Diffusion dynamics and Persistence probability of an active asymmetric Brownian particle in two dimensions

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First Passage Phenomena and Persistence

- First passage properties is extended to simple to one or few degrees of freedom non-equilibrium systems, random walk, random acceleration, ABP, surface growth and many more.
- First passage probability is the probability that a random walk or a diffusing particle hits a specified point for the first time at t.
- Persistence is defined as the prob that any stochastic variable x has not changed its sign upto time t.
- The probability density of the first time at which the process crosses $x=0$ is $F(t)=-dP(t)/dt$
- Persistence properties are non trivial in these systems as the effective underline process is non-Markovian.

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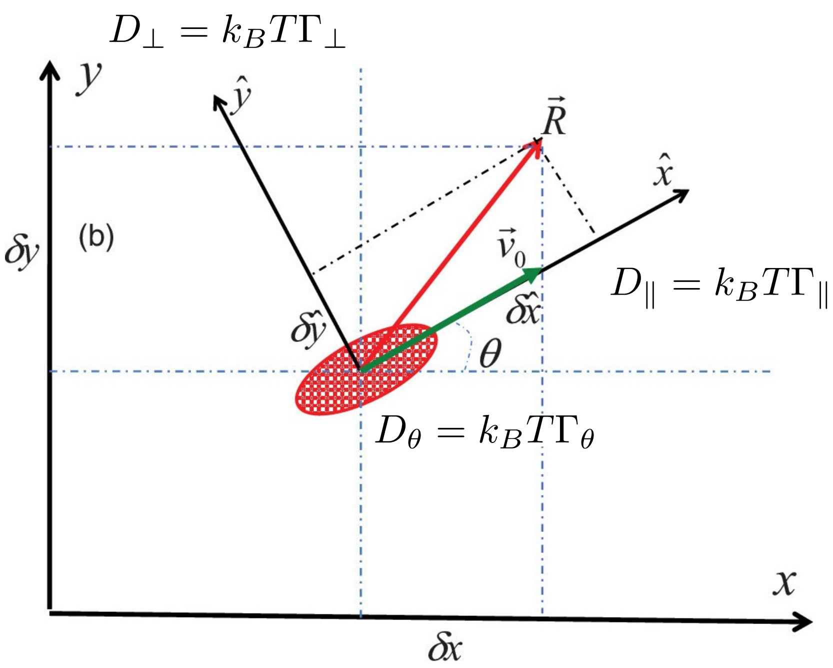
- The probability density of the first time at which the process crosses x=0 is F(t)=-dP(t)/dt
- Persistence properties are non trivial in these systems as the effective underline process is non-Markovian.
- survival probability for diffusing particle in an absorbing boundary at x=0 $p(t) = erf(x/\sqrt{4Dt})$
- In asymptotic time limit $p(t) = x/\sqrt{\pi Dt}$ So the dependence is $t^{-\theta}$, when $\theta = 1/2$

Langevin model of an active asymmetric Brownian particle



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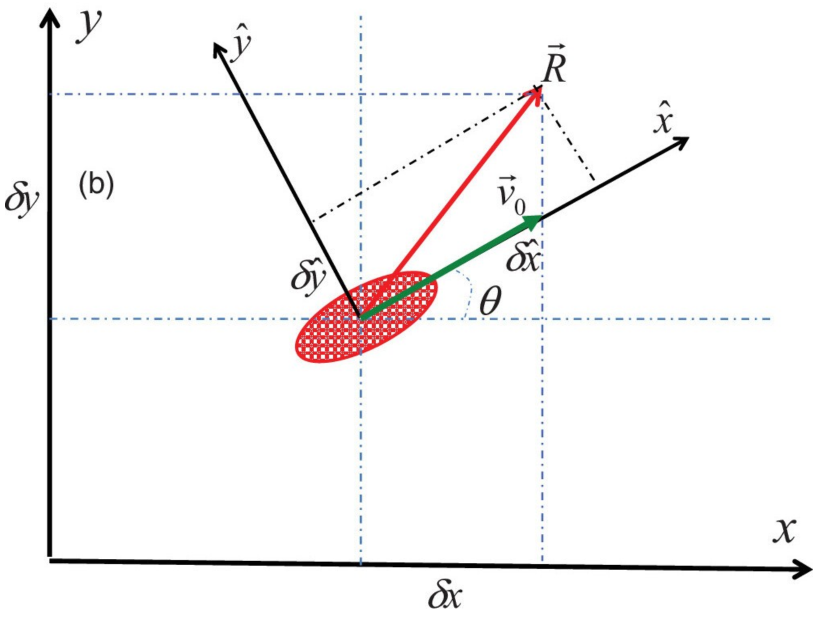

Equation of motion for the C.M. in body frame

$$\Gamma_x^{-1}\frac{\partial \tilde{x}}{\partial t} = F_x\cos\theta(t) + F_y\sin\theta(t) + v_0/\Gamma_x + \tilde{\eta}_x(t)$$
$$\Gamma_y^{-1}\frac{\partial \tilde{y}}{\partial t} = F_y\cos\theta(t) - F_x\sin\theta(t) + \tilde{\eta}_y(t)$$
$$\Gamma_\theta^{-1}\frac{\partial \theta}{\partial t} = \tau + \tilde{\eta}_\theta$$

Thermal fluctuations in the body frame

$$\langle\tilde{\eta}\rangle = 0$$
$$\langle\tilde{\eta}_i(t)\tilde{\eta}_j(t')\rangle = 2D_i\delta_{ij}\delta(t-t')$$

Body frame to Lab frame transformation

Transformation relation

$$\delta x = \cos\theta\delta\tilde{x} - \sin\theta\delta\tilde{y}$$
$$\delta y = \cos\theta\delta\tilde{y} + \sin\theta\delta\tilde{x}$$

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Transformed Langevin Equation

$$\frac{\partial x}{\partial t} = v_0\cos\theta(t) + F_x[\bar{\Gamma} + \frac{\Delta\Gamma}{2}\cos 2\theta(t)] + \frac{\Delta\Gamma}{2}F_y\sin 2\theta(t) + \eta_x(t)$$
$$\frac{\partial y}{\partial t} = v_0\sin\theta(t) + F_y[\bar{\Gamma} - \frac{\Delta\Gamma}{2}\cos 2\theta(t)] + \frac{\Delta\Gamma}{2}F_x\sin 2\theta(t) + \eta_y(t)$$
$$\frac{\partial\theta(t)}{\partial t} = \Gamma_3\tau + \eta_\theta(t)$$

$$\bar{\Gamma} = (\Gamma_\parallel + \Gamma_\perp)/2$$
$$\Delta\Gamma = (\Gamma_\parallel - \Gamma_\perp)$$

