MP2F12 method

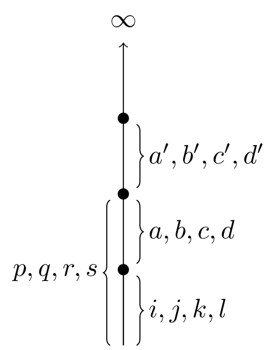
mg20240013

September 2024

1 Notation and Convection

1.1 Orbital

Let an orthonormal basis $\{\phi_\kappa\}$ of spin orbitals be given. This basis has usually a finite dimentsion d,but it should be chosen $d \to \infty$.



The RI approximation is that

$$I \equiv \frac{1}{2}|\kappa\gamma\rangle\langle\kappa\gamma| \approx \frac{1}{2}|pq\rangle\langle pq| + \frac{1}{2}|a'b'\rangle\langle a'b'| \tag{1.1.1}$$

Here the coefficient $\frac{1}{2}$ is due to Einstein Summation Convention. We do not restrict $\kappa < \gamma$ and the summation range of each repeated index is in full range,and stick to this convection throughout the whole report .

1.2 Hamiltonian

In this report, normal ordered Hamiltonian is

$$\hat{H} = E_0 + \hat{F} + \hat{G} \tag{1.2.1}$$

The E_0 is reference state energy. In this case the Hartree Fock Energy.

The fock operator $\hat{F}$ is

$$\hat{F} = \hat{t} + \hat{v}_n + \hat{j} - \hat{k} \tag{1.2.2}$$

where t is kinetic energy operator, $\hat{v}_n$ is nuclear potential operator .and $\hat{j}$ and $\hat{k}$ is Coulomb operator and exchange operator respectively.

$$\hat{F} = f^p_q a^\dagger_q a_p \quad f^p_q \equiv \langle p|f|q\rangle \tag{1.2.3}$$

The normal ordered two particle operator is

$$\hat{G} = \frac{1}{4}\bar{g}^{pq}_{rs} a^\dagger_r a^\dagger_s a_q a_p \quad \bar{g}^{pq}_{rs} = \langle rs||pq\rangle = \langle rs|pq\rangle - \langle sr|pq\rangle \tag{1.2.4}$$

the $\bar{g}^{pq}_{rs}$ is antisymmetrized two electron repulsion integral (eri).

2 Work equation

2.1 f12 geminal basis

In first quantization

$$|\Psi^{kl}_{ij}\rangle = \hat{S}_{kl}\hat{Q}_{12} f_{12}|\phi_k\phi_l\rangle\langle\phi_i\phi_j|0\rangle \tag{2.1.1}$$

$$f_{12} = -\frac{1}{\gamma}e^{-\gamma r_{12}} \tag{2.1.2}$$

The projector the

$$\hat{Q}_{12} = (1-\hat{O}_1)(1-\hat{O}_2) - \hat{V}_1\hat{V}_2 \tag{2.1.3}$$

ensure the f12 geminal is orthogonal to convetional excitation. The rational generator

$$\hat{S}_{kl} = \frac{3}{8} - \frac{1}{8}\hat{P}_{kl} \tag{2.1.4}$$

In second quantization

$$|\Psi^{kl}_{ij}\rangle = \frac{1}{2}\mathcal{F}^{kl}_{\alpha\beta}|\Psi^{\alpha\beta}_{ij}\rangle \tag{2.1.5}$$

where

$$\mathcal{F}^{kl}_{\alpha\beta} = \langle\alpha\beta|\hat{S}_{kl}\hat{Q}_{12} f_{12}|kl\rangle \tag{2.1.6}$$

We define the antisymmetrized integral

$$\bar{r}^{\alpha\beta}_{kl} = \langle\alpha\beta|f_{12}|kl\rangle = r^{\alpha\beta}_{kl} - r^{\beta\alpha}_{kl} \tag{2.1.7}$$

The first order wavefunction is

$$|\Psi^{(1)}\rangle = \frac{1}{4}t^{ij}_{ab}|\Psi^{ab}_{ij}\rangle + \frac{1}{4}c^{ij}_{kl}|\Psi^{kl}_{ij}\rangle \tag{2.1.8}$$

