WEEK 2

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Exercise 1. *Consider the Langevin dynamics splitting parts in the harmonic potential case,*

$$\begin{aligned} \mathcal{U}_h^A(\boldsymbol{q},\boldsymbol{p}) &= (\boldsymbol{q} + h\boldsymbol{M}^{-1}\boldsymbol{p}, \boldsymbol{p}), \\ \mathcal{U}_h^B(\boldsymbol{q},\boldsymbol{p}) &= (\boldsymbol{q}, \boldsymbol{p} - h\boldsymbol{q}), \\ \mathcal{U}_h^O(\boldsymbol{q},\boldsymbol{p}) &= (\boldsymbol{q}, e^{-\gamma h}\boldsymbol{p} + \sqrt{kT(1-e^{-2\gamma h})\boldsymbol{M}^{1/2}\boldsymbol{R}}). \end{aligned} \tag{1}$$

Show that method $[\![OABA]\!]$ *and* $[\![BAOAB]\!]$ *are conjugates.*

Without loss of generality, we prove that the algorithm works in one dimension. In the base case $n = 0$,

$$\begin{aligned} [\![OABA]\!] &= [\![OAB]\!](q + hp/2m, p) \\ &= [\![OA]\!](q + hp/2m, p - h(q + hp/2m)) \\ &= [\![O]\!](q + hp/2m + h(p - h(q + hp/2m))/2m, p - h(q + hp/2m)) \end{aligned}$$