FPE: $\frac{\partial}{\partial t} P = \mathcal{L} P$, $\mathcal{L} = \sum_{ij} \frac{\partial^2}{\partial x_i \partial x_j} D^{(2)}_{ij} - \sum_i \frac{\partial}{\partial x_i} D^{(1)}_i$

$\Leftrightarrow$ Langevin eq.

$$\underbrace{\frac{d}{dt} x_i = D^{(1)}_i + f_i(t)}_{\text{formal way of writing}} \qquad \langle f_i(t) f_j(t') \rangle = 2 D^{(2)}_{ij} \delta(t-t')$$

$$\longrightarrow x_i(t+\tau) = x_i(t) + D^{(1)}_i \tau + \sqrt{2\tau}\, r_i \qquad t \to 0$$

$$\langle r_i \rangle = 0, \quad \langle r_i r_j \rangle = D^{(2)}_{ij}$$

so-called

ITO interpretation

$$\vec{v} = \frac{1}{\xi}\vec{F} \qquad \vec{F} = \xi \vec{v}$$

Brownian Dynamics with Hydrodynamic Interactions (BD + HI)

$\underline{D_{ij}}$ has non-vanishing off-diagonal elements

correlations from the flow field

$$\mathcal{L} = \sum_{ij} \frac{\partial^2}{\partial x_i \partial x_j} D_{ij} - \sum_i \frac{\partial}{\partial x_i} \phi_i$$

determ. displacement

$$D_{ij} = D_{ij}(\{x\})$$

<u>Ito Langevin:</u>

$$\frac{d}{dt} x_i = \phi_i + f_i \qquad \langle f_i(t) f_j(t') \rangle = 2 \underline{D_{ij}}\, \delta(t - t')$$

$$\mathcal{L} \exp(-\beta \mathcal{H}) = 0$$

$\mathcal{H} = U$

$$\frac{\partial}{\partial x_i}\frac{\partial}{\partial x_j} D_{ij} = \underline{\frac{\partial}{\partial x_i} D_{ij} \frac{\partial}{\partial x_j}} + \text{something}$$

$$\frac{\partial}{\partial x_j}\left(D_{ij} P\right) = \frac{\partial D_{ij}}{\partial x_j} P + \underline{D_{ij}\frac{\partial}{\partial x_j} P}$$

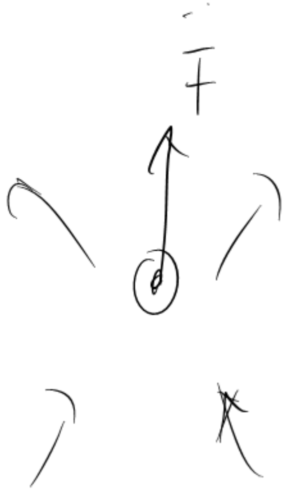
$$\mathcal{L} = \sum_i \frac{\partial}{\partial x_i}\left\{\sum_j \left(\frac{\partial D_{ij}}{\partial x_j} + D_{ij}\frac{\partial}{\partial x_j}\right) - \phi_i\right\} \Rightarrow 0 = \mathcal{L}\exp(-\beta\mathcal{H})$$

$$= \sum_i \frac{\partial}{\partial x_i}\left\{\sum_j \left(\frac{\partial D_{ij}}{\partial x_j} - \beta D_{ij}\frac{\partial \mathcal{H}}{\partial x_j}\right) - \phi_i\right\}\exp(-\beta\mathcal{H})$$

$$\Rightarrow \phi_i = \sum_j \left(\frac{\partial D_{ij}}{\partial x_j} - \beta D_{ij} \frac{\partial U}{\partial x_j} \right) =$$

$$= \underbrace{\sum_j \frac{\partial D_{ij}}{\partial x_j}}_{\text{often zero}} + \sum_j \underbrace{\beta D_{ij}}_{\underset{\approx}{\mu_{ij}}\ \text{mobility tensor}} F_j \checkmark$$

force on particle j generates velocity at particle i, of size $\underline{\underline{\mu_{ij} F_j}}$ $\qquad \underline{\underline{\tilde{\mu} = ??}}$



