Translational diffusion

- Brown: particle in suspension
- molecular theory of heat.

$$\frac{m}{2}\langle x_i^2 \rangle = \frac{k_B T}{2}$$

Einstein 1905.

- minimal model for undirected transport, stock prices, ...

Albert Einstein 1905.

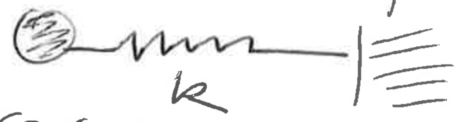
$\dot{x} = \sqrt{2D}\,\xi$. $\Rightarrow$ $\dot{c} = D\nabla^2 c$

Langevin eqn. for single part. — diffusion eqn.

SDE — FPE

What is D?

- Way #1: by equi-partition theorem



$\gamma = 6\pi\eta a$

$$\gamma \dot{x} = -kx + \gamma\xi$$

$$\langle \xi(t)\xi(t')\rangle = 2D\,\delta(t-t')$$

Ornstein-Uhlenbeck process

Stored energy

$$\frac{k_BT}{2} \overset{!}{=} \langle E\rangle = \frac{k}{2}\langle x^2\rangle = \frac{k}{2}\frac{2D}{2k/\gamma} = \frac{D\gamma}{2}$$

$$\Rightarrow D = \frac{k_BT}{\gamma} \equiv \text{Stokes Einstein rel.}$$

Rotational diffusion

$$\dot{\varphi} = \xi$$

$$\langle \xi(t)\,\xi(t') \rangle = 2 D_{rot}\, \delta(t-t').$$

Sphere: $$D_{rot} \sim \frac{k_B T}{8\pi \eta a^3}$$

disk:

Units: $[\xi]\ \frac{1}{s}$, $[D_{rot}]\ \frac{1}{s}$ Note: $[\delta(t)]\ \frac{1}{s}$.

$\longrightarrow$ rotational diffusion in 3D?

$\longrightarrow$ coupling of translations + rotations.

Lie group
- group + smooth manifold
- group operations are smooth

Reminder group
- multiplication $G \times G \longrightarrow G$
- unit element $1 \in G$
- inverse : $^{-1}: G \longrightarrow G$

examples: permutations, geometric transformations, i.e. rotations

Reminder: smooth manifold

M topological space (2nd countable = countable base for open sets, Hausdorff = points separable by open sets)

$$M = \bigcup_{j \in J} U_j = \text{open cover}$$

atlas: $f_j : U_j \xrightarrow{\sim} V_j \subseteq \mathbb{R}^n$ charts

smooth coordinate transformations

$$f_k \circ f_j^{-1} : f_j(U_j \cap U_k) \longrightarrow V_k$$

must be smooth

examples Lie groups:

- translations in 1D: $\mathbb{R}$

- rotations in 2D:

$$SO(2) = \left\{ \begin{pmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{pmatrix} \middle| \varphi \in \mathbb{R} \right\}.$$

- rotations in 3D.

$$SO(3) = \{ G \in \mathbb{R}^{3\times 3} \text{ with } \cancel{\det} \, G G^T = \mathbb{1} \}.$$

⚠ not commutative

- rigid body transformations in 3D

$$SE(3) \equiv \text{translations} + \text{rotations}$$

$$\mathbb{R}^{4\times 4} \supseteq SO(3) \ni G = \begin{pmatrix} \underline{\underline{R}} & \underline{V} \\ 0 & 1 \end{pmatrix}$$

$\underline{\underline{R}} \equiv$ rotation matrix

$\underline{V} \equiv$ translation vector.

How does this work?

* $\underline{d} \in R^3$ ≡ direction vector.
  - affine coordinates: write as $\begin{pmatrix} \underline{d} \\ 0 \end{pmatrix} \in R^4$.
  - transformation rule
$$\begin{pmatrix} \underline{d} \\ 0 \end{pmatrix} \longmapsto \underline{\underline{G}} \begin{pmatrix} \underline{d} \\ 0 \end{pmatrix}.$$

* $\underline{r} \in R^3$ ≡ position vector
  - affine coordinates write as $\begin{pmatrix} \underline{r} \\ 1 \end{pmatrix} \in R^4$
  - transformation rule
$$\begin{pmatrix} \underline{r} \\ 1 \end{pmatrix} \longmapsto \underline{\underline{G}} \begin{pmatrix} \underline{r} \\ 1 \end{pmatrix}$$

