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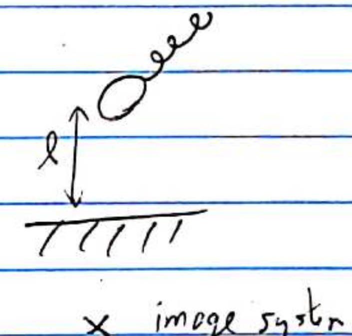
# Lost in configuration space

7/20/21

Microswimmers and active particles often interact with boundaries.

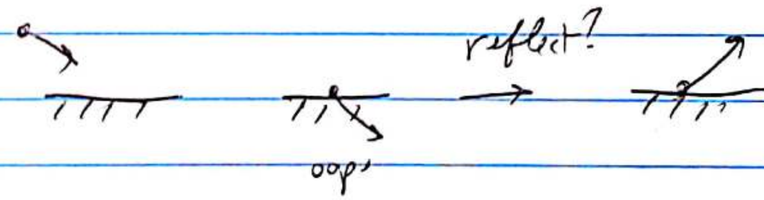
$\begin{cases} \text{hydrodynamic} \\ \text{steric (contact)} \end{cases}$

Hydrodynamic is well-understood:




Particle feels its "image" in the boundary.
Use Stokes flow, for most part

Steric is trickier: lots of ad-hoc models, experimentally motivated & validated.

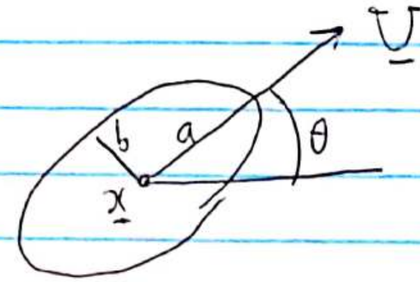



Or use a confining potential

Flagella & shape play crucial roles.

Is there a "mathematically sound" way of modeling steric interactions? Can we include effect of shape of swimmer?

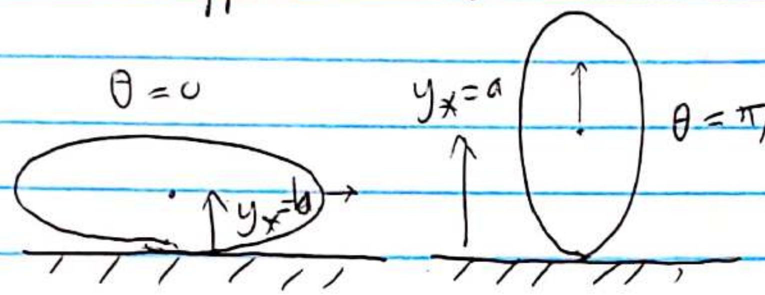
A model: elliptical swimmer (2D)




Center is at $\underline{x} = (x, y)$

CONFIGURATION $(x, y, \theta)$.

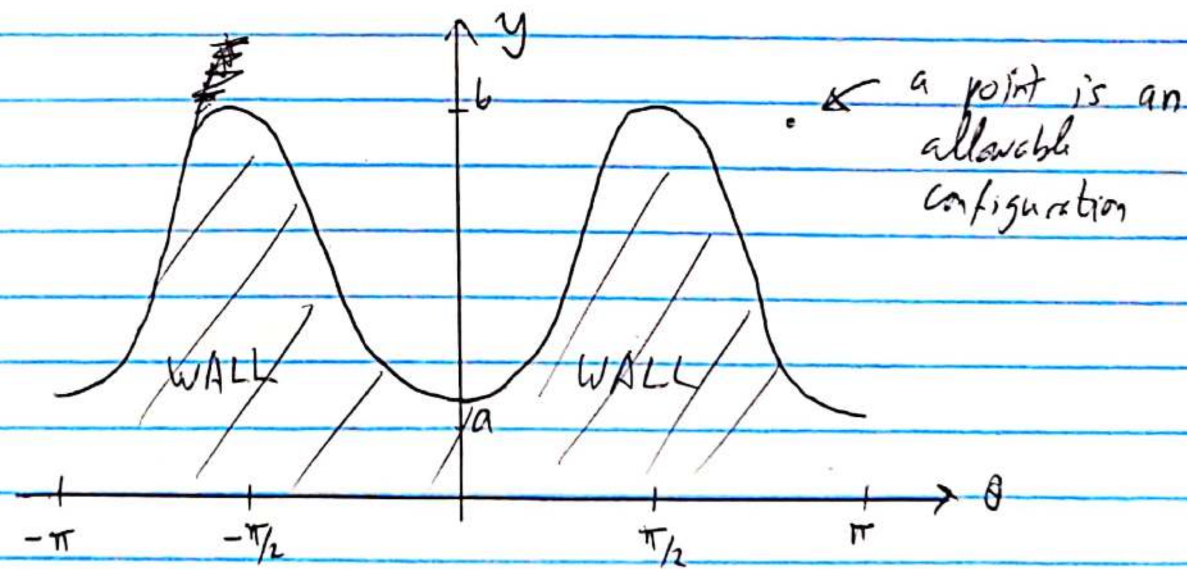
What happens when we make contact with a plane wall?




