Mimicking heterogeneous diffusion with time dependent random diffusivity.

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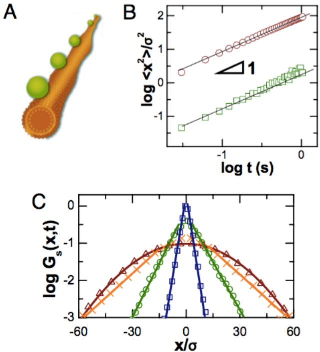
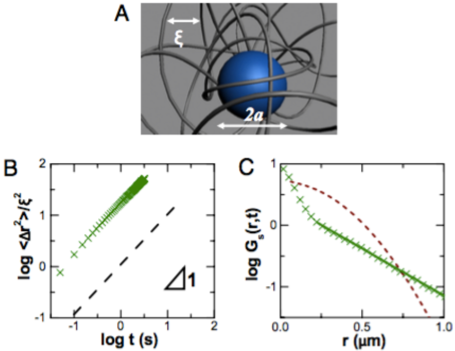
Outline

Brownian yet non-gaussian diffusion (BnG)





$$\langle (x(t) - x_0)^2 \rangle = 2\langle D \rangle t$$

$$P(x,t) \propto exp\left(-\frac{|x - x_0|}{\lambda(t)}\right) \longrightarrow P(x,t) \propto \exp\left(-\frac{(x - x_0)^2}{4\langle D \rangle t}\right)$$

[1] Wang B, Anthony S M, Bae S C & Granick S 2009, PNAS, **106** 15160 – 64
[2] Wang B, Kuo J, Bae S C & Granick S 2012, *Nat. Mater.* **11** 481– 5

How can the Brownian scaling of the MSD be reconciled with non-gaussian PDF?

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

Brownian motion

Heterogeneity

Heterogeneity of tracers → **Both** ← **Heterogeneity in the environment**

- ggBM-like models;
- superstatistics;
- diffusing diffusivity.

Generalised grey Brownian motion (ggBM)

It is possible to define ggBM model through the stochastic representation

$$X_{\mathrm{ggBM}} = \sqrt{\Lambda}\, X_g$$

where Λ is an independent non-negative random variable and X_g is a Gaussian process.

The PDF of the stochastic variable X_{ggBM} can be evaluated by means of the integral

$$P_{\mathrm{ggBM}}(x,t) = \int_0^\infty P_{X_g}\left(\frac{x}{\lambda^{1/2}}\right) P_\Lambda(\lambda)\, \frac{d\lambda}{\lambda^{1/2}}$$

where $P_{\mathrm{X_g}}$ and P_Λ are the distributions of X_g and Λ respectively.

[3] Mura A & Pagnini G 2008, *J. Phys. A: Math. Theor.*, **41** 285003

Generalised grey Brownian motion

- If X_g is fractional Brownian motion and Λ is distributed according to a Mainardi-Wright function $\implies$ stochastic process used to model both slow and fast diffusion;

- if X_g is Brownian motion and Λ is an independent non-negative random variable $\implies$ stochastic process that models BnG diffusion.

↓

Ensemble of Brownian particles with random diffusivities from the distribution $p_D(D)$

$$X_{\mathrm{ggBM}}(t) = \sqrt{2D}\, W(t),$$

$$P_{\mathrm{ggBM}}(x,t) = \int_0^\infty \frac{1}{\sqrt{2\pi t}} \exp\left(-\frac{(x/\sqrt{2D})^2}{2t}\right) p_D(D) \frac{dD}{\sqrt{2D}}$$

Superstatistical Brownian motion

$\downarrow$

"Statistics of a statistics" $\rightarrow$ based on two statistical levels describing:

1. the fast jiggly dynamics of the Brownian particle;
2. the slow environmental fluctuations with spatially local patches of given diffusivity.

