interazione di configurazione

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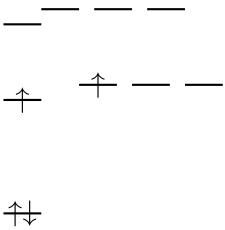
correlazione e interazione di configurazione

$$\Psi = \sum_k a_k \Psi_k$$

dove Ψ_k sono determinanti di slater.

determinanti



$$|1, 1, 1, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0\rangle$$

$$|1, 1, 1, 0, 1\rangle$$

$$T_{4,5}|1, 1, 1, 1\rangle$$

quanti!

ALLDET

$$N_{\mathrm{det}} = \binom{n}{N}$$

$$\binom{20}{10} = 184756$$

ancora algebra lineare

$$\begin{bmatrix} H_{00} & H_{01} \\ H_{10} = H_{01} & H_{11} \end{bmatrix} \begin{bmatrix} a_{00} \\ a_{10} \end{bmatrix} = \epsilon_0 \begin{bmatrix} a_{00} \\ a_{10} \end{bmatrix}$$

$$\begin{bmatrix} H_{00} & H_{01} \\ H_{10} = H_{01} & H_{11} \end{bmatrix} \begin{bmatrix} a_{01} \\ a_{11} \end{bmatrix} = \epsilon_1 \begin{bmatrix} a_{01} \\ a_{11} \end{bmatrix}$$

possiamo riscrivere tutto riallineando le colonne:

$$\begin{bmatrix} E_1 & \delta \\ \delta & E_2 \end{bmatrix} \begin{bmatrix} a_{00} & a_{01} \\ a_{10} & a_{11} \end{bmatrix} = \begin{bmatrix} \epsilon_0 & 0 \\ 0 & \epsilon_1 \end{bmatrix} \begin{bmatrix} a_{00} & a_{01} \\ a_{10} & a_{11} \end{bmatrix}$$

$$A^{-1} \begin{bmatrix} E_1 & \delta \\ \delta & E_2 \end{bmatrix} A = \begin{bmatrix} \epsilon_0 & 0 \\ 0 & \epsilon_1 \end{bmatrix}$$

ancora algebra lineare

$$A^{-1}\begin{bmatrix} E_1 & \delta \\ \delta & E_2 \end{bmatrix} A = \begin{bmatrix} \epsilon_0 & 0 \\ 0 & \epsilon_1 \end{bmatrix}$$

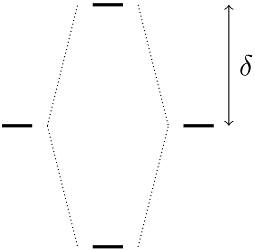
$$\det \begin{bmatrix} E_1-\epsilon & \delta \\ \delta & E_2-\delta \end{bmatrix} = \epsilon^2 + E_1E_2 - \epsilon(E_1+E_2) - \delta^2 = 0$$

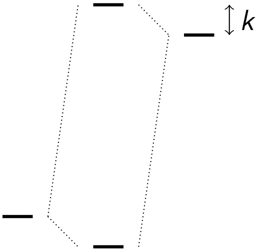
che ha soluzioni

$$\epsilon = \frac{E_1 + E_2 \pm \sqrt{(E_2-E_1)^2 + 4\delta^2}}{2}$$

ancora algebra lineare, soluzione

$$\epsilon = \frac{E_1 + E_2 \pm \sqrt{(E_2 - E_1)^2 + 4\delta^2}}{2}$$





degenerazione $\epsilon = \frac{E_1+E_2}{2} \pm \delta$

perturbazione $\begin{cases} \epsilon_1 = E_1 - k \\ \epsilon_2 = E_2 + k \end{cases}$

perchè...

$$\epsilon = \frac{E_1 + E_2}{2} \pm \frac{E_2 - E_1}{2}\sqrt{1 + 4\frac{\delta^2}{(E_2 - E_1)^2}} \approx \begin{cases} E_1 - k \\ E_1 + k \end{cases}$$

$$k = \frac{\delta^2}{(E_2 - E_1)}$$