdt$$

$$= \frac{1}{2}[\tilde{\Psi}(u+ikv) + \tilde{\Psi}(u-ikv)] = \mathrm{Re}\tilde{\Psi}(u+ikv) \qquad \tilde{\Psi}(u) = \frac{1-\psi(u)}{u}$$

- Levy walks with 1<$\boldsymbol{\alpha}$<2: a superdiffusive Levy walk

$$\langle t \rangle \equiv \tau < \infty \qquad\qquad \langle t^2 \rangle \sim \langle x^2 \rangle = \infty$$

$$\psi(u) = 1 - \tau u - C_1 u^\alpha$$

$$\psi(k,u) = 1 - \tau u - C_1 u^\alpha + \frac{C_1\alpha(\alpha-1)k^2v^2}{2}u^{\alpha-2} + \cdots \approx 1 - \tau u + \frac{C_1\alpha(\alpha-1)k^2v^2}{2}u^{\alpha-2}$$

small-*k* expansion $kv \ll u \leftrightarrow vu^{-1} \ll k^{-1}$

$$\Psi(k,u) = \tau + \frac{1}{2}C_1[(u+ikv)^{\alpha-1} + (u-ikv)^{\alpha-1}] \overset{kv \ll u}{\approx} \tau + C_1 u^{\alpha-1} - \frac{C_1(\alpha-1)(\alpha-2)k^2v^2}{2}u^{\alpha-3}$$

$$P(k,u) \approx u^{-1} - C_2 k^2 u^{\alpha-4}$$

- Ensemble-averaged MSD

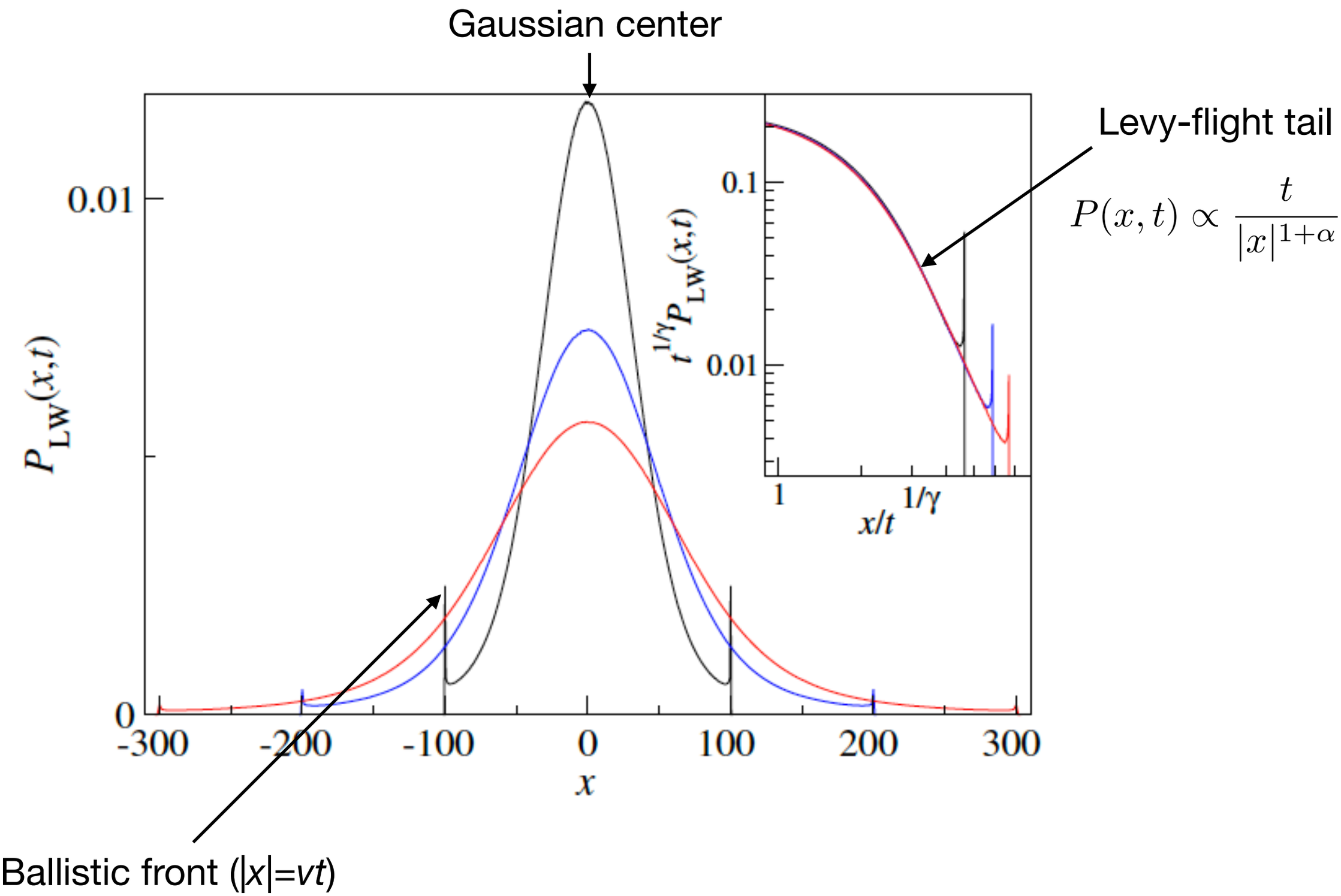
$$\langle x^2(u)\rangle = -\partial_k^2 P(k,u)|_{k=0} = 2C_2 u^{\alpha-4}$$

Using the Tauberian theorem

$$\langle x^2(t)\rangle = \frac{2C_2}{\Gamma(4-\alpha)}t^{3-\alpha} \qquad 1 < \alpha < 2$$

at large *t*

Superdiffusion



$$P_{\text{front}}(x,t) = \frac{1}{2}\Psi(t)\delta(|x| - vt)$$

- Levy walks with 0<α<1: a ballistic Levy walk

$$\langle t \rangle = \infty \qquad \langle t^2 \rangle = \infty$$

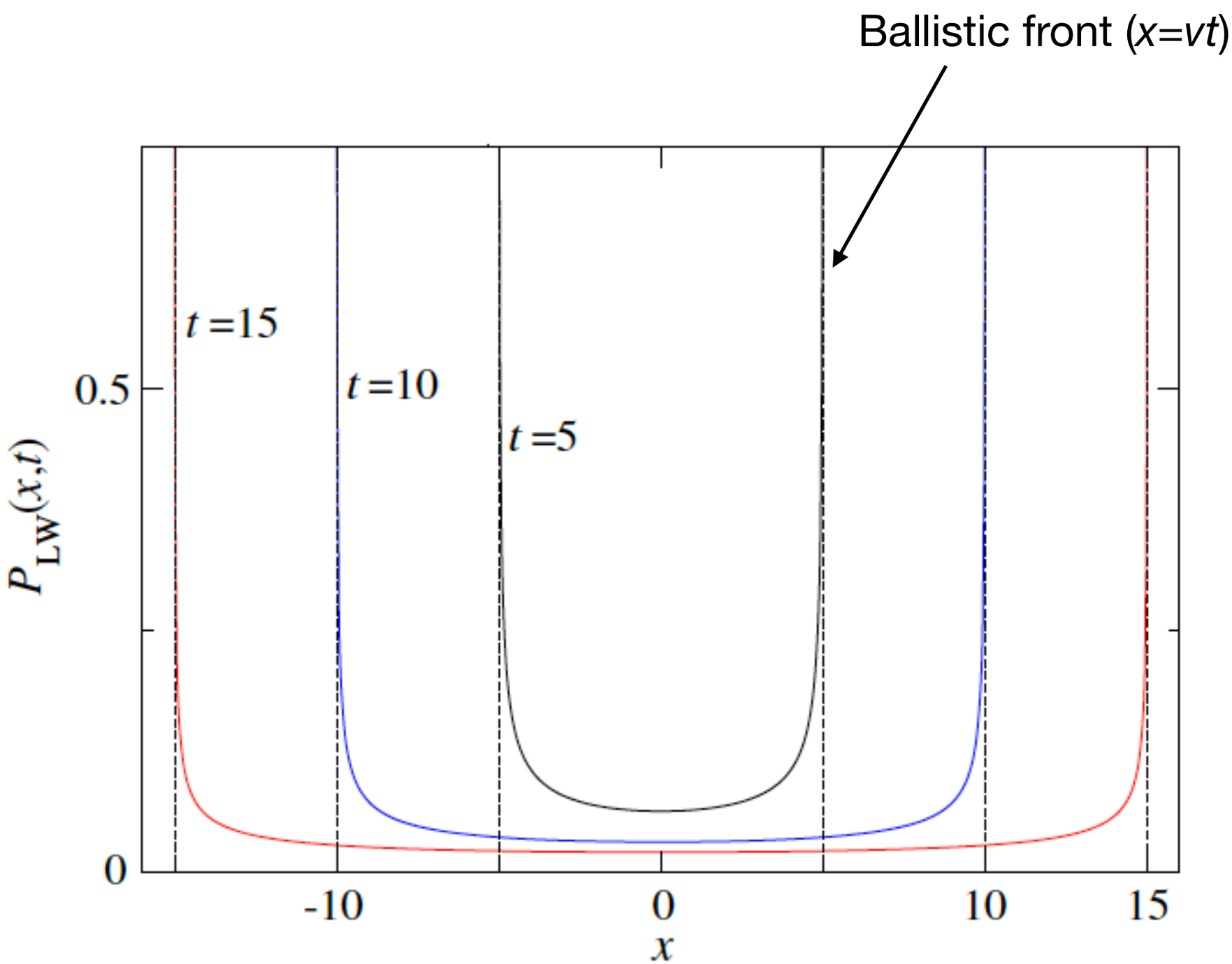
$$\psi(u) = 1 - C_1 u^\alpha \quad \tilde{\Psi}(u) = C_1 u^{\alpha-1}$$