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Mobility tensor

$$\Gamma_{ij} = \bar{\Gamma}\delta_{ij} + \frac{\Delta\Gamma}{2}\begin{pmatrix}\cos 2\theta & \sin 2\theta \\ \sin 2\theta & -\cos 2\theta\end{pmatrix}$$

$$\langle\eta_3(t)\eta_3(t')\rangle = 2D_\theta\delta(t-t')$$
$$\langle\eta_i(t)\eta_j(t')\rangle = 2k_BT\Gamma_{ij}\delta(t-t')$$

MSD of free ABP

General Solution

$$x(t) = v_0 \cos\theta(t) + \eta_x(t)$$
$$y(t) = v_0 \sin\theta(t) + \eta_y(t)$$

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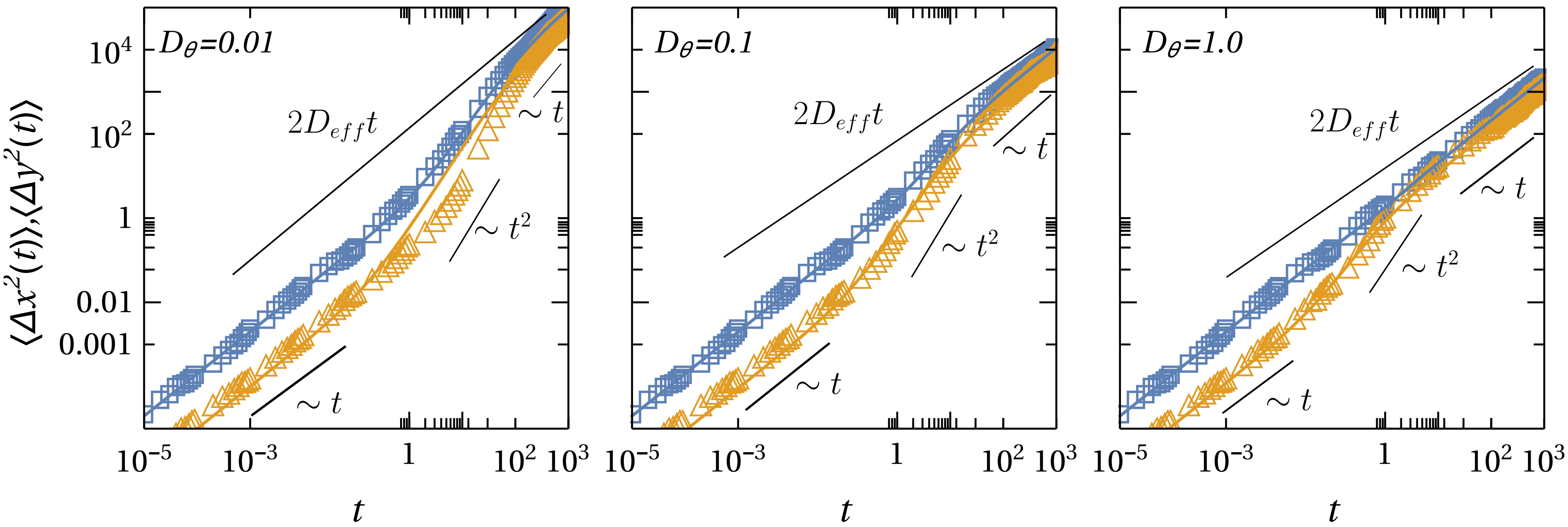
MSD -x

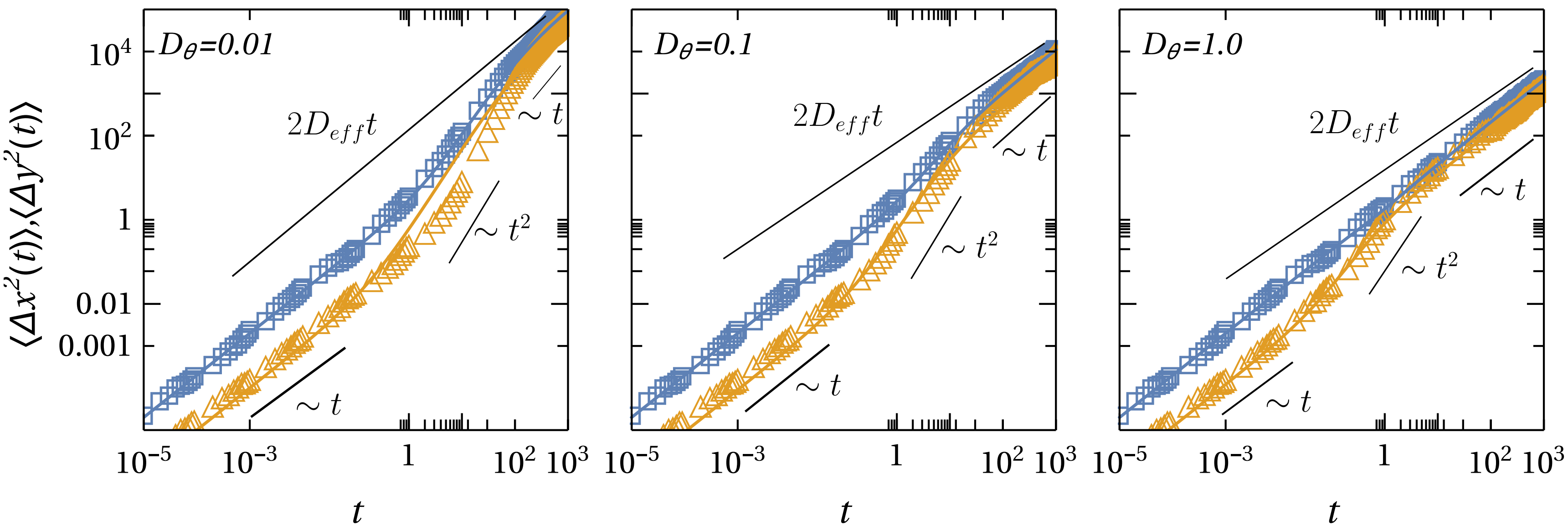
$$\langle \Delta x^2(t) \rangle_{\eta,\theta} = 2k_B T \left[\bar{\Gamma} t + \frac{\Delta\Gamma}{2} \cos 2\theta_0 \left(\frac{1 - e^{-4D_\theta t}}{4D_\theta} \right) \right] + \frac{v_0^2 \cos 2\theta_0}{12 D_\theta^2} \left(3 - 4e^{-D_\theta t} + e^{-4D_\theta t} \right) + \frac{v_0^2}{D_\theta^2} \left(D_\theta t + e^{-D_\theta t} - 1 \right)$$

