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Modeling a Brownian microswimmer interacting with walls

(Marseille - IRPHE)
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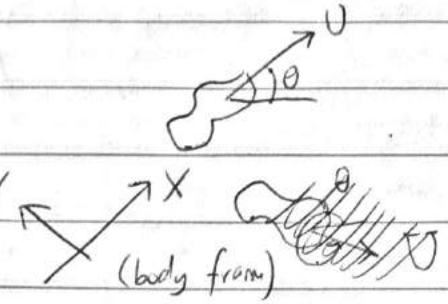
Simple model: Constant speed, Brownian angle

SDEs:



$$dX = U\,dt + \sqrt{2D_X}\,dW_1$$
$$dY = \sqrt{2D_Y}\,dW_2$$
$$d\theta = \sqrt{2D_\theta}\,dW_3$$

dW_i Gaussian white noise.

Rotate to convert to lab (absolute) frame

$$dx = \left(U\,dt + \sqrt{2D_X}\,dW_1\right)\cos\theta - \sin\theta\sqrt{2D_Y}\,dW_2$$
$$dy = \left(U\,dt + \sqrt{2D_X}\,dW_1\right)\sin\theta + \cos\theta\sqrt{2D_Y}\,dW_2$$
$$d\theta = \sqrt{2D_\theta}\,dW_3$$

Already not trivial to solve! Also used in polymer physics
(See Kurzthaler and Franosch, 2017, for Intermediate Scattering Function)

Turn this into a PDE in the usual manner.
(NOT multiplicative noise: $F(\theta)\,dW_{1,2}$.) ← Itô, Strat, whatever
Get Fokker-Planck (Kolmogorov backward) eq'n.

$p(x,y,\theta,t)$ = probability density

$$\underline{\mu} = \begin{pmatrix} U\cos\theta \\ U\sin\theta \\ 0 \end{pmatrix}, \quad \mathbb{B} = \begin{pmatrix} \sqrt{2D_x}\cos\theta & -\sqrt{2D_Y}\sin\theta & 0 \\ \sqrt{2D_x}\sin\theta & \sqrt{2D_Y}\cos\theta & 0 \\ 0 & 0 & \sqrt{2D_\theta} \end{pmatrix}$$

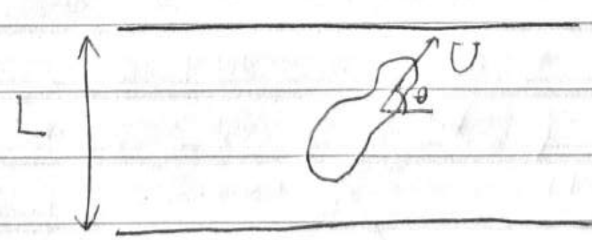
$$\begin{pmatrix} dx \\ dy \\ d\theta \end{pmatrix} = \underline{\mu}\, dt + \mathbb{B}(\theta) \begin{pmatrix} dW_1 \\ dW_2 \\ dW_3 \end{pmatrix}$$

$$\partial_t p = -\nabla \cdot \underbrace{(\underline{\mu} p - \mathbb{D} \nabla p)}_{\underline{f}\ (\text{flux})}$$

$$\mathbb{D} = \frac{1}{2} BB^T = \begin{pmatrix} D_X\cos^2\theta + D_Y\sin^2\theta & \frac{1}{2}(D_X - D_Y)\sin 2\theta & 0 \\ \frac{1}{2}(D_X - D_Y)\sin 2\theta & D_X\sin^2\theta + D_Y\cos^2\theta & 0 \\ 0 & 0 & D_\theta \end{pmatrix}$$

Note: $D_X = D_Y \Rightarrow \mathbb{D} = \begin{pmatrix} D_X & & \\ & D_Y & \\ & & D_\theta \end{pmatrix}$

Solve for Green's function, etc. But consider a swimmer in a channel:



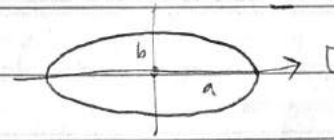
It cannot enter the wall: probability must be conserved.

