EXERCISES 3

DAVID LI

1. Langevin Dynamics Splitting Scheme

The equation for Langevin dynamics is

$$\begin{aligned} d\boldsymbol{q} &= \boldsymbol{M}^{-1}\boldsymbol{p}dt, \\ d\boldsymbol{p} &= -\nabla U(\boldsymbol{q})dt - \gamma\boldsymbol{p}dt + \sqrt{2\gamma k_B T}\boldsymbol{M}^{1/2}d\mathbf{W}. \end{aligned} \tag{1}$$

Equation (1) may be reformulated into the Ito formula,

$$d\phi(\boldsymbol{q},\boldsymbol{p}) = \nabla\phi \cdot [\boldsymbol{a}(\boldsymbol{q},\boldsymbol{p})dt + \boldsymbol{B}d\mathbf{W}] + \frac{1}{2}\mathrm{Tr}[\boldsymbol{B}^T\phi''\boldsymbol{B}]dt,$$

where

$$\begin{aligned} \boldsymbol{a}(\boldsymbol{q},\boldsymbol{p}) &= (\boldsymbol{M}^{-1}\boldsymbol{p}, -\nabla U(\boldsymbol{q}) - \gamma\boldsymbol{p}) \\ \boldsymbol{B} &= (0, \sqrt{2\gamma k_B T}M^{1/2}d\mathbf{W}), \end{aligned}$$

to yield its corresponding generator,

$$\mathcal{L}_{\mathrm{LD}}\phi = \nabla_q\phi \cdot (\boldsymbol{M}^{-1}\boldsymbol{p}) + \nabla_p\phi \cdot (-\nabla U(\boldsymbol{q}) - \gamma\boldsymbol{p}) + \gamma k_B T\Delta_M\phi, \tag{2}$$

where $\Delta_M = \sum_{i=1}^{N_C} m_i \dfrac{\partial}{\partial p_i}$ is the mass-weighted Laplacian. We split the generator into three separate components, (I separated the dels from the piecewise operators, because it seems that they were not considered in 7.7.1)

$$\mathcal{L}_{\mathrm{LD}}\phi = \mathcal{L}_A \cdot \nabla_q + \mathcal{L}_B \cdot \nabla_p + \mathcal{L}_O\Delta_M,$$

where operators

$$\mathcal{L}_A = \boldsymbol{M}^{-1}\boldsymbol{p}, \tag{3}$$

$$\mathcal{L}_B = -\nabla U(\boldsymbol{q}), \tag{4}$$

$$\mathcal{L}_O = \gamma\boldsymbol{p} \cdot \nabla_p + \gamma k_B T, \tag{5}$$

mirrors the three splitting parts,

$$\mathcal{U}_h^A(\boldsymbol{q},\boldsymbol{p}) = (\boldsymbol{q} + h\boldsymbol{M}^{-1}\boldsymbol{p}, \boldsymbol{p}), \tag{6}$$

$$\mathcal{U}_h^B(\boldsymbol{q},\boldsymbol{p}) = (\boldsymbol{q}, \boldsymbol{p} - h\nabla U(\boldsymbol{q})), \tag{7}$$

$$\mathcal{U}_h^O(\boldsymbol{q},\boldsymbol{p}) = (\boldsymbol{q}, e^{-\gamma h}\boldsymbol{p} + \sqrt{k_B T(1 - e^{-2\gamma h})}\boldsymbol{M}^{1/2}\mathbf{R}). \tag{8}$$

Recall that

$$e^{t\mathcal{L}_f}\phi = (\mathrm{Id} + t\mathcal{L}_f + \frac{t^2}{2}\mathcal{L}_f^2 + \cdots)\phi$$

Since $\mathcal{L}_A = \boldsymbol{M}^{-1}\boldsymbol{p}$, then

$$e^{t\mathcal{L}_A}\phi(\boldsymbol{q},\boldsymbol{p}) = (\mathrm{Id} + t\mathcal{L}_A + \cdots)\phi = \phi(\boldsymbol{q} + t\boldsymbol{M}^{-1}\boldsymbol{p}, \boldsymbol{p}).$$

Likewise for $\mathcal{L}_B$,

$$e^{t\mathcal{L}_B}\phi(\boldsymbol{q},\boldsymbol{p}) = \phi(\boldsymbol{q}, \boldsymbol{p} - t\nabla U(\boldsymbol{q})).$$

In the case of $\mathcal{L}_O$,

$$
\begin{aligned}
e^{t\mathcal{L}_O}\phi(\boldsymbol{q},\boldsymbol{p}) &= (\mathrm{Id} + t\mathcal{L}_O + \frac{t^2}{2}\cdots)\phi \\
&= ??? \\
&= \int_{\mathcal{P}} \phi(\boldsymbol{q}, e^{-\gamma t} + \xi \boldsymbol{M}^{1/2}\boldsymbol{x}) \frac{e^{-|\boldsymbol{x}|^2/2}}{(2\pi)^{\mathrm{N}_c/2}} d\boldsymbol{x}.
\end{aligned}
$$