MSD- y

$$\langle \Delta y^2(t) \rangle_{\eta,\theta} = 2k_B T \left[\bar{\Gamma} t - \frac{\Delta\Gamma}{2} \cos 2\theta_0 \left(\frac{1 - e^{-4D_\theta t}}{4D_\theta} \right) \right] - \frac{v_0^2 \cos 2\theta_0}{12 D_\theta^2} \left(3 - 4e^{-D_\theta t} + e^{-4D_\theta t} \right) + \frac{v_0^2}{D_\theta^2} \left(D_\theta t + e^{-D_\theta t} - 1 \right)$$



$$D_{eff} = \bar{D} + \frac{v_0^2}{2D_\theta}$$



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Small time $t < D_\theta^{-1}$ regime

$$\langle \Delta x^2(t)\rangle = 2D_\parallel t + (v_0^2 - 2D_\theta \Delta D)t^2$$
$$\langle \Delta y^2(t)\rangle = 2D_\perp t + 2D_\theta \Delta D t^2$$

Particle in Harmonic trap

Basic Langevin equation

$$U(x) = \frac{1}{2}\kappa(x^2 + y^2)$$

$$\frac{\partial x}{\partial t} = -\kappa x\left(\bar{\Gamma} + \frac{1}{2}\Delta\Gamma\cos\theta(t)\right) - \frac{1}{2}\kappa y\Delta\Gamma\sin\theta(t) + v_0\cos\theta(t) + \eta_x(t)$$

$$\frac{\partial y}{\partial t} = -\frac{1}{2}\kappa x\Delta\Gamma\sin\theta(t) - \kappa y\left(\bar{\Gamma} - \frac{1}{2}\Delta\Gamma\cos\theta(t)\right) + v_0\sin\theta(t) + \eta_y(t)$$

$$\frac{\partial \theta}{\partial t} = \Gamma_3\tau + \eta_\theta(t)$$

- Correction due to asymmetry comes in the combination of $\kappa\Delta\Gamma/2$
- Coupling is proportional $\Delta\Gamma$

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- Coupling is proportional $\Delta\Gamma$

$$\dot{\boldsymbol{R}} = -\kappa\left[\bar{\Gamma}1 + \frac{\Delta\Gamma}{2}\overline{\overline{\mathcal{R}}}(t)\right]\boldsymbol{R}(t) + v_0\hat{n} + \eta(t)$$

Perturbative Expansion

$$\boldsymbol{R}(t) = \boldsymbol{R}_0(t) - \left(\frac{\kappa\Delta\Gamma}{2}\right)\boldsymbol{R}_1(t) + \left(\frac{\kappa\Delta\Gamma}{2}\right)^2\boldsymbol{R}_2(t) + \mathcal{O}\left(\frac{\kappa\Delta\Gamma}{2}\right)^3$$

Langevin equation related to different orders

$$\begin{aligned}
\dot{\boldsymbol{R}}_0 &= -\kappa\overline{\Gamma}\boldsymbol{R}_0(t) + v_0\hat{n} + \eta(t) \\
\dot{\boldsymbol{R}}_1 &= -\kappa\overline{\Gamma}\boldsymbol{R}_1(t) + \overline{\overline{\mathcal{R}}}(t)\boldsymbol{R}_0(t) \\
\dot{\boldsymbol{R}}_2 &= -\kappa\overline{\Gamma}\boldsymbol{R}_2(t) + \overline{\overline{\mathcal{R}}}(t)\boldsymbol{R}_1(t)
\end{aligned}$$

Solution

$$\boldsymbol{R}_0(t) = \int_0^t dt' e^{-\kappa\overline{\Gamma}(t-t')}[\eta(t') + v_0\hat{n}(t')]$$

$$\boldsymbol{R}_1(t) = \int_0^t dt' e^{-\kappa\overline{\Gamma}(t-t')}\overline{\overline{\mathcal{R}}}(t')\boldsymbol{R}_0(t')$$

$$\boldsymbol{R}_2(t) = \int_0^t dt' e^{-\kappa\overline{\Gamma}(t-t')}\overline{\overline{\mathcal{R}}}(t')\boldsymbol{R}_1(t')$$

Explicit form of the correlation matrix in equal time

$$\langle R_i(t)R_j(t)\rangle_{\eta,\theta} = \langle R_{0,i}(t)R_{0,j}(t)\rangle_{\eta,\theta} - (\kappa\Delta\Gamma)\langle R_{0,i}(t)R_{1,j}(t)\rangle_{\eta,\theta} + (\kappa\Delta\Gamma/2)^2[2\langle R_{0,i}(t)R_{2,j}(t)\rangle_{\eta,\theta} + 2\langle R_{1,i}(t)R_{1,j}(t)\rangle_{\eta,\theta}] + \mathcal{O}(\kappa\Delta\Gamma/2)^3$$

Solution

$$\boldsymbol{R}_0(t) = \int_0^t dt' e^{-\kappa\overline{\Gamma}(t-t')}[\eta(t') + v_0\hat{n}(t')]$$

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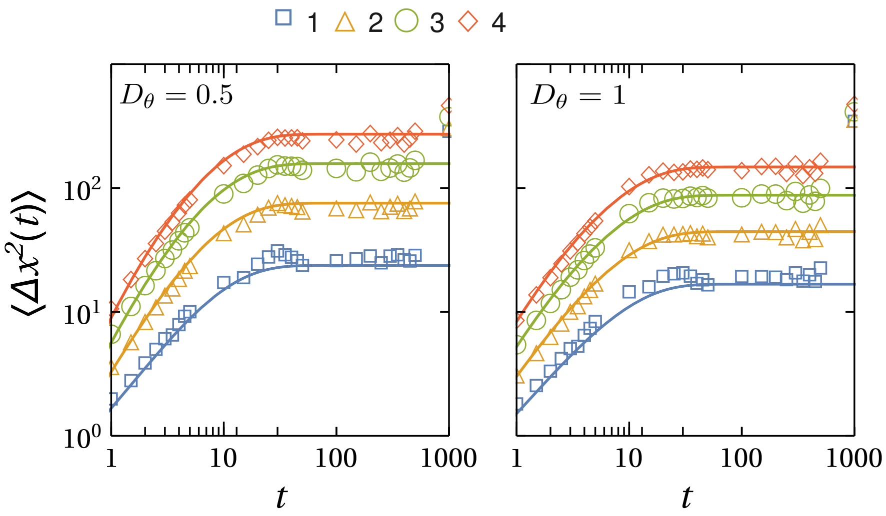
MSD along x-axis

$$\langle x^2(t)\rangle_{\eta,\theta} = \langle x_0^2(t)\rangle_{\eta,\theta} - \kappa\Delta\Gamma\langle x_0(t)x_1(t)\rangle_{\eta,\theta}$$

