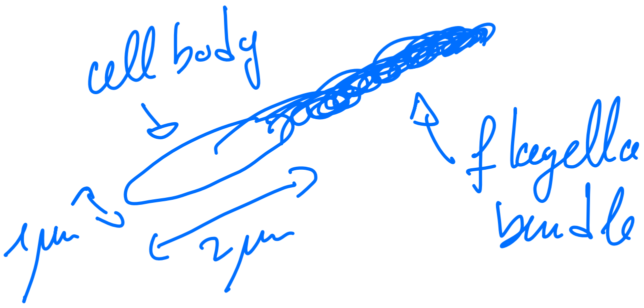
Chapter 8: Active Particles

8.1) Run and Tumble Particles (RTPs)

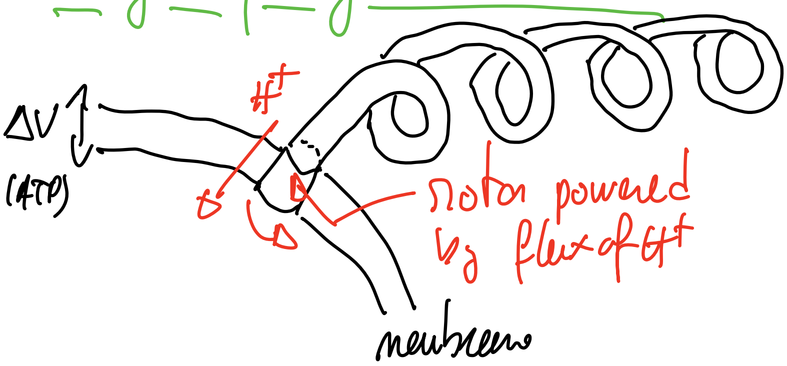
8.1.1) Runs



E. coli: 5-10 flagella

- More for other bacteria
- Sometimes 0 or 1 flagella
- Many other locomotion mode

Why do flagella rotate?



chiral flagella rotate

$\Downarrow$

hydrodynamic coupling between the flagella

$\Downarrow$

formation of a bundle

Rotation of the bundle $\Rightarrow$ forward swimming.

Q: why so complicated $\to$ zero Reynolds swimming

Navier-Stokes $\vec{v}(\vec{r},t)$

$$\rho D_t \vec{v} = \underbrace{\rho \partial_t \vec{v}}_{①} + \underbrace{\rho \vec{v}\cdot\vec{\nabla}\vec{v}}_{①'} = -\vec{\nabla} p + \vec{f}_{vol} + \underbrace{\rho \nu \Delta \vec{v}}_{②}$$

① & ①' $\Leftrightarrow$ inertial forces / terms

2 $\Leftrightarrow$ viscous force

If the flow has a typical scale L and speed U

$$\left.\begin{array}{l} 1 \sim 1' \sim \rho \dfrac{U^2}{L} \\ 2 \sim \rho \nu \dfrac{U}{L^2} \end{array}\right\} \quad \frac{1}{2} \sim \frac{UL}{\nu} \equiv \text{Reynold's number}$$

The Reynold's number measures the ratio between viscous and inertial forces.

Human:

$$\left.\begin{array}{l} L = 1\,m \\ U = 1\,m/s \\ \nu = 10^{-6}\,m^2/s \end{array}\right\} Re = 10^{6}$$

Bacteria:

$$\left.\begin{array}{l} L = 10^{-6}\,m \\ U = 10^{-5}\,\mu m/s \\ \nu = 10^{-6}\,m^2/s \end{array}\right\} Re = 10^{-5}$$

Inertia is 10^{11} times less important for swimming bacteria than for us.

Coasting length: length you travel after bringing the self propulsion force from f_0 to 0.

Human: 2-3 m $\Rightarrow$ Bacteria: 0,2-0,3 Å 1/10th water molecule.

