Diffusion on fractals and space-fractional diffusion equations

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Vortrag im Rahmen des Promotionsverfahrens

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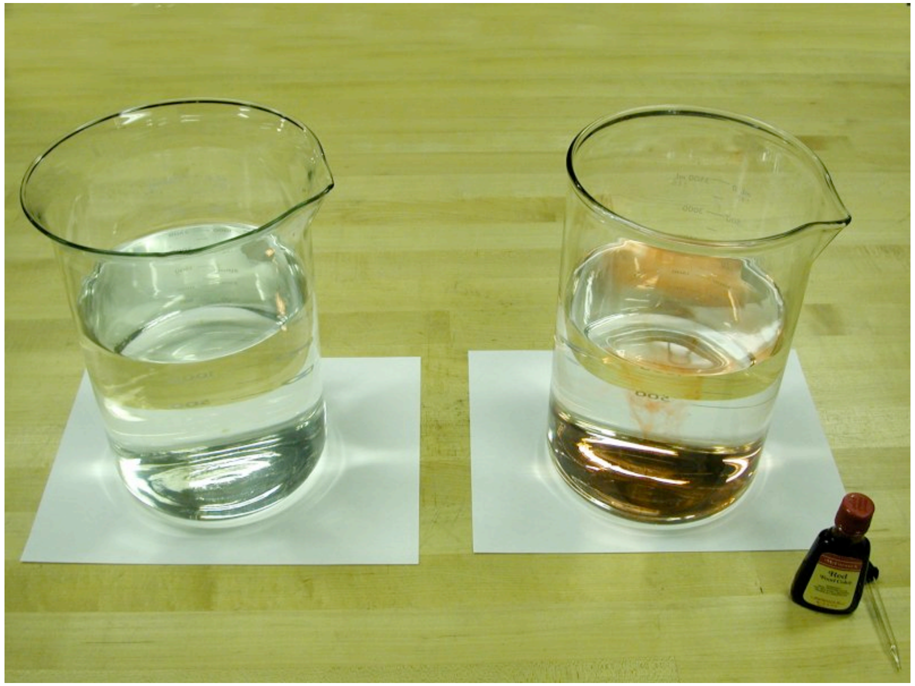
Outline

Normal diffusion



- Size of particle cloud $\langle r^2(t) \rangle = D\, t$

$$D: \ \text{Diffusion constant}$$

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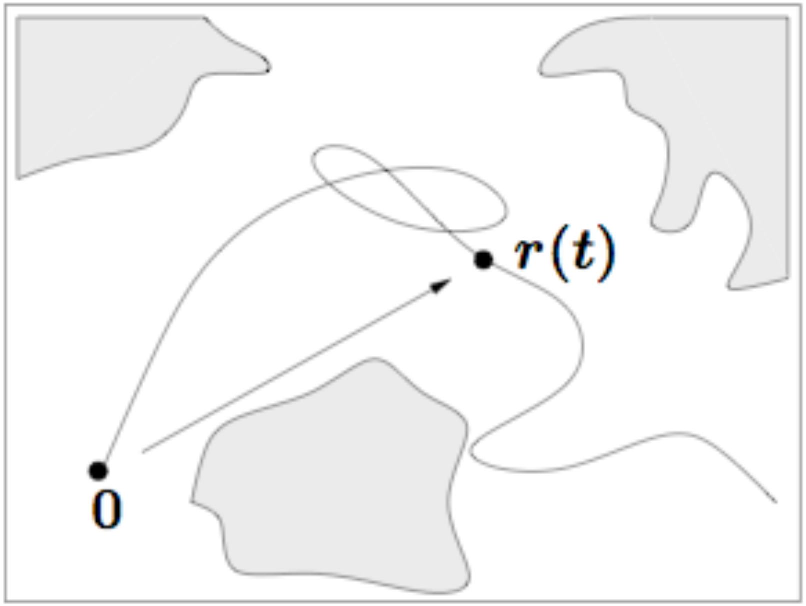
Anomalous Diffusion

- Diffusion of particles in disordered materials
  - inside a bulk
  - on the surface (deposit)



$$\langle r^2(t)\rangle \sim t^\gamma \qquad \gamma > 0$$

$\gamma < 1$	Subdiffusion
$\gamma = 1$	Normal diffusion
$\gamma > 1$	Superdiffusion