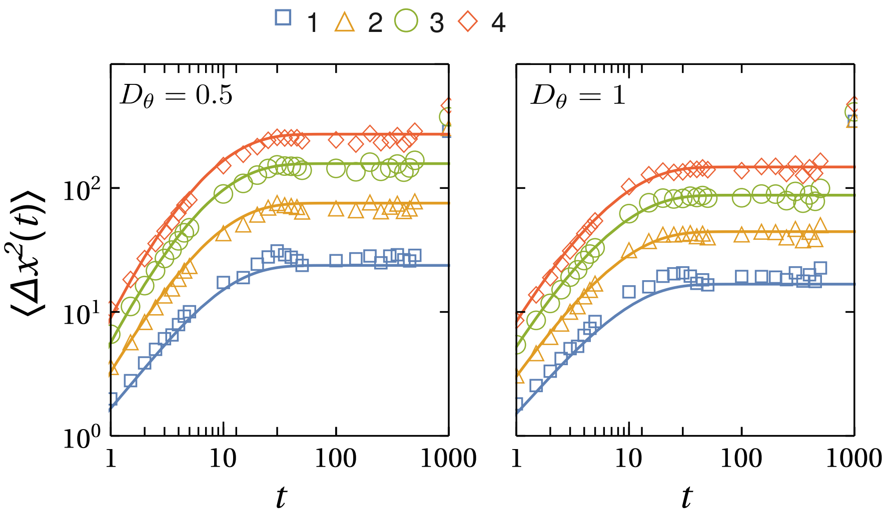
Exact expression of MSD

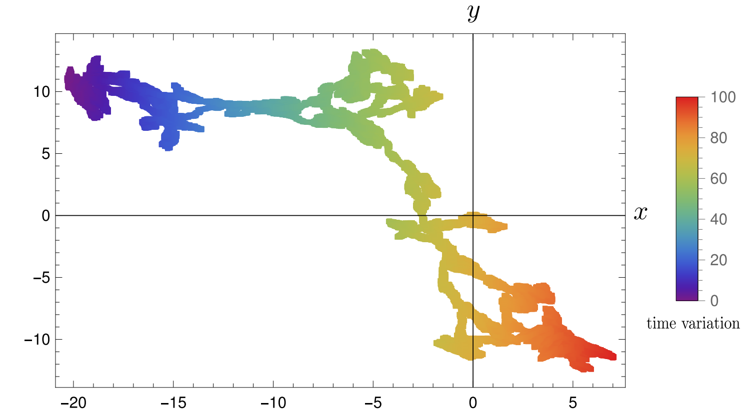
$$
\begin{aligned}
\langle x^2(t)\rangle =\; & \frac{k_B T}{\kappa}(1-e^{-2\kappa\bar{\Gamma}t}) + \frac{\Delta D}{4D_\theta}\left[e^{-2\kappa\bar{\Gamma}t} - e^{-(2\kappa\bar{\Gamma}+4D_\theta)t} + \kappa\Delta\Gamma\frac{e^{-\kappa\bar{\Gamma}t}-e^{-(2\kappa\bar{\Gamma}+4D_\theta)t}}{\kappa\bar{\Gamma}+4D_\theta}\right] \\
& + \frac{v_0^2\cos 2\theta_0}{2}\left[\frac{D_\theta(e^{-4D_\theta t}-e^{-2\kappa\bar{\Gamma}t})}{(\kappa\bar{\Gamma}-D_\theta)(\kappa\bar{\Gamma}-2D_\theta)(\kappa\bar{\Gamma}-3D_\theta)} + \frac{e^{-4D_\theta t}-2e^{-(\kappa\bar{\Gamma}+D_\theta)t}+e^{-2\kappa\bar{\Gamma}t}}{(\kappa\bar{\Gamma}-D_\theta)(\kappa\bar{\Gamma}-3D_\theta)}\right] \\
& + \frac{v_0^2}{2}\left[\frac{1-2e^{-(\kappa\bar{\Gamma}+D_\theta)t}+e^{-2\kappa\bar{\Gamma}t}}{(\kappa\bar{\Gamma}-D_\theta)(\kappa\bar{\Gamma}+D_\theta)} - \frac{D_\theta(1-e^{-2\kappa\bar{\Gamma}t})}{\kappa\bar{\Gamma}(\kappa\bar{\Gamma}-D_\theta)(\kappa\bar{\Gamma}+D_\theta)}\right] \\
& + (\kappa\Delta\Gamma)\sinh\kappa\bar{\Gamma}te^{-\kappa\bar{\Gamma}t}\left[\frac{3v_0^2 D_\theta}{2\kappa\bar{\Gamma}(\kappa\bar{\Gamma}+D_\theta)(\kappa\bar{\Gamma}-D_\theta)(\kappa\bar{\Gamma}+2D_\theta)} - \frac{\Delta D}{2\kappa\bar{\Gamma}(\kappa\bar{\Gamma}+2D_\theta)}\right]
\end{aligned}
$$

If $\kappa \to 0$ it reproduces the correct result for the free diffusion of anisotropic ABP

