

Detailed balance for Markov processes.

(1)

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

Trajectory level

$$P(\{q(t)\}) = P(q_1) \prod_{i=1}^{N-1} \Omega(q_i) e^{-|t_i - t_{i-1}| \Omega(q_i)} W(q_i \rightarrow q_{i+1}) \times e^{-|t_N - t_{N-1}| \Omega(q_N)}$$
$$= P(q_1^N = q_N) \prod_{i=1}^N \Omega(q_i^N = q_{N+1-i}) e^{-|t_i^N - t_{i-1}^N| \Omega(q_i^N)} \times e^{-|t_N^N - t_{N-1}^N| \Omega(q_N^N)}$$

using  $|t_i^N - t_{i-1}^N| = |t_{N-i} - t_{N-i+1}|$

Comments If we sum over all possible trajectories between  $q_1$  &  $q_N$ , we find

$$P_S(q_1, t_0) P(q_N, t_f | q_1, t_0) = P_S(q_N, t_f) P(q_1, t_f | q_N, t_0)$$

### 5.3) At the transition matrix level

Vector  $|P(t)\rangle$  of dimension cardinal  $\{\Omega(q)\}$  whose  $i^{\text{th}}$  component is

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

Master equation:

$$\partial_t P(q, t) = \sum_{q' \neq q} W(q' \rightarrow q) P(q', t) - \left[ \sum_{q' \neq q} W(q \rightarrow q') \right] P(q, t)$$

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

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

$\Rightarrow \partial_t |P\rangle = M |P\rangle \Rightarrow$  like a Fokker-Planck equation in finite dimension.

## Detailed balance

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

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

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

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

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

Similarly:  $M^{\dagger} = P^{-1/2} M P^{1/2}$  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



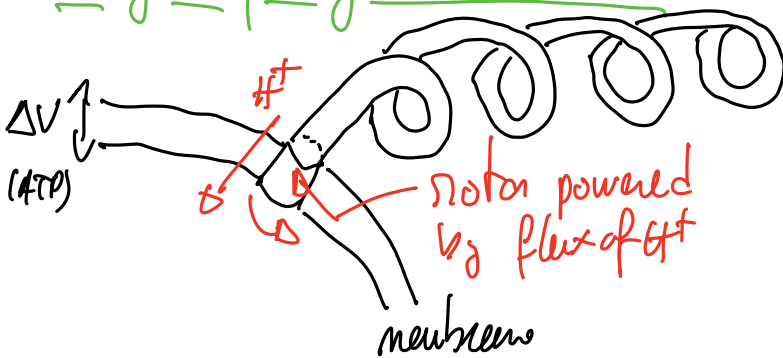
E. coli : 5-10 flagella

More for other bacteria

Sometimes 0 or 1 flagella

Many other locomotion mode

### Why do flagella rotate?



drinal 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  $\vec{v}(\vec{x}, t)$

$$\rho \frac{D \vec{v}}{D t} = \underbrace{\rho \partial_t \vec{v}}_{(1)} + \underbrace{\rho \vec{v} \cdot \nabla \vec{v}}_{(1')} = -\nabla p + \underbrace{\vec{f}_{vol}}_{(2)} + \underbrace{\rho \nabla^2 \vec{v}}_{(2)}$$

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

②  $\leftrightarrow$  viscous force

If the flow has a typical scale  $L$  and speed  $U$

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

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

Human:

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

Bacteria:

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

Inertia is  $10^6$  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  $\mu\text{m}$   $\approx$  1/10th water molecule.

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

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

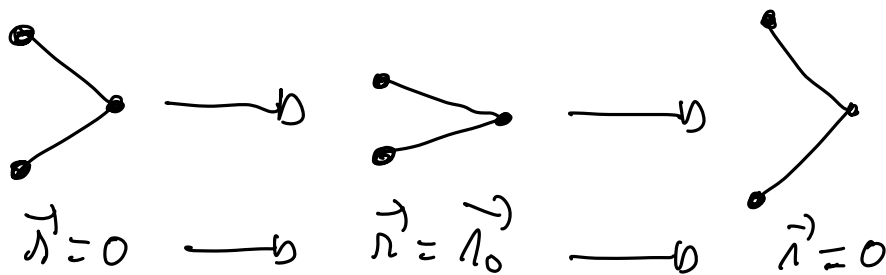
$\rightarrow$  wait  $\frac{U}{10^{-3}} = 10^{-5} \Rightarrow U = 10^{-8} \text{ m/s} \approx 10^{-6} \text{ cm/s} \approx \frac{1 \text{ cm}}{10 \text{ days}}$

[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 sequence of flags of the bacterium 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 & Yanada, 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.