$$P(k,u) = \frac{1}{u} \frac{C_1 u^\alpha - (\alpha-1)(\alpha-2)k^2 v^2 u^{\alpha-2}/2}{C_1 u^\alpha - \alpha(\alpha-1)k^2 v^2 u^{\alpha-2}/2}$$

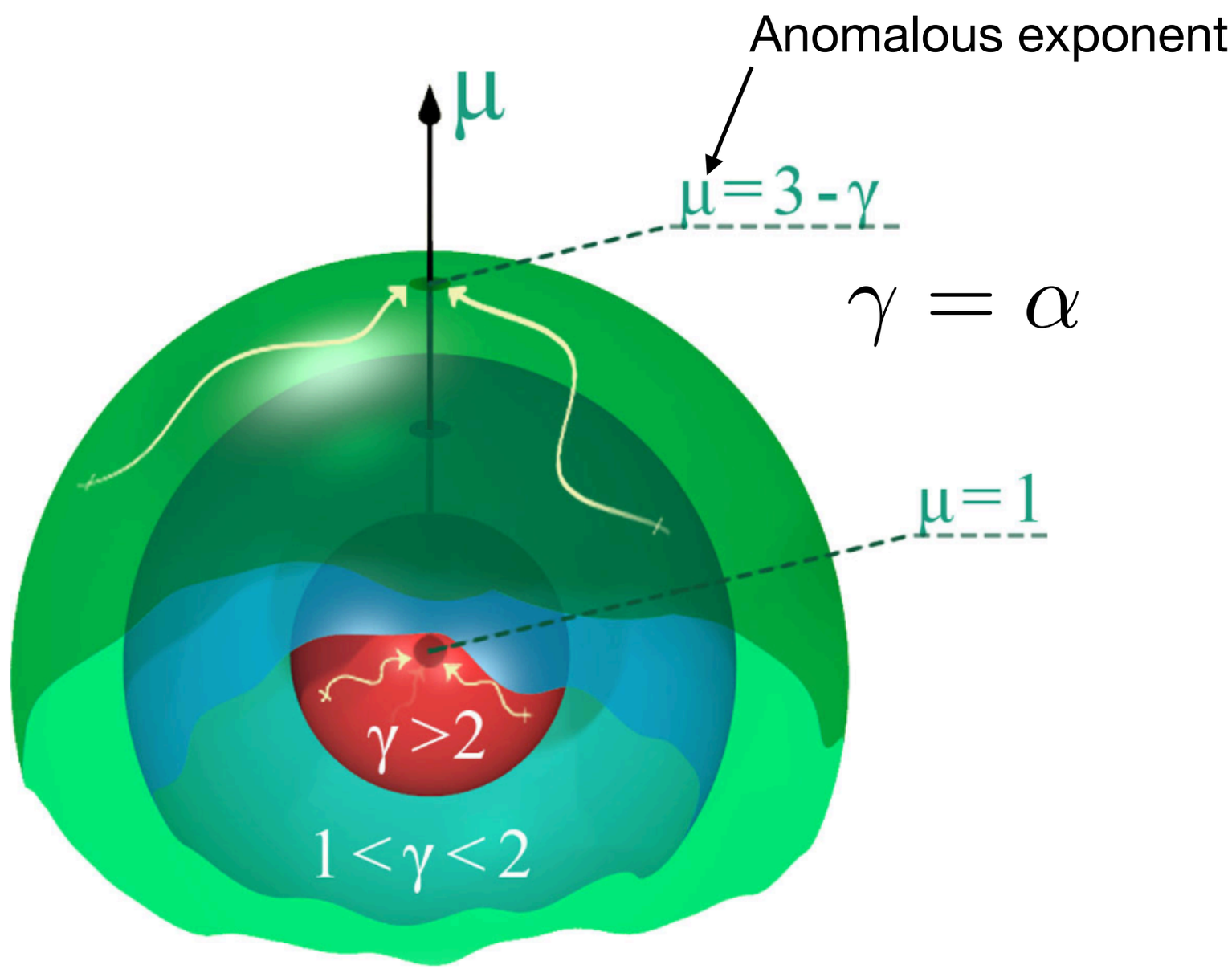
$$\downarrow$$

$$\langle x^2(t) \rangle \simeq (1-\alpha) v^2 t^2$$ Ballistic diffusion

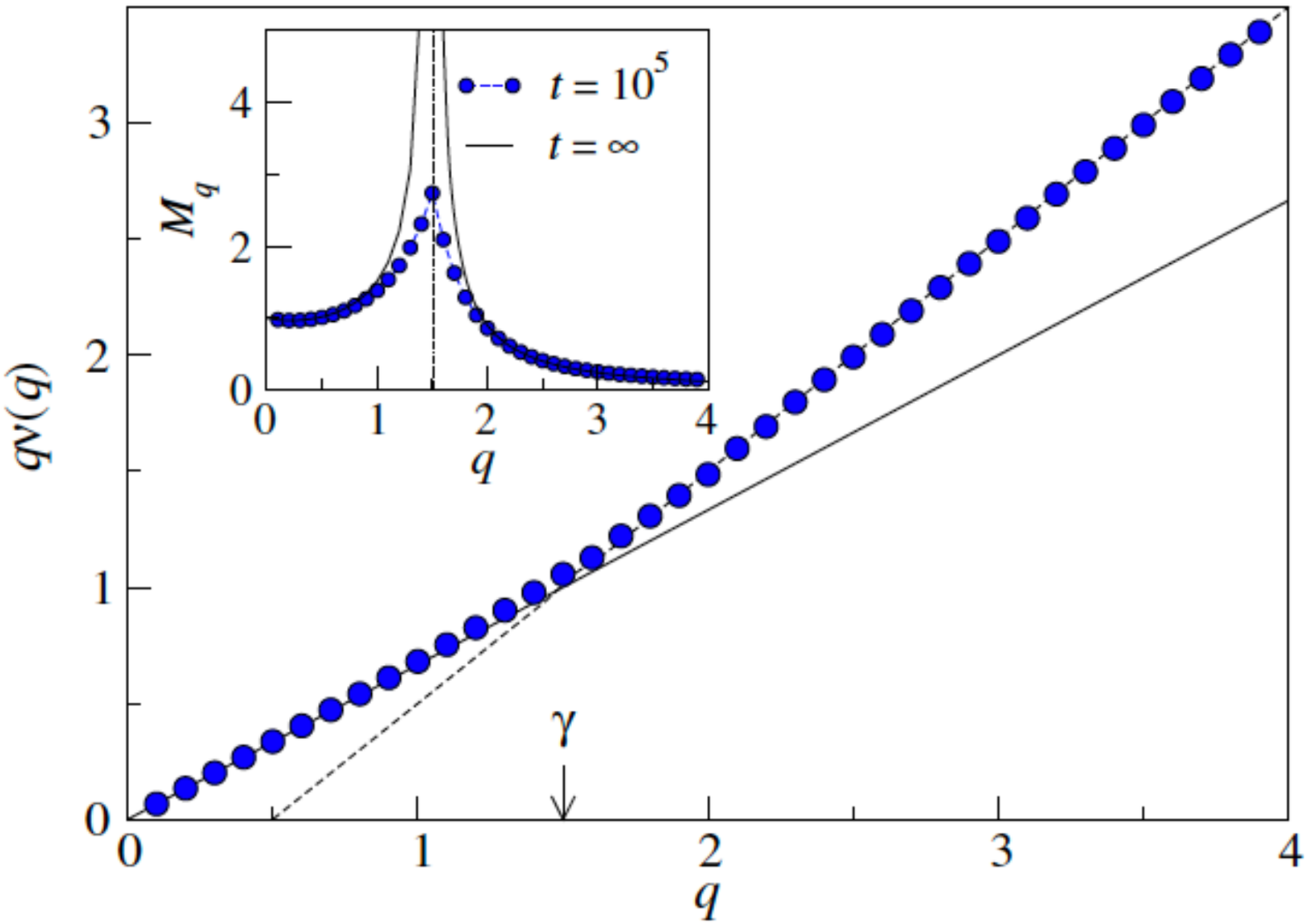
at large *t*


Ballistic front (x=vt)
t =15
t =10
t =5
0.5
0
$P_{LW}(x,t)$
-10
0
10
15
x

- For all α>2: the random walks become Gaussian (the CLT)



from Zaburdaev, Denisov, & Klafter, Phys Mod Phy 87, 483 (2015)


$t = 10^5$
$t = \infty$
M_q
q
$qV(q)$
γ
0
1
2
3
4

4. Fractional diffusion equations

4.1 Riemann-Liouville derivatives

- Heuristic approach of fractional-order differentiation

For integers *m*, *n* with *m* ≥ *n*

$$\frac{d^n x^m}{dx^n} = \frac{\Gamma(m+1)}{\Gamma(m-n+1)} x^{m-n}$$

⇨

For real values μ, ν with $\mu \geq \nu$

$$\frac{d^\nu x^\mu}{dx^\nu} = \frac{\Gamma(\mu+1)}{\Gamma(\mu-\nu+1)} x^{\mu-\nu}$$

Application to some functions

$$\frac{d^\nu}{dx^\nu} e^{-x} = \frac{d^\nu}{dx^\nu} \sum_{n=0}^{\infty} \frac{(-t)^n}{\Gamma(n+1)} = (-1)^\nu e^{-x}$$

HW: show this using incomplete gamma function

fractional derivative of exponential is exponential.

$$\frac{d^\nu}{dx^\nu} 1 = \frac{1}{\Gamma(1-\nu)} x^{-\nu}$$

only zero for natural values of ν.

- Riemann-Liouville fractional integral

Let us recall the Cauchy formula of *n*-fold repeated integration (*n*≥1):

$$\int_a^t \int_a^{t_1} \cdots \int_a^{t_{n-2}} \int_a^{t_{n-1}} f(t_n) dt_n dt_{t-1} \cdots dt_2 dt_1 = \frac{1}{(n-1)!} \int_a^t (t-t')^{n-1} f(t') dt'$$

$$\equiv {}_a I_t^n f(t)$$

Generalizing this formula, we define fractional-order integral by the following way:

order

$${}_a I_t^{\alpha} f(t) = \frac{1}{\Gamma(\alpha)} \int_a^t (t-t')^{\alpha-1} f(t') dt'$$ for real value $\boldsymbol{\alpha}$>0

start point end point

- Riemann-Liouville fractional derivative

Fractional derivative is defined from the fractional integral by the following way:

$$ {}_a\mathcal{D}_t^{\alpha} f(t) = \frac{d^n}{dt^n}\ {}_aI_t^{n-\alpha} f(t) \quad \text{with } n-1 \leq \alpha < n $$

start point

the variable of differentiation

