Exercise 8

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1 Rates formulas

Consider a one-dimensional system governed by the overdamped Langevin equation

$$dx_t = -\frac{1}{m\gamma}\frac{d}{dx}V(x)dt + \sqrt{2D}\eta\,, \tag{1}$$

where m is the mass, γ is the friction, $D = \frac{k_B T}{m\gamma}$ is the diffusion constant and $V(x)$ is the potential energy function. The corresponding Fokker-Planck equation is written as

$$LP(x,t) = \frac{\partial P}{\partial t} = \left\{\frac{\partial}{\partial x}\left[\frac{1}{m\gamma}\frac{d}{dx}V(x)\right] + D\frac{\partial^2}{\partial x^2}\right\}P(x,t)\,, \tag{2}$$

and the backward Kolmogorov equation is written as

$$L^\dagger P(x,t) = \frac{\partial P}{\partial t} = \left\{\frac{\partial}{\partial x}\left[-\frac{1}{m\gamma}\frac{d}{dx}V(x)\right] + D\frac{\partial^2}{\partial x^2}\right\}P(x,t)\,. \tag{3}$$

From eq. 3 is possible derive the differential equation

$$-\frac{1}{m\gamma}\frac{d}{dx}V(x)\frac{d}{dx_0}\langle\tau\rangle + D\frac{\partial^2}{\partial x_0^2}\langle\tau\rangle = -1\,, \tag{4}$$

where $\langle\tau\rangle$ is the Mean First Passage Time (MFPT) requested by the system to reach a final destination x_F starting at x_0.

Pen-and-paper exercise

1. Solve eq. 4, find the Pontryagin formula for the MFPT

$$\langle\tau\rangle = \frac{1}{D}\int_{x_0}^{x_F} dx\, e^{\beta V(x)}\int_{-\infty}^{x} dx'\, e^{-\beta V(x')} \tag{5}$$

and the transition rate

$$k = \frac{1}{\langle\tau\rangle}\,. \tag{6}$$

2. Assume that the potential energy function $V(x)$ is a double well potential whose product region (left well) can be approximated by an harmonic potential

$$V(x) \approx V(x_A) + \frac{1}{2}\omega_A^2 m(x-x_A)^2\,, \tag{7}$$

around the minimum of the left well x_A and by

$$V(x) \approx V(x_B) - \frac{1}{2}\omega_B^2 m(x-x_B)^2\,, \tag{8}$$

close to the barrier x_B. Show that eq 6 can be approximated as

$$k \quad = \quad \frac{\omega_B}{\gamma}\cdot\frac{\omega_A}{2\pi}\exp\left(-\beta E_{AB}\right)\,, \tag{9}$$

with $E_{AB} = V(x_B) - V(x_A)$.

3. The Kramers rate for moderate friction is written as

$$k_{AB} = \frac{\gamma}{\omega_B}\left(\sqrt{\frac{1}{4}+\frac{\omega_B^2}{\gamma^2}} - \frac{1}{2}\right)\cdot\frac{\omega_A}{2\pi}\exp\left(-\beta E_{AB}\right)\,. \tag{10}$$

Show that eq. 10 can be approximated as eq. 9 in the high-friction regime.

2 Stochastic calculus

Consider the stochastic integral

$$\int_0^t W_s \, dW_s \,, \tag{11}$$

where W_s represents a Wiener process.

Pen-and-paper exercise

1. Solve eq. 11 using the Ito's integral
2. Solve eq. 11 using the Stratonovich integral.