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Han-sur-Lesse 2022

- Lecture 1a : Slides on active matter - introduction (from course materials)

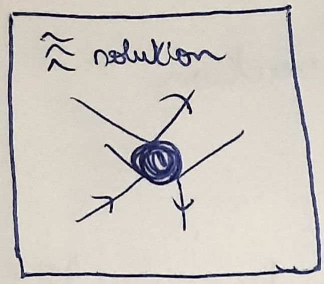
- Lecture 1b : • Brownian motion : Langevin equation - $\langle v^2 \rangle$ - equipartition - MSD - Stokes-Einstein skipping the calculations.
  • Introduce ABPs conceptually, including equation of motion

- Lecture 2a : • ABP'S : motion of a single ABP result for MSD, effective diffusion coefficient

  2b • Collective motion of ABP'S : Phenomenology, MIPS, overview of results (try to squeeze in more some experiments)
  (if there is time) : ABP'S as a cell model

Exercise Class : • Introduce Euler-Maruyama for ABP's [note: update slides] - efficient factors of 2 ...
• Write single ABP code and compute MSD
• Let people play with Brown.py collective code

Lecture 1b: Brownian motion (ask for student background)



Consider: . particle with radius R, mass m

. subject to constant collisions with H_2O molecules, on time scales of $\sim 10^{-14}$ s

random, very fast -

. density matched (to simplify)

Equations of motion:

$$\boxed{m \frac{d\vec{V}}{dt} = \vec{F}_{tot} = -\zeta \vec{V} + \vec{f}(t)}$$ Langevin equation

↳ Stokes drag: $\zeta = 6\pi\eta R$

$\vec{f}(t)$: random stochastic force: $\langle \vec{f}(t) \rangle = 0$

. zero on average $\qquad \langle \vec{f}(t) \cdot \vec{f}(t') \rangle = 2d\gamma\, \delta(t-t')$

. no time correlation $\qquad \langle\ \rangle$ statistical average

Stochastic ODE: We can solve this, e.g. (not focus here)

$$\vec{V}(t) = \vec{V}(0)\, e^{-t\zeta/m} + \frac{1}{m}\int_0^t e^{-(t-t')\zeta/m} f(t')\, dt'$$

In particular, we can now calculate:

$\langle f(t') \rangle = 0$

$$\langle \vec{V}(t) \rangle = \langle V(0) \rangle e^{-t\boxed{\zeta/m}} + 0 = \underline{0}$$ going nowhere on average

mean velocity $\qquad$ also 0 on average $\qquad \tau = \frac{m}{\zeta}$

short for 1μm colloid

$$\langle V(t)^2 \rangle = \langle V(t) \cdot V(t) \rangle = \ldots$$

$$= V(0)^2 e^{-2t\zeta/m} + \frac{\gamma}{m\zeta}\left(1 - e^{-2t\zeta/m}\right)$$

$$\xrightarrow[t\to\infty]{} \frac{\gamma}{m\zeta} \quad \text{constant.}$$

Thermal equilibrium: $\langle T \rangle = \langle U \rangle = \frac{1}{2} kT$

and therefore: $\frac{1}{2} m \langle v^2 \rangle = \frac{1}{2} \frac{\gamma}{\zeta} = \frac{1}{2} kT$

or: $\boxed{\gamma = \zeta k T}$ fluctuation - dissipation relation

noise amplitude = friction × temperature

Diffusion:

. random trajectory: How far have I gone?

$$\Delta x(t) = x(t) - x(0) = \int_0^t dt' \, v(t')$$

$\langle \Delta x(t) \rangle = \cdots 0$ going nowhere on average

. Calculate the mean-square displacement:

$MSD(t) = \langle \Delta x^2(t) \rangle$ average square width of trajectory plot

$= \cdots$ relatively involved calculation $\cdots$

$$= \frac{3\gamma}{\zeta^2} \left[2t + \frac{m}{\zeta} \left(-2 + 2 e^{-t\zeta/m} \right) \right]$$

$$\to \frac{6\gamma}{\zeta^2} t \quad \text{as } t \to \infty$$

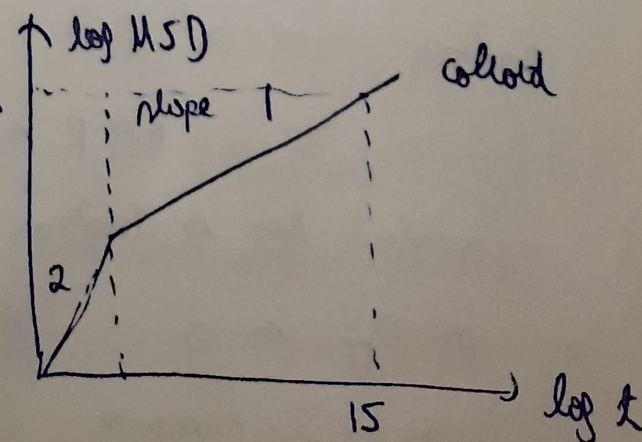
Stokes - Einstein relation:

diffusion coefficient

$$\gamma = \zeta k_B T \to MSD(t) = 2 \frac{3 k_B T}{\zeta} t := 2 D t$$

Hence: $\boxed{D = d \frac{k_B T}{\zeta}}$

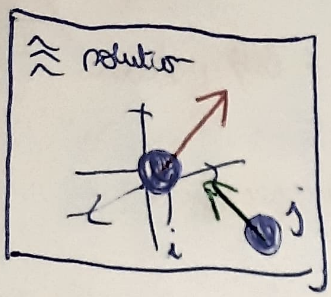
Stokes - Einstein relation



1 μm colloid: $MSD = 6Dt = R^2$

$D = \frac{k_B T}{6\pi \eta R} \sim 1$ $\Rightarrow \tau = 1$ second

Active Brownian motion



- Consider now a particle either in solution or on a substrate
- Could be cell ($\sim 10\,\mu m$), colloid ($\sim 1\,\mu m$) or swimming bacterium ($1\,\mu m$)

- Assume that it is (somehow) driven internally

Biologically → crawling cell
→ swimming using flagella

Chemically → Janus particle
→ Electrophoresis / Light + H_2O_2
→ Magnetic Quincke rollers
→ ... (many)

- Equations of motion:

$$m\frac{d\vec{V}_i}{dt} = \vec{F}_i = \underbrace{-\zeta\vec{V}_i}_{\text{friction force}} + \underbrace{\vec{F}_{act}}_{\text{active force}} + \underbrace{\vec{\eta}_i^{\,T}}_{\text{thermal fluctuations } (\equiv \vec{\xi}(t))} + \underbrace{\sum_{j=1}^{N}\vec{F}_{ij}}_{\text{pair interactions}}$$

- Simplification:

1) Overdamped dynamics: recall $\langle V(t)\rangle \sim e^{-\zeta t/m}$

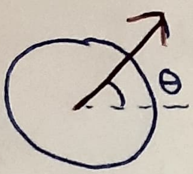
for $t > \tau = \frac{m}{\zeta}$, mass term is irrelevant

scaling: $\left.\begin{array}{l} m \sim R^3 \\ \zeta = 6\pi\eta R \sim R \end{array}\right\} \tau = \frac{m}{\zeta} \sim R^2 \to 0$ as $R \to 0$

⇒ neglect the acceleration term

$m\frac{d\vec{V}}{dt} \triangleq 0$ define: $\frac{F^i_{act}}{\zeta} = \underbrace{v_0\,\hat{n}_i}_{\text{active velocity}}$

divide by ζ, rearrange

2)  where $\hat{n}_i = (\cos\theta_i, \sin\theta_i)$ is a unit vector (2d version, 3d can also be done)

we will restrict ourself to motion on a surface (2d)
O.K. for most artificial particles and most cells

Equations of motion for ABP's:

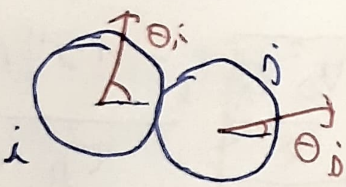
$$\boxed{\frac{d\vec{r}_i}{dt} = \underbrace{v_0 \hat{n}_i}_{\text{self-propulsion}} + \underbrace{\frac{1}{\xi}\sum_{j=1}^{N} \vec{F}_{ij}}_{\text{interactions}} + \underbrace{\vec{\eta}_i^{\,T}}_{\text{noise}}}$$

where: $\langle \vec{\eta}_i^{\,T}(t)\, \vec{\eta}_j^{\,T}(t') \rangle = \underset{2d}{4}\, \delta_{ij}\, \delta(t-t') \frac{k_B T}{\xi}$

Stokes-Einstein

Angular dynamics

We have one new variable: θ_i, particle orientation in plane



Need to specify equation of motion too!

Newton: $\overset{\text{moment of inertia}}{I}\, \ddot{\theta}_i = T_i$ torque

$$T_i = \underbrace{-\xi^r \dot{\theta}_i}_{\text{rotational friction}} + \underbrace{\eta^R}_{\text{rotational noise}} + \underbrace{\sum_{j=1}^{N} T_{ij}}_{\text{pair torques}}$$

· Make the same overdamped dynamics assumption: $I\ddot{\theta}_i \simeq 0$

$$\boxed{\frac{d\theta_i}{dt} = \frac{1}{\xi^r}\sum_{j=1}^{N} T_{ij} + \hat{\eta}_i^R}$$

$\langle \hat{\eta}_i^R(t)\, \eta_j^R(t') \rangle = 2 \boxed{D_r}\, \delta_{ij}\, \delta(t-t')$

rotational diffusion constant

· Non-aligning (standard) ABP's

$T_{ij} = 0$

$\tau_r = \frac{1}{D_r}$ reorientation time

Motion of a single ABP

$$\boxed{\frac{d\vec{r}}{dt} = v_0 \hat{n} + \vec{\eta}^T} \quad \text{and} \quad \boxed{\frac{d\theta}{dt} = \tilde{\eta}^R}$$

$$\langle \vec{\eta}^T(t)\, \vec{\eta}(t') \rangle = 4 D_t\, \delta(t-t') \qquad D_t = \frac{k_B T}{\xi}$$

$$\langle \tilde{\eta}^R(t)\, \tilde{\eta}^R(t') \rangle = 2 D_r\, \delta(t-t')$$

$$= \frac{2}{\tau_r}\, \delta(t-t')$$

Solve this motion (sketch of derivation):

- $\frac{d\theta}{dt} = \tilde{\eta}^R \rightarrow \theta(t) = \int_0^t \tilde{\eta}^R(t')\, dt'$ formal solution

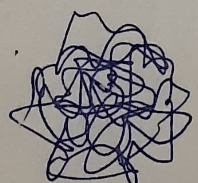
Can calculate $\hat{n}(t) = (\cos\theta, \sin\theta)$ and its moments

Final result: $\langle \hat{n}(t) \rangle = 0$

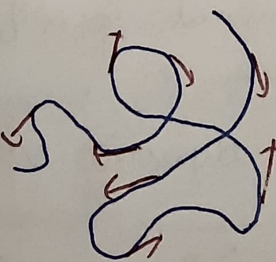
$$\langle v_0 \hat{n}(t) \cdot v_0 \hat{n}(t') \rangle = 2 \boxed{\frac{v_0^2 \tau_r}{2}}\, \frac{e^{-|t-t'|/\tau_r}}{\tau_r}$$

What does that mean? D_a effective diffusion constant

$\vec{n}(t)$ is time-correlated noise with persistence time τ_r



thermal random walk



persistent random walk

ABP does persistent trajectory

- persistence time τ_r
- persistence length

$$\boxed{\xi = v_0 \tau_r}$$

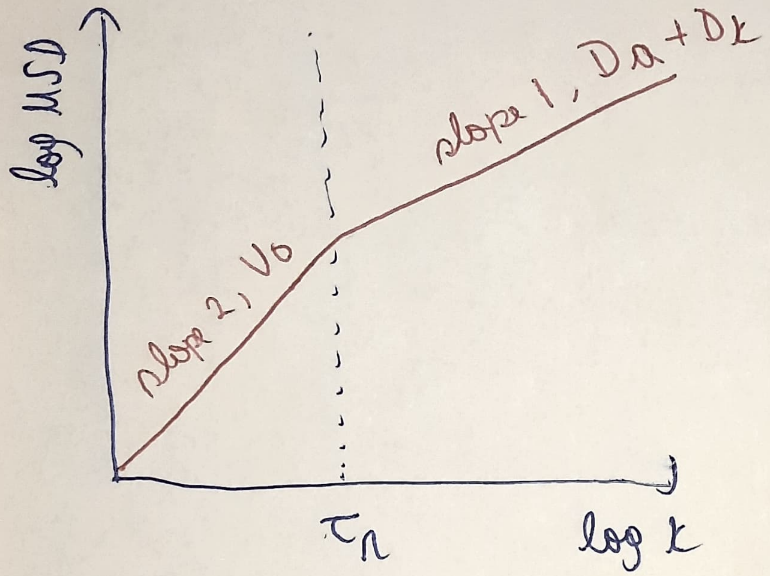
- $\lim \tau_r \to 0$: $\langle v_0 \vec{n} \cdot v_0 \vec{n} \rangle \rightarrow 2 \boxed{\frac{v_0^2 \tau_r}{2}}\, \delta(t-t')$

normal random walk $\boxed{\frac{k_B T_{eff}}{\xi}}$ effective active temperature

Can calculate the MSD here as well:

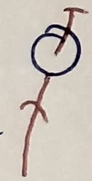
$$MSD(t) = \langle |\vec{r}(t) - \vec{r}(0)|^2 \rangle = \dots$$

$$\boxed{MSD(t) = 4 D_t t + 2 v_0^2 \tau_r \left[t - \tau_r \left(1 - e^{-t/\tau_r}\right)\right]}$$



- for $t \ll \tau_r$

$$\boxed{MSD(t) \simeq v_0^2 t^2}$$



ballistic straight motion

- for $t \gg \tau_r$

$$\boxed{MSD(t) \simeq 4 \left[D_t + D_a \right] t}$$

$$\boxed{D_a = \frac{v_0^2 \tau_r}{2} = \frac{k_B T_{eff}}{\zeta}}$$

behaves like thermal particle, but with effective active temperature!

<u>Exercise class</u>:

- Numerically integrate equations of motion for single ABP using Euler-Maruyama algorithm
- Compute MSD numerically.