

Detailed balance for Markov processes.

(1)

Rates level $W(q \rightarrow q') P(q) = W(q' \rightarrow q) P(q')$

Trajectory level

$$P\{q(t_f)\} = P(q_i) \prod_{i=r}^{N-1} n(q_i) e^{-\epsilon_i - \epsilon_{i+1}} \alpha(q_i) w(q_i \rightarrow q_{i+1}) \times e^{-(\epsilon_N - \epsilon_{N+1})} \alpha(q_N)$$
$$= P(q_i^n = q_N) \prod_{i=r}^N n(q_i^n = \epsilon_{N+1-i}) e^{-\epsilon_i^n - \epsilon_{i+1}^n} \ln(q_i^n) \times e^{-(\epsilon_N^n - \epsilon_{N+1}^n)} n(q_N^n)$$

using $|\epsilon_i^n - \epsilon_{i+1}^n| = |\epsilon_{N-i} - \epsilon_{N-i+1}|$

Comments If we sum over all possible trajectories between q_i & q_N , we find

$$P_{ss}(q_i, t_0) P(q_N, t_f | q_i, t_0) = P_{ss}(q_N, t_f) P(q_i, t_f | q_N, 0)$$

5.3) At the Transition matrix level

Vector $|P(\epsilon)|$ of dimension cardinal $\{q\}$ whose i^{th} component is

$$P_i(\epsilon) \equiv P(q_i, \epsilon) \equiv P_{q_i}(\epsilon)$$

Master equation:

$$\frac{\partial}{\partial \epsilon} P(q, \epsilon) = \sum_{q' \neq q} W(q' \rightarrow q) P(q', \epsilon) - \left[\sum_{q' \neq q} W(q \rightarrow q') \right] P(q, \epsilon)$$

$$\Leftrightarrow \frac{\partial}{\partial \epsilon} P_q = \sum_{q'} M_{qq'} P_{q'} \quad \text{with} \quad M_{qq} = - \sum_{q' \neq q} W(q \rightarrow q')$$

$$\text{and} \quad M_{qq'} = W(q' \rightarrow q) \quad \text{if} \quad q' \neq q$$

$\Rightarrow \frac{\partial}{\partial \epsilon} |P\rangle = M |P\rangle \Rightarrow$ like a Fokker-Planck equation in finite dimension.

Detailed balance

$$\forall q \neq q', P(q) W(q \rightarrow q') = P(q') W(q' \rightarrow q)$$

$$\Leftrightarrow M_{q'q} P_q = M_{qq'} P_{q'} \Leftrightarrow M_{q'q} = P_q^{-1} M_{qq'} P_{q'}$$

$$\Leftrightarrow M_{qq'}^+ = P_q^{-1} M_{qq'} P_{q'} \quad (**)$$

Let's define $P = \text{diag}(P_q)$, then $(**)$ can be rewritten as

$$M^+ = P^{-1} M P \quad (\Leftrightarrow H^+ = P^{-1} H P)$$

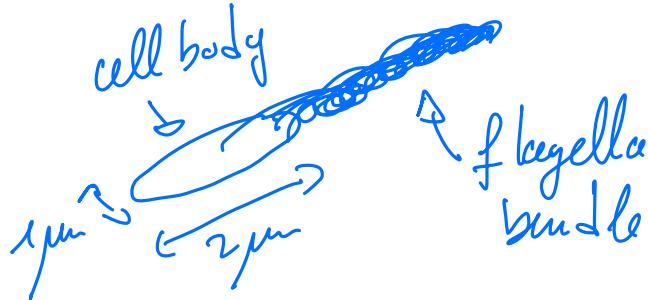
Similarly: $M^H = P^{-1/2} M P^{1/2}$ is hermitian \Rightarrow diagonalizable with real eigenvalues in an orthonormal basis.

$\Rightarrow M$ is diagonalizable, with real eigenvalues, but not in an orthonormal basis.