How can I experience the Reynold's number of the bacteria:

$\Rightarrow$ swim in Honey $\nu \simeq 10^{-3}\,m^2/s$

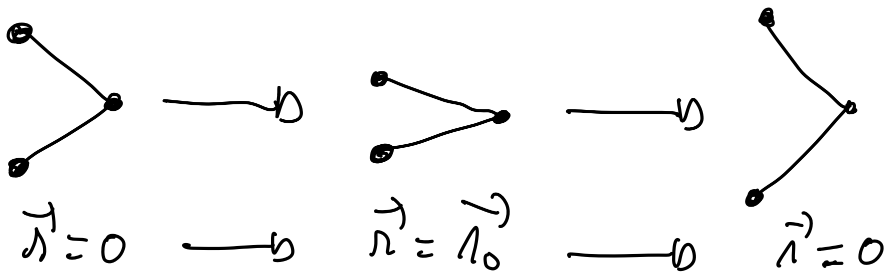
$\Rightarrow$ wait $\dfrac{U}{10^{-3}} = 10^{-5} \Rightarrow U = 10^{-8}\,m/s \Leftrightarrow 10^{-6}\,cm/s \Leftrightarrow \dfrac{1\,cm}{10\,days}$

[Life at low Reynold's, Purcell 1977, Am. J. Phys. 45, p3]

Comment: The flow around a swimming bacterium is given by Stokes equation $\Rightarrow$ this is a <u>reversible</u> equation

If a protocole $\{x_i(t)\}$ for the degrees of freedom of the bacteria lead to a flow $\vec{u}(t)$, then $\{x_i(t_f - t)\}$ leads to $-\vec{u}(t)$.

Reciprocal motion (protocole invariant by $t \to -t$) <u>cannot</u> lead to net motion.



<u>Formal proof</u>: Ishimoto & Yamada, arXiv: 1107.5938

You cannot swim at zero Reynolds using reciprocal motion (Scallop theorem).

$\to$ this is why the rotation of a chiral helix is used

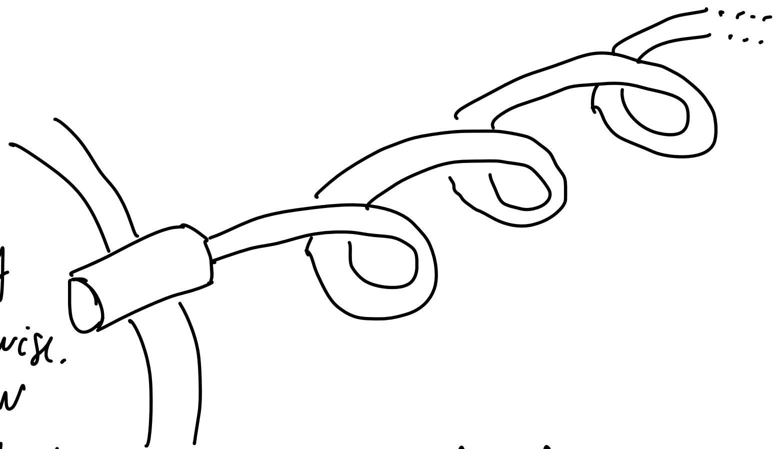
$\to$ non reciprocal under time reversal

This is the microscopic origin of the runs in quasi straight line.

rotation of the motor $\Rightarrow$ $O(\varepsilon)$ non-reciprocal $\to$ breaking TRS.

shape of the helix: $\dot{O}(\varepsilon)$ $\Rightarrow$ force along the axis of the helix. $\Rightarrow$ break L/R symmetry.

8.12) The tumble



* the rotor is spontaneously rotating counter clockwise. CCW
* protein CheY can bind to the rotor and change the direction of rotation to clock-wise rotation (CW).

$$\text{CheY}\ ,\ \overset{\text{Motor}}{\text{CCW}} \ \underset{\beta}{\overset{\alpha}{\rightleftharpoons}}\ \text{CheY-Motor}\ ,\ \text{CW}$$

* 1 flagellum rotating CW break the flagella bundle $\Rightarrow$ reorientation of the cell
* When CCW rotation resumes $\Rightarrow$ swimming in straight line resumes

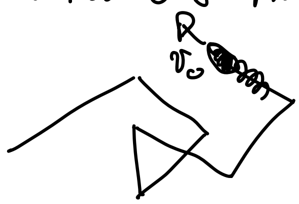
[E. coli in Motion, H. Berg]

Tumbles occur at rate $\alpha \simeq 1\,\text{Hz}$ for E. coli

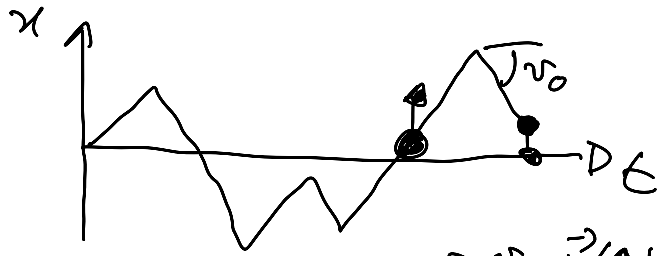
Swimming resumes at rate $\beta = 10\,\text{Hz}$

In practice we assume instantaneous tumbles.