integer

NOTE: the fractional derivative needs the starting point of evaluation.

Using this, let us write down the fractional derivative for 0<$\boldsymbol{\alpha}$<1.

(we mostly use $\boldsymbol{\alpha}$ in this range of values; e.g., the one-sided Levy PDF of waiting times)

$$ {}_a\mathcal{D}_t^{\alpha} f(t) = \frac{d}{dt}\frac{1}{\Gamma(1-\alpha)}\int_a^t (t-t')^{-\alpha} f(t')dt' $$

Note that the fractional derivative is a non-local operator. The outcome of the operation depends on the starting point.

- Examples (& Exercise)

Power-law functions

$$ {}_0\mathcal{D}_t^\alpha t^\mu = \frac{d^n}{dt^n}\ {}_0I_t^{n-\alpha} t^\mu = \frac{d^n}{dt^n}\frac{1}{\Gamma(n-\alpha)}\int_0^t (t-z)^{n-\alpha-1} z^\mu dz $$

HW: show this using beta function $n-1 \leq \alpha < n$

$$ = \frac{\Gamma(\mu+1)}{\Gamma(\mu-\alpha+1)} t^{\mu-\alpha} $$

Consistent result with the heuristic approach above.

$$ {}_0\mathcal{D}_t^\alpha 1 = \frac{1}{\Gamma(1-\alpha)} t^{-\alpha} $$

NOTE: However, we may get a different result if the staring point *a* is not zero.

To see this, look at the next example.

Exponential functions

$$ {}_0\mathcal{D}_t^{\alpha} e^t = e^t \frac{\gamma(-\alpha, t)}{\Gamma(-\alpha)} $$

HW: show this

where incomplete gamma function is

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

In this case, fractional derivative of exponential function is not exponential.

$$ {}_{-\infty}\mathcal{D}_t^{\alpha} e^t = e^t $$

HW: show this

A special case: Riemann-Liouville derivative with a→-∞, called the Weyl derivative, which gives exponential function.

- Laplace transform

When the starting point is 0, the Laplace transformed form of the R-L integro-differential operators is obtained.

$$L[{}_0I_t^\alpha f(t)] = L\left[\frac{1}{\Gamma(\alpha)}\int_0^t (t-t')^{\alpha-1} f(t')dt'\right] = u^{-\alpha} f(u)$$ for α>0

HW: show this using convolution and the Gamma function

fractional derivatives with 0<α<1

$$L[{}_0\mathcal{D}_t^\alpha f(t)] = L\left[\frac{d}{dt}\frac{1}{\Gamma(1-\alpha)}\int_0^t (t-t')^{-\alpha} f(t')dt'\right] = u^{\alpha} f(u)$$

HW: show this

NOTE: information on *f*(*t*=0) is not involved.