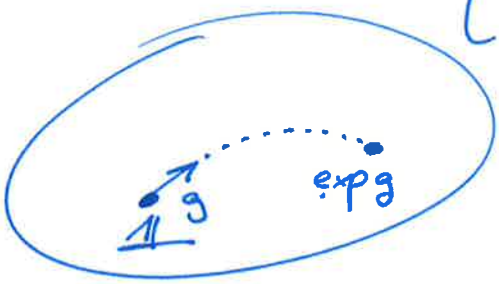
* Concatenation
$$\underline{\underline{G}}_1 = \begin{pmatrix} \underline{\underline{R}}_1 & \underline{V}_1 \\ \underline{0}^T & 1 \end{pmatrix}, \quad \underline{\underline{G}}_2 = \begin{pmatrix} \underline{\underline{R}}_2 & \underline{V}_2 \\ \underline{0}^T & 1 \end{pmatrix}.$$
$$\underline{\underline{G}}_2 \circ \underline{\underline{G}}_1 = \begin{pmatrix} \underline{\underline{R}}_2 \cdot \underline{\underline{R}}_1 & \underline{V}_2 + \underline{\underline{R}}_1 \cdot \underline{V}_2 \\ \underline{0}^T & 1 \end{pmatrix}$$

The exponential map:

$$\exp : T_{\mathbb{1}} M \longrightarrow M$$

$$g \longmapsto G(1) \quad \text{with}$$

$$\begin{cases} G(0) = \mathbb{1} \\ \dot{G} = G g. \end{cases} \equiv \text{initial value problem}$$



Q: Why does this mathematical trick work?

A: Group action allows us to identify all $T_G M$ (natural connection)

- $T_{\mathbb{1}} M$ is called Lie algebra of M.

How to compute the exponential map?

- for matrix groups, use matrix exponential

$$\exp g := \sum_{n=0}^{\infty} \frac{1}{n!} g^n .$$

<u>Proof:</u>

- $G(t) = \exp tg$
- $\frac{d}{dt} G(t) = \frac{d}{dt} \sum_{n=0}^{\infty} \frac{1}{n!} t^n g^n$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} n t^{n-1} g^{n-1} \cdot g$$

$$= G(t) \cdot g .$$

- $G(0) = \mathbb{1}$. q.e.d.

Example: $SO(2)$.

$$\exp: \quad \begin{array}{ccc} so(2) & \longrightarrow & SO(2) \\ \cong & & \\ \varphi \in \mathbb{R} & \longmapsto & \begin{pmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{pmatrix} \end{array}.$$

- infinitesimal rotation: $\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = E_1$

$E_1^2 = -\mathbb{1}$, $E_1^3 = -E_1$, $E_1^4 = \mathbb{1}$.

$so(2) = \{\varphi \underline{\underline{E}}_1 \mid \varphi \in \mathbb{R}\}$.

Proof:

$$\exp \varphi \underline{\underline{E}}_1 = \sum_{n=0}^{\infty} \frac{1}{n!} (\varphi \underline{\underline{E}}_1)^n$$

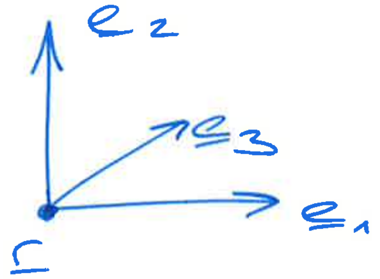
$$= \sum_{\substack{n=0 \\ 2 \nmid n}}^{\infty} \frac{1}{n!} \underline{\underline{E}}_1 \varphi^n (-1)^{\frac{n-1}{2}}$$

$$+ \sum_{\substack{n=0 \\ 2 \mid n}}^{\infty} \frac{1}{n!} \varphi^n (-1)^{n/2} \mathbb{1}.$$

$$= \sin\varphi \, \underline{\underline{E}}_1 + \cos\varphi \, \underline{\underline{\mathbb{1}}}$$

q.e.d.

Kinematics



material frame

$\underline{V} = v_1 \underline{e}_1 + v_2 \underline{e}_2 + v_3 \underline{e}_3 \equiv$ propulsion velocity.