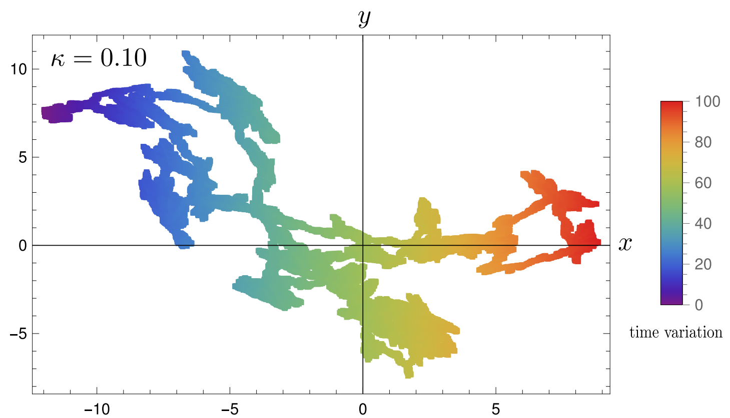


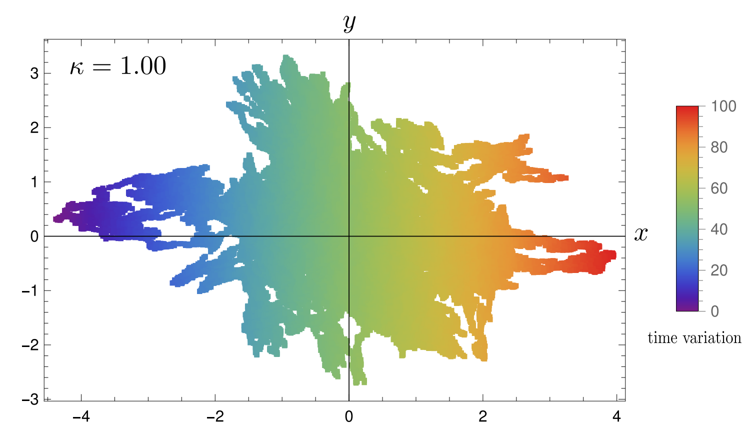
1
2
3
4
$D_\theta = 0.5$
$D_\theta = 1$
$\langle \Delta x^2(t) \rangle$
10^0
10^1
10^2
1
10
100
1000
t

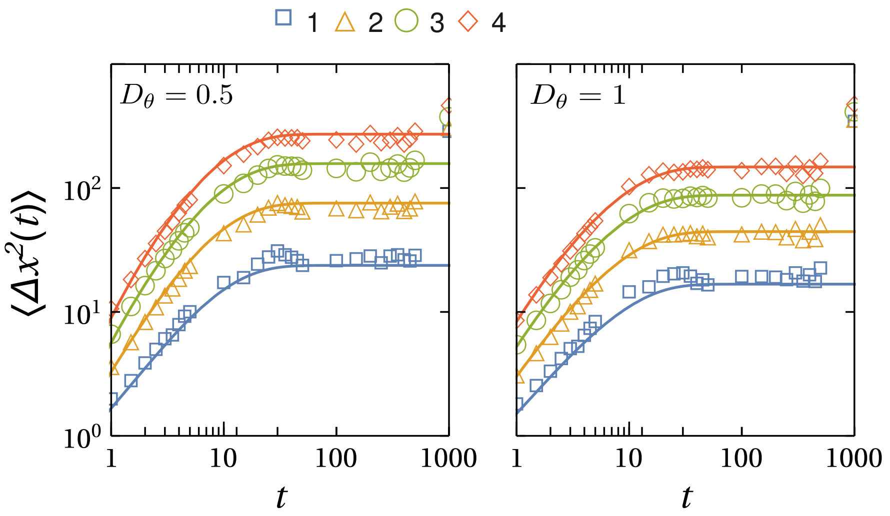


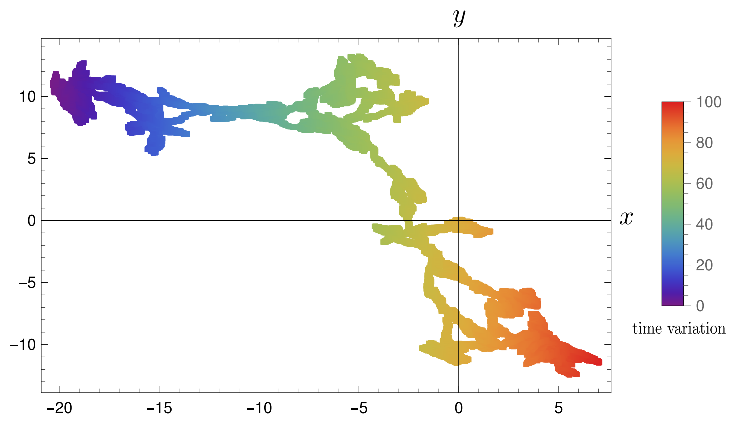


Free particle









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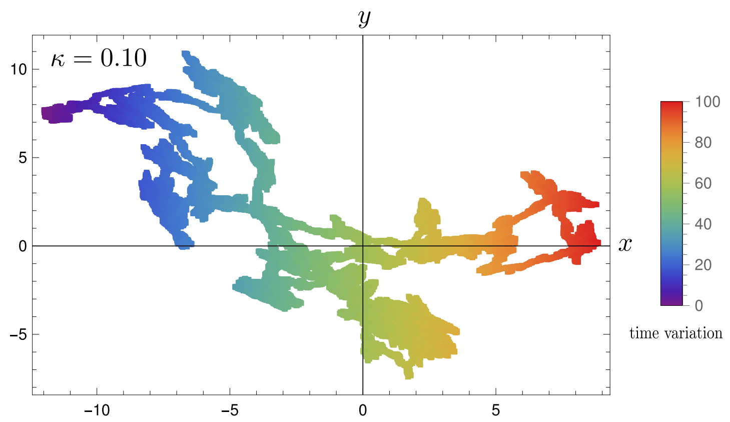

