1)

i) $$\langle \chi_j \chi_1 | H | \chi_1 \chi_1 \rangle = \int dx \int dy\, \chi_j(x)\chi_1(y)\left(h(x) + h(y) + a x^4 y^4\right) \chi_1(x)\chi_1(y).$$

$$= \int dx\, \chi_j(x) \int dy\, \chi_1(y) \left(h(x) + h(y) + a x^4 y^4\right) \chi_1(x)\chi_1(y)$$

$$= \int dx\, \chi_j(x) \int dy\, \chi_1(y) \left(h(x)\chi_1(x)\chi_1(y) + \chi_1(x)\, h(y)\, \chi_1(y) + a x^4 \chi_1(x) y^4 \chi_1(y)\right)$$

$$= \int dx\, \chi_j(x)\, h(x)\chi_1(x) \langle \chi_1(y) | \chi_1(y)\rangle + \chi_1(x) \langle \chi_1(y) | h(y) | \chi_1(y)\rangle + a \langle \chi_1(y) | y^4 | \chi_1(y)\rangle x^4 \chi_1(x).$$

$$= \int dx\, \chi_j(x) \left(\left(h(x) + a\langle \chi | y^4 | \chi\rangle x^4\right) \chi_1(x) + \langle \chi | h | \chi\rangle \chi_1(x)\right)$$

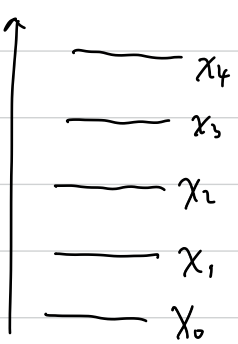
$$= \int dx\, \chi_j(x)\, \epsilon_1 \chi_1(x) + \langle \chi | h | \chi\rangle \chi_1(x).$$

$$= \epsilon_1 \langle \chi_j | \chi_1 \rangle + \langle \chi | h | \chi\rangle \langle \chi_j | \chi_1 \rangle$$

$$= \epsilon_1 \delta_{j,1} + \langle \chi | h | \chi \rangle \delta_{j1}.$$

ii) From eq 27, large $\langle \chi_i \chi_j | H | \chi_1 \chi_1 \rangle$ terms give greater contribution to E^{CI}.
& lower energies E_{ij} contribute more to E^{CI}.

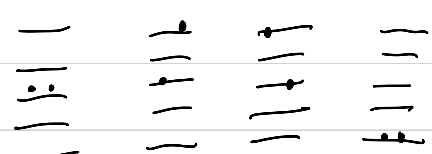
iii) 0-index here for sake of notation:



$$\operatorname*{argmax}_{ij} \langle \chi_i \chi_j | H | \chi_0 \chi_0 \rangle = \{(0,0), (2,2), (2,4), (4,2)\}.$$

I would expect:

Configs: $\Rightarrow$



contribute the most.

3.

i) Define $|\Phi_{ij}\rangle :=$ the Slater determinant of $|\chi_i\rangle$ & $|\chi_j\rangle$, then $\langle \Phi_{ij}|H|\Phi_{kl}\rangle$

$$= \tfrac{1}{2}\langle \chi_i(x)\chi_j(y) - \chi_j(x)\chi_i(y) \,|\, H \,|\, \chi_k(x)\chi_l(y) - \chi_l(x)\chi_k(y)\rangle$$

$$= \tfrac{1}{2}\Big(\underline{\int dx \int dy\, \chi_i\chi_j H \chi_k\chi_l} - \int dx\int dy\, \chi_i\chi_j H\chi_l\chi_k - \int dx\int dy\, \chi_j\chi_i H\chi_k\chi_l \qquad (1)$$

$$+ \int dx\int dy\, \chi_j\chi_i H\chi_l\chi_k \Big).$$

Consider the term in red:

$$\int dx\int dy\, \chi_i(x)\chi_j(y)\,[h(x) + h(y) + a x^4 y^4]\,\chi_k(x)\chi_l(y)$$

we have:

$$\int dx\, \chi_i(x)\int dy\, \chi_j(y)\,[h(x) + h(y) + a x^4 y^4]\,\chi_k(x)\chi_l(y)$$

$$= \int dx\, \chi_i(x)\Big(\big(h(x)\delta_{jl} + a\langle\chi_j|y^4|\chi_l\rangle x^4\big)\chi_k(x) + \langle\chi_j|h|\chi_l\rangle\chi_k(x)\Big)$$

$$= \langle\chi_i|h|\chi_k\rangle\delta_{jl} + a\langle\chi_j|y^4|\chi_l\rangle\langle\chi_i|x^4|\chi_k\rangle + \langle\chi_j|h|\chi_l\rangle\delta_{ik}.$$

