Problem Set 3: Solutions

(warning: I used q instead of x)

1.1 a.) $V(x)$

$$i\mathcal{L} g = \frac{\partial g}{\partial t} \Rightarrow \frac{\partial g}{\partial p}\frac{\partial p}{\partial t} + \frac{\partial g}{\partial q}\frac{\partial q}{\partial t} = i\mathcal{L} g$$

$$-\frac{\partial g}{\partial p}\frac{\partial H}{\partial q} + \frac{\partial g}{\partial q}\frac{\partial H}{\partial p} = i\mathcal{L} g$$

$$\{H, g\} = i\mathcal{L} g$$

Verlet:
$$e^{i\mathcal{L}\Delta t} g(p(0), q(0)) = g(p(\Delta t), q(\Delta t))$$

can write: $i\mathcal{L} = i\mathcal{L}_p + i\mathcal{L}_q$

$$\rightarrow i\mathcal{L}_p g = \frac{\partial g}{\partial p}\frac{\partial p}{\partial t}$$

$$i\mathcal{L}_q g = \frac{\partial g}{\partial q}\frac{\partial q}{\partial t}$$

$$e^{i\mathcal{L}\Delta t} \sim e^{i\mathcal{L}_p\frac{\Delta t}{2}} e^{i\mathcal{L}_q\Delta t} e^{i\mathcal{L}_p\frac{\Delta t}{2}}$$

$$e^{i\mathcal{L}_p\frac{\Delta t}{2}} e^{i\mathcal{L}_q\Delta t} \underline{e^{i\mathcal{L}_p\frac{\Delta t}{2}} g(p(0), q(0))}$$

$$\left[1 + \frac{i\mathcal{L}_p\Delta t}{2} + \frac{(i\mathcal{L}_p)^2\Delta t^2}{2\cdot 2^2} + \dots\right] g(p(0), q(0))$$

$$i\mathcal{L}_p g(p(0), q(0)) = \frac{\partial g(p(0), q(0))}{\partial p}\frac{\partial p}{\partial t}$$

$$(i\mathcal{L}_p)^2 g(p(0), q(0)) = \frac{\partial^2 g(p(0), q(0))}{\partial p^2}\left(\frac{\partial p}{\partial t}\right)^2$$

$$\Rightarrow e^{i\mathcal{L}_p\frac{\Delta t}{2}} g(p(0), q(0)) = g\left(p(0) + \Delta t\frac{\partial p(0)}{\partial t}, q(0)\right)$$

$$= g\left(p(0) + \frac{\Delta t}{2}\hat{F}(0), q(0)\right) = g\left(p\left(\tfrac{\Delta t}{2}\right), q(0)\right)$$

Similarly: $e^{i\mathcal{L}_a \Delta t} g(p(\frac{\Delta t}{2}), q(0)) = g(p(\frac{\Delta t}{2}), q(\Delta t))$ ②

Verlet algorithm:

- start with $p(0),\ q(0)$
- using $q(0) \to F(q(0))$, calculate $p(\frac{\Delta t}{2})$

$$p(\tfrac{\Delta t}{2}) = q(0) + \tfrac{\Delta t}{2} F(q(0))$$

- using $p(\frac{\Delta t}{2}) \to$ calculate $q(\Delta t)$

$$q(\Delta t) = q(0) + \frac{p(\frac{\Delta t}{2})}{m} \Delta t$$

- using $q(\Delta t) \to$ calculate $p(\Delta t) = p(\frac{\Delta t}{2}) + \frac{\Delta t}{2} F(q(\Delta t))$

b.) $$V(x, X) + \frac{p^2}{2m} + \frac{P^2}{2M} = H(p, P, x, \cancel{X})$$

$$g(p, P, x, X) \to g(p(0), P(0), x(0), X(0))$$

$$i\mathcal{L}g = \frac{\partial g}{\partial p}\frac{\partial p}{\partial t} + \frac{\partial g}{\partial P}\frac{\partial P}{\partial t} + \frac{\partial g}{\partial x}\frac{\partial x}{\partial t} + \frac{\partial g}{\partial X}\frac{\partial X}{\partial t}$$

$$i\mathcal{L}_m = \frac{\partial g}{\partial p}\frac{\partial p}{\partial t} + \frac{\partial g}{\partial x}\frac{\partial x}{\partial t}$$ → Lagrangian for small mass particle