Closest approach $y_*(\theta)$ depends on angle.

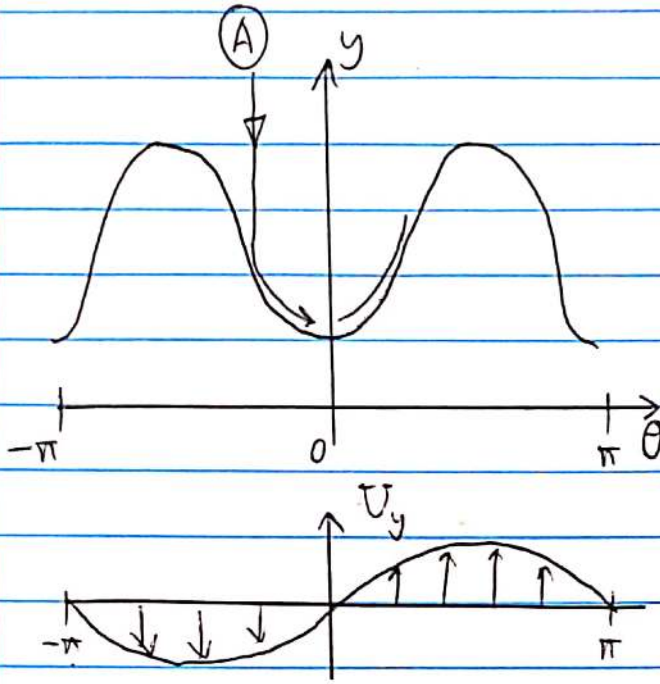
The range of allowable $(x, y, \theta)$ is called
<u>configuration space</u>

ellipse: $y_*(\theta) = \sqrt{a^2 \sin^2\theta + b^2 \cos^2\theta}$




$x$ is unconstrained (not shown)

Scanned with CamScanner




Add some dynamics:

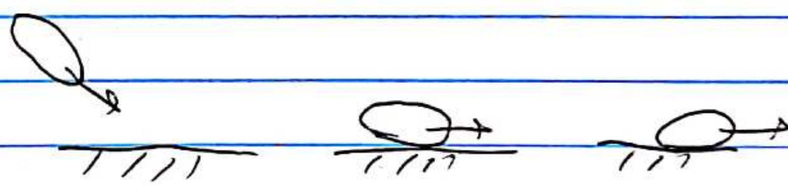
$\underline{U} = U(\cos\theta, \sin\theta)$

constant speed of swimming

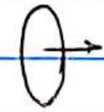
Trajectory A: moves down, encounters wall "constraint" keeps it from entering, but still has downward drift.

The swimmer must rotate ~~...~~ to horizontality.

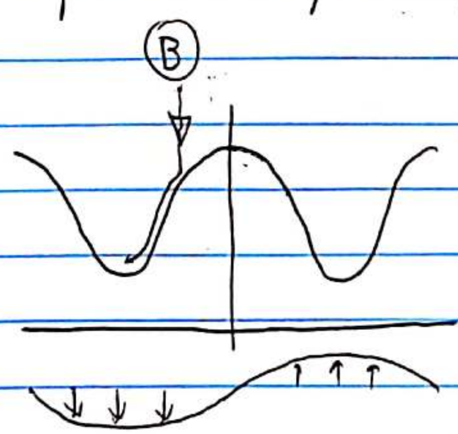
A.

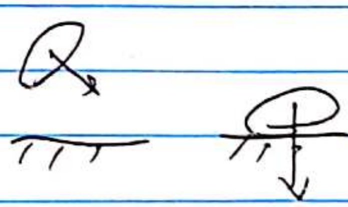


Depends on shape!



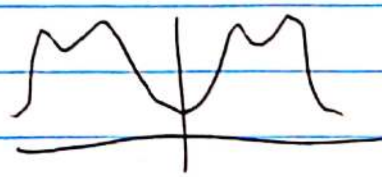
"prolate"



oops, stuck!

Some shapes have strange landscapes.



