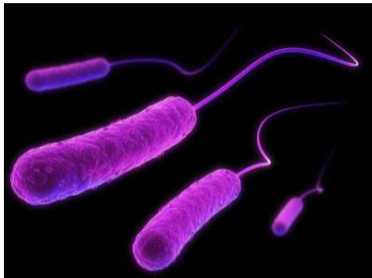




## Circle swimmers, gravitaxis, and the harmonic oscillator

Thomas Franosch  
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Universität Innsbruck

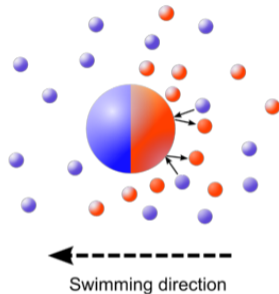
# Self-propelled agents



Bacteria using flagella to swim



Paramecium uses cilia

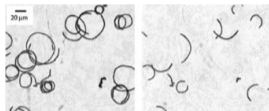
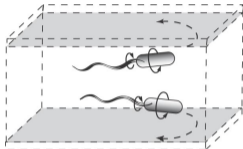


self-propelled Janus particle

- Swimming mechanism by shape deformations or induced gradients in the fluid
- intrinsically far from equilibrium
- recent **experimental progress** to build artificial self-propelled particles
- plethora of collective phenomena (flocking, swarms, phase separation, trapping,...)
- mostly **simulational studies**
- lacking: **complete characterization** of single particle motion

# Circle swimmers

## *Escherichia coli*

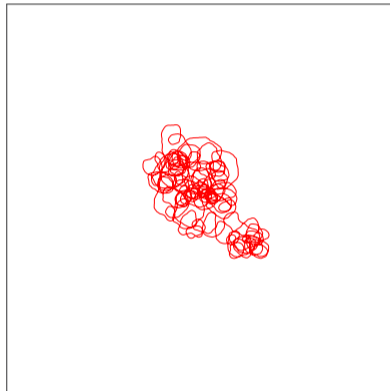


DiLuzio

Lauga

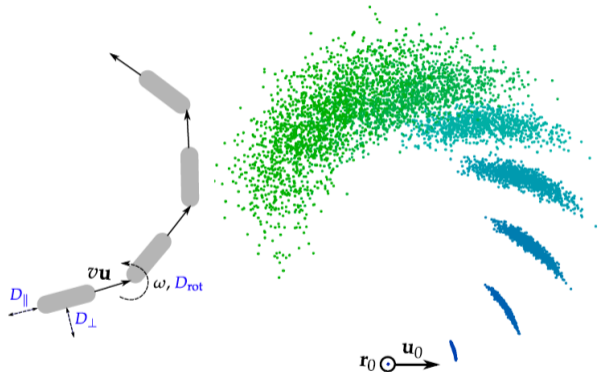
- Chirality of flagellar motion
- Hydrodynamic coupling close to boundaries  
→ circular motion
- angular drift velocity  $\omega$

$$\frac{d}{dt}\vartheta(t) = \omega + \zeta(t)$$
$$\langle \zeta(t)\zeta(t') \rangle = 2D_{\text{rot}}\delta(t - t')$$



# Model set-up

## Active Brownian Particle – circle swimmer



- Active propulsion with constant velocity  $v$  along the long axis  $\mathbf{u}$ ,  $|\mathbf{u}| = 1$
- Rotational diffusion  $D_{\text{rot}}$
- Anisotropic translational diffusion  $D_{\parallel}, D_{\perp}$
- possibly angular drift  $\omega$
- ignores microscopic origin of propulsion, effective description
- simplistic model encoding persistent random walk  
persistence length  $\ell = v/D_{\text{rot}}$   
persistence time  $\tau_{\text{rot}} = 1/D_{\text{rot}}$   
period  $T = 2\pi/\omega$

# Stochastic equations

## Circle swimmer

$$\frac{d}{dt} \vartheta(t) = \omega + \zeta(t)$$
$$\frac{d}{dt} \mathbf{r}(t) = v \mathbf{u}(t) + \boldsymbol{\eta}(t) = v \begin{pmatrix} \cos \vartheta(t) \\ \sin \vartheta(t) \end{pmatrix} + \boldsymbol{\eta}(t)$$

angular drift

position

fixed velocity

orientation

$$\langle \zeta(t) \zeta(t') \rangle = 2D_{\text{rot}} \delta(t - t'), \quad \langle \eta_i(t) \eta_j(t') \rangle = [2D_{\perp} \delta_{ij} + 2(D_{\parallel} - D_{\perp}) u_i(t) u_j(t)] \delta(t - t')$$

independent Gaussian white noise

- translational anisotropy  $\Delta D = D_{\parallel} - D_{\perp}$ , mean diffusion coefficient  $\bar{D} = (D_{\parallel} + D_{\perp})/2$
- characteristic length  $a = \sqrt{3\bar{D}/D_{\text{rot}}}/2$  replaces radius of the particle
- dimensionless parameters

anisotropy  $\Delta D/\bar{D}$

Péclet number  $Pe = va/\bar{D}$

quality factor  $M = \omega/2\pi D_{\text{rot}}$

# Circle swimmer – angular motion

## angular diffusion with drift

- conditional probability  $\mathbb{P}(\vartheta, t|\vartheta_0), t > 0$

$$\partial_t \mathbb{P} = D_{\text{rot}} \partial_{\vartheta}^2 \mathbb{P} - \omega \partial_{\vartheta} \mathbb{P}$$

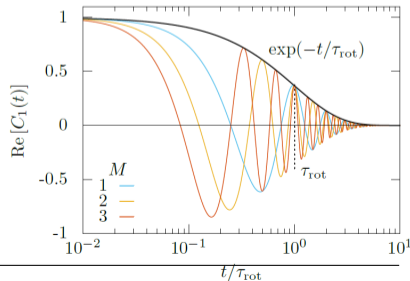
- $2\pi$ -periodic solution: **wrapped normal distribution with drift**

$$\mathbb{P}(\vartheta, t|\vartheta_0) = \frac{1}{\sqrt{4\pi D_{\text{rot}} t}} \sum_{n=-\infty}^{\infty} \exp\left\{-\frac{(\vartheta - \vartheta_0 - \omega t + 2\pi n)^2}{4D_{\text{rot}} t}\right\} = \sum_{\nu=-\infty}^{\infty} e^{-\nu^2 D_{\text{rot}} t} e^{i\nu(\vartheta - \vartheta_0 - \omega t)}$$

- angular correlation functions,  $\nu, \mu \in \mathbb{Z}, t > 0$

$$\langle e^{i\nu\vartheta(t)} e^{-i\mu\vartheta(0)} \rangle = \int_0^{2\pi} d\vartheta \int_0^{2\pi} \frac{d\vartheta_0}{2\pi} e^{i\nu\vartheta} e^{-i\mu\vartheta_0} \mathbb{P}(\vartheta|t|\vartheta_0)$$

$$\langle e^{i\nu\vartheta(t)} e^{-i\mu\vartheta(0)} \rangle = \delta_{\mu\nu} \exp(-\nu^2 D_{\text{rot}} t + i\nu\omega t)$$



# Circle swimmer - mean-square displacement

## pedestrian calculation

- increment

$$\Delta x(t) := x(t) - x(0) = \int_0^t [v \cos \vartheta(t') + \eta_x(t')] dt' \quad \Delta y(t) := y(t) - y(0) = \int_0^t [v \sin \vartheta(t') + \eta_y(t')] dt'$$