$|\underline{v}| \equiv$ speed $[\frac{m}{s}]$.

$\underline{\Omega} = \Omega_1 \underline{e}_1 + \Omega_2 \underline{e}_2 + \Omega_3 \underline{e}_3 \equiv$ Darboux vector

rotation vector

$|\underline{\Omega}| \equiv$ angular velocity $[\frac{rad}{s}]$

$$\underline{e}_1 \longrightarrow \underline{\underline{E}}_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}$$

$\equiv$ infinitesimal rotation around $\underline{e}_1$- axis.

$$(\underline{\underline{E}}_1)_{ij} = \varepsilon_{ijk}, \quad k=1$$

$\equiv$ ~~Kle~~ Levi-Civita-symbol

$$\hat{\underline{\underline{\Omega}}} = \Omega_1 \underline{\underline{E}}_1 + \Omega_2 \underline{\underline{E}}_2 + \Omega_3 \underline{\underline{E}}_3$$

$\equiv$ rotation matrix

- express material frame wrt lab frame

$$\underline{\underline{H}} = \begin{pmatrix} \underline{e}_1 & \underline{e}_2 & \underline{e}_3 & \underline{r} \\ 0 & 0 & 0 & 1 \end{pmatrix} \in \mathbb{R}^{4\times 4}.$$

$$\dot{\underline{\underline{H}}} = \underline{\underline{H}} \cdot \underline{\underline{g}},$$

$$\underline{\underline{g}} = \begin{pmatrix} \hat{\underline{\Omega}} & \underline{v} \\ 0 & 1 \end{pmatrix} \equiv \text{infinitesimal transformation}$$

- constant propulsion

$$\underline{\underline{H}}(t) = \exp(\underline{\underline{g}} \cdot t)$$

$\longrightarrow$ helix.

- time-varying propulsion

$\longrightarrow$ time-ordered exponential integrals.

$$G(t) = T\exp \int_0^t dt' \, g(t')$$
$$= \sum_{n=0} \int_{0<t_1<\dots<t_n<t} dt_1 \cdots dt_n \, g(t_1) \cdots g(t_n).$$

- exercise: physical units of $\exp(gt)$?

Helical swimming

- assume constant propulsion

$$\left.\begin{matrix} V_1(t),\ V_2(t),\ V_3(t), \\ \Omega_1(t),\ \Omega_2(t),\ \Omega_3(t) \end{matrix}\right\}\ \text{all const.}$$

- The tangent vector

$$v_0 \underline{t} = \underline{V} = V_1 \underline{e}_1 + V_2 \underline{e}_2 + V_3 \underline{e}_3 .$$

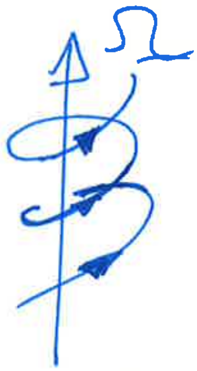
$$\dot{\underline{V}} = \underline{\Omega} \times \underline{V}$$

- The rotation vector stays constant

$$\dot{\underline{\Omega}} = \underline{\Omega} \times \underline{\Omega} = \underline{0}.$$

- Resulting swimming path is a helix. with helix axis $\underline{\Omega}$

torsion $= \tau = \Omega_{\parallel} / v_0$



curvature $\kappa = |\underline{\Omega}_{\perp}| / v_0 .$

$$\underline{\Omega} = \Omega_{\parallel} \underline{t} + \underline{\Omega}_{\perp}$$

geometric interpretation:

- $k = \frac{1}{R}$,

  $R \equiv$ radius of osculating ~~plane~~ circle

- $\tau v_0 \equiv$ rotation rate of osculating plane

- helix radius

  $$r = \frac{k}{k^2+\tau^2}$$

  helix pitch

  $$2\pi h = \frac{2\pi\tau}{k^2+\tau^2}.$$

angular helix frequency $|\Omega|$.