2.2 Hylleraas functional

The hyllerass functional is defined as

$$J = \langle \Psi^{(1)} | \hat{F} | \Psi^{(1)} \rangle + 2 \langle \Psi^{(1)} | \hat{G} | \Psi^{(0)} \rangle \tag{2.2.1}$$

And the residue is defined as

$$R^{ab}_{ij} = \langle \Psi^{ab}_{ij} | \hat{F} | \Psi^{(1)} \rangle + \langle \Psi^{ab}_{ij} | \hat{G} | \Psi^{(0)} \rangle \tag{2.2.2}$$

$$R^{kl}_{ij} = \langle \Psi^{kl}_{ij} | \hat{F} | \Psi^{(1)} \rangle + \langle \Psi^{kl}_{ij} | \hat{G} | \Psi^{(0)} \rangle \tag{2.2.3}$$

Thus the functional can be writeen as

$$J = \frac{1}{4} t^{ij}_{ab} (R^{ab}_{ij} + V^{ab}_{ij}) + \frac{1}{4} c^{ij}_{kl} (R^{kl}_{ij} + V^{kl}_{ij}) \tag{2.2.4}$$

2.3 Evalutate of Residue

2.3.1 R^{ab}_{ij}

for R^{ab}_{ij} we need consider four terms:

First and the easist is

$$\begin{aligned} V^{ab}_{ij} &= \langle \Psi^{ab}_{ij} | \hat{G} | \Psi^{(0)} \rangle \\ &= \frac{1}{4} \langle 0 | i^\dagger j^\dagger b a \bar{g}^{pq}_{rs} r^\dagger s^\dagger q p | 0 \rangle \\ &= \frac{1}{4} \bar{g}^{pq}_{rs} (\delta^{pq}_{ij} \delta^{rs}_{ab} - \delta^{pq}_{ij} \delta^{sr}_{ab} - \delta^{qp}_{ij} \delta^{rs}_{ab} + \delta^{qp}_{ij} \delta^{sr}_{ab}) = \bar{g}^{ij}_{ab} \end{aligned}$$

The second is

$$\frac{1}{4} t^{kl}_{cd} \langle \Psi^{ab}_{ij} | \hat{F} | \Psi^{cd}_{kl} \rangle \tag{2.3.1}$$

The contraction of type $\bar{c}^{kl}_{cd} \langle \Psi^{ab}_{ij} | \hat{F} | \Psi^{cd}_{kl} \rangle$ is used several times in this report ,thus we give it here explicitly

$$\begin{aligned} \bar{c}^{kl}_{cd} \langle \Psi^{ab}_{ij} | \hat{F} | \Psi^{cd}_{kl} \rangle &= f^p_q \bar{c}^{kl}_{cd} \langle 0 | i^\dagger j^\dagger b a q^\dagger p c^\dagger d^\dagger l k | 0 \rangle \\ &= f^p_q \bar{c}^{kl}_{cd} [(\bar{\delta}^{ij}_{kl})(\bar{\delta}^{pb}_{cd} \delta^a_q + \bar{\delta}^{ap}_{cd} \delta^b_q) - (\bar{\delta}^{cd}_{ab})(\bar{\delta}^{iq}_{kl} \delta^j_p + \bar{\delta}^{qj}_{kl} \delta^i_p)] \\ &= f^p_q \bar{c}^{kl}_{cd} 4 [(\delta^{ij}_{kl})(\delta^{pb}_{cd} \delta^a_q + \delta^{ap}_{cd} \delta^b_q) - (\delta^{cd}_{ab})(\delta^{iq}_{kl} \delta^j_p + \delta^{qj}_{kl} \delta^i_p)] \\ &= 4 (f^c_a \bar{c}^{ij}_{cb} + f^d_b \bar{c}^{ij}_{cb} - f^j_l \bar{c}^{il}_{ab} - f^i_k \bar{c}^{kj}_{ab}) \end{aligned}$$

Use the above formula

$$\frac{1}{4} t^{kl}_{cd} \langle \Psi^{ab}_{ij} | \hat{F} | \Psi^{cd}_{kl} \rangle = f^c_a t^{ij}_{cb} + f^d_b t^{ij}_{cb} - f^j_l t^{il}_{ab} - f^i_k t^{kj}_{ab} \tag{2.3.2}$$

