Existence of a conserved "Hamiltonian" for the Verlet dynamics

In the Verlet dynamics

$$e^{iL\Delta t} \rightarrow e^{iL_p\Delta t/2}\, e^{iL_q \Delta t}\, e^{iL_p \Delta t/2}$$

We can use the Baker-Campbell-Hausdorff formula to put this three terms together.

$$e^{B} e^{A} e^{B} = \exp\Big(A + 2B + \frac{1}{6}[A,[A,B]] + \frac{1}{6}[B,[A,B]] + \ldots \text{higher-order nested commutators}\Big)$$

$$e^{iL_p \Delta t/2}\, e^{iL_q \Delta t}\, e^{iL_p \Delta t/2} =$$

$$= \exp\Big[i(L_p+L_q)\Delta t + \frac{\Delta t^3}{12}[iL_q,[iL_q,iL_p]] + \frac{\Delta t^3}{24}[iL_p,[iL_q,iL_p]] + O(\Delta t^4)\Big]$$

Now we want to show that ~~term~~ in brackes can be written as $i\hat{L}$, where

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

$i\hat{L}$ is a Liouvillian and $\hat{H}$ is the corresponding Hamiltonian. [which is <u>not</u> CANONICAL $\hat{H} \neq \frac{p^2}{2m} + \text{fun}(q)$]

Thus

$$e^{iLt} \xrightarrow[\text{Verlet}]{} e^{i\hat{L}t} \qquad \hat{H} \text{ is conserved}$$

The proof uses two results

$$\begin{cases} iL_1 \longrightarrow H_1 & iL_2 \longrightarrow H_2 \\ iL_1 + iL_2 \longrightarrow (H_1 + H_2) \end{cases}$$

The sum of two Liouvillians is a Liouvillian

$$\begin{aligned} iL_1 + iL_2 &= -\frac{\partial H_1}{\partial q}\frac{\partial}{\partial p} + \frac{\partial H_1}{\partial p}\frac{\partial}{\partial q} \\ &\quad -\frac{\partial H_2}{\partial q}\frac{\partial}{\partial p} + \frac{\partial H_2}{\partial p}\frac{\partial}{\partial q} \\ &= -\frac{\partial (H_1 + H_2)}{\partial q}\frac{\partial}{\partial p} + \frac{\partial (H_1 + H_2)}{\partial p}\frac{\partial}{\partial q} \end{aligned}$$

THE COMMUTATOR OF LIOUVILLIAN IS A LIOUVILLIAN

Given $\begin{array}{l} L_1 \longrightarrow H_1 \\ L_2 \longrightarrow H_2 \end{array} \Longrightarrow [iL_1, iL_2] = iL_3$ with L_3 associated with H_3

We give the proof for one particle in 1D.

$$iL_1 = -\frac{\partial H_1}{\partial q}\frac{\partial}{\partial p} + \frac{\partial H_1}{\partial p}\frac{\partial}{\partial q} \qquad iL_2 \equiv \text{same with } 2 \rightarrow 1.$$

We compute (f is a generic function of p, q)

$$iL_1(iL_2 f) = \left(-\frac{\partial H_1}{\partial q}\frac{\partial}{\partial p} + \frac{\partial H_1}{\partial p}\frac{\partial}{\partial q}\right)\left(-\frac{\partial H_2}{\partial q}\frac{\partial f}{\partial p} + \frac{\partial H_2}{\partial p}\frac{\partial f}{\partial q}\right)$$

$$\left.\begin{aligned} = &+\frac{\partial H_1}{\partial q}\frac{\partial H_2}{\partial q}\frac{\partial^2 f}{\partial p^2} - \frac{\partial H_1}{\partial p}\frac{\partial H_2}{\partial q}\frac{\partial^2 f}{\partial p \partial q} \\ &-\frac{\partial H_1}{\partial q}\frac{\partial H_2}{\partial p}\frac{\partial^2 f}{\partial p \partial q} + \frac{\partial H_1}{\partial p}\frac{\partial H_2}{\partial p}\frac{\partial^2 f}{\partial q^2} \end{aligned}\right\} (a)$$