Chapter 8 : Active Particles

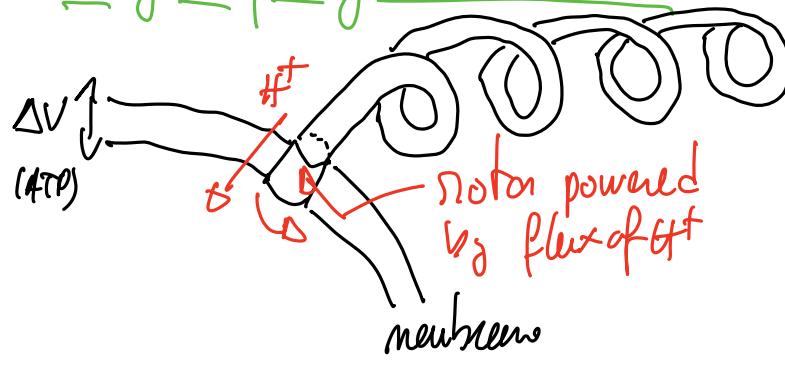
8.1) Run and Tumble Particles (RTPs)

8.1.1) Runs



E. coli : 5-10 flagella
 Many for other bacteria
 - Sometimes 0 or 1 flagella
 Many other locomotion mode

Why do flagella rotate?



→ chiral flagella rotates

hydrodynamic coupling
between the flagella
formation of a bundle

Rotation of the bundle \Rightarrow forward swimming.

Q: why so complicated \rightarrow zero Reynolds swimming

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

$$\rho \frac{D}{Dt} \vec{v} = \underbrace{\rho \partial_t \vec{v}}_{(1)} + \underbrace{\rho \vec{v} \cdot \vec{\nabla} \vec{v}}_{(1')} = -\vec{\nabla} p + \vec{f}_{\text{vol}} + \underbrace{\rho \partial \Delta \vec{v}}_{(2)}$$

(1) & (1') \Leftrightarrow inertial forces/terms

② \leftrightarrow viscous force

If the flow has a typical scale L and speed U

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

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

Human:

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

Bacteria:

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

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 \AA $\ell/10^6$ water molecule.

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

\rightarrow swim in Honey $D \approx 10^{-3} \text{ m}^2/\text{s}$

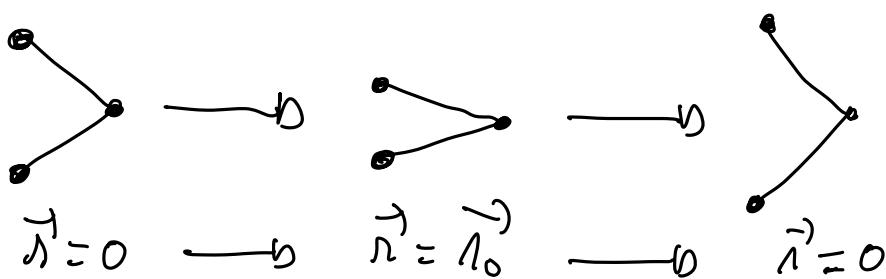
\rightarrow wait $\frac{U}{10^{-3}} = 10^{-5} \Rightarrow U = 10^{-8} \text{ m/s} \Leftrightarrow 10^{-6} \text{ cm/s} \Leftrightarrow \frac{1 \text{ cm}}{10 \text{ days}}$

[life at low Reynolds', Purcell 1977, Am. J. Phys. 45, p3] (5)

Comment: The flow around a swimming bacterium is given by Stokes equation \Rightarrow this is a reversible equation

If a protocol $\{x_i(t)\}$ 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 (protocol invariant by $t \rightarrow -t$) cannot lead to net motion.



Formal proof: Ishimoto & Yamada, arXiv: 1107.5938

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

\rightarrow this is why the rotation of a chiral helix is used
 \rightarrow non reciprocal under time reversal

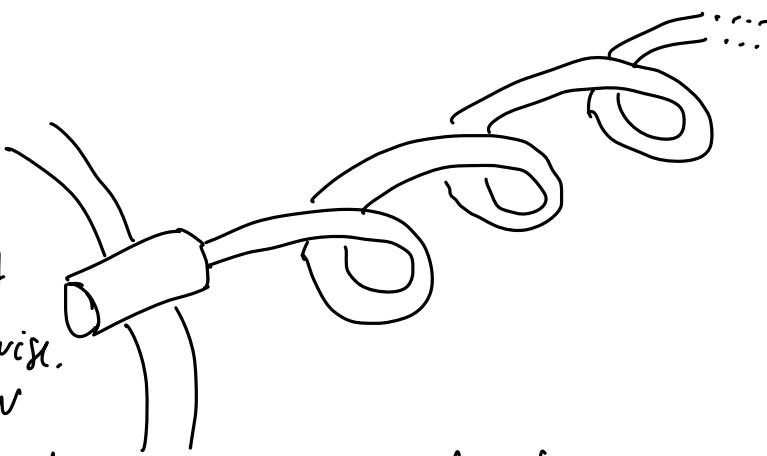
This is the microscopic origin of the runs in quasi straight line.