The final term is coupling terms

$$
\begin{aligned}
\frac{1}{4}c^{kl}_{mn}\langle\Psi^{ab}_{ij}|\hat{F}|\Psi^{mn}_{kl}\rangle &= \frac{1}{4}c^{kl}_{mn}\frac{1}{2}\mathcal{F}^{mn}_{\alpha\beta}\langle\Psi^{ab}_{ij}|\hat{F}|\Psi^{\alpha\beta}_{kl}\rangle \\
&= \frac{1}{4}c^{kl}_{mn}\frac{1}{2}\mathcal{F}^{mn}_{\alpha\beta}f^{p}_{q}[(\bar{\delta}^{ij}_{kl})(\bar{\delta}^{pb}_{\alpha\beta}\delta^{a}_{q}+\bar{\delta}^{ap}_{\alpha\beta}\delta^{b}_{q})-(\bar{\delta}^{\alpha\beta}_{ab})(\bar{\delta}^{iq}_{kl}\delta^{j}_{p}+\bar{\delta}^{qj}_{kl}\delta^{i}_{p})] \\
&= \frac{1}{4}c^{kl}_{mn}\frac{1}{2}\mathcal{F}^{mn}_{\alpha\beta}f^{p}_{q}(\bar{\delta}^{ij}_{kl})(\bar{\delta}^{pb}_{\alpha\beta}\delta^{a}_{q}+\bar{\delta}^{ap}_{\alpha\beta}\delta^{b}_{q}) \\
&= \frac{1}{2}c^{ij}_{mn}(\mathcal{F}^{mn}_{\alpha b}f^{\alpha}_{a}+\mathcal{F}^{mn}_{a\beta}f^{\beta}_{b}) \\
&= c^{ij}_{mn}C^{mn}_{ab}
\end{aligned}
$$

Defination of C term

$$
C^{mn}_{ab} = \frac{1}{2}(\mathcal{F}^{mn}_{\alpha b}f^{\alpha}_{a}+\mathcal{F}^{mn}_{a\beta}f^{\beta}_{b}) \tag{2.3.3}
$$

$$
R^{ab}_{ij} = \bar{g}^{ab}_{ij}+f^{c}_{a}t^{ij}_{cb}+f^{d}_{b}t^{ij}_{cb}-f^{j}_{l}t^{il}_{ab}-f^{i}_{k}t^{kj}_{ab}+c^{ij}_{mn}C^{mn}_{ab} \tag{2.3.4}
$$

2.3.2 R^{mn}_{kl}

V term

$$
\begin{aligned}
V^{mn}_{kl} &= \langle\Psi^{mn}_{kl}|\hat{G}|\Psi^{(0)}\rangle \\
&= \frac{1}{2}\mathcal{F}^{\alpha\beta}_{mn}\langle\Psi^{\alpha\beta}_{kl}|\hat{G}|\Psi^{(0)}\rangle \\
&= \frac{1}{2}\mathcal{F}^{\alpha\beta}_{mn}\bar{g}^{\alpha\beta}_{kl}
\end{aligned}
$$

Copuling term

$$
\begin{aligned}
\frac{1}{4}t^{ij}_{ab}\langle\Psi^{mn}_{kl}|\hat{F}|\Psi^{ab}_{ij}\rangle &= \frac{1}{4}t^{ij}_{ab}\frac{1}{2}\mathcal{F}^{\alpha\beta}_{mn}\langle\Psi^{\alpha\beta}_{kl}|\hat{F}|\Psi^{ab}_{ij}\rangle \\
&= \frac{1}{4}t^{ij}_{ab}\frac{1}{2}\mathcal{F}^{\alpha\beta}_{mn}f^{p}_{q}(\bar{\delta}^{ij}_{kl})(\bar{\delta}^{pb}_{\alpha\beta}\delta^{a}_{q}+\bar{\delta}^{ap}_{\alpha\beta}\delta^{b}_{q}) \\
&= \frac{1}{2}t^{kl}_{ab}\frac{1}{2}\mathcal{F}^{\alpha\beta}_{mn}f^{p}_{q}(\bar{\delta}^{pb}_{\alpha\beta}\delta^{a}_{q}+\bar{\delta}^{ap}_{\alpha\beta}\delta^{b}_{q}) \\
&= \frac{1}{2}t^{kl}_{ab}(\mathcal{F}^{a\beta}_{mn}f^{\beta}_{b}+\mathcal{F}^{\alpha b}_{mn}f^{\alpha}_{a}) \\
&= t^{kl}_{ab}C^{ab}_{mn}
\end{aligned}
$$