Configuration space: take $\rho = \rho(y, \theta, t)$ (ignore x)

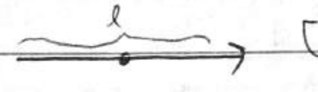
What values of θ and y are accessible to swimmer?

NOW GEOMETRY OF SWIMMER MATTERS!

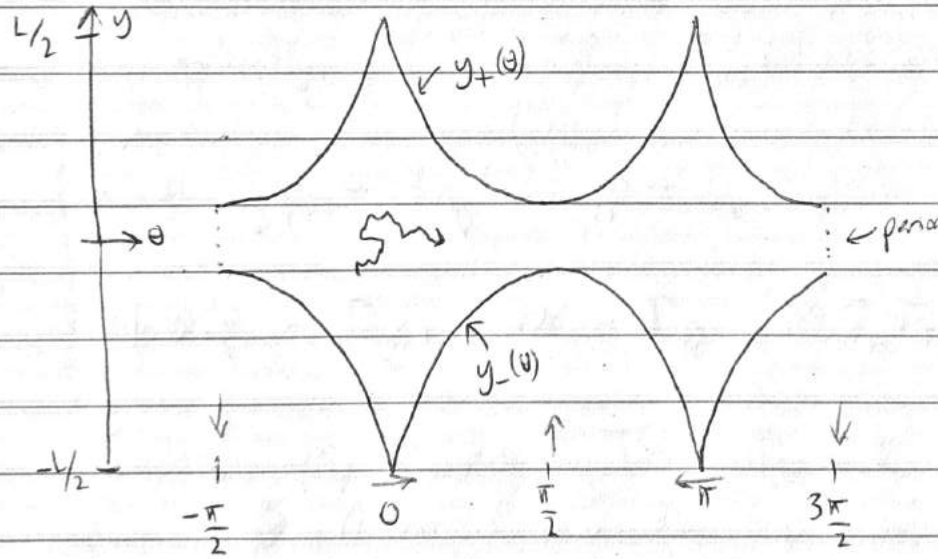
__examples:__ ellipse



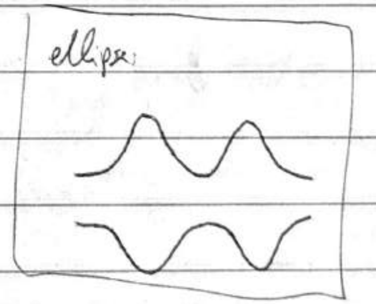
needle



For needle, domain is $-\pi < \theta < \pi$, $y_-(\theta) < y < y_+(\theta)$

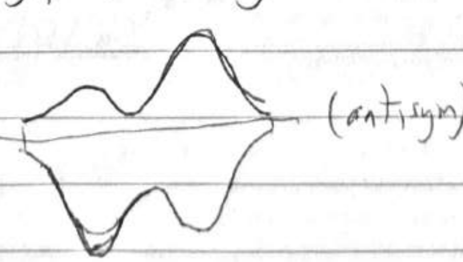


$$y_\pm(\theta) = \pm\left(\frac{L}{2} - \frac{\ell}{2}|\sin\theta|\right)$$



For general shape, $y_\pm(\theta)$ depends on __convex hull__ of swimmer

But always have: $y_+(\theta) = -y_-(\theta)$



Now we want to solve the F-P equation in our configuration space Ω
What BC? Need to conserve probability:

$$\underline{f} \cdot \hat{n} = 0 \quad \text{on } \partial\Omega \quad \left(\underline{f} = \underline{\mu}\, p - \mathbb{D} \nabla p\right)$$

So we have Robin (mixed) BCs at the walls.