rotation of the motor $\Rightarrow \mathcal{O}(E)$ non-reciprocal \Rightarrow breaking TRS.

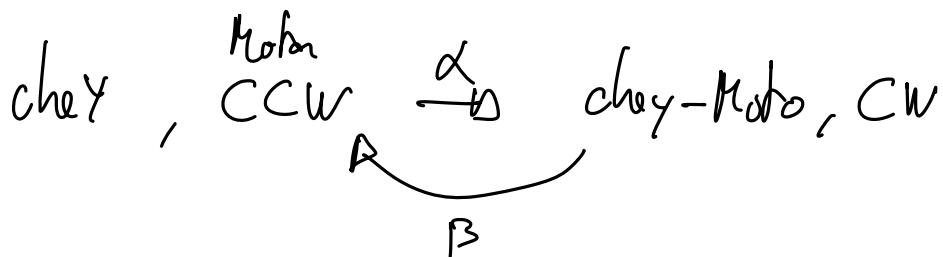
shape of the helix: $\mathcal{O}(E) \Rightarrow$ face along the axis of the helix. \Rightarrow break L/R symmetry.

8.12 The tumble

⑥



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



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

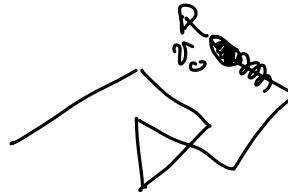
[E. coli in Motion, H. Berg]

Tumbles occur at rate $\alpha = 1/t_0$ for E. coli

Swimming resumes at rate $\beta = 10/t_0$

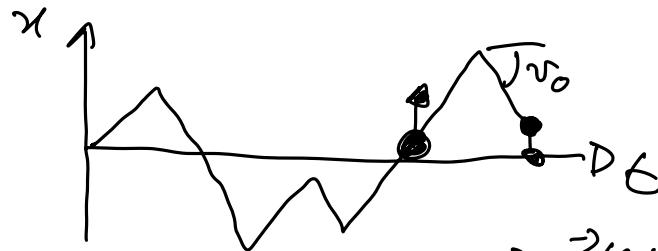
In practice we assume instantaneous tumbles.

- * Typical trajectories: 2D

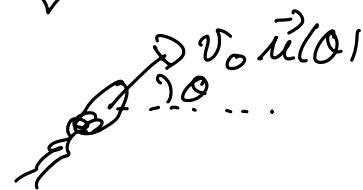


8.1.3) Models

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



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



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

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

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

$P(\vec{r}, \theta; t)$ 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.

$$\frac{\partial}{\partial t} P(\vec{r}, \theta; t) = - \frac{\partial}{\partial x} J_x - \frac{\partial}{\partial y} J_y - \alpha P(\vec{r}, \theta, t) + \frac{\alpha}{2\pi} \int d\theta' P(\vec{r}, \theta', t)$$

represents $\vec{r} = v_0 \vec{u}(\theta) + \sqrt{2D} \vec{z}$ $\theta \xrightarrow{\alpha} \theta'$ $\theta' \xrightarrow{\alpha} \theta$ $P(\theta') = \frac{1}{2\pi}$

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

$$\frac{\partial}{\partial t} P(\vec{r}, \theta; t) = - \vec{\nabla} \cdot \left[v_0 \vec{u}(\theta) P(\vec{r}, \theta) - D \vec{\nabla} P \right] - \alpha P + \frac{\alpha}{2\pi} \int d\theta' P(\vec{r}, \theta')$$

probability current due to swimming $\xrightarrow{\text{contribution of diffusion}}$ gain & loss due to tumbles in and out of θ .

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

$L(x, t)$: α_L left

Master equation:

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

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