$\vec{u}(\vec{r}) = ?$ $\rho = \text{const.}$

$$\vec{\nabla} \cdot \vec{u} = 0$$

$$\underbrace{\rho \frac{\partial \vec{u}}{\partial t}}_{=0} = -\vec{\nabla} p + \eta \vec{\nabla}^2 \vec{u} + \vec{F}\delta(\vec{r})$$

$$\longrightarrow \vec{u}(\vec{r}) = \frac{1}{(2\pi)^3} \int d^3\vec{k}\; \vec{v}(\vec{k})\, e^{-i\vec{k}\cdot\vec{r}}$$

$$p(\vec{r}) = \frac{1}{(2\pi)^3} \int d^3\vec{k}\; \tilde{p}(\vec{k})\, e^{-i\vec{k}\cdot\vec{r}}$$

$$\delta(\vec{r}) = \frac{1}{(2\pi)^3} \int d^3\vec{k}\, e^{-i\vec{k}\vec{r}}$$

$$-i\vec{k}\cdot\vec{v} = 0 \qquad \hat{k} = \frac{\vec{k}}{k}$$

$$0 = +i\vec{k}\tilde{p} - \eta k^2 \vec{v} + \vec{F} \quad \Big| \cdot i\vec{k}\cdot \qquad \hat{r} = \frac{\vec{r}}{r}$$

$$0 = -k^2\tilde{p} + i\vec{k}\cdot\vec{F} \qquad \tilde{p} = \frac{i\vec{k}\cdot\vec{F}}{k^2}$$

$$i\vec{k}\tilde{p} = -\frac{1}{k^2}\vec{k}(\vec{k}\cdot\vec{F}) = -\hat{k}\otimes\hat{k}\,\vec{F}$$

$$\vec{v} = \frac{1}{\eta k^2}\left(\mathbb{1} - \hat{k}\otimes\hat{k}\right)\vec{F} \qquad \vec{u}(\vec{r}) = \vec{\mu}(\vec{r})\,\vec{F}$$

$$\boxed{\vec{\mu}(\vec{r}) = \frac{1}{(2\pi)^3}\frac{1}{\eta}\int d^3\vec{k}\,\frac{1}{k^2}\left(\mathbb{1} - \hat{k}\otimes\hat{k}\right)e^{-i\vec{k}\vec{r}}}$$

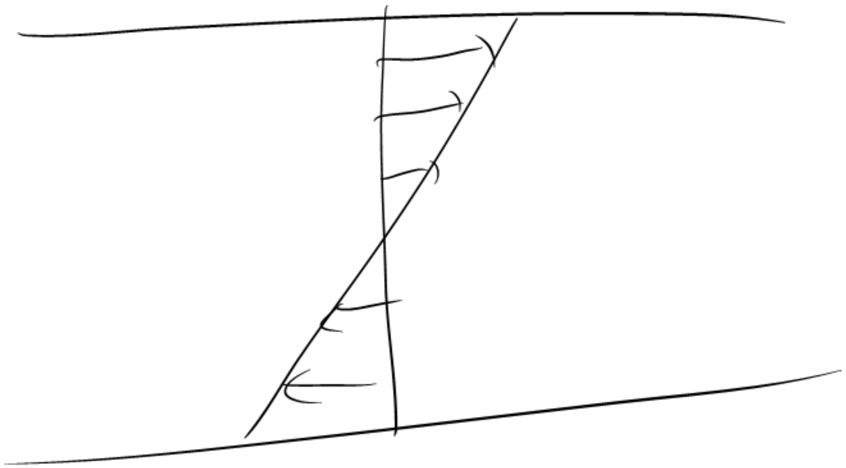
$$\mu_{\alpha\beta} = A(r)\,\delta_{\alpha\beta} + B(r)\,\hat{r}_\alpha \hat{r}_\beta$$

$$\mu_{\alpha\beta}\delta_{\alpha\beta} = \mu_{\alpha\alpha} = \mathrm{tr}(\overleftrightarrow{\mu}) = 3A(r) + B(r)$$

