$$w = \begin{pmatrix} q_1^x \\ q_1^y \\ q_1^z \\ p_1^x \\ \vdots \\ q_2^x \\ \vdots \end{pmatrix} = \begin{pmatrix} q_i^a \\ p_i^a \end{pmatrix} \quad \text{where} \quad \begin{array}{l} a \in \{x, y, z\} \text{ is spatial coordinates} \\ i \in \{1, 2, \dots, n\} \text{ is particle label} \end{array}$$

$$\frac{dw}{dt} = \sum_{ai} \left[\frac{\partial w}{\partial q_i^a} \frac{dq_i^a}{dt} + \frac{\partial w}{\partial p_i^a} \frac{dp_i^a}{dt} \right]$$

$$= \sum_{ai} \left[\frac{p_i^a}{m_i} \frac{\partial w}{\partial q_i^a} + f_i^a \frac{\partial w}{\partial p_i^a} \right]$$

$$\Rightarrow \left\{ \begin{array}{l} \hat{T} \equiv \sum_{ai} \frac{p_i^a}{m_i} \frac{\partial}{\partial q_i^a} = \sum_{ai} \frac{\partial T}{\partial p_i^a} \frac{\partial}{\partial q_i^a} \quad , \text{ where } T = \sum_{ai} \frac{{p_i^a}^2}{2m_i} \\ \hat{V} = \sum_{ai} f_i^a \frac{\partial}{\partial p_i^a} = -\sum_{ai} \frac{\partial V}{\partial q_i^a} \frac{\partial}{\partial p_i^a} \quad , \text{ where } V = \sum_{i,j<i} \frac{G m_i m_j}{|\vec{r}_i - \vec{r}_j|} \end{array} \right.$$

$$[\hat{T}, \hat{V}] = \hat{T}\hat{V} - \hat{V}\hat{T}$$

$$= \sum_{ai} \frac{p_i^a}{m_i} \frac{\partial}{\partial q_i^a} \sum_{bj} f_j^b \frac{\partial}{\partial p_j^b} - \sum_{bj} f_j^b \frac{\partial}{\partial p_j^b} \sum_{ai} \frac{p_i^a}{m_i} \frac{\partial}{\partial q_i^a}$$

$$= \sum_{abij} \left\{ \frac{p_i^a}{m_i} \left(\frac{\partial f_j^b}{\partial q_i^a} \right) \frac{\partial}{\partial p_j^b} + \cancel{\frac{p_i^a}{m_i} f_j^b \frac{\partial^2}{\partial q_i^a \partial p_j^b}} - \frac{f_j^b}{m_i} \underbrace{\frac{\partial p_i^a}{\partial p_j^b}}_{\downarrow\ \delta_{ij}\,\delta^{ab}} \frac{\partial}{\partial q_i^a} - \cancel{\frac{f_j^b}{m_i} p_i^a \frac{\partial^2}{\partial q_i^a \partial p_j^b}} \right\}$$

$$= \underbrace{\sum_{abij} \frac{p_i^a}{m_i} \frac{\partial f_j^b}{\partial q_i^a} \frac{\partial}{\partial p_j^b}}_{\hat{A}} - \underbrace{\sum_{ai} \frac{f_i^a}{m_i} \frac{\partial}{\partial q_i^a}}_{\hat{B}}$$

$$[\hat{V}, \hat{A}] = \sum_{ck} f_k^c \frac{\partial}{\partial p_k^c} \sum_{abij} \frac{p_i^a}{m_i} \frac{\partial f_j^b}{\partial q_i^a} \frac{\partial}{\partial p_j^b} - \sum_{abij} \frac{p_i^a}{m_i} \frac{\partial f_j^b}{\partial q_i^a} \frac{\partial}{\partial p_j^b} \sum_{ck} f_k^c \frac{\partial}{\partial p_k^c}$$

$$= \sum_{abcijk} \left\{ \frac{f_k^c}{m_i} \left(\frac{\partial p_i^a}{\partial p_k^c} \right) \frac{\partial f_j^b}{\partial q_i^a} \frac{\partial}{\partial p_j^b} + \cancel{\frac{f_k^c p_i^a}{m_i} \frac{\partial f_j^b}{\partial q_i^a} \frac{\partial^2}{\partial p_j^b \partial p_k^c}} - \cancel{\frac{p_i^a}{m_i} \frac{\partial f_j^b}{\partial q_i^a} f_k^c \frac{\partial^2}{\partial p_j^b \partial p_k^c}} \right\}$$

$$= \sum_{abij} \frac{f_i^a}{m_i} \frac{\partial f_j^b}{\partial q_i^a} \frac{\partial}{\partial p_j^b}$$

$$[\hat{V}, -\hat{B}] = -\sum_{ck} f_k^c \frac{\partial}{\partial p_k^c} \sum_{ai} \frac{f_i^a}{m_i} \frac{\partial}{\partial q_i^a} + \sum_{ai} \frac{f_i^a}{m_i} \frac{\partial}{\partial q_i^a} \sum_{ck} f_k^c \frac{\partial}{\partial p_k^c}$$

$$= \sum_{acik} \left\{ -\cancel{\frac{f_i^a f_k^c}{m_i} \frac{\partial^2}{\partial q_i^a \partial q_k^c}} + \frac{f_i^a}{m_i} \frac{\partial f_k^c}{\partial q_i^a} \frac{\partial}{\partial p_k^c} + \cancel{\frac{f_i^a}{m_i} f_k^c \frac{\partial^2}{\partial q_i^a \partial p_k^c}} \right\}$$

$$= \sum_{abij} \frac{f_i^a}{m_i} \frac{\partial f_j^b}{\partial q_i^a} \frac{\partial}{\partial p_j^b}$$

$$[\hat{V},[\hat{T},\hat{V}]] = [\hat{V},\hat{A}-\hat{B}] = 2\sum_{abij} \frac{f_i^a}{m_i}\frac{\partial f_j^b}{\partial q_i^a}\frac{\partial}{\partial p_j^b}$$

