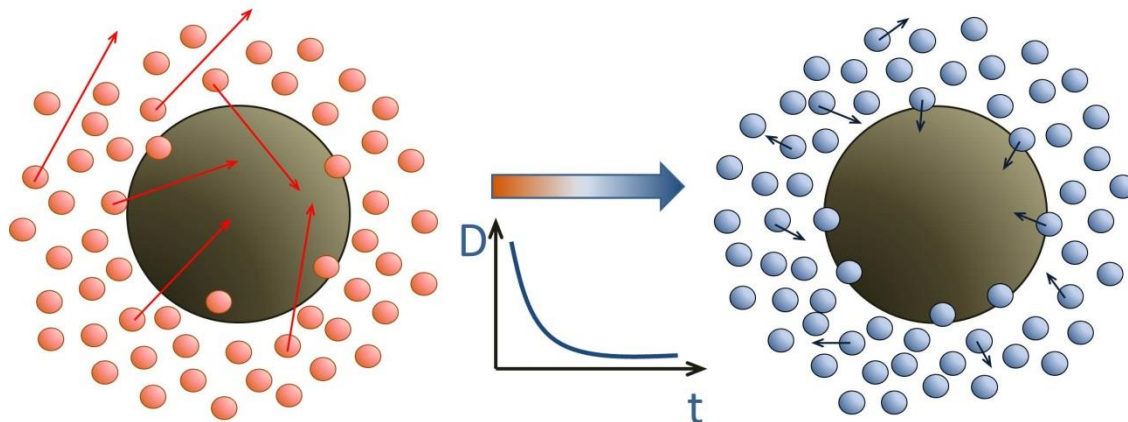


Brownian motion with time-dependent diffusion coefficient

Anna Bodrova

Skolkovo Institute of Science and Technology



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Andrey Cherstvy



Alexei Chechkin



Nikolay Brilliantov
University of Leicester,
United Kingdom



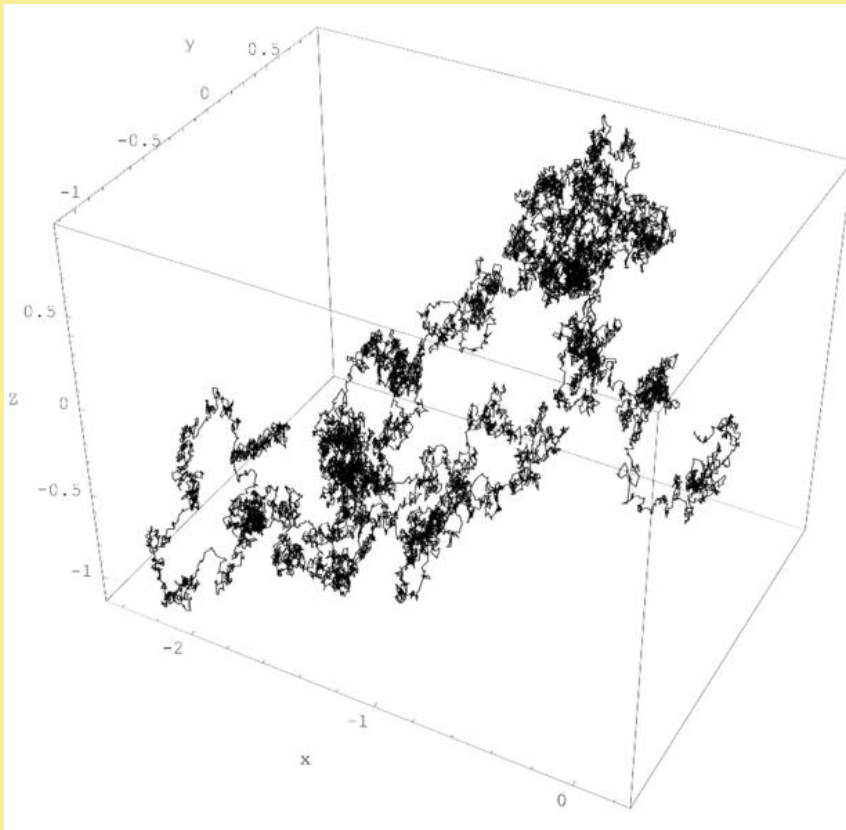
Igor Sokolov
Humboldt University,
Berlin, Germany

Normal diffusion

A. Einstein (1905)

$$\langle R^2(t) \rangle = 6Dt$$

D – diffusion coefficient

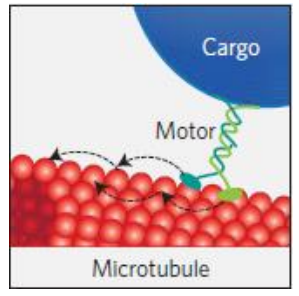
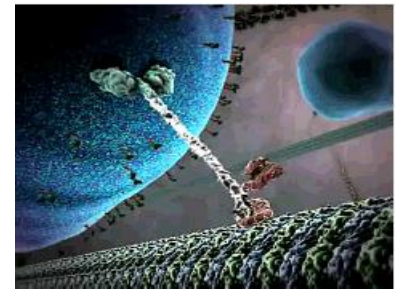


Anomalous diffusion

$$\langle R^2(t) \rangle \sim t^\alpha \quad \alpha \neq 1$$

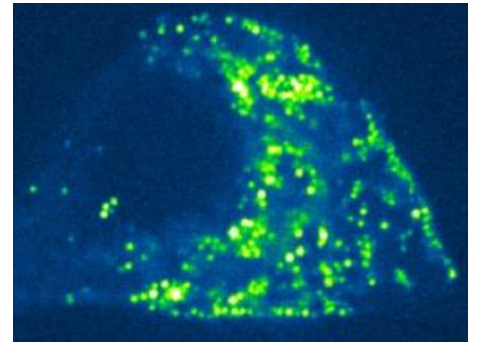
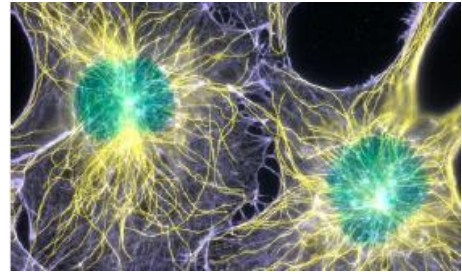
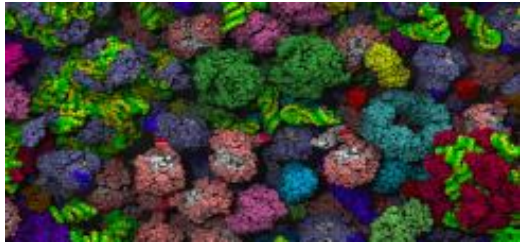
$$\alpha > 1$$

Superdiffusion



$$\alpha < 1$$

Subdiffusion



$$\alpha = 1$$

Normal diffusion

Anomalous diffusion in biology

Superdiffusion

- Flight of albatrosses.
- Movement of spider monkeys.
- Molecular motors: active motion of motor proteins with cargo along the filaments in the cytoskeleton.



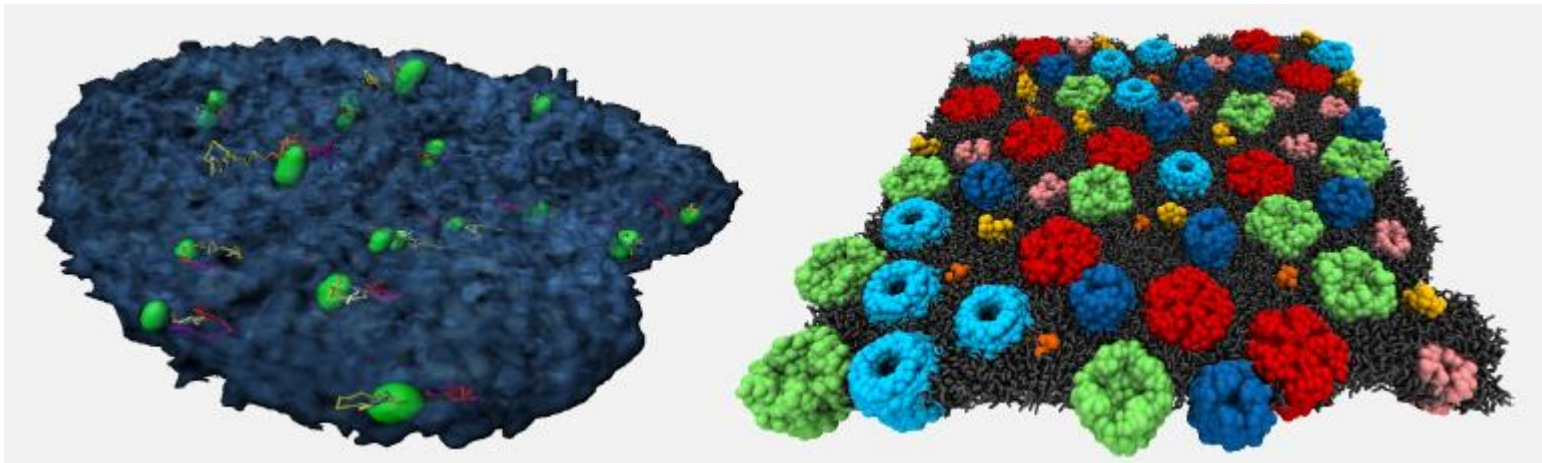
Advantages of superdiffusion in biology

- Superdiffusion leads to the effective search strategy for finding randomly located objects.

Anomalous diffusion in biology

Subdiffusion

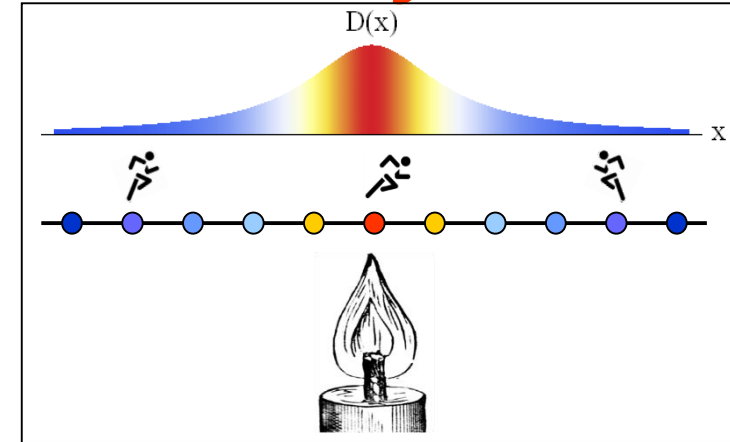
- Diffusion of **channel proteins** in cell membranes.
- Diffusion of **telomers** (chromosomal end parts) in human cell nuclei.
- Motion of **messenger RNA** in bacteria cells.
- Anomalous diffusion of large molecules due to **high density** of the **cell environment**.



Some sources of anomaly

Geometrical constraints

- Diffusion in crowded systems
- Diffusion on fractal structures



Diffusion in inhomogeneous environment

- Heterogeneous diffusion process (motion with space-dependent diffusion coefficient)

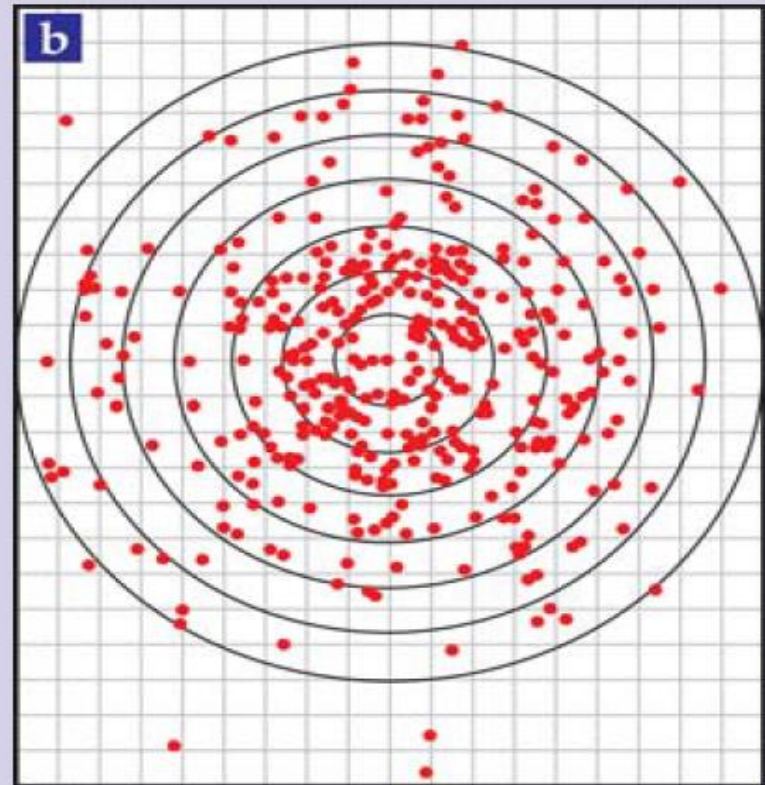
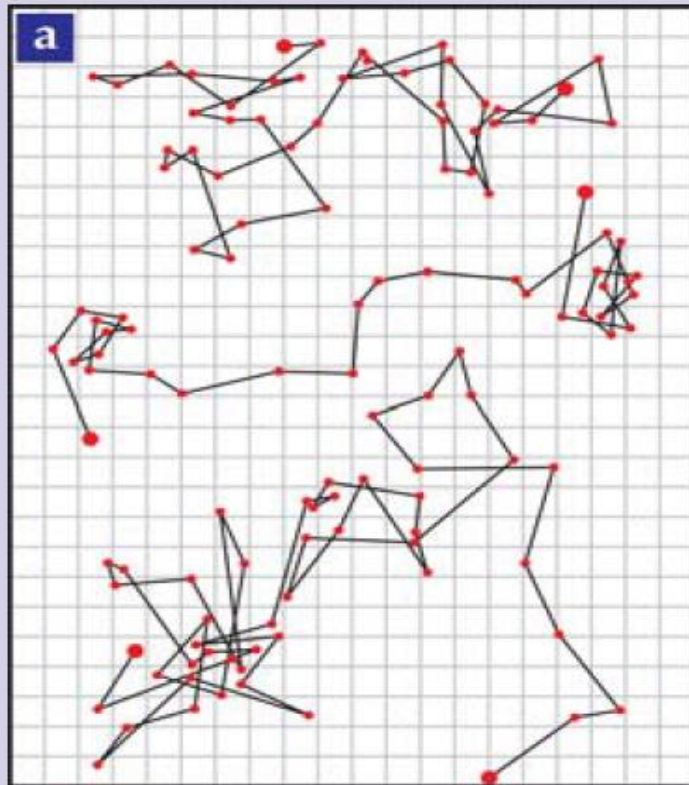
Diffusion in non-stationary environment

- Scaled Brownian motion (motion with time-dependent diffusion coefficient)

Ergodicity breaking

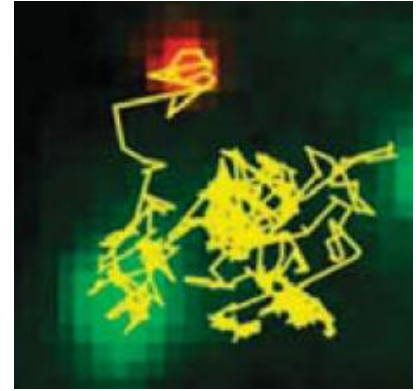
Ensemble averaged mean-squared displacement (MSD) is not equal to the ensemble-averaged MSD.

$$\langle \overline{\delta^2(\Delta)} \rangle \neq \langle x^2(\Delta) \rangle$$



Time-averaged mean-squared displacement (MSD)