- mean-square displacement

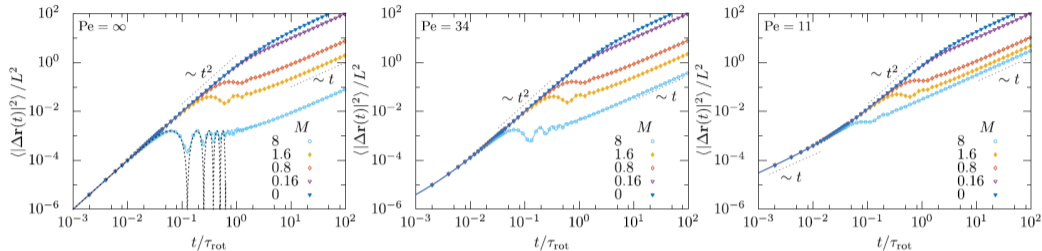
$$\langle \Delta x(t)^2 \rangle + \langle \Delta y(t)^2 \rangle = \int_0^t dt' \int_0^t dt'' [v^2 \underbrace{\langle \cos \vartheta(t') \cos \vartheta(t'') + \sin \vartheta(t') \sin \vartheta(t'') \rangle}_{\langle \cos[\vartheta(t'') - \vartheta(t')] \rangle = \exp(-D_{\text{rot}}|t' - t''|) \cos[\omega(t' - t'')]} + \underbrace{\langle \eta_x(t') \eta_x(t'') + \eta_y(t') \eta_y(t'') \rangle}_{4\bar{D}\delta(t' - t'')}]$$

$$\langle |\Delta \mathbf{r}(t)|^2 \rangle = 4\bar{D}t + \frac{2v^2}{(D_{\text{rot}}^2 + \omega^2)} \left[ D_{\text{rot}}^2(D_{\text{rot}}t - 1) + \omega^2(D_{\text{rot}}t + 1) + e^{-D_{\text{rot}}t} [(D_{\text{rot}}^2 - \omega^2) \cos(\omega t) - 2D_{\text{rot}}\omega \sin(\omega t)] \right] \xrightarrow{t \rightarrow \infty} 4D_{\text{eff}}t$$

**rotational time**  $\tau_{\text{rot}} = 1/D_{\text{rot}}$ , **effective diffusion coefficient**  $D_{\text{eff}} = \bar{D} + v^2 D_{\text{rot}} / [2(D_{\text{rot}}^2 + \omega^2)]$

- higher moments  $\langle |\Delta \mathbf{r}(t)|^n \rangle$  become tedious

# Circle swimmer – mean-square displacement



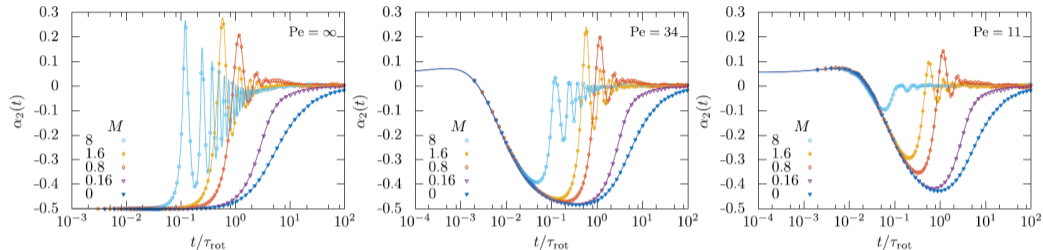
- oscillatory behavior for larger quality factor  $M \gtrsim 1$
- without noise  $D_{\text{rot}} = \bar{D} = 0$  deterministic motion  $|\Delta \mathbf{r}(t)| = 2R |\sin(\omega t/2)|$  with radius  $R = v/\omega$
- crossover to long-time diffusion  $D_{\text{eff}} = \bar{D} + v^2 D_{\text{rot}} / [2(D_{\text{rot}}^2 + \omega^2)]$  ✓

$$D_{\text{eff}}/\bar{D} = 1 + \frac{2}{3} \frac{\text{Pe}^2}{1 + 4\pi^2 M^2}$$

→ **enhanced diffusion** but suppressed by **angular drift**



# Circle swimmer – non-Gaussian parameter



- lengthy explicit expression for

$$\alpha_2(t) = \frac{1}{2} \frac{\langle |\Delta \mathbf{r}|^4 \rangle}{\langle |\Delta \mathbf{r}(t)|^2 \rangle^2} - 1$$

- $\alpha_2(t) \rightarrow 0$  for  $t \rightarrow \infty$  by central limit theorem
- without noise  $D_{\text{rot}} = \bar{D} = 0$  deterministic motion  $|\Delta \mathbf{r}(t)| = 2R|\sin(\omega t/2)| \rightarrow \alpha_2(t) = -1/2$ .
- initial value with noise  $\alpha_2(t \rightarrow 0) = \Delta D^2 / 8\bar{D}^2$
- oscillatory behavior for larger quality factor  $M \gtrsim 1$

# Fokker-Planck equation

**conditional probability density**  $\mathbb{P}(\mathbf{r}, \vartheta, t | \vartheta_0)$  (Green function)

Perrin equation (Markov process)

$$\partial_t \mathbb{P} = D_{\text{rot}} \partial_{\vartheta}^2 \mathbb{P} - \omega \partial_{\vartheta} \mathbb{P} - \mathbf{v} \mathbf{u} \cdot (\partial_{\mathbf{r}} \mathbb{P}) + \partial_{\mathbf{r}} \cdot [D_{\parallel} (\partial_{\mathbf{r}} \mathbb{P}) - \Delta D (\mathbb{I} - \mathbf{u} \mathbf{u}) \cdot (\partial_{\mathbf{r}} \mathbb{P})]$$

orientational diffusion   angular drift   active propulsion   anisotropic diffusion  $\Delta D = D_{\parallel} - D_{\perp}$

- Fokker-Planck equation for non-equilibrium dynamics
- coupling between **orientational diffusion**, **angular drift**, **active propulsion**, and **translation**
- spatial Fourier transform  $\tilde{\mathbb{P}}(\mathbf{k}, \vartheta, t | \vartheta_0) = \int d^2 r \exp(-i\mathbf{k} \cdot \mathbf{r}) \mathbb{P}(\mathbf{r}, \vartheta, t | \vartheta_0)$

$$\partial_t \tilde{\mathbb{P}} = D_{\text{rot}} \partial_{\vartheta}^2 \tilde{\mathbb{P}} - \omega \partial_{\vartheta} \tilde{\mathbb{P}} - i \mathbf{v} \mathbf{u} \cdot \mathbf{k} \tilde{\mathbb{P}} - [D_{\perp} k^2 + \Delta D (\mathbf{u} \cdot \mathbf{k})^2] \tilde{\mathbb{P}}$$

- solution for intermediate scattering function

$$F(\mathbf{k}, t) = \langle \exp(-i\mathbf{k} \cdot \Delta \mathbf{r}(t)) \rangle = \int_0^{2\pi} d\vartheta \int_0^{2\pi} \frac{d\vartheta_0}{2\pi} \tilde{\mathbb{P}}(\mathbf{k}, \vartheta, t | \vartheta_0)$$

Christina Kurzthaler et al, *Soft Matter* (2017)

# Generalized Mathieu functions

## Separation ansatz

- choose coordinates  $k$  in  $x$ -direction

$$\partial_t \tilde{\mathbb{P}} = \left[ D_{\text{rot}} \partial_{\vartheta}^2 - \omega \partial_{\vartheta} - ivk \cos \vartheta - \left( D_{\perp} k^2 + \Delta D k^2 \cos^2 \vartheta \right) \right] \tilde{\mathbb{P}}$$

- separation ansatz  $\exp(-\lambda t) z(\vartheta)$

**eigenvalue problem**  $\left( \frac{d^2}{d\vartheta^2} - 2\pi M \frac{d}{d\vartheta} - \frac{ivk}{D_{\text{rot}}} \cos \vartheta - \frac{\Delta D k^2}{D_{\text{rot}}} \cos^2 \vartheta - \frac{D_{\perp} k^2}{D_{\text{rot}}} + \frac{\lambda}{D_{\text{rot}}} \right) z(\vartheta) = 0$

- substitution  $x = \vartheta/2$ , **non-Hermitian** eigenvalue problem  $Lz(x) = az(x)$

**Sturm-Liouville operator**  $L = L(q, c, M) = \frac{d^2}{dx^2} - 2q \cos(2x) - c^2 \cos^2(2x) - 4\pi M \frac{d}{dx}$

**deformation parameters**  $q = 2ivk/D_{\text{rot}}$ ,  $c^2 = 4\Delta D k^2/D_{\text{rot}}$ ,  $M = \omega/2\pi D_{\text{rot}}$

**eigenvalue**  $a = 4(\lambda - D_{\perp} k^2)/D_{\text{rot}}$

# Generalized Mathieu functions

## Summary of properties

- scalar product for  $\pi$ -periodic functions

$$\langle \varphi | \psi \rangle = \frac{1}{\pi} \int_0^\pi \varphi(x)^* \psi(x) dx$$

adjoint operator  $L^+ = L^+(q, c, M) = \frac{d^2}{dx^2} - 2q^* \cos(2x) - c^2 \cos^2(2x) + 4\pi M \frac{d}{dx}$