$r(t)$: Distance a particle has traversed in time *t* from its origin

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Anomalous diffusion

- Anomalous subdiffusion in living cells

  M. Weiss, et al.; *Biophys. J.*, **87 (2004)**:3518--3524.

- Diffusion in disordered materials

  S. Havlin and D. Ben-Avraham; *Adv. Phys.*, **36 (1987)**:695--798.

- Spreading of diseases

  A. L. Lloyd; *Science*, **292 (2001)**:1316--1317

- Foraging behavior of wandering albatrosses

  G. M. Viswanathan, et al.; *Nature*, **381(1996)**:413--415

➢ Investigating anomalous diffusion of great interest for various field of science

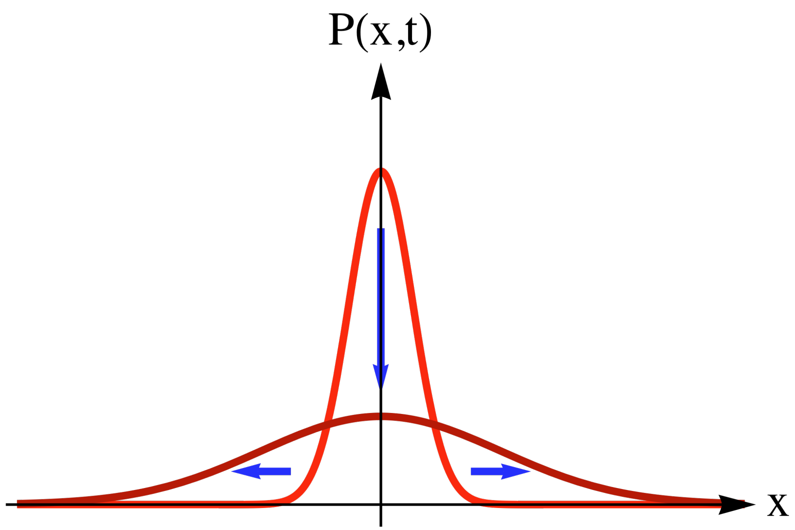
Diffusion equation

- Normal diffusion equation (one dimensional)

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

$P(x,t)$: Probability to be at position x at time t

- Initial condition $P(x, t=0) = \delta(x)$



$$\langle r^2(t) \rangle = D\, t \sim t^{\gamma} \quad \text{with } \gamma = 1$$

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Generalized diffusion equations

- In the literature known:

  Time-fractional diffusion equation

$$\frac{\partial^{\gamma}}{\partial t^{\gamma}} P(x,t) = D \frac{\partial^2}{\partial x^2} P(x,t) \qquad 1 < \gamma < 2$$

  – Represents superdiffusive processes

$$\langle r^2(t) \rangle \sim t^{\gamma} \quad \text{with } \gamma > 1$$

  – Due to the choice of γ , a bridging regime between

Diffusion equation $\gamma \to 1$ → Wave equation $\gamma \to 2$

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Bridging regime

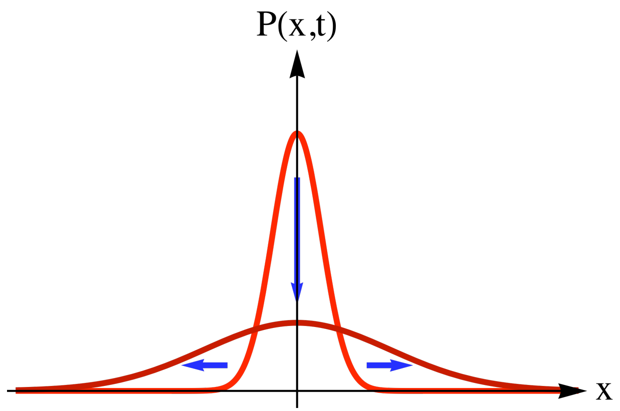
Diffusion equation → Wave equation

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

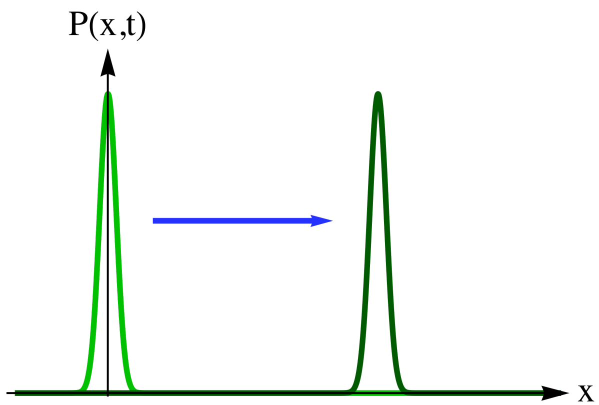
D : Diffusion constant

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

$\sqrt{D}$: speed of propagating wave



Iconic for irreversibility



Iconic for reversibility

Space-fractional diffusion equations

- Extending space derivatives to fractional order, instead of time derivatives

$$\frac{\partial}{\partial t} P(x,t) = D \frac{\partial^{\alpha}}{\partial x^{\alpha}} P(x,t)$$

$$1 < \alpha \leq 2$$
$$-\infty < x < \infty$$
$$0 \leq t < \infty$$

Represents same bridging regime:

Half wave equation → Diffusion equation

reversible process → irreversible process

$$\alpha \to 1$$

$$\frac{\partial}{\partial t} P(x,t) = D \frac{\partial}{\partial x} P(x,t)$$

$$\alpha \to 2$$

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

Space-fractional diffusion equation

➢ I investigated the bridging regime due to the thermodynamical aspect of irreversibility

- Natural measure of irreversibility:

Entropy production rate

(Half) wave equation → Diffusion equation

low entropy production rates | high entropy production rates

Intuitive expectation:

Moving from the wave regime to the diffusion regime the entropy production rate should increase!

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Space-fractional diffusion equations

1. What is a fractional derivative?

2. How to solve a space-fractional diffusion equation?

3. What happens with the entropy production rate?

1. What is a fractional derivative

- Definition via Fourier transformation:
  - Fourier transformation: $$\tilde{f}(k) = \mathcal{F}\left\{f(x)\right\} = \int_{-\infty}^{\infty} f(x)\, e^{ikx}\, \mathrm{d}x$$
    $$f(x) = \mathcal{F}^{-1}\left\{\tilde{f}(k)\right\} = \frac{1}{2\,\pi} \int_{-\infty}^{\infty} \tilde{f}(k)\, e^{-ikx}\, \mathrm{d}k$$
  - Example: First derivative:

$$\frac{\partial}{\partial x} f(x) = \frac{\partial}{\partial x}\left\{\frac{1}{2\,\pi}\int_{-\infty}^{\infty} \tilde{f}(k)\, e^{-ikx}\, \mathrm{d}k\right\} = \frac{1}{2\,\pi}\int_{-\infty}^{\infty} (-i\,k)\,\tilde{f}(k)\, e^{-ikx}\, \mathrm{d}k$$

$$\frac{\partial}{\partial x} f(x) = \mathcal{F}^{-1}\left\{(-i\,k)\,\mathcal{F}\left\{f(x)\right\}\right\}$$

  - Fractional derivative: $$\frac{\partial^\alpha}{\partial x^\alpha} P(x,t) = \mathcal{F}^{-1}\left\{(-i\,k)^\alpha\,\mathcal{F}\left\{P(x,t)\right\}\right\}$$

➢ Fractional derivative becomes a multiplication

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2. How to solve a space-fractional diffusion equation?

$$\frac{\partial}{\partial t} P(x,t) = D \frac{\partial^\alpha}{\partial x^\alpha} P(x,t) \qquad \begin{array}{c} 1 < \alpha \le 2 \\ -\infty < x < \infty \\ 0 \le t < \infty \end{array}$$

- Applying the Fourier transformation:

$$\frac{\partial}{\partial t} P(x,t) = D \frac{\partial^\alpha}{\partial x^\alpha} P(x,t) \quad \rightarrow \quad \frac{\partial}{\partial t} \tilde{P}(k,t) = D\,(-i\,k)^\alpha\, \tilde{P}(k,t)$$

- Choosing initial condition:

$$P(x,t=0) = \delta(x) \quad \rightarrow \quad \tilde{P}(k,t=0) = \mathcal{F}\left\{\delta(x)\right\} = 1$$

- Leads to:

$$\tilde{P}(k,t) = \exp\left(D\,t\,(-i\,k)^\alpha\right)$$

$$\tilde{P}(k,t) = \exp\left(D\,t\,|k|^\alpha \cos\left(\frac{\alpha\,\pi}{2}\right)\left[1 - i\,\mathrm{sign}(k)\,\tan\left(\frac{\alpha\,\pi}{2}\right)\right]\right)$$

2. How to solve a space-fractional diffusion equation?

- Characteristic function of solution of space-fractional diffusion equations:

$$\tilde{P}(k,t) = \exp\left(D\,t\,|k|^{\alpha}\,\cos\left(\frac{\alpha\,\pi}{2}\right)\,\left[1 - i\,\mathrm{sign}(k)\,\tan\left(\frac{\alpha\,\pi}{2}\right)\right]\right)$$

➢ Problem: Closed form of the inverse Fourier transformation is not know!