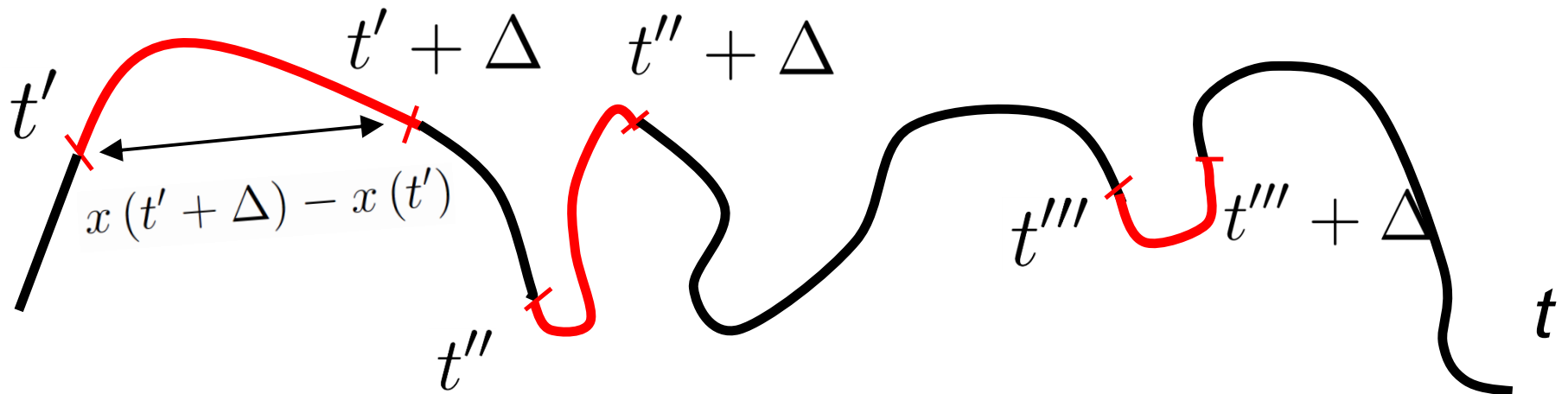
Single particle tracking experiments



$$\overline{\delta^2(\Delta)} = \frac{1}{t - \Delta} \int_0^{t-\Delta} [x(t' + \Delta) - x(t')]^2 dt'$$

Δ – lag time

t – trajectory length



Time-dependent diffusion coefficient $D(t)$

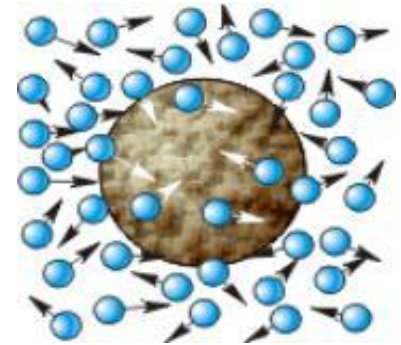
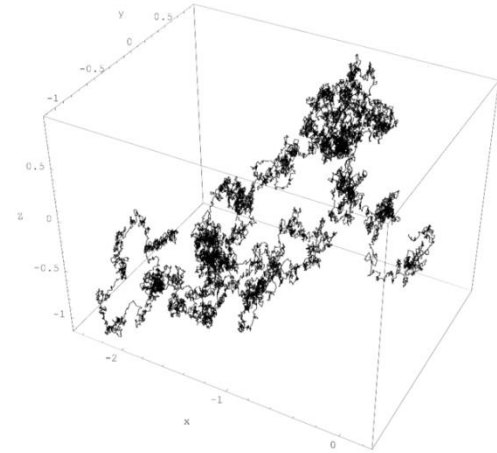
*I. Brownian motion in a bath with
time-dependent temperature*

II. Snow melt dynamics

III. Diffusion in turbulence

*IV. Water diffusion in **brain** tissue*

*V. Free cooling **granular** gases*



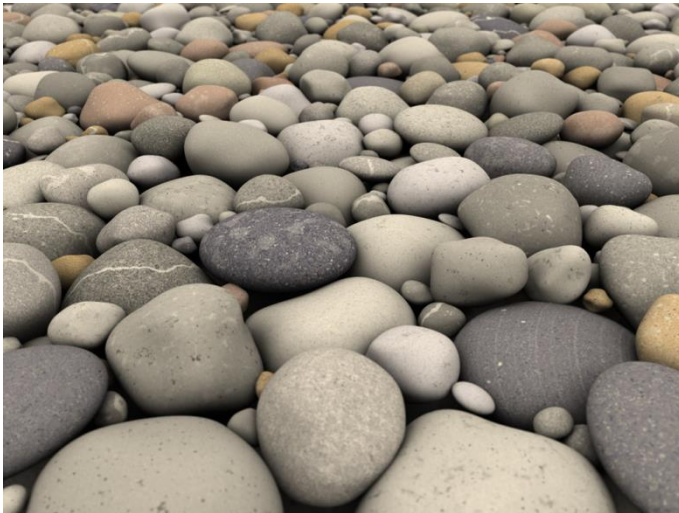
Granular systems



Powders



Sand



Stones



Nuts

Granular solids

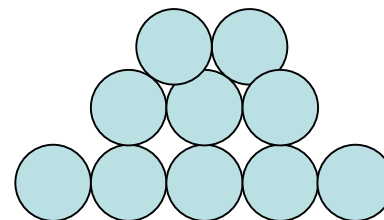
For **small loads** granular systems behave like **solids**:
resist the load and **preserve** their **form**



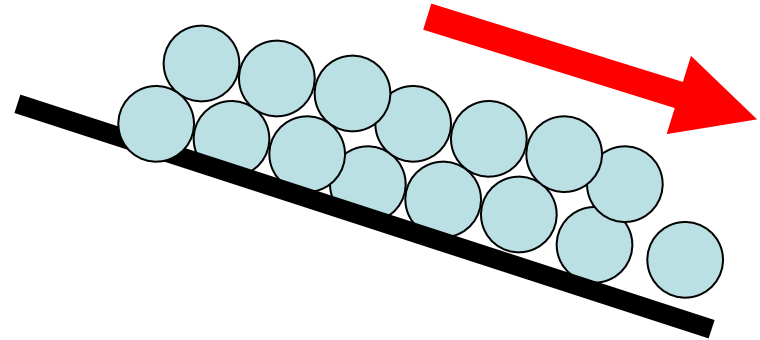
Sand



Stones

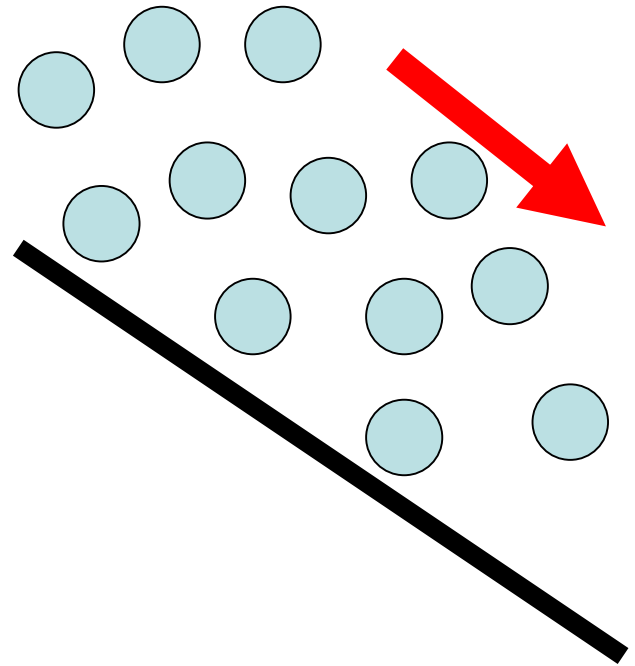


Granular liquids



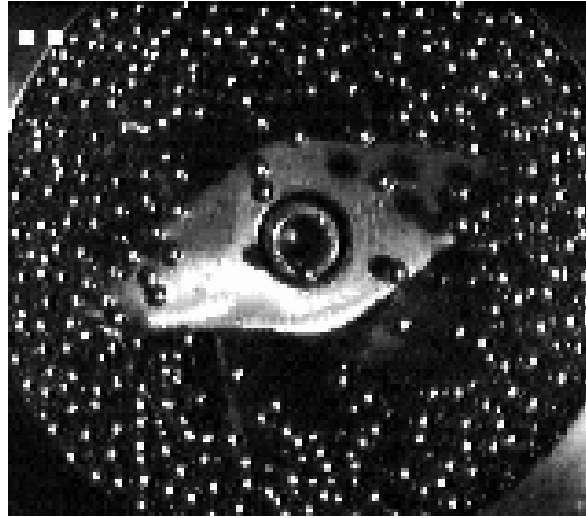
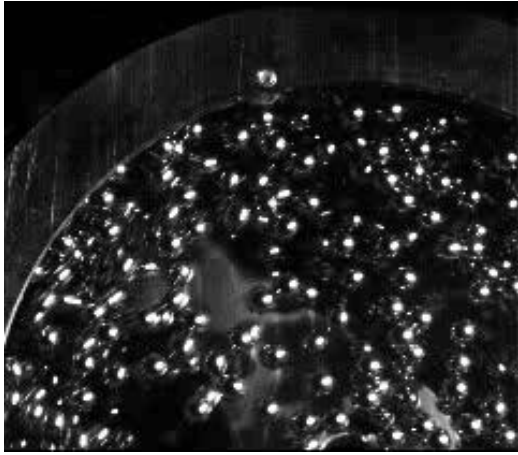
For **lager loads** they **flow** like **liquids** and **preserve** their **volume**

Granular gases

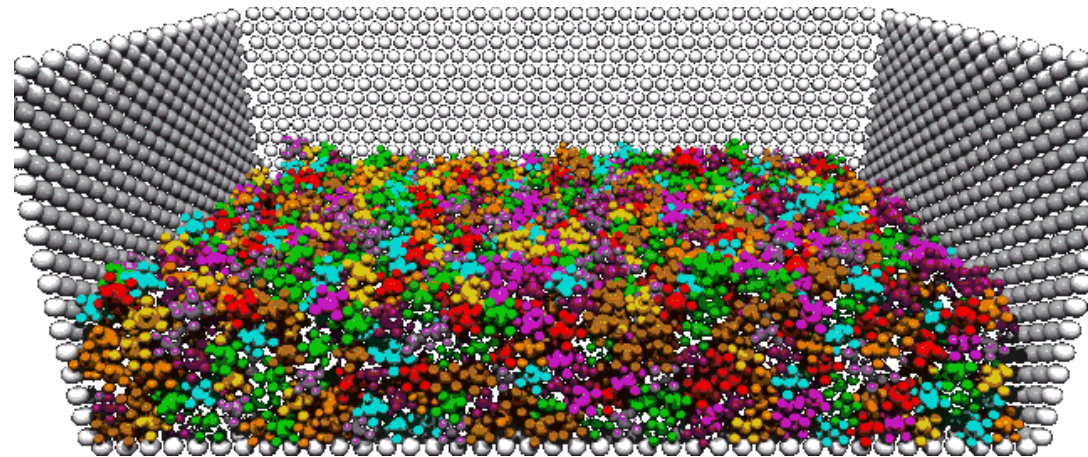


For **larger loads** they form rapid granular flows, where they behave like **gases**





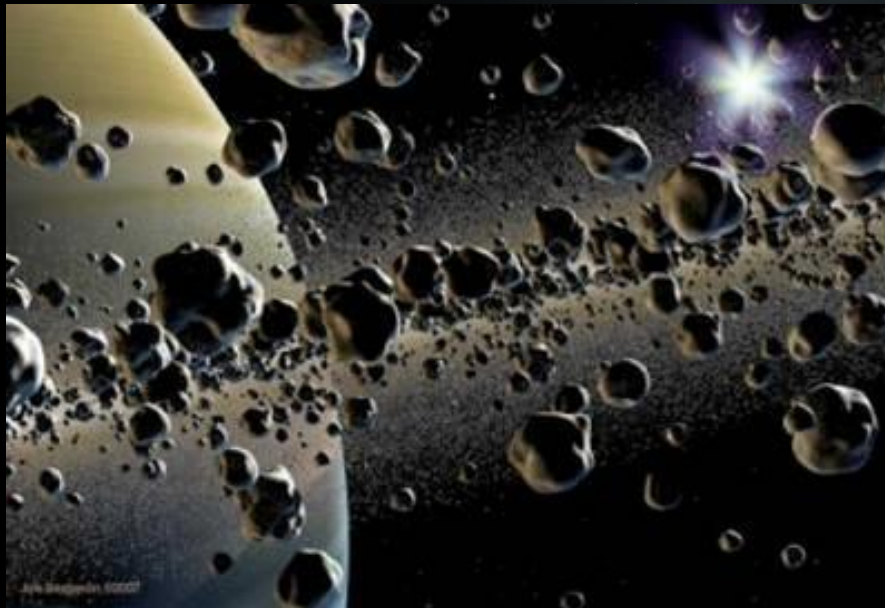
Granular gas – *rarefied* system of *macroscopic* particles, which collide with *loss of energy*



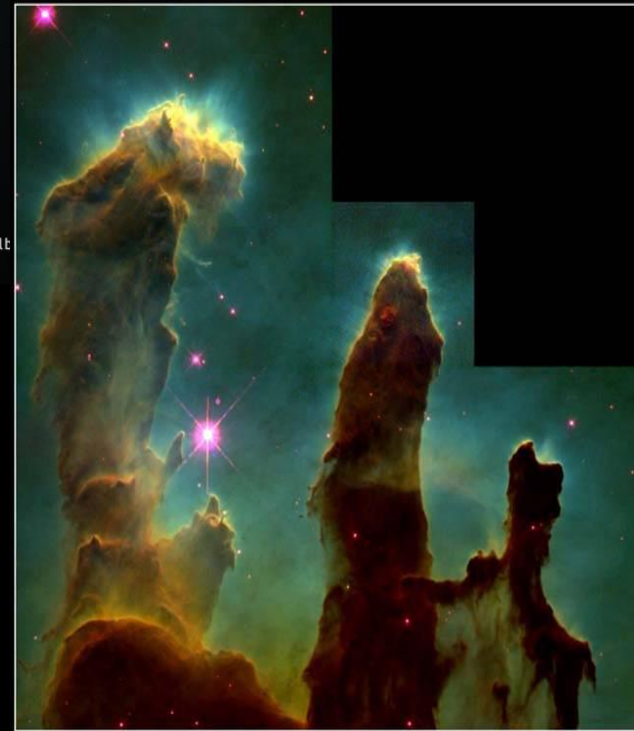
Granular gas: space



Protoplanetary disc



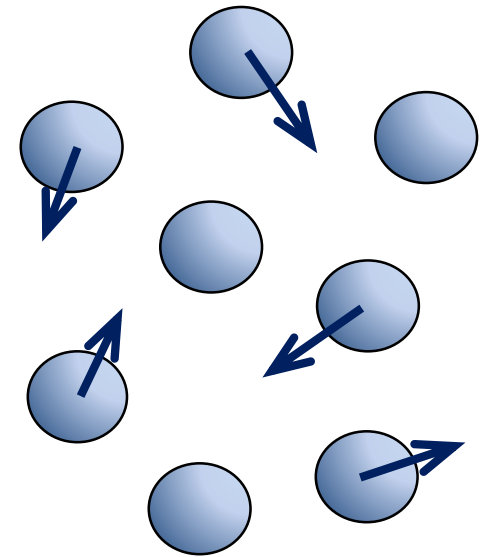
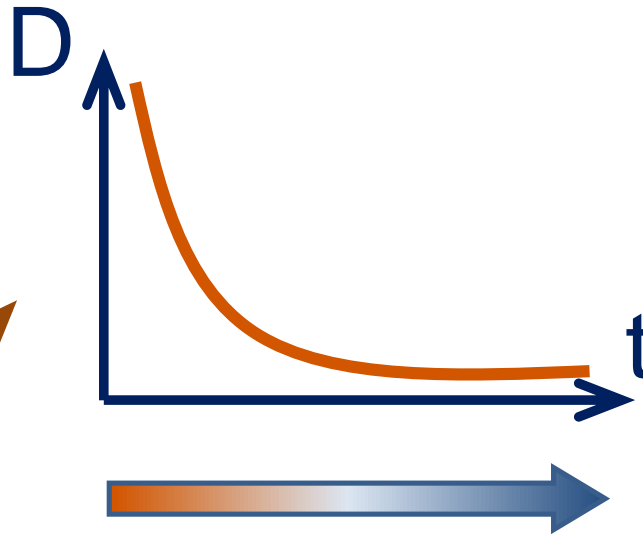
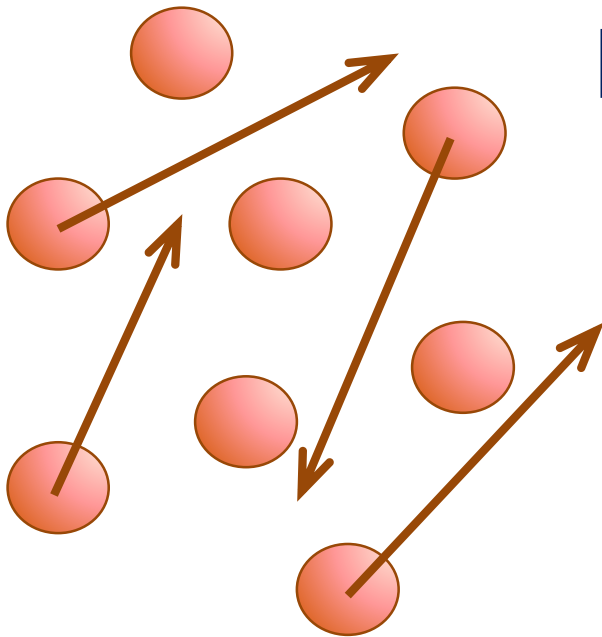
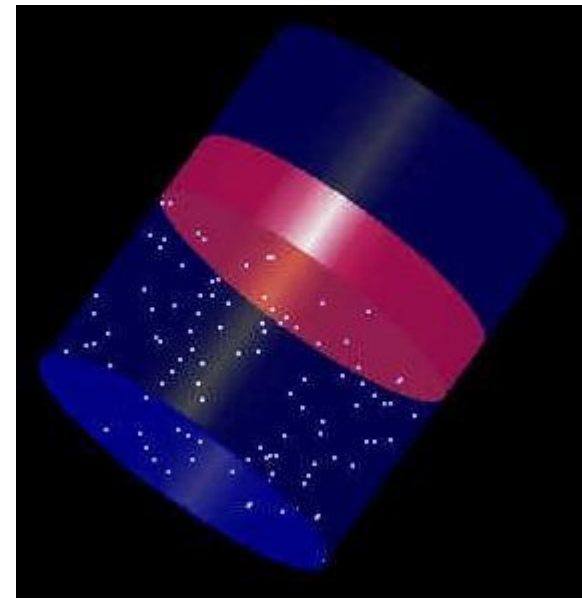
Planetary rings



