Introduction to

Stochastic Thermodynamics

Lecture 1

The 22nd KIAS-APCTP Winter School on Statistical Physics

January 6 ~10, 2025

Jae Sung Lee

Korea Institute for Advanced Study

imagine the impossible

KIAS KOREA INSTITUTE FOR ADVANCED STUDY

Lecture Overview

Lecture 1

1) Langevin & Fokker-Planck equation
2) Stochastic calculus

Lecture 2

1) Heat & Work
2) Stochastic trajectory

Lecture 3

1) Entropy production
2) Thermodynamic Uncertainty Relations

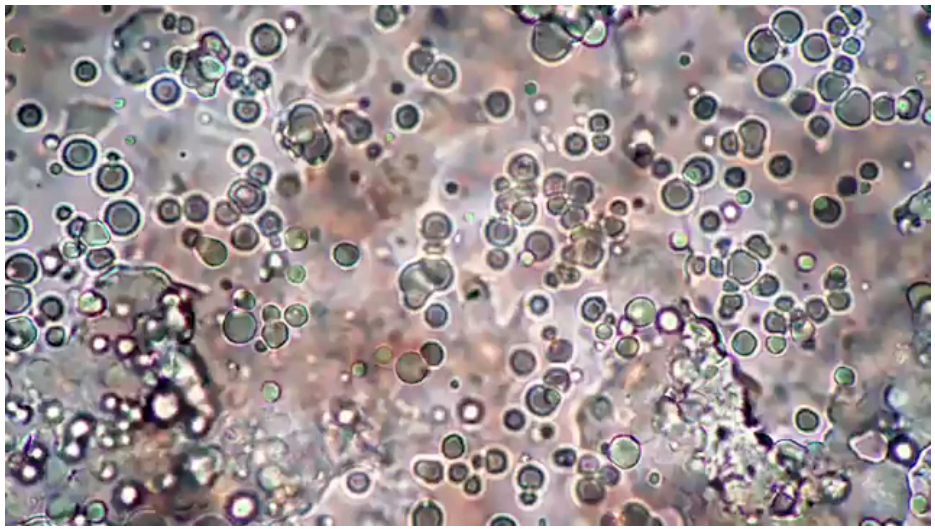
Lecture 4

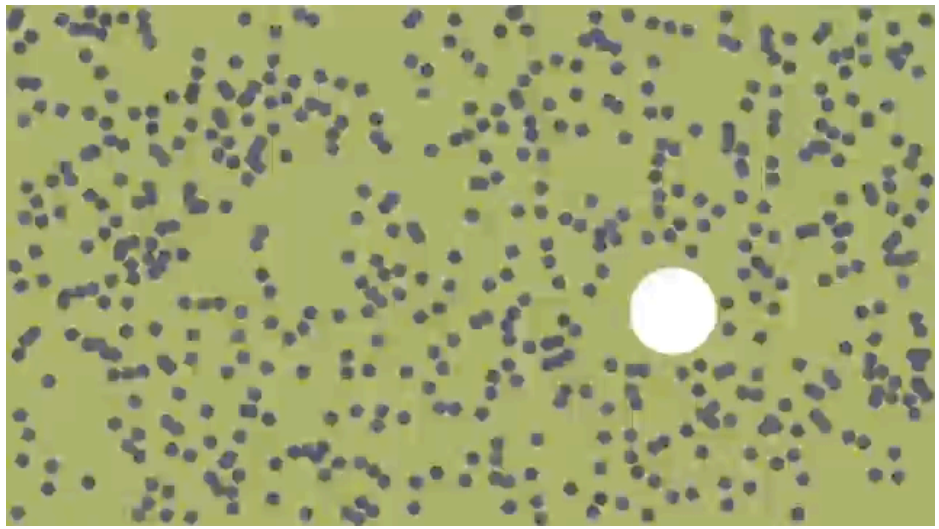
1) Eigenfunction of Fokker-Planck equation
2) Calculation of mean & variance of observables

Brownian Motion

https://www.youtube.com/watch?v=ZNzoTGv_XiQ

: motion connecting mesoscopic and microscopic worlds

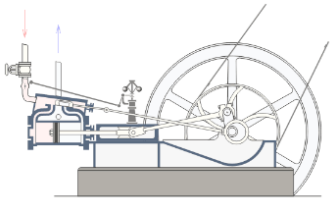




Brownian Motion: When Does It Occur?

