$$\frac{1}{12}\begin{pmatrix} -f'(q)p \\ f'.f + f''(p,p) \end{pmatrix}$$

$M = Id$.

$f(q) = -\nabla V(q)$

$$F_3(qp) = \frac{1}{12}\begin{pmatrix} +2\nabla^2 V(q)\,p \\ \nabla^2 V.\nabla V + D^3V : p\otimes p \end{pmatrix}$$

$(D^3V : p \otimes p)_i$

$= \partial_{q_i}(p^T \nabla^2 V p)$

$V^{(3)} p^2$

$$\overset{?}{=} \begin{pmatrix} \partial_p \tilde{H} \\ -\partial_q \tilde{H} \end{pmatrix}$$

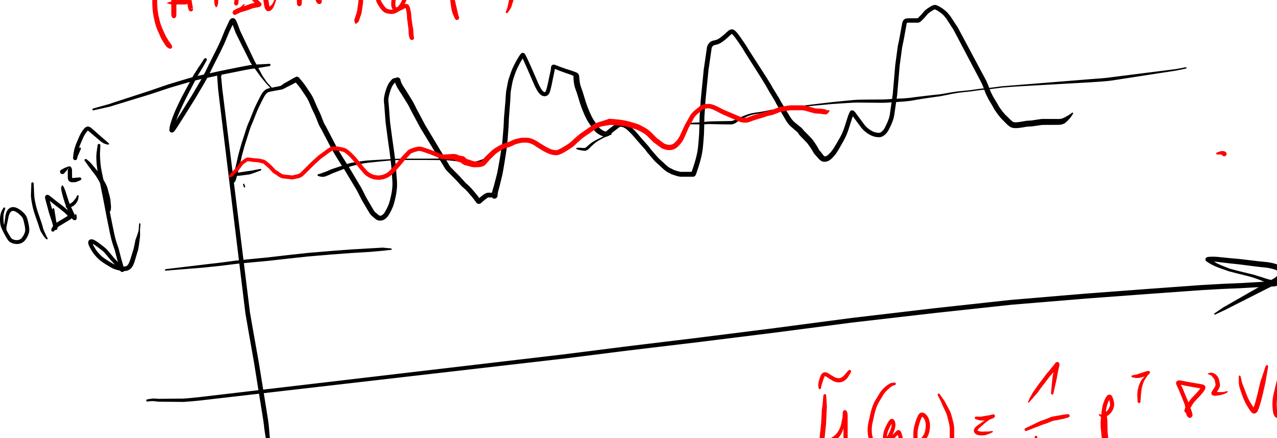
$\frac{1}{12} p^T(\nabla^2 V)p$

1D

$\rightarrow \frac{1}{12} D^3 V : p \otimes p - \frac{1}{24} |\nabla V|^2$

$$H(q^n p^n) = H(q^0 p^0) + O(\Delta t^2)$$

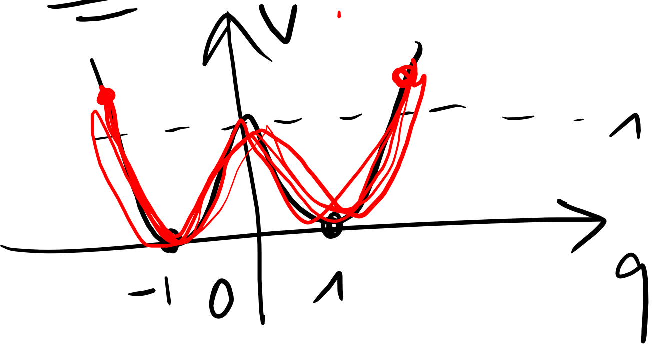
$$(H + \Delta t^2 \tilde{H})(q^n p^n) = \;- - -\; + O(\Delta t^4)$$



$$\tilde{H}(q p) = \frac{1}{12} p^T \nabla^2 V(q) p - \frac{1}{24} |\nabla V(q)|^2$$