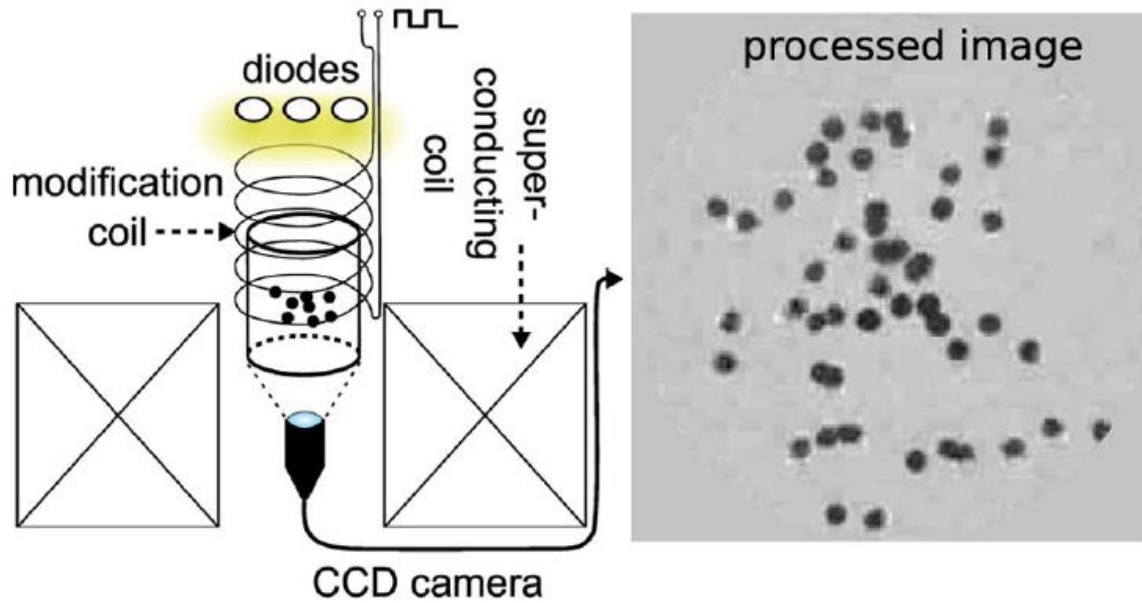
Interstellar dust

Free granular gas

If no external forces act on the granular system, it evolves freely and the particles slow down.



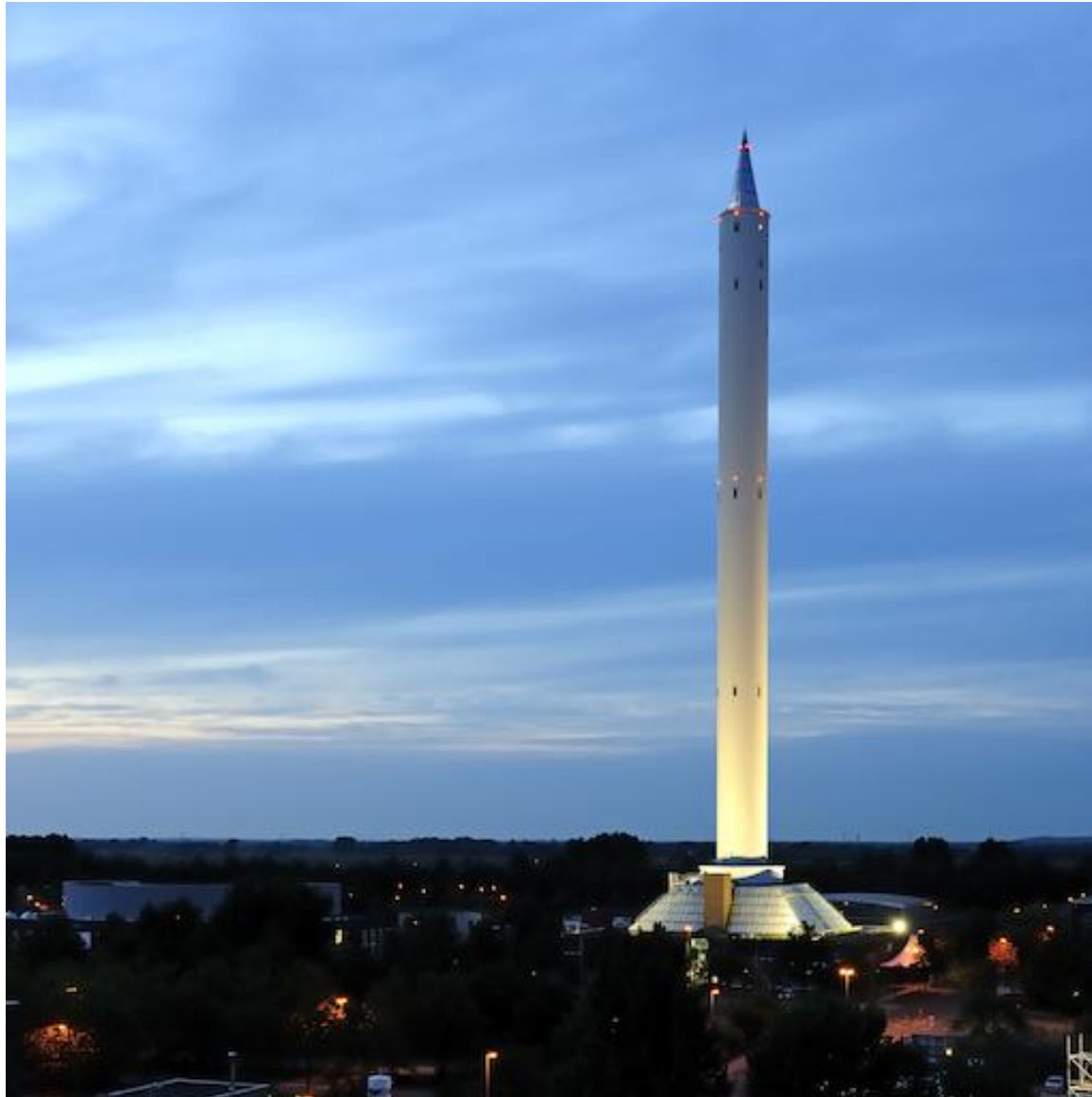
Magnetic levitation



Georg Maret, University of Konstanz, Germany

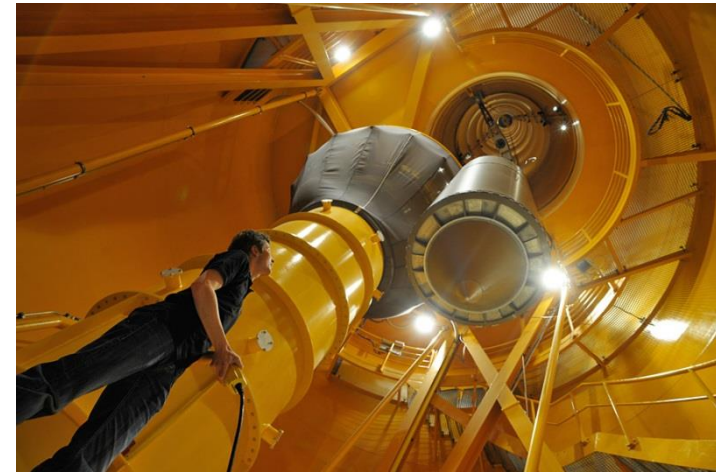
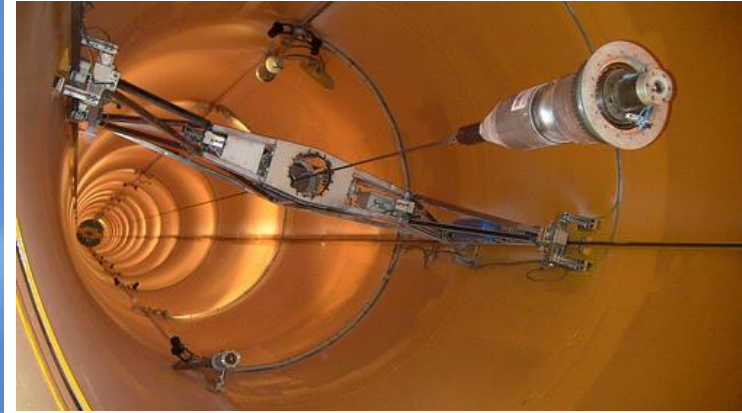


The Bremen Drop-tower



146 m

9.3 s of weightlessness

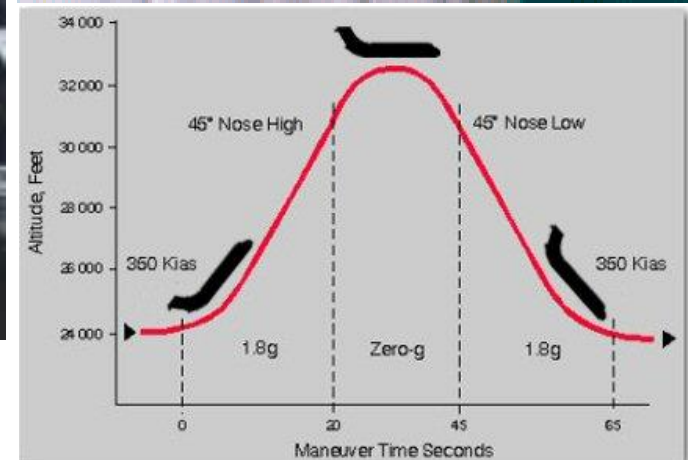


Low gravity environment



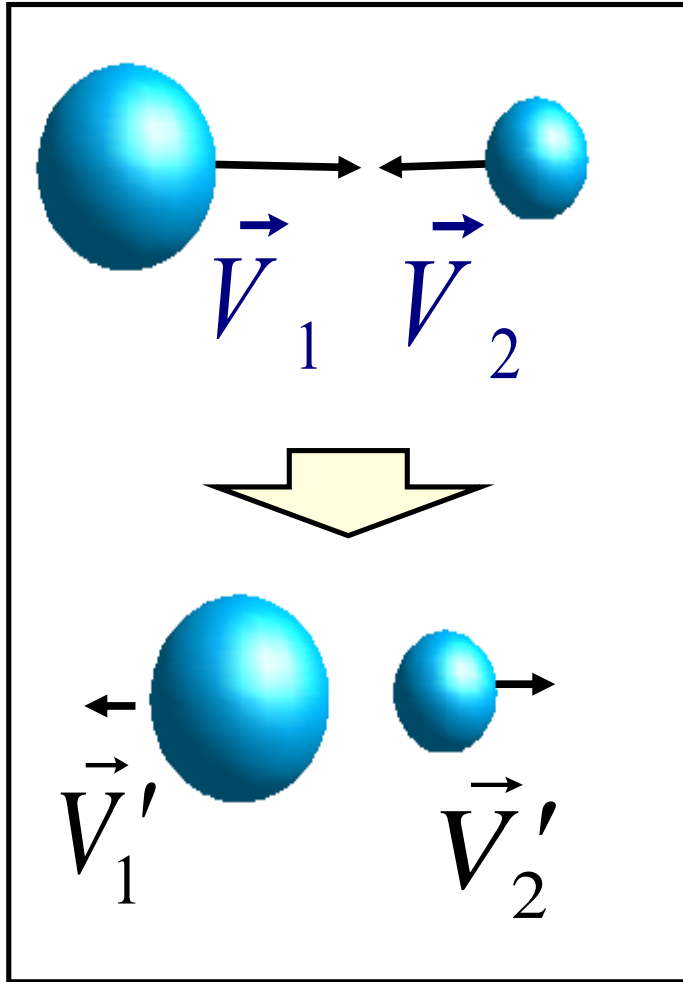
Rocket experiments (12 min of microgravity)

Eric Falcon, Univ Paris Diderot,
Sorbonne Paris Cité, Paris, France



*Parabolic flights
(30 parabolas,
20 s of reduced gravity)*

Restitution coefficient ε



$$\varepsilon = \frac{|\vec{V}_1' - \vec{V}_2'|}{|\vec{V}_1 - \vec{V}_2|} = \frac{|\vec{V}_{12}'|}{|\vec{V}_{12}|}$$



Energy loss:

$$\Delta E = -\frac{1}{4}(1 - \varepsilon^2)mV_{12}^2$$

$$0 \leq \varepsilon \leq 1$$

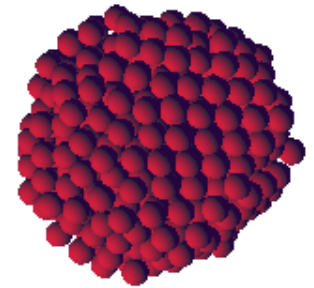
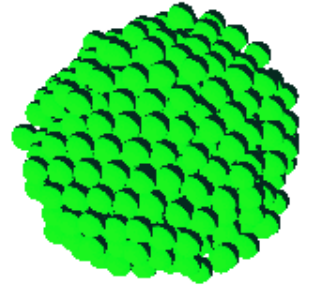
perfectly **inelastic**
collision

perfectly **elastic**
collision

Restitution coefficient ε

Dependence of ε on the relative velocity V_{12} :

$$\varepsilon(V_{12}) = 1 - C_1 V_{12}^{1/5} + C_2 V_{12}^{2/5} \mp \dots$$



Coefficients C_1 , C_2 depend on *Young's modulus*, *Poisson ratio*, *viscosity*, *density* and *sizes* of colliding particles