Recalling $f_j^b = -\partial V/\partial q_j^b$, $\partial f_j^b/\partial q_i^a = -\dfrac{\partial^2 V}{\partial q_i^a\,\partial q_j^b} = \partial f_i^a/\partial q_j^b$

Comparing $\hat{V} = \sum_{bj} f_j^b\,\partial/\partial p_j^b$, it is natural to define

$$\tilde{f}_j^b \equiv 2\sum_{ai}\frac{f_i^a}{m_i}\frac{\partial f_j^b}{\partial q_i^a} = 2\sum_{ai}\frac{f_i^a}{m_i}\frac{\partial f_i^a}{\partial q_j^b} = \frac{\partial}{\partial q_j^b}\sum_{ai}\frac{(f_i^a)^2}{m_i}$$

$$V = \sum_{i,\, j<i} - \frac{G m_i m_j}{|r_i - r_j|}$$, assume $a = x$

$$f_i^x = -\frac{\partial V}{\partial x_i} = + \sum_{i \neq j} G m_i m_j \frac{\partial}{\partial x_i} \frac{1}{|r_i - r_j|}$$

$$= -\sum_{i \neq j} \frac{G m_i m_j}{|r_i - r_j|^2} \frac{\partial}{\partial x_i} |r_i - r_j|$$

$$= -\sum_{i \neq j} \frac{G m_i m_j}{|r_i - r_j|^3} (x_i - x_j)$$

$$\Rightarrow \quad f_i^a = -\sum_{i \neq j} \frac{G m_i m_j}{|r_i - r_j|^3} (q_i^a - q_j^a)$$

$$\frac{\partial f_i^a}{\partial q_j^b} = \frac{-\partial}{\partial q_j^b} \sum_{i \neq k} \frac{G m_i m_k}{|r_i - r_k|^3} (q_i^a - q_k^a)$$

if $i = j$, $$\frac{\partial f_i^a}{\partial q_j^b} = -\sum_{j \neq k} \frac{G m_j m_k}{|r_j - r_k|^3} \delta^{ab} + \sum_{j \neq k} \frac{+3 G m_j m_k}{|r_j - r_k|^5} (q_j^a - q_k^a)(q_j^b - q_k^b)$$

if $i \neq j$, $$\frac{\partial f_i^a}{\partial q_j^b} = + \frac{G m_i m_j}{|r_i - r_j|^3} \delta^{ab} + 3 \frac{G m_i m_j}{|r_i - r_j|^5} (q_i^a - q_j^a)(q_j^b - q_i^b)$$

$$= + \frac{G m_i m_j}{|r_i - r_j|^3} \delta^{ab} - 3 \frac{G m_i m_j}{|r_i - r_j|^5} (q_j^a - q_i^a)(q_j^b - q_i^b)$$

$$\tilde{f}_j^b \equiv 2 \sum_{ai} \frac{f_i^a}{m_i} \frac{\partial f_j^b}{\partial q_i^a} = 2 \sum_{ai} \frac{f_i^a}{m_i} \frac{\partial f_i^a}{\partial q_j^b}$$

$$= 2 \sum_a \left[\frac{f_j^a}{m_j} \frac{\partial f_j^a}{\partial q_j^b} + \sum_{i \neq j} \frac{f_i^a}{m_i} \frac{\partial f_i^a}{\partial q_j^b} \right]$$

$$= 2 \sum_a \left\{ - \frac{f_j^a}{m_j} \sum_{i \neq j} \frac{G m_i m_j}{|r_i - r_j|^3} \left[\delta^{ab} - 3 \frac{(q_i^a - q_j^a)(q_i^b - q_j^b)}{|r_i - r_j|^2} \right] \right.$$

$$\left. + \sum_{i \neq j} \frac{f_i^a}{m_i} \frac{G m_i m_j}{|r_i - r_j|^2} \left[\delta^{ab} - 3 \frac{(q_i^a - q_j^a)(q_i^b - q_j^b)}{|r_i - r_j|^2} \right] \right\}$$

$$= 2 \sum_a \sum_{i \neq j} \left(-\frac{f_j^a}{m_j} + \frac{f_i^a}{m_i} \right) \frac{G m_i m_j}{|r_i - r_j|^3} \left[\delta^{ab} - 3 \frac{(q_i^a - q_j^a)(q_i^b - q_j^b)}{|r_i - r_j|^2} \right]$$

$$\frac{\tilde{f}_i^b}{m_i} = -2 \sum_{j \neq i} \frac{G m_j}{|r_j - r_i|^3} \sum_a \left(\frac{f_j^a}{m_j} - \frac{f_i^a}{m_i} \right) \left(3 \frac{(q_j^a - q_i^a)(q_j^b - q_i^b)}{|r_j - r_i|^2} - \delta^{ab} \right)$$