- left and right eigenfunctions

$$L r_m = a_m r_m, \quad L^+ l_m = a_m^* l_m, \quad \langle l_m | r_n \rangle = \delta_{mn}$$

$$\rightarrow l_m(q, c, M, x)^* = r_n(q, c, M, -x)$$

# Generalized Mathieu functions – cont'd

- Define *your own eigenfunctions* (call them generalized Mathieu functions)  $\pi$ -periodic for  $x$  deformation of complex exponential functions  $\exp(2i\pi nx)$

$$\text{Fourier expansion} \quad ee_{2n}(q, c, M, x) = \sum_{m=-\infty}^{\infty} A_{2m}^{2n} e^{2mix} \quad n \in \mathbb{Z}$$

- **orthogonality and normalization**

$$\int_0^{\pi} ee_{2m}(q, c, M, x) ee_{2n}(q, c, M, -x) dx = \pi \delta_{mn} \quad n, m \in \mathbb{Z}$$

- **completeness**

$$\pi\text{-periodic} \quad f(x) = \sum_{n=-\infty}^{\infty} \gamma_{2n} ee_{2n}(q, c, M, x)$$

$$\text{Fourier coefficients} \quad \gamma_{2n} = \frac{1}{\pi} \int_0^{\pi} f(x) ee_{2n}(q, c, M, -x) dx$$

# Anisotropic self-propulsion

- Solution Fokker-Planck equation

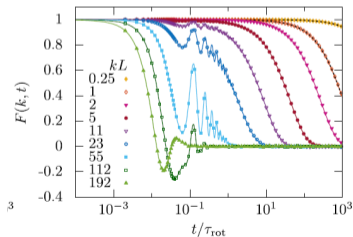
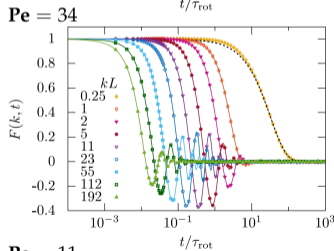
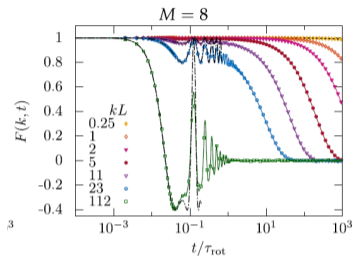
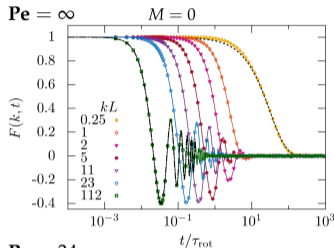
$$\tilde{\mathbb{P}}(k, \vartheta, t | \vartheta_0) = \frac{e^{-k^2 D_{\perp} t}}{2\pi} \sum_{n=-\infty}^{\infty} e^{-a_{2n}(q) D_{\text{rot}} t / 4} e e_{2n}(q, c, M, \vartheta / 2) e e_{2n}(q, c, M, -\vartheta_0 / 2)$$

- **intermediate scattering** function (ISF) after averaging and marginalizing

$$F(k, t) = \frac{e^{-k^2 D_{\perp} t}}{4\pi^2} \sum_{n=-\infty}^{\infty} e^{-a_{2n}(q) D_{\text{rot}} t / 4} \left[ \int_0^{2\pi} d\vartheta e e(q, c, M, \vartheta / 2) \right]^2$$

C Kurzthaler et al, Soft Matter (2017)

# Circle swimmer – intermediate scattering function



- ISF in 2D for isotropic motion

$$F(k, t) = \langle J_0(k|\Delta\mathbf{r}(t)|) \rangle$$

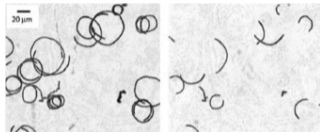
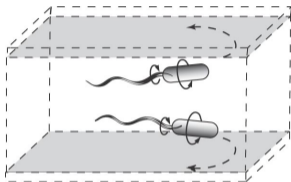
- chiral swimming pattern leads to **oscillations** around a plateau
- **ideal motion**  
 $|\Delta\mathbf{r}(t)| = 2R|\sin(\omega t/2)|$

$$\rightarrow F(k, t) = J_0(2kR|\sin(\omega t/2)|)$$

$\rightarrow$  oscillations between 1 and  $J_0(2kR)$

# Circle swimmers

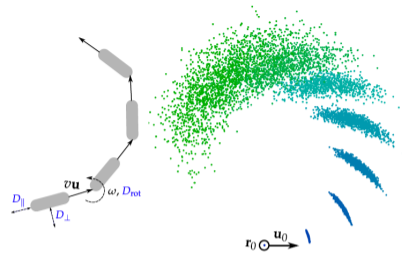
## *Escherichia coli*



### DiLuzio

- Chirality of flagellar motion
- Hydrodynamic coupling close to boundaries  
→ circular motion
- angular drift velocity  $\omega$
- quality factor  $M = \frac{\omega/2\pi}{D_{\text{rot}}}$
- exact solution of intermediate scattering function in terms of generalizations of Mathieu functions

### Lauga

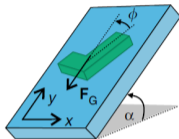
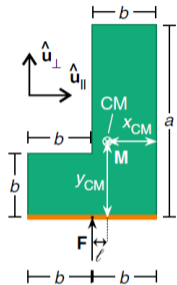


$$\begin{aligned}\frac{d}{dt}\mathbf{r}(t) &= v\mathbf{u}(t) \\ \frac{d}{dt}\vartheta(t) &= \omega + \zeta(t) \\ \langle \zeta(t)\zeta(t') \rangle &= 2D_{\text{rot}}\delta(t-t')\end{aligned}$$

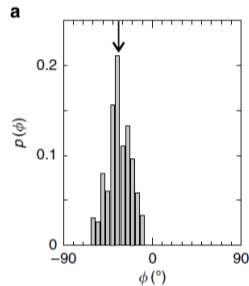
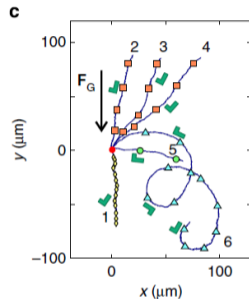
Kurzthaler *et al* Soft Matter (2017)



# Gravitaxis



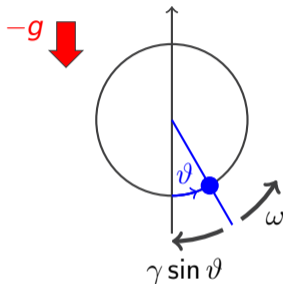
- active L-shaped particles are **circle swimmers**
- can move upwards against **gravity**
- transition from a **locked** to **periodic** phase



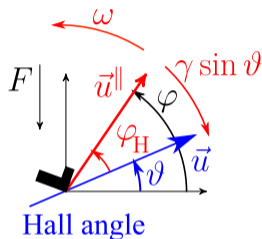
ten Hagen *et al*, Nature Communications (2014)

# Minimal model for gravitaxis

$$\frac{d}{dt} \mathbf{r}(t) = v \mathbf{u}(t) := v \begin{pmatrix} \cos \vartheta(t) \\ \sin \vartheta(t) \end{pmatrix}$$
$$\frac{d}{dt} \vartheta(t) = \omega - \gamma \sin \vartheta(t) + \zeta(t)$$
$$\langle \zeta(t) \zeta(t') \rangle = 2D_{\text{rot}} \delta(t - t')$$



driven pendulum



- simplified model of [ten Hagen et al, Nature Communications \(2014\)](#)
- maps to overdamped noisy driven pendulum / tilted washboard ... but geometry is rotated
- without noise  $D_{\text{rot}} = 0$  and drive  $\omega = 0$  the active particle moves **horizontally**

# Fold bifurcation

## Classical motion (without noise)

$$\frac{d}{dt}\vartheta = \omega - \gamma \sin \vartheta$$

- **locked phase**: stable fixed point, locked angle  $\vartheta_* \in [0, \pi/2]$  for  $\gamma \geq \omega$  (unstable fixed point at  $\pi - \vartheta_*$ )

$$\sin \vartheta_* = \omega/\gamma \quad \text{constant **drift velocity**} \quad \mathbf{v} \mathbf{u} = v \begin{pmatrix} \cos \vartheta_* \\ \sin \vartheta_* \end{pmatrix} = v \begin{pmatrix} \sqrt{1 - \omega^2/\gamma^2} \\ \omega/\gamma \end{pmatrix}$$