$$P_S(x,t) = \int p_D(D) P(x,t|D) dD$$

$$\Downarrow$$

$$P_S(x,t) = P_{\mathrm{ggBM}}(x,t)$$

[4] Beck C & Cohen E D B 2003, *Physica A*, **322** 267 – 275

ggBM-like models & Superstatistical models

- Describe heterogeneity of the tracers and/or heterogeneity in the medium;
- At the single-trajectory level $\rightarrow$ standard Brownian motion;
- At the ensemble level $\rightarrow$ BnG diffusion;
- They are described through the same stochastic representation:

$$X = \sqrt{2D} \times X_g,$$

(where D is random and X_g is Brownian motion)

- **Not able to explain transition to Gaussian diffusion!**

$\downarrow$

Diffunsing Diffusivity

Minimal diffusing diffusivity model (mDD)

$$\begin{cases} \frac{d}{dt}X(t) &= \sqrt{2D(t)}\,\xi_1(t) \\ D(t) &= \mathbf{Y}^2(t) \\ \frac{d}{dt}\mathbf{Y}(t) &= -\mathbf{Y}(t) + \xi_{\mathbf{2}}(t) \end{cases} \quad \xrightarrow{\text{(subordination)}} \quad \begin{cases} \frac{d}{dt}X(\tau) &= \sqrt{2}\,\xi_1(\tau) \\ \frac{d}{dt}\tau(t) &= D(t) \end{cases}$$

where the n-dimensional OU process starts from its equilibrium distribution, such that $p_D(D) = \frac{D^{n/2-1}}{\Gamma(n/2)} \exp(-D)$.

$$P_{\mathrm{DD}}(x,t|x_0) = \int_0^\infty G(x,\tau|x_0, D=1)\, T_n(\tau,t)\, d\tau,$$

where $T_n(\tau,t)$ is the PDF of the process $\tau(t) = \int_0^t \mathbf{Y}^2(t')dt'$, defined via its Laplace transform

$$\tilde{T}_n(s,t) = \frac{\exp(n\,t/2)}{\left[\frac{1}{2}(\sqrt{1+2s^2} + \frac{1}{\sqrt{1+2s^2}})\sinh\left(t\sqrt{1+2s^2}\right) + \cosh\left(t\sqrt{1+2s^2}\right)\right]^{n/2}}.$$

A more general minimal diffusing diffusivity model

$$\gamma^{\mathrm{gen}}_{\nu,\eta}(D) = \frac{\eta}{D_\star^{\nu}\,\Gamma(\nu/\eta)} D^{\nu-1} e^{-(D/D_\star)^{\eta}}, \qquad \langle D^n \rangle_{\mathrm{st}} = D_\star^n \frac{\Gamma\left(\frac{\nu+n}{\eta}\right)}{\Gamma\left(\frac{\nu}{\eta}\right)},$$

where $D_\star$, ν and η are positive constants.
If $\eta = 1$ and $2\nu \in \mathbb{N} \implies$ Gamma distribution.

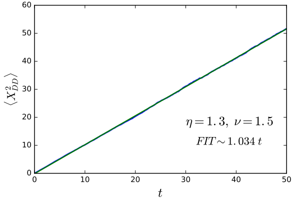
$$\downarrow$$

$$X_{\mathrm{DD}}(t) = \int_0^t \sqrt{2D(s)}\,\xi(s)ds,$$

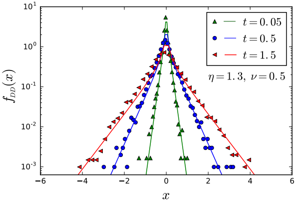
$$D(t) = Y^2(t),$$

$$\boxed{dY = \frac{\sigma^2}{2\,Y}\left[2\nu - 1 - 2\,\eta\,\left(\frac{Y}{\sqrt{D_\star}}\right)^{2\eta}\right] dt + \sigma\; dW(t).}$$

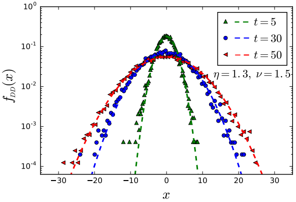
- linear dispersion of the mean-squared displacement with time $\langle X^2(t)\rangle = 2\langle D\rangle_{\rm st}\, t$;



- full consistency in the short time limit with the superstatistical approach, describing non-gaussian diffusion;



- explicit derivation of the crossover to Gaussian diffusion at long times.



