

Asymmetric [Ellipsoid] active particle:

An asymmetric active particle undergoes self-propulsion with a velocity $v_p \hat{\mathbf{n}}(t)$ along its longer axis in 2-dimension. The angle between the x -axis of the lab frame and long axis of the ellipsoid at time t is represented by $\theta(t)$. The component of the orientation vector $\hat{\mathbf{n}}(t)$ w.r.t the lab frame can be expressed as $\hat{\mathbf{n}}(t) \equiv (\cos \theta(t), \sin \theta(t))$.

In the body frame, the equation of motion of the centre of mass of the particle is given as

$$\begin{aligned} \frac{\partial \tilde{x}}{\partial t} &= v_p + \Gamma_{\parallel} F_x \cos \theta(t) + \Gamma_{\parallel} F_y \sin \theta(t) + \Gamma_{\parallel} \tilde{\eta}_x(t) \\ \frac{\partial \tilde{y}}{\partial t} &= \Gamma_{\perp} F_x \cos \theta(t) + \Gamma_{\perp} F_y \sin \theta(t) + \Gamma_{\perp} \tilde{\eta}_y(t) \\ \frac{\partial \theta}{\partial t} &= \Gamma_{\theta} \tau + \tilde{\eta}_{\theta} \end{aligned} \quad (1)$$

where F_x and F_y are the forces acting on the particle along the x and y directions (in the lab frame), respectively and τ is the torque acting on the particle.

In the lab frame, the displacements are related to the body frame as

$$\begin{aligned} \delta x &= \cos \theta \delta \tilde{x} - \sin \theta \delta \tilde{y}, \\ \delta y &= \sin \theta \delta \tilde{x} + \cos \theta \delta \tilde{y}. \end{aligned} \quad (2)$$

Substituting equation(1) in equation(2), we have

$$\frac{\partial \mathbf{x}_i}{\partial t} = \Gamma_{ij} \mathbf{F}_j + v_p \hat{\mathbf{n}}_i(t) + \xi_i(t) \quad (3)$$

where

$$\begin{bmatrix} \xi_x(t) \\ \xi_y(t) \end{bmatrix} = \begin{bmatrix} \Gamma_{\parallel} \\ \Gamma_{\perp} \end{bmatrix} \begin{bmatrix} \cos \theta(t) & -\sin \theta(t) \\ \sin \theta(t) & \cos \theta(t) \end{bmatrix} \begin{bmatrix} \tilde{\eta}_x(t) \\ \tilde{\eta}_y(t) \end{bmatrix} \quad (4)$$

The correlation of thermal fluctuation in the body frame are

$$\begin{aligned} \langle \tilde{\eta} \rangle &= 0 \text{ and } \langle \tilde{\eta}_i(t) \tilde{\eta}_j(t') \rangle = 2D_i \delta_{ij} \delta(t - t') \\ \text{where } D_{\parallel} &= K_B T \Gamma_{\parallel}, D_{\perp} = K_B T \Gamma_{\perp} \end{aligned}$$

The coupled Langevin equation in the presence of an external force F and torque τ are

$$\begin{aligned} \partial_t r_i &= \Gamma_{ij}(\theta(t)) F_j + v_p \hat{n}_i(t) + \xi_i(t), \\ \text{where } \Gamma_{ij}(\theta(t)) &= \bar{\Gamma} \delta_{ij} + \frac{\Delta \Gamma}{2} M_{ij}(\theta(t)) \\ \partial_t \theta &= \Gamma_{\theta} \tau + \xi_{\theta}(t) \end{aligned} \quad (5)$$

$$\bar{\Gamma} = \frac{\Gamma_{\parallel} + \Gamma_{\perp}}{2}, \Delta \Gamma = \Gamma_{\parallel} - \Gamma_{\perp} \text{ and } M_{ij}(\theta(t)) = \begin{bmatrix} \cos 2\theta(t) & \sin 2\theta(t) \\ \sin 2\theta(t) & -\cos 2\theta(t) \end{bmatrix} \quad (6)$$