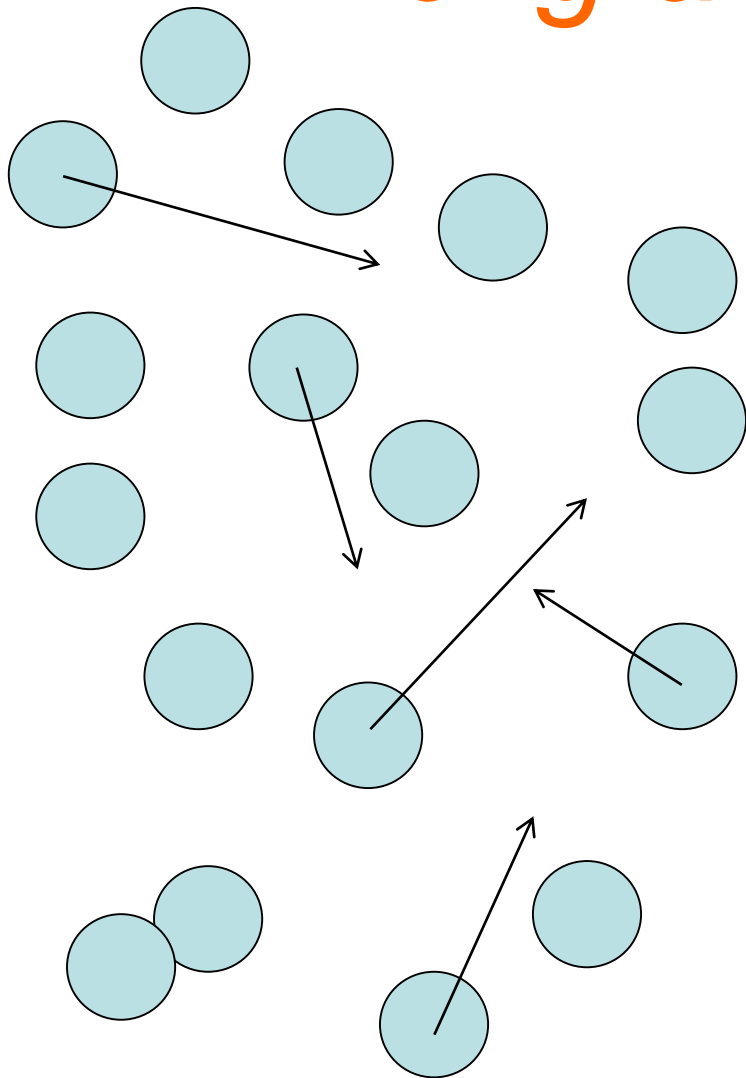
For *small* collisional relative velocities

$$V_{12} \rightarrow 0$$

collisions become *more elastic*:

$$\varepsilon \rightarrow 1$$

Event-driven simulations of granular gases



Restitution coefficient $\varepsilon = -\frac{(\vec{v}'_{12} \cdot \vec{n})}{(\vec{v}_{12} \cdot \vec{n})}$

$$\vec{v}'_1 = \vec{v}_1 - \frac{1}{2}(1 + \varepsilon)(\vec{v}_{12} \cdot \vec{n})\vec{n}$$
$$\vec{v}'_2 = \vec{v}_2 + \frac{1}{2}(1 + \varepsilon)(\vec{v}_{12} \cdot \vec{n})\vec{n}$$

Instantaneous binary collisions of particles

Granular temperature

$$T(t) = \frac{2}{3} \int d\vec{v} \frac{mv^2}{2} f(\vec{v}, \tau)$$

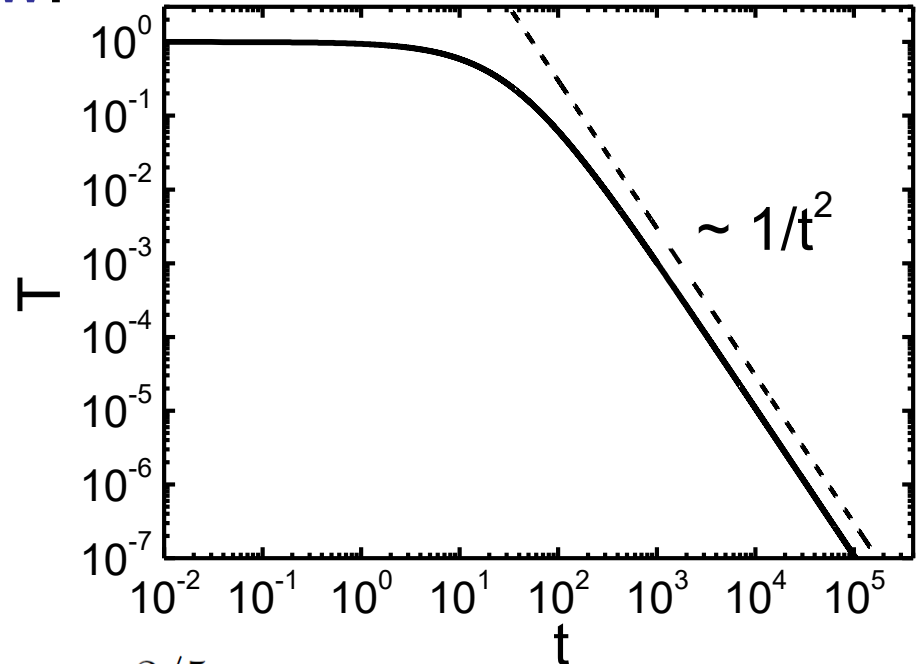
The mean kinetic energy (**granular temperature**) in a granular gas **decreases** due to inelastic collisions according to the **Haff's law**:

$$T(t) = \frac{T_0}{(1 + t / \tau_0)^2}$$

for $\varepsilon = \text{const}$

$$T(t) = \frac{T_0}{(1 + t / \tau_0)^{5/3}}$$

for $\varepsilon(V_{12}) = 1 - C_1 V_{12}^{1/5} + C_2 V_{12}^{2/5} \mp \dots$



Diffusion coefficient

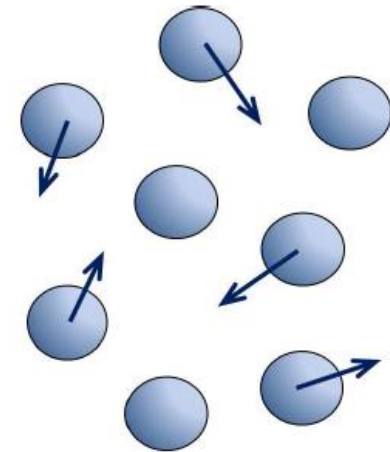
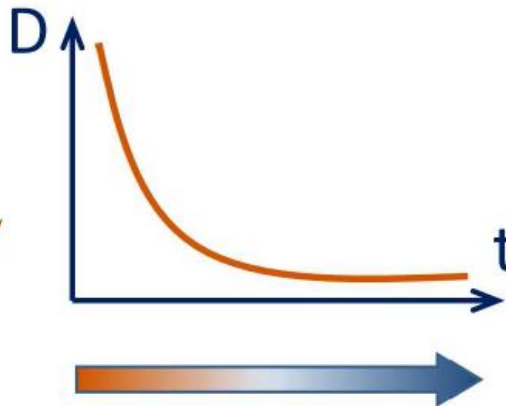
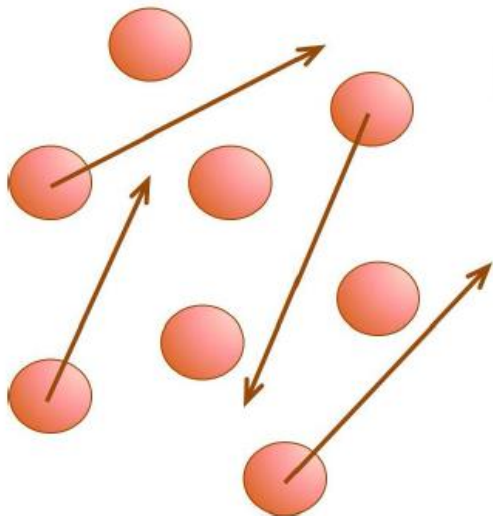
Diffusion coefficient of granular particles is time-dependent:

$$D(t) = \frac{d \langle r^2(t) \rangle}{dt}$$

$$D(t) = \frac{T(t)\tau_v(t)}{m} \quad \tau_v(t) - \text{velocity correlation time}$$

$$\tau_v^{-1}(t) = \frac{2}{3} \sqrt{\pi} \sigma^2 n \sqrt{\frac{T(t)}{m}} (1 + \varepsilon)^2$$

$$D(t) \sim \sqrt{T(t)}$$



Diffusion coefficient of rough granular particles

$$D(t) = \frac{T(t)}{m} \left(\frac{2}{3} \tau_c^{-1}(t) \left(\frac{1 + \varepsilon}{2} + \frac{q(1 + \beta)}{2(1 + q)} \right) - \frac{1}{2} \xi \right)^{-1}$$

Moment of inertia

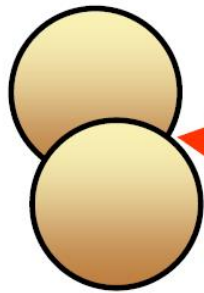
$$I = \frac{qm\sigma^2}{4}$$

Tangential restitution coefficient $\beta = -\frac{g_t'}{g_t}$

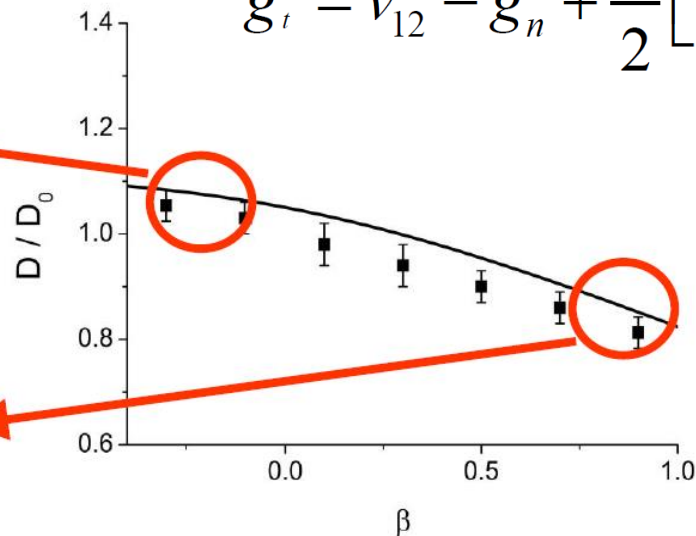
Tangential velocity

$$\vec{g}_t = \vec{v}_{12} - \vec{g}_n + \frac{\sigma}{2} [\vec{e} \times (\vec{\omega}_1 + \vec{\omega}_2)]$$

Smooth particles



Rough particles



Diffusion coefficient of granular gases

Constant
restitution coefficient

$$\varepsilon = \textit{const}$$

Velocity-dependent
restitution coefficient

$$\varepsilon(V_{12}) = 1 - C_1 V_{12}^{1/5} + C_2 V_{12}^{2/5} \mp \dots$$

Granular temperature
(mean kinetic energy of granular particles)

$$T(t) = T_0 \frac{1}{(1 + t/\tau_0)^2}$$

$$T(t) = \frac{T_0}{(1 + t/\tau_0)^{5/3}}$$

Diffusion coefficient

$$D(t) = \frac{T(t)\tau_v(t)}{m} = \frac{D_0}{1 + t/\tau_0}$$

$$D(t) = \frac{D_0}{(1 + t/\tau_0)^{5/6}}$$

Overdamped Langevin equation

$$\cancel{m \frac{dy}{dt}} + \gamma(t)v = \sqrt{2D(t)}\gamma(t)\xi(t)$$

White Gaussian noise

$$v = \sqrt{2D(t)}\xi(t)$$

$$\langle \xi(t_1)\xi(t_2) \rangle = \delta(t_1 - t_2)$$

Scaled Brownian motion (SBM)

Ultraslow SBM

Diffusion coefficient

$$D(t) = \frac{\alpha D_0}{t^{1-\alpha}} \quad \alpha > 0$$

$$D(t) = \frac{D_0}{1+t/\tau_0} \sim \frac{1}{t} \quad \alpha = 0$$

Mean-squared displacement (MSD)

$$\langle x^2(t) \rangle = 2D_0 t^\alpha$$

$$\langle x^2(t) \rangle = 2D_0 \tau_0 \log(1+t/\tau_0)$$

Underdamped Langevin equation with time-dependent temperature

$$m \frac{dv}{dt} + \gamma(t)v = \sqrt{2D(t)\gamma(t)}\xi(t)$$

Friction coefficient

$$\gamma(t) = \frac{m}{\tau_v(0)} \sqrt{\frac{T(t)}{T(0)}}$$

Temperature

$$T(t) = \frac{T(0)}{(1 + t/\tau_0)^{2-2\alpha}}$$

Diffusion coefficient

$$D(t) = \frac{D_0}{(1 + t/\tau_0)^{1-\alpha}}$$

Mean-squared displacement

$$\langle x^2(t) \rangle = 2D_0 \left[\frac{\tau_0}{\alpha} \left(\left(1 + \frac{t}{\tau_0}\right)^\alpha - 1 \right) + \tau_v(0) \left(\exp \left(-\frac{\tau_0}{\alpha\tau_v(0)} \left[\left(1 + \frac{t}{\tau_0}\right)^\alpha - 1 \right] \right) - 1 \right) \right]$$

For large times $t \gg \tau_0$ *SBM result* $\langle x^2(t) \rangle = \frac{2D_0\tau_0^{1-\alpha}}{\alpha} t^\alpha$

For small times $t \ll \tau_0$ *ballistic behavior* $\langle x^2(t) \rangle = \frac{D_0 t^2}{\tau_v(0)}$

Time-averaged MSD

$$\langle \overline{\delta^2(\Delta)} \rangle = \langle \overline{\delta_0^2(\Delta)} \rangle + \langle \Xi(\Delta) \rangle$$

Underdamped

Overdamped

$$\langle \overline{\delta_0^2(\Delta)} \rangle = \frac{2D_0\tau_0^2}{\alpha(\alpha+1)(t-\Delta)} \times \left[1 + \left(1 + \frac{t}{\tau_0}\right)^{\alpha+1} - \left(1 + \frac{\Delta}{\tau_0}\right)^{\alpha+1} - \left(1 + \frac{t-\Delta}{\tau_0}\right)^{\alpha+1} \right]$$

$$\langle \Xi(\Delta) \rangle = \frac{2D_0\tau_v(0)}{t-\Delta} \int_0^{t-\Delta} dt' \left[\exp\left(-\frac{\hat{\tau}}{\alpha} \left[\left(1 + \frac{t'+\Delta}{\tau_0}\right)^\alpha - \left(1 + \frac{t'}{\tau_0}\right)^\alpha \right]\right) - 1 \right]$$

For large lag times $\Delta \gg \tau_v(0) (t/\tau_0)^{1-\alpha}$

the underdamped and overdamped limits become comparable:

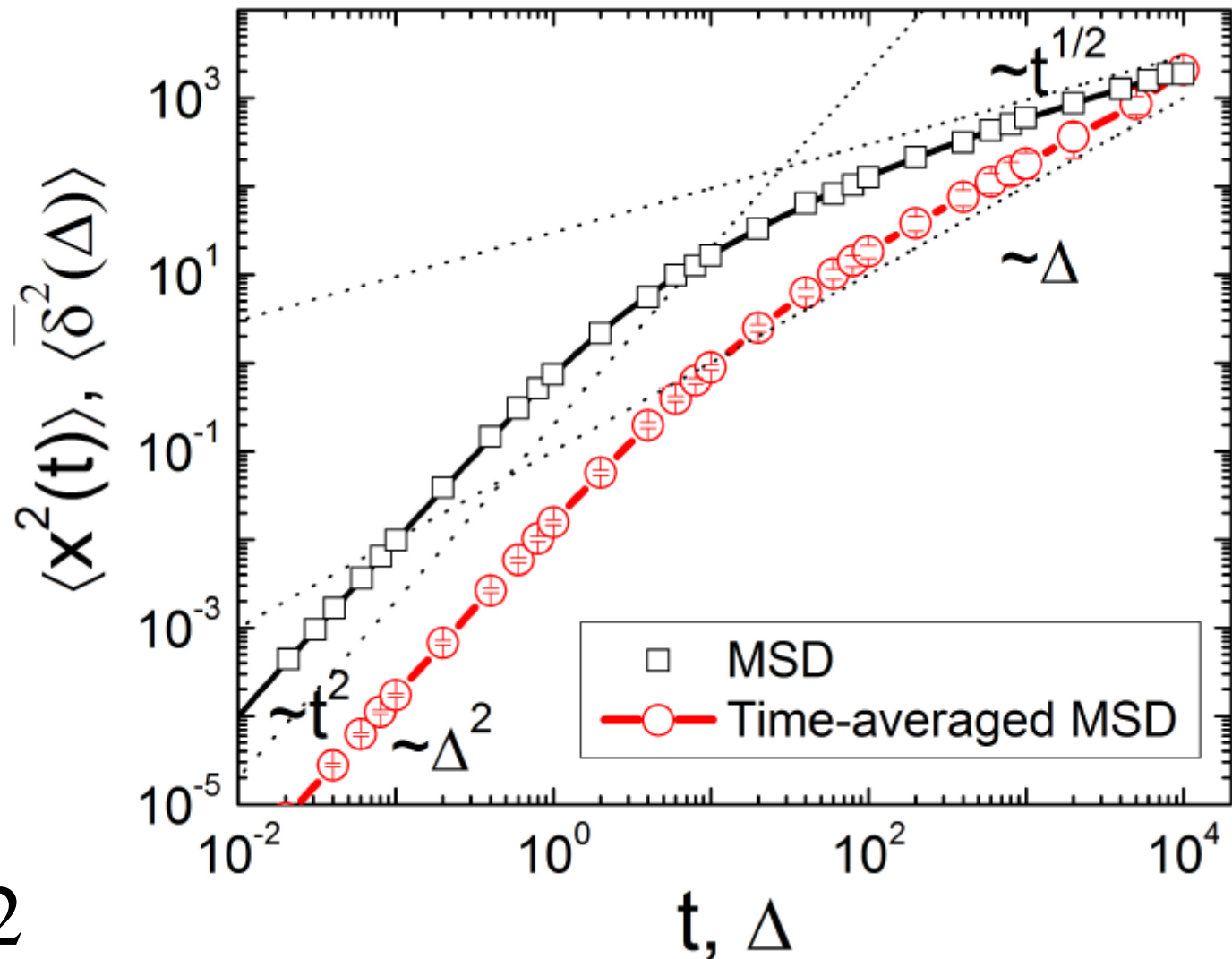
$$\langle \overline{\delta^2(\Delta)} \rangle \simeq \langle \overline{\delta_0^2(\Delta)} \rangle \simeq \frac{2D_0\tau_0^{1-\alpha}\Delta}{\alpha t^{1-\alpha}}$$

