$$\langle c'|H|c'\rangle = \left(1 + \sum_{ai} |\delta c_{ai}|^2\right)\langle c|H|c\rangle$$

$$+ \underbrace{\sum_{ai} |\delta c_{ai}|^2 (\varepsilon_a^{HF} - \varepsilon_i^{HF})} + \cdots$$

$$\sum_{ai} \delta c_{ai}^* \delta c_{ai} (\varepsilon_a^{HF} - \varepsilon_i^{HF})$$

$$= \sum_{\substack{ai \\ bj}} \delta c_{ai}^* \delta c_{bj} (\varepsilon_a^{HF} - \varepsilon_i^{HF}) \delta_{ab} \delta_{ij}$$

ph-config $\quad I = \{ai\}$

$\quad J = \{bj\}$

$$= \sum_{IJ} \delta c_I^* \delta c_J \Delta\varepsilon_{IJ}$$

$$\Delta\varepsilon_{IJ} = (\varepsilon_a^{HF} - \varepsilon_i^{HF}) \delta_{ab} \delta_{ij}$$

$$\delta c^* \begin{bmatrix} \Delta\varepsilon_{11} & & \\ & \Delta\varepsilon_{22} & \\ & & \ddots \Delta_{pH} \end{bmatrix} \delta c$$

$$\sum_{a_i'} \sum_{b_j} \delta C^*_{a_i'} \delta C_{b_j} A_{a_i' b_j}$$

$$\underline{I} \quad \underline{J}$$

$$A_{a_i' b_j} = - \langle a_i' | w | b_j \rangle$$

$$\underline{I} \quad \underline{J}$$

$$= A_{\underline{I}\underline{J}}$$

$$\sum_{\underline{I}\underline{J}} \delta C^*_{\underline{I}} \delta C_{\underline{J}} A_{\underline{I}\underline{J}}$$

$$= \delta C^* A \delta C$$

$$\Delta E = \frac{1}{2} \left[\delta C^* \delta C \right]$$

$$\times \begin{bmatrix} \Delta\varepsilon + A & B \\ B^* & \Delta\varepsilon + A^* \end{bmatrix} \begin{bmatrix} \delta C \\ \delta C^* \end{bmatrix}$$