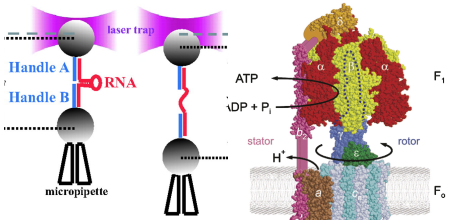
10^0 m 10^{-3} m 10^{-6} m 10^{-9} m

meso/microscopic system



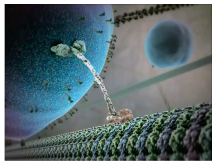
Motion is deterministic.

Brownian particle,
many biological systems



RNA folding
/unfolding

F1-motor



kinesin

In microscopic scale, motion is not deterministic,
but random or stochastic.



YouTube: Myosin V molecular motor

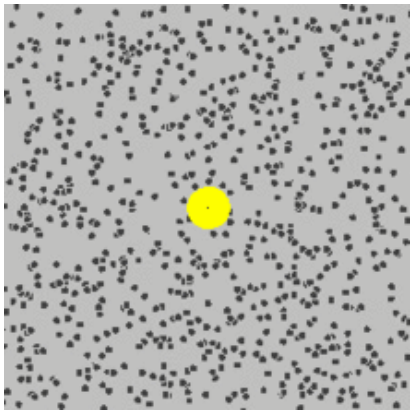
Brownian Motion

Source of stochasticity - environment

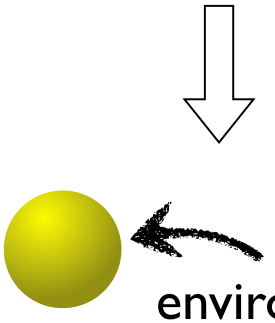
: interaction between a system and environmental particles

→ In principle, the motion is deterministic.

→ But, practically infeasible to keep track of all degrees of freedom of environmental particles.



Wikipedia: Brownian motion

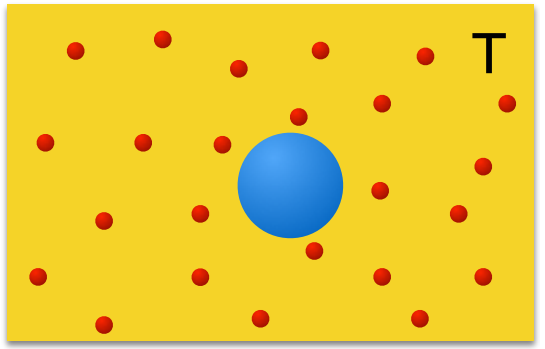


→ treat the environmental interaction as a simple random noise

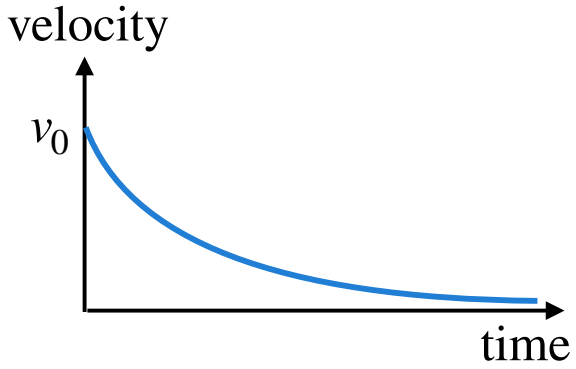
- Langevin equation (continuous state)
- master equation (discrete state)