How does heterogeneity affect the first passage properties of the diffusion process?

↓

We would expect that, rare events, represented by the exponential tails of the particles displacement distribution, may dominate triggered actions.

First passage problem for BM

$$\begin{cases} \frac{\partial}{\partial t} P_{\mathrm{BM}}(x,t|x_0) &= D\frac{\partial^2}{\partial x^2} P_{\mathrm{BM}}(x,t|x_0), \\ P_{\mathrm{BM}}(x,0|x_0) &= \delta(x-x_0), \\ P_{\mathrm{BM}}(0,t|x_0) &= P_{\mathrm{BM}}(L,t|x_0) = 0. \end{cases}$$

Survival probability: $S(t|x_0) = \int_0^L P(x,t|x_0)dx$

First passage time density function: $\wp(t|x_0) = -\frac{d}{dt} S(t|x_0)$

$\rightarrow$ L finite

- $S_{\mathrm{BM}}(t|x_0) = \frac{4}{\pi} \sum_{n=0}^{\infty} \sin\left(\frac{\pi(2n+1)}{L} x_0\right) \frac{\exp\left(-D\lambda_{2n+1}^2 t\right)}{(2n+1)}, \quad \lambda_n = n\pi/L.$
- $\wp_{\mathrm{BM}}(t|x_0) \sim \exp(-t/\tau_1), \quad \tau_1 = L^2/\pi^2 D \quad \Longrightarrow \langle t_{\mathrm{BM}} \rangle < \infty.$

$\rightarrow$ $L = \infty$

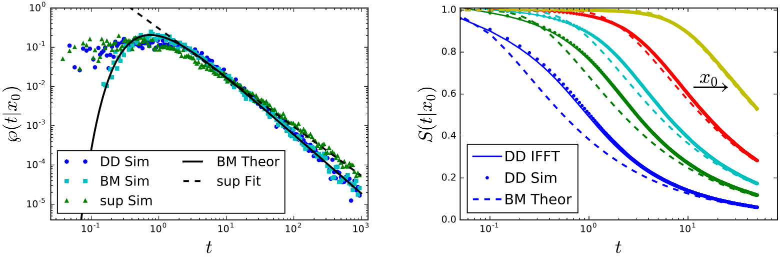
- $S_{\mathrm{BM}}(t|x_0) = \mathrm{erf}\left(\frac{x_0}{\sqrt{4Dt}}\right).$
- $\wp_{\mathrm{BM}}(t|x_0) = \frac{x_0}{\sqrt{4\pi D t^3}} \exp\left(-\frac{x_0}{\sqrt{4Dt}}\right) \quad \Longrightarrow \langle t_{\mathrm{BM}} \rangle = \infty.$

First passage problem for mDD: semi-infinite interval

$$
\begin{aligned}
S_{\mathrm{DD}}(t|x_0) &= \int_0^\infty T(\tau, t) S_{\mathrm{BM}}(\tau|x_0) d\tau \\
&= \int_0^\infty dx \int_{-\infty}^{+\infty} \frac{dk}{2\pi} e^{-ikx} \left(e^{ikx_0} - e^{-ikx_0}\right) \tilde{T}(k^2, t),
\end{aligned}
$$

