

Shape Matters

A Brownian microswimmer interacting with walls

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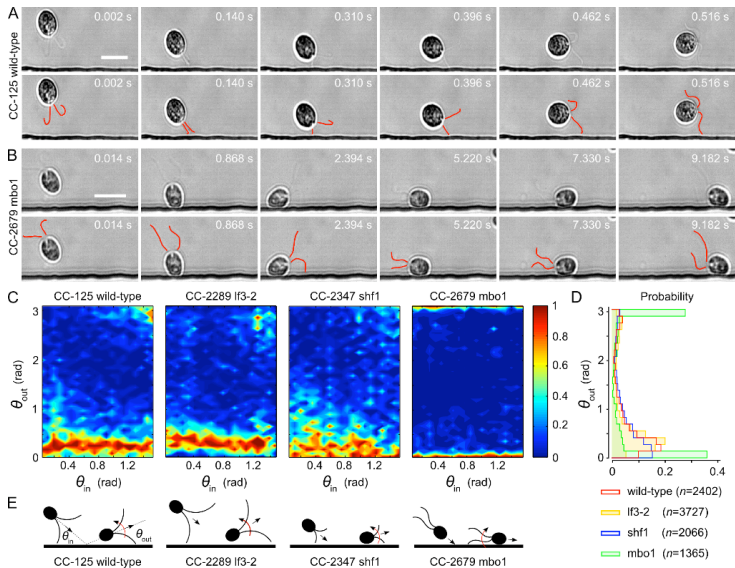
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Microswimmer scattering off a surface

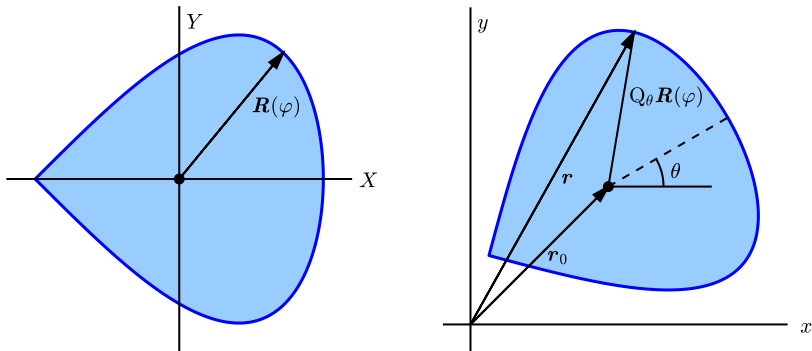




- Swimmers have a **distribution of scattering angles**, but peak at a preferred angle.
- Angle depends strongly on the type of swimmers.
- Steric interaction with boundary is important.
- Hydrodynamic interaction with boundary can also be important.
- It's biology: everything is important.

- Kantsler, V., Dunkel, J., Polin, M., & Goldstein, R. E. (2013). *Proc. Natl. Acad. Sci. USA*, **110** (4), 1187–1192
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The shape of a 2D swimmer



Convex swimmer in its frame (X, Y) and the fixed lab frame (x, y) .

The **swimming direction** corresponds to $\varphi = 0$.

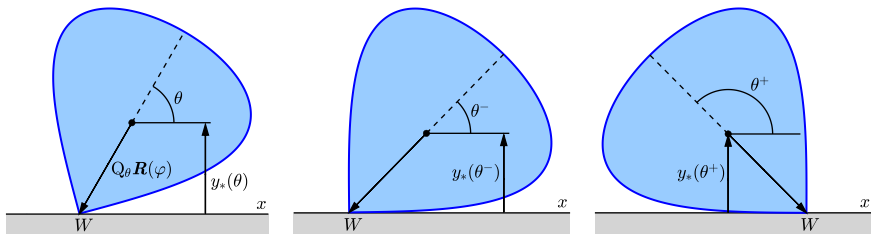
Q_θ is a **rotation matrix** about a given **center of rotation**.