So what's the mathematical model?

spatial diffusion
Take $D_x = D_y$ for simplicity

ABP (Active Brownian Particle)

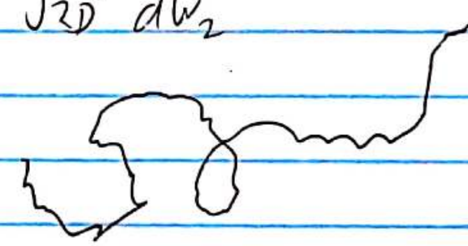
$$d\underline{X} = \underline{U}\,dt + \sqrt{2D}\,d\underline{W}_1$$

$$d\theta = \Omega\,dt + \sqrt{2D_r}\,dW_2$$

rotational diffusion
($1/\text{time}$)

$W_i(t)$ are Brownian motion.

Lab frame:
$$dx = U\cos\theta\,dt + \sqrt{2D}\,dW_1$$
$$dy = U\sin\theta\,dt + \sqrt{2D}\,dW_2$$



"Smoother" than Brownian motion.
Persistence length $U/D_r$.

(like some simple polymer models)

Because of boundaries, better to solve for probability density

$p(x,y,\theta,t)$ Fokker-Planck eq'n
(Smoluchowski)

$$\partial_t p + \nabla\cdot(\underline{U}p) + \partial_\theta(\Omega p) = D\nabla^2 p + D_r\partial_\theta^2 p$$

Flux form: ← probability flux

$$\partial_t p + \nabla \cdot \underline{f} = 0 \qquad \underline{f} = \underline{U} p + \Omega \hat{\theta} p$$

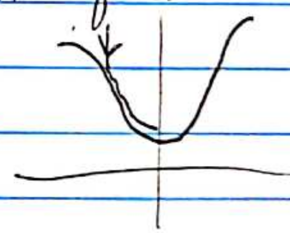
$$\text{in } \Omega \text{ (domain)} \qquad - D \nabla p - D_r \partial_\theta p \, \hat{\theta}$$

Now we can impose a natural, flux preserving BC:

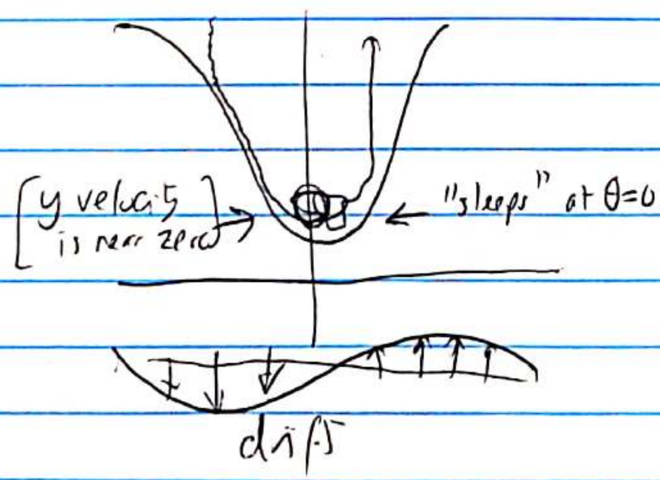
$$\underline{f} \cdot \hat{n} = 0 \quad \text{on } \partial\Omega \text{ (boundary of configuration space)}$$

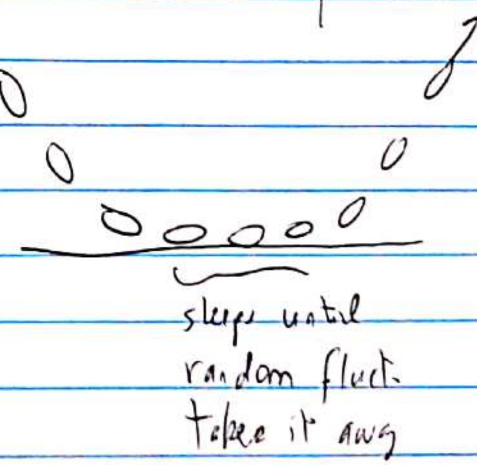
This is so that $\frac{d}{dt} \int_\Omega p \, dV = - \int_{\partial\Omega} \underline{f} \cdot d\underline{S} = 0$ Conservation of probability

At boundaries, the normal velocity is balanced by a diffusive flux. This gives the effect described before:



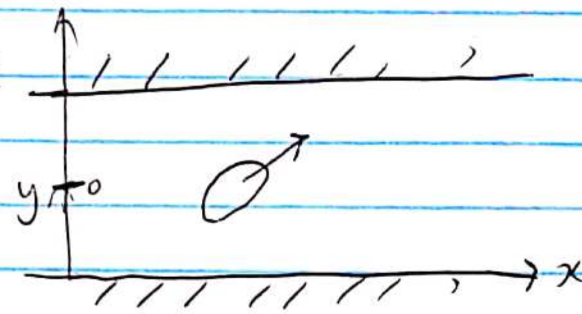
With noise, typical trajectory:



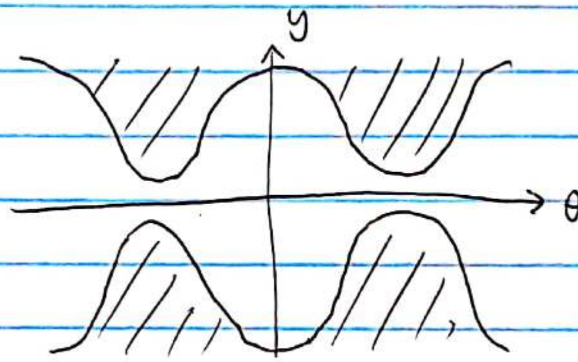
With this technology, we can complicate the domain.