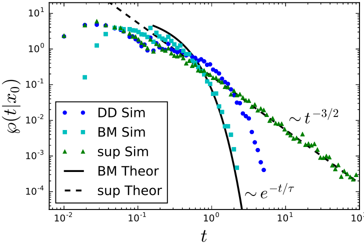
where

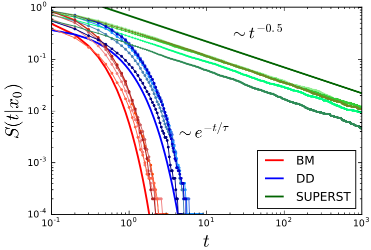
$$
\tilde{T}(k^2, t) = e^{t/2} \Bigg/ \left[\frac{1}{2}\left(\sqrt{1+2k^2} + \frac{1}{\sqrt{1+2k^2}}\right) \sinh\left(t\sqrt{1+2k^2}\right) + \cosh\left(t\sqrt{1+2k^2}\right)\right]^{1/2}
$$



First passage problem for mDD: finite interval

$$S_{\mathrm{DD}}(t|x_0) = \int_0^\infty T(\tau, t) S_{\mathrm{BM}}(\tau|x_0) d\tau = \frac{4}{\pi} \sum_{n=0}^{\infty} \sin\left(\frac{\pi(2n+1)}{L} x_0\right) \frac{\tilde{T}(\lambda_{2n+1}^2, t)}{(2n+1)}$$





NB: $\wp_s(t|x_0) \sim t^{-1.5} \implies \langle t_S \rangle = \infty$

Superstatistical model shows an infinite mean first passage time even in a finite interval! → Caused by the non 0 value of $p_D(D)$ at the origin which introduces immobile particles.

Summary I

- ggBM-like models and superstatistical models describe heterogenous ensemble of particles or diffusion in heterogenous medium where:
  - ✓ BnG diffusion is observed;
  - ✓ there is no crossover to gaussian diffusion.
- DD models describe systems with slowly varying and heterogenous fluctuations of the environment where:
  - ✓ the validity of the superstatistical assumption in the short time regime allows for a description of BnG diffusion;
  - ✓ in the long time regime the sampling of the entire diffusivity space leads to gaussian diffusion with an effective value for the diffusivity;
  - ✓ the underlying stochastic process describing the diffusivity fluctuations is responsible for the shape of the non-gaussian displacement distribution in the short time regime.

Summary II

- In general heterogeneities in the environment do not improve the mean first passage result, in fact some of the particles are slowed down;
- thanks to the heterogeneity some particles have a diffusion coefficient greater than the average, thus an increase in the speed of target location for these particles is observed;
- the amount of fast particles is independent on the initial position and they are responsible for the faster decrease of the survival probability at short times;
- at long times the results for the DD model approach the BM ones, as expected;
- the superstatistical model results deviates drastically from the BM ones showing a slower decay of the survival probability in the long times.

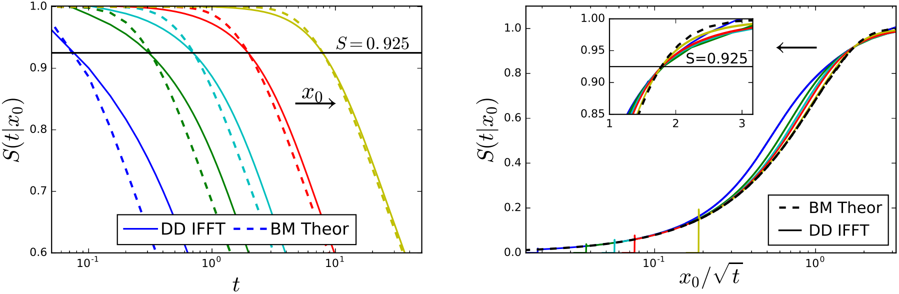
Thank you for your attention!

