The role of shape for a Brownian microswimmer interacting with walls

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Microswimmer scattering off a surface

[Kantsler et al. (2013)]
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.
- A small sample of papers on this topic:
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 \(\varphi = 0\).

\(Q_\theta\) is a rotation matrix about a given center of rotation.
Swimmer touching a wall at $y = 0$

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

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

The angle $\theta$ can vary from the \textbf{right-tangency} angle $\theta^-$ to the \textbf{left-tangency} angle $\theta^+$. 

Range of $y$ values:

$$y_*(\theta) = -\sin \theta X(\varphi) - \cos \theta Y(\varphi), \quad \theta^- \leq \theta \leq \theta^+. $$
Wall distance function $y_*(\theta)$: 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.
Wall distance function: needle with $X_{\text{rot}} < 0$

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

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

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

\( \zeta_\pm \) are related by the channel symmetry

\[
\zeta_+(\theta) = -\zeta_-(\theta + \pi).
\]
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 rotating reference frame.

In terms of absolute \( x \) and \( y \) coordinates, this becomes

\[ dx = (U \, dt + \sqrt{2D_X} \, dW_1) \cos \theta - \sin \theta \sqrt{2D_Y} \, dW_2 \]
\[ dy = (U \, dt + \sqrt{2D_X} \, dW_1) \sin \theta + \cos \theta \sqrt{2D_Y} \, dW_2 \]
\[ d\theta = \sqrt{2D_\theta} \, dW_3 \]
The F–P equation for the probability density $p(x, y, \theta, t)$:

$$\partial_t p = -\nabla \cdot (u p - \nabla \cdot D p) + \partial^2_{\theta}(D_{\theta} p)$$

where the drift vector and diffusion tensor are respectively

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

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

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

BCs: No probability flux at the boundaries.
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.
Reduced equation

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 PDE for $p(\theta, y, t) = P(\theta, T) e^{\sigma(\theta)y}$

\[
\partial_T P + \partial_\theta (\mu(\theta) P - \partial_\theta P) = 0
\]

\[
T := D_\theta t,
\]

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

\[
\mu(\theta) := \frac{\sigma(\theta)}{2 \sinh \Delta(\theta)} \left( e^{\Delta(\theta)} \zeta_+'(\theta) - e^{-\Delta(\theta)} \zeta_-'(\theta) \right)
\]

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

The shape of the swimmer enters through drift $\mu(\theta)$.
What is the natural invariant density $P(\theta)$ for the swimmer? For open channel, $2\pi$-periodic solution to

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

Integrate once:

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

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

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

$\omega$ 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: ellipse

\[ L = 2.00 \]

\[ \int \tilde{p}_0(\theta, y) \, d\theta \]
Invariant density examples: teardrop

$L = 2.00$

play movie
Mean reversal time

The mean time for a swimmer to go from $\theta = 0$ to $\theta = \pm \pi$.

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.

See Holcman & Schuss (2014) for the case without drift.
The diffusive needle

For a purely-diffusive \((U = 0)\) needle of length \(\ell\) 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 \(\delta\) 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 \(D_\theta\), theirs for small \(\delta\).

Different scaling in \(D_\theta\)! (Ours: \(D_\theta^{-1}\); theirs: \(D_\theta^{-3/2}\).)
Numerical simulation of needle reversal

$U = 0, \: D_X = D_Y = 1, \: \lambda = 0.9, \: L = 1 \: (\delta = 0.1)$
• 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 $\theta$.
• 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 (lots of boundary layers!);
  • Compare to experiments;
  • Other confined geometries.