Stable distribution

- P. Lévy: In the 1920's characterization of a class of probability distributions
  - Include skewness, heavy tails, mathematical intriguing properties
  - Defined via their characteristic function

➢ Stable distribution $\mathbf{S}\left(x|\alpha,\beta,\gamma,\delta;n\right)$

$\alpha \in (0,2]$	$\rightarrow$	characteristic exponent
$\beta \in [-1,1]$	$\rightarrow$	skewness parameter
$\gamma \in [0,\infty)$	$\rightarrow$	scaling of distribution
$\delta \in \mathbb{R}$	$\rightarrow$	localization or shift of distribution
$n = \{0,1\}$	$\rightarrow$	parameterization

Stable distribution

- Characteristic function of stable distribution for $n = 1$:

$$\mathcal{F}\{\mathbf{S}(x|\alpha,\beta,\gamma,\delta_1;1)\}$$

$$= \exp\left(-\gamma^{\alpha}\,|k|^{\alpha}\left[1 - i\,\beta\,\mathrm{sign}(k)\,\tan\left(\frac{\alpha\pi}{2}\right)\right] + i\,\delta_1\,k\right),\quad \alpha \neq 1$$

- Characteristic function of solution of space-fractional diffusion equation:

$$\tilde{P}(k,t) = \exp\left(D\,t\,\cos\left(\frac{\alpha\,\pi}{2}\right)|k|^{\alpha}\left[1 - i\,\mathrm{sign}(k)\;1\,\tan\left(\frac{\alpha\,\pi}{2}\right)\right] + 0\right)$$

Both equation are identical for:

$$\alpha \in (1,2] \qquad \beta = 1$$

$$\gamma = \left(-D\,t\,\cos\left(\frac{\alpha\,\pi}{2}\right)\right)^{1/\alpha} = (D_{\alpha}\,t)^{1/\alpha} \qquad \delta_1 = 0$$

Stable distribution

- Problem:

  For this stable distribution the inverse Fourier transform is not known!

- But, we know:
  - Asymptotic heavy tail behavior in closed form
  - Location of mean of distribution is $\delta_1 = 0$
  - Location of mode of distribution is indicated by $\delta_0 = \delta_1 - \gamma\,\beta\,\tan\left(\frac{\alpha\,\pi}{2}\right)$

➢ Numerical calculation of
$$P(x,t) = \mathbf{S}\left(x|\alpha,\beta,\gamma,\delta;n\right)$$

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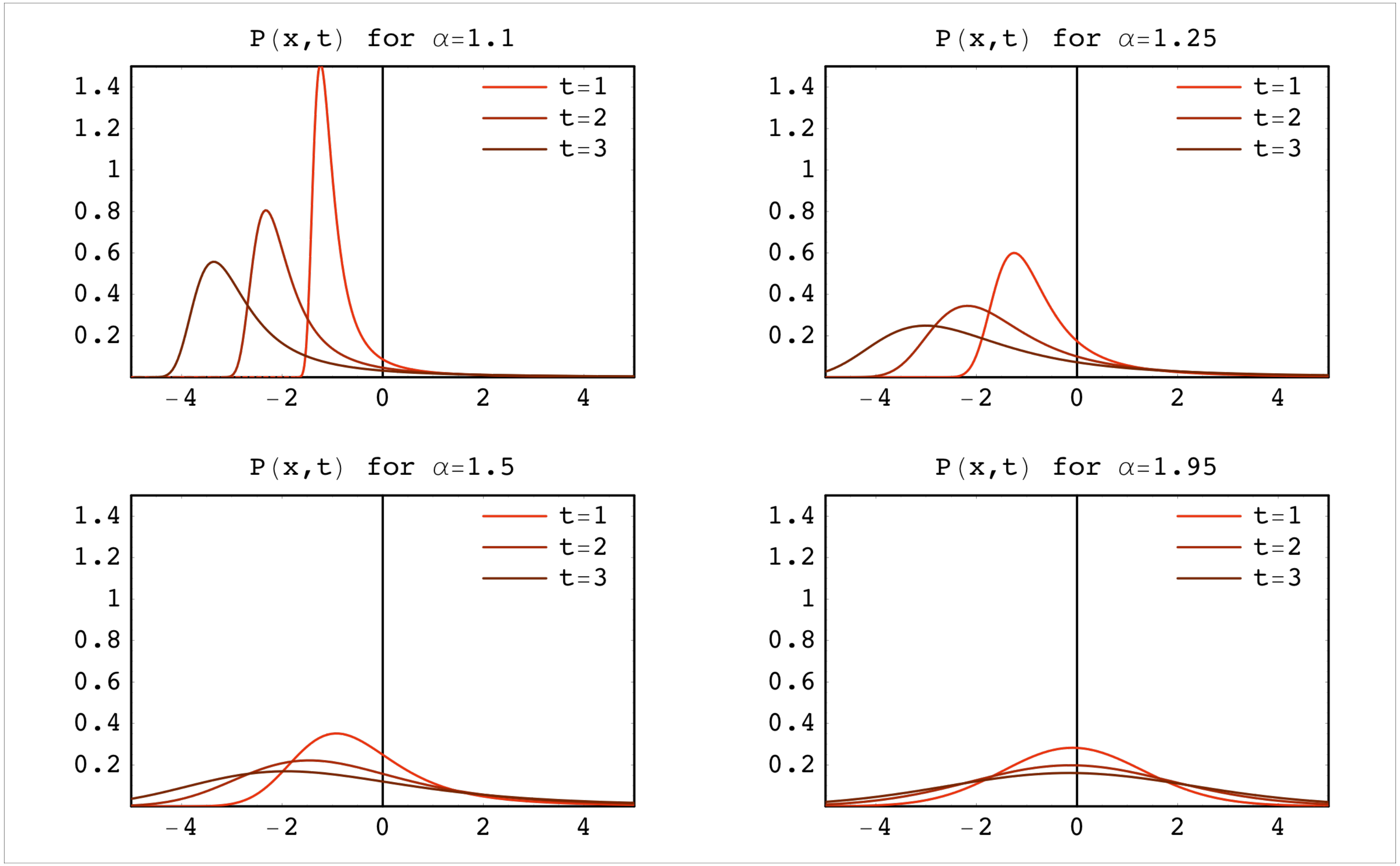
Examples of probability distribution $P(x,t)$