For more details:

Beck C & Cohen E D B 2003, *Physica A*, **322** 267 – 275
Mura A & Pagnini G 2008, *J. Phys. A: Math. Theor.*, **41** 285003
Chechkin A V, Seno F, Metzler R & Sokolov I 2017, PRX **7**, 021002
VS, Chechkin A V, Seno F, Pagnini G & Metzler R 2018, *New. J. Phys.* **20**, 043044
VS, Chechkin A V & Metzler R 2019, *J. Phys. A: Math. Theor.* **52**, 04LT01

First passage problem for mDD: semi-infinite interval

ST $\rightarrow$ $\tilde{T}(k^2,t) \sim \left(k^2 t + 1\right)^{-1/2}$



$$S_{\mathrm{DD}}(t|x_0) = \frac{x_0}{\sqrt{t}}\left[K_0\left(\frac{x_0}{\sqrt{t}}\right)L_{-1}\left(\frac{x_0}{\sqrt{t}}\right) + K_1\left(\frac{x_0}{\sqrt{t}}\right)L_0\left(\frac{x_0}{\sqrt{t}}\right)\right] = S_{\mathrm{S}}(t|x_0)$$

$K_\nu(z)$ modified Bessel function of second kind

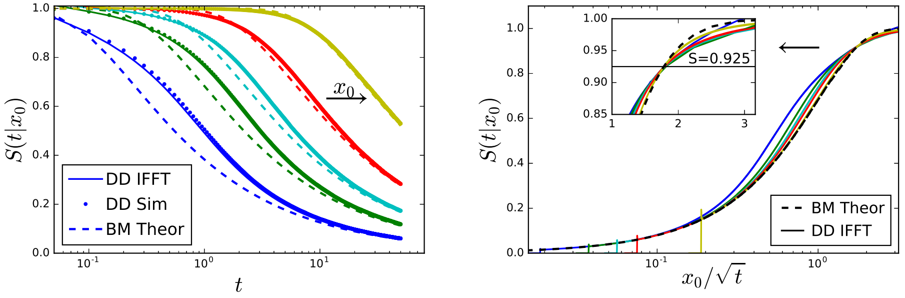
$L_\nu(z)$ modified Struve function

$$S_{\mathrm{DD}}(t|x_0) \overset{t\rightarrow 0}{\sim} 1 - \frac{\sqrt{2}e^{-(x_0/\sqrt{t})}}{\sqrt{\pi x_0}}t^{1/4} + \frac{5e^{-(x_0/\sqrt{t})}}{4\sqrt{2\pi x_0^3}}t^{3/4}$$

$$S_{\mathrm{BM}}(t|x_0) \overset{t\rightarrow 0}{\sim} 1 - \frac{\sqrt{2}e^{-(x_0^2/2t)}}{\sqrt{\pi}x_0}t^{1/2}$$

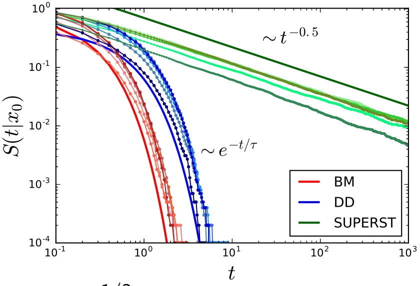
First passage problem for mDD: semi-infinite interval

LT $\rightarrow$ $\tilde{T}(k^2, t) \sim \exp\left(-\frac{k^2 t}{2}\right)$



$$S_{\mathrm{DD}}(t|x_0) = \mathrm{erf}\left(\frac{x_0}{\sqrt{4\langle D\rangle_{\mathrm{st}}\, t}}\right) = S_{\mathrm{BM}}(t|x_0)$$

First passage problem for mDD: finite interval



$$\text{ST} \rightarrow \tilde{T}(k^2, t) \sim \left(k^2 t + 1\right)^{-1/2}$$

$$S_{\mathrm{DD}}(t|x_0) \sim \frac{4}{\pi} \sum_{n=0}^{\infty} \sin\left(\frac{\pi(2n+1)}{L} x_0\right) \frac{1}{(2n+1)\sqrt{\lambda_{2n+1}^2 t + 1}} = S_{\mathrm{S}}(t|x_0)$$