- **periodic phase**: no fixed point

$$\text{period} \quad T = \int_0^{2\pi} \frac{d\vartheta}{\omega - \gamma \sin \vartheta} = \frac{2\pi}{\sqrt{\omega^2 - \gamma^2}} \quad \text{diverges as} \quad \gamma \uparrow \omega$$

$$\text{average drift} \quad \frac{1}{T} \int_0^T v \begin{pmatrix} \cos \vartheta(t) \\ \sin \vartheta(t) \end{pmatrix} dt = \frac{v}{T} \int_0^{2\pi} \begin{pmatrix} \cos \vartheta \\ \sin \vartheta \end{pmatrix} \frac{d\vartheta}{\omega - \gamma \sin \vartheta} = v \begin{pmatrix} 0 \\ \omega/\gamma - \sqrt{(\omega/\gamma)^2 - 1} \end{pmatrix}$$

- **bifurcation** at  $\gamma_c = \omega$

# Tilted-washboard potential

- motion in effective potential

$$\frac{d}{dt}\vartheta = -\frac{D_{\text{rot}}}{k_B T} \partial_{\vartheta} U + \zeta(t)$$

$$\frac{D_{\text{rot}}}{k_B T} U(\vartheta) = -\omega\vartheta - \gamma \cos \vartheta$$

non-periodic due to angular drift  $\rightarrow$  **nonequilibrium**

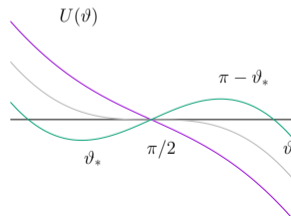
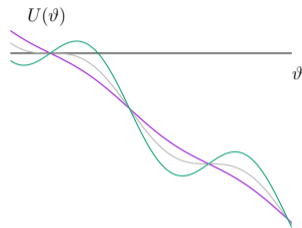
local **barrier** for  $\gamma > \omega \rightarrow$  crossing by **fluctuations**

**no barrier** for  $0 < \gamma < \omega$

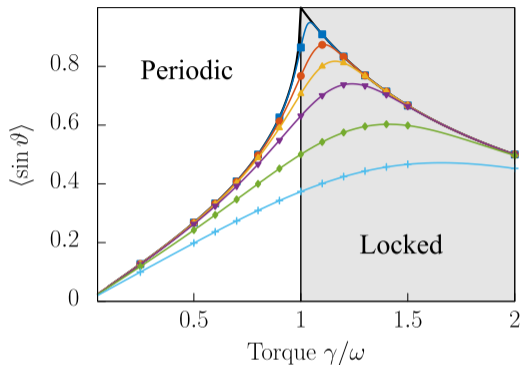
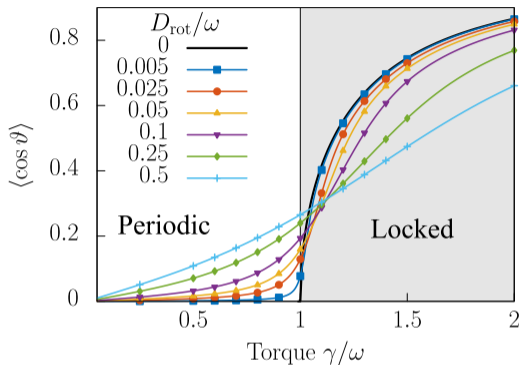
- harmonic approximation close in the locked phase

$$\frac{D_{\text{rot}}}{k_B T} U(\vartheta) = \frac{D_{\text{rot}}}{k_B T} U(\vartheta_*) + \frac{(\vartheta - \vartheta_*)^2}{2} \sqrt{\gamma^2 - \omega^2} + O(\vartheta - \vartheta_*)^3$$

becomes **soft** upon approaching the bifurcation  $\gamma \downarrow \omega$



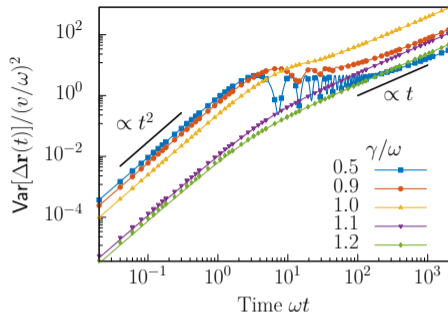
# Mean drift



- analytic solution for stationary state  $p^{\text{st}}(\vartheta)$  known  
→ calculate numerically the mean drift and compare to simulation
- fluctuations smooths out the transition
- net horizontal motion in the periodic phase only due to fluctuations

Risken, *The Fokker-Planck equation*

# Fluctuations

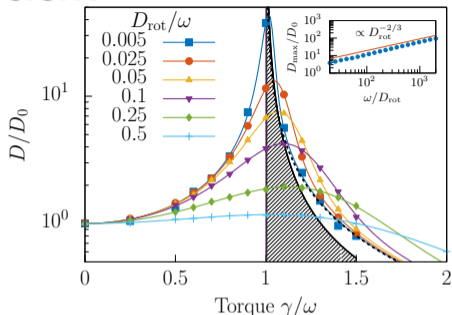


**variance**  $\text{Var}[\Delta \mathbf{r}(t)] := \langle [\Delta \mathbf{r}(t) - \langle \Delta \mathbf{r}(t) \rangle]^2 \rangle$

with increment  $\Delta \mathbf{r}(t) := \mathbf{r}(t) - \mathbf{r}(0)$

- results for **stochastic simulations**
- initially  $\text{Var}[\Delta \mathbf{r}(t)]^2$  grows  $\propto t^2$
- prefactor depends drastically on the torque  $\gamma$
- oscillations below the classical bifurcation
- long-time behavior diffusive  $\propto t$

# Diffusion coefficient



**diffusion coefficient**  $D := \lim_{t \rightarrow \infty} \frac{1}{2} \frac{d}{dt} \text{Var}[\Delta \mathbf{r}(t)]$

- normalize by free circle swimmer  $D_0 = v^2 D_{\text{rot}} / [2(D_{\text{rot}}^2 + \omega^2)] \propto D_{\text{rot}}$  as  $D_{\text{rot}} \rightarrow 0$
- **resonance** emerging close to bifurcation as  $D_{\text{rot}} \downarrow 0$
- maximal relative diffusivity scales  $\propto D_{\text{rot}}^{-2/3}$  on parametric curve
- **goal:** rationalize the resonance and the scaling **analytically!**

# Fokker-Planck equation

**conditional probability density**  $\mathbb{P}(\mathbf{r}, \vartheta, t | \vartheta_0)$  (Green function)

Fokker-Planck equation (Markov process)

$$\partial_t \mathbb{P} = D_{\text{rot}} \partial_{\vartheta}^2 \mathbb{P} - \partial_{\vartheta} [(\omega - \gamma \sin \vartheta) \mathbb{P}] - \mathbf{v} \mathbf{u} \cdot (\partial_{\mathbf{r}} \mathbb{P})$$

orientational diffusion

angular drift

active propulsion

- spatial Fourier transform  $\tilde{\mathbb{P}}(\mathbf{k}, \vartheta, t | \vartheta_0) = \int d^2 r \exp(-i\mathbf{k} \cdot \mathbf{r}) \mathbb{P}(\mathbf{r}, \vartheta, t | \vartheta_0)$

$$\partial_t \tilde{\mathbb{P}} = D_{\text{rot}} \partial_{\vartheta}^2 \tilde{\mathbb{P}} - \partial_{\vartheta} [\omega - \gamma \sin \vartheta] \tilde{\mathbb{P}} - i \mathbf{v} \mathbf{u} \cdot \mathbf{k} \tilde{\mathbb{P}} =: (\mathcal{L} + \delta \mathcal{L}_{\mathbf{k}}) \tilde{\mathbb{P}}$$

- solution for intermediate scattering function

$$F(\mathbf{k}, t) = \langle \exp(-i\mathbf{k} \cdot \Delta \mathbf{r}(t)) \rangle = \int_0^{2\pi} d\vartheta \int_0^{2\pi} d\vartheta_0 \tilde{\mathbb{P}}(\mathbf{k}, \vartheta, t | \vartheta_0) p^{\text{st}}(\vartheta_0)$$

average with respect to **stationary distribution**



# Eigenfunctions

## Matrix representation

- Hilbert space of periodic square-integrable functions  $f(\vartheta) \in L^2[0, 2\pi]$

$$\text{scalar product} \quad \langle f|g \rangle = \int_0^{2\pi} d\vartheta f(\vartheta)^* g(\vartheta)$$

- make isomorphism manifest by generalized eigenstates  $f(\vartheta) = \langle \vartheta|f \rangle$   
 $\{|n\rangle : n \in \mathbb{Z}\}$  ONB in  $\mathcal{H}$  with real-space representation  $\langle \vartheta|n \rangle = \exp(in\vartheta)/\sqrt{2\pi}$ .