- Fourier transform

$$F[{}_{-\infty}\mathcal{D}_x^\alpha f(x)] = (ik)^\alpha f(k)$$

4.2 Subdiffusive CTRW

- Recall the Laplace-Fourier transformed PDF $0 < \alpha < 1$

$$P(k,u) = \frac{P_0(k)}{u + \frac{k^2\langle \delta x^2 \rangle}{2\tau^\alpha} u^{1-\alpha}} = \frac{P_0(k)}{u + k^2 D_\alpha u^{1-\alpha}}$$

$$\downarrow$$

$$uP(k,u) - P_0(k) = -k^2 u^{1-\alpha} D_\alpha P(k,u)$$

$$\downarrow$$

$$uP(x,u) - \underbrace{P_0(x)}_{= \delta(x) \text{ (for } P(x,t) = \delta(x)\delta(t))} = D_\alpha u^{1-\alpha} \frac{\partial^2}{\partial x^2} P(x,u) \qquad 0 < \alpha < 1$$

$$\downarrow$$ using $L[{}_0\mathcal{D}_t^\alpha f(t)] = u^\alpha f(u)$

$$\boxed{\frac{\partial}{\partial t} P(x,t) = {}_0\mathcal{D}_t^{1-\alpha} D_\alpha \frac{\partial^2}{\partial x^2} P(x,t)}$$

fractional diffusion eq.

$$\boxed{\frac{\partial}{\partial t}P(x,t) = \frac{D_\alpha}{\Gamma(\alpha)}\frac{\partial}{\partial t}\int_0^t (t-t')^{\alpha-1}\frac{\partial^2 P(x,t')}{\partial x^2}dt' \qquad 0<\alpha<1}$$

Alternatively, we can write down the same fractional equation in this way:

$$P(x,u) - \delta(x)/u = D_\alpha u^{-\alpha}\frac{\partial^2}{\partial x^2}P(x,u)$$

$$\downarrow$$

$$P(x,t) - \delta(x) = {}_0\mathcal{D}_t^{-\alpha} D_\alpha \frac{\partial^2}{\partial x^2}P(x,t)$$

$$\equiv {}_0I_t^\alpha$$

$$\downarrow$$

$${}_0\mathcal{D}_t^\alpha P(x,t) - \frac{t^{-\alpha}}{\Gamma(1-\alpha)}\delta(x) = D_\alpha\frac{\partial^2}{\partial x^2}P(x,t)$$

More generally, we can suggest the following fractional diffusion equation in the presence of potential (next page).

4.3 Fractional Fokker-Planck equation

$$\frac{\partial}{\partial t}P(x,t) = {}_0\mathcal{D}_t^{1-\alpha}\left[-\mu_\alpha \frac{\partial}{\partial x}F(x) + D_\alpha \frac{\partial^2}{\partial x^2}\right]P(x,t)$$

generalized mobility external force

$$= {}_0\mathcal{D}_t^{1-\alpha}\left[\mu_\alpha \frac{\partial}{\partial x}U'(x) + D_\alpha \frac{\partial^2}{\partial x^2}\right]P(x,t)$$

external potential *U*(*x*)

$$= {}_0\mathcal{D}_t^{1-\alpha}\mathcal{L}_{FP}(x)P(x,t)$$

- Equilibrium distribution (at $t \to \infty$)

$$P_{\mathrm{st}}(x) = \mathcal{N}\exp\left(-\frac{\mu_\alpha}{D_\alpha}U(x)\right)$$

confining potential

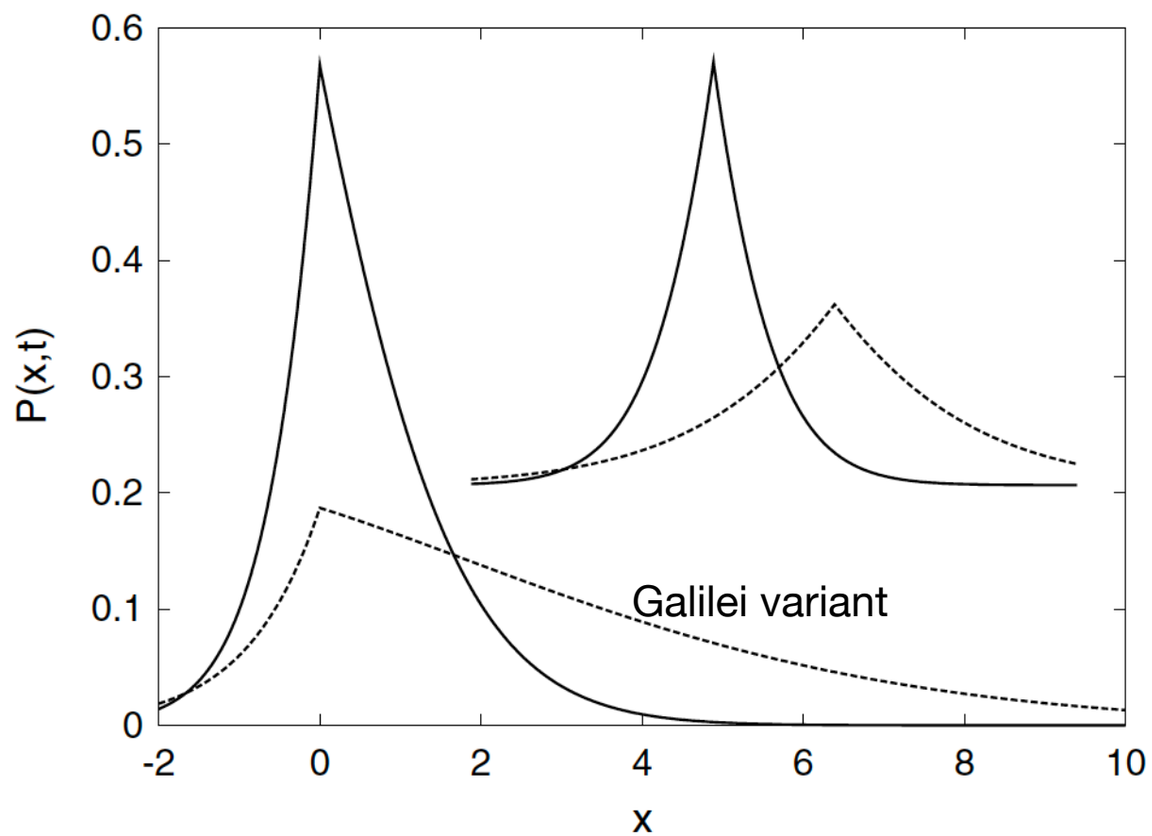
- Generalized Stokes-Einstein relation

$$\exp\left(-\frac{\mu_\alpha}{D_\alpha}U(x)\right) = \exp\left(-U(x)/[k_B T]\right) \quad \Rightarrow \quad D_\alpha = \mu_\alpha k_B T = \frac{k_B T}{\gamma_\alpha}$$

- Under a constant force (fractional diffusion-advection equation)

$$\frac{\partial}{\partial t}P(x,t) = {}_0\mathcal{D}_t^{1-\alpha}\left[-V_\alpha\frac{\partial}{\partial x} + D_\alpha\frac{\partial^2}{\partial x^2}\right]P(x,t)$$

$$V_\alpha = \mu_\alpha F$$



$$\langle x(t)\rangle = \frac{V_\alpha t^\alpha}{\Gamma(1+\alpha)}$$

$$\langle x^2(t)\rangle = \frac{2V_\alpha^2 t^{2\alpha}}{\Gamma(1+2\alpha)} + \frac{2D_\alpha t^\alpha}{\Gamma(1+\alpha)}$$

Galilei variant

$$\langle \Delta x^2(t)\rangle = \frac{2D_\alpha t^\alpha}{\Gamma(1+\alpha)} + \left(\frac{2}{\Gamma(1+2\alpha)} - \frac{1}{\Gamma^2(1+\alpha)}\right) V_\alpha^2 t^{2\alpha} \neq \langle x^2(t)\rangle_0$$

⇨ Generalized 2nd Einstein relation is satisfied.

$$\langle x(t)\rangle_F = \frac{1}{2}\frac{\mu_\alpha F}{D_\alpha}\langle x^2(t)\rangle_0 = \frac{F}{2k_B T}\langle x^2(t)\rangle_0$$

4.4 Eigenfunction expansion method

Fractional FPE with a time-independent force

$$\frac{\partial}{\partial t}P(x,t) = {}_0\mathcal{D}_t^{1-\alpha}\mathcal{L}_{FP}(x)P(x,t)$$

- We look for the solution of FFPE in the form of eigenfunction expansion

$$P(x,t) = \sum_{n=0}^{\infty} A_n(x_0,t_0)\phi_n(x)T_n(t)$$

separation of variables

- Here, $\phi_n(x)$ is an eigenfunction satisfying

$$\mathcal{L}_{FP}\phi_n(x) = -\lambda_n\phi_n(x)$$

eigenvalue

(In this lecture, we do not go over the general method of solving the above eigenvalue equation of a given Fokker-Planck operator. For this part, see some standard textbooks (e.g., Stochastic Methods (Gardiner), Fokker-Planck equation (Risken), etc).