Bridging regime from wave equation to diffusion equation

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Remember:

- Natural measure of irreversibility:

Entropy production rate

Intuitive expectation:

Moving from the wave regime to the diffusion regime the entropy production rate should increase!

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3. What happens with the entropy production rate?

- Standard definition – Shannon entropy:

$$S = -\int_{-\infty}^{\infty} P(x,t)\,\ln(P(x,t))\,\mathrm{d}x$$

➢ Group method approach

- One-parameter group: $x = \lambda^{-1/\alpha}\,\tilde{x},\;\; t = \lambda\,\tilde{t}$
- Normalization: $P(x,t) = t^{-\frac{1}{\alpha}}\,G_\alpha(\eta)$ mit $\eta = x\,t^{-\frac{1}{\alpha}}$

$$S = \frac{1}{\alpha}\ln t - \int_{-\infty}^{\infty} G_\alpha(\eta)\,\ln(G_\alpha(\eta))\,\mathrm{d}\eta \;\;\rightarrow\;\; \underbrace{\dot{S} = \frac{1}{\alpha\,t}}_{\text{Entropy production rate}}$$

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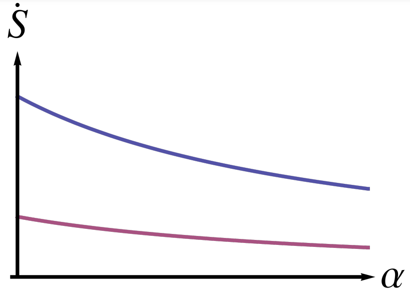
Entropy production paradox

- Entropy production rate: $\dot{S} = \dfrac{1}{\alpha\, t}$



> ➢ For increasing α $\dot{S}$ is monotonically decreasing
> Paradoxical behavior to intuitive expectation

- Same paradox also appears for generalized entropy definitions:
  - Tsallis entropy:

$$S_q^T \equiv -\frac{1}{1-q} \int_{-\infty}^{\infty} P(x,t)\,(1 - P^{q-1}(x,t))\mathrm{d}x \quad \text{mit } q \in \mathbb{R} \setminus \{1\}$$

  - Renyi entropy:

$$S_q^R \equiv \frac{1}{1-q} \ln \left(\int_{-\infty}^{\infty} P^q(x,t)\,\mathrm{d}\eta \right) \quad \text{mit } q > 0$$

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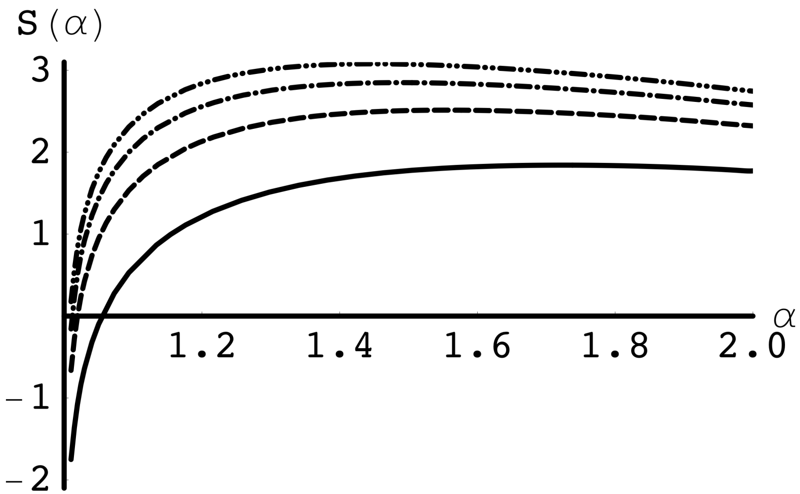
Entropy production paradox