$\therefore$, for all four terms in eq(1), we have:

$$\Rightarrow \tfrac{1}{2}\Big(2\delta_{jl}\langle\chi_i|h|\chi_k\rangle + 2\delta_{ik}\langle\chi_j|h|\chi_l\rangle - 2\delta_{il}\langle\chi_j|h|\chi_k\rangle - 2\delta_{jk}\langle\chi_i|h|\chi_l\rangle$$

$$+ 2a\langle\chi_j|y^4|\chi_l\rangle\langle\chi_i|x^4|\chi_k\rangle - 2a\langle\chi_i|y^4|\chi_l\rangle\langle\chi_j|x^4|\chi_k\rangle\Big)$$

$$\Rightarrow \langle\chi_i\chi_j|H|\chi_k\chi_l\rangle = \delta_{jl}\langle\chi_i|h|\chi_k\rangle + \delta_{ik}\langle\chi_j|h|\chi_l\rangle - \delta_{il}\langle\chi_j|h|\chi_k\rangle - \delta_{jk}\langle\chi_i|h|\chi_l\rangle$$

$$+ a\langle\chi_j|y^4|\chi_l\rangle\langle\chi_i|x^4|\chi_k\rangle - a\langle\chi_i|y^4|\chi_l\rangle\langle\chi_j|x^4|\chi_k\rangle. \quad \blacksquare$$

ii).

From, previous part, we know the individual terms when H is acted on a Slater determinant.

Consider one of the terms:

$$\langle \chi_i \chi_j | H | \chi_k \chi_l \rangle.$$

From previous part, we know it is equal to:

$$\Rightarrow \langle \chi_i | h | \chi_k \rangle \delta_{jl} + a \langle \chi_j | y^4 | \chi_l \rangle \langle \chi_i | x^4 | \chi_k \rangle + \langle \chi_j | h' \chi_l \rangle \delta_{ik}.$$

$$\langle \chi_i | h | \chi_k \rangle = \langle \textstyle\sum_A C_{Ai} \phi_A | h | \sum_B C_{Bk} \phi_B \rangle \delta_{jl}$$

$$= \left(\textstyle\sum_A C_{Ai} C_{Ak} \langle \phi_A | h | \phi_B \rangle \right) \delta_{jl}.$$

$$= \left(\textstyle\sum_A \sum_B C_{Ai} C_{Bk} \langle \phi_A | h | \phi_B \rangle \right) \delta_{jl}.$$

$$= \left(\underline{C}_i^T \underline{\underline{h}} \underline{c}_k \right) \delta_{jl}, \text{ where } \underline{\underline{h}}_{AB} = \langle \phi_A | h | \phi_B \rangle.$$

Similarly, $\langle \chi_j | y^4 | \chi_l \rangle$

$$= \textstyle\sum_A \sum_B C_{Aj} C_{Bl} \langle \phi_A | y^4 | \phi_B \rangle.$$

$$= \underline{c}_j^T \underline{\underline{G}} \underline{c}_i \text{ , where } \underline{\underline{G}}_{AB} = \langle \phi_A | y^4 | \phi_B \rangle.$$

Then, altogether we get

$$\langle \Phi_{ij} | H | \Phi_{kl} \rangle = \delta_{jl} \underline{C}_i^T \underline{\underline{h}} \underline{c}_k^T + \delta_{ik} \underline{C}_i^T \underline{\underline{h}} \underline{c}_l - \delta_{il} \underline{c}_j^T \underline{\underline{h}} \underline{c}_k - \delta_{jk}^T \underline{c}_i \underline{\underline{h}} \underline{c}_l$$

$$+ a \left((\underline{c}_j^T \underline{\underline{G}} \underline{c}_l)(\underline{c}_i^T \underline{\underline{G}} \underline{c}_k) \right) - a \left((\underline{c}_i^T \underline{\underline{G}} \underline{c}_l)(\underline{c}_j^T \underline{\underline{G}} \underline{c}_k) \right) \quad \blacksquare$$