- Then we have the eigenvalue equation for time part:

$$\frac{d}{dt}T_n(t) = -\lambda_n \; {}_0\mathcal{D}_t^{1-\alpha} T_n(t)$$

In Laplace space:

$$uT_n(u) - T_n(0) = -\lambda_n u^{1-\alpha} T_n(u)$$

initial value = 1

$$\Rightarrow \qquad T_n(u) = \frac{1}{u + \lambda_n u^{1-\alpha}}$$

inverse Laplace (Mittag-Leffler function)

$$\Rightarrow \qquad T_n(t) = E_\alpha(-\lambda_n t^\alpha) \qquad \alpha = 1: \; T_n(t) = \exp(-\lambda_n t)$$

As we found in *P*(*k*,*u*) (subdiffusive CTRW), each mode has a strange relaxation descried by Mittag-Leffler functions —> long relaxation!

$$= \begin{cases} \exp\left(-\dfrac{-\lambda_n t^\alpha}{\Gamma(1+\alpha)}\right) & \text{stretched exponential (short-time)} \\[2ex] \dfrac{1}{\Gamma(1-\alpha)\lambda_n t^\alpha} & \text{power-law (long-time)} \end{cases}$$

- Recall *P*(*x*,*t*) in the form of the eigenfunction expansion (in the ordinary FPE)

$$P(x,t) = e^{[\Phi(x_0)-\Phi(x)]/2} \sum_{n=0}^{\infty} \psi_n(x)\psi_n(x_0)e^{-\lambda_n t}$$

where $P_{\rm st}(x) = \mathcal{N} e^{-\Phi(x)}$ and ψ_n is the eigenfunction of a Hermitian operator

$$\mathcal{L}_s = -e^{\Phi/2}\mathcal{L}_{FP}e^{-\Phi/2}$$

$$= -D_\alpha \frac{\partial^2}{\partial x^2} + D_\alpha[\frac{1}{4}(\Phi'(x))^2 - \frac{1}{2}\Phi''(x)]$$

and $\mathcal{L}_s\psi_n = \lambda_n\psi_n$ & $\psi_n = e^{\Phi/2}\phi_n(x)$

- Replacing the time part, we have

$$\boxed{P(x,t) = e^{[\Phi(x_0)-\Phi(x)]/2} \sum_{n=0}^{\infty} \psi_n(x)\psi_n(x_0)E_\alpha(-\lambda_n t^\alpha)}$$

- Example: The fractional harmonically bound particle

(We skip the derivation of solving the FPE for a Brownian particle in a harmonic trap; see Gardiner)

$$U(x) = \frac{1}{2} m\omega^2 x^2$$

$$P(x,t|x_0) = \sqrt{\frac{m\omega^2}{2\pi k_B T}} \sum_n \frac{E_\alpha[-n(t/\tau)^\alpha]}{2^n n!} H_n(\frac{\tilde{x}_0}{\sqrt{2}}) H_n(\frac{\tilde{x}}{\sqrt{2}}) e^{-\tilde{x}^2/2}$$

Hermite polynomial

where $\tilde{x} = x\sqrt{m\omega^2/[k_B T]}$ & $\tau^{-\alpha} = m\omega^2/\gamma_\alpha$

At $t \to \infty$: the particle is fully equilibrated (NB: even though the mean waiting time is diverging, the system is thermalized after infinite time. (We called it weak ergodicity breaking in earlier our lecture).

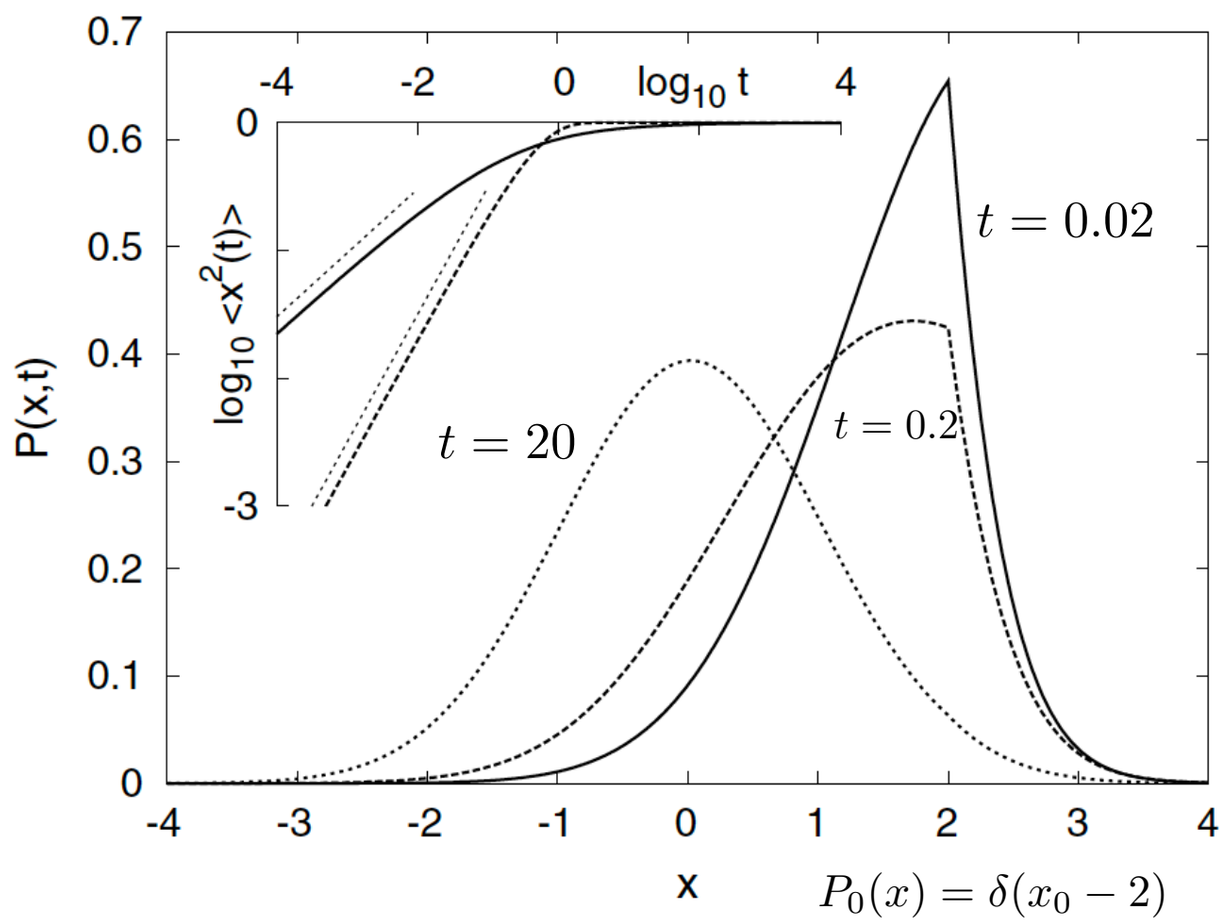
$$\Rightarrow \quad P_{\rm st}(x) = \sqrt{\frac{m\omega^2}{2\pi k_B T}} \exp\left(-\frac{m\omega^2 x^2}{2k_B T}\right)$$

$$\frac{\partial}{\partial t}P(x,t) = {}_0\mathcal{D}_t^{1-\alpha}\left[\mu_\alpha \frac{\partial}{\partial x}U'(x) + D_\alpha \frac{\partial^2}{\partial x^2}\right]P(x,t)$$

