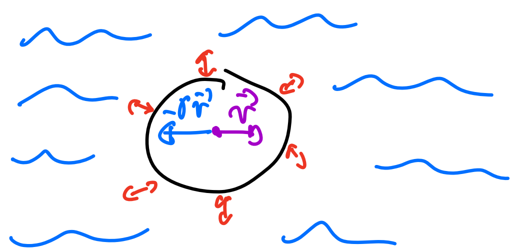
Chapter I: Active Matter at the microscopic scale

1. From passive to active particles

1.1 Energetics of passive particles

Schematic of colloid in fluid



Dynamics

$$\dot{\vec{r}} = \vec{v}\,; \qquad m\dot{\vec{v}} = -\vec{\nabla} V - \gamma \vec{v} + \sqrt{2\gamma k_B T}\,\vec{\eta}$$

average force exerted by fluid

↳ fluctuations around the mean. Assumed Gaussian.

Energetics $E = E_k + E_p = \frac{1}{2} m \vec{v}^2 + V(\vec{r}, \lambda(t))$

controlled externally e.g. amplitude of optical trap.

$$\frac{dE_p}{dt} = \sum_i \frac{\partial V(\vec{r})}{\partial x_i} \dot{x}_i + \frac{\partial V}{\partial \lambda} \dot{\lambda} = \vec{\nabla} V \cdot \vec{v} + \dot{\lambda} \frac{\partial V}{\partial \lambda}$$

$\frac{dE_k}{dt} = ?$ $\quad E_c(v(t))$

↳ stochastic, irregular variable (C^0 but not differentiable)

Itō formula: $\frac{d}{dt} f(v(t)) = ?$ (1d for simplicity)

Time increments in $[t, t+dt)$

- $d\eta = \int_0^{dt} \eta(s)\,ds \qquad \langle d\eta \rangle = 0\,; \quad \langle d\eta^2 \rangle = \int_0^t ds \int_0^t du \underbrace{\langle \eta(s)\eta(u) \rangle}_{\delta(s-u)} = dt$
- $dv = v(t+dt) - v(t) = \int_0^t ds\, \dot{v}(s)$

Taylor-expand $f(v)$ and keep terms to order dt:

$$f(v(t+dt)) - f(v(t)) = \sum_{k=1}^{\infty} \frac{dv^k}{k!} f^{(k)}(v(t)) = dv\, f'(v) + \frac{1}{2} dv^2 f''(v(t)) + o(dv^2)$$

① $dv \simeq \dot{v}(t)dt + o(dt)$

② $dv^2 = \left(-\frac{1}{m}\partial_x V\, dt - \frac{\gamma v}{m}dt + \frac{\sqrt{2\gamma kT}}{m}d\eta\right)^2$

$= 2\gamma kT\, d\eta^2 + o(dt)$

$d\eta^2 = \langle d\eta^2\rangle + B$ where $B = d\ ^2 - \langle d\eta^2\rangle$

All moments of B are $= 0 + o(dt) \Rightarrow d\eta^2 = \langle d\eta^2\rangle + o(dt)$
$= dt + o(dt)$

$\Rightarrow \frac{d}{dt} f(v(t)) = f'(v)\,\dot{v} + \frac{\gamma kT}{m^2} f''(v)$

Application to $E_c = \frac{1}{2}m\vec{v}^2$

$$\frac{dE_c}{dt} = \sum_i \left[\frac{\partial}{\partial v_i}\left(\frac{1}{2}m\vec{v}^2\right).\dot{v}_i + \frac{\gamma kT m}{m^2}\right]$$

$$= \vec{v}.m\dot{\vec{v}} + d\frac{\gamma kT}{m}$$

$$= \left(-\vec{\partial}V - \gamma\vec{v} + \sqrt{2\gamma kT}\,\vec{\eta}\right).\vec{v} + d\frac{\gamma kT}{m}$$

$$\frac{d}{dt}E_c(v(t)) = -\vec{v}.\vec{\partial}V + \vec{v}.\left[-\gamma\vec{v} + \sqrt{2\gamma kT}\,\vec{\eta}\right] + d\frac{\gamma kT}{m}$$

$$\frac{dE_{tot}}{dt} = \underbrace{-\gamma\vec{v}^2 + d\frac{\gamma kT}{m} + \sqrt{2\gamma kT}\,\vec{\eta}.\vec{v}}_{-\frac{dQ}{dt}} + \underbrace{\dot{\lambda}\frac{\partial V}{\partial\lambda}}_{\frac{dW}{dt}}$$