$\xi_i(t)$ and ξ_{θ} are the Gaussian random noise with zero mean and

$$\langle \xi_{\theta}(t) \xi_{\theta}(t') \rangle = 2K_B T \Gamma_{\theta} \delta(t - t') = 2D_{\theta} \delta(t - t')$$

for a fixed angle $\theta(t)$,

$$\langle \xi_i(t) \xi_j(t') \rangle = 2K_B T \Gamma_{ij}(\theta(t)) \delta(t - t')$$

Calculation of $\langle \hat{n}_i(t_1) \hat{n}_j(t_2) \rangle_{\theta_0}$, the average is taken for fixed initial angle θ_0

$$\theta(t_1) \equiv \theta_1, \theta(t_2) \equiv \theta_2$$

$$\langle \hat{n}_i(t_1) \hat{n}_j(t_2) \rangle_{\theta_0} = \begin{bmatrix} \langle \cos \theta_1 \cos \theta_2 \rangle & \langle \cos \theta_1 \sin \theta_2 \rangle \\ \langle \sin \theta_1 \cos \theta_2 \rangle & \langle \sin \theta_1 \sin \theta_2 \rangle \end{bmatrix} \quad (7)$$

$$2\langle \cos \theta_1 \cos \theta_2 \rangle = e^{-D_r(t_1+t_2-2\min(t_1,t_2))} + \cos 2\theta_0 e^{-D_r(t_1+t_2+2\min(t_1,t_2))}$$

$$2\langle \sin \theta_1 \sin \theta_2 \rangle = e^{-D_r(t_1+t_2-2\min(t_1,t_2))} - \cos 2\theta_0 e^{-D_r(t_1+t_2+2\min(t_1,t_2))}$$

$$2\langle \cos \theta_1 \sin \theta_2 \rangle = \sin 2\theta_0 e^{-D_r(t_1+t_2+2\min(t_1,t_2))}$$

$$2\langle \cos \theta_2 \sin \theta_1 \rangle = \sin 2\theta_0 e^{-D_r(t_1+t_2+2\min(t_1,t_2))}$$

Substituting, we have

$$\langle \hat{n}_i(t_1) \hat{n}_j(t_2) \rangle_{\theta_0} = \frac{\delta_{ij}}{2} e^{-D_r(t_1+t_2-2\min(t_1,t_2))} + \frac{M_{ij}(\theta_0)}{2} e^{-D_r(t_1+t_2+2\min(t_1,t_2))} \quad (8)$$

Langevin equation without trap:

$$\frac{\partial r_i}{\partial t} = v_p \hat{n}_i(t) + \xi_i(t) \quad (9)$$

$$\implies r_i(t) - r_i(0) = \int_0^t v_p \hat{n}_i(t') dt' + \int_0^t \xi_i(t') dt'$$

$$\implies \Delta r_i(t) = \int_0^t v_p \hat{n}_i(t') dt' + \int_0^t \xi_i(t') dt'$$

Mean Square Displacement (MSD) :-

$$\langle \Delta x^2(t) \rangle_{\theta_0} = v_p^2 \int_0^t dt'_1 \int_0^t dt'_2 \langle \hat{n}_i(t'_1) \hat{n}_i(t'_2) \rangle_{\theta_0} + \int_0^t dt'_1 \int_0^t dt'_2 \langle \xi_i(t'_1) \xi_i(t'_2) \rangle_{\theta_0} \quad (10)$$

$$\langle \Delta x^2(t) \rangle_{\theta_0} = v_p^2 \int_0^t dt'_1 \int_0^t dt'_2 \left[\frac{1}{2} e^{-D_r(t'_1+t'_2-2\min(t'_1,t'_2))} + \frac{M_{xx}(\theta_0)}{2} e^{-D_r(t'_1+t'_2+2\min(t'_1,t'_2))} \right] +$$

$$2K_B T \int_0^t dt'_1 \int_0^t dt'_2 \langle \Gamma_{xx}(\theta(t'_1)) \rangle_{\theta_0} \delta(t'_1 - t'_2)$$