In the above FFPE $P \to \int x^n P(x,t)dx$

$$\frac{d}{dt}\langle x(t)\rangle = -\,{}_0\mathcal{D}_t^{1-\alpha} m\mu_\alpha\omega^2\langle x(t)\rangle \quad \Rightarrow \quad \langle x(t)\rangle = x_0 E_\alpha[-(t/\tau)^\alpha]$$

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



$P_0(x) = \delta(x_0 - 2)$

Langevin equation for FFPE

<u>Idea of subordination</u>

$$P(x,t) = \sum_{n=0}^{\infty} P_n(x) Q_n(t) \; = \int_0^{\infty} P_1(x,s) \mathcal{E}_\alpha(s,t) ds$$

By matching L.H.S and R.H.S in the Laplace-Fourier space

$$\mathcal{E}_\alpha(s,t) = \frac{\tau^{1/\alpha} t}{\alpha s^{1+1/\alpha} \tau} L_{\alpha,0}\left(\frac{t}{(s\tau^{\alpha-1})^{1/\alpha}}\right)$$

Coupled Langevin equation (Forgedby 1994)

$$\frac{dx(s)}{ds} = \frac{D}{k_B T} F(x) + \eta(s)$$

$$\frac{dt(s)}{ds} = \omega(s)$$

5. Time-averaging and aging

- Ensemble-averaged (EA) mean squared displacement (MSD)

$$\langle x^2(\Delta)\rangle = \int x^2 P(x,\Delta)dx \simeq \frac{1}{N}\sum_{i=1}^{N} x_i^2(\Delta)$$

- Time-averaged (TA) mean squared displacement (MSD)

$$\overline{\delta^2(\Delta,T)} = \frac{1}{T-\Delta}\int_0^{T-\Delta}[x(t+\Delta)-x(t)]^2 dt$$

Length of observation time

lag time

EA TAMSD (fluctuation-free): $\langle\overline{\delta^2(\Delta,T)}\rangle = \frac{1}{N}\sum_{i=1}^{N}\overline{\delta_i^2(\Delta,T)}$

$$\langle \overline{\delta^2(\Delta, T)} \rangle = \frac{1}{T-\Delta} \int_0^{T-\Delta} \langle [x(t+\Delta) - x(t)]^2 \rangle dt$$

$$\Rightarrow \langle \delta x^2 \rangle \langle n(t+\Delta, t) \rangle$$

$$\Rightarrow \langle n(t+\Delta, t) \rangle = \langle n(t+\Delta) \rangle - \langle n(t) \rangle$$

- Normal diffusion

$$\langle \delta x^2 \rangle \langle n(t+\Delta, t) \rangle = \langle \delta x^2 \rangle \frac{\Delta}{\tau}$$

$$\langle \overline{\delta^2(\Delta, T)} \rangle = 2\langle \delta x^2 \rangle \frac{\Delta}{2\tau} = 2D\Delta \quad \Leftrightarrow \quad \langle x^2(\Delta) \rangle$$

Ergodicity is satisfied.

- Subdiffusive CTRW processes $\psi(t) \sim \frac{\alpha}{\Gamma(1-\alpha)} \frac{\tau^\alpha}{t^{1+\alpha}} \quad 0 < \alpha < 1$

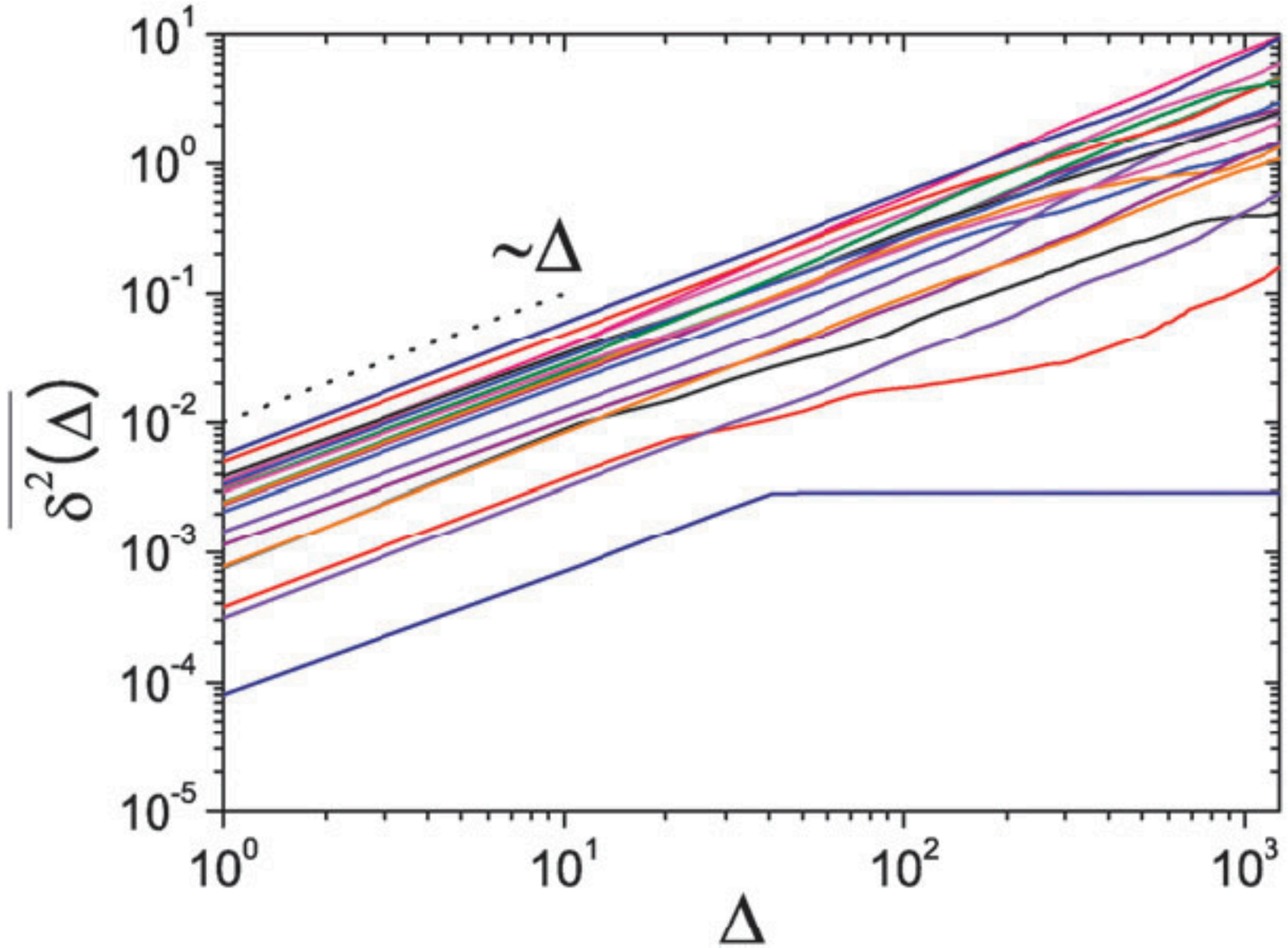
Using $\langle n(t) \rangle = \frac{1}{\Gamma(1+\alpha)} \frac{t^\alpha}{\tau^\alpha}$ we can obtain the TA MSD as such:

$$\langle \overline{\delta^2(\Delta, T)} \rangle = \frac{1}{T-\Delta} \frac{\langle \delta x^2 \rangle}{\tau^\alpha \Gamma(1+\alpha)} \int_0^{T-\Delta} [(t+\Delta)^\alpha - t^\alpha] dt$$

$$\simeq \frac{2D_\alpha}{\Gamma(1+\alpha)} \frac{\Delta}{T^{1-\alpha}} \qquad \Delta \ll T$$

<u>Weak ergodicity breaking</u>

$$\langle \overline{\delta^2(\Delta, T)} \rangle \neq \langle x^2(\Delta) \rangle = \frac{2D_\alpha}{\Gamma(1+\alpha)} \Delta^\alpha$$


10^1
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
$\overline{\delta^2(\Delta)}$
$\sim\Delta$
10^0
10^1
10^2
10^3
Δ

- By measuring TA MSDs (e.g. single-particle tracking experiments), we seemingly observe a Fickian dynamics for the subdiffusive CTRW process.

$$\langle \overline{\delta^2(\Delta, T)} \rangle \simeq \frac{2D_\alpha}{\Gamma(1+\alpha)} \frac{\Delta}{T^{1-\alpha}} \equiv 2D_{\mathrm{eff}}(T)\Delta$$

aging effect

- However, this process is different from ordinary Fickian dynamics (normal diffusion) in the sense that the effective diffusivity depends on the observation time *T*.

