$Z \quad \zeta \quad \zeta \quad \zeta \quad \zeta$ zeta

#1

#15

x_i

friction coefficient

Langevin

$$m_x \ddot{x} = f(x, v, t) - \frac{\partial E(x)}{\partial x} - \gamma \dot{x} + \xi$$

external force

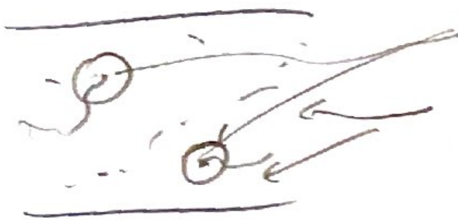
$$\sigma_\xi^2 = \frac{2\gamma}{\beta} \delta(t)$$

Delta correlated white noise.

overdamped Langevin
(Brownian

$0 =$

[Free energy as function of coordinate is Potential of Mean Force] #2



x slow

y fast

F_{xy}

$E(x,y)$ Joint energy

Mean force on x $= \left\langle \frac{\partial E}{\partial x} \right\rangle = \int dy \, P(y|x) \frac{\partial E}{\partial x}$

$$P(y|x) = \frac{P(x,y)}{P(x)} = \frac{e^{-\beta E(x,y) + \cancel{\beta F_{xy}}}}{\int dy \, e^{-\beta E(x,y) + \cancel{\beta F_{xy}}}}$$

Pointwise free energy

define $F_{XY}(x) = -\frac{1}{\beta} \ln \int dy \, e^{-\beta E(x,y)}$

$$\frac{\partial F_{xy}(x)}{\partial x} = \frac{\int dy \, e^{-\beta E(x,y)} \frac{\partial E}{\partial x}}{\int dy \, e^{-\beta E(x,y)}} = \int dy \, P(y|x) \frac{\partial E}{\partial x} = \left\langle \frac{\partial E}{\partial x} \right\rangle$$

$= E^{MF}$

#3

Berezhkovskii & Szabo 2011

(Klein-Kramers = Fokker-Planck underdamped
= Smoluchowski eq

$$m\ddot{x} = f_x(t) - \frac{\partial E(x,y)}{\partial x} = -\frac{\partial}{\partial x}E^{MF}(x) + \delta f_x$$

$$\delta f_x = -\frac{\partial E(x,y)}{\partial x} + \left\langle \frac{\partial E(x,y)}{\partial x} \right\rangle_y$$

Approximations $\delta f_x = 0$

Friction wrt to displacement

or δf_x is delta correlated white noise

force $\gamma = \beta \int_0^\infty \langle \delta f_x(0)\, \delta f_x(t) \rangle \, dt$

Sivak et al 2012

$\delta\left(\frac{\partial F(x)}{\partial x}\right)$

$$\delta f_x \approx -\gamma \dot{x} + c\,\xi$$

$c \downarrow \sqrt{\frac{2\gamma}{\beta}}$ Fluctuation dissipation Theorem

$D = \frac{\mu}{\beta}$ ← mobility $= \frac{\langle v \rangle}{F^{ex}} = \frac{1}{\beta\gamma}$

diffusion coeffn

Einstein Relation

$(\beta\gamma)^{-1} = D$ (γ could be matrix)

low Reynolds number Re

(Ratio of inertial to viscous forces)

(Micro bodies at low Reynolds #)

Stokes - Einstein eq. $D = \frac{1}{\beta\, 6\pi\eta r}$ ← Radius

↑ Viscosity

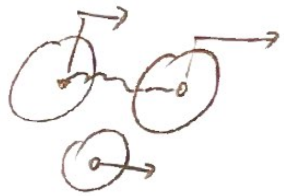
$\gamma = 6\pi\eta r$ ← friction scale ∝ Radius.

Effective Mass $P(v) \propto \frac{e^{-\frac{\beta}{2} m_x v^2}}{\sqrt{2\pi/\beta m_x}}$

#5

Problems → Aggradation of N particles Radius ~ $N^{1/3}$ $D \sim \frac{1}{N^{1/3}}$

But in Langevin does not work



everyone has to move in same direction! $D \overset{?}{\sim} \frac{1}{e^N}$

Why? Langevin breaks Galileon symmetries No absolute frame of rest.

Potential Solution Dissipative Particle Dynamics

dissipative - fluctuating force between particles.

Langevin Path Action

Hunt & Ross 1981

$$m\ddot{x}(t) = f(x) - \gamma(x)\dot{x}(t) + \xi(t) \qquad \langle \xi_i \rangle = 0 \qquad \langle \xi_i(0)\,\xi_j(t) \rangle = \frac{2\gamma}{\beta}\delta(t)$$

$$P[x\,|\,x(0)] \propto e^{-A^{\text{action (or } S)}} \propto e^{-\int \mathcal{L}(t)\,dt}$$

$$P[\xi(t)] = \left(\frac{\beta}{\pi}\right)^{\frac{d}{2}} |\gamma|^{-1/2}\, e^{-\frac{\beta}{4}\xi^T(t)\,\gamma^{-1}\,\xi(t)}$$

[Multidimensional Normal]

$$P[\xi] \propto \exp\left(-\frac{\beta}{4}\int \xi^T \gamma^{-1} \xi \, dt\right)$$

$$P[x\,|\,x(0)] \propto J\, e^{-\int dt\, \mathcal{L}(t)}$$

Jacobian is path independent

$$\mathcal{L} \propto \frac{1}{4}\beta\left(m\ddot{x} - f(x) + \gamma\dot{x}\right)^T \gamma^{-1}\left(m\ddot{x} - f(x) + \gamma\dot{x}(t)\right) + C$$

$$+ \frac{1}{2}\ln|\beta\gamma^{-1}|$$

Sekimoto 1998

$$A = \int \mathcal{L}\, dt, \quad \mathcal{L} = \frac{1}{2}\beta\left(m\ddot{x} - f(x)\right)\dot{x} \qquad ①$$

$$+ \frac{1}{4}\beta\left[m\ddot{x} - f(x)\right]^T \gamma^{-1}\left[m\ddot{x} - f(x)\right] \qquad ②$$ low friction

$$+ \frac{1}{4}\beta\dot{x}^T \gamma\, \dot{x} \qquad ③$$ high friction

$$+ \frac{1}{2}\ln|\beta\gamma^{-1}| \qquad ④$$

①

$$\cancel{Q =} \frac{\partial E}{\partial x}\frac{\partial x}{\partial t}\frac{d}{\partial \lambda} E(x, \dot{x}, \lambda) = \frac{\partial E}{\partial x}\frac{dx}{dt} + \frac{\partial\left(\frac{1}{2}m\dot{x}^2\right)}{\partial \dot{x}}\frac{d\dot{x}}{dt} + \underbrace{\frac{dE}{\partial \lambda}\frac{\partial \lambda}{\partial t}}_{W}$$

$$-f\dot{x} \qquad m\ddot{x}\dot{x}$$

$$\underbrace{(m\ddot{x} - f)\dot{x}}_{Q} + W$$

$$\frac{A - \tilde{A}}{2} = \beta Q$$

~~[illegible]~~ friction, ~~[illegible]~~ ② dominates

$$m\ddot{x} \cancel{=} - f(x) = 0$$

(classical