Considering $t'_1 > t'_2$,

$$\langle \Delta x^2(t) \rangle_{\theta_0} = 2v_p^2 \int_0^t dt'_2 \int_{t'_2}^t dt'_1 \left[\frac{1}{2} e^{-D_r(t'_1-t'_2)} \right] + 2v_p^2 \int_0^t dt'_2 \int_{t'_2}^t dt'_1 \frac{M_{xx}(\theta_0)}{2} e^{-D_r(t'_1+3t'_2)}$$

$$+ 2K_B T \int_0^t dt'_1 \int_0^t dt'_2 [\bar{\Gamma} + \frac{\Delta \Gamma}{2} \langle \cos 2\theta(t'_1) \rangle_{\theta_0}] \delta(t'_1 - t'_2)$$

$$\langle \Delta x^2(t) \rangle_{\theta_0} = 2v_p^2 \int_0^t dt'_2 \int_{t'_2}^t dt'_1 \left[\frac{1}{2} e^{-D_r(t'_1-t'_2)} \right] + 2v_p^2 \int_0^t dt'_2 \int_{t'_2}^t dt'_1 \frac{M_{xx}(\theta_0)}{2} e^{-D_r(t'_1+3t'_2)}$$

$$+ 2K_B T \int_0^t dt'_1 \int_0^t dt'_2 \bar{\Gamma} \delta(t'_1 - t'_2) + 2K_B T \frac{\Delta \Gamma}{2} \int_0^t dt'_1 \int_0^t dt'_2 \cos 2\theta_0 e^{-4D_r t'_1} \delta(t'_1 - t'_2)$$

$$\text{Take } \tau_r = \frac{1}{2D_r}, \tau_1(t) = \frac{1 - e^{-D_r t}}{D_r}, \tau_4(t) = \frac{1 - e^{-4D_r t}}{4D_r}$$

$$\langle \Delta x^2(t) \rangle_{\theta_0} = 2\tau_r v_p^2 [t - \tau_1(t)] + \frac{2\tau_r v_p^2}{3} \cos 2\theta_0 [\tau_1(t) - \tau_4(t)] + 2K_B T \bar{\Gamma} t + K_B T \Delta \Gamma \cos 2\theta_0 \tau_4(t)$$

Similarly,

$$\langle \Delta y^2(t) \rangle_{\theta_0} = 2\tau_r v_p^2 [t - \tau_1(t)] - \frac{2\tau_r v_p^2}{3} \cos 2\theta_0 [\tau_1(t) - \tau_4(t)] + 2K_B T \bar{\Gamma} t - K_B T \Delta \Gamma \cos 2\theta_0 \tau_4(t) \quad (11)$$

Generalising, we have

$$\langle \Delta x_i(t) \Delta x_j(t) \rangle_{\theta_0} = \{2\bar{D}t + 2\tau_r v_p^2 [t - \tau_1(t)]\} \delta_{ij} + \left[\frac{2\tau_r v_p^2}{3} [\tau_1(t) - \tau_4(t)] + \Delta D \tau_4(t) \right] M_{ij}(\theta_0) \quad (12)$$

Therefore,

$$\langle \Delta r^2(t) \rangle_{\theta_0} = \langle \Delta x^2(t) \rangle_{\theta_0} + \langle \Delta y^2(t) \rangle_{\theta_0} \quad (13)$$

$$\langle \Delta r^2(t) \rangle_{\theta_0} = 4(K_B T \bar{\Gamma} + \tau_r v_p^2) t - 4\tau_r v_p^2 \tau_1(t)$$

$$\text{Take } \bar{D} = K_B T \bar{\Gamma},$$

The MSD for the untrapped active asymmetric particle is given as

$$\langle \Delta r^2(t) \rangle_{\theta_0} = 4\bar{D}t + 4\tau_r v_p^2 (t - 2\tau_r (1 - e^{-\frac{t}{2\tau_r}}))$$

