Lecture 7 "back to physics" ...

$\boxed{\text{Ornstein - Uhlenbeck process}}$

General SDE: $dx_t = \mu(x,t)\,dt + \sigma(x,t)\,dW$

Normalised Wiener process

O-U process is when

$$\boxed{dx_t = -\underbrace{\theta}_{}(x-\underbrace{x_0}_{})\,dt + \underbrace{\sigma}_{\text{constants}}\,dW}$$

we are familiar with

$$m\dot{v} = -\underbrace{\gamma v}_{\text{friction}} + \underbrace{\sqrt{2kT\gamma}}_{\text{thermal noise}} \cdot \xi(t)$$

Also overdamped:

$$\gamma\dot{x} = \underbrace{-k(x-x_0)}_{\text{spring force}} + \sqrt{2kT\gamma}\,\xi(t)$$

All physical systems near equilibrium....
So standard form

$$dx_t = -\frac{k}{\gamma}(x-x_0)\,dt + \sqrt{\frac{2kT}{\gamma}}\,dW$$

Note: $$X(t) = \int_0^t V(s)\, ds$$

$$\langle x^2(t) \rangle = \int_0^t ds_1 \int_0^t ds_2 \, \langle V(s_1) V(s_2) \rangle$$

$$\frac{d}{dt}\langle x^2(t)\rangle = 2 \int_0^t ds \, \underbrace{\langle V(t) V(s) \rangle}_{\text{ensemple averaging at fixed } t.}$$

$$\boxed{\text{for free diffusion} \quad \langle x^2 \rangle = 2Dt}$$

$$D = \int_0^t \langle V(t) V(s) \rangle ds = \int_0^t \langle V(\tilde{s}) V(0) \rangle d\tilde{s}$$

depends on $t - s = \tilde{s}$

Also: go back to free-diffusion SDE

multiply it by $V_0 = \text{const}$, $\langle \ldots \rangle$

$\langle V_0 \xi \rangle = 0$

$$m \frac{d}{dt} \langle V(t) \cdot V_0 \rangle = -\gamma \langle V(t) V_0 \rangle, \text{ hence}$$

$$\langle V(t) V(0) \rangle = V_0^2 \cdot e^{-\gamma/m \, t}$$

$\langle V_0^2 \rangle$: ensemble average with $P(v)$

"Memory" of initial velocity V_0 decays with $\tau_v = m/\gamma$

Then...

$$D = \langle v_0^2 \rangle \int_0^t ds\, e^{-\frac{\gamma}{m}s} = \langle v_0^2 \rangle \frac{m}{\gamma}\left(1 - e^{-\frac{\gamma}{m}t}\right)$$

"Diffusion" is constant only at

$t \gg m/\gamma$, then

$$\boxed{D = \langle v_0^2 \rangle \frac{m}{\gamma} = \frac{k_B T}{\gamma}}$$

But $\boxed{\left\langle \frac{mv^2}{2} \right\rangle = \frac{1}{2} kT}$

This is called Green-Kubo formula

$$\boxed{D = \int_0^{\infty} \langle v(t) v(0) \rangle \, dt}$$

Multiple variables in O-U proc.

$$\boxed{dx_i = -\theta_{ik} x_k \, dt + \sigma_{ik} \, dW_k}$$

(or equivalently $\frac{d}{dt} x_i = -\theta_{ik} x_k + \sigma_{ik} \xi_k$)

Don't need to be symmetric

Just like we did in 1D diffusion, solve this SDE set via Green's function:

$$X_i(t) = \int_{\underset{\text{initial}}{0}}^{t} e^{-\theta_{ik}(t-s)}\, \sigma_{kl}\, \xi_l(s)\, ds$$

Matrix elements $\begin{pmatrix} e^{-\theta_{11}(t-s)} & \cdots \\ \vdots & \ddots \end{pmatrix}$

Check by differentiation!

Construct a correlation function

$$M_{ik} = \langle X_i(t)\, X_k(t) \rangle$$

$$M_{ik} = \int_0^t ds_1 \int_0^t ds_2\; e^{-\theta_{ia}(t-s_1)}\, \sigma_{ab} \cdot e^{-\theta_{kp}(t-s_2)}\, \sigma_{pq} \cdot \underbrace{\langle \xi_b(s_1)\, \xi_q(s_2) \rangle}_{\delta_{bq} \cdot \delta(s_1 - s_2)}$$

$$= \int_0^t ds\; e^{-\theta_{ia}(t-s)}\, \sigma_{ab}\, \sigma^T_{bp}\, e^{-\theta^T_{pk}(t-s)}$$

So we have

$$M_{ik} = \int_0^t ds\, e^{-\theta_i (t-s)} \sigma_{\flat} \sigma^T_{bp} e^{-\theta^T_{pk}(t-s)}$$

(Recall $\int_0^t ds \, \langle v_0^2 \rangle e^{-\frac{\gamma}{m} t}$)

Call $t - s \to \tilde{s}$

$$\boxed{M_{ik} = \int_0^t d\tilde{s}\, e^{-\underline{\underline{\theta}}\tilde{s}} \sigma \sigma^T e^{-\underline{\underline{\theta}}^T \tilde{s}}}$$

take this to ∞

for 1D case: $M = \langle x^2 \rangle = \int_0^\infty dt\, e^{-2\theta t} \cdot \sigma^2 = \dfrac{\sigma^2}{2\theta}$

⊙ $m\dot{v} = -\gamma v + A(t)$

$\sqrt{2kT\gamma}\, \xi(t)$

$\downarrow$

$$\langle v_\infty^2 \rangle = \frac{2kT\gamma}{m^2 \cdot 2\gamma/m} = \frac{kT}{m} \quad ✓$$

⊙ $\gamma \dot{x} = -\varkappa x + \sqrt{\dfrac{2kT\gamma}{\gamma}}\, \xi(t)$

$\downarrow$

$$\langle x^2 \rangle = \frac{2kT\gamma}{\gamma^2 \cdot 2\varkappa/\gamma} = \frac{kT}{\varkappa} \quad ✓$$

in potential well

Let us construct

$$\underline{\underline{\theta}} \cdot \underline{\underline{M}} + \underline{\underline{M}} \cdot \underline{\underline{\theta}}^T$$

$$= \int_0^\infty \left(\underline{\underline{\theta}} \cdot e^{-\underline{\underline{\theta}} t} \cdot \underline{\underline{\sigma}}\,\underline{\underline{\sigma}}^T \cdot e^{-\underline{\underline{\theta}}^T t} + e^{-\underline{\underline{\theta}} t} \underline{\underline{\sigma}}\,\underline{\underline{\sigma}}^T e^{-\underline{\underline{\theta}}^T t} \underline{\underline{\theta}}^T \right) dt$$

this is the full $\frac{d}{dt}\left(e^{-\theta t} \sigma \sigma^T e^{-\theta^T t}\right)$

$$= -\int_0^\infty dt \frac{d}{dt}\left(e^{-\underline{\underline{\theta}} t} \underline{\underline{\sigma}}\,\underline{\underline{\sigma}}^T e^{-\underline{\underline{\theta}}^T t} \right) = \underline{\underline{\sigma}}\,\underline{\underline{\sigma}}^T$$

only at lower limit

General (multi-variable) form of Fluctuation - Dissipation relation

$$\boxed{\theta_{ik} \langle X_k X_l \rangle_{eq.} + \langle X_i X_k \rangle_{eq.} \theta_{lk} = \sigma_{ik} \sigma_{lk}}$$