Comments:

* Q: heat released in the thermostat

$-\gamma\vec{v}^2 < 0 \Rightarrow$ dissipation
$d\frac{\gamma kT}{m} > 0 \Rightarrow$ injection of NRG
$\sqrt{2\gamma kT}\,\vec{\eta}.\vec{v} \Rightarrow$ fluctuations

} power injected by the fluid / dissipated

* W: work injected in the system by the operator.

$\dot{\lambda}\frac{\partial V}{\partial\lambda}$: power injected by operator when changing $\lambda(t)$

* If $\lambda(t) \in \mathbb{R}$ (i.e. is a constant), $V(\vec{r})$ does not enter $\frac{d}{dt} E_{tot}(\vec{r}(t), \vec{v}(t)) \Rightarrow \vec{\nabla} V$ is then a conservative force.

Equipartition: $\dot{\lambda} = 0$; steady state.

$$\frac{d}{dt} \left\langle \frac{dE_{tot}}{dt} \right\rangle = 0 = -\gamma \langle v^2 \rangle + d\frac{\gamma k T}{m}$$

$$\Rightarrow \left\langle \frac{1}{2} m v^2 \right\rangle = \langle E_c \rangle = d\frac{kT}{2}$$

1.2) Green-Kubo relation and fluctuation-dissipation theorem

Green-Kubo and diffusivity

Let's characterise the stochastic motion of $\vec{r}(t)$ without external potential, starting from $\vec{r}(t) = \vec{v}(t) = 0$.

① $\langle \vec{r}(t) \rangle = \langle \vec{v}(t) \rangle = 0$

② Fluctuations? MSD $\langle \vec{r}^{\,2}(t) \rangle = ?$

Two strategies:

. $\vec{v}(t) = \vec{v}_0 e^{-\frac{\gamma t}{m}} + \int_0^t ds\, e^{-\frac{\gamma}{m}(t-s)} \frac{\sqrt{2\gamma k T}}{m} \vec{\eta}(s)$; $r(t) = \int_0^t du\, v(u)$

$$\Rightarrow \langle r(t)^2 \rangle = \int_0^t du \int_0^t ds \, \langle v(u) v(s) \rangle$$

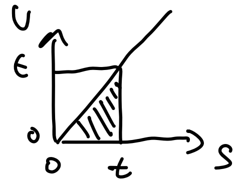
$\rightarrow$ 4 integrals $\rightarrow$ long & painful

. alternative: Green-Kubo formula

Goal: compute $D = \lim_{t \to \infty} \frac{1}{2dt} \langle (\vec{r}(t) - \vec{r}(0))^2 \rangle$

Start from $\vec{r}(t) - \vec{r}(0) = \int_0^t ds\, \vec{v}(s)$ and $C_v(s-u) \equiv \langle \vec{v}(s) \cdot \vec{v}(u) \rangle$
$= C_v(u-s)$

$$\left\langle \frac{|\vec{r}(t)-\vec{r}(0)|^2}{2dt} \right\rangle = \frac{1}{2dt}\int_0^t ds \int_0^t du \, \langle \vec{v}(s)\cdot\vec{v}(u)\rangle$$



$$= \frac{1}{dt}\int_0^t ds \int_0^s du \; C_v(\underbrace{s-u}_{r})$$

$$= \frac{1}{dt}\int_0^t ds \underbrace{\int_0^s dr \; C_v(r)}_{g(s)} = \frac{1}{dt}\int_0^t ds \; g(s)\times 1$$

$$\overset{IBP}{=} \frac{1}{dt}\left\{ \left[s\, g(s)\right]_0^t - \int_0^t ds \; s\, C_v(s)\right\}$$

$$= \frac{1}{dt}\left\{ t\int_0^t ds \; C_v(s) - \int_0^t ds \; s\, C_v(s)\right\}$$

$$= \frac{1}{d}\int_0^t ds \; C_v(s)\left(1-\frac{s}{t}\right)$$

Note that $C_v(s) \xrightarrow[s\to\infty]{} 0$ typically as $e^{-*\cdot s}$ $\Rightarrow \lim_{t\to\infty} \frac{1}{t}\int_0^t ds \, C_v(s)\, s = 0$

$$\lim_{t\to\infty} \left\langle \frac{(\vec{r}(t)-\vec{r}(0))^2}{2dt} \right\rangle = \boxed{\frac{1}{d}\int_0^\infty ds \langle \vec{v}(s)\cdot\vec{v}(0)\rangle = D}$$

