

## EXERCISES 3

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### 1. LANGEVIN DYNAMICS SPLITTING SCHEME

The equation for Langevin dynamics is

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

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

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

where

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

to yield its corresponding generator,

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

where  $\Delta_M = \sum_{i=1}^{N_C} m_i \frac{\partial}{\partial p_i}$  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)

$$\mathcal{L}_{\text{LD}}\phi = \mathcal{L}_A \cdot \nabla_{\mathbf{q}} + \mathcal{L}_B \cdot \nabla_{\mathbf{p}} + \mathcal{L}_O \Delta_M,$$

where operators

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

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

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

mirrors the three splitting parts,

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

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

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

Recall that

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

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

$$e^{t\mathcal{L}_A}\phi(\mathbf{q}, \mathbf{p}) = (\text{Id} + t\mathcal{L}_A + \dots)\phi = \phi(\mathbf{q} + t\mathbf{M}^{-1}\mathbf{p}, \mathbf{p}).$$

Likewise for  $\mathcal{L}_B$ ,

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

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

$$e^{t\mathcal{L}_O}\phi(\mathbf{q},\mathbf{p}) = (\text{Id} + t\mathcal{L}_O + \frac{t^2}{2}\cdots)\phi$$