I. Langevin equation

: phenomenological description of the interaction of environmental particles



1) dissipation

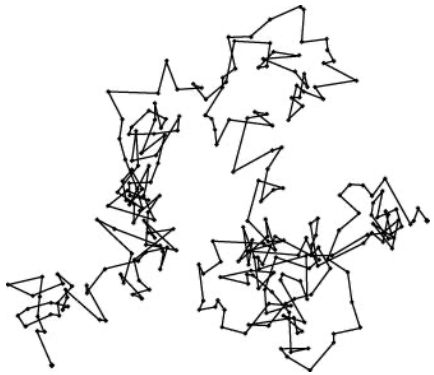


$$m\dot{v} = -\gamma v$$

(m : mass, γ : dissipation coefficient)

$$\therefore\ v(t) = v(0)e^{-\gamma t/m} \quad \rightarrow \quad v = 0 \text{ in the long time limit?}$$

2) random motion



$$m\dot{v} = -\gamma v + \sigma\xi \quad (\xi : \text{white} - \text{Gaussian random noise})$$

i) $\langle\xi\rangle = 0 \quad \Rightarrow \quad m\langle\dot{v}\rangle = -\gamma\langle v\rangle$

ii) $\langle\xi(t)\xi(t')\rangle = \delta(t-t')$ (Markovian noise)

$$\therefore\ v(t) = v(0)e^{-\gamma t/m} + e^{-\gamma t/m}\int_0^t dt' e^{\gamma t'/m}\sigma\xi(t')/m$$

$$\rightarrow \lim_{t\to\infty}\langle v^2(t)\rangle = \frac{\sigma^2}{2\gamma m} = \frac{k_B T}{m} \qquad \Rightarrow D \equiv \frac{\sigma^2}{2} = \gamma k_B T$$

(equipartition) (Einstein)

I. Langevin equation

1) underdamped Langevin equation

$$\dot{x} = v, \quad m\dot{v} = -\partial_x U(\lambda, x) + f_{\rm nc} - \gamma v + \sigma\xi \quad \Rightarrow \quad \dot{x} = v, \quad \dot{v} = \frac{1}{m}\left[-\partial_x U(\lambda, x) + f_{\rm nc} - \gamma v + \sigma\xi\right]$$

force from the heat bath

$$\langle \xi \rangle = 0 \qquad \langle \xi(t)\xi(t') \rangle = \delta(t - t')$$

2) overdamped Langevin equation

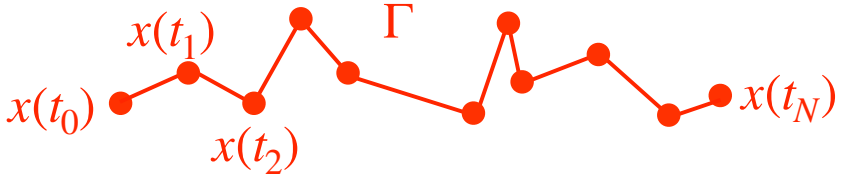
Velocity relaxation time: $\tau_{\rm r} = \dfrac{m}{\gamma} \ll \tau_{\rm obs}$

$$(m\dot{v} = -\gamma v)$$

→ velocity is always in equilibrium

Schematic of a stochastic system

$t_n \equiv n\tau_{\rm obs} + t_0 \quad (t_N = \tau)$



$$m\dot{v} = -\partial_x U(\lambda, x) + f_{\rm nc} - \gamma v + \sigma\xi$$

neglect inertia term $\qquad = -\gamma\dot{x}$

$$\gamma\dot{x} = -\partial_x U(\lambda, x) + f_{\rm nc} + \sigma\xi \quad \Rightarrow \quad \dot{x} = \frac{1}{\gamma}\left[-\partial_x U(\lambda, x) + f_{\rm nc} + \sigma\xi\right]$$

1. Langevin equation

1) underdamped Langevin equation

$$\dot{x} = v$$

$$\dot{v} = \frac{1}{m}\left[-\partial_x U(\lambda, x) + f_{\mathrm{nc}} - \gamma v + \sigma\xi\right]$$

2) overdamped Langevin equation

$$\dot{x} = \frac{1}{\gamma}\left[-\partial_x U(\lambda, x) + f_{\mathrm{nc}} + \sigma\xi\right]$$

(1 dim) $\dot{z} = A + B\xi$

ex) overdamped

$$z = x$$

$$A = \frac{1}{\gamma}\left[-\partial_x U(\lambda, x) + f_{\mathrm{nc}}\right] \qquad B = \frac{\sigma}{\gamma}$$