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$$e^{i\mathcal{L}\Delta t} \cong e^{i\mathcal{L}_M \frac{\Delta t}{2}} \underbrace{e^{i\mathcal{L}_m \Delta t}} e^{i\mathcal{L}_M \frac{\Delta t}{2}}$$

$$e^{i\mathcal{L}_m \Delta t} = \left[e^{i\mathcal{L}_m \delta t}\right]^n$$

$\cancel{e^{i\mathcal{L}_m \delta t}} =$

Now apply usual break up:

$$i\mathcal{L}_m = i\mathcal{L}_m^{(p)} + i\mathcal{L}_m^{(x)}$$
$$i\mathcal{L}_M = i\mathcal{L}_M^{(P)} + i\mathcal{L}_M^{(X)}$$

Start with: $\rho(p(0), P(0), x(0), X(0))$

$$e^{iL_M \frac{\Delta t}{2}} \sim e^{iL_M^{(x)} \frac{\Delta t}{4}} e^{iL_M^{(p)} \frac{\Delta t}{2}} e^{iL_M^{(x)} \frac{\Delta t}{2}}$$

$$e^{iL_m \delta t} \sim e^{iL_m^{(x)} \frac{\delta t}{2}} e^{iL_m^{(p)} \delta t} e^{iL_m^{(x)} \frac{\delta t}{2}}$$

propagation:

$$e^{iL_M \frac{\Delta t}{2}} e^{iL_m \Delta t} e^{iL_M \frac{\Delta t}{2}} \rho(p(0), P(0), x(0), X(0))$$

$$= e^{iL_M \frac{\Delta t}{2}} \underbrace{e^{iL_m \Delta t}} \rho(p(0), P(\tfrac{\Delta t}{2}), x(0), X(\tfrac{\Delta t}{2}))$$

$\left[e^{iL_m \delta t}\right]^n$ propagated in n small steps (δt)

$$\rho(p(\delta t), P(\tfrac{\Delta t}{2}), x(\delta t), X(\tfrac{\Delta t}{2}))$$

$$\vdots$$

$$\rho(p(\Delta t), P(\tfrac{\Delta t}{2}), x(\Delta t), X(\tfrac{\Delta t}{2}))$$

apply $e^{iL_M \frac{\Delta t}{2}}$ (propagate heavy degrees of freedom)

$$\rightarrow \rho(p(\Delta t), P(\Delta t), x(\Delta t), X(\Delta t))$$

Note: the small step propagations were done such that the small degrees of freedom ~~were~~ was propagated but the heavy one was stationary.

Problem 2:

a) $P(x)\,T(x|x') = P(x')\,T(x'|x)$ (detailed balance)

symmetric matrix $M(x|x')$

$T(x|x') = M(x|x')\,A(x|x')$

$\rightarrow P(x)\,A(x|x') = P(x')\,A(x'|x)$

$A(x|x') = \min\left[1, \frac{P(x')}{P(x)}\right]$ (acceptance probability)

b.) matrix $M(x|x')$ is not symmetric

$$P(x)\,M(x|x')\,A(x|x') = P(x')\,M(x'|x)\,A(x'|x)$$

$$A(x|x') = \min\left[1, \frac{P(x')\,M(x'|x)}{P(x)\,M(x|x')}\right]$$

check! $P(x')\,M(x'|x) > P(x)\,M(x|x')$

in this case

$A(x|x') = 1$

$A(x'|x) = \frac{P(x)\,M(x|x')}{P(x')\,M(x'|x)}$

$\Downarrow$

$$P(x)\,M(x|x') = P(x')\,M(x'|x)\,\frac{P(x)\,M(x|x')}{P(x')\,M(x'|x)} \checkmark$$

or $P(x')\,M(x'|x) < P(x)\,M(x|x')$

$\rightarrow A(x'|x) = 1 \qquad A(x|x') = \frac{P(x')\,M(x'|x)}{P(x)\,M(x|x')}$

$\rightarrow$ ~~$P(x)\,M(x|x') = P(x)$~~

$\rightarrow$ detailed balance gives $\frac{P(x)\,M(x|x')\,P(x')\,M(x'|x)}{P(x)\,M(x|x')} = P(x')\,M(x'|x)$