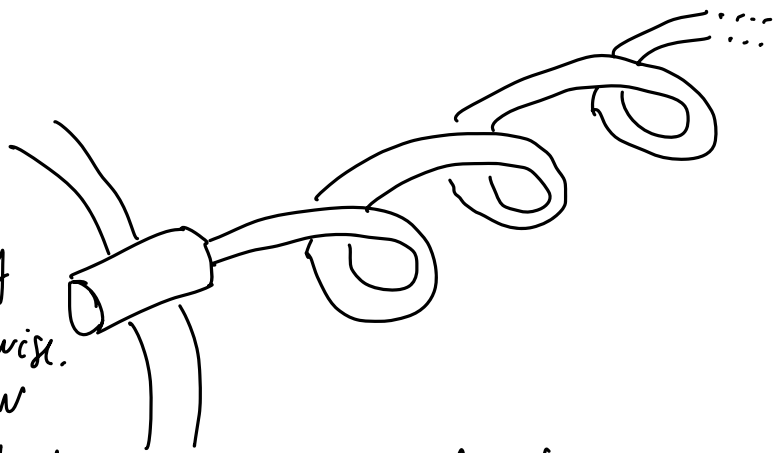
rotation of the motor  $\Rightarrow O(\epsilon)$  non-reciprocal  $\Rightarrow$  breaking TRS.

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

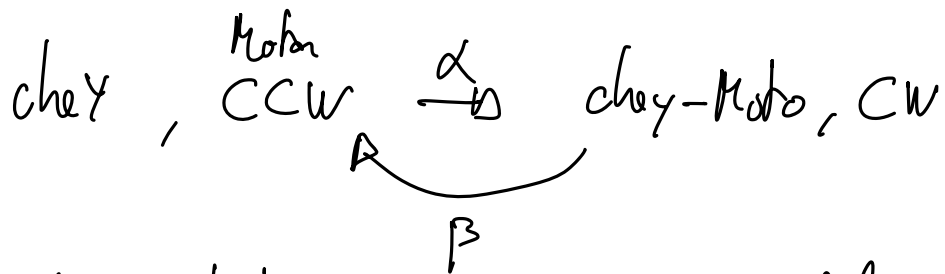
## 8.12 \ The tumble

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- \* the motor is spontaneously rotating counter clockwise. CCW



- \* protein CheY can bind to the motor and change the direction of rotation to clockwise rotation (CW).



- \* If 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  $\alpha \approx 1 \text{ Hz}$  for E. coli

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

In practice we assume instantaneous tumbles.

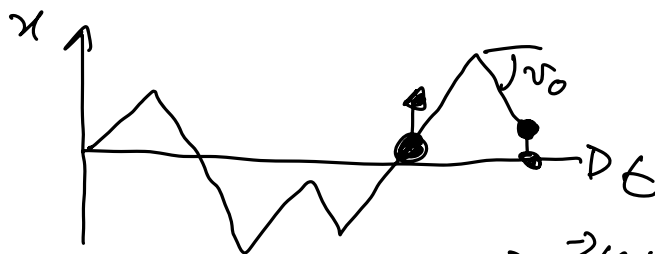
- \* Typical trajectories: 2D



# 8.1.3) Models

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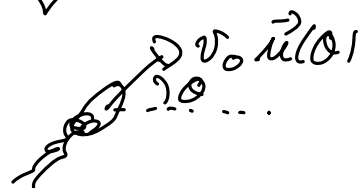
1D:  $v_0 \vec{\mu}_x \xrightarrow{\alpha} -v_0 \vec{\mu}_x$



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

$\theta \rightarrow \theta'$  at rate  $\alpha$

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



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

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

Comment:  $\theta$  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.

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

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

$$\frac{\partial}{\partial t} P(\vec{r}, \theta; t) = - \vec{\nabla} \cdot \left[ \underbrace{v_0 \vec{\mu}(\theta) P(\vec{r}, \theta)}_{\text{probability current due to swimming}} - \underbrace{D \vec{\nabla} P(\vec{r}, \theta)}_{\text{contribution of diffusion}} \right] - \alpha P + \frac{\alpha}{2\pi} \int d\theta' P(\vec{r}, \theta')$$

probability current due to swimming

contribution of diffusion

gain/loss terms due to tumbles in and out of  $\theta$ .

## One-dimensional case:

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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  $\alpha_R$

left  $\alpha_L$

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

$L(x, t)$ : left

Master equation:

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

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