Frenet equations

$$\dot{\underline{r}} = v_0 \underline{t}$$

$$\dot{\underline{t}} = v_0 k \underline{n}$$

$$\dot{\underline{n}} = -v_0 k \underline{t} + v_0 T \underline{b}$$

$$\dot{\underline{b}} = -v_0 T \underline{n}.$$

- relationship to kinematic description

$$v_0 \underline{t} = \underline{v}.$$

$$(k \underline{b} + T \underline{t}) v_0 = \underline{\Omega}$$

$$\longrightarrow \quad \dot{\underline{t}} = \underline{\Omega} \times \underline{t}, \quad \dot{\underline{n}} = \underline{\Omega} \times \underline{n}$$
$$\dot{\underline{b}} = \underline{\Omega} \times \underline{b}$$

- fancy matrix notation

$$\underline{\underline{H}}(t) = \begin{pmatrix} \underline{t} & \underline{n} & \underline{b} & \underline{r} \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

$$\dot{\underline{\underline{H}}}(t) = \underline{\underline{H}}(t) \cdot \underline{\underline{g}}$$

$$\hat{\Omega} = \begin{pmatrix} 0 & -\Omega_3 & \Omega_2 \\ \Omega_3 & 0 & -\Omega_1 \\ -\Omega_2 & \Omega_1 & 0 \end{pmatrix} \in so(3), \quad \underline{\underline{g}} = \begin{pmatrix} \underline{\hat{\Omega}} & \underline{v} \\ 0 & 1 \end{pmatrix}.$$

Ito vs. Stratonovich

- Q: Given an ODE, e.g.

$$\dot{x} = f(x):$$

What does it mean?

A: Constructive approach:
estimate $x_i = x(i\,dt)$, numerically,
then let $dt \to 0$.

- Possibility no 1: explicite Euler scheme

$$x_i = x_{i-1} + f(x_{i-1}) \cdot dt.$$

- Possibility no 2: implicite

$$x_i = x_{i-1} + f(x_i)\,dt.$$

- Possibility no 3: mixed

$$x_i = x_{i-1} + \tfrac{1}{2}\left[f(x_{i-1}) + f(x_i)\right] dt.$$

$\Rightarrow$ For deterministic ODEs different schemes differ only in terms of numerical performance, stability, etc. Not in the limit result

- What about SDEs?

$$\dot{x} = f(x) + \sqrt{2D(x)}\,\xi$$

$$\langle \xi(t)\,\xi(t') \rangle = \delta(t-t').$$

- Explicit Euler scheme:

$$x_i = x_{i-1} + f(x_{i-1})\,dt + \sqrt{2D(x_{i-1})}\,\mathcal{N}\cdot\sqrt{dt}.$$

$\equiv$ normally distributed normal variable mean 0, variance 1

$\equiv$ Wiener increment

$\longrightarrow$ Ito

- Mixed scheme:

$$x_i = x_{i-1} + \tfrac{1}{2}[f(x_{i-1}) + f(x_i)]\,dt + \tfrac{1}{2}\left[\sqrt{2D(x_{i-1})} + \sqrt{2D(x_i)}\right]\mathcal{N}\cdot\sqrt{dt}.$$

$\longrightarrow$ Stratonovich

$$x_i = x_{i-1} + f(x_{i-1})\cdot dt + O(dt^{3/2}) + g(x_{i-1})\cdot\mathcal{N}\cdot\sqrt{dt} + g'(x_{i-1})\cdot g(x_{i-1})\cdot\mathcal{N}^2\cdot dt + O(dt^{3/2})$$

$\Rightarrow \langle \mathcal{N}^2 \rangle = 1 \neq 0$

$\Rightarrow$ Itô vs. Stratonovich interpretation give different drift terms.

Wrap-up

- stating a nonlinear SDE without specifying its interpretation does not make sense (it's like writing a text and not specifying in which language it was written)

  $\longrightarrow$ Many more interpretations:
  - Itô - thermal
  - alpha - calculus by Lau & Lubensky PRE

- A Stratonovich SDE $\dot{x} = f(x) + g(x)\xi$ can be rewritten as Itô SDE $\dot{x} = f(x) + g(x)\xi + \frac{1}{2} g' g$ and vice versa.

  Use interpretation most suitable for a given task.

- finance loves Ito:
  not looking back into the past.

- Physics: often Stratonovich used, often Wong-Zakai-theorem applies:

Theorem (Wong-Zakai):

If $\dot{x} = f(x) + g(x)\,\xi$ is an SDE with colored noise of finite correlation time τ, then taking the limit $\tau \to 0$ will yield a Stratonovich SDE with Gaussian white noise ξ.

