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,

$$dX = -\gamma X dt + \sigma dW. \tag{1}$$

The corresponding Fokker-Planck equation is,

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

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

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

Exercise 2. *Show that $[\![OABA]\!]$ and $[\![BAOAB]\!]$ are conjugates, i.e., show that*

$$\left(\mathcal{U}_h^{[\![OABA]\!]}\right)^{n+1} = \mathcal{U}_{h/2}^A \circ \mathcal{U}_{h/2}^B \circ \left(\mathcal{U}_h^{[\![BAOAB]\!]}\right)^n \circ \mathcal{U}_{h/2}^B \circ \mathcal{U}_{h/2}^A \circ \mathcal{U}_h^O \tag{4}$$

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 γ.*

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

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

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

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

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

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

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

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,

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

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

$$Z = \frac{1}{\Omega}\frac{2\pi}{\beta}\sqrt{\frac{2\pi m}{\beta}} = \frac{2\pi\sqrt{m}}{\Omega\beta} \tag{9}$$

This solves the probability density function,

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

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 $q\exp(-\beta\Omega^2q^2/2)$ is an odd, integrable function, so $\int_{-\infty}^{\infty} dq[q\exp(-\beta\Omega^2q^2/2)] = 0$, 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 $x^2 = \beta\Omega^2q^2/2$, 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,

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

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

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

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

Exercise 6. *Show from example (7.2) that* $\mathbb{E}(\mu_{n,1}q_n) = \mathbb{E}(\mu_{n,2}q_n) = 0$, $\mathbb{E}(\mu_{n,1}p_n) = \kappa_1\kappa_3$, $\mathbb{E}(\mu_{n,1}\mu_{n,2}) = \kappa_1\kappa_2$, *and* $\mathbb{E}(\mu_{n,2}^2) = \kappa_2^2 + \kappa_3^2$.

Proof. The proof is straightforward. We find $\mathbb{E}(\mu_{n,2}^2)$ as an example:

$$\mathbb{E}(\mu_{n,2}^2) = \mathbb{E}((\kappa_2 R_n + \kappa_3 R_{n+1})^2) = \kappa_2^2 + \kappa_3^2.$$

□

Exercise 7. *Demonstrate equation (7.4).*