- Aging effect: $D_{\mathrm{eff}}(T) \to 0$ as $T \to \infty$

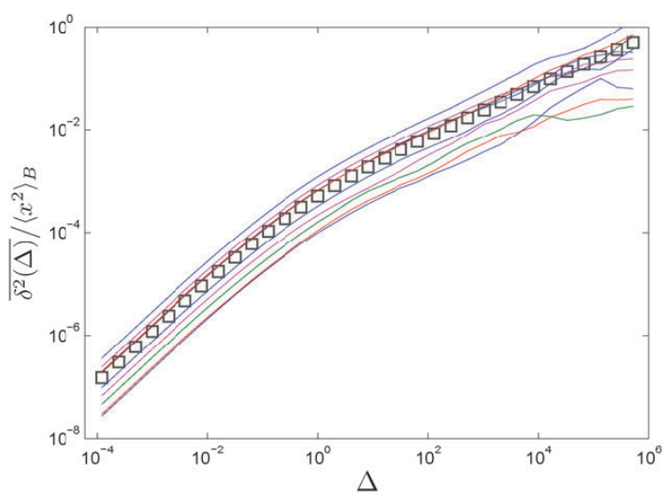
  The process looks *slower* as we observe it with *longer* observation time *T*.

  $\alpha \to 1$: no aging (normal diffusion)

* PROJECT

- Confined subdiffusive CTRW processes were shown to have TA MSD of the following form:

$$\langle \overline{\delta^2(\Delta, T)} \rangle \sim (\langle x^2 \rangle_B - \langle x \rangle_B^2) \frac{2\sin(\pi\alpha)}{(1-\alpha)\pi\alpha} \left(\frac{\Delta}{T}\right)^{1-\alpha}$$



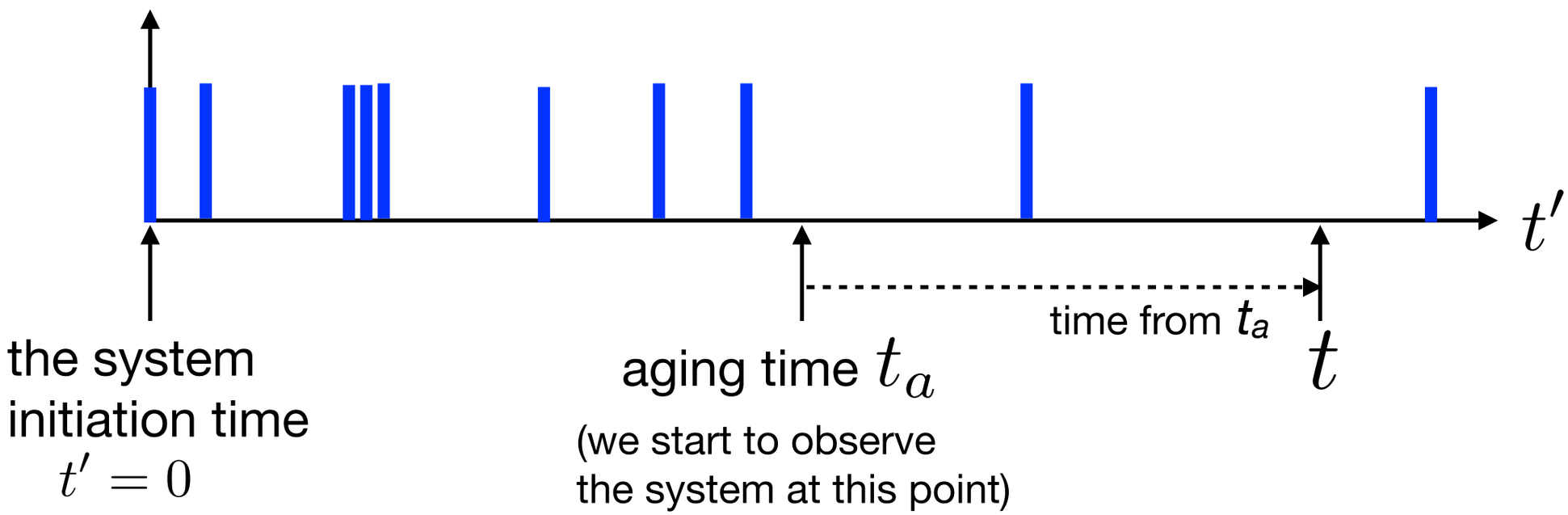
thermal average with ($P_{\rm st}(x)$)

lag time: $(1/[D_\alpha \lambda_1])^{1/\alpha} \ll \Delta \ll T$

the lowest eigenvalue of $\mathcal{L}_{FP}$

- Seemingly, TA MSD does not saturate towards the thermal value (for any observation time T). This is also WEB.

Aging phenomena



- Now we define time *t* from the aging time and see the dynamics of the process.

$$\langle x^2(t; t_a)\rangle$$

aging time dependence

- $t_a = 0$: the usual setting that we observe the process when the system is made

$$\langle x^2(t; t_a = 0)\rangle = \langle x^2(t)\rangle$$

aging-free MSD

- Aged EA MSD

$$\langle x^2(t;t_a)\rangle = \int x^2 P(x,t;t_a)dx$$

$$= \langle x^2(t+t_a)\rangle - \langle x^2(t_a)\rangle$$

$$= \frac{2D_\alpha}{\Gamma(1+\alpha)}\left[(t_a+t)^\alpha - t_a^\alpha\right] \qquad 0<\alpha<1$$

* No aging for normal diffusion $\alpha \to 1$

CASE 1: $t_a/t \gg 1$ (strong aging)

$$\langle x^2(t;t_a)\rangle \simeq \frac{2\alpha D_\alpha}{\Gamma(1+\alpha)}\frac{t}{t_a^{1-\alpha}}$$

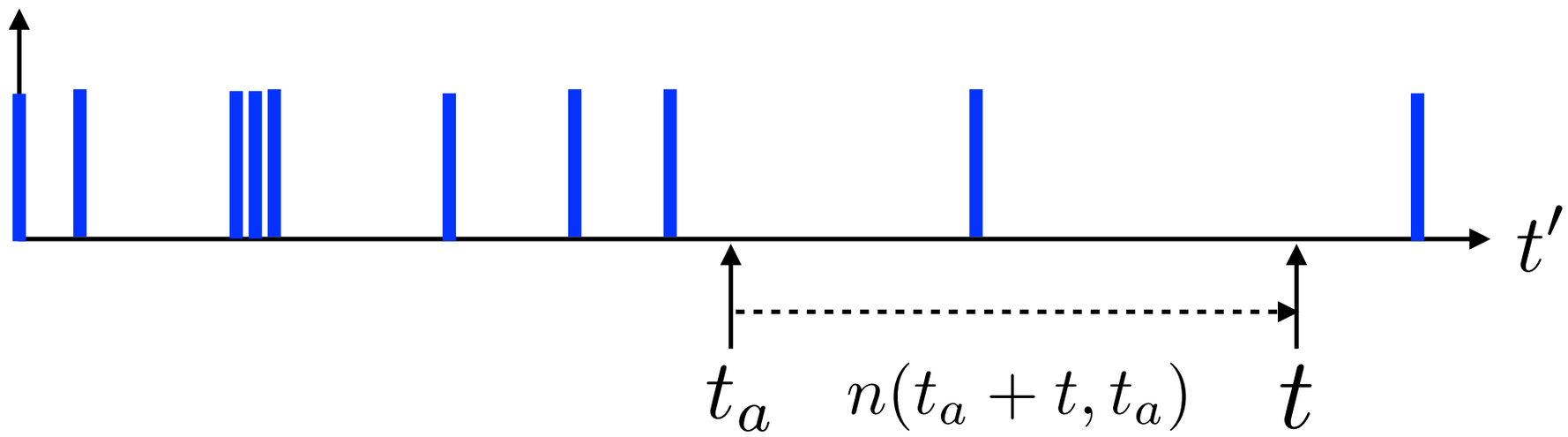
Exactly same behavior shown in TA MSD

CASE 2: $t_a/t \ll 1$ (weak aging)