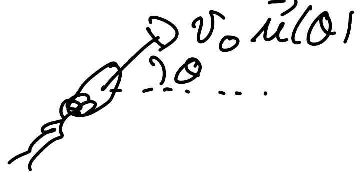
* Typical trajectories: 2D



8.1.3) Models



1D: $v_0 \vec{u}_x \xrightarrow{\alpha} -v_0 \vec{u}_x$



2D: $\dot{\vec{r}} = v_0 \vec{u}(\theta) + \sqrt{2D}\,\vec{\eta}$

$\theta \xrightarrow{\alpha} \theta'$ at rate α

$\vec{u}(\theta) = (\cos\theta, \sin\theta)$

$P(\theta') = \frac{1}{2\pi}$ (approximation)

$P(\vec{r},\theta;t)$ the probability density of finding the bacteria at position $\vec{r}$ and angle θ at time t.

Comment: θ is not the angle between $\vec{r}$ and $\vec{e}_x$

The dynamics is a mixture between a Langevin dynamics for $\vec{r}(t)$ in 2D and a Markov process in continuous space for the orientation.

$$\partial_t P(\vec{r},\theta;t) = \underbrace{-\frac{\partial}{\partial x}J_x - \frac{\partial}{\partial y}J_y}_{\text{represents } \dot{\vec{r}} = v_0\vec{u}(\theta)+\sqrt{2D}\vec{\eta}} \; \underbrace{-\alpha P(r,\theta,t)}_{\theta \xrightarrow{\alpha} \theta'} + \underbrace{\frac{\alpha}{2\pi}\int d\theta' P(r,\theta',t)}_{\theta' \xrightarrow{\alpha} \theta \;\&\; P(\theta)=\frac{1}{2\pi}}$$

$$= -\frac{\partial}{\partial x}\left[v_0\cos\theta\, P(\vec{r},\theta) - D\partial_x P\right] - \frac{\partial}{\partial y}\left[v_0\sin\theta\, P(\vec{r},\theta) - D\partial_y P\right] - \alpha P + \frac{\alpha}{2\pi}\int d\theta' P(\vec{r},\theta')$$

$$\partial_t P(\vec{r},\theta;t) = -\vec{\nabla}\cdot\Big[\underbrace{v_0\vec{u}(\theta)\, P(\vec{r},\theta)}_{\text{probability current due to swimming}} \underbrace{- D\vec{\nabla} P(\vec{r},\theta)}_{\text{contribution of diffusion}}\Big] \underbrace{-\alpha P + \frac{\alpha}{2\pi}\int d\theta' P(r,\theta')}_{\text{gain and loss terms due to tumbles in and out of } \theta.}$$

One-dimensional case:

Particles go to the right at speed v_R $\Leftrightarrow$ $\dot{x} = v_R$
——— left at ——— v_L $\Leftrightarrow$ $\dot{x} = -v_L$

Right-going particles pick a new direction at rate α_R
left ——— α_L

$R(x,t)$: proba density to find the particles at x & t going to the right
$L(x,t)$: ——— left

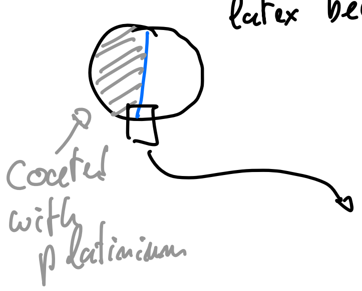
Master equation:

$$(1)\quad \partial_t R(x,t) = -\partial_x \cdot J_R - \frac{\alpha_R}{2} R(x,t) + \frac{\alpha_L}{2} L(x,t) = -\partial_x\left[v_R R(x,t)\right] - \frac{\alpha_R}{2}R + \frac{\alpha_L}{2} L$$