For intermediate lag times $\Delta \ll \tau_v(0) (t/\tau_0)^{1-\alpha} \ll t$

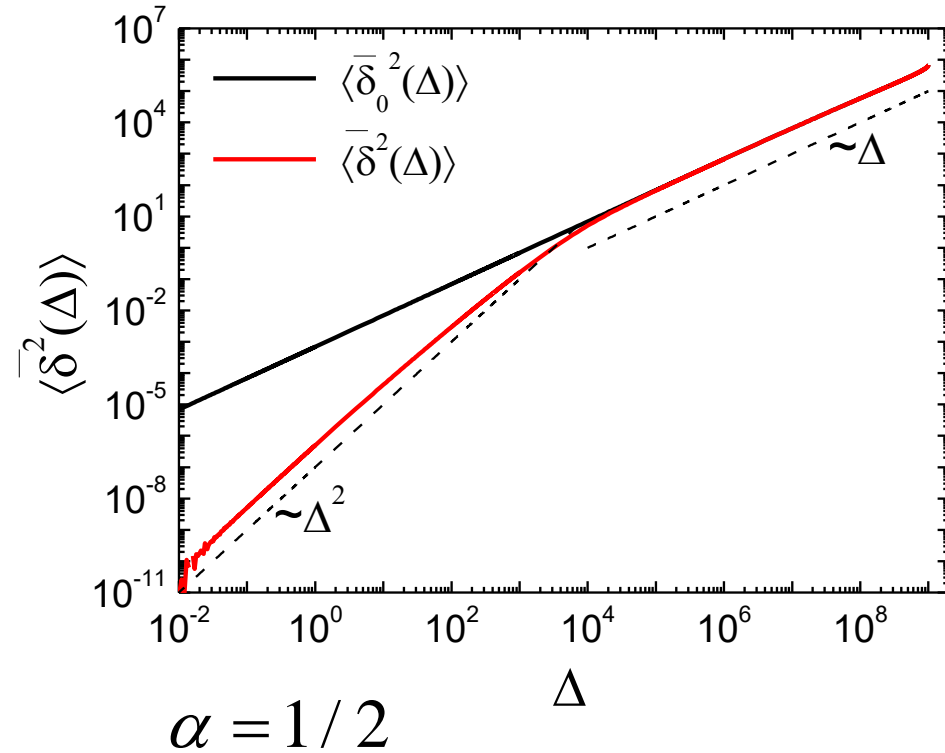
$$\langle \overline{\delta^2(\Delta)} \rangle \simeq \frac{2D_0\tau_0^{1-\alpha}\Delta^{\alpha+1}}{\alpha t}$$

Underdamped SBM

MSD and time-averaged MSD



Time-averaged MSD: overdamped and underdamped limits

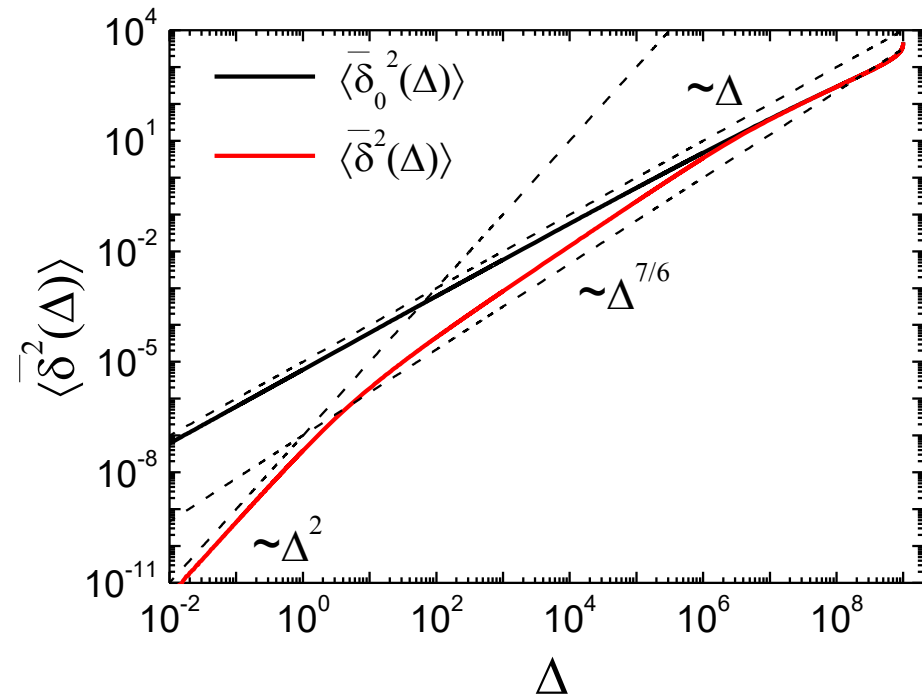


$$\langle \delta^2(\Delta) \rangle \simeq \langle \delta_0^2(\Delta) \rangle \simeq \frac{2D_0\tau_0^{1-\alpha}\Delta}{\alpha t^{1-\alpha}}$$

Underdamped Overdamped

$$\alpha = 1/6$$

$$\langle \delta^2(\Delta) \rangle \simeq \frac{2D_0\tau_0^{1-\alpha}\Delta^{\alpha+1}}{\alpha t}$$



Underdamped Langevin equation: ultraslow limit

$$\frac{dv}{dt} + \frac{\tau_v^{-1}(0)}{(1 + t/\tau_0)} v = \sqrt{\frac{2D_0}{1 + t/\tau_0}} \frac{\tau_v^{-1}(0)}{(1 + t/\tau_0)} \xi(t)$$

Friction coefficient

$$\gamma(t) = \frac{m}{\tau_v(0)} \sqrt{\frac{T(t)}{T(0)}}$$

Temperature

$$T(t) = T_0 \frac{1}{(1 + t/\tau_0)^2}$$

Diffusion coefficient

$$D(t) = \frac{D_0}{1 + t/\tau_0}$$

Mean-squared displacement

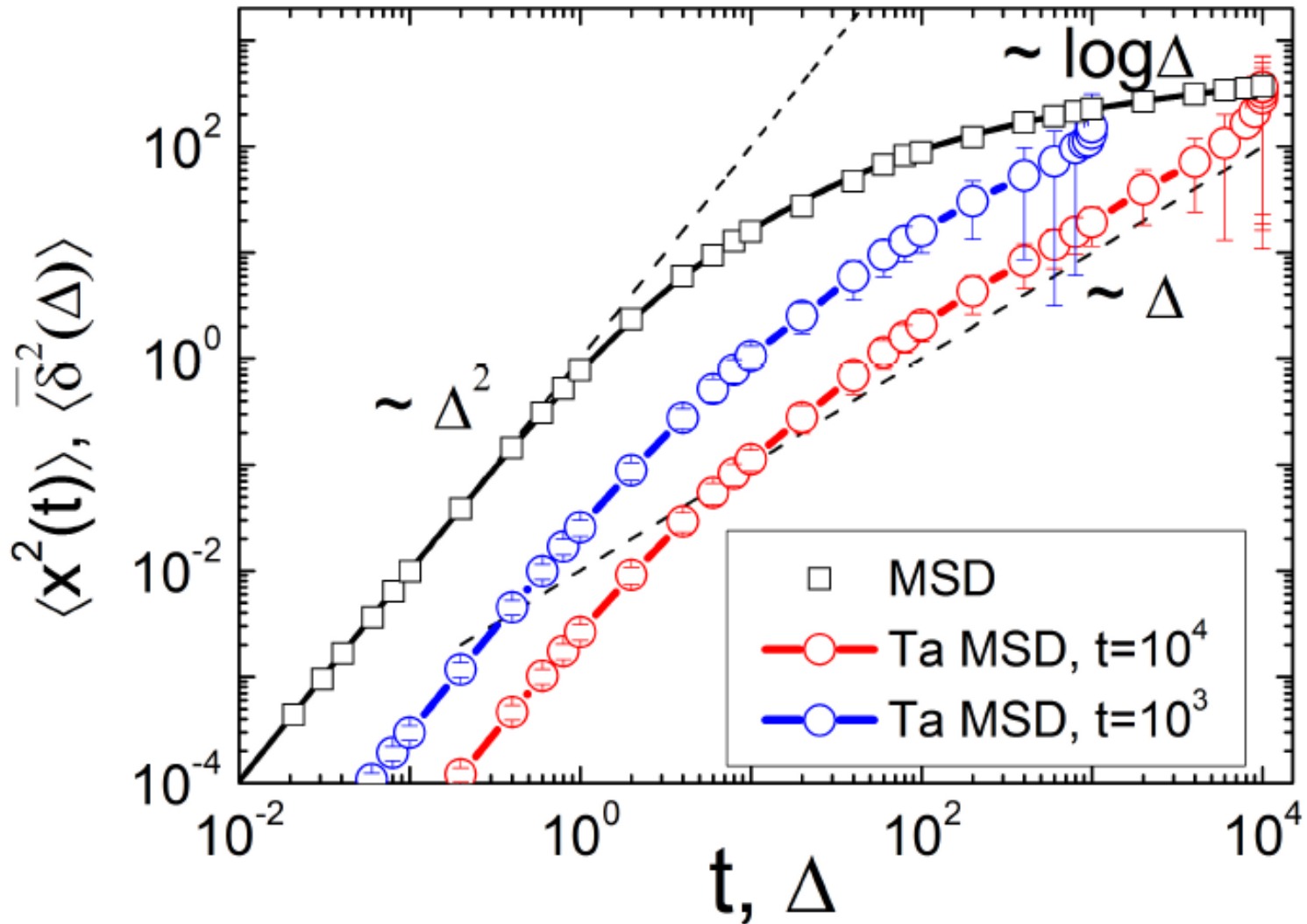
$$\langle x^2(t) \rangle = \frac{2D_0\tau_0^3}{\tau_v^2(0) (\hat{\tau} - 1)^2} \left[\log \left(1 + \frac{t}{\tau_0} \right) + \frac{1}{\hat{\tau} - 1} \left(\left(1 + \frac{t}{\tau_0} \right)^{1-\hat{\tau}} - 1 \right) \right]$$

Time-averaged mean-squared displacement

$$\langle \overline{\delta^2(\Delta)} \rangle \sim \frac{D_0 \Delta}{t} \quad \text{for} \quad \tau_0 \ll \Delta \ll t \quad \hat{\tau} = \frac{\tau_0}{\tau_v(0)}$$