Swimmer touching a wall at $y = 0$



Denote by $y_*(\theta)$ the **vertical coordinate** of a swimmer with orientation θ when it touches the wall.

Convex swimmer touching a horizontal wall at a corner point W :

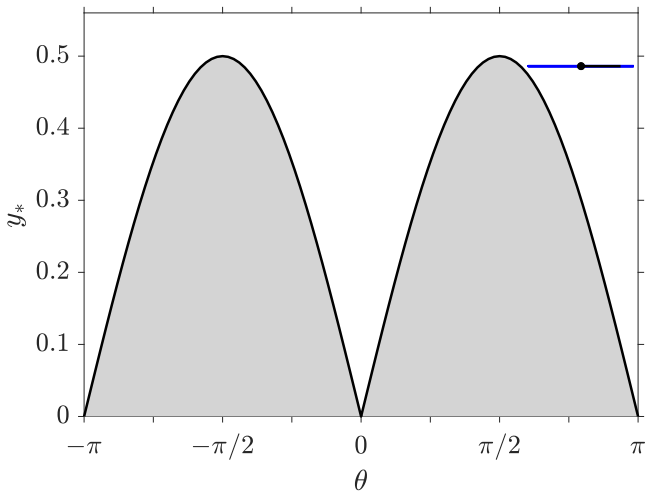


The angle θ can vary from the **right-tangency** angle θ^- to the **left-tangency** angle θ^+ .

Range of y values:

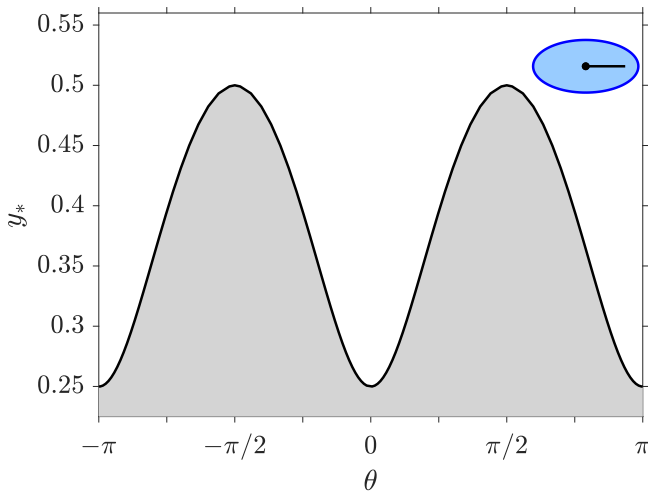
$$y_*(\theta) = -\sin \theta X(\varphi) - \cos \theta Y(\varphi), \quad \theta^- \leq \theta \leq \theta^+.$$

Wall distance function $y_*(\theta)$: needle



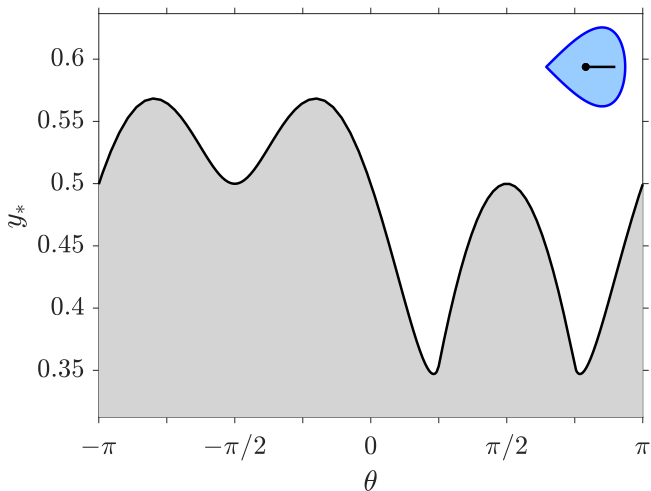
The needle is all corners; $y_*(\theta) = \frac{1}{2}\ell|\sin \theta|$

Wall distance function $y_*(\theta)$: ellipse



The ellipse has no corners; $y_*(\theta) = \sqrt{a^2 \sin^2 \theta + b^2 \cos^2 \theta}$