Now geminal-germinal part

$$
\begin{aligned}
\frac{1}{4}c^{ij}_{xy}\langle\Psi^{mn}_{kl}|\hat{F}|\Psi^{xy}_{ij}\rangle &= \frac{1}{4}c^{ij}_{xy}\frac{1}{2}\mathcal{F}^{\alpha\beta}_{mn}(\langle\Psi^{\alpha\beta}_{kl}|\hat{F}|\Psi^{\kappa\lambda}_{ij}\rangle)\frac{1}{2}\mathcal{F}^{xy}_{\kappa\lambda} \\
&= \frac{1}{4}c^{ij}_{xy}\frac{1}{2}\mathcal{F}^{\alpha\beta}_{mn}f^{p}_{q}[(\bar{\delta}^{kl}_{ij})(\bar{\delta}^{p\beta}_{\kappa\lambda}\delta^{\alpha}_{q}+\bar{\delta}^{\alpha p}_{\kappa\lambda}\delta^{\beta}_{q})-(\bar{\delta}^{\kappa\lambda}_{\alpha\beta})(\bar{\delta}^{kq}_{ij}\delta^{l}_{p}+\bar{\delta}^{ql}_{ij}\delta^{k}_{p})]\frac{1}{2}\mathcal{F}^{xy}_{\kappa\lambda}
\end{aligned}
$$

We split this into two part.The first is p-p contraction

$$
\begin{aligned}
&\frac{1}{4}c_{xy}^{ij}\frac{1}{2}\mathcal{F}_{mn}^{\alpha\beta}f_q^p[(\bar{\delta}_{ij}^{kl})(\bar{\delta}_{\kappa\lambda}^{p\beta}\delta_q^\alpha+\bar{\delta}_{\kappa\lambda}^{\alpha p}\delta_q^\beta)]\frac{1}{2}\mathcal{F}_{\kappa\lambda}^{xy}\\
&=\frac{1}{2}c_{xy}^{kl}\frac{1}{2}\mathcal{F}_{mn}^{\alpha\beta}f_q^p[(\bar{\delta}_{\kappa\lambda}^{p\beta}\delta_q^\alpha+\bar{\delta}_{\kappa\lambda}^{\alpha p}\delta_q^\beta)]\frac{1}{2}\mathcal{F}_{\kappa\lambda}^{xy}\\
&=\frac{1}{2}c_{xy}^{kl}\frac{1}{2}\mathcal{F}_{mn}^{\alpha\beta}[f_\alpha^\kappa\mathcal{F}_{\kappa\beta}^{xy}+f_\beta^\lambda\mathcal{F}_{\alpha\lambda}^{xy}]\\
&=\frac{1}{2}c_{xy}^{kl}B_{mn}^{xy}
\end{aligned}
$$

The B term is defined as

$$
B_{mn}^{xy}=\frac{1}{2}\mathcal{F}_{mn}^{\alpha\beta}f_\alpha^\kappa\mathcal{F}_{\kappa\beta}^{xy}+\frac{1}{2}\mathcal{F}_{mn}^{\alpha\beta}f_\beta^\lambda\mathcal{F}_{\alpha\lambda}^{xy}=\mathcal{F}_{mn}^{\alpha\beta}f_\alpha^\kappa\mathcal{F}_{\kappa\beta}^{xy} \tag{2.3.5}
$$