Example : rotational diffusion in 2D.

$$\dot\varphi = \xi .$$

$$e_1 = \begin{pmatrix}\cos\varphi \\ \sin\varphi\end{pmatrix}, \quad e_2 = \begin{pmatrix}-\sin\varphi \\ \cos\varphi\end{pmatrix}.$$

$SO(2)$: $\quad \frac{d}{dt}[e_1, e_2] = [e_1, e_2]\cdot \xi \cdot \begin{pmatrix}0 & -1 \\ +1 & 0\end{pmatrix}$

$$(S) \quad \begin{cases} \dot e_1 = \xi\, e_2 \\ \dot e_2 = -\xi\, e_1 \end{cases}$$

$$\Downarrow$$

$$(I) \quad \begin{cases} \dot e_1 = \xi\, e_2 + \frac{1}{2}\underbrace{\langle \xi\, \frac{\partial e_2}{\partial e_1}\cdot \dot e_1 \rangle}_{0} + \underbrace{\frac{1}{2}\langle \xi\, \frac{\partial e_2}{\partial e_2}\cdot \dot e_2 \rangle}_{\frac{1}{2}(2D_{rot})\cdot(-e_1)} \\ \quad = \xi\, e_2 + \cancel{\xi} - D_{rot}\, e_1 \\ \dot e_2 = -\xi\, e_1 - D_{rot}\, e_2 . \end{cases}$$

Exercise :

Run simulations for

$$(I) \quad \begin{aligned} \dot e_1 &= \xi e_2 - D_{rot}\, e_1 \\ \dot e_2 &= -\xi e_1 - D_{rot}\, e_2 \end{aligned}$$

and

$$(I) \quad \begin{aligned} \dot e_1 &= \xi e_2 \\ \dot e_2 &= -\xi e_1 \end{aligned}$$

Extended example:

Persistent random walk (2D).

$$\dot{\underline{r}} = v_0 \underline{e}_1$$

$$\underline{e}_1 = \begin{pmatrix} \cos\varphi \\ \sin\varphi \end{pmatrix}, \quad \dot{\varphi} = \xi, \quad \langle \xi(t_1)\xi(t_2)\rangle = 2D_{rot}\delta(t_1-t_2)$$

Proposition

$$C(t) = \langle \underline{e}_1(0)\cdot\underline{e}_1(t)\rangle = \exp(-D_{rot}\,t)$$

$$t_p = \frac{1}{D_{rot}} \equiv \text{persistence time}$$

$$\ell_p = v_0 t_p \equiv \text{persistence length}$$

Proof:

$$\frac{d}{dt}C(t) = \langle \underline{e}_1(0)\,\dot{\underline{e}}_1(t)\rangle$$

$$= \langle [\underline{e}_1(0)\cdot\underline{e}_1(t)][\underline{e}_1(t)\cdot\dot{\underline{e}}_1(t)]\rangle$$
$$+ \langle [\underline{e}_1(0)\cdot\underline{e}_2(t)][\underline{e}_2(t)\cdot\dot{\underline{e}}_1(t)]\rangle.$$

Itô calculus: factors independent

$$= \langle \underline{e}_1(0)\cdot\underline{e}_1(t)\rangle\cdot\langle \underline{e}_1(t)\cdot\dot{\underline{e}}_1(t)\rangle.$$
$$+ \langle \underline{e}_1(0)\cdot\underline{e}_2(t)\rangle\,\langle \underline{e}_2(t)\cdot\dot{\underline{e}}_1(t)\rangle$$

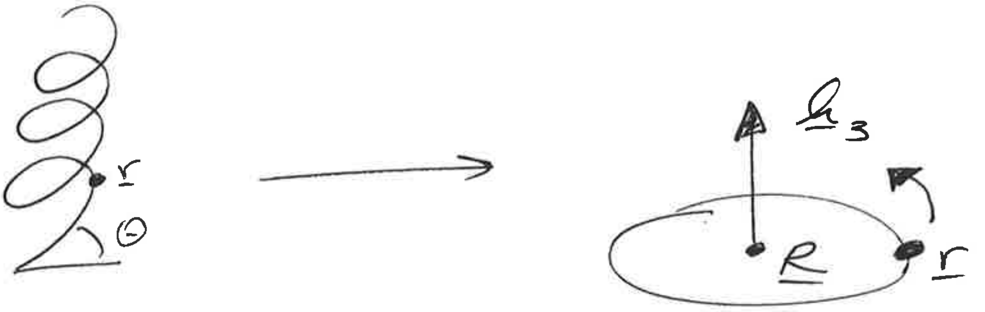
$$= C(t)\cdot(-D_{rot}) + \sqrt{1-C^2}\cdot\underbrace{\langle\xi\rangle}_{=0}.$$

$$= -D_{rot}\,C(t).$$

q.e.d.