Channel:




Swimmer bounces around between two parallel plane walls.

Configuration space:




In the small $D_r$ limit, we derived a "reduced equation" that allows us to derive quantities such as the invariant density of swimmers. They tend to cluster at walls but not always, depending on shape. Hydrodynamic interactions are also important but can be easily included.

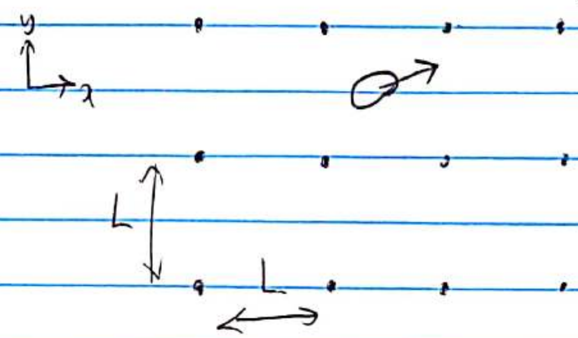
(Chen & Thiffeault, JFM, 2021)

Can also define configuration space for multiple particles. One point in that space is the location and orientation of all particles. Very complex! Topology not well understood.

(Volume of configuration space related to phase transitions.)

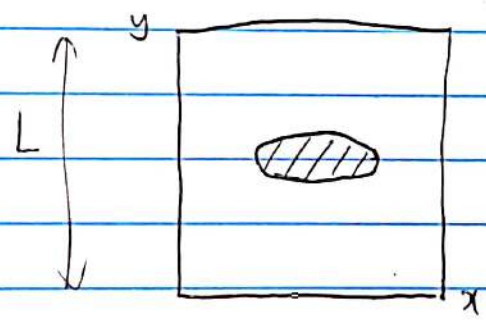
## Swimmer in a lattice:

← posts (fibers)




What's the configuration space?

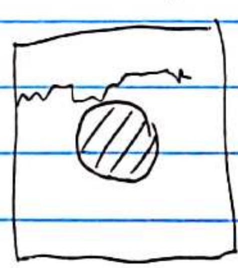
First consider a fixed orientation. We can imagine the lattice is moving around the swimmer.




Configuration space reproduces the shape of swimmer.

~~bi-periodic~~

We can already answer some interesting questions: a nonswimming particle will diffuse through a lattice of posts following exactly the same equation as heat conduction in a perforated domain, a problem solved by Rayleigh using a reflection method.

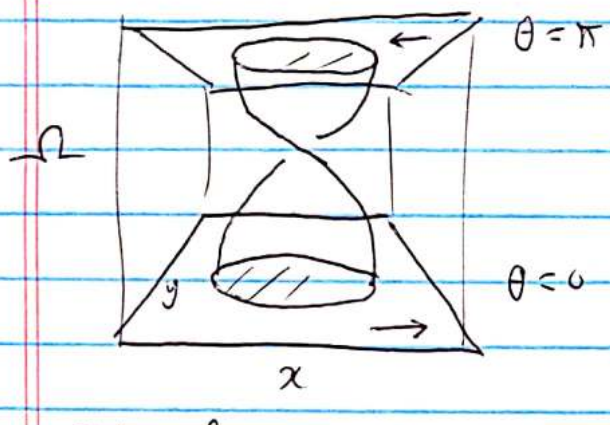


$$D_{eff} = \frac{D}{1+\phi}$$

$\phi$ = volume (area) fraction of swimmers (small)

for a circular particle.

This was for fixed orientation. If the angle changes randomly, need to include $\theta$:




Take the previous picture and twist it in $\theta$

3D periodic cell in $(x, y, \theta)$

Solve heat equation in $\Omega$, with a tubular obstacle $\partial\Omega$ that describes shape. $\underline{f} \cdot \hat{n} = 0$ on $\partial\Omega$

Adding a swimming velocity imposes a drift that can create boundary layers along the tubular obstacle.

Rayleigh's theory $(\underline{U} = 0)$, or tools from homogenization theory allow us to compute the transport coefficients in the lattice.

This is ongoing work with Hongfei Chen & Zihong Zhang.

<u>Some further work:</u> Full 3D, multiparticle, deformable particles and boundaries, computational methods, random environments, run-and-tumble dynamics...