The <u>invariant density</u> $p(y,\theta)$ satisfies:

$$\nabla \cdot \left(\underline{\mu}\, p - \mathbb{D} \nabla p\right) = 0 \qquad \begin{array}{l} \text{Unique } p \geq 0 \\ \int_\Omega p \, dV = 1 \end{array}$$

More explicitly: $(U = 1)$ $D_{yy}(\theta) = D_X \sin^2\theta + D_Y \cos^2\theta$

$$\begin{cases} \sin\theta \, \partial_y p - D_{yy}(\theta)\, \partial_{yy} p - D_\theta \, \partial_{\theta\theta} p = 0 \,, & (\theta, y) \in \Omega \\ \sin\theta \, p - D_{yy}(\theta)\, \partial_y p + D_\theta \, y_\pm'(\theta)\, \partial_\theta p = 0 \,, & y = y_\pm(\theta) \end{cases}$$

Solve! ok, not easy. Take $D_\theta = \varepsilon$ small.

<u>$O(\varepsilon^0)$:</u> $\sin\theta \, \partial_y p_0 - D_{yy}(\theta)\, \partial_{yy} p_0 = 0 \qquad (\theta, y) \in \Omega$

$$\sin\theta \, p_0 - D_{yy}(\theta)\, \partial_y p_0 = 0 \,, \qquad y = y_\pm(\theta)$$

$$\Rightarrow \quad p_0 = \mathbb{P}(\theta)\, e^{\sigma(\theta) y} \,, \qquad \sigma(\theta) \equiv \frac{\sin\theta}{D_{yy}(\theta)}$$

(No flux in y direction)

$$p = p_0 + \varepsilon p_1 + \cdots$$

$O(\varepsilon^1)$: $\sin\theta\, \partial_y p_1 - D_{yy}(\theta)\, \partial_{yy} p_1 = \partial_{\theta\theta} p_0$ (PDE)

$$\sin\theta\, p_1 - D_{yy}(\theta)\, \partial_y p_1 = -y_\pm'(\theta)\, \partial_\theta p_0 \,, \quad y = y_\pm(\theta) \quad \text{(BC)}$$

Integrate PDE in y from $y_-(\theta)$ to $y_+(\theta)$; apply BC.

After manipulation we get:

$$\partial_\theta \int_{y_-(\theta)}^{y_+(\theta)} \partial_\theta p_0\, dy = 0 \qquad p_0 = P(\theta)\, e^{\sigma(\theta) y}$$

carry out y integrals

$$\boxed{\left(w(\theta)\, P'(\theta) - \nu(\theta)\, P(\theta) \right)' = 0}$$

$y_+ \geq y_-$

$$w(\theta) = \int_{y_-(\theta)}^{y_+(\theta)} e^{\sigma(\theta) y}\, dy = \frac{e^{\sigma y_+} - e^{\sigma y_-}}{\sigma} \geq 0$$

(equality only when $y_+ = y_-$)

Solve: $P(\theta) = \left(c_1 + c_2 F(\theta)\right) e^{\Phi(\theta)}$

$$\Phi(\theta) = \int_{\theta_0}^{\theta} \frac{\nu(\tilde\theta)}{w(\tilde\theta)}\, d\tilde\theta \,, \qquad F(\theta) = \int_{\theta_0}^{\theta} \frac{e^{-\Phi(\tilde\theta)}}{w(\tilde\theta)}\, d\tilde\theta$$

BC in θ is periodicity: $P(-\pi) = P(\pi)$, $\theta_0 = -\pi$:

$$P(\theta) = c_1 e^{\Phi(\theta)} \left(1 - \left(1 - e^{-\Phi(\pi)}\right) F(\theta) / F(\pi) \right)$$

(choose c_1 so $\int_{-\pi}^{\pi} w P\, d\theta = 1$)