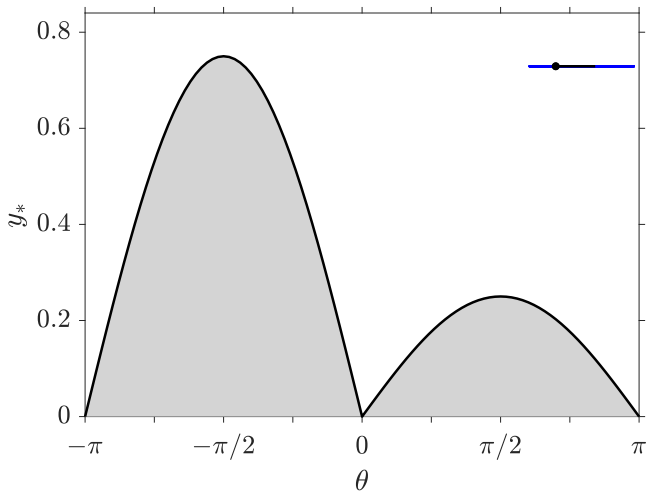
Wall distance function $y_*(\theta)$: teardrop



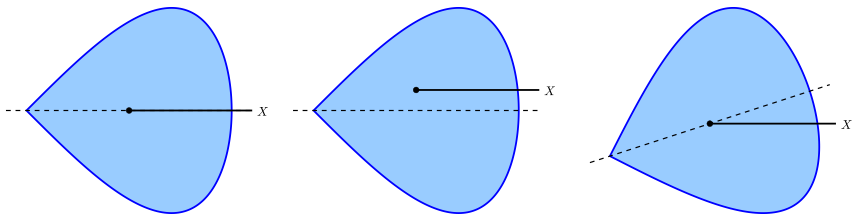
The teardrop has a corner and a smooth boundary.

Note **local min** at $\theta = -\pi/2$ (important later).

Wall distance function: needle with $X_{\text{rot}} < 0$



Center of rotation moved towards the rear ($X_{\text{rot}} < 0$).



A swimmer with an axis of symmetry along its swimming direction has

$$y_*(\theta) = y_*(\pi - \theta)$$

that is, reflection-symmetry about $\pm\pi/2$.

All the swimmers presented so far have that symmetry.

This symmetry is easily broken by moving the center of rotation.

So far we have considered only one wall.

For two parallel walls at $y = \pm L/2$, we have

$$\zeta_-(\theta) \leq y \leq \zeta_+(\theta)$$

where

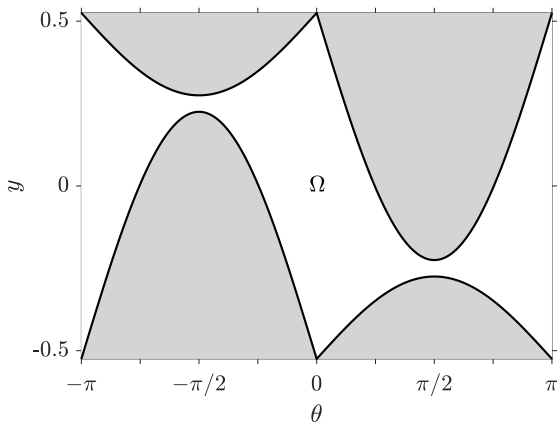
$$\zeta_-(\theta) = y_*(\theta) - L/2, \quad \zeta_+(\theta) = -y_*(\theta + \pi) + L/2.$$