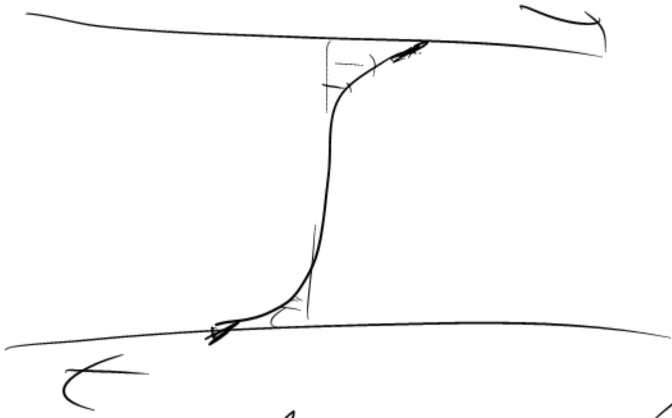
$$\mu_{\alpha\beta}\hat{r}_\alpha \hat{r}_\beta = A(r) + B(r) \Rightarrow \dots \Rightarrow$$

$$\overleftrightarrow{\mu}(\vec{r}) = \frac{1}{8\pi\eta r}\left(\mathbb{1} + \hat{r}\otimes\hat{r}\right)$$ Oseen tensor

const



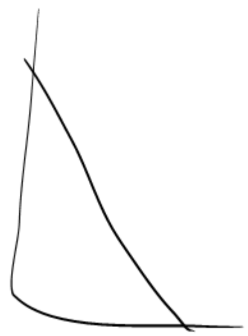
artifact of SD:



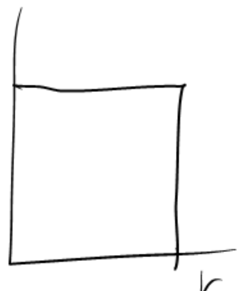
scr. length $\sim \frac{1}{r_\xi}$

$\xi(r)$

or $\xi(r)$

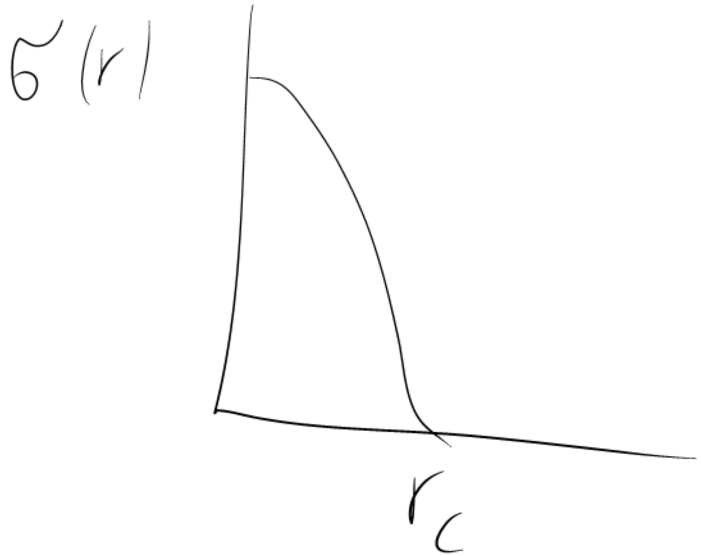


or $\xi(r)$



$\xi > 0$

compact support



$\sigma(r)$: same properties

(same r_c, $\sigma > 0$)

FDT $\longrightarrow$ $\sigma^2 = k_B T \xi$