

## EXERCISES

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**Exercise 1.** *Derive the Fokker-Planck operator  $\mathcal{L}$  for the OU process.*

The Ornstein-Uhlenbeck SDE is the equation,

$$dX = -\gamma X dt + \sigma dW. \quad (1)$$

The corresponding Fokker-Planck equation is,

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x}(\gamma x \rho) + \frac{1}{2} \frac{\partial^2}{\partial x^2}(\sigma^2 \rho). \quad (2)$$

Therefore, the Fokker-Planck operator for the OU process is

$$\mathcal{L}^\dagger \rho = \frac{\partial}{\partial x}(\gamma x \rho) + \frac{1}{2} \frac{\partial^2}{\partial x^2}(\sigma^2 \rho). \quad (3)$$

**Exercise 2.** *Show that  $\llbracket OABA \rrbracket$  and  $\llbracket BAOAB \rrbracket$  are conjugates, i.e., show that*

$$\left(\mathcal{U}_h^{\llbracket OABA \rrbracket}\right)^{n+1} = \mathcal{U}_{h/2}^A \circ \mathcal{U}_{h/2}^B \circ \left(\mathcal{U}_h^{\llbracket BAOAB \rrbracket}\right)^n \circ \mathcal{U}_{h/2}^B \circ \mathcal{U}_{h/2}^A \circ \mathcal{U}_h^O \quad (4)$$

It's not obvious how these two operations are conjugate pairs.

**Exercise 3.** *Explain why Stochastic Position Verlet (SPV) is unsuitable for large choices of  $\gamma$ .*

As  $\gamma \rightarrow \infty$ ,  $\eta \rightarrow 0$  diminishes the force evaluation term.

**Exercise 4.** *With the Hamiltonian of a one-dimensional harmonic oscillator with spring potential  $U(q) = \Omega^2 q^2/2$ ,*

$$H(q, p) = \frac{p^2}{2m} + \frac{\Omega^2 q^2}{2}, \quad (5)$$

*where  $(q, p) \in \mathbb{R}^2$ , show that  $\langle q \rangle = \langle p \rangle = 0$ ,  $\langle \Omega^2 q^2 \rangle = \langle p^2/m \rangle = k_B T$ , and  $\langle qp \rangle = 0$ .*

We first solve for the distribution,

$$\rho_\beta = \frac{1}{Z} \exp(-\beta H),$$

where the partition function is

$$Z = \iint d\omega \exp(-\beta H).$$

Separating integrands for  $q$  and  $p$  yields

$$Z = \int_{-\infty}^{\infty} dq \exp(-\beta \Omega^2 q^2/2) \int_{-\infty}^{\infty} dp \exp(-\beta p^2/2m).$$

We know

$$\int_{-\infty}^{\infty} dx \exp(-x^2) = \sqrt{\pi}. \quad (6)$$

Let  $x^2 = \beta \Omega^2 q^2/2$ , then  $x = q\sqrt{\beta \Omega^2/2}$  and  $dx = \sqrt{\beta \Omega^2/2} dq$ , so that

$$\int_{-\infty}^{\infty} dq \exp(-\beta \Omega^2 q^2/2) = \frac{1}{\sqrt{\beta \Omega^2/2}} \int_{-\infty}^{\infty} dx \exp(-x^2) = \frac{1}{\Omega} \sqrt{\frac{2\pi}{\beta}}. \quad (7)$$

Next, we solve for the  $p$  integrand factor. Let  $y^2 = \beta p^2/2m$ , then  $y = p\sqrt{\beta/2m}$  and  $dy = dp\sqrt{\beta/2m}$ . Therefore,

$$\int_{-\infty}^{\infty} dp \exp(-\beta p^2/2m) = \sqrt{2m/\beta} \int_{-\infty}^{\infty} dy \exp(-y^2) = \sqrt{\frac{2\pi m}{\beta}} \quad (8)$$

Substituting (8) and (7) into  $Z$  gives our partition function,

$$Z = \frac{1}{\Omega} \frac{2\pi}{\beta} \sqrt{\frac{2\pi m}{\beta}} = \frac{2\pi\sqrt{m}}{\Omega\beta} \quad (9)$$