ζ_{\pm} are related by the **channel symmetry**

$$\zeta_+(\theta) = -\zeta_-(\theta + \pi).$$

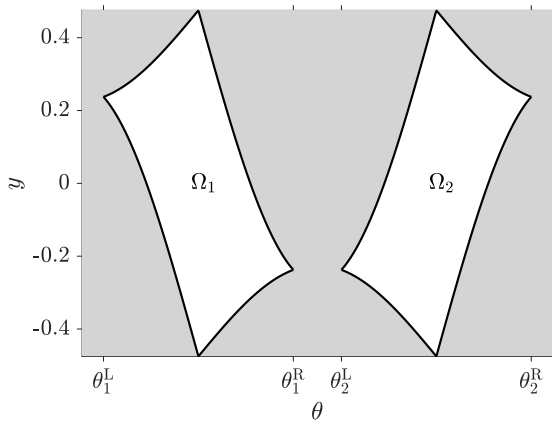
The channel symmetry is always satisfied, **even for an asymmetric swimmer**.

Open channel configuration space



Configuration space for the needle in of length $\ell = 1$ in an **open** channel of width $L = 1.05$. (x not shown.)

A point in this space specifies the **position and orientation** of the swimmer.



Configuration space for the needle in of length $\ell = 1$ in a **closed** channel of width $L = 0.95$.

The swimmer **cannot reverse direction**.

The Brownian swimmer obeys the SDE

$$dX = U dt + \sqrt{2D_X} dW_1$$

$$dY = \sqrt{2D_Y} dW_2$$

$$d\theta = \sqrt{2D_\theta} dW_3$$

in its own **moving reference frame**.

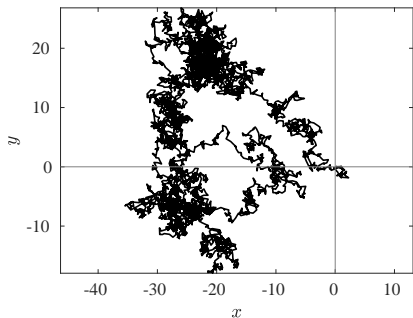
In terms of **absolute x and y coordinates**, this becomes

$$dx = (U dt + \sqrt{2D_X} dW_1) \cos \theta - \sin \theta \sqrt{2D_Y} dW_2$$

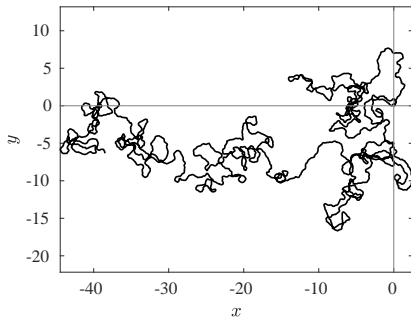
$$dy = (U dt + \sqrt{2D_X} dW_1) \sin \theta + \cos \theta \sqrt{2D_Y} dW_2$$

$$d\theta = \sqrt{2D_\theta} dW_3.$$

- Swimmer **swims** a distance U/D_θ in a time $1/D_\theta$.
- Swimmer **diffuses** a distance $\sqrt{D_X/D_\theta}$ in a time $1/D_\theta$.
- $Pe_{\theta,X} := \frac{U}{D_\theta} / \sqrt{\frac{D_X}{D_\theta}} = \frac{U}{\sqrt{D_\theta D_X}}$ measures the **smoothness of the path**.



$Pe_{\theta,X} \ll 1$



$Pe_{\theta,X} \gg 1$

The F–P equation for the probability density $p(x, y, \theta, t)$:

$$\partial_t p = -\nabla \cdot (\mathbf{u} p - \nabla \cdot \mathbb{D} p) + \partial_\theta^2 (D_\theta p)$$

where the **drift vector** and **diffusion tensor** are respectively

$$\mathbf{u} = \begin{pmatrix} U \cos \theta \\ U \sin \theta \end{pmatrix}$$

$$\mathbb{D} = \begin{pmatrix} D_X \cos^2 \theta + D_Y \sin^2 \theta & \frac{1}{2}(D_X - D_Y) \sin 2\theta \\ \frac{1}{2}(D_X - D_Y) \sin 2\theta & D_X \sin^2 \theta + D_Y \cos^2 \theta \end{pmatrix}.$$

Note that $\nabla := \hat{\mathbf{x}} \partial_x + \hat{\mathbf{y}} \partial_y$ (no θ).