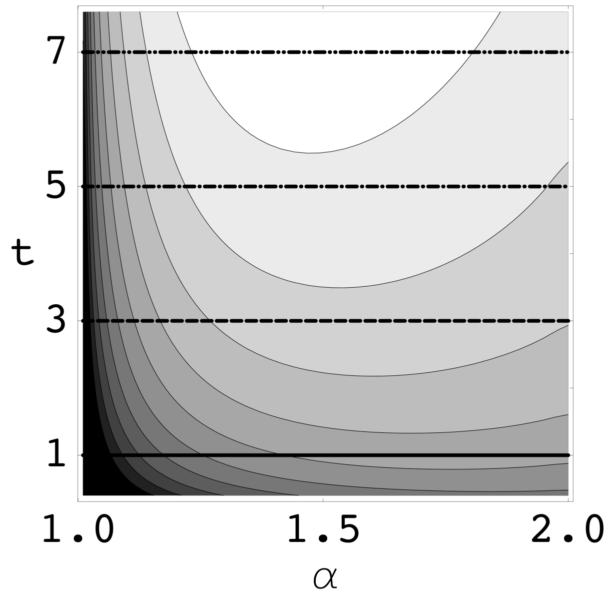
- How to explain the entropy production paradox?

➢ Considering the full α-dependence of the entropy

$$S = \frac{1}{\alpha} \ln t - \int_{-\infty}^{\infty} G_\alpha(\eta) \ln(G_\alpha(\eta))\, d\eta$$

➢ From intuitive expectation: Comparing entropies at equal times, the entropy for $\alpha \to 1$ should be smaller than for $\alpha \to 2$





$t = 1(—), 3(- -), 5(- \cdot -),$ and $7(- \cdot \cdot -)$

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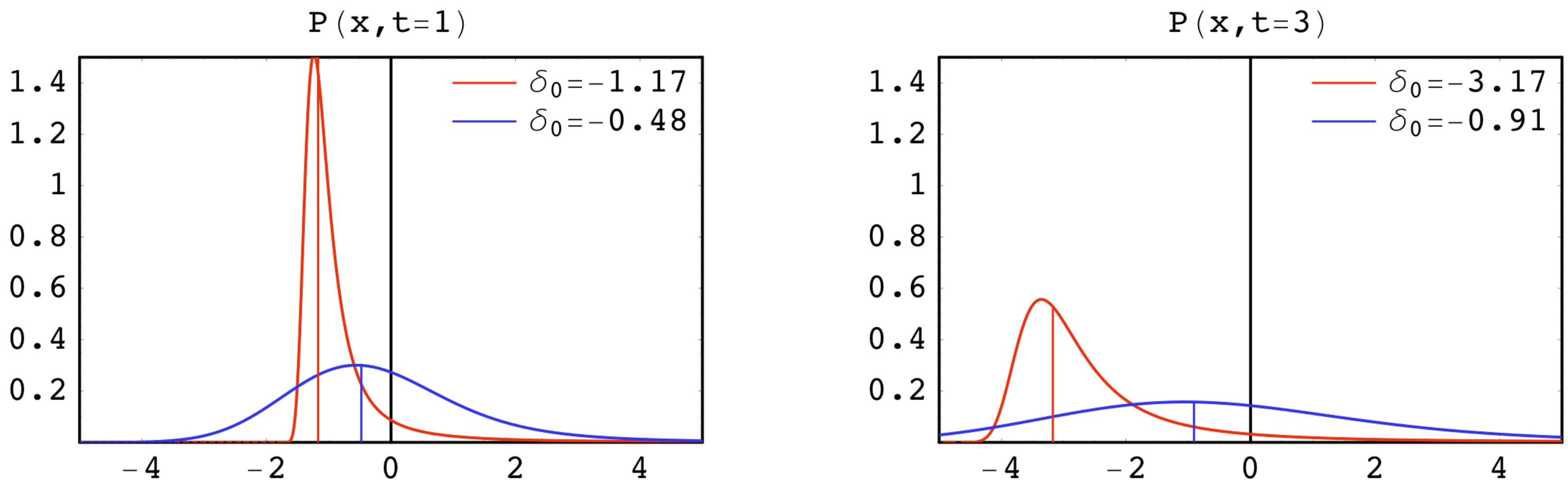
Why does the paradox appear?