$$\langle x^2(t;t_a)\rangle \simeq \frac{2D_\alpha}{\Gamma(1+\alpha)} t^\alpha$$

Exactly aging-free MSD

<u>Origin for the aging from the viewpoint of renewal process</u>



# of events in [t_a +t, t_a]

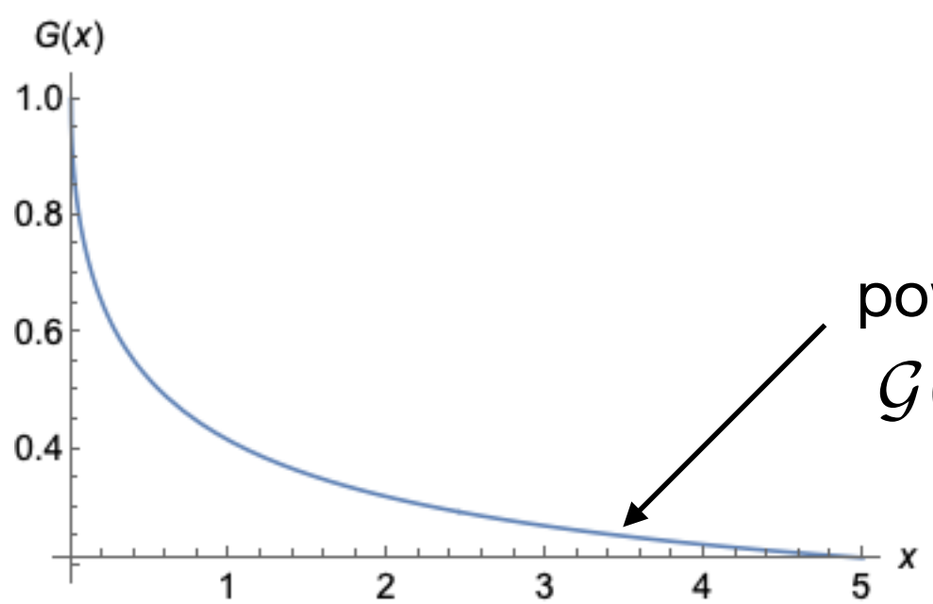
- The process does not reach a stationary state

$$\langle n(t_a + t, t_a)\rangle \neq \langle n(t)\rangle$$

$$\langle n(t)\rangle = \frac{1}{\Gamma(1+\alpha)}\frac{t^\alpha}{\tau^\alpha}$$

$$\langle n(t_a + t, t_a)\rangle = \langle n(t)\rangle \underbrace{\left\{\left(1+\frac{t_a}{t}\right)^\alpha - \left(\frac{t_a}{t}\right)^\alpha\right\}}_{\text{scaling function}}$$

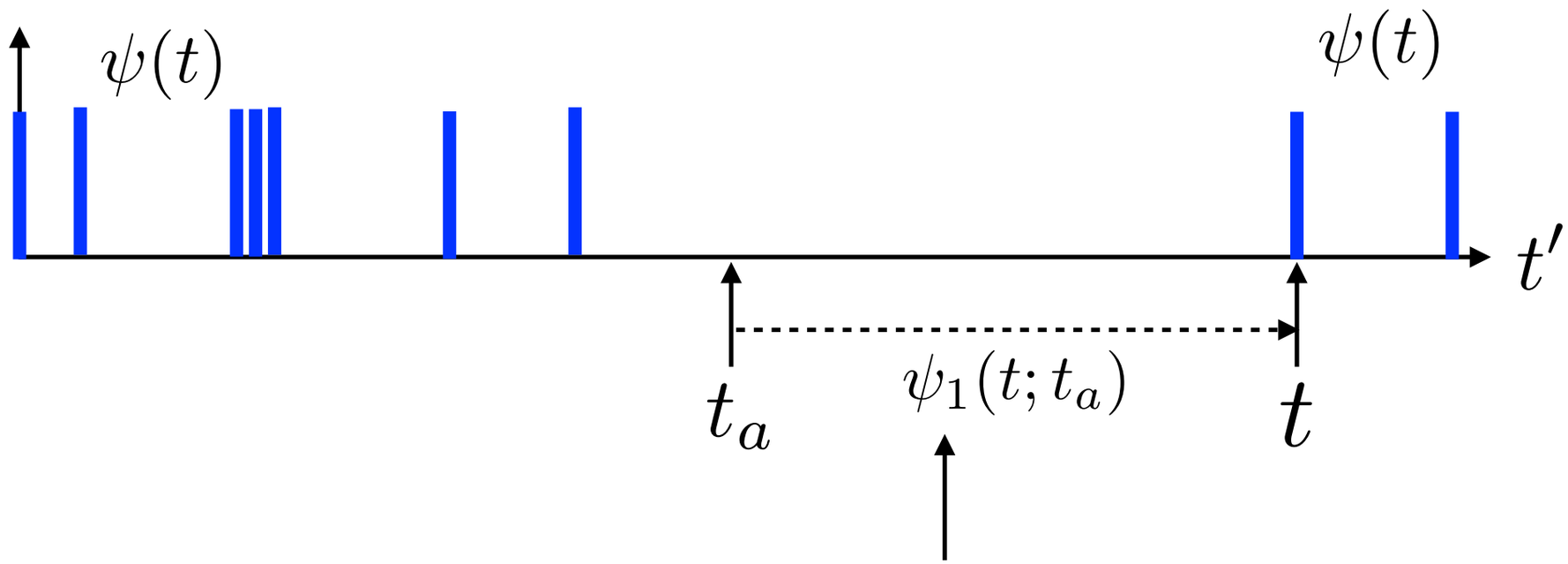
$$\mathcal{G}(x) = (1+x)^\alpha - x^\alpha \qquad x = t_a/t$$



power-law decay

$$\mathcal{G}(x) \simeq \alpha x^{\alpha-1}$$

- Forward waiting time PDF $\psi_1(t; t_a)$



The PDF that the *first* event occurs at *t* under given aging time t_a.

$$\psi_1(t; t_a) = \sum_{n=0}^{\infty} \int_0^{t_a} \psi_n(t')\psi(t_a - t' + t)dt'$$

$$\downarrow \quad \downarrow$$

$$\psi_1(s; u) = \frac{1}{1 - \psi(u)} \frac{\psi(u) - \psi(s)}{s - u}$$

double Laplace transformed form

- Processes with a heavy-tailed waiting PDF

using $\psi(u) = 1 - \tau^\alpha u^\alpha$ $\qquad \psi_1(s;u) = \dfrac{s^\alpha - u^\alpha}{u^\alpha(s-u)}$

$$\psi_1(t;t_a) = \frac{\sin(\pi\alpha)}{\pi}\frac{t_a^\alpha}{t^\alpha(t+t_a)}$$

CASE 1: $t_a/t \gg 1$ (strong aging)

$$\psi_1(t;t_a) \sim t_a^{\alpha-1} t^{-\alpha}$$

probability density smaller with t_a $\qquad$ the aged PDF is heavier than $\psi(t)$

CASE 2: $t_a/t \ll 1$ (weak aging) $\qquad \psi_1(t;t_a) \sim t_a^\alpha t^{-(1+\alpha)}$