(*N* dim) $\dot{z}_i = A_i + \sum_{j=1}^{N} B_{ij}\xi_j$

ex) underdamped

$$\begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} x \\ v \end{bmatrix} \qquad \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} = \begin{bmatrix} v \\ \dfrac{-\partial_x U(\lambda, x) + f_{\mathrm{nc}} - \gamma v}{m} \end{bmatrix}$$

$$\begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & \sigma/m \end{bmatrix}$$

2. Langevin equation & Fokker-Planck equation

(1 dim) $\dot{z} = A + B\xi$

$P(z, t)$: probability distribution of z at time t

Governing equation for $P(z, t)$: Fokker-Planck (FP) equation

$$\partial_t P(z,t) = -\partial_z (A - \partial_z D) P(z,t) \qquad D = B^2/2$$

Risken, The Fokker-Planck equation

Gardiner, Stochastic Methods

Probability current $J(z, t)$

$$\partial_t P(z,t) = -\partial_z J(z,t) \qquad J(z,t) = (A - \partial_z D) P(z,t)$$

(ex1) Write FP equation for $\gamma \dot{x} = -kx + \sqrt{2k_B \gamma T}\,\xi$

2. Langevin equation & Fokker-Planck equation

(*N* dim) $\dot{z}_i = A_i + \sum_{j=1}^{N} B_{ij}\xi_j$

$P(z,t)$: probability distribution of z at time t $\qquad z = (z_1, z_2, \cdots, z_N)$

Governing equation for $P(z,t)$: Fokker-Planck (FP) equation

$$\partial_t P(z,t) = -\sum_{i=1}^{N} \partial_{z_i}\left(A_i - \sum_{j=1}^{N} \partial_{z_j} D_{ij}\right) P(z,t) \qquad D = \frac{1}{2}BB^{\mathrm{T}} \qquad J_i(z,t) = \left(A_i - \sum_{j=1}^{N} \partial_{z_j} D_{ij}\right) P(z,t)$$

(ex1) Write FP equation for $\gamma\dot{x} = -kx + \epsilon y + \sqrt{2k_{\mathrm{B}}\gamma T_x}\xi_x$, $\gamma\dot{y} = -ky + \delta x + \sqrt{2k_{\mathrm{B}}\gamma T_y}\xi_y$

(ex2) Write FP equation for $\dot{x} = v$, $\dot{v} = \frac{1}{m}\left[f(x,t) - \gamma v + \sqrt{2k_{\mathrm{B}}\gamma T}\xi\right]$

3. Stochastic Calculus

1) Wiener process: pure Brownian motion

$$\dot{z} = A + B\xi \qquad (z = x,\ \ A = 0,\ \ B = 1)$$

$$\rightarrow \dot{x} = \xi$$

Define $\quad W(t) \equiv x(t) - x(0) = \int_0^t \xi(s)ds \ = \int_0^t dW(s)$

Autocorrelation of $W(t)$

$$\langle W(t)W(t')\rangle \ = \min\{t, t'\}$$

$$\langle dW(t)dW(t)\rangle = dt$$

$$\therefore \langle \xi(t)\xi(t)\rangle \rightarrow 1/dt$$

3. Stochastic Calculus

2) Stochastic product

$$\dot{z} = A + B\xi \qquad (A = f(z(t)),\ \ B = 0)$$

$$\rightarrow \dot{z} = f(z(t))$$

regular function product

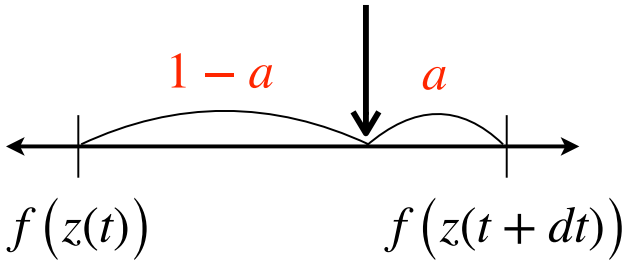
$$\left\langle f\left(z(t)\right)\dot{z}(t)\right\rangle \underset{?}{=} \left\langle f\left(z(t+dt)\right)\dot{z}(t)\right\rangle = \left\langle \left[f\left(z(t)\right) + \partial_z f\left(z(t)\right)\dot{z}(t)dt\right]\dot{z}(t)\right\rangle$$