### non-Hermitian matrix representation

$$[\mathcal{L}]_{mn} = \langle m|\mathcal{L}n \rangle = \int_0^{2\pi} \frac{d\vartheta}{2\pi} e^{-im\vartheta} \mathcal{L} e^{in\vartheta} = (-D_{\text{rot}} m^2 - im\omega) \delta_{mn} + \frac{\gamma}{2} m (\delta_{m,n+1} - \delta_{m,n-1})$$

$$[\delta\mathcal{L}_{\mathbf{k}}]_{mn} = \langle m|\delta\mathcal{L}_{\mathbf{k}}n \rangle = \int_0^{2\pi} \frac{d\vartheta}{2\pi} e^{-im\vartheta} \delta\mathcal{L}_{\mathbf{k}} e^{in\vartheta} = -\frac{ik_x v}{2} (\delta_{m,n+1} + \delta_{m,n-1}) - \frac{k_y v}{2} (\delta_{m,n+1} - \delta_{m,n-1})$$

→ **tridiagonal matrix** easy to diagonalize

- right and left **eigenstates**

$$\mathcal{L}|r_\lambda\rangle = \lambda|r_\lambda\rangle \quad \mathcal{L}^\dagger|l_\lambda\rangle = \lambda|l_\lambda\rangle$$

# Formal solution

- stationary state  $\rho^{\text{st}}(\vartheta) = \langle \vartheta | r_0 \rangle$  is eigenstate with eigenvalue 0,  $\langle \vartheta | l_0 \rangle = 1$

$$\rightarrow F(\mathbf{k}, t) = \int_0^{2\pi} d\vartheta \int_0^{2\pi} d\vartheta_0 \langle l_0 | \vartheta \rangle \langle \vartheta | e^{(\mathcal{L} + \delta\mathcal{L}_{\mathbf{k}})t} \vartheta_0 \rangle \langle \vartheta_0 | r_0 \rangle = \langle l_0 | e^{(\mathcal{L} + \delta\mathcal{L}_{\mathbf{k}})t} r_0 \rangle$$

- Expansion in powers of the wave vector yield moments

$$F(\mathbf{k}, t) = \langle \exp[i\mathbf{k} \cdot \Delta\mathbf{r}(t)] \rangle = 1 - i\mathbf{k} \cdot \langle \Delta\mathbf{r}(t) \rangle - \frac{1}{2} \langle [\mathbf{k} \cdot \Delta\mathbf{r}(t)]^2 \rangle + O(|\mathbf{k}|^3)$$

- time-dependent **perturbation theory** in  $\delta\mathcal{L}_{\mathbf{k}}$

$$\begin{aligned} \text{Dyson representation} \quad e^{(\mathcal{L} + \delta\mathcal{L}_{\mathbf{k}})t} &= e^{\mathcal{L}t} + \int_0^t ds e^{\mathcal{L}(t-s)} \delta\mathcal{L}_{\mathbf{k}} e^{(\mathcal{L} + \delta\mathcal{L}_{\mathbf{k}})s} \\ &= e^{\mathcal{L}t} + \int_0^t ds e^{\mathcal{L}(t-s)} \delta\mathcal{L}_{\mathbf{k}} e^{\mathcal{L}s} + \int_0^t ds \int_0^s du e^{\mathcal{L}(t-s)} \delta\mathcal{L}_{\mathbf{k}} e^{\mathcal{L}(s-u)} \delta\mathcal{L}_{\mathbf{k}} e^{\mathcal{L}u} + O(\delta\mathcal{L}_{\mathbf{k}})^3 \end{aligned}$$

**Born series**

## ...collecting results

- with  $e^{\mathcal{L}t}|r_0\rangle = |r_0\rangle$ ,  $\langle e^{\mathcal{L}^\dagger}l_0| = \langle l_0|$

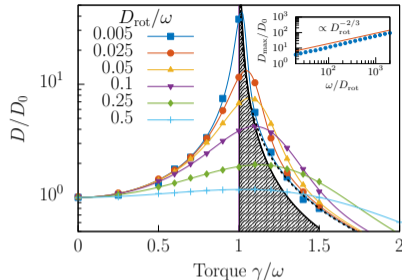
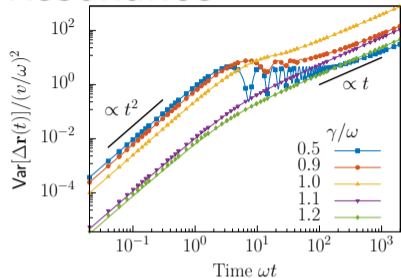
$$\begin{aligned}F(\mathbf{k}, t) &= 1 + \int_0^t ds \langle l_0|e^{\mathcal{L}(t-s)}\delta\mathcal{L}_{\mathbf{k}}e^{\mathcal{L}s}r_0\rangle + \int_0^t ds \int_0^s du \langle l_0|e^{\mathcal{L}(t-s)}\delta\mathcal{L}_{\mathbf{k}}e^{\mathcal{L}_{\mathbf{k}}(s-u)}\delta\mathcal{L}_{\mathbf{k}}e^{\mathcal{L}u}r_0\rangle + O(|\mathbf{k}|^3) \\&= 1 + t\langle l_0|\delta\mathcal{L}_{\mathbf{k}}r_0\rangle + \sum_{\lambda} \int_0^t ds \int_0^s du \langle l_0|\delta\mathcal{L}_{\mathbf{k}}e^{\mathcal{L}(s-u)}r_{\lambda}\rangle \langle l_{\lambda}|\delta\mathcal{L}_{\mathbf{k}}r_0\rangle + O(|\mathbf{k}|^3) \\&= 1 + t\langle l_0|\delta\mathcal{L}_{\mathbf{k}}r_0\rangle + \sum_{\lambda} \int_0^t ds \int_0^s du e^{-\lambda(s-u)} \langle l_0|\delta\mathcal{L}_{\mathbf{k}}r_{\lambda}\rangle \langle l_{\lambda}|\delta\mathcal{L}_{\mathbf{k}}r_0\rangle + O(|\mathbf{k}|^3) \\&= 1 + t\langle l_0|\delta\mathcal{L}_{\mathbf{k}}r_0\rangle + \sum_{\lambda} \frac{e^{-\lambda t} + \lambda t - 1}{\lambda^2} \langle l_0|\delta\mathcal{L}_{\mathbf{k}}r_{\lambda}\rangle \langle l_{\lambda}|\delta\mathcal{L}_{\mathbf{k}}r_0\rangle + O(|\mathbf{k}|^3)\end{aligned}$$

- mean drift and variance along  $\mathbf{n} = \mathbf{k}/k$

$$\mathbf{n} \cdot \frac{d}{dt} \langle \Delta \mathbf{r}(t) \rangle = \frac{i}{k} \langle l_0 | \delta \mathcal{L}_{\mathbf{k}} r_0 \rangle$$

$$\text{Var}[\mathbf{n} \cdot \Delta \mathbf{r}(t)] = \frac{2}{k^2} \sum_{\lambda \neq 0} \frac{1 - \lambda t - e^{-\lambda t}}{\lambda^2} \langle l_0 | \delta \mathcal{L}_{\mathbf{k}} r_{\lambda} \rangle \langle l_{\lambda} | \delta \mathcal{L}_{\mathbf{k}} r_0 \rangle$$

# Resonance



- **analytic theory** describes all data
- diffusion coefficient for motion along  $\mathbf{n} = \mathbf{k}/k$

$$D_{\mathbf{n}} := \lim_{t \rightarrow \infty} \frac{1}{2} \frac{d}{dt} \text{Var}[\mathbf{n} \cdot \Delta \mathbf{r}(t)] = \frac{-1}{k^2} \sum_{\lambda \neq 0} \frac{1}{\lambda} \langle I_0 | \delta \mathcal{L}_{\mathbf{k}} r_{\lambda} \rangle \langle I_{\lambda} | \delta \mathcal{L}_{\mathbf{k}} r_0 \rangle$$

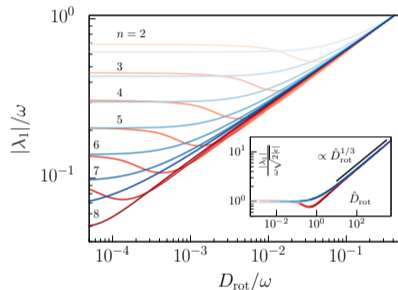
- discarded terms due to translational diffusion and noise can be readily **included**, only  $\delta \mathcal{L}_{\mathbf{k}}$  changes
- How to explain the **resonance**?