$$\text{LT} \rightarrow \tilde{T}(k^2, t) \sim \frac{\sqrt{2}\exp\left(\frac{t}{2}\left(1-\sqrt{1+2k^2}\right)\right)}{\left(1+\frac{1}{2}\left(\sqrt{1+2k^2}+\frac{1}{\sqrt{1+2k^2}}\right)\right)^{1/2}} \quad \xrightarrow{k \ll 1} \quad \exp\left(-\frac{k^2 t}{2}\right)$$

$$S_{\mathrm{DD}}(t|x_0) \sim \frac{4\sqrt{2}}{\pi} \sum_{n=0}^{\infty} \frac{\sin\left(\frac{\pi(2n+1)}{L} x_0\right)}{(2n+1)} \frac{\exp\left(\frac{t}{2}\left(1-\sqrt{1+2\lambda_{2n+1}^2}\right)\right)}{\sqrt{1+\frac{1}{2}\left(\sqrt{1+2\lambda_{2n+1}^2}+\frac{1}{\sqrt{1+2\lambda_{2n+1}^2}}\right)}}$$

Generalisation to 2D and 3D

Subordination: $P_{\mathrm{DD}}(\mathbf{r},t|\mathbf{r}_0)=\int_0^\infty G(\mathbf{r},\tau|\mathbf{r}_0,D=1)\,T_d(\tau,t)d\tau$,

$$\tilde{T}_d(s,t)=\frac{\exp(d\,t/2)}{\left[\frac{1}{2}\left(\sqrt{1+2s^2}+\frac{1}{\sqrt{1+2s^2}}\right)\sinh\left(t\sqrt{1+2s^2}\right)+\cosh\left(t\sqrt{1+2s^2}\right)\right]^{d/2}}.$$

Superstatistics: $P_{\mathrm{S}}(\mathbf{r},t|\mathbf{r}_0)=\int_0^\infty G(\mathbf{r},t|\mathbf{r}_0,D)p_D(D)dD$,

$$p_D(D)=\begin{cases} e^{-D} & d=2,\\ \frac{2\sqrt{D}}{\sqrt{\pi}}e^{-D} & d=3.\end{cases}$$

$S_{\mathrm{DD}}(t|\mathbf{r}_0)=\int_0^\infty S_{\mathrm{BM}}(t|\mathbf{r}_0)\,T_d(\tau,t)d\tau$; $\quad S_{\mathrm{S}}(t|\mathbf{r}_0)=\int_0^\infty S_{\mathrm{BM}}(t|\mathbf{r}_0)p_D(D)dD$

- $S_{\mathrm{BM}}(t|\mathbf{r}_0)$ in a semi-infinite 2 and 3 dimensional space;
- $S_{\mathrm{BM}}(t|\mathbf{r}_0)$ for isotropic diffusion in concentric circles and spheres.

Comparison of different DD models

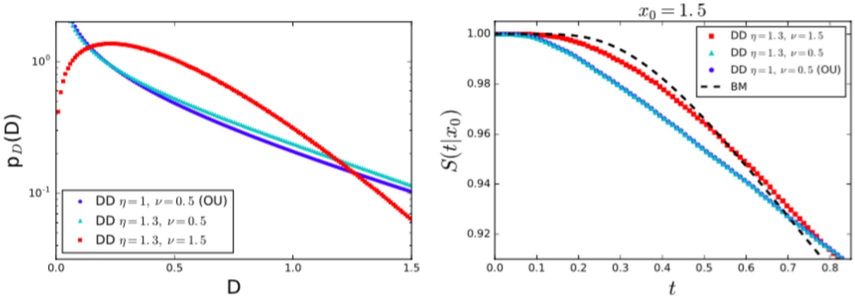


Figure 3. Comparison of the DD model based on the Ornstein–Uhlenbeck (OU) process with the generalised DD model from [24] based on the generalised Gamma distribution. Left: depending on the parameters ν and η the distribution $p(D)$ may be significantly different. Right: survival probability for the different models, demonstrating that for certain parameter values the first passage behaviour remains faster while for others the performance is getting close to that of Brownian–Gaussian motion. Note that the results for the two cases with $\nu = 0.5$ almost coincide.