Comparing two $P(x,t)$ two two different times $t=1,3$



For $\alpha = 1.1(—)$ and $1.7(—)$

– We know: $\delta_1 = 0 \rightarrow$ mean is zero

➢ Each process exhibits a change of shape of $P(x,t)$

➢ Each process has its internal quickness ➢ moving bulk

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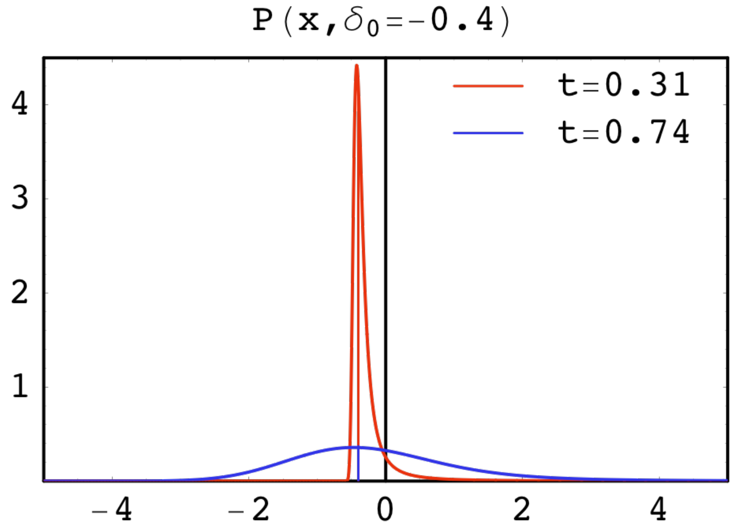
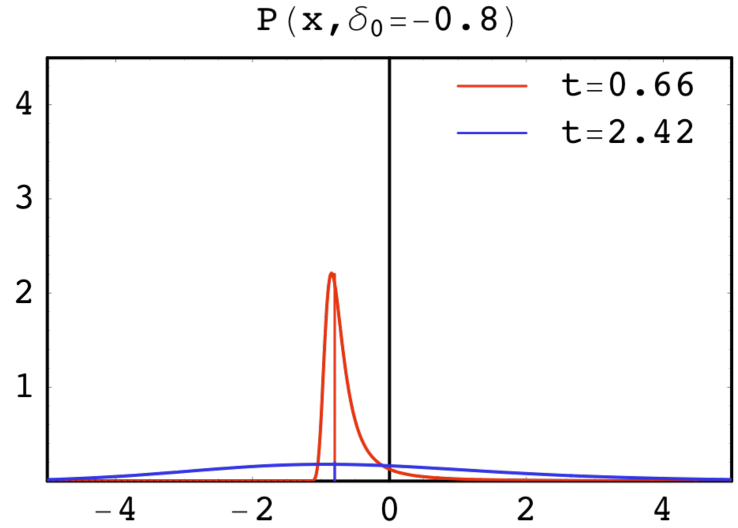
Eliminating effects of bulk movement

- What we know about stable distribution:
  - Localization of mode of distribution indicated by

$$\delta_0 = \gamma\,\beta\,\tan\left(\frac{\alpha\,\pi}{2}\right) = (D_\alpha\,t_\alpha)^{1/\alpha}\,\tan\left(\frac{\alpha\,\pi}{2}\right)$$