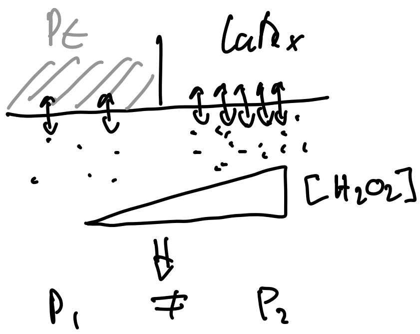
$$(2)\quad \partial_t L(x,t) = -\partial_x \cdot J_L - \frac{\alpha_L}{2} L(x,t) + \frac{\alpha_R}{2} R(x,t) = \partial_x\left[v_L L(x,t)\right] + \frac{\alpha_R}{2}R - \frac{\alpha_L}{2} L$$

8.2) Active Brownian Particles

8.2.1) Model self diffusiophoretic Janus colloids



$$H_2O_2 \xrightarrow{Pt} H_2O + \frac{1}{2} O_2$$



Interactions between bead and solute $\Leftrightarrow$ transfer of momentum
Gradient of interaction strength
$\Leftrightarrow$ gradient of pressure in the fluid
$\Rightarrow$ flow $\Rightarrow$ advect the particle
$\Rightarrow$ self-propulsion

Everything you may want to know can be found in the R. Golestanian lecture notes
[Golestanian, arxiv: 1909.03747]

In practice, many more ingredients (e.g. electrostatic interactions)
$\to$ hard to predict speed or even direction of self propulsion

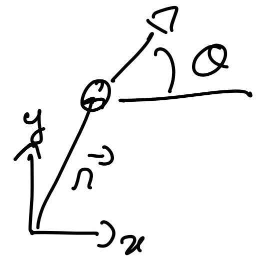
Philosophically: . chemical reaction break time-reversal symmetry
. Asymmetric coating break parity $(x \to -x)$
$\Big\} \Rightarrow$ ratchet.

Experimental reference

Latex / Pt : [Palacci et al, PRL 2010]

Au / Pt : [Theurkauff et al, PRL 2012]

8.2.2) The model



2D $\quad \dot{\vec{r}} = v_0 \vec{u}(\theta) + \sqrt{2D_t}\,\vec{\eta} \quad (1)$

$\vec{u}(\theta) = (\cos\theta, \sin\theta)$

rotational diffusion $\quad \dot{\theta} = \sqrt{2D_r}\,\xi \quad (2)$

η_x, η_y and ξ are three Gaussian white noises.

$P(\vec{r},\theta) = P(x,y,\theta)$ the probability to find the particle at x,y going in the direction θ at time t. (1)&(2) are Langevin dynamics $\Rightarrow$ dynamics of $P(\vec{r},t)$ is a Fokker-Planck equation.

$$\partial_t P(x,y,\theta) = -\frac{\partial}{\partial x} J_x - \frac{\partial}{\partial y} J_y - \frac{\partial}{\partial \theta} J_\theta$$

$$= -\frac{\partial}{\partial x}\left[v_0 \cos\theta\, P - \frac{\partial}{\partial x}(D_t P)\right] - \frac{\partial}{\partial y}\left[v_0 \sin\theta\, P - \frac{\partial}{\partial y}(D_t P)\right] + \frac{\partial^2}{\partial \theta^2}(D_r P)$$

$$\boxed{\partial_t P(x,y,\theta) = -\vec{\nabla}\cdot\Big[\underbrace{v_0\, \vec{u}(\theta)\, P - \vec{\nabla}(D_t P)}_{\text{Probability current in } \vec{r} \text{ space}}\Big] - \frac{\partial}{\partial \theta}\Big[\underbrace{-\frac{\partial}{\partial \theta} D_r P}_{\text{proba current in } \theta\text{-space}}\Big]}$$

Comment: If D_t and D_r have as an origin the collision of the particle with an equilibrated fluid, they will be related. If D_r has an active origin, they need not be.

8.3 The relevant scales of active dynamics

8.3.1) The persistence time

Active particle starts with some orientation $\vec{u}_0$.
For how long does $\vec{u}(t)$ remains correlated to $\vec{u}_0$?