This is an example of Green-Kubo formula which relates transport parameters, here D, to correlation functions.

Application to an Brownian colloids

$$\vec{v}(s)\cdot\vec{v}(0) = \vec{v}(0)^2 e^{-\frac{\gamma}{m}s} + \int_0^s du \; e^{-\frac{\gamma}{m}(s-u)} \, \vec{\eta}(u)\cdot\vec{v}(0)$$

$$\langle \vec{v}(s)\cdot\vec{v}(0)\rangle = \underbrace{\langle \vec{v}(0)^2\rangle}_{d\frac{kT}{m}} e^{-\frac{\gamma}{m}s} + 0$$

$$D = \frac{1}{d}\,\frac{d\,kT}{m}\underbrace{\int_0^\infty ds\; e^{-\frac{\gamma}{m}s}}_{\frac{m}{\gamma}} = \frac{kT}{\gamma} = \mu\, kT \quad \text{where } \mu = \gamma^{-1}$$

$D = \mu k T$ is the fluctuation dissipation relation

Comment: μ is called the mobility of the particle. It is a response coefficient. Applying a constant force $\vec{F}$ leads to

$$m\dot{\vec{v}} = -\gamma\vec{v} + \vec{F}$$

In steady state $\langle\dot{\vec{v}}\rangle = 0$ so that $\langle\vec{v}\rangle = \frac{1}{\gamma}\vec{F} = \mu\vec{F}$

μ measures how fast a particle moves when you push on it. Hence the name.

$D = \mu k T$ is the Stokes-Einstein relation, it ensures that the balance between the dissipation, controled by γ, and the injection of energy, controled by $\sqrt{2D}\,\vec{\eta}$ leads to an equilibrium dynamics and the Boltzmann weight.

1.3) Active particles and the overdamped limit

Active particles dissipate some internal source of energy to exert a propelling force on the environment. Newton's 3rd law means that the particle experience an equal & opposite force: the self-propulsion force $\vec{f_p}$.

Langevin dynamics becomes:

$$m\dot{\vec{v}} = -\gamma\vec{v} + \vec{f_p} - \vec{\nabla}V + \sqrt{2\gamma kT}\,\vec{\eta}$$

Constant potential $V(\vec{r})$:

$$\frac{dE}{dt} = -\gamma\vec{v}^2 + d\,\frac{\gamma kT}{m} + \sqrt{2\gamma kT}\,\vec{\eta}\cdot\vec{v} + \vec{f_p}\cdot\vec{v}$$

$$\frac{d}{dt}\langle E\rangle = \underbrace{-\gamma\langle \vec{v}^2\rangle}_{\text{dissipation}} + \underbrace{d\frac{\gamma k_B T}{m} + \underbrace{\langle \vec{f}_p\cdot\vec{v}\rangle}_{w_p}}_{\text{injection}}$$

In general, it is natural to expect that $\vec{v}$ closely follows $\vec{f}_p$ so that $\vec{f}_p\cdot\vec{v} > 0$. w_p measures the power injected in the system by the active force.

This disconnection between injection and dissipation of energy drives active particles out of equilibrium.

Comments:

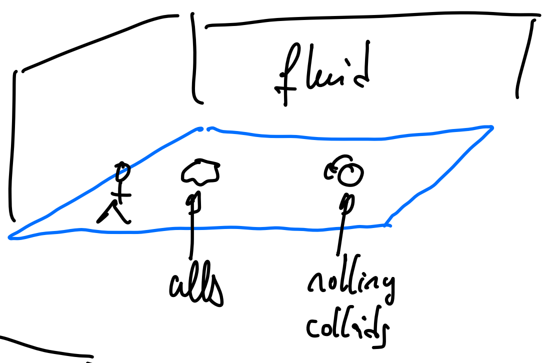
* $\vec{f}_p(t)$ enters $\frac{dE}{dt}$ through the dissipated power $w_p = \vec{f}_p\cdot\vec{v}$

  $\Rightarrow \vec{f}_p$ is a non-conservative force

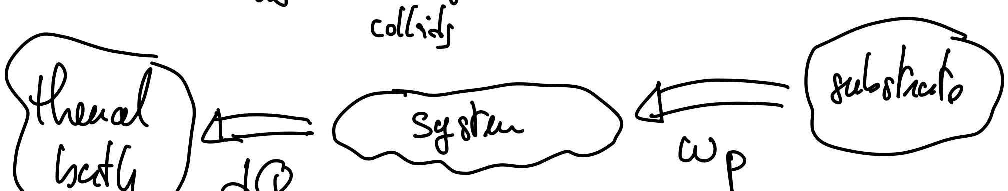
* $\left\langle \frac{dE}{dt}\right\rangle = 0$ in steady-state

$$\langle \gamma v^2\rangle - d\frac{\gamma k_B T}{m} = \frac{dQ}{dt} = \langle \vec{f}_p\cdot\vec{v}\rangle \equiv w_p$$

On average, the power injected by the active force w_p is balanced by the energy dissipated in the thermal bath.



the particles are self-propelled by exchanging momentum with a substrate, and also interact with a surrounding fluid.

*


$\frac{d\mathcal{Q}}{dt}$

In this sense, the dissipation w_p characterizes the departure from thermal equilibrium of the system and it thus attracted a lot of interest.

[Etienne Fodor, Mike Cates]

The overdamped limit:

In practice, inertia is always negligible for micron-size self-propelled particles $\Rightarrow$ most studies work in the large γ limit.

The 1d case

↳ Not done in class

$$m \frac{d^2}{dt^2} x(t) = -\gamma \frac{d}{dt} x(t) - V'(x) + \sqrt{2\gamma k_B T}\, \eta(t) + f_p$$

Large $\gamma \Rightarrow$ nothing happens when $t \underset{\gamma\to\infty}{\sim} \mathcal{O}(1)$

$$t = \gamma \tau \quad \text{with} \quad \tau \underset{\gamma\to\infty}{\sim} \mathcal{O}(1)$$

$$\frac{m}{\gamma^2} \frac{d^2}{d\tau^2} x(\tau) = -\frac{d}{d\tau} x(\tau) - V'(x) + \sqrt{2\gamma k_B T}\, \underbrace{\eta(\gamma\tau)}_{?} + f_p(x)$$

$$\langle \eta(\gamma\tau)\, \eta(\gamma\tau') \rangle = \delta(\gamma\tau - \gamma\tau') = \frac{1}{\gamma} \delta(\tau - \tau')$$

$$\left[\int_{-\infty}^{+\infty} dt\, \delta(\gamma t)\, f(t) \underset{u=\gamma t}{=} \frac{1}{\gamma} \int_{-\infty}^{+\infty} du\, \delta(u)\, f\!\left(\frac{u}{\gamma}\right) = \frac{1}{\gamma} f(0) = \frac{1}{\gamma} \int_{-\infty}^{+\infty} dt\, \delta(t) f(t) \right]$$

$$\Rightarrow \delta(\gamma t) = \frac{1}{\gamma} \delta(t)$$

$\Rightarrow \langle \eta(\gamma\tau)\,\eta(\gamma\tau')\rangle = \frac{1}{\gamma}\langle \tilde{\eta}(\tau)\,\tilde{\eta}(\tau')\rangle$

$\Rightarrow \eta(\gamma\tau) = \frac{1}{\sqrt{\gamma}}\,\tilde{\eta}(\tau)$

$\lim_{t\to\infty} (*)$: $0 = -\frac{d}{d\tau}x(\tau) - V'(x) + \sqrt{2kT}\,\tilde{\eta}(\tau) + f_p$

$$\frac{dx}{d\tau} = -V'(x) + \sqrt{2kT}\,\tilde{\eta}(\tau) + f_p$$

Dimensions are clearly wrong! $[\tau] = \left[\frac{t}{\gamma}\right] = \frac{T^2}{M}$

Restore initial units $\tau = \gamma t$ $\tilde{\eta}(\tau) = \sqrt{\gamma}\,\tilde{\eta}(t)$

$$\gamma\frac{dx}{dt} = -V'(x) + f_p + \sqrt{2\gamma kT}\,\eta(t)$$

$$\Leftrightarrow \frac{dx}{dt} = \dot{x} = -\mu V'(x) + v_p + \sqrt{2D}\,\eta(t)$$

$$v_p \equiv \mu f_p \quad ; \quad D = \frac{kT}{\gamma} = \mu kT$$

Comment: D is the diffusivity when $f_p = V = 0$ only.

In d dimensions

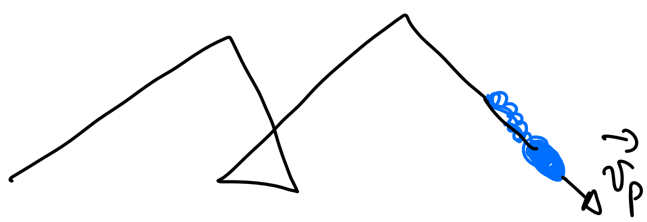
$$\dot{\vec{r}} = \mu\vec{f}_p - \vec{\nabla}V + \sqrt{2D}\,\vec{\eta} \Rightarrow$$ 90% of the models in the literature.

Definition of active particles $\Longleftrightarrow$ Dynamics of $\vec{f}_p$

2) Standard models of active particles

2.1) Run and Tumble particles

e.g. swimming bacteria like E. Coli, whose dynamics alternate between quasi-straight runs & sudden reorientations.



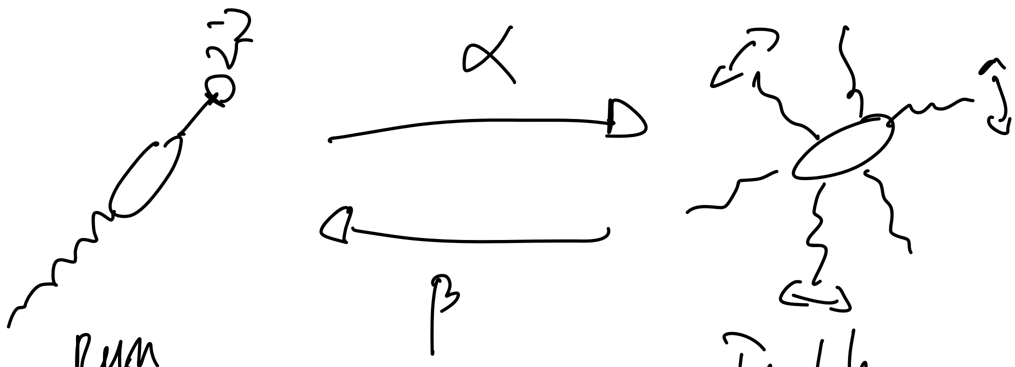
particle size $\sim 1\text{-}2\,\mu m$

speed $\sim 10\text{-}30\,\mu m/s$

tumbling rate $\sim 1\ s^{-1}$

duration $\sim 0{,}1\ s$

Two-state model



P_R: proba that the particle is running

P_T: ——————— tumbling

Master equation: $\partial_t P_R(t) = \beta P_T(t) - \alpha P_R(t)$

$$\partial_t P_T(t) = \alpha P_R(t) - \beta P_T(t)$$

$P_R(t) = 1 - P_T(t) \Rightarrow \partial_t P_T(t) = \alpha - (\alpha+\beta) P_T(t)$

$$P_T(t) = P_T(0)\, e^{-(\alpha+\beta)t} + \frac{\alpha}{\alpha+\beta}\left(1 - e^{-(\alpha+\beta)t}\right)$$

In practice, β is much larger than α.

$$P_T(t) \simeq P_T(0)\, e^{-\beta t} + \frac{\alpha}{\alpha+\beta}\left(1 - e^{-\beta t}\right)$$

To describe the system on time-scales $\gg \frac{1}{\beta}$, one gets

$P_T(t) \simeq \frac{\alpha}{\alpha+\beta} \simeq \frac{1}{\beta}$ and $P_T(t) \simeq \frac{\beta}{\alpha+\beta} \simeq 1 - \frac{1}{\beta} \gg P_R(t)$

$\Rightarrow$ Assume tumbles instantaneous.

Run and Tumble dynamics

$\dot{\vec{r}} = v_p \vec{u}$, $\|\vec{u}\| = 1$ is the orientation of the particle

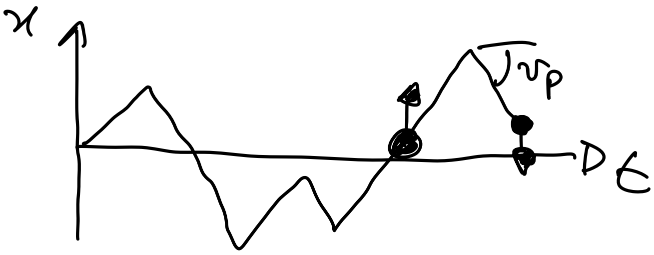
$\vec{u} \xrightarrow{\alpha} \vec{u}'$ uniformly.

2d: $\vec{u} = (\cos\theta, \sin\theta)$ $\quad \theta \xrightarrow{\alpha} \theta'$; $p(\theta') = \frac{1}{2\pi}$

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

1D: $\dot{x} = \sigma v_p$

$\sigma \xrightarrow{\alpha} -\sigma$



Master equation:

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

The dynamics is a mixture between zero-noise Langevin dynamics for $\vec{r}(t)$ in 2D and Markov process in continuous space (a.k.a. jump process).

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

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

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

Translational noise:

$$\dot{\vec{r}} = v_0 \vec{u}(\theta) + \underline{\sqrt{2D}\,\vec{\eta}} \; ; \quad \theta \xrightarrow{\alpha} \theta' \quad \text{with } p(\theta') = \frac{1}{2\pi}$$

$$\partial_t P(\vec{r},\theta,t) = -\vec{\nabla}\cdot\left[v_0 \vec{u}(\theta) P(\vec{r},\theta)\right] - \alpha P(\vec{r},\theta) + \frac{\alpha}{2\pi}\int d\theta' P(r,\theta')$$
$$\underbrace{+ \frac{\partial}{\partial x}\left[\frac{\partial}{\partial x} DP\right] + \frac{\partial}{\partial y}\left[\frac{\partial}{\partial y} DP\right]}_{\underline{D\Delta P}}$$

One-dimensional case with asymmetric speeds & tumbling rates

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

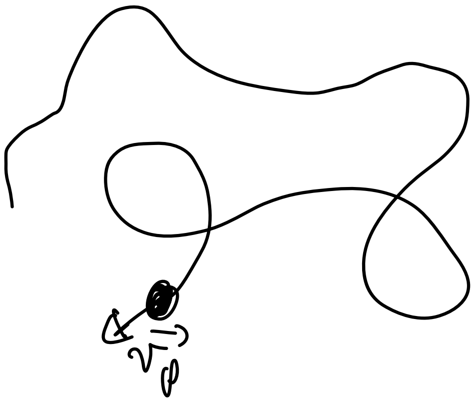
Master equation:

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

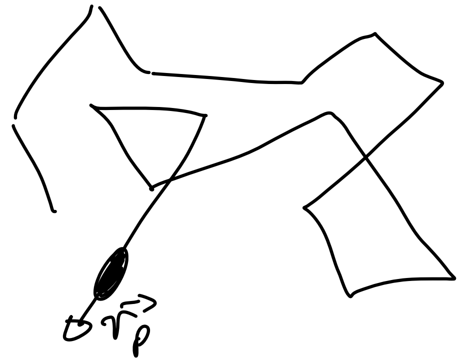
$$(2) \quad \partial_t L(x,t) = -\partial_x \cdot J_L - \frac{\alpha_L}{2} L(x,t) + \frac{\alpha_R}{2} R(x,t) = \partial_x\left[v_L L(x,t)\right] + \frac{\alpha_R}{2} R - \frac{\alpha_L}{2} L$$

2.2) Active Brownian Particles

Some bacterial strains do not tumble ⎫ reorientation due
Self propelled colloids ——— ⎭ to rotational diffusion



vs



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

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

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