For $\alpha = 1.1(—)$ and $1.7(—)$

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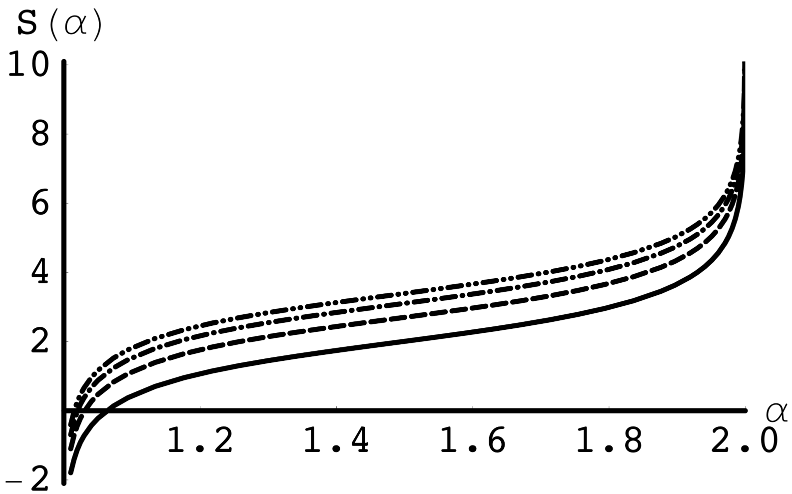
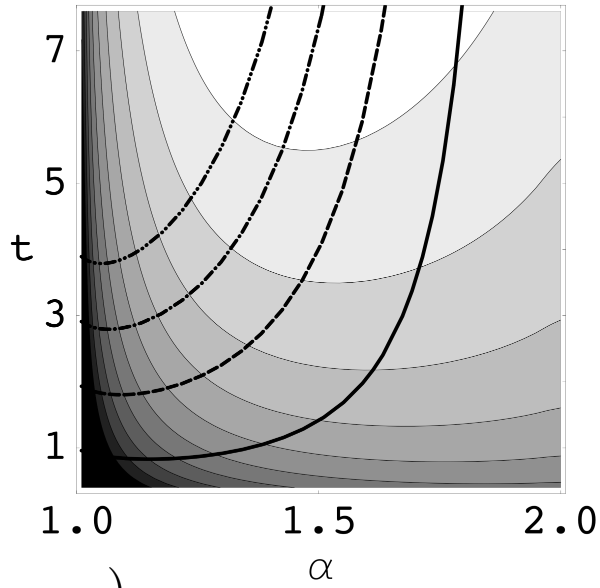
Resolving of the paradox

- Comparing entropies at fixed bulk positions δ_0 resolves the paradox:





$\delta_0 = -1(—), -3(- -), -5(- \cdot -),$ and $-7(- \cdot \cdot -)$

➢ The paradox is solved!

➢This new basis of comparison does also work for the Tsallis and Rényi entropy definiton.

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Summary

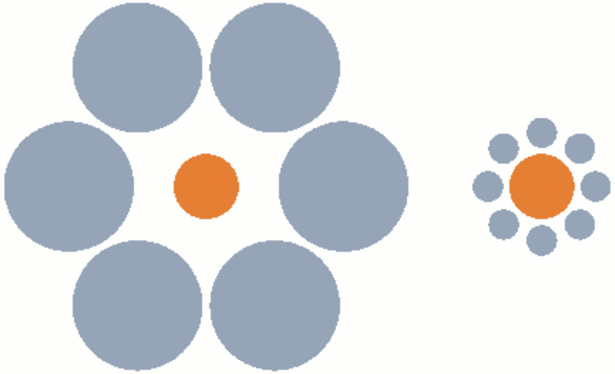
- Introduction of space-fractional diffusion equations as bridging regime between reversibility and irreversibility
- Expressing solution of space-fractional diffusion equations in terms of a stable distribution
- Numerical calculation of entropy and entropy production rate for different entropy definitions
- Observation of an entropy production paradox
- Resolution of the paradox by taking internal quickness and the change of the shape into account.

The end

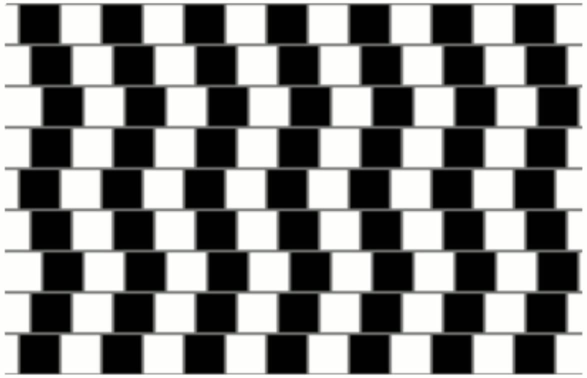
Thank you for your attention.

Questions?

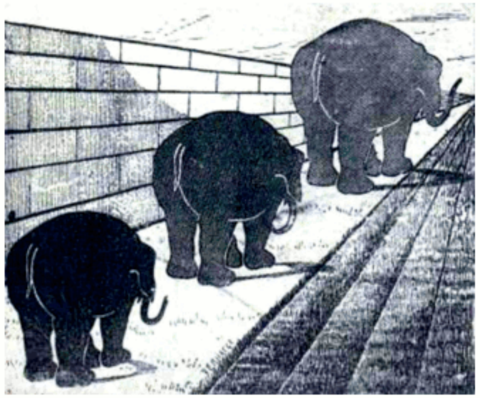
Optical Illusions



The right inner circle appears to be bigger



The horizontal lines look slanted



The elephants seem to be of different size

The ball appears to be in the goal.

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