The time dependent displacement diffusion tensor for a fixed initial angle θ_0 are

$$D_{ij}(t, \theta_0) = \frac{\langle \Delta x_i(t) \Delta x_j(t) \rangle_{\theta_0}}{2t} \quad (14)$$

Asymmetric Brownian particle

$$D_{ij}(t, \theta_0) = \bar{D} \delta_{ij} + \frac{\Delta D}{2} \frac{\tau_4(t)}{t} M_{ij}(\theta_0)$$

Asymmetric Active particle without harmonic trap

$$D_{ij}(t, \theta_0) = [\bar{D} + \tau_r v_p^2 - \frac{\tau_r v_p^2}{t} \tau_1(t)] \delta_{ij} + \left[\frac{2\tau_r v_p^2}{3} [\tau_1(t) - \tau_4(t)] + \Delta D \tau_4(t) \right] \frac{M_{ij}(\theta_0)}{2t}$$

If we average D_{ij} over all the initial angles θ_0 ,

$$\text{Asymmetric Brownian particle} \quad (15)$$

$$D_{ij}(t) = \frac{1}{2\pi} \int_0^{2\pi} d\theta_0 D_{ij}(t, \theta_0) = \bar{D} \delta_{ij}$$

Asymmetric Active particle without harmonic trap

$$D_{ij}(t) = \frac{1}{2\pi} \int_0^{2\pi} d\theta_0 D_{ij}(t, \theta_0) = [\bar{D} + \tau_r v_p^2 - \frac{\tau_r v_p^2}{t} \tau_1(t)] \delta_{ij}$$

For $t \gg \tau_r$, $D_{ij}(t) \sim [\bar{D} + \tau_r v_p^2] \delta_{ij}$, which means that the asymmetry is lost at long times and the system behave like a passive brownian particle but with an enhanced diffusion.

For $t \ll \tau_r$, $D_{ij}(t) \sim [\bar{D} + \frac{v_p^2}{4}] \delta_{ij}$, $\langle \Delta r^2(t) \rangle_{\theta_0} = 4\bar{D}t + v_p^2 t^2$, which shows ballistic behaviour at short times.

The correlation $\langle \Delta x(t_1) \Delta x(t_2) \rangle_{\theta_0}$

$$\begin{aligned}
\langle \Delta x(t_1) \Delta x(t_2) \rangle_{\theta_0} &= v_p^2 \int_0^{t_1} dt_1' \int_0^{t_2} dt_2' \langle \hat{n}_x(t_1') \hat{n}_x(t_2') \rangle_{\theta_0} + \int_0^{t_1} dt_1' \int_0^{t_2} dt_2' \langle \xi_x(t_1') \xi_x(t_2') \rangle_{\theta_0} \quad (16) \\
\langle \Delta x(t_1) \Delta x(t_2) \rangle_{\theta_0} &= v_p^2 \int_0^{t_1} dt_1' \int_0^{t_2} dt_2' \left[\frac{1}{2} e^{-D_r(t_1' + t_2' - 2 \min(t_1', t_2'))} + \frac{M_{xx}(\theta_0)}{2} e^{-D_r(t_1' + t_2' + 2 \min(t_1', t_2'))} \right] \\
&\quad + 2K_B T \int_0^{t_1} dt_1' \int_0^{t_2} dt_2' \langle \Gamma_{xx}(\theta(t_1')) \rangle_{\theta_0} \delta(t_1' - t_2') \\
\langle \Delta x(t_1) \Delta x(t_2) \rangle_{\theta_0} &= v_p^2 \int_0^{t_2} dt_2' \int_{t_2'}^{t_2} dt_1' \frac{1}{2} e^{-D_r(t_1' - t_2')} + v_p^2 \int_0^{t_2} dt_2' \int_{t_2'}^{t_1} dt_1' \frac{1}{2} e^{-D_r(t_1' - t_2')} \\
&\quad + v_p^2 \frac{M_{xx}(\theta_0)}{2} \int_0^{t_2} dt_2' \int_{t_2'}^{t_2} dt_1' e^{-D_r(t_1' + 3t_2')} + v_p^2 \frac{M_{xx}(\theta_0)}{2} \int_0^{t_2} dt_2' \int_{t_2'}^{t_1} dt_1' e^{-D_r(t_1' + 3t_2')} \\
&\quad + 2K_B T \int_0^{t_1} dt_1' \int_0^{t_2} dt_2' \left[\bar{\Gamma} + \frac{\Delta \Gamma}{2} \langle \cos 2\theta(t_1') \rangle_{\theta_0} \right] \delta(t_1' - t_2') \\
\langle \Delta x(t_1) \Delta x(t_2) \rangle_{\theta_0} &= v_p^2 \tau_r \left[2t_2 - \tau_1(t_2) - 2\tau_r \left(e^{\frac{-(t_1 - t_2)}{2\tau_r}} - e^{\frac{-t_1}{2\tau_r}} \right) \right] \\
&\quad + \cos 2\theta_0 \tau_r v_p^2 \left[\frac{2\tau_4(t_2)}{3} - \frac{\tau_1(t_2)}{3} - e^{\frac{-t_1}{2\tau_r}} \tau_3(t_2) \right] \\
&\quad + 2K_B T \bar{\Gamma} t_2 + K_B T \Delta \Gamma \cos 2\theta_0 \tau_4(t_2)
\end{aligned}$$

