THE VERLET APPROXIMATION

Let $t = n\Delta t$

$$\begin{pmatrix} p(t) \\ q(t) \end{pmatrix} = e^{iLt} \begin{pmatrix} p(0) \\ q(0) \end{pmatrix} = e^{iLn\Delta t} \begin{pmatrix} p(0) \\ q(0) \end{pmatrix}$$

$$= e^{iL\Delta t} \cdot e^{iL\Delta t} \cdot e^{iL\Delta t} \cdots e^{iL\Delta t} \begin{pmatrix} p(0) \\ q(0) \end{pmatrix}$$

We approximate $e^{iL\Delta t}$.

$$iL = -\sum_i \frac{\partial H}{\partial \bar{q}_i} \cdot \frac{\partial}{\partial \bar{p}_i} + \sum_i \frac{\partial H}{\partial \bar{p}_i} \cdot \frac{\partial}{\partial \bar{q}_i}$$

$$= \underbrace{\sum_i \bar{F}_i \cdot \frac{\partial}{\partial \bar{p}_i}}_{iL_p} + \underbrace{\sum_i \frac{\bar{p}_i}{m} \cdot \frac{\partial}{\partial \bar{q}_i}}_{iL_q} = iL_p + iL_q$$

$\boxed{\text{$i$ runs over all particles of the system}}$

Approximation

$$e^{iL\Delta t} = e^{iL_p\Delta t + iL_q\Delta t}$$

$$= e^{iL_p\Delta t/2}\, e^{iL_q\Delta t}\, e^{iL_p\Delta t/2} + O(\Delta t^3)$$

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 $e^{iL_q t}$ <u>EXACTLY</u>

Computation (one particle in 1D)

$$e^{iL_p \alpha} A(p,q) =$$

$$= e^{i\alpha F \frac{\partial}{\partial p}} A(p,q) = \sum_n \frac{\alpha^n}{n!} F^n \frac{\partial^n A}{\partial p^n}$$

$$= A(p+\alpha F, q)$$ ← Taylor expansion

[here we use that fact that F only depends on r, $[F, \frac{\partial}{\partial p}] = 0$]

$$e^{iL_q \alpha} A(p,q) =$$

$$= e^{\alpha \frac{p}{m} \frac{\partial}{\partial q}} A(p,q) = \sum_n \frac{\alpha^n}{n!} \left(\frac{p}{m}\right)^n \frac{\partial^n A}{\partial q^n}$$

($[p, \frac{\partial}{\partial q}] = 0$ of course)

$$= A\left(p, q + \frac{\alpha p}{m}\right)$$ ↔ Taylor expansion

Now let's work out the time step

a) $$e^{iL_p \Delta t/2} \begin{pmatrix} p \\ q \end{pmatrix} = \begin{pmatrix} p + \frac{\Delta t}{2} F(q) \\ q \end{pmatrix}$$

b) $$e^{iL_q \Delta t} e^{iL_p \Delta t/2} \begin{pmatrix} p \\ q \end{pmatrix} = e^{iL_q \Delta t} \begin{pmatrix} p + \frac{\Delta t}{2} F(q) \\ q \end{pmatrix}$$

$$= \begin{pmatrix} p + \frac{\Delta t}{2} F\left(q + \frac{p}{m}\Delta t\right) \\ q + \frac{p}{m}\Delta t \end{pmatrix}$$

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c)

$$e^{iL_p \Delta t/2}\, e^{iL_q \Delta t}\, e^{iL_p \Delta t/2} \begin{pmatrix} p \\ q \end{pmatrix} =$$

$$e^{iL_p \Delta t/2} \begin{pmatrix} p + \frac{\Delta t}{2} F\left(q + \frac{p}{m}\Delta t\right) \\ q + \frac{p}{m}\Delta t \end{pmatrix} =$$

$$\left[\begin{array}{l} \text{We should replace} \\ p \to p + \frac{\Delta t}{2} F(q) \end{array} \right]$$

$$= \begin{pmatrix} p + \frac{\Delta t}{2} F(q) + \frac{\Delta t}{2} F\left(q + \frac{p\Delta t}{m} + \frac{\Delta t^2}{2m} F(q)\right) \\ q + \frac{p\Delta t}{m} + \frac{\Delta t^2}{2m} F(q) \end{pmatrix}$$

The result is our approximate $e^{iL\Delta t}$ which corresponds to moving forward in time by Δt.
Thus, for q we have (second line)

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

$$p(t+\Delta t) = p + \frac{\Delta t}{2} F(q(t)) + \frac{\Delta t}{2} F\Big(\underbrace{q(t) + \frac{\Delta t}{m} p(t) + \frac{\Delta t^2}{2m} F(q(t))}_{q(t+\Delta t)}\Big)$$

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

THIS IS EXACTLY THE VERLET EVOLUTION

VERLET EVOLUTION = UNITARY EVOLUTION IN PHASE SPACE