$$z(t+dt) = z(t) + \dot{z}(t)dt$$

$$= \left\langle f\left(z(t)\right)\dot{z}(t)\right\rangle + \left\langle \partial_z f\left(z(t)\right)\dot{z}^2(t)\right\rangle dt$$

$$\left\langle \partial_z f\left(z(t)\right)\dot{z}^2(t)\right\rangle dt = 0 \quad (dt \rightarrow 0 \text{ limit})$$

$$f^a(t) \equiv (1-a)f\left(z(t+dt)\right) + af\left(z(t)\right)$$



$$\left\langle f\left(z(t)\right) \odot_a \dot{z}(t)\right\rangle \equiv \langle f^a(t)\dot{z}(t)\rangle$$

$$= (1-a)\left\langle f\left(z(t+dt)\right)\dot{z}(t)\right\rangle + a\left\langle f\left(z(t)\right)\dot{z}(t)\right\rangle$$

$$= \left\langle f\left(z(t)\right)\dot{z}(t)\right\rangle$$

3. Stochastic Calculus

2) Stochastic product

$$\dot{z} = A + B\xi \qquad (A = f(z(t)),\ \ B = 1)$$

$$\rightarrow \dot{z} = f(z(t)) + \xi$$

Stochastic function product

$$\left\langle f\left(z(t)\right)\xi(t)\right\rangle \underset{?}{=} \left\langle f\left(z(t+dt)\right)\xi(t)\right\rangle$$

$$\langle f\left(z(t)\right)\xi(t)\rangle = \langle f\left(z(t)\right)\rangle\langle\xi(t)\rangle = 0$$

$$\left\langle f\left(z(t+dt)\right)\xi(t)\right\rangle = \left\langle \left[f\left(z(t)\right) + \partial_z f\left(z(t)\right)\dot{z}(t)dt\right]\xi(t)\right\rangle$$

$$= z(t) + \dot{z}(t)dt$$

$$= \left\langle f\left(z(t)\right)\xi(t)\right\rangle + \left\langle \partial_z f\left(z(t)\right)\dot{z}(t)\xi(t)\right\rangle dt$$

$$= \left\langle \partial_z f\left(z(t)\right) f\left(z(t)\right)\xi(t)\right\rangle dt + \partial_z f\left(z(t)\right)\underbrace{\left\langle \xi^2(t)\right\rangle dt}_{=1}$$

$$= \partial_z f\left(z(t)\right)$$

3. Stochastic Calculus

2) Stochastic product

$$\dot{z} = A + B\xi \qquad (A = f(z(t)),\ \ B = 1)$$

$$\rightarrow \dot{z} = f(z(t)) + \xi$$

Stochastic function product

$$\left\langle f\left(z(t)\right)\xi(t)\right\rangle \underset{?}{=} \left\langle f\left(z(t+dt)\right)\xi(t)\right\rangle$$

$$\langle f\left(z(t)\right)\xi(t)\rangle = \langle f\left(z(t)\right)\rangle\langle\xi(t)\rangle = 0$$

$$\left\langle f\left(z(t+dt)\right)\xi(t)\right\rangle = \partial_z f\left(z(t)\right)$$

$$\left\langle f\left(z(t)\right)\odot_a \xi(t)\right\rangle = (1-a)\left\langle f\left(z(t+dt)\right)\xi(t)\right\rangle + a\left\langle f\left(z(t)\right)\xi(t)\right\rangle = (1-a)\partial_z f\left(z(t)\right)$$

Stratonovich : $a = 1/2$ $(\circ \equiv \odot_{1/2})$ e . g . $f\left(z(t)\right)\circ\xi(t)$

Ito : $a = 1$ $(\bullet \equiv \odot_1)$ e . g . $f\left(z(t)\right)\bullet\xi(t)$