If $\Phi(\theta)$ is periodic, then

$$\boxed{P(\theta) = c_1 e^{\Phi(\theta)}} \quad (c_2 = 0)$$

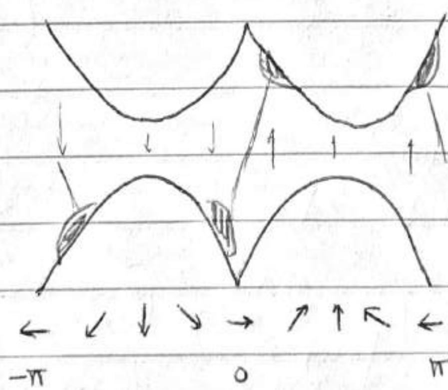
This is the case when $y_+(\theta) = -y_-(-\theta)$!

Flux of swimmers (horizontal)

$$-\int_{y_-}^{y_+} \partial_\theta p \, dy = -(wP' - \nu P) = -c_2$$

Thus, $c_2 = 0$ is the statement that there is no net flux of swimmers in the channel. C_2 could be nonzero if the swimmer interacts differently with the two walls!

What do solutions look like? Have to integrate numerically, given a wall shape.



- $\sin\theta$ drift pushes against ~~wall~~ wall.
- See "transitions" between top and bottom wall.
- Swimmer spends most of its time pointing a bit towards a wall

Now can compute averages:

$$p(y) = \int_{-\pi}^{\pi} P(\theta)\, e^{\sigma(\theta) y} \, d\theta$$ ← marginal distribution in y (collect at walls, but not always)

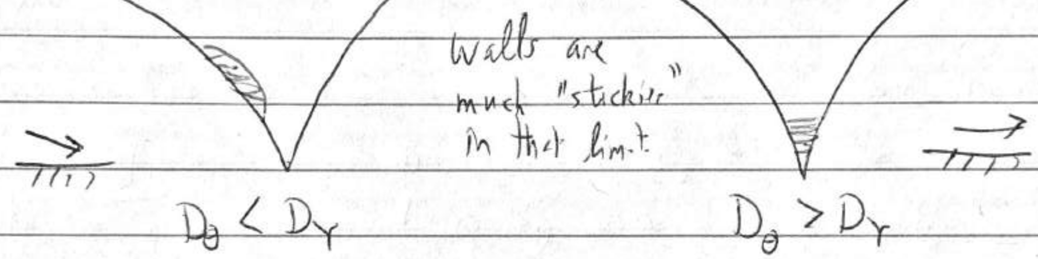
$\mathbb{E}\cos\theta = 0$ (horizontal drift)

$\mathbb{E}\cos^2\theta$ varies ($\sim .8$) (horizontal diffusion)

Much remains to be done to characterize the range of behavior.
Also Green's function, etc.

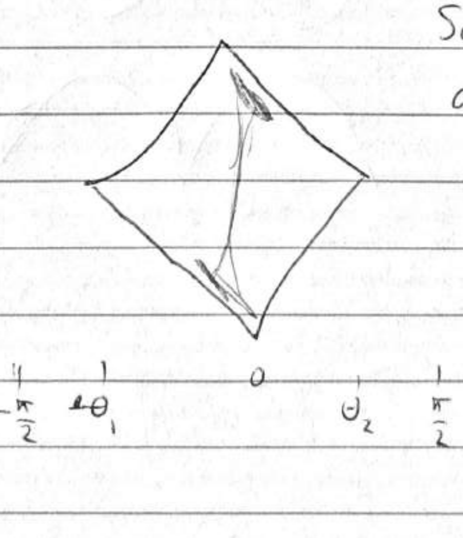
The expansion presented breaks down if $D_\theta > D_Y$, which I feel is the more interesting limit.

Much harder!



Unfortunately, the case $D_\theta > D_Y$ seems to require two nested boundary layers and lots of Airy functions.
I'm sure we'll figure it out eventually...

<u>Closed</u>:



Swimmer cannot turn around in channel

Again, $c_2 = 0$, this time because we impose no net flux. Also gets rid of singularities in w.