The h-h contraction part is

$$
\begin{aligned}
&\frac{1}{4}c_{xy}^{ij}\frac{1}{2}\mathcal{F}_{mn}^{\alpha\beta}f_q^p[-(\bar{\delta}_{\alpha\beta}^{\kappa\lambda})(\bar{\delta}_{ij}^{kq}\delta_p^l+\bar{\delta}_{ij}^{ql}\delta_p^k)]\frac{1}{2}\mathcal{F}_{\kappa\lambda}^{xy}\\
&=-\frac{1}{4}c_{xy}^{ij}\frac{1}{2}\mathcal{F}_{mn}^{\alpha\beta}f_q^p[(\bar{\delta}_{ij}^{kq}\delta_p^l+\bar{\delta}_{ij}^{ql}\delta_p^k)]\mathcal{F}_{\alpha\beta}^{xy}\\
&=-\frac{1}{4}c_{xy}^{ij}f_q^p[(\bar{\delta}_{ij}^{kq}\delta_p^l+\bar{\delta}_{ij}^{ql}\delta_p^k)](\frac{1}{2}\mathcal{F}_{mn}^{\alpha\beta}\mathcal{F}_{\alpha\beta}^{xy})\\
&=-\frac{1}{2}(c_{xy}^{kj}f_j^l+c_{xy}^{il}f_i^k)X_{mn}^{xy}
\end{aligned}
$$

The X term is defined as

$$
X_{mn}^{xy}=\frac{1}{2}\mathcal{F}_{mn}^{\alpha\beta}\mathcal{F}_{\alpha\beta}^{xy} \tag{2.3.6}
$$

We collect all term to form residue

$$
R_{kl}^{mn}=V_{kl}^{mn}+t_{ab}^{kl}C_{mn}^{ab}+\frac{1}{2}c_{xy}^{kl}B_{mn}^{xy}-\frac{1}{2}(c_{xy}^{kj}f_j^l+c_{xy}^{il}f_i^k)X_{mn}^{xy} \tag{2.3.7}
$$

2.3.3 Evaluate Energy

We optimize convential amplitude t_{ab}^{ij},and let c_{mn}^{kl} fix In canonical orbital

$$
R_{ij}^{ab}=\bar{g}_{ij}^{ab}+(f_a^a+f_b^b-f_i^i-f_j^j)t_{ab}^{ij}+c_{mn}^{ij}C_{ab}^{mn} \tag{2.3.8}
$$

$$
R_{kl}^{mn}=V_{kl}^{mn}+\frac{1}{2}c_{xy}^{kl}B_{mn}^{xy}-\frac{1}{2}(f_l^l+f_k^k)c_{xy}^{kl}X_{mn}^{xy}+t_{ab}^{kl}C_{mn}^{ab} \tag{2.3.9}
$$

Let $R_{ij}^{ab}=0$

$$
t_{ab}^{ij}=\frac{1}{\Delta_{ij}^{ab}}(\bar{g}_{ij}^{ab}+c_{mn}^{ij}C_{ab}^{mn}) \tag{2.3.10}
$$

$$
t_{ab}^{kl}C_{mn}^{ab}=\frac{1}{\Delta_{kl}^{ab}}(\bar{g}_{kl}^{ab}+c_{mn}^{kl}C_{ab}^{mn})C_{mn}^{ab} \tag{2.3.11}
$$

We Define

$$\Delta_{ij}^{ab} \equiv f_i^i + f_j^j - f_a^a - f_b^b \tag{2.3.12}$$

$$J = E_1 + E_2 = \frac{1}{4} t_{ab}^{ij} (R_{ij}^{ab} + V_{ij}^{ab}) + \frac{1}{4} c_{kl}^{ij} (R_{ij}^{kl} + V_{ij}^{kl})$$

$$E_1 = \frac{1}{4} \frac{1}{\Delta_{ij}^{ab}} (\bar{g}_{ij}^{ab} + c_{mn}^{ij} C_{ab}^{mn}) \bar{g}_{ij}^{ab}$$

$$E_2 = \frac{1}{4} c_{kl}^{ij} (V_{ij}^{kl} + t_{ab}^{ij} C_{kl}^{ab} + \frac{1}{2} c_{xy}^{ij} B_{kl}^{xy} - \frac{1}{2} (c_{xy}^{in} f_n^j + c_{xy}^{mj} f_m^i) X_{kl}^{xy} + V_{ij}^{kl})$$