Interaction with boundaries



How to handle the interaction of the swimmer with boundaries?

Volpe *et al.* (2014) use a specular reflection model (**point swimmer**):

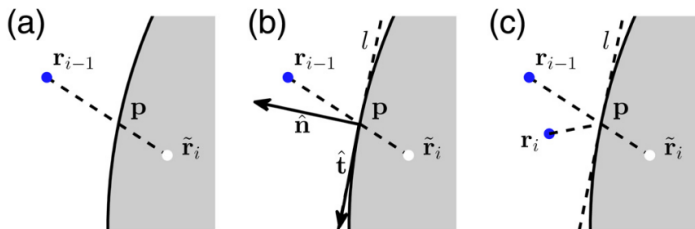


Fig. 3. Implementation of reflective boundary conditions. At each time step, the algorithm (a) checks whether a particle has moved inside an obstacle; if so: (b) the boundary of the obstacle is approximated by its tangent l at the point \mathbf{p} where the particle entered the obstacle, and (c) the particle position is reflected on this line.

For any fixed volume V we have

$$\begin{aligned}\partial_t \int_V p \, dV &= - \int_V (\nabla \cdot (\mathbf{u} p - \nabla \cdot (\mathbb{D} p)) - \partial_\theta^2 (D_\theta p)) \, dV \\ &= - \int_{\partial V} \mathbf{f} \cdot d\mathbf{S},\end{aligned}$$

where ∂V is the boundary of V , and the **flux vector** is

$$\mathbf{f} = \mathbf{u} p - \nabla \cdot (\mathbb{D} p) - \hat{\boldsymbol{\theta}} \partial_\theta (D_\theta p).$$

Thus, on the **reflecting** (impermeable) parts of the boundary we require the no-flux condition

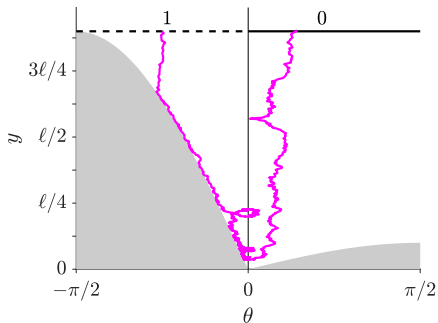
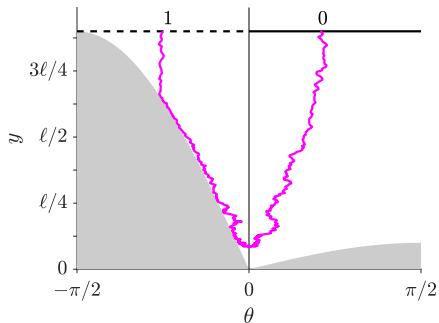
$$\mathbf{f} \cdot \mathbf{n} = 0, \quad \text{on } \partial V_{\text{refl}}$$

where \mathbf{n} is normal to the boundary.

Configuration space and drift in θ - y plane



Drift is $U \sin \theta \hat{y}$; no-flux condition forces swimmer to align with the wall.



Once the particle crosses $\theta = 0$ (parallel to wall), it is pushed upward by the drift.

The F–P equation is challenging to solve because of the **complicated boundary shape**.

Tractable limit $D_\theta \ll 1$ (**small rotational diffusivity**)

Get a (1+1)D PDE¹ for $p(\theta, y, t) = P(\theta, T) e^{\sigma(\theta)y}$

$$\partial_T P + \partial_\theta(\mu(\theta) P - \partial_\theta P) = 0, \quad T := D_\theta t,$$

$$\sigma(\theta) := U \sin \theta / D_{yy}(\theta)$$

$$\mu(\theta) := \frac{\sigma(\theta)}{2 \sinh \Delta(\theta)} \left(e^{\Delta(\theta)} \zeta'_+(\theta) - e^{-\Delta(\theta)} \zeta'_-(\theta) \right)$$

$$\Delta(\theta) := \frac{1}{2} \sigma(\theta) (\zeta_+(\theta) - \zeta_-(\theta)).$$

The **shape of the swimmer** enters through drift $\mu(\theta)$.

