THE VERLET APPROXIMATION

Let \( t = n \Delta t \)

\[
(p(t)) = e^{iL\Delta t} (p(0)) = e^{iL\Delta t} (q(0))
\]

\[
= e^{i\Delta t} \cdot e^{iL\Delta t} \cdot e^{i\Delta t} \cdot e^{iL\Delta t} (p(0))
\]

We approximate \( e^{iL\Delta t} \).

\[
L = -\sum_i \frac{\partial H}{\partial q_i} \cdot \frac{\partial}{\partial p_i} + \sum_i \frac{\partial H}{\partial p_i} \cdot \frac{\partial}{\partial q_i}
\]

\[
= \sum_i \frac{\ddot{q}_i}{m} \cdot \frac{\partial}{\partial q_i} + \sum_i \frac{\ddot{p}_i}{m} \cdot \frac{\partial}{\partial q_i} = L_p + L_q
\]

Approximation

\[
e^{iL\Delta t} = e^{iL_p\Delta t} \cdot e^{iL_q\Delta t}
\]

\[
= \left( e^{iL_p\Delta t/2} \right)^{\frac{n}{2}} \cdot 
\left( e^{iL_p\Delta t/2} \right)^{\frac{n}{2}} \cdot \left( e^{iL_q\Delta t} \right)^{\frac{n}{2}} \cdot \left( e^{iL_q\Delta t} \right)^{\frac{n}{2}} + O(\Delta t^3)
\]

The advantage of the factorization:

(a) We are not able to compute \( e^{iL\Delta t} \) exactly. It is equivalent to solving the equations of motion

(b) We know how to compute \( e^{iL_p\Delta t/2} \) and \( e^{iL_q\Delta t} \) EXACTLY
Computation (one particle in 1D)
\[ e^{iL_{p,q} \alpha} A(p, q) = \]
\[ = e^{i \alpha \frac{\partial^2}{\partial p^2} A(p, q)} = \sum_n \frac{\alpha^n}{n!} F^n \frac{\partial^n A}{\partial p^n} \]
\[ = A(p + \alpha F, q) \quad \text{Taylor expansion} \]
\[ \text{here we use that} \]
\[ \text{fact that} \]
\[ F \text{ only depends on} \]
\[ r, \quad [F, \frac{\partial}{\partial p}] = 0 \]
\[ \]
\[ e^{iL_{p,q} \alpha} A(p, q) = \]
\[ = e^{\alpha \frac{\partial}{\partial q}} A(p, q) = \sum_n \frac{\alpha^n}{n!} \left( \frac{p}{m} \right)^n \frac{\partial^n A}{\partial q^n} \]
\[ = A(p, q + \frac{\alpha p}{m}) \quad \text{Taylor expansion} \]
\[ \text{of course} \]

Now let's work out the time step

a) \[ e^{iL_{p,q} \Delta t/2} \left( \begin{array}{c} p \\ q \end{array} \right) = \left( \begin{array}{c} p + \frac{\Delta t}{2} F(q) \\ q \end{array} \right) \]

b) \[ e^{iL_{q} \Delta t} e^{iL_{p,q} \Delta t/2} \left( \begin{array}{c} p \\ q \end{array} \right) = e^{i \Delta t/2} F(q + \frac{p}{m} \Delta t) \]
\[ = \left( \begin{array}{c} p + \frac{\Delta t}{2} F(q + \frac{p}{m} \Delta t) \\ q + \frac{p}{m} \Delta t \end{array} \right) \]
\[ e^{iL\Delta t/2} e^{iL\Delta t} e^{-iL\Delta t/2}(P) = e^{iL\Delta t/2} \left( p + \frac{\Delta t}{2} F(q + \frac{p}{m} \Delta t) \right) \left( q + \frac{p}{m} \Delta t \right) \]
\[ = \left( p + \frac{\Delta t}{2} F(q) + \frac{\Delta t}{2} F\left(q + \frac{p \Delta t}{m} + \frac{\Delta t^2}{2m} F(q)\right) \right) \]
\[ q + \frac{p \Delta t}{m} + \frac{\Delta t^2}{2m} F(q) \]

The result is our approximate \( e^{iL\Delta t} \) which corresponds to moving forward in time by \( \Delta t \).
Thus, for \( q \) we have (second line)
\[ q(t+\Delta t) = q(t) + \frac{\Delta t}{m} p(t) + \frac{\Delta t^2}{2m} F(q(t)) \]
\[ p(t+\Delta t) = p + \frac{\Delta t}{2} F(q(t)) + \frac{\Delta t}{2} F\left(q(t) + \frac{p(t)}{m} + \frac{\Delta t^2}{2m} F(q(t))\right) \]
\[ = p + \frac{\Delta t}{2} F(q(t)) + \frac{\Delta t}{2} F(q(t+\Delta t)) \]

THIS IS EXACTLY THE VERLET EVOLUTION

VERLET EVOLUTION = UNITARY EVOLUTION IN PHASE SPACE