# Eigenvalues

- **all eigenvalues** go to **zero** as  $D_{\text{rot}} \rightarrow 0$  upon approaching the resonance  $\varepsilon = (\gamma - \omega)/\omega \rightarrow 0$
- all curves have the same shape  
→ **scaling behavior** with reduced rotational diffusion coefficient  $\hat{D}_{\text{rot}} := |\varepsilon|^{-3/2} D_{\text{rot}}/\omega$

$$\lambda_n/\omega = \sqrt{2|\varepsilon|} \Lambda_{n,\pm}(\hat{D}_{\text{rot}})$$

- close to resonance in locked phase  
 $\lambda_n \propto n$  **harmonic potential**  
→  $\Lambda_{+,n}(\hat{D}_{\text{rot}}) \rightarrow n$  for  $\hat{D}_{\text{rot}} \rightarrow 0$



separation parameter  $\varepsilon = (\gamma - \omega)/\omega = \pm 10^{-n/3}$

# Harmonic approximation

- linearize around fixed point  $\vartheta_*$  for small **separation parameter**  $\varepsilon = (\gamma - \omega)/\omega \ll 1$

$$\dot{\vartheta}(t) = -\frac{1}{\tau}[\vartheta(t) - \vartheta_*] + \zeta(t), \quad \langle \zeta(t)\zeta(t') \rangle = 2D_{\text{rot}}\delta(t - t')$$

**relaxation rate**  $\frac{1}{\tau} = \sqrt{\gamma^2 - \omega^2} \propto \omega\sqrt{2\varepsilon}$  for  $\varepsilon \rightarrow 0^+$

- eigenvalues**  $\lambda_n = n/\tau, n \in \mathbb{N}_0$  approach zero
- perturbing operator** upon linearization in harmonic approximation

$$\delta\mathcal{L}_{\mathbf{k}} = i\mathbf{v} \cdot \mathbf{k} = -ik_x v \cos \vartheta_* - ik_y v \sin \vartheta_* + (ik_x v \sin \vartheta_* - ik_y v \cos \vartheta_*)(\vartheta - \vartheta_*) + O(\dots)$$

→ drift velocity approaches classical value

- relevant transition matrix elements couple only to excited state

$$\langle l_0 | \delta\mathcal{L}_{\mathbf{k}} r_\lambda \rangle = \langle l_\lambda | \delta\mathcal{L}_{\mathbf{k}} r_0 \rangle = iv\sqrt{D_{\text{rot}}\tau}(k_x \sin \vartheta_* - k_y \cos \vartheta_*)\delta_{\lambda,1}.$$

→ only a single term contributes

# Harmonic approximation

- ...within harmonic approximation

$$\text{Var}[\mathbf{n} \cdot \Delta \mathbf{r}(t)] = 2 \left( \frac{t}{\tau} - 1 + e^{-t/\tau} \right) (v\tau)^2 D_{\text{rot}} \tau (n_x \sin \vartheta_* - n_y \cos \vartheta_*)^2$$

$$D_{\mathbf{n}} = (v\tau)^2 D_{\text{rot}} (n_x \sin \vartheta_* - n_y \cos \vartheta_*)^2$$

- picture should hold if relaxation rate  $1/\tau$  large to **Kramer's escape rate**  $\propto \exp(-\Delta U/k_B T)$

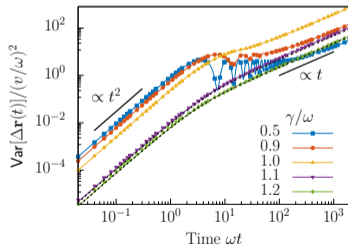
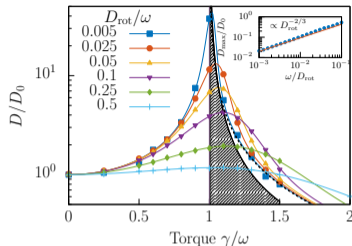
**large barrier**  $1 \ll \frac{\Delta U}{k_B T} = \frac{4\sqrt{2}}{3} \frac{\omega}{D_{\text{rot}}} \varepsilon^{3/2} + O(\dots)$

define **reduced rotational diffusion coefficient**

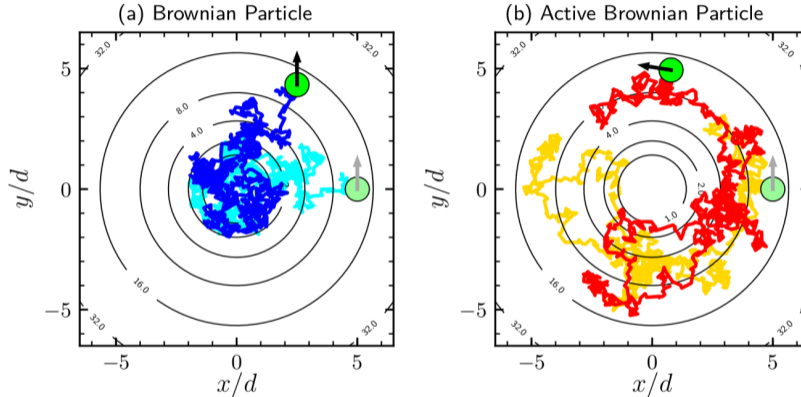
$$\hat{D}_{\text{rot}} := |\varepsilon|^{-3/2} D_{\text{rot}} / \omega$$

→ harmonic picture should hold for  $\varepsilon > 0$  and  $\hat{D}_{\text{rot}} \ll 1$

**maximal enhancement**  $D_{\text{max}}/D_0 \propto |\varepsilon|^{-1} \propto D_{\text{rot}}^{-2/3}$



# Active Brownian Particle – harmonic well



- passive particle is most likely in the center, Boltzmann distribution  $\propto \exp(-U(\mathbf{r})/k_B T)$
- **active particle** is off-center, non-equilibrium process



# Stochastic differential equations

## Active Brownian particle

$$\frac{d}{dt}\mathbf{r} = -\mu k\mathbf{r} + v\mathbf{u} + \boldsymbol{\eta}(t), \quad \frac{d\vartheta}{dt} = \zeta(t)$$

harmonic  
restoring force

fixed velocity

orientation  
 $\mathbf{u} = (\cos \vartheta, \sin \vartheta)$

$$\langle \eta_i(t)\eta_j(t') \rangle = 2D\delta_{ij}\delta(t-t'), \quad \langle \zeta(t)\zeta(t') \rangle = 2D_{\text{rot}}\delta(t-t')$$

independent Gaussian white noise

- Einstein relation  $D = \mu k_B T$  defines temperature of the bath
- thermal oscillator length  $d = \sqrt{k_B T/k}$ , trap relaxation time  $\tau = 1/\mu k$
- dimensionless parameters

rotationality  $D_{\text{rot}}\tau$

Péclet number  $Pe = vd/D$

# Fokker-Planck equation

**conditional probability density**  $\mathbb{P}(\mathbf{r}, \vartheta, t | \mathbf{r}_0, \vartheta_0)$  (Green function)

Fokker-Planck equation (Markov process)

$$\partial_t \mathbb{P} = \Omega \mathbb{P} := \underbrace{\nabla \cdot (\mu \mathbf{k} \mathbb{P}) + D \nabla^2 \mathbb{P}}_{\text{passive particle in harmonic well}} + \underbrace{D_{\text{rot}} \partial_{\vartheta}^2 \mathbb{P}}_{\text{orientational diffusion}} - \underbrace{\mathbf{v} \mathbf{u} \cdot \nabla \mathbb{P}}_{\text{active propulsion}}$$

- Fokker-Planck equation for non-equilibrium dynamics
- coupling between **translational motion** and **orientational diffusion** via **active propulsion**  $\mathbf{u} = (\cos \vartheta, \sin \vartheta)$

steady state solution by Malakar *et al.*, PRE **101**, 022610 (2020)