Ultraslow underdamped SBM

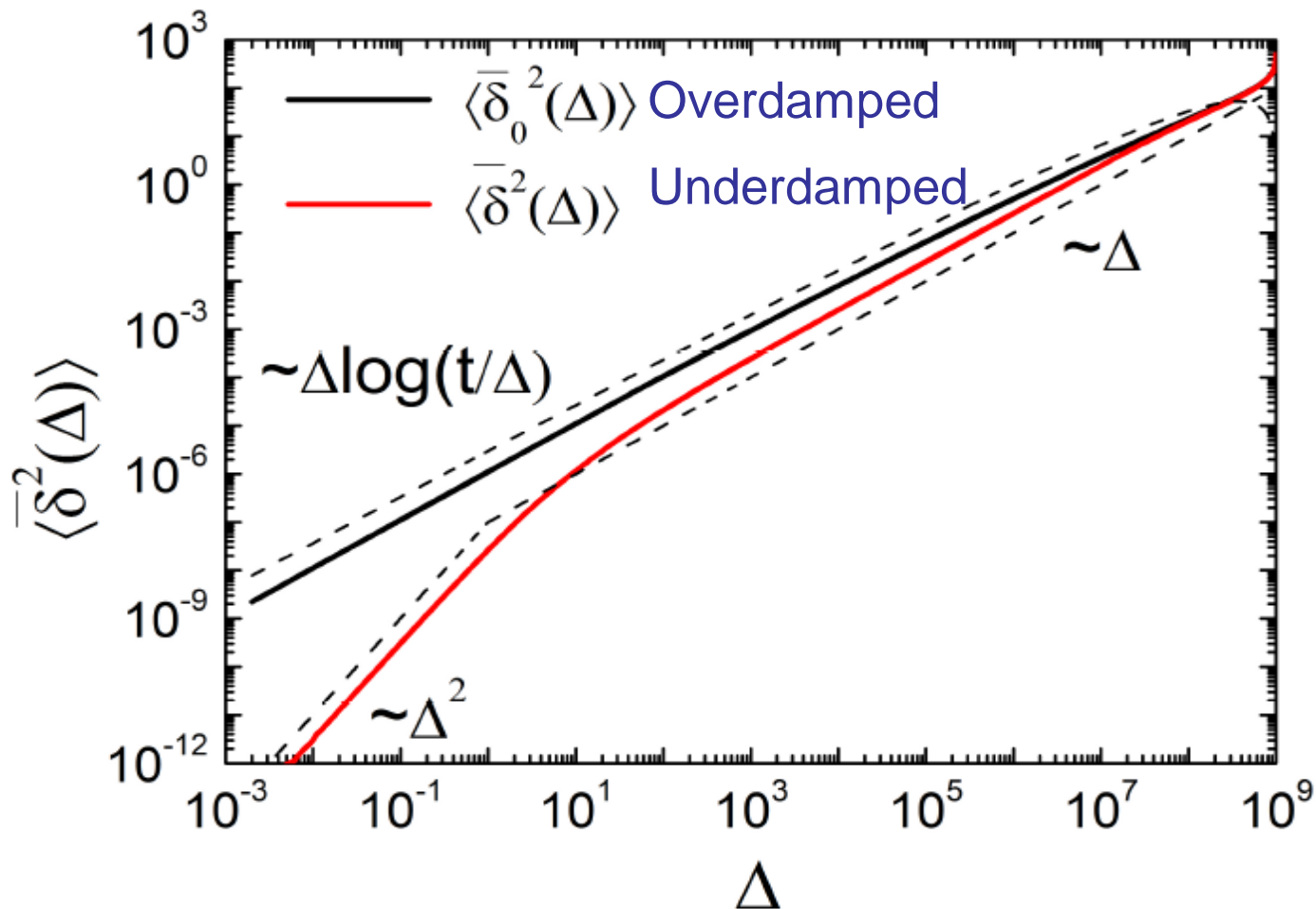
MSD and time-averaged MSD



Ultraslow underdamped SBM

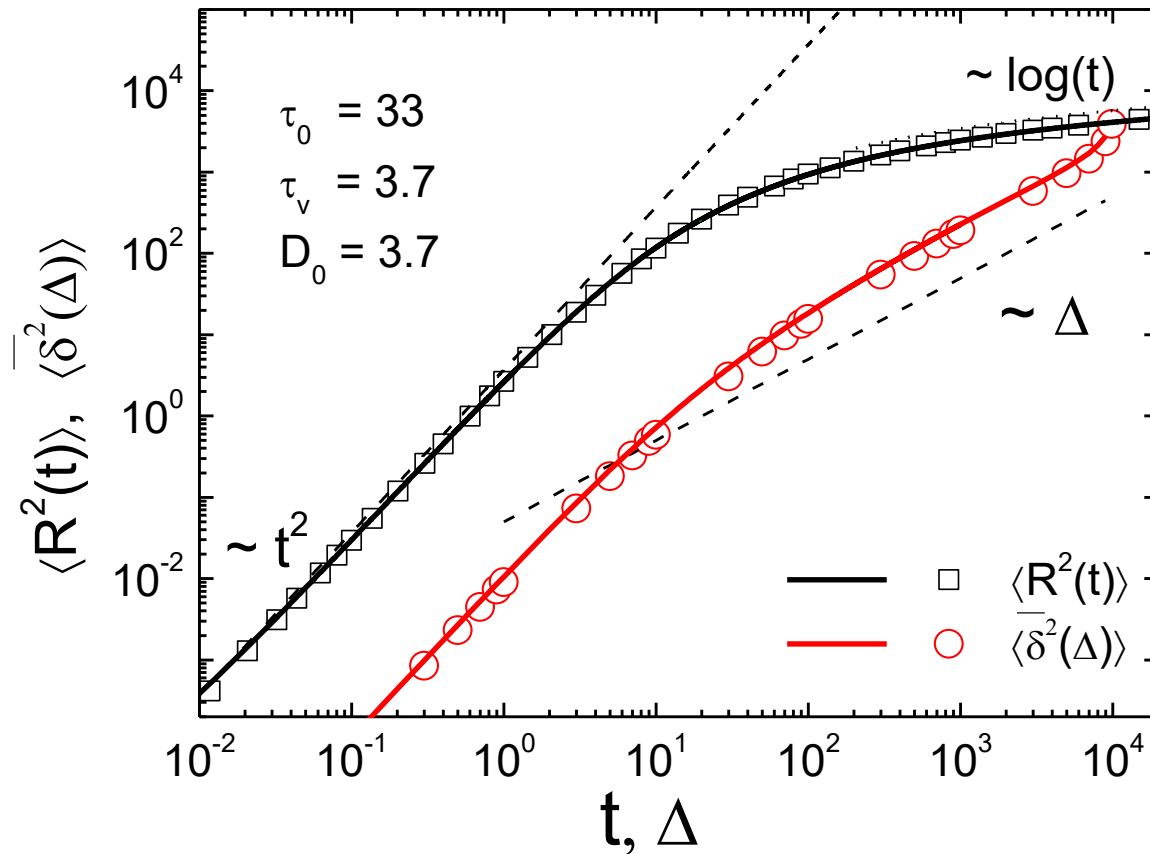
Time-averaged MSD:

overdamped and underdamped limits



Granular gas with constant restitution coefficient

$$\varepsilon(v_{12}) = \text{const}$$



Mean-squared displacement (MSD):

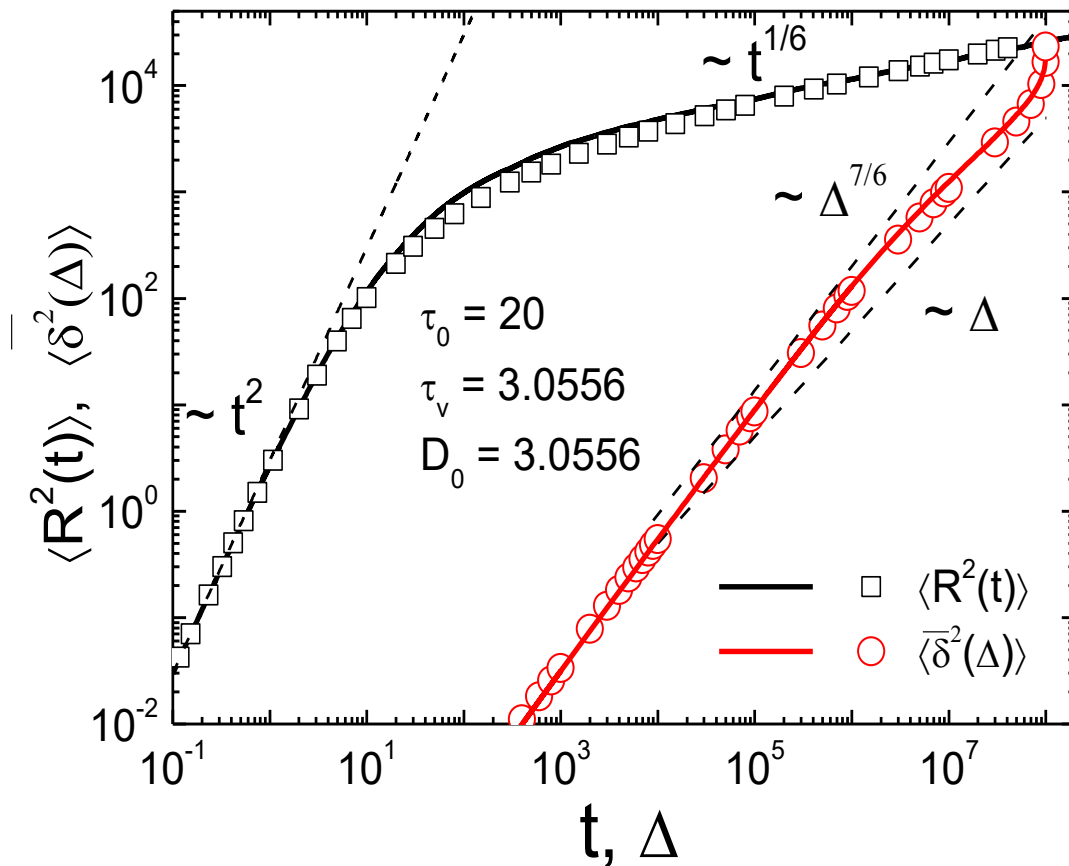
$$\langle R^2(t) \rangle \sim \log t$$

Time-averaged MSD:

$$\langle \overline{\delta^2(\Delta)} \rangle \sim \Delta/t$$

Granular gas with velocity-dependent restitution coefficient

$$\varepsilon(v_{12}) = 1 - C_1 v_{12}^{1/5} + C_2 v_{12}^{2/5} \mp \dots$$



Mean-squared displacement (MSD):

$$\langle R^2(t) \rangle \sim t^{1/6}$$

Time-averaged MSD:

Crossover from

$$\langle \delta^2(\Delta) \rangle \sim \Delta^{7/6} / t$$

to $\langle \delta^2(\Delta) \rangle \sim \Delta / t^{5/6}$

Resetting



If one **searches** for a **goal** and is lost, sometimes it is useful to **return** to **starting point** and to start the search from the beginning.

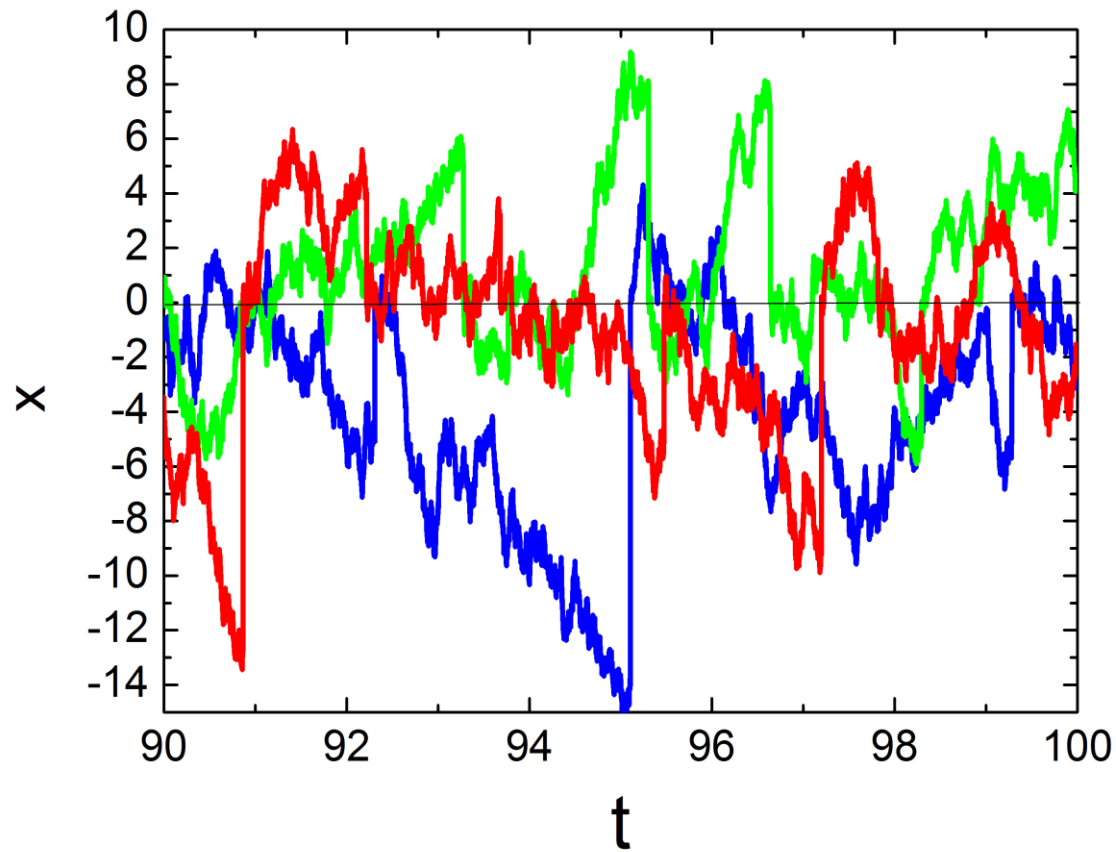
Resetting

- Foraging animals

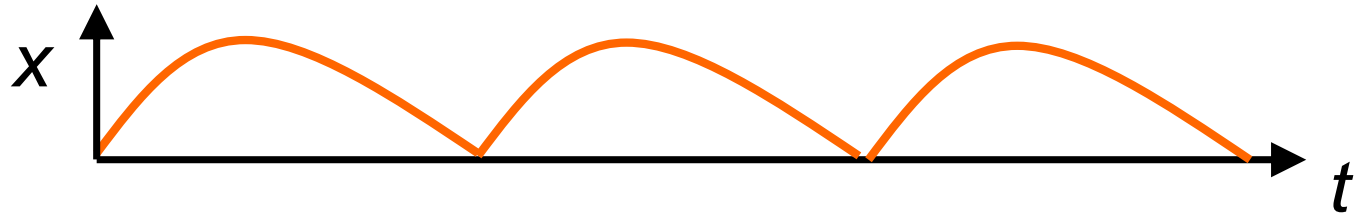
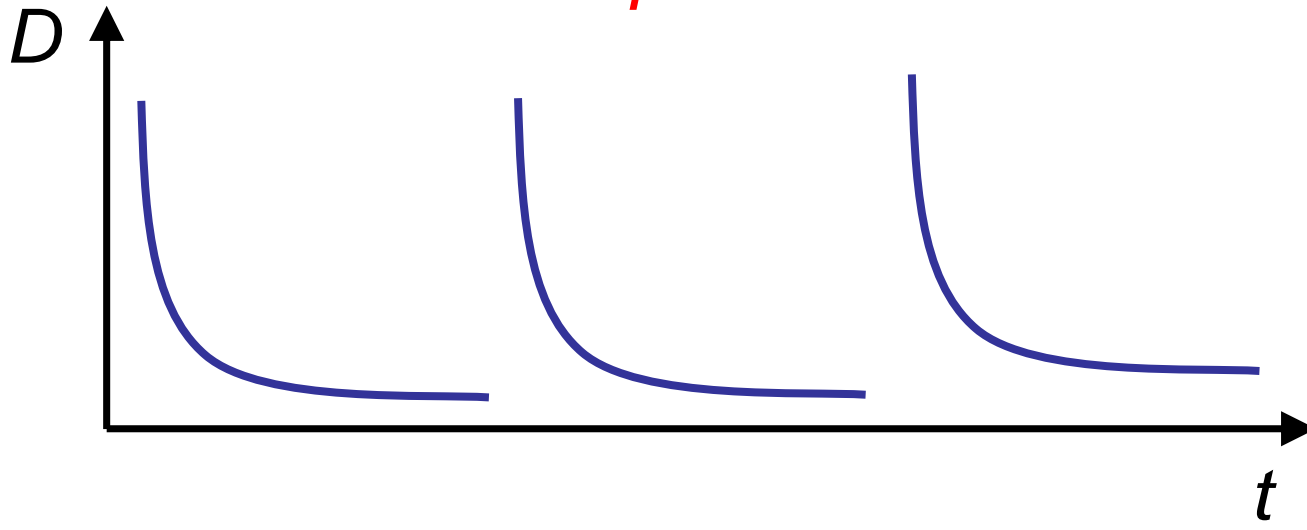


- Optimizing search algorithms

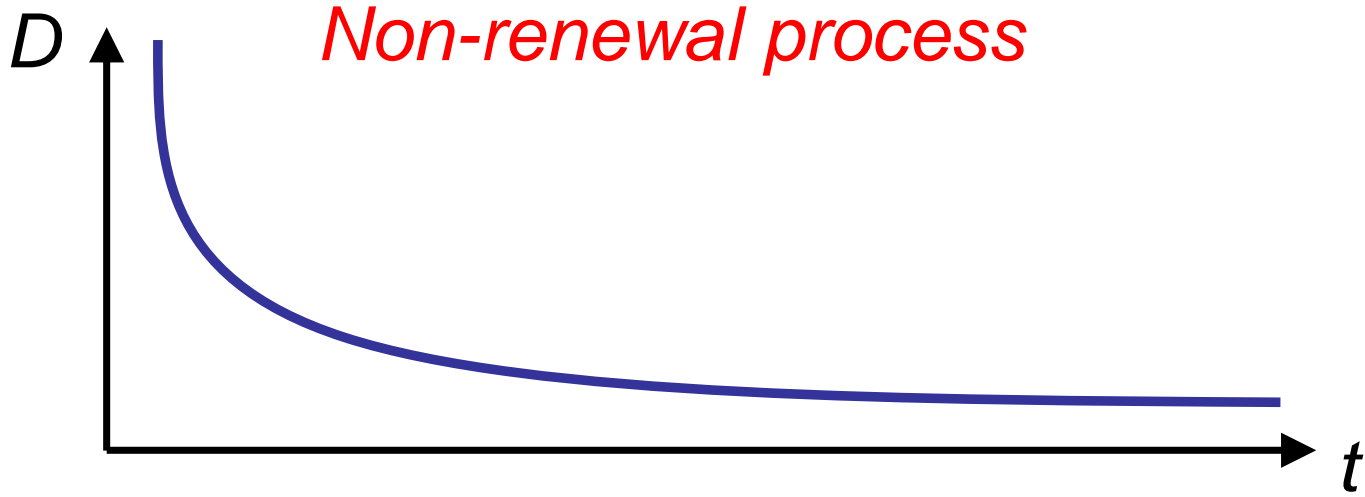
Typical trajectories for scaled Brownian motion with resetting



Renewal process



Non-renewal process



Scaled Brownian motion

$$\frac{dx(t)}{dt} = \sqrt{2D(t)}\eta(t)$$

White Gaussian noise

$$\langle \eta(t_1)\eta(t_2) \rangle = \delta(t_1 - t_2)$$

Diffusion coefficient

$$D(t) = \alpha K_\alpha t^{\alpha-1}$$

Mean-squared displacement

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

$\alpha > 1$ *Superdiffusion*

$$0 < \alpha < 1$$

Subdiffusion

$\alpha = 1$ *Ordinary Brownian motion*

Probability distribution function

$$p_0(x, t) = \frac{1}{\sqrt{4\pi K_\alpha t^\alpha}} \exp\left(-\frac{x^2}{4K_\alpha t^\alpha}\right)$$