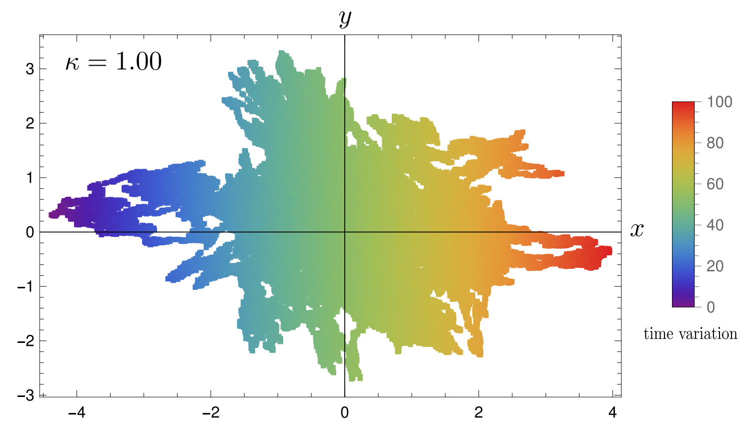

- Stronger confinement, earlier steady state
- More localized

Two-time correlation of free particle

Considering $t_1 > t_2$

$$\langle x(t_1)x(t_2)\rangle = 2k_BT\bar{\Gamma}t_2\Big[1+\frac{\Delta\Gamma}{2\bar{\Gamma}}\cos 2\theta_0\Big(\frac{1-e^{-4D_\theta t_2}}{4D_\theta t_2}\Big)\Big] + v_0^2\Bigg[\cos 2\theta_0\Big(\frac{1-e^{-D_\theta t_2}}{6D_\theta^2}+\frac{1-e^{-4D_\theta t_2}}{12D_\theta^2} - e^{-D_\theta t_1}\frac{1-e^{-3D_\theta t_2}}{6D_\theta^2}\Big) - \frac{1-e^{-D_\theta t_2}}{2D_\theta^2} + \frac{t_2}{D_\theta} - e^{-D_\theta t_1}\frac{1-e^{D_\theta t_2}}{D_\theta^2}\Bigg]$$

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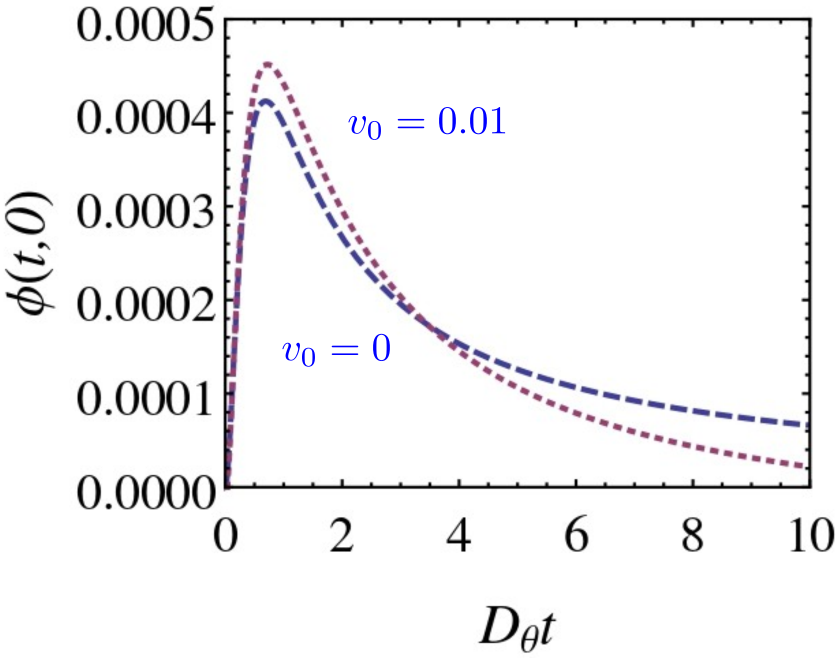
Approximation is at asymptotic time limit when $t_1 >> t_2$

$$\langle x(t_1)x(t_2)\rangle_{\theta_0=0} = 2D_{eff}t_2[1 + \frac{\Delta D_{eff}\tau_4(t_2)}{2D_{eff}t_2} - \frac{v_0^2\tau_1(t_2)}{6D_\theta D_{eff}t_2}]$$

$$D_{eff} = \bar{D} + \frac{v_0^2}{2D_\theta}$$

$$\Delta D_{eff} = \Delta D + \frac{v_0^2}{3D_\theta}$$

Non-Gaussian Parameter



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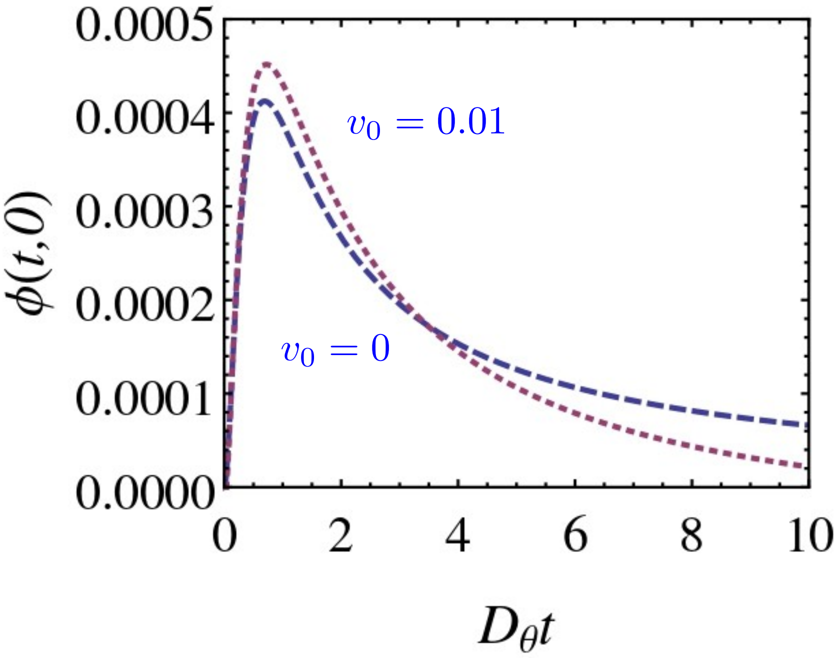

$$\phi(t, \theta_0) = \frac{C^4_{\theta_0}(t)}{3(\langle \Delta x(t)^2 \rangle)^2}$$

$$C^4_{\theta_0} = \langle [\Delta x(t) - \langle \Delta x(t) \rangle]^4 \rangle - 3(\langle [\Delta x(t) - \langle \Delta x(t) \rangle]^2 \rangle)^2$$