This solves the probability density function,

$$\rho_\beta = \frac{\Omega\beta}{2\pi\sqrt{m}} \exp(-\beta p^2/2m) \exp(-\beta\Omega^2 q^2/2). \quad (10)$$

We find  $\langle q \rangle$ :

$$\begin{aligned} \langle q \rangle &= \frac{\Omega\beta}{2\pi\sqrt{m}} \int d\omega \exp(-\beta p^2/2m) q \exp(-\beta\Omega^2 q^2/2) \\ &= \frac{\Omega\beta}{2\pi\sqrt{m}} \int_{-\infty}^{\infty} dp [\exp(-\beta p^2/2m)] \int_{-\infty}^{\infty} dq [q \exp(-\beta\Omega^2 q^2/2)], \end{aligned}$$

but  $q \exp(-\beta\Omega^2 q^2/2)$  is an odd, integrable function, so  $\int_{-\infty}^{\infty} dq [q \exp(-\beta\Omega^2 q^2/2)] = 0$ , and  $\langle q \rangle = 0$ . Similarly,  $\langle p \rangle = 0$ .

Next, we find  $\langle \Omega^2 q^2 \rangle$ :

$$\begin{aligned} \langle \Omega^2 q^2 \rangle &= \frac{\Omega\beta}{2\pi\sqrt{m}} \int d\omega \exp(-\beta p^2/2m) \Omega^2 q^2 \exp(-\beta\Omega^2 q^2/2) \\ &= \frac{\Omega\beta}{2\pi\sqrt{m}} \int_{-\infty}^{\infty} dp [\exp(-\beta p^2/2m)] \int_{-\infty}^{\infty} dq [\Omega^2 q^2 \exp(-\beta\Omega^2 q^2/2)] \\ &= \frac{\Omega\beta}{2\pi\sqrt{m}} \frac{\sqrt{2\pi m}}{\sqrt{\beta}} \int_{-\infty}^{\infty} dq [\Omega^2 q^2 \exp(-\beta\Omega^2 q^2/2)]. \end{aligned}$$

Let  $x^2 = \beta\Omega^2 q^2/2$ , then  $x = q\sqrt{\beta\Omega^2/2}$  and  $dx = \sqrt{\beta\Omega^2/2} dq$ , and

$$\int_{-\infty}^{\infty} dq [\Omega^2 q^2 \exp(-\beta\Omega^2 q^2/2)] = \frac{1}{\sqrt{\beta^3\Omega^2/2}} \int_{-\infty}^{\infty} dx [2x^2 \exp(-x^2)] = \sqrt{\frac{\pi}{\beta^3\Omega^2/2}}.$$

Then,

$$\langle \Omega^2 q^2 \rangle = \frac{1}{\beta} = k_B T. \quad (11)$$

By similar methods, we also find  $\langle p^2/m \rangle = k_B T$ .

Finally, we find  $\langle qp \rangle$ :

$$\begin{aligned} \langle qp \rangle &= \frac{\Omega\beta}{2\pi\sqrt{m}} \int d\omega p \exp(-\beta p^2/2m) q \exp(-\beta\Omega^2 q^2/2) \\ &= \frac{\Omega\beta}{2\pi\sqrt{m}} \int_{-\infty}^{\infty} dp [p \exp(-\beta p^2/2m)] \int_{-\infty}^{\infty} dq [q \exp(-\beta\Omega^2 q^2/2)]. \end{aligned}$$

Since each integral equals zero by symmetry,  $\langle qp \rangle = 0$ .

**Exercise 5.** Show that the expectations of Equation (7.12) are  $\langle q \rangle_h^{[ABO]} = \langle p \rangle_h^{[ABO]} = 0$ .

Taking the expectations of (7.12), we have

$$\begin{aligned} \langle q \rangle &= \langle q \rangle + h \langle p \rangle / m \\ \langle p \rangle &= -\Omega^2 h e^{-h\gamma} \langle q \rangle + (1 - \Omega^2 h^2 / m) e^{-h\gamma} \langle p \rangle. \end{aligned}$$

From the first equation,  $\langle p \rangle = 0$ . Substituting into the second equation gives  $\langle q \rangle = 0$ .