Noisy helices

From the Frenet frame to the helix frame



Spinning + translating

$$\underline{h}_3 = \frac{\underline{\Omega}}{|\underline{\Omega}|} = \sin\Theta\, \underline{t} + \cos\Theta\, \underline{b}$$

$$\underline{n} \perp \underline{h}_3 \Rightarrow \underline{h}_1 = -\underline{n}, \quad \underline{h}_2 = \underline{h}_3 \times \underline{h}_1$$

Why? $v_0 k \underline{n} = \dot{\underline{t}} = \underline{\Omega} \times \underline{t}$ q.e.d.

$$\underline{R} = \underline{r} + r_0 \underline{n}.$$

$$\underline{\underline{F}} = (\underline{t}, \underline{n}, \underline{b})$$

$$\dot{\underline{\underline{F}}} = \underline{\underline{F}} \cdot \underline{\underline{f}}, \quad \underline{\underline{f}} = v_0 (k \underline{\underline{E}}_3 + \tau \underline{\underline{E}}_1)$$

$$\underline{\underline{H}} = (\underline{h}_1, \underline{h}_2, \underline{h}_3).$$

$$\dot{\underline{\underline{H}}} = \underline{\underline{H}} \cdot \underline{\underline{h}}$$

$$\underline{\underline{H}} = \underline{\underline{G}}^{-1} \cdot \underline{\underline{F}} \cdot \underline{\underline{G}} \quad \text{with} \quad \underline{\underline{G}} = \begin{pmatrix} 0 & \cos\Theta & \sin\Theta \\ -1 & 0 & 0 \\ 0 & -\sin\Theta & \cos\Theta \end{pmatrix}$$

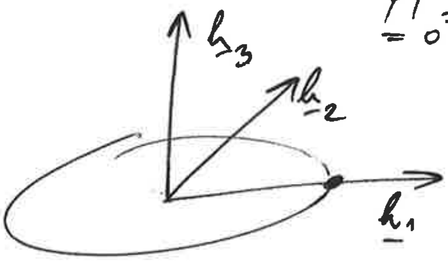
$$\Rightarrow \underline{\underline{h}} = \underline{\underline{G}}^{-1} \underline{\underline{f}} \cdot \underline{\underline{G}}$$

$$k(t) = k_0 + \xi_k$$
$$T(t) = T_0$$

$\xi_k \equiv$ weak noise, stationary
power spectrum $\bar{S}_k(\omega)$.

The helix frame

$$\left.\begin{aligned} \underline{\underline{h}}_0 &= \omega_0 \underline{\underline{E}}_3 \\ \underline{\underline{H}}_0 &= \exp t \underline{\underline{h}}_0 . \end{aligned}\right\} \text{ without noise.}$$



$$\underline{\underline{h}} = \omega_0 \underline{\underline{E}}_3 + \xi_j \underline{\underline{E}}_j$$

Einstein summation convention

$\xi_1 = 0.$

$$\xi_2 = -v_0 \sin\Theta\, \xi_k$$
$$\xi_3 = v_0 \cos\Theta\, \xi_k .$$

with noise

$$\underline{\underline{H}}(nT) = \exp(\Xi_j \underline{\underline{E}}_j)$$

How to compute Ξ_j ?

$$\underline{\underline{H}}(nT) = T\exp \int_0^{nT} dt \left[(\omega_0 + \xi_3) \underline{\underline{E}}_3 + \xi_2 \underline{\underline{E}}_2 \right]$$

$$= \sum_{k=0}^{\infty} \int_{0<t_1<\dots<t_k<nT} dt_1 \cdots dt_k \left[(\omega_0 + \xi_3(t_1)) \underline{\underline{E}}_3 + \xi_2(t_1) \underline{\underline{E}}_2 \right] \cdots \left[(\omega_0 + \xi_3(t_k)) \underline{\underline{E}}_3 + \xi_2(t_k) \underline{\underline{E}}_2 \right]$$

~~[illegible]~~

⚠ $\underline{\underline{E}}_2$ and $\underline{\underline{E}}_3$ do <u>not</u> commute

$\Rightarrow$ exact computation hopeless

$\Rightarrow$ approximation ~~[illegible]~~ for weak noise.

