$$(\nabla^2 V)_{ij} = \frac{\partial^2 V}{\partial q_i q_j} = \frac{\cdots\cdots}{|q_j - q_i|^3}$$

$$\in \mathbb{R}^{N\times N}$$

$$= \partial_{q_i}\left(\frac{q_j - q_i}{|q_j - q_i|^2}\right)$$

$$V(q) \propto \sum_{l<k} \frac{1}{|q_k - q_l|} \longrightarrow \partial^2_{q_i q_j}\left(\frac{1}{|q_i - q_j|}\right)$$

bei $N=3$:

$$\partial_{q_2}\partial_{q_1}\left(\frac{1}{|q_1 - q_2|} + \cancel{\frac{1}{|q_1 - q_3|}}\right) + \cancel{\frac{1}{|q_2 - q_3|}}$$

$$\partial^2_{q_1}$$

$$\partial^2_{q_i} \longrightarrow N \text{ tems}$$

$$\partial_{q_i q_j} \longrightarrow 1 \text{ tem}$$

1. calculer $N = 2$

Débuggage :

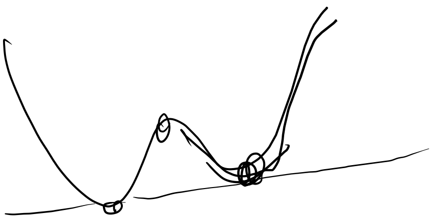
2. $$V(q + \sigma G) - 2V(q) + V(q - \sigma G)$$

$$\simeq G^T \nabla^2 V G \, \sigma^2 + O(\sigma^4)$$

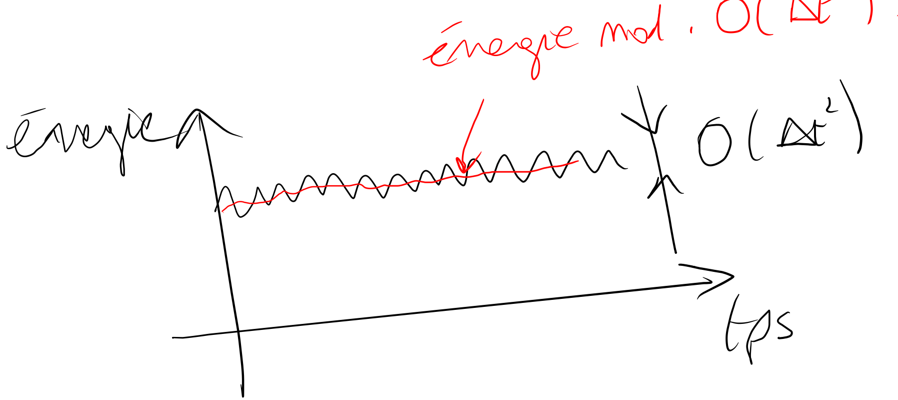
(G aléatoire)

$$V(q + \sigma G) + \nabla V(q) \cdot \sigma G + \frac{\sigma^2}{2} G^T \nabla^2 V G + O(\sigma^3)$$

Option "renormalisée" : cas 1D



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



" débougage des fonds d'en. "modifiée" "

$$H(q^m p^m)$$

$$+ a\, p^m \nabla^2 V(q^m)\, p^m$$

$$+ b\, |\nabla V(q^m)|^2$$

$$\min_{a,b} \sum \left(H + a \cdots + b \cdots\right)^2$$

$\longrightarrow a, b = ?$
(minimiser)

$\Rightarrow$ varie $O(\Delta t^4)$

Faire régression linéaire !

$$\underset{D_3}{F_3}(q,p) = \frac{1}{12}\begin{pmatrix} -\frac{\cancel{}}{2}\nabla^2 V \cdot p \\ \nabla^2 V \cdot \nabla V \cancel{+} \underbrace{- D^3 V : p \otimes p}_{\text{vecteur de composante } p^T \nabla^2(\partial_i V)\, p} \end{pmatrix}$$

$$\Omega = \mathrm{Id}$$

$$= J \nabla H_3 = \begin{pmatrix} +\nabla_p H_3 \\ -\nabla_q H_3 \end{pmatrix}$$

avec $H_3 = \frac{1}{12} p^T \nabla^2 V p - \frac{1}{24} |\nabla V|^2$

$$\longrightarrow \quad \nabla_p H_3 = \frac{1}{6} \nabla^2 V \cdot p$$

$$\nabla_q H_3 = -\frac{1}{12} \nabla^2 V \cdot \nabla V - \frac{1}{12} D^3 V : p \otimes p$$

On doit trouver

$$\boxed{H_2(qp) = \frac{1}{12} p^T \Omega^{-1} D^2 V \Omega^{-1} p - \frac{1}{24} \nabla V^T \Omega^{-1} \nabla V}$$

$\frac{1}{m^2}$

$\frac{1}{m}$

1D $\longrightarrow$ vérifier scaling / t m