$$\left.\begin{aligned} &+\frac{\partial H_1}{\partial q}\frac{\partial^2 H_2}{\partial p \partial q}\frac{\partial f}{\partial p} - \frac{\partial H_1}{\partial q}\frac{\partial^2 H_2}{\partial p^2}\frac{\partial f}{\partial q} \\ &-\frac{\partial H_1}{\partial p}\frac{\partial^2 H_2}{\cancel{\partial p}\partial q^2}\frac{\partial f}{\partial p} + \frac{\partial H_1}{\partial p}\frac{\partial^2 H_2}{\partial q \partial p}\frac{\partial f}{\partial q} \end{aligned}\right\} (b)$$

Now we consider terms (a) that involve second-order derivatives of f.

We subtract the analogous contributions due to $iL_2(iL_1 f)$ [it is enough to change 1 with 2]

$$\frac{\partial H_1}{\partial q}\frac{\partial H_2}{\partial q}\frac{\partial^2 f}{\partial p^2} - \frac{\partial H_1}{\partial p}\frac{\partial H_2}{\partial q}\frac{\partial^2 f}{\partial p \partial q}$$

$$- \frac{\partial H_1}{\partial q}\frac{\partial H_2}{\partial p}\frac{\partial^2 f}{\partial p \partial q} + \frac{\partial H_1}{\partial p}\frac{\partial H_2}{\partial p}\frac{\partial^2 f}{\partial q^2}$$

$$- \Big[\frac{\partial H_2}{\partial q}\frac{\partial H_1}{\partial q}\frac{\partial^2 f}{\partial p^2} - \frac{\partial H_2}{\partial p}\frac{\partial H_1}{\partial q}\frac{\partial^2 f}{\partial p \partial q}$$

$$- \frac{\partial H_2}{\partial q}\frac{\partial H_1}{\partial p}\frac{\partial^2 f}{\partial p \partial q} - \frac{\partial H_2}{\partial p}\frac{\partial H_1}{\partial p}\frac{\partial^2 f}{\partial q^2}\Big] = 0$$

All these terms cancel.

Terms (b) can be written as

$$(b) \quad \left(\frac{\partial H_1}{\partial q}\frac{\partial^2 H_2}{\partial p \partial q} - \frac{\partial H_1}{\partial p}\frac{\partial^2 H_2}{\partial q^2} \right)\frac{\partial f}{\partial p} \qquad (b1)$$

$$- \left(\frac{\partial H_1}{\partial q}\frac{\partial^2 H_2}{\partial p^2} - \frac{\partial H_1}{\partial p}\frac{\partial^2 H_2}{\partial p \partial q} \right)\frac{\partial f}{\partial q} \qquad (b2)$$

Now consider term (b1) and subtract the contribution $1 \leftrightarrow 2$:

$$\left(\frac{\partial H_1}{\partial q}\frac{\partial^2 H_2}{\partial p \partial q} - \frac{\partial H_1}{\partial p}\frac{\partial^2 H_2}{\partial q^2} - \frac{\partial H_2}{\partial q}\frac{\partial^2 H_1}{\partial p \partial q} + \frac{\partial H_2}{\partial p}\frac{\partial^2 H_1}{\partial q^2} \right)\frac{\partial f}{\partial p}$$

$$= \left[\frac{\partial}{\partial q}\left(\frac{\partial H_1}{\partial q}\frac{\partial H_2}{\partial p} - \frac{\partial H_1}{\partial p}\frac{\partial H_2}{\partial q} \right) \right] \frac{\partial f}{\partial p}$$

We define $H_3 = - \frac{\partial H_1}{\partial q}\frac{\partial H_2}{\partial p} + \frac{\partial H_1}{\partial p}\frac{\partial H_2}{\partial q}$

$\boxed{\text{Check}}$

$$(b2) - (1 \leftrightarrow 2) = \frac{\partial H_3}{\partial p}\frac{\partial f}{\partial q}$$