Distribution of waiting times between the resetting events

Exponential (Poissonian) resetting

$$\psi(t) = r e^{-rt}$$

Power-law resetting

$$\psi(t) = \frac{\beta/\tau_0}{(1 + t/\tau_0)^{1+\beta}}$$

Survival probability

$$\Psi(t) = e^{-rt}$$

$$\Psi(t) = (1 + t/\tau_0)^{-\beta}$$

The probability that an event occurs at time t

$$\phi(t) = r$$

constant rate

$$\beta > 1$$
$$\phi(t) = \frac{\beta - 1}{\tau_0}$$

$$0 < \beta < 1$$
$$\phi(t) = \frac{t^{\beta-1} \tau_0^{-\beta}}{\Gamma(\beta)\Gamma(1-\beta)}$$

Probability distribution function

The probability to find the particle at location x at time t :

$$p(x, t) = \underbrace{\Psi(t)}_{\text{No resetting}} p_0(x, t, 0) + \int_0^t dt' \phi(t') \underbrace{\Psi(t - t')}_{\text{Last resetting at time } t' } p_0(x, t, t')$$

Mean-squared displacement

$$\langle x^2(t) \rangle = 2K_\alpha t^\alpha \Psi(t) + 2K_\alpha \int_0^t dt' \phi(t') \Psi(t - t') (t^\alpha - t'^\alpha)$$

Renewal process: diffusion coefficient also resets to initial value D_0

Non-renewal process: diffusion coefficient is not affected by the resetting events

Mean-squared displacement

Exponential resetting

$$\psi(t) = r e^{-rt}$$

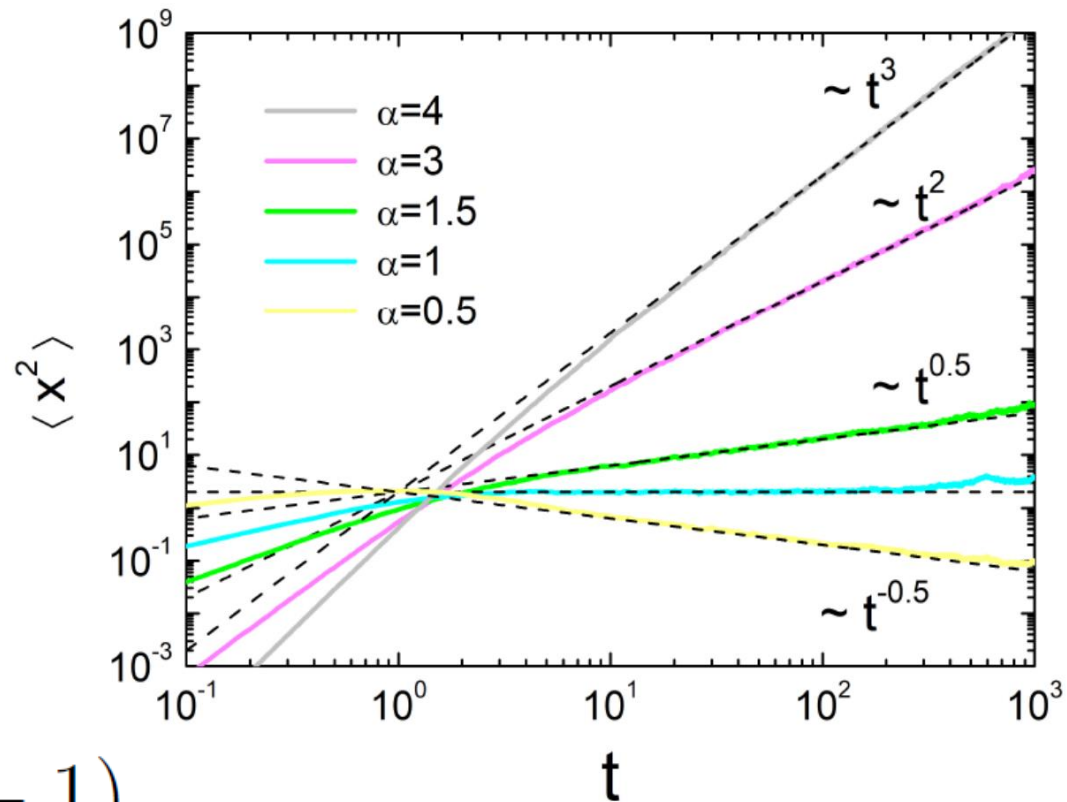
Non-renewal process:

$$\langle x^2(t) \rangle = \frac{2\alpha K_\alpha}{r} t^{\alpha-1}$$

Renewal process:

Steady state:

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

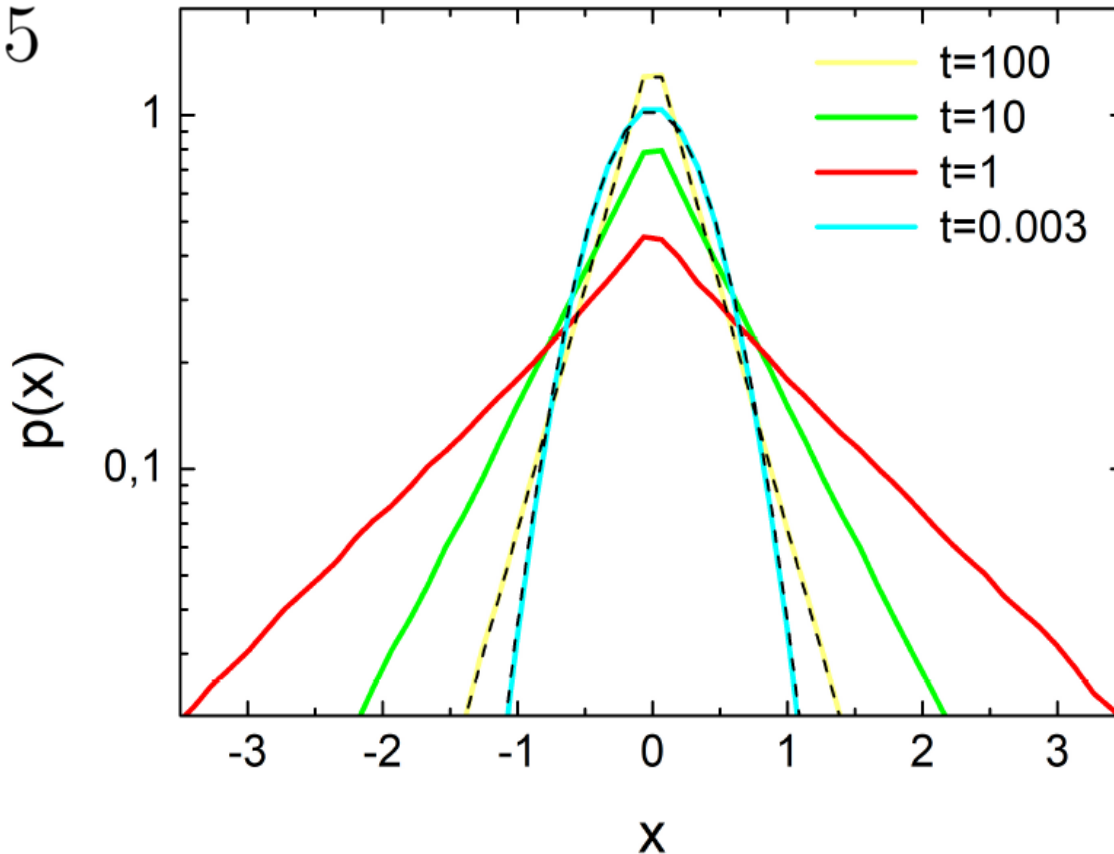


Probability distribution function

Exponential resetting: non-renewal process

$$p(x, t) = \frac{1}{2} \sqrt{\frac{r}{\alpha K_\alpha}} t^{\frac{1-\alpha}{2}} \exp\left(-\sqrt{\frac{r}{\alpha K_\alpha}} |x| t^{\frac{1-\alpha}{2}}\right)$$

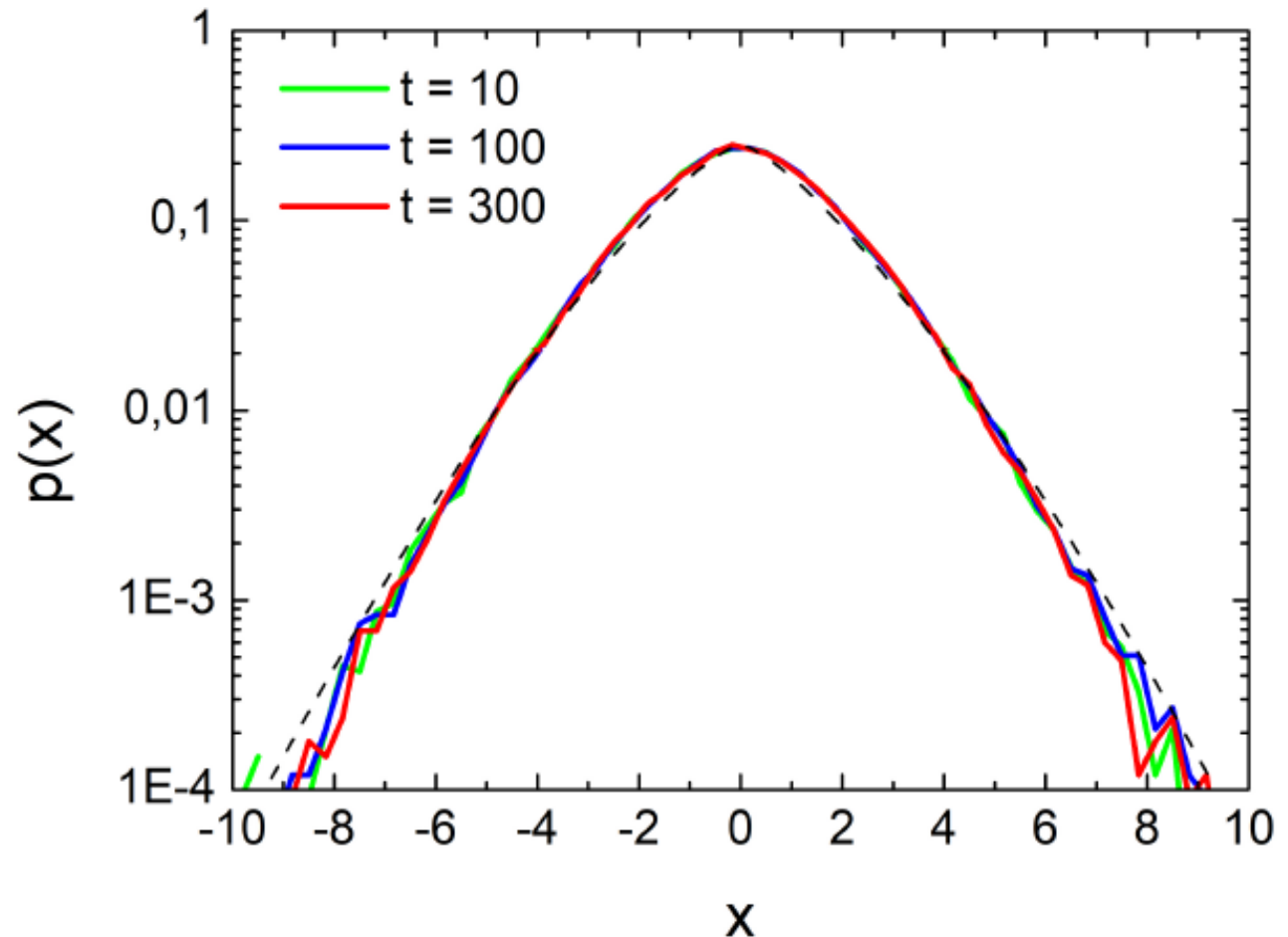
$\alpha = 0.5$



Probability distribution function

Exponential resetting: renewal process

$$p(x, t) = \frac{r\sqrt{2}}{\sqrt{\alpha(\alpha+1)}} \left(\frac{\alpha}{4K_\alpha r}\right)^{\frac{1}{\alpha+1}} x^{\frac{1-\alpha}{2(\alpha+1)}} \exp\left(-\left(\frac{x^2 r^\alpha}{4K_\alpha}\right)^{\frac{1}{\alpha+1}} \left(\alpha^{\frac{1}{\alpha+1}} + \alpha^{-\frac{\alpha}{\alpha+1}}\right)\right)$$



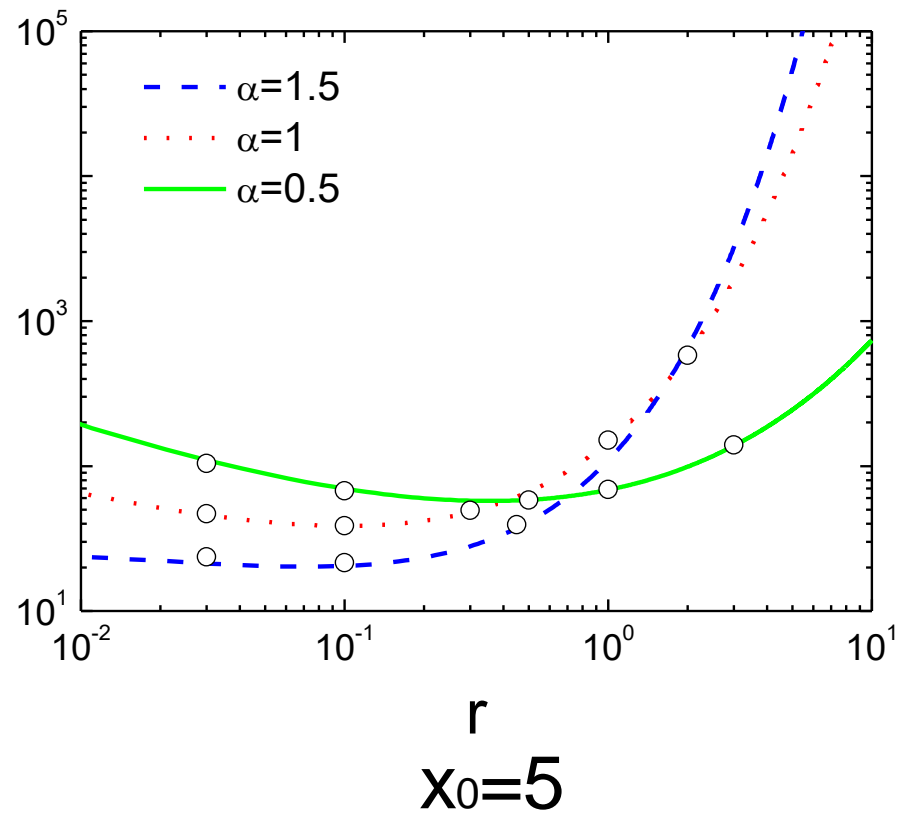
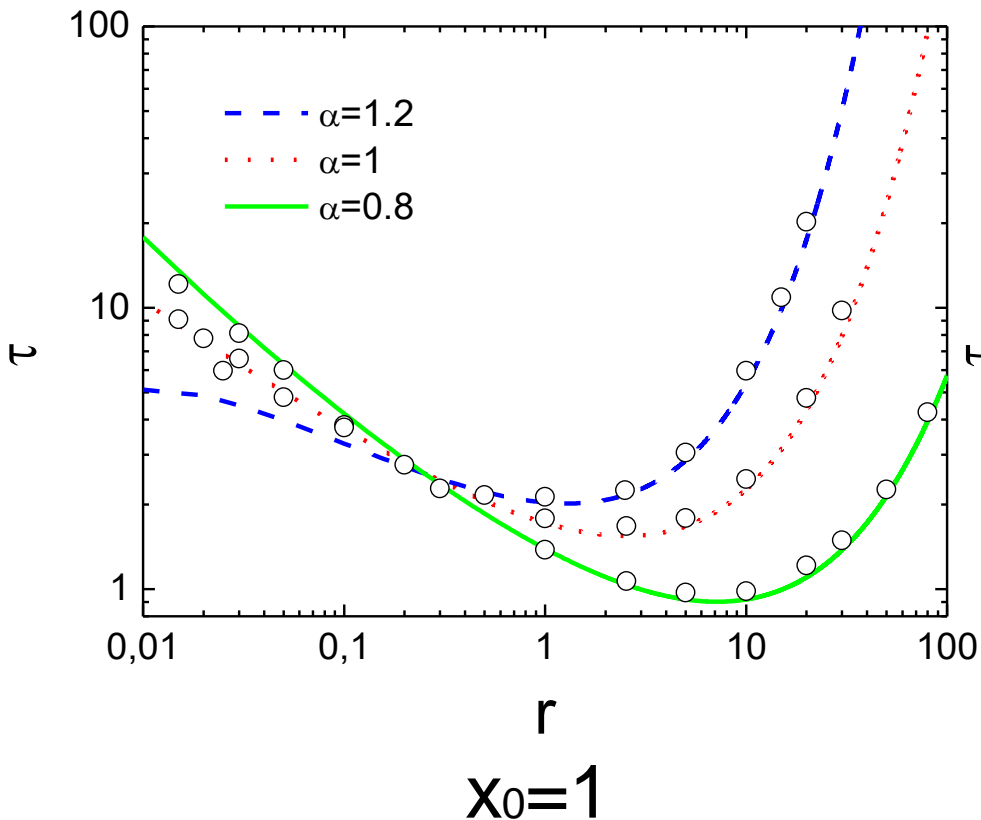
Steady state

$$\alpha = 0.5$$

First passage time

Exponential resetting: renewal process

$$\tau = \frac{1}{r} \left\{ \sqrt{\frac{\alpha + 1}{2\alpha}} \exp \left[r^{\frac{\alpha}{\alpha+1}} \left(\frac{x_0^2}{4K_\alpha} \right)^{\frac{1}{\alpha+1}} \left(\alpha^{\frac{1}{1+\alpha}} + \alpha^{-\frac{\alpha}{1+\alpha}} \right) \right] - 1 \right\}$$



