G0W0

Patryk Kozlowski

November 24, 2023

1 Derivation of Factors

Initially, we have the expression

$$A_{iajb} = \delta_{ij}\delta_{ab}\left(\varepsilon_a - \varepsilon_i\right) + (\underline{ia}|\underline{jb}) \tag{1}$$

all is in terms of spin orbitals. We want to derive the conversion into spatial orbitals.

$$(\underline{ia}|\underline{jb}) = \sum_{\sigma_1\sigma_2\sigma_3\sigma_4} \int dr_1 \int dr_2 \phi_{i,\sigma_1}(r_1)\phi^*_{a,\sigma 2}(r_1)\frac{1}{r_{12}}\phi_{j,\sigma 3}(r_2)\phi^*_{b,\sigma 4}(r_2) \tag{2}$$

The spin at a given index has to be the same, So

$$= \sum_{\sigma_1\sigma_2} \int dr_1 \int dr_2 \phi_{i,\sigma_1}(r_1)\phi^*_{a,\sigma_1}(r_1)\frac{1}{r_{12}}\phi_{j,\sigma_2}(r_2)\phi^*_{b,\sigma_2}(r_2) \tag{3}$$

Because we are working in a direct approximation, we only care about the Coloumb ones of

$$(ia|jb) \to (i_\alpha a_\alpha|j_\beta b_\beta), (i_\beta a_\beta|j_\alpha b_\alpha); (i_\alpha a_\alpha|j_\alpha b_\alpha), (i_\beta a_\beta|j_\beta b_\beta) \tag{4}$$

which 2 does this correspond to and is my logic correct? Next, we have:

$$W_{p,q,i,a} = \sum_{\underline{p,q,i,a}} (\underline{pq}|\underline{ia}) \tag{5}$$

which is the same as

$$W_{p,q,i,a} = \sum_{p,q,i,a} \sum_{\sigma_1\sigma_2\sigma_3\sigma_4} \int dr_1 \int dr_2 \phi_{p\sigma_1}(r_1)\phi^*_{q\sigma_2}(r_1)\frac{1}{r_{12}}\phi_{i\sigma_3}(r_2)\phi^*_{a\sigma_4}(r_2) \tag{6}$$

I am not sure where to go from here.