$\Rightarrow$ keep only terms linear in ξ_j

$$\underline{\underline{H}}(nT) = \underbrace{\exp nT \omega_0 \underline{\underline{E}}_3}_{\mathbb{1}} + O(\xi_3) + O(\xi_2) + \text{h.o.t.}$$

• First, take care of ξ_3:

$$\underline{\underline{H}}(nT) = \sum_{k=0}^{\infty} \int_{0<t_1<\dots<t_k<nT} dt_1 \cdots dt_k \prod_{\ell=1}^{k} \left(\omega_0 + \xi_3(t_\ell)\right) \underline{\underline{E}}_3 + \mathcal{O}(\xi_2)$$

$$= \sum_{k=0}^{\infty} \frac{1}{k!} \int_0^{nT} dt_1 \cdots \int_0^{nT} dt_k \prod_{\ell=1}^{k} \left(\omega_0 + \xi_3(t_\ell)\right) \underline{\underline{E}}_3$$

$$= \sum_{k=0}^{\infty} \frac{1}{k!} \left[\int_0^{nT} dt \left(\omega_0 + \xi_3(t)\right) \underline{\underline{E}}_3 \right]^k$$

$$= \exp \int_0^{nT} dt \left(\omega_0 + \xi_3(t)\right) \underline{\underline{E}}_3 . \quad + \mathcal{O}(\xi_2)$$

$$= \exp \int_0^{nT} dt \; \xi_3(t) \; \underline{\underline{E}}_3 . \quad + \mathcal{O}(\xi_2)$$

That was easy, now comes the hard part.

• let's tackle $\mathcal{O}(\xi_2)$

Simplify life using complex notation:

$$\underline{\underline{Y}} = \underline{\underline{E}}_1 + i\,\underline{\underline{E}}_2$$

$$\xi_Y = \xi_1 - i\,\xi_2$$

$\underline{\underline{Y}}$ and $\underline{\underline{E}}_3$ do not commute, but we can prove

$$\underline{\underline{E}}_3 \cdot \underline{\underline{Y}} = \underline{\underline{Y}} \cdot (\underline{\underline{E}}_3 - i\,\mathbb{1}), \quad \text{hence}$$

$$\underline{\underline{E}}_3^{\,e} \cdot \underline{\underline{Y}} = \underline{\underline{Y}}\,(\underline{\underline{E}}_3 - i\,\mathbb{1})^e$$

Now, we are ready

$$\underline{\underline{H}}(nT) = T\exp \int_0^{nT} \omega_0 \underline{\underline{E}}_3 + \xi_Y(t)\,\underline{\underline{Y}} + \mathcal{O}(\xi_3)$$

$$= \sum_{k=-1}^{\infty} \int_{0<t_1<\dots<t_{k+1}<nT} dt_1 \dots dt_{k+1} \prod_{e=0}^{k+1} \left(\omega_0 \underline{\underline{E}}_3 + \xi_Y(t_{e+1})\,\underline{\underline{Y}}\right)$$

$$= \mathbb{1} + \sum_{k=0}^{\infty} \int_{0<t_1<\dots<t_{k+1}<nT} dt_1 \dots dt_{k+1} \sum_{e=0}^{k} (\omega_0 \underline{\underline{E}}_3)^e \cdot \xi_Y(t_{e+1})\,\underline{\underline{Y}}\,(\omega_0 \underline{\underline{E}}_3)^{k-e}$$

$$= \mathbb{1} + \sum_{k=0}^{\infty} \int_0^{nT} dt \sum_{e=0}^{k} \frac{t^e}{e!} \frac{(nT-t)^{k-e}}{(k-e)!}\, \omega_0^{\,k}\, \xi_Y(t) \cdot \underbrace{\underline{\underline{E}}_3^{\,e} \cdot \underline{\underline{Y}} \cdot \underline{\underline{E}}_3^{\,k-e}}_{\underline{\underline{Y}} \cdot (\underline{\underline{E}}_3 - i\mathbb{1})^e \cdot \underline{\underline{E}}_3^{\,k-e}} + \text{h.o.t.}$$

Do you see the binomial formula?

$$\sum_{l=0}^{k} \frac{t^l}{l!} \frac{(nT-t)^{k-l}}{(k-l)!} (\underline{\underline{E}}_3 - i\mathbb{1})^{l} \underline{\underline{E}}_3^{k-l}$$

$$= \frac{1}{k!} \sum_{l=0}^{k} \binom{k}{l} (t\,\underline{\underline{E}}_3 - i t\,\mathbb{1})^l [(nT-t)\underline{\underline{E}}_3]^{k-l}$$

$$= \frac{1}{k!} \quad nT\,(\underline{\underline{E}}_3 - i t\,\mathbb{1})^k$$

Back to work:

$$\underline{\underline{H}}(nT) = \ldots =$$

$$= \mathbb{1} + \sum_{k=0}^{\infty} \frac{1}{k!} \int_0^{nT} dt \;\; \xi_Y(t) \underline{\underline{Y}} (2\pi n \underline{\underline{E}}_3 - i\omega_0 t\,\mathbb{1})^k$$

$$+ h.o.t$$

$$= \mathbb{1} + \int_0^{nT} dt \;\; \xi_Y(t)\, \underline{\underline{Y}} \cdot \underbrace{\sum_{k=0}^{\infty} (2\pi n\,\underline{\underline{E}}_3 - i\omega_0 t\,\mathbb{1})^k \frac{1}{k!}}$$

$$= \exp(2\pi n \underline{\underline{E}}_3 - i\omega_0 t\,\mathbb{1})$$

$$= \exp(2\pi n\,\underline{\underline{E}}_3) \cdot \exp(-i\omega_0 t\,\mathbb{1})$$

$$= \mathbb{1} \exp(-i\omega_0 t) \cdot \mathbb{1}.$$

$$= \mathbb{1} + \underbrace{\int_0^{nT} dt \;\; \xi_Y(t)\; e^{-i\omega_0 t}}_{\Xi_Y} \cdot \underline{\underline{Y}} \quad + h.o.t.$$

$$\approx \exp \Xi_Y \cdot \underline{\underline{Y}} \qquad + h.o.t.$$

with

$$\Xi_Y = \int_0^{nT} dt \;\; \xi_Y(t)\, e^{-i\omega_0 t}.$$

Almost done.
What is

$\langle \Xi_y \Xi_y^* \rangle$?

$$\langle \Xi_y \Xi_y^* \rangle = (v_0 \sin\theta)^2 \int_0^{nT} dt_1 \int_0^{nT} dt_2 \, \underbrace{\underbrace{\langle \zeta_k(t_1)\, \zeta_k(t_2) \rangle}_{\text{auto-correlation fct.}} e^{-i\omega_0(t_1-t_2)}}_{\approx \text{ Fourier trf. of auto-correlation function. (WIENER-KHICHINE)}}$$

$$= (v_0 \sin\theta)^2 \, nT \cdot \tilde{S}_k(\omega)$$

On the other hand:

$$C_{11} = \langle \Xi_1^2 \rangle \approx 2D_{rot} \cdot t$$

for $T_k \ll t \ll \frac{1}{D_{rot}}$

$$C_{22} = \langle \Xi_2^2 \rangle \approx 2D_{rot} \cdot t$$

$\Rightarrow$

$$4D_{rot} = (v_0 \sin\theta)^2 \tilde{S}_k(\omega_0).$$

$\Rightarrow$ persistence length

$$l_p = w_0 h_0 t_p, \quad t_p = \frac{1}{2D_{rot}}.$$

$$\langle \underline{h}_3(0) \cdot \underline{h}_3(t) \rangle = \exp\left(-\, t/t_P\right).$$

<u>Outlook</u>

- coupling rotation + translation
- coupling with steering

$$\dot{\psi} = -\beta \sin\psi + \xi + D_{rot} \cot\psi.$$

$$\langle \xi(t_1)\, \xi(t_2) \rangle = 2 D_{rot}\, \delta(t_1 - t_2).$$