# Solution strategy

- formal solution  $\mathbb{P}(\mathbf{r}, \vartheta, t | \mathbf{r}_0, \vartheta_0) = e^{\Omega t} \delta(\mathbf{r} - \mathbf{r}_0) \delta(\vartheta - \vartheta_0)$
- Boltzmann equilibrium without self-propulsion

$$p^{\text{eq}}(\mathbf{r}, \vartheta) = \frac{\exp(-r^2/2d^2)}{4\pi d^2}, \quad \int d\mathbf{r} \int_0^{2\pi} d\vartheta p^{\text{eq}}(\mathbf{r}, \vartheta) = 1$$

thermal oscillator length  $d = \sqrt{k_B T/k}$

- splitting off the equilibrium reference state

$$\Omega[\psi(\mathbf{r}, \vartheta) p^{\text{eq}}(\mathbf{r}, \vartheta)] =: p^{\text{eq}}(\mathbf{r}, \vartheta) \mathcal{L}\psi(\mathbf{r}, \vartheta)$$

- decompose  $\mathcal{L} = \mathcal{L}_0 + \text{Pe} \mathcal{L}_1$  with Péclet number  $\text{Pe} := vd/D$   
in polar coordinates  $\mathbf{r} = r(\cos \varphi, \sin \varphi)$

$$\mathcal{L}_0 \psi = \frac{1}{\tau} \left[ \frac{d^2}{r} \partial_r (r \partial_r \psi) + \frac{d^2}{r^2} \partial_\varphi^2 \psi + D_{\text{rot}} \tau \partial_\vartheta^2 \psi - r \partial_r \psi \right]$$
$$\mathcal{L}_1 \psi = \frac{d}{\tau} \left[ -\cos(\chi) \partial_r \psi - \frac{1}{r} \sin(\chi) \partial_\varphi \psi + \frac{r}{d^2} \cos(\chi) \psi \right]$$

with relative angle  $\chi = \angle(\mathbf{u}, \mathbf{r}) = \vartheta - \varphi$

# Hilbert space formulation

- Kubo scalar product

$$\langle \phi | \psi \rangle := \int d\mathbf{r} \int_0^{2\pi} d\vartheta \rho^{\text{eq}}(\mathbf{r}, \vartheta) \phi(\mathbf{r}, \vartheta) \psi(\mathbf{r}, \vartheta)$$

reference operator is Hermitian  $\langle \phi | \mathcal{L}_0 \psi \rangle = \langle \mathcal{L}_0 \phi | \psi \rangle$

$$\text{eigenvalue problem } \mathcal{L}_0 \psi = -\lambda \psi$$

→ eigenvalues are real

- Hilbert space basis  $|\psi_\Lambda\rangle$

$$\langle \psi_\Lambda | \psi_M \rangle = \delta_{\Lambda M}$$

$$\sum_{\Lambda} \rho^{\text{eq}}(\mathbf{r}, \vartheta) \psi_\Lambda(\mathbf{r}, \vartheta) \psi_\Lambda(\mathbf{r}_0, \vartheta_0)^* = \delta(\mathbf{r} - \mathbf{r}_0) \delta(\vartheta - \vartheta_0)$$

- generalized position-orientation eigenstates  $|\mathbf{r}, \vartheta\rangle$  with  $\psi(\mathbf{r}, \vartheta) = \langle \mathbf{r}, \vartheta | \psi \rangle$   
to make isomorphism  $|\psi\rangle \leftrightarrow \psi(\mathbf{r}, \vartheta)$  manifest

$$\text{orthogonal} \quad \rho^{\text{eq}}(\mathbf{r}, \vartheta) \langle \mathbf{r}, \vartheta | \mathbf{r}_0, \vartheta_0 \rangle = \delta(\mathbf{r} - \mathbf{r}_0) \delta(\vartheta - \vartheta_0)$$

$$\text{complete} \quad \int d\mathbf{r} d\vartheta \rho^{\text{eq}}(\mathbf{r}, \vartheta) |\mathbf{r}, \vartheta\rangle \langle \mathbf{r}, \vartheta| = \mathbb{I}$$

# Formal expression for propagator

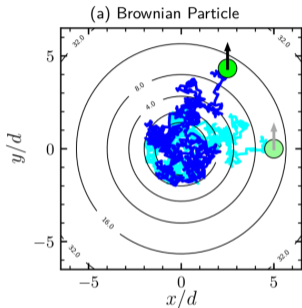
- use orthogonality and completeness relations...

$$\begin{aligned}\mathbb{P}(\mathbf{r}, \vartheta, t | \mathbf{r}_0 \vartheta_0) &= e^{\Omega t} \delta(\mathbf{r} - \mathbf{r}_0) \delta(\vartheta - \vartheta_0) = e^{\Omega t} \sum_{\Lambda} \rho^{\text{eq}}(\mathbf{r}, \vartheta) \psi_{\Lambda}(\mathbf{r}, \vartheta) \psi_{\Lambda}(\mathbf{r}_0, \vartheta_0)^* \\ &= \rho^{\text{eq}}(\mathbf{r}, \vartheta) e^{\mathcal{L}t} \sum_{\Lambda} \psi_{\Lambda}(\mathbf{r}, \vartheta) \psi_{\Lambda}(\mathbf{r}_0, \vartheta_0)^* = \rho^{\text{eq}}(\mathbf{r}, \vartheta) e^{\mathcal{L}t} \sum_{\Lambda} \langle \mathbf{r}, \vartheta | \psi_{\Lambda} \rangle \langle \psi_{\Lambda} | \mathbf{r}_0, \vartheta_0 \rangle \\ &= \rho^{\text{eq}}(\mathbf{r}, \vartheta) \sum_{\Lambda} \langle \mathbf{r}, \vartheta | e^{\mathcal{L}t} \psi_{\Lambda} \rangle \langle \psi_{\Lambda} | \mathbf{r}_0, \vartheta_0 \rangle\end{aligned}$$

$$\mathbb{P}(\mathbf{r}, \vartheta, t | \mathbf{r}_0 \vartheta_0) = \rho^{\text{eq}}(\mathbf{r}, \vartheta) \langle \mathbf{r}, \vartheta | e^{\mathcal{L}t} \mathbf{r}_0 \vartheta_0 \rangle$$

→ propagates initial state to final state

# Symmetries



- rotation of the position  $\mathbf{r}$  around the center

generator  $L = -i\partial_\varphi$  'orbital momentum'

- rotation of the orientation  $\mathbf{u}$

generator  $S = -i\partial_\vartheta$  'spin'

- simultaneous rotation of position and orientation

generator  $J = -i\partial_\varphi - i\partial_\vartheta = L + S$  'total angular momentum'

- total angular momentum  $J$  **conserved** for active Brownian particle, 'good quantum number'  
for passive particles orbital momentum  $L$  and spin  $S$  are conserved separately

# Passive Brownian particle

- eigenvalue problem**  $\mathcal{L}_0\psi = -\lambda\psi$   
separation ansatz  $\psi(r, \varphi, \vartheta) = \exp(i\ell\varphi) \exp[i(j - \ell)\vartheta]R(r)$   $j = l + s$  reflects conservation laws

$$\rightarrow \frac{d^2}{dr^2} \frac{d}{dr} \left( r \frac{dR(r)}{dr} \right) - \frac{d^2\ell^2}{r^2} R(r) - D_{\text{rot}}\tau(j - \ell)^2 R(r) - r \frac{dR(r)}{dr} + \lambda\tau R(r) = 0$$

- orbital angular momentum barrier dominates for  $r \rightarrow 0 \rightarrow R(r) \propto r^{|\ell|}$   
thermal oscillator length  $d$  sets the scale

$$\text{ansatz} \quad R(r) = r^{|\ell|} L(\rho^2), \quad \text{with } \rho = r/d\sqrt{2}$$

$$xL''(x) + (1 + |\ell| - x)L'(x) + [\lambda\tau/2 - D_{\text{rot}}\tau(j - \ell)^2/2 - |\ell|/2]L(x) = 0$$

solutions are **associated Laguerre polynomials**  $L_n^{|\ell|}(x)$

$$\text{eigenvalue} \quad \lambda_{n\ell j} = \frac{1}{\tau} (2n + |\ell|) + D_{\text{rot}}(j - \ell)^2$$