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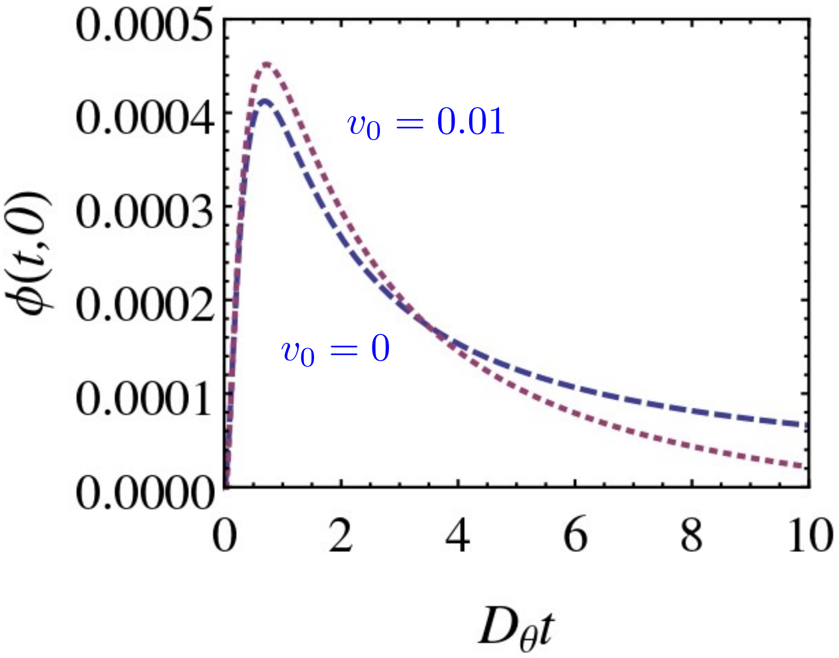

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- Non-Gaussian parameter depends on $\Delta D^2/\bar{D}^2$ and $v_0^2/\bar{D}^2$
- Weak asymmetry, NG parameter small.
- Large t, NG parameter decays as t^{-1}

Way to Calculate persistence probability

- Route to calculate the persistence probability is through the non-stationary two-time correlation function.
- The Lamperti transformation converts the non-stationary correlator to a stationary process.
- For a Gaussian stochastic process, the persistence probability can be directly calculated using Slepian's theorem.

Transformation in the spatial coordinate $\tilde{X}(t) = \frac{x(t)}{\sqrt{\langle x^2(t) \rangle}}$

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Rescaled two-time correlation $\langle \tilde{X}(t_1)\tilde{X}(t_2)\rangle = \sqrt{\frac{2D_{eff}t_2[1+\frac{\Delta D_{eff}\tau_4(t_2)}{2D_{eff}} - \frac{v_0^2\tau_1(t_2)}{6D_\theta t_2 D_{eff}}]}{2D_{eff}t_1[1+\frac{\Delta D_{eff}\tau_4(t_1)}{2D_{eff}} - \frac{v_0^2\tau_1(t_1)}{6D_\theta t_1 D_{eff}}]}}$

Define the transformation in time $e^T = 2D_{eff}t[1 + \frac{\Delta D_{eff}\tau_4(t)}{2D_{eff}} - \frac{v_0^2\tau_1(t)}{6D_\theta D_{eff}t}]$

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Now $\tilde{X}(t)$ is stationary Gaussian process with purely exponential correlation

$$\langle \tilde{X}(t_1)\tilde{X}(t_2)\rangle = e^{-(T_1-T_2)/2}$$

Persistence probability of free particle

Since the stationary correlation function now decays exponentially for all times, following Slepian, the asymptotic form of the persistence probability is found to be

$$p(T) \sim e^{-\lambda T}$$

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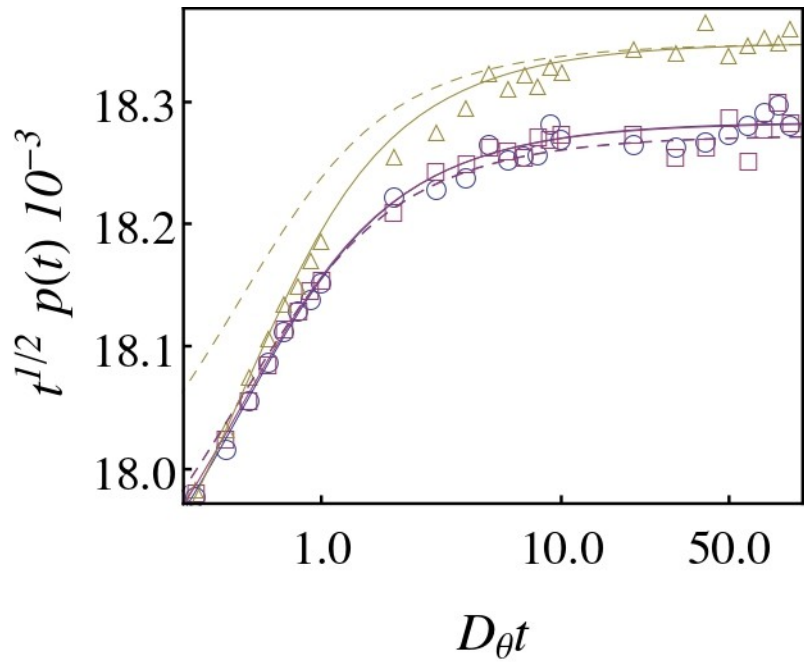
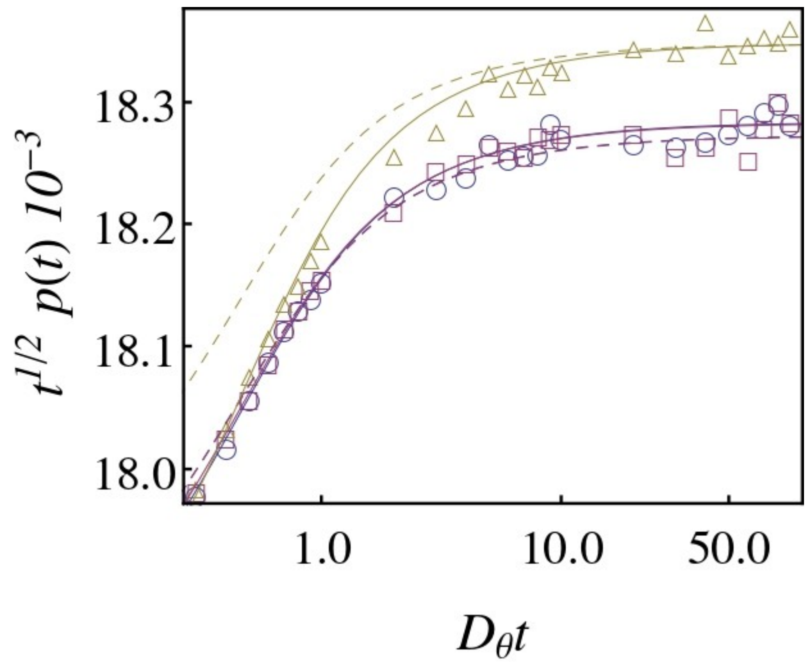
Transforming back to real-time

$$p(t, \theta_0 = 0) = \frac{1}{\sqrt{2D_{eff}t}}\left[1 + \frac{\Delta D_{eff}\tau_4(t)}{2D_{eff}} - \frac{v_0^2\tau_1(t)}{6D_\theta D_{eff}t}\right]^{-1/2}$$



Plot for different choices of propulsion velocity $v_0 = 0$ (open circles), $v_0 = 0.01$ (open square) $v_0 = 0.1$ (open triangles). Dashed lines are analytical plots, where as solid lines are fit to the data.