Tests : ① cas 1D

$q \in \mathbb{R}, \; p \in \mathbb{R}, \; m = 1$



$$V(q) = (q^2 - 1)^2$$

ES / Verlet

$H, \quad H + \Delta t^{\alpha} \tilde{H} \quad (\alpha = 1 \text{ ou } 2)$

$$V'(q) = 4q(q^2 - 1)$$

② syst. solaire

→ ES

→ Verlet $\quad \nabla^2 V(q)$

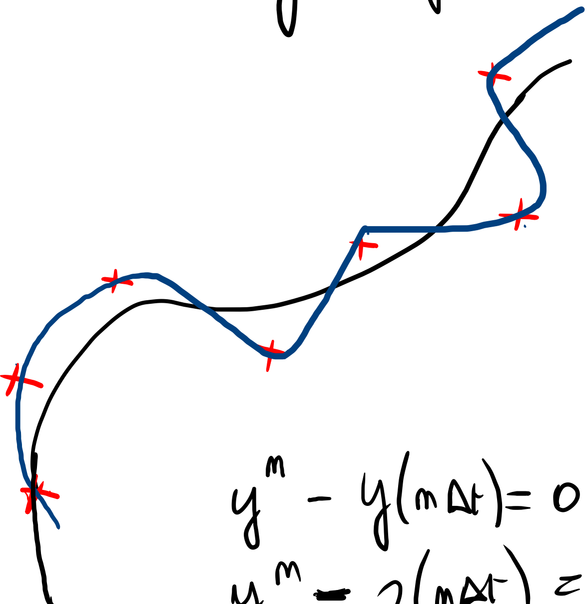
$$y^n - y(n\Delta t) \approx z(n\Delta t) - y(n\Delta t)$$

z (donc y^n) $\qquad\qquad$ $H_{\Delta t}$ - - - - - H

préserve $H_{\Delta t}$ exactement

$\longleftrightarrow$ y^n préserve H de manière approchée

$$\dot y = f(y) \quad - - - - - \quad y^{n+1} = \Phi_{\Delta t}(y^n)$$



$$F_1 \longrightarrow O(\Delta t^{\alpha+1})$$

$$F_2 \longrightarrow O(\Delta t^{\alpha+2})$$

$$= f + \Delta t F_1 + \dots$$

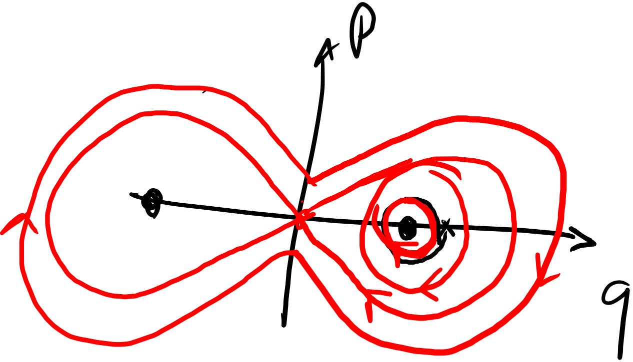
$$\dot z = \boxed{f_{\Delta t}}(z)$$

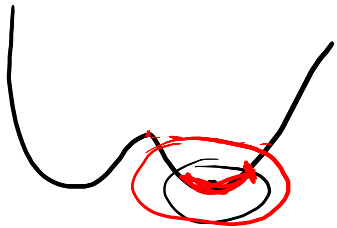
$$\boxed{y^n = z(n\Delta t)}$$

$$y^n - y(n\Delta t) = O(\Delta t^{\alpha})$$

$$y^n - z(n\Delta t) = O(\Delta t^{\cancel{\alpha+1}\ +\infty}) = 0$$

avec

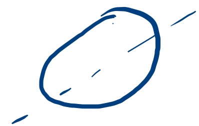




$q = 1$
$p = 0$

- faux pour $\Delta t > 0$. — pas Verlet $\delta t \ll 1$

ES $\longrightarrow$



- intégrat° "exacte" pour $H + \Delta t \tilde{H}$

1. $\{y^n\}$ avec Δt

2. trajectoire "continue" ($\delta t \ll \Delta t$)

pour $$\dot{z} = J\nabla(H + \Delta t\, \tilde{H})(z)$$