Run and tumble particles in 2D:

$$\frac{d}{dt}\langle \vec{u}(\theta(t)) \cdot \vec{u}(0)\rangle = \frac{d}{dt}\langle \vec{u}(\theta(t))\rangle \cdot \vec{u}(0)$$

$$= \frac{d}{dt}\int d^2\vec{r}\, d\theta\; P(\vec{r},\theta,t)\, \vec{u}(\theta)\cdot\vec{u}(0)$$

$$= \int d^2\vec{r}\, d\theta\; \frac{dP}{dt}\; \vec{u}(\theta)\cdot\vec{u}(0)$$

$$\frac{dP}{dt} = \underbrace{-\nabla_{\vec{r}}\cdot\left[v_p \vec{u}(\theta) P\right]}_{\int d^2\vec{r}\,[\dots]=0 \text{ since } P \xrightarrow[\vec{r}\to\infty]{} 0} - \alpha P + \frac{\alpha}{2\pi}\rho(\vec{r})\,; \quad \rho(\vec{r}) = \int d\theta\, P(\vec{r},\theta)$$

$\rho(\vec{r})$ term $\Rightarrow \int d\theta\, \rho(\vec{r})\,\vec{u}(\theta) = 0$ (symmetry)

$$\Rightarrow \frac{d}{dt}\langle \vec{u}(\theta(t))\cdot\vec{u}(\theta_0)\rangle = -\alpha\int d^2r\, d\theta\, P(\vec{r},\theta,t)\,\vec{u}(\theta)\cdot\vec{u}(\theta_0)$$

$$= -\alpha\langle \vec{u}(\theta(t))\cdot\vec{u}(\theta_0)\rangle$$

$$\Rightarrow \langle \vec{u}(\theta(t))\cdot\vec{u}(\theta_0)\rangle = \langle \vec{u}^{\,2}(\theta_0)\rangle e^{-\alpha t}$$

$$= e^{-\alpha t}$$

RTPs forget their orientation after a typical time $\tau = \frac{1}{\alpha}$

Active Brownian Particles

2D: $\dot{\theta} = \sqrt{2D_r}\,\xi$ Itô formula $\frac{d}{dt}\vec{u}(\theta(t)) = \frac{d\vec{u}}{d\theta}\dot{\theta} + D_r \frac{d^2\vec{u}}{d\theta^2}$

$\vec{u} = (\cos\theta, \sin\theta) \Rightarrow \frac{d\vec{u}}{d\theta} = (-\sin\theta, \cos\theta) \equiv \vec{u}^{\perp}(\theta) \Rightarrow \frac{d^2\vec{u}}{d\theta^2} = -\vec{u}$

$\Rightarrow \frac{d}{dt}\vec{u} = \vec{u}^{\perp}\sqrt{2D_r}\,\xi - D_r\vec{u}$

$\frac{d}{dt}\langle\vec{u}\rangle \overset{\text{Itô}}{=} 0 - D_r\langle\vec{u}\rangle$ since $\langle\vec{u}^{\perp}(\theta(t))\,\xi(t)\rangle \overset{\text{Itô}}{=} \langle\vec{u}^{\perp}(\theta(t))\rangle \times \underbrace{\langle\xi(t)\rangle}_{=0}$

Again $\langle\vec{u}(\theta(t))\rangle = e^{-t/\tau}\langle\vec{u}(\theta_0)\rangle$

Here $\tau = \frac{1}{D_r}$ ([rotational diffusivity] $= T^{-1}$)

d dimension: Same path as RTPs & $\Delta_{\vec{u}}\vec{u} = -(d-1)\vec{u}$

leads to $\tau = \frac{1}{(d-1)D_r}$

8.3.2) Persistence length

$\dot{\vec{r}} = \vec{v}_p(t)$ with $\vec{v}_p = v_p\,\vec{u}(\theta)$ & $v_p \in \mathbb{R}^+$ for ABPs, RTPs

$$\vec{r}(t) - \vec{r}(0) = \int_0^t ds\, \vec{v}_p(s)$$

$$\langle\vec{r}(t) - \vec{r}(0)\rangle = \int_0^t ds\,\langle\vec{v}_p(s)\rangle = \int_0^t ds\, e^{-t/\tau}\langle\vec{v}_p(0)\rangle$$

$$= \langle\vec{v}_p(0)\rangle \cdot \left[-\tau e^{-s/\tau}\right]_0^t$$

$$= \langle\vec{v}_p(0)\rangle\tau(1 - e^{-t/\tau})$$