Mean-squared displacement

Power-law resetting
non-renewal process

$$\psi(t) = \frac{\beta/\tau_0}{(1 + t/\tau_0)^{1+\beta}}$$

$$0 < \beta < 1 \quad \langle x^2(t) \rangle = 2K_\alpha t^\alpha \left(1 - \frac{1}{\alpha B(\alpha, \beta)} \right)$$

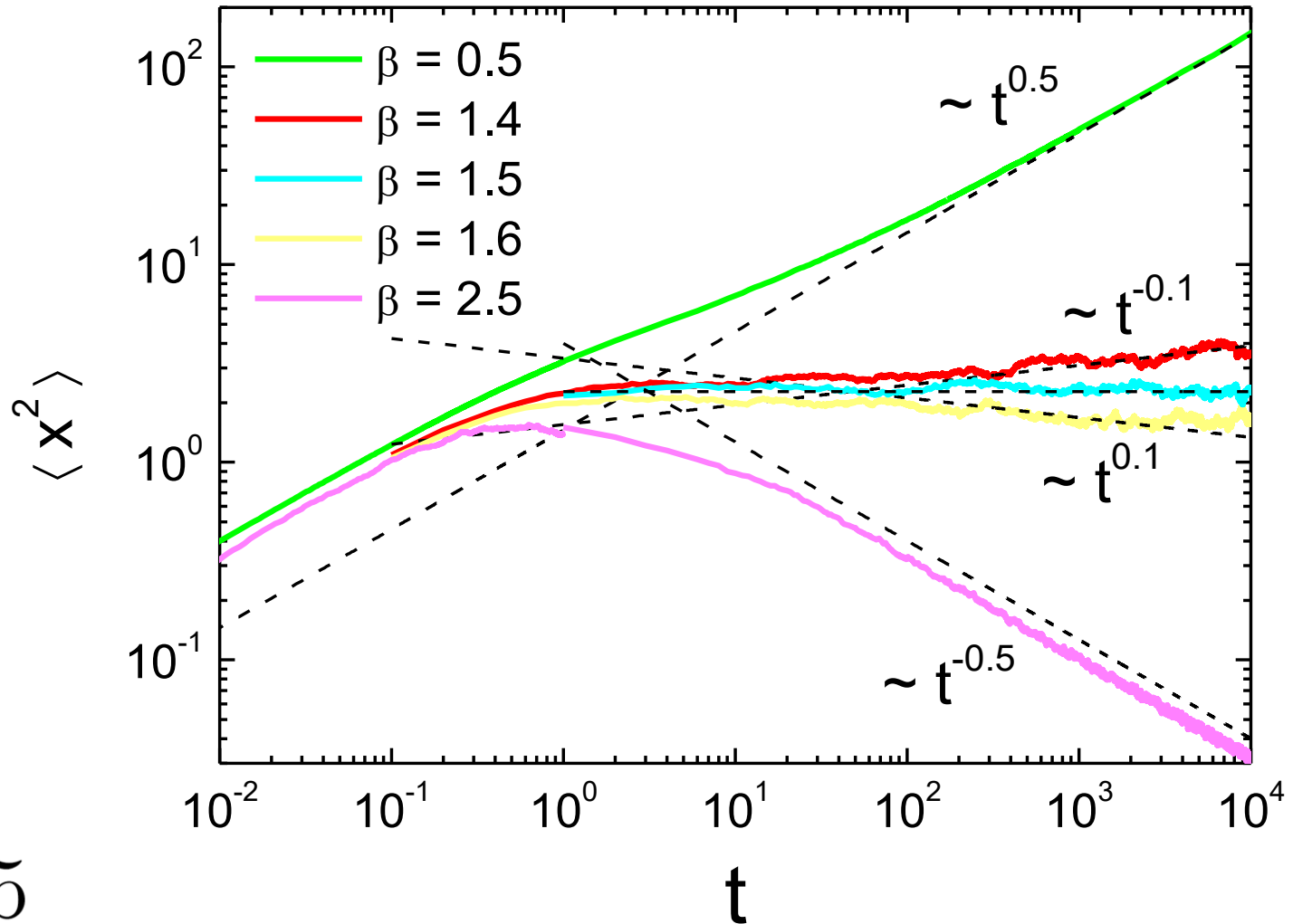
$$1 < \beta < 2$$

$$\langle x^2(t) \rangle = 2K_\alpha t^{1+\alpha-\beta} \tau_0^{\beta-1} (\alpha B(\alpha, 2-\beta) - 1)$$

$$\beta > 2 \quad \langle x^2(t) \rangle = \frac{2\alpha K_\alpha \tau_0}{\beta - 2} t^{\alpha-1}$$

Mean-squared displacement

Power-law resetting
non-renewal process



$\alpha = 0.5$

Mean-squared displacement

Power-law resetting: renewal process

$$0 < \beta < 1$$

$$\langle x^2(t) \rangle = \frac{2K_\alpha t^\alpha}{\Gamma(\beta) \Gamma(1-\beta)} \int_0^1 d\tau \tau^{\beta-1} (1-\tau)^{\alpha-\beta}$$

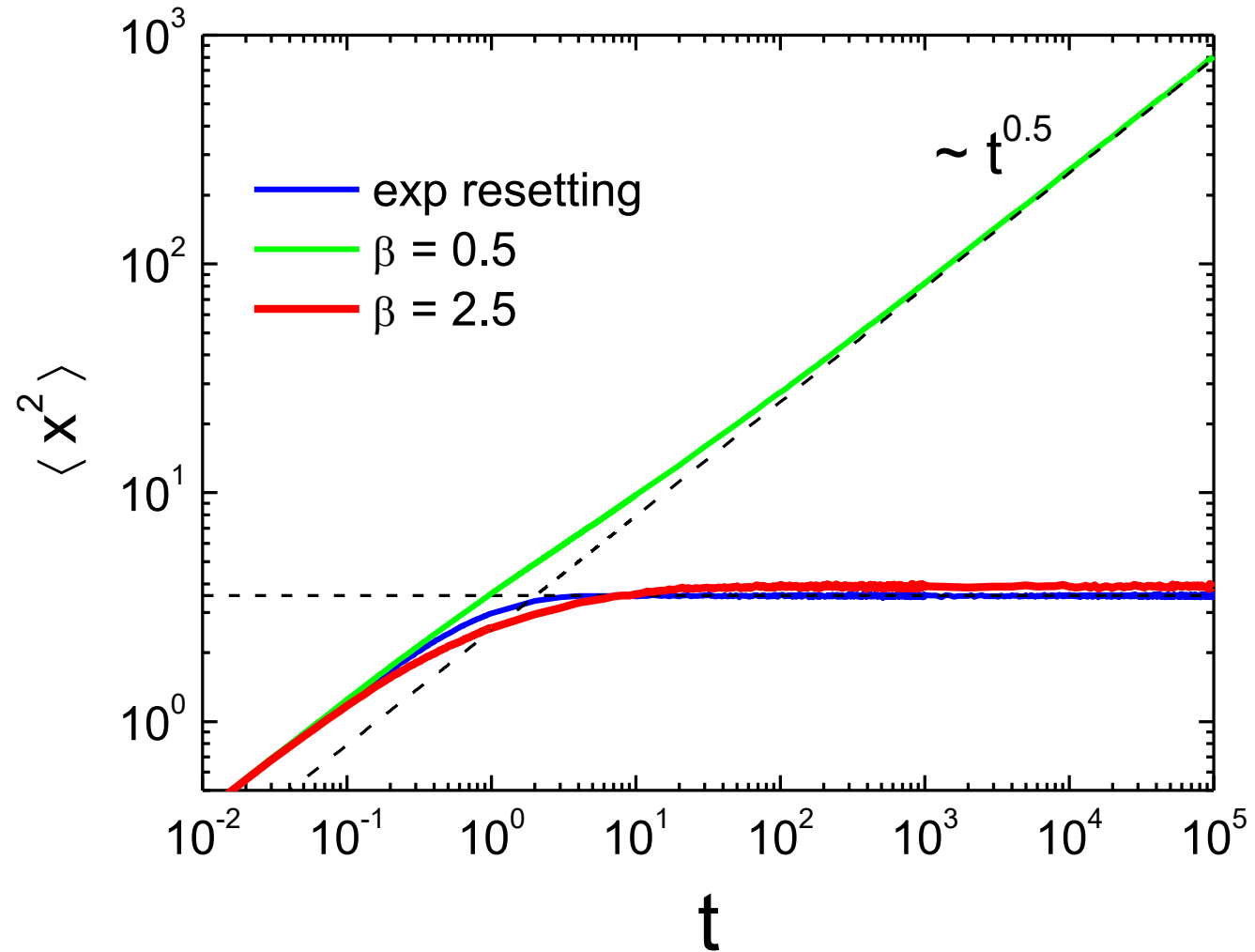
$$1 < \beta < 2$$

$$\langle x^2(t) \rangle = \frac{2K_\alpha \tau_0^{\beta-1} (\beta-1)}{\alpha-\beta+1} t^{\alpha-\beta+1}$$

$$\beta > 2 \quad \langle x^2(t) \rangle = \frac{\alpha K_\alpha \tau_0}{\beta-2}$$

Mean-squared displacement

Power-law resetting
renewal process

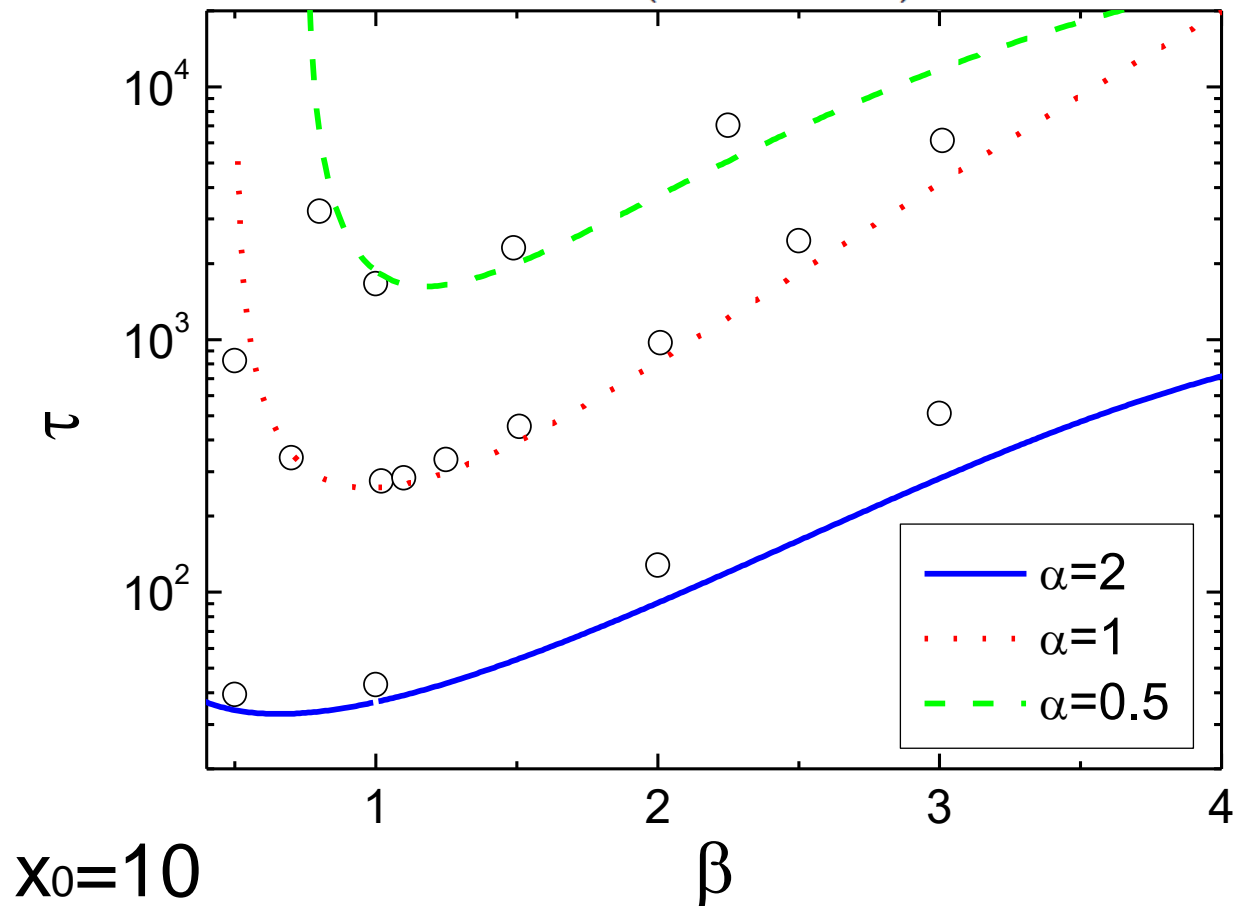


$$\alpha = 0.5$$

First passage time

Power-law resetting: renewal process

$$\tau \simeq \frac{\tau_0}{\beta - 1} \times \frac{\sqrt{\pi} \operatorname{erf}(\sqrt{A}) - A^{1-\beta} \gamma\left(A, \frac{\beta-1}{\alpha} + \frac{1}{2}\right)}{A^{-\beta} \gamma\left(A, \frac{\beta}{\alpha} + \frac{1}{2}\right) + \sqrt{\pi} \operatorname{erfc}(\sqrt{A})}$$



Conclusions

- The **underdamped scaled Brownian motion**, a novel anomalous diffusion process governed by **Langevin equation** with **time-dependent diffusion** and **friction** coefficients, describes the diffusion in **bath** with **time-dependent temperature** and in **granular gases**.
- The **overdamped** limit of the Langevin equation does not capture all properties of the system
- **Resetting** significantly affects the behavior of Brownian motion with **time-dependent** diffusion coefficient

1. Bodrova A., Chechkin A. V., Cherstvy A. G., Metzler R., *Quantifying non-ergodic dynamics of force-free granular gases*. **PCCP** 17, 21791 (2015).
2. Bodrova A., Chechkin A. V., Cherstvy A. G., Metzler R., *Ultraslow scaled Brownian motion*. **New J. Phys.** 17, 063038 (2015)
3. Bodrova A., Chechkin A. V., Cherstvy A. G., Safdari H., Sokolov I.M., Metzler R., *Underdamped scaled Brownian motion: (non-)existence of the overdamped limit in anomalous diffusion*. **Sci. Rep.** 6, 30520 (2016)
4. Bodrova A.S., Chechkin A. V., Sokolov I.M. *Non-renewal resetting of scaled Brownian motion*. Submitted to **Phys. Rev. E** (2018)
5. Bodrova A.S., Chechkin A. V., Sokolov I.M. *Scaled Brownian motion with renewal resetting*. Submitted to **Phys. Rev. E** (2018)