¹See Hongfei's specialty exam on 11/19 for more details.

Invariant density and mean drift (open channel)



What is the natural invariant density $\mathcal{P}(\theta)$ for the swimmer? For open channel, 2π -periodic solution to

$$\partial_{\theta}(\mu(\theta) \mathcal{P} - \partial_{\theta} \mathcal{P}) = 0.$$

Integrate once:

$$\mu(\theta) \mathcal{P} - \partial_{\theta} \mathcal{P} = c_2.$$

Integrate this from $-\pi$ to π to find

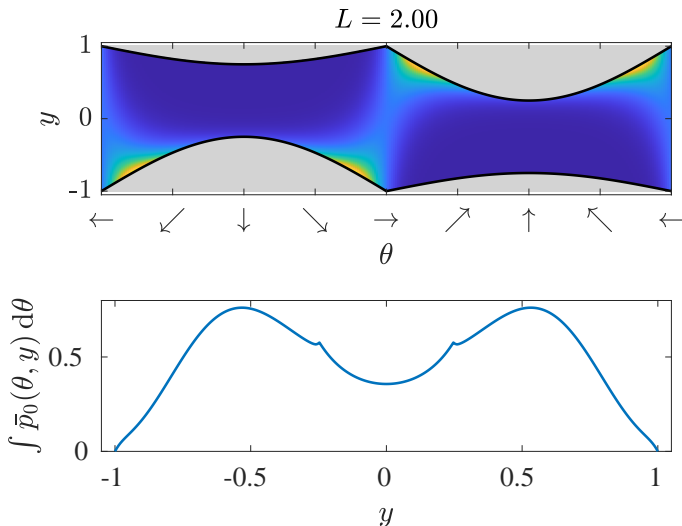
$$\mathbb{E}\mu(\theta) = \int_{-\pi}^{\pi} \mu(\theta) \mathcal{P} d\theta = 2\pi c_2 =: \omega.$$

ω is the **mean drift** or **mean rotation rate** of the swimmer.

Easy to show: if the swimmer is left-right symmetric, then $\omega = 0$ and the probability satisfies **detailed balance**.

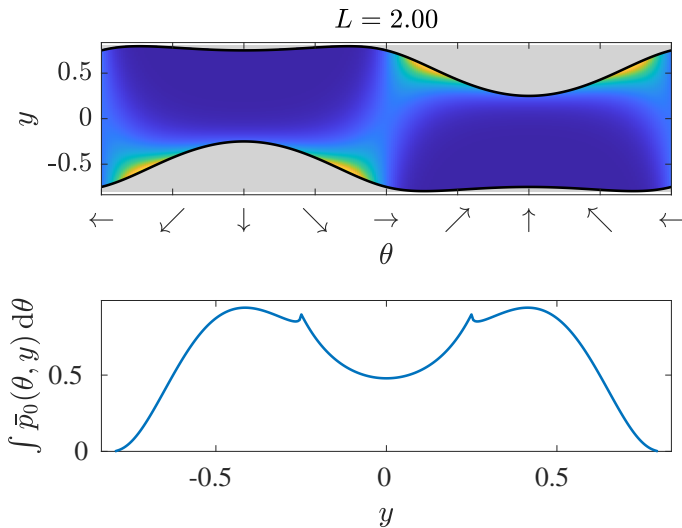
An asymmetric swimmer thus picks up a **mean rotation!**