Plot for different choices of propulsion velocity $v_0 = 0$ (open circles), $v_0 = 0.01$ (open square) $v_0 = 0.1$ (open triangles). Dashed lines are analytical plots, where as solid lines are fit to the data.

- For small propulsion velocities, $t^{1/2}p(t)$ is unable to Pick up the activity of the particle.

- In the asymptotic limit it goes to constant value and the persistence probability goes like $t^{-1/2}$ decay, which is exactly like isotropic case in asymptotic limit.

Two-time Correlation in Harmonic trap

We have restricted up to first order correction

$$\langle x(t_1)x(t_2)\rangle_{\eta,\theta} = \langle x_0(t_1)x_0(t_2)\rangle_{\eta,\theta} - \left(\frac{\kappa\Delta\Gamma}{2}\right)\left[\langle x_0(t_1)x_1(t_2)\rangle_{\eta,\theta} + \langle x_0(t_2)x_1(t_1)\rangle_{\eta,\theta}\right]$$

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$$\langle x(t_1)x(t_2)\rangle_{\eta,\theta} = \langle x_0(t_1)x_0(t_2)\rangle_{\eta,\theta} - (\kappa\Delta\Gamma)\left[\langle x_0(t_1)x_1(t_2)\rangle_{\eta,\theta}\right]$$

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Exact expression of two-time correlation

$$\langle x(t_1)x(t_2)\rangle_{\theta_0=0} = e^{-\kappa\bar{\Gamma}t_1}\left[\left(\frac{2k_BT}{\kappa'}\right)\sinh\kappa\bar{\Gamma}t_2 + \frac{v_0^2(e^{-\kappa\bar{\Gamma}t_2} - e^{-D_\theta t_2})}{(\kappa\bar{\Gamma} - 3D_\theta)(\kappa\bar{\Gamma} + D_\theta)} + (k_BT\Delta\Gamma)\frac{1 - e^{-4D_\theta t_2}}{4D_\theta}\right]$$

effective trap constant $\quad {\kappa'}^{-1} = \kappa^{-1}[1 - \frac{v_0^2 D_\theta}{\bar{D}(\kappa\bar{\Gamma} - D_\theta)(\kappa\bar{\Gamma} + D_\theta)} + \frac{\kappa\Delta\Gamma}{2}\frac{3v_0^2 D_\theta}{2\bar{D}(\kappa\bar{\Gamma} - D_\theta)(\kappa\bar{\Gamma} + D_\theta)(\kappa\bar{\Gamma} + 2D_\theta)}]$

Persistence in harmonic trap

$$p(t)|_{\theta_0=0} = e^{-\kappa\bar{\Gamma}t/2}\left[\left(\frac{2k_BT}{\kappa'}\right)\sinh\kappa\bar{\Gamma}t + \frac{v_0^2(e^{-\kappa\bar{\Gamma}t} - e^{-D_\theta t})}{(\kappa\bar{\Gamma} - 3D_\theta)(\kappa\bar{\Gamma} + D_\theta)} + (\Delta D)\frac{1 - e^{-4D_\theta t}}{4D_\theta}\right]^{-1/2}$$

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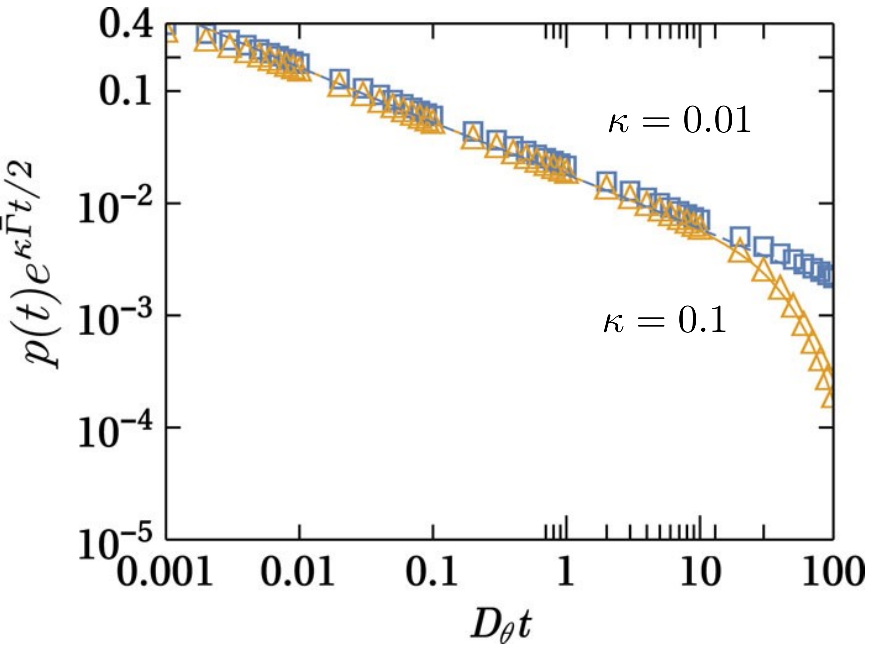

$D_\theta = 1, \theta_0 = 0, D_{\|} = 1, D_\perp = 0.5$

- In the limit of $v_0 = 0$, the equation correctly reproduces the result for a passive anisotropic particle.

- When $\kappa = 0$, and $\Delta D = 0$ the results for passive isotropic Brownian particle is found in the long time.

Summary

- MSD of an asymmetric ABP has been calculated in absence of any potential and in the presence of a harmonic potential.

- We have calculated the persistence probability along the x-axis of an active anisotropic particle in two dimensions in the absence of any potential and in the presence of a harmonic potential.

- The two-time correlation function has been calculated in both the cases. In the case of the harmonic trapped particle, we have used a perturbative solution for calculating the correlation functions.

- The persistence probability has been calculated with suitable space and time transformations.

Talk based on

Ghosh et. al. J. Chem. Phys. 157, 194905 (2022)

S. Mandal, A. Ghosh arXiv preprint arXiv:2308.03451 (2023)

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Torque and rotational diffusion