3. Stochastic Calculus

3) differentiation

$$\dot{z} = A + B\xi \qquad (A = f(z(t)),\ \ B = 1)$$

$$\rightarrow \dot{z} = f(z(t)) + \xi$$

$$df\left(z(t)\right) = f\left(z(t+dt)\right) - f\left(z(t)\right) = f\left(z(t) + dz(t)\right) - f\left(z(t)\right)$$

$$\approx f\left(z(t)\right) + \frac{\partial f}{\partial z}dz(t) + \frac{1}{2}\frac{\partial^2 f}{\partial z^2}dz^2(t) - f\left(z(t)\right)$$

$$= \left[\frac{\partial f}{\partial z} + \frac{1}{2}\frac{\partial^2 f}{\partial z^2}dz\right]dz$$

$dz^2(t) = \underbrace{(f^2 + 2f\xi)dt^2}_{O(dt^2)} + \underbrace{\xi^2 dt^2}_{O(dt)}$

$$= \frac{1}{2}\left[\frac{\partial}{\partial z}f\left(z(t+dt)\right) + \frac{\partial}{\partial z}f\left(z(t)\right)\right]dz = \frac{\partial}{\partial z}f\left(z(t)\right) \circ dz$$

expansion should be Stratonovich!

Revisit: Langevin equation & Fokker-Planck equation

(1 dim) $\dot{z} = A + B\xi \;\rightarrow \dot{z} = A(z(t)) + B(z(t))\xi$

Ito? Stratonovich?

$$\dot{z} = A(z(t)) + B(z(t)) \bullet \xi \quad \text{(Ito)}$$

$$\rightarrow z(t+dt) = z(t) + A(z(t))dt + B(z(t))dW(t)$$

$$\dot{z} = A(z(t)) + B(z(t)) \circ \xi \quad \text{(Stratonovich)}$$

$$\rightarrow z(t+dt) = z(t) + A(z(t))dt + \frac{1}{2}\left[B(z(t+dt)) + B(z(t))\right] dW(t)$$

$$= \frac{1}{2}\left[B(z(t)) + \partial_z B dz(t) + B(z(t))\right] dW(t)$$

$$= B(z(t))dW(t) + \frac{1}{2}\partial_z B dz(t) dW(t)$$

$$= B(z(t))dW(t) + \frac{1}{2}\partial_z B(A dt dW(t) + B\underbrace{dW^2(t)}_{dt})$$

$$= B(z(t))dW(t) + \frac{1}{2}B\partial_z B dt$$

$$\rightarrow z(t+dt) = z(t) + \left[A(z(t)) + \frac{1}{2}B\partial_z B\right] dt + B(z(t))dW(t)$$

Summary of Lecture 1

1. Langevin & FP equation

Langevin (1 dim): $\dot{z} = A + B\xi$

FP (1 dim): $\partial_t P(z,t) = -\partial_z (A - \partial_z D) P(z,t) \qquad D = B^2/2$

Langevin (N dim): $\dot{z}_i = A_i + \sum_{j=1}^{N} B_{ij}\xi_j$

FP (N dim): $\partial_t P(\boldsymbol{z},t) = -\sum_{i=1}^{N} \partial_{z_i} \left(A_i - \sum_{j=1}^{N} \partial_{z_j} D_{ij} \right) P(\boldsymbol{z},t) \qquad D = \frac{1}{2} B B^{\mathrm{T}}$

2. Stochastic calculus

Wiener process: $\langle dW(t) dW(t) \rangle = dt, \qquad \langle \xi(t)\xi(t) \rangle \to 1/dt$

Function product:

$$\left\langle f\left(z(t)\right) \odot_a \xi(t) \right\rangle = (1-a)\left\langle f\left(z(t+dt)\right)\xi(t) \right\rangle + a\left\langle f\left(z(t)\right)\xi(t) \right\rangle = (1-a)\partial_z f\left(z(t)\right)$$

Differentiation: $df\left(z(t)\right) = \frac{\partial}{\partial z} f\left(z(t)\right) \circ dz$