Invariant density examples: needle



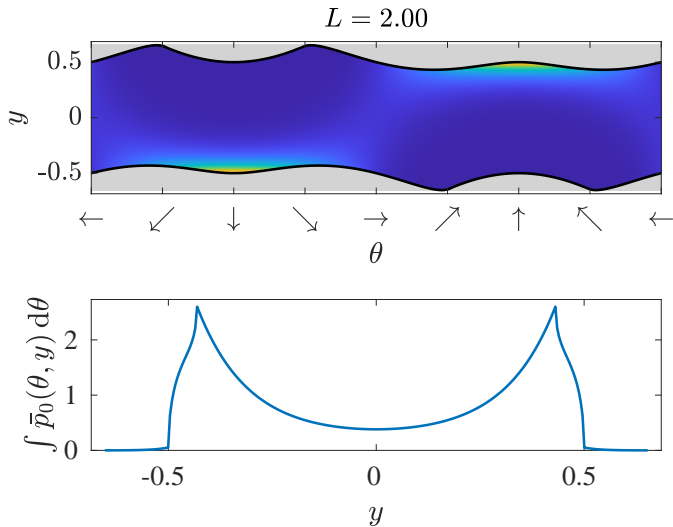
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Invariant density examples: ellipse



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Invariant density examples: teardrop



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From our reduced equation, we can derive an adjoint equation for the **mean exit time** of swimmer starting at orientation θ to reach the “exit” $\theta = \theta^L$ or $\theta = \theta^R$ for the first time:

$$\begin{aligned}\mu(\theta) \tau' + \tau'' &= -1, & \theta^L < \theta < \theta^R; \\ \tau(\theta^L) &= \tau(\theta^R) = 0.\end{aligned}$$

The **mean reversal time** is the special case $\tau(0)$ for $-\theta^L = \theta^R = \pi$.

It gives the expected time for the swimmer to **completely reverse direction** in the channel. See Holcman & Schuss (2014) for the case without drift.

For a reflection-symmetric swimmer, the mean reversal time takes the simple form

$$\tau_{\text{rev}} = \frac{1}{4} \int_0^\pi \frac{d\vartheta}{\mathcal{P}(\vartheta)}$$

where $\mathcal{P}(\theta)$ is the **invariant density**.

Intuitively, small \mathcal{P} corresponds to **"bottlenecks"** that dominate the reversal time.

The diffusive needle



For a **purely-diffusive** ($U = 0$) needle of length ℓ in a channel of width L , the mean reversal time is

$$\tau_{\text{rev}} = \frac{(\pi - 2\lambda)(\pi - \arccos \lambda)}{D_\theta \sqrt{1 - \lambda^2}}, \quad \lambda := \ell/L < 1.$$

The '**narrow exit**' limit corresponds to $\lambda = 1 - \delta$, with δ small:

$$\tau_{\text{rev}} = \frac{\pi(\pi - 2)}{D_\theta \sqrt{2\delta}} + O(\delta^0), \quad \delta \ll 1.$$

This is **similar but not identical** to Holcman & Schuss (2014, Eq. (5.13)):

$$\tau_{\text{rev}}^{(\text{HS})} = \frac{\pi(\pi - 2)}{D_\theta \sqrt{\delta}} \sqrt{\frac{D_X}{L^2 D_\theta}} + O(\delta^0),$$

Our result holds for **small** D_θ , theirs for **small** δ .

Different scaling in D_θ ! (Ours: D_θ^{-1} ; theirs: $D_\theta^{-3/2}$.)



- Simple model for a **Brownian swimmer** or interacting with walls.
- The boundary conditions are naturally dictated by **conservation of probability** in **configuration space**.
- **Swimmer geometry** plays a role as it affects the shape of configuration space.
- This opens up the analysis to **PDE methods** (**Fokker–Planck equation**).
- (1+1)D reduced PDE when y dynamics are fast compared to θ .
- Lots more to look at:
 - Effective diffusivity in terms of mean reversal time;
 - Scattering angle distribution;
 - 3D swimmers;
 - The $D_\theta \gg D_X$ limit (hard boundary layers!);
 - Compare to experiments;
 - Other confined geometries.
- More at Hongfei's specialty exam on 11/19.

- Contino, M., Lushi, E., Tuval, I., Kantsler, V., & Polin, M. (2015). *Phys. Rev. Lett.* **115** (25), 258102.
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