# Passive Brownian particle – cont'd

- Laguerre polynomials

**orthogonal**  $\int_0^\infty x^k e^{-x} L_m^k(x) L_n^k(x) dx = \delta_{mn} \frac{(n+k)!}{n!}$

**complete**  $x^k e^{-x} \sum_{n=0}^\infty \frac{n!}{(n+k)!} L_n^k(x) L_n^k(x_0) = \delta(x - x_0)$

- eigenfunctions

$$\langle \mathbf{r} \vartheta | \psi_{n,\ell,j} \rangle = \psi_{n,\ell,j}(\mathbf{r}, \vartheta) = \sqrt{\frac{n!}{(n+|\ell|)!}} \left( \frac{r}{d\sqrt{2}} \right)^{|\ell|} L_n^{|\ell|} \left( \frac{r^2}{2d^2} \right) e^{i\ell\varphi} e^{i(j-\ell)\vartheta}$$

$$\langle \psi_{n',\ell',j'} | \psi_{n,\ell,j} \rangle = \delta_{nn'} \delta_{\ell\ell'} \delta_{jj'}$$

$$p^{\text{eq}}(\mathbf{r}, \vartheta) \sum_{n=0}^\infty \sum_{\ell=-\infty}^\infty \sum_{j=-\infty}^\infty \psi_{n,\ell,j}(\mathbf{r}, \vartheta) \psi_{n,\ell,j}(\mathbf{r}_0, \vartheta_0)^* = \delta(\mathbf{r} - \mathbf{r}_0) \delta(\vartheta - \vartheta_0)$$

**propagator**  $\mathbb{P}_0(\mathbf{r}, \vartheta, t | \mathbf{r}_0, \vartheta_0) = p^{\text{eq}}(\mathbf{r}, \vartheta) \sum_{n=0}^\infty \sum_{\ell=-\infty}^\infty \sum_{j=-\infty}^\infty e^{-\lambda_{n,\ell,j} t} \psi_{n,\ell,j}(\mathbf{r}, \vartheta) \psi_{n,\ell,j}(\mathbf{r}_0, \vartheta_0)^*$



# Active Brownian particle – spectrum

- eigenvalues in perturbation theory – **action** of the active propulsion

$$\mathcal{L}_1 |\psi_{n,\ell,j}\rangle = \frac{1}{\sqrt{2\tau}} \begin{cases} \sqrt{n+\ell+1} |\psi_{n,\ell+1,j}\rangle - \sqrt{n+1} |\psi_{n+1,\ell-1,j}\rangle & \text{if } \ell > 0, \\ \sqrt{n+1} |\psi_{n,\ell+1,j}\rangle + \sqrt{n+1} |\psi_{n,\ell-1,j}\rangle & \text{if } \ell = 0, \\ \sqrt{n-\ell+1} |\psi_{n,\ell-1,j}\rangle - \sqrt{n+1} |\psi_{n+1,\ell+1,j}\rangle & \text{if } \ell < 0. \end{cases}$$

**rotational invariance** →  $j$  is unchanged ✓

activity **couples** different orbital momenta

one of the quantum numbers  $n$ ,  $|\ell|$  increases by 1

→ sort states such that matrix  $\langle \psi_{n',\ell',j} | \mathcal{L}_1 | \psi_{n,\ell,j} \rangle$  is **strictly lower-diagonal !!!**

eigenvalues independent of Péclet number – harmonic oscillator is **isospectral**

# Propagator

- formal expression for propagator

$$\begin{aligned}\mathbb{P}(\mathbf{r}, \vartheta, t | \mathbf{r}_0, \vartheta_0) &= p^{\text{eq}}(\mathbf{r}, \vartheta) \langle \mathbf{r}, \vartheta | e^{\mathcal{L}t} \mathbf{r}_0 \vartheta_0 \rangle \quad \text{insert completeness} \quad \sum_{n,\ell,j} |\psi_{n,\ell,j}\rangle \langle \psi_{n,\ell,j}| = \mathbb{I} \\ &= p^{\text{eq}}(\mathbf{r}, \vartheta) \sum_{n,\ell,j} \langle \mathbf{r}, \vartheta | \psi_{n,\ell,j} \rangle \underbrace{\langle \psi_{n,\ell,j} | e^{\mathcal{L}t} \mathbf{r}_0 \vartheta_0 \rangle}_{=: M_{n,\ell,j}(\mathbf{r}_0, \vartheta_0, t)}\end{aligned}$$

expansion in eigenfunctions  $\mathbb{P}(\mathbf{r}, \vartheta, t | \mathbf{r}_0, \vartheta_0) = p^{\text{eq}}(\mathbf{r}, \vartheta) \sum_{n,\ell,j} M_{n,\ell,j}(\mathbf{r}_0, \vartheta_0, t) \psi_{n,\ell,j}(\mathbf{r}, \vartheta)$

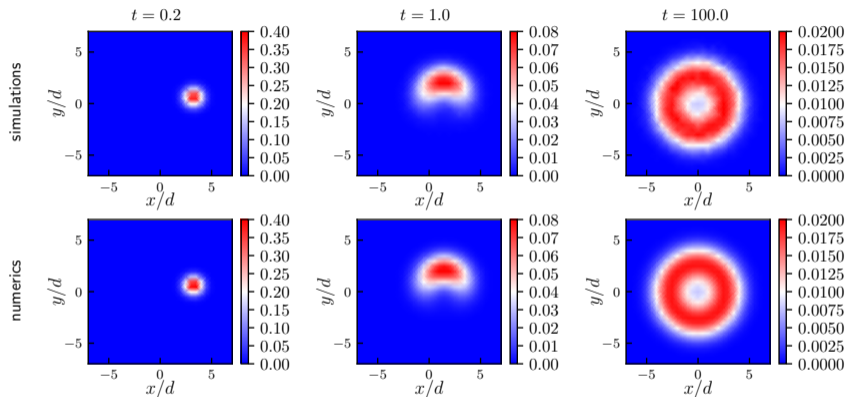
- Dyson equation (perturbation identity)

$$e^{\mathcal{L}t} = e^{\mathcal{L}_0 t} + \text{Pe} \int_0^t ds e^{\mathcal{L}(t-s)} \mathcal{L}_1 e^{\mathcal{L}s}$$

- recursion relation** (use angular momentum conservation)

$$M_{n,\ell,j}(\mathbf{r}_0, \vartheta_0, t) = e^{-\lambda_{n,\ell,j} t} \langle \psi_{n,\ell,j} | \mathbf{r}_0, \vartheta_0 \rangle + \text{Pe} \int_0^t ds e^{-\lambda_{n,\ell,j}(t-s)} \sum_{n',\ell'} \langle \psi_{n,\ell,j} | \mathcal{L}_1 | \psi_{n',\ell',j} \rangle M_{n',\ell',j}(\mathbf{r}_0, \vartheta_0, s)$$

# Propagator – cont'd



- analytics corroborated by simulation ✓
- stationary distribution **non-Gaussian** – pile-up of probability on the edge

# Correlation functions

- Perturbation  $\mathcal{L}_1$  'upper diagonal'
  - no chains, no term appears twice
  - scheme terminates for simple correlation functions: **integrable**
- Positional autocorrelation function (PAF)

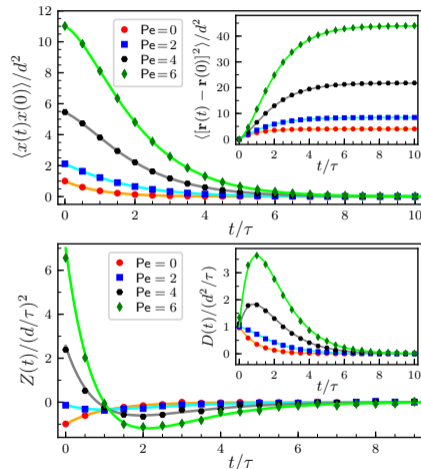
$$\langle x(t)x(0) \rangle = d^2 \left[ e^{-t/\tau} - \frac{\text{Pe}^2}{2} \frac{D_{\text{rot}}\tau e^{-t/\tau} - e^{-D_{\text{rot}}t}}{1 - (D_{\text{rot}}\tau)^2} \right]$$

eigenvalues are unchanged!

- Velocity autocorrelation function (VACF)

$$Z(t) = -\frac{d^2}{dt^2} \langle x(t)x(0) \rangle$$

not a completely monotone function → fingerprint of **non-equilibrium dynamics**



M. Caraglio and T. Franosch, PRL (2022)

# Summary and Conclusions

## Circle swimmer

- exact solution in terms of generalized Mathieu functions
- ISF displays non-trivial plateau due to circular motion

## Gravitaxis

- formal solution of Fokker-Planck equation
- generates low-order moments
- **resonance** close to classical bifurcation for small noise
- rationalized in terms of **harmonic approximation**

## Active Brownian particle in a harmonic well

- **isospectral**: eigenvalues remain unchanged
- perturbative scheme for **propagator**
- **closed expressions** for low-order correlation functions