$$\begin{aligned}
E = E_1 + E_2 = & \frac{1}{4} \frac{1}{\Delta_{ij}^{ab}} \bar{g}_{ij}^{ab} \\
& + \frac{1}{4} \frac{1}{\Delta_{ij}^{ab}} c_{mn}^{ij} C_{ab}^{mn}) \bar{g}_{ij}^{ab} \\
& + \frac{1}{4} c_{kl}^{ij} V_{ij}^{kl} \\
& + \frac{1}{4} c_{kl}^{ij} \frac{1}{\Delta_{ij}^{ab}} \bar{g}_{ij}^{ab} C_{kl}^{ab} \\
& + \frac{1}{4} c_{kl}^{ij} \frac{1}{\Delta_{ij}^{ab}} c_{mn}^{ij} C_{ab}^{mn} C_{kl}^{ab} \\
& + \frac{1}{4} c_{kl}^{ij} \frac{1}{2} c_{xy}^{ij} B_{kl}^{xy} \\
& - \frac{1}{4} c_{kl}^{ij} \frac{1}{2} c_{xy}^{ij} (f_j^j + f_i^i) X_{kl}^{xy} \\
& + \frac{1}{4} c_{kl}^{ij} V_{ij}^{kl} \\
& = E_{mp2} + \frac{1}{4} c_{kl}^{ij} (2 * \tilde{V}_{ij}^{kl}) + \frac{1}{4} c_{kl}^{ij} \tilde{B}_{kl}^{xy}(i,j) \frac{1}{2} c_{xy}^{ij}
\end{aligned}$$

Here

$$\tilde{V}_{ij}^{kl} = V_{ij}^{kl} + \frac{1}{\Delta_{ij}^{ab}} C_{kl}^{ab} \bar{g}_{ij}^{ab} \tag{2.3.13}$$

$$\tilde{B}_{kl}^{xy}(i,j) = B_{kl}^{xy} - (f_i^i + f_j^j) X_{kl}^{xy} + 2 \frac{1}{\Delta_{ij}^{ab}} C_{ab}^{xy} C_{kl}^{ab} \tag{2.3.14}$$

3 Matrix Element

3.1 V term and X term

$$\hat{V}_1 = |a\rangle\langle a| \quad \hat{O}_2 = |i\rangle\langle i| \tag{3.1.1}$$

$$
\begin{aligned}
\hat{Q}_{12} &= (1-\hat{O}_1)(1-\hat{O}_2) - \hat{V}_1\hat{V}_2 \\
&= 1 - \hat{O}_1 - \hat{O}_2 + \hat{O}_1\hat{O}_2 - \hat{V}_1\hat{V}_2 \\
&\approx 1 - \hat{O}_1(\hat{P}_2 + \hat{P}_2') - (\hat{P}_1 + \hat{P}_1')\hat{O}_2 + \hat{O}_1\hat{O}_2 - \hat{V}_1\hat{V}_2 \\
&= 1 - \hat{O}_1\hat{O}_2 - \hat{O}_1\hat{V}_2 - \hat{O}_1\hat{P}_2' - \hat{O}_1\hat{O}_2 - \hat{V}_1\hat{O}_2 - \hat{P}'\hat{O}_2 + \hat{O}_1\hat{O}_2 - \hat{V}_1\hat{V}_2 \\
&= 1 - \hat{O}_1\hat{P}_2' - \hat{P}_1'\hat{O}_2 - \hat{P}_1\hat{P}_2
\end{aligned}
$$

We need to check the space of $\hat{Q}_{12}$ on antisymmetrized two electron space.The range and image of the operator is different.

$$\hat{P}_1\hat{P}_2 = \frac{1}{2}|pq\rangle\langle pq| \tag{3.1.2}$$

$$\hat{O}_1\hat{P}_2' + \hat{P}_1'\hat{O}_2 = |ia'\rangle\langle ia'| \tag{3.1.3}$$

$$
\begin{aligned}
\hat{O}_1\hat{P}_2' + \hat{P}_1'\hat{O}_2|ia'\rangle &= (\hat{O}_1\hat{P}_2' + \hat{P}_1'\hat{O}_2)\frac{1}{\sqrt{2}}(\phi_i\phi_{a'} - \phi_{a'}\phi_i) \\
&= \frac{1}{\sqrt{2}}[(\hat{O}_1\hat{P}_2' + \hat{P}_1'\hat{O}_2)(\phi_i\phi_{a'}) - (\hat{O}_1\hat{P}_2' + \hat{P}_1'\hat{O}_2)\phi_{a'}\phi_i] \\
&= \frac{1}{\sqrt{2}}[(\phi_i\phi_{a'} - \phi_{a'}\phi_i] \\
&= |ia'\rangle
\