The two time correlation for a fixed initial angle θ_0 ,

Asymmetric brownian particle (17)

Taking $t_1 > t_2$

$$\langle \Delta x(t_1) \Delta x(t_2) \rangle_{\theta_0} = 2\bar{D}t_2 \left[1 + \frac{\Delta \Gamma}{2\bar{\Gamma}} \cos 2\theta_0 \tau_4(t_2) \right]$$

Asymmetric Active brownian particle

$$\begin{aligned}
\langle \Delta x(t_1) \Delta x(t_2) \rangle_{\theta_0} &= 2\bar{D}t_2 \left[1 + \frac{\Delta \Gamma}{2\bar{\Gamma}} \cos 2\theta_0 \tau_4(t_2) \right] + v_p^2 \tau_r \left[2t_2 - \tau_1(t_2) - 2\tau_r \left(e^{\frac{-(t_1 - t_2)}{2\tau_r}} - e^{\frac{-t_1}{2\tau_r}} \right) \right] \\
&\quad + \cos 2\theta_0 \tau_r v_p^2 \left[\frac{2\tau_4(t_2)}{3} - \frac{\tau_1(t_2)}{3} - e^{\frac{-t_1}{2\tau_r}} \tau_3(t_2) \right]
\end{aligned}$$

Average over all the initial angles θ_0 , we have a non stationary correlation,

Asymmetric brownian particle (18)

$$\langle \Delta x(t_1) \Delta x(t_2) \rangle = 2\bar{D} \min(t_1, t_2)$$

Asymmetric Active brownian particle,

$$\langle \Delta x(t_1) \Delta x(t_2) \rangle = 2\bar{D} \min(t_1, t_2) + v_p^2 \tau_r \min(t_1, t_2) (2 - \tau_1) - 2v_p^2 \tau_r^2 \left(e^{-D_r |t_1 - t_2|} - e^{-D_r t_1} \right)$$

when $t_1, t_2 \rightarrow \infty$, $|t_1 - t_2| \rightarrow \text{finite}$,

$$\langle \Delta x(t_1) \Delta x(t_2) \rangle = 2\bar{D}t_2 + v_p^2 \tau_r t_2 (2 + t_1 + \frac{t_1^2 D_r}{2}) - 2v_p^2 \tau_r^2 \left(e^{\frac{-|t_1 - t_2|}{2\tau_r}} - \left[1 - D_r t_1 + \frac{(D_r t_1)^2}{2} \right] \right) \quad (19)$$

Putting $t_1 = t, t_2 = 0$,

$$\langle \Delta x(t) \Delta x(0) \rangle = 2v_p^2 \tau_r^2 \left(\left[1 - D_r t + \frac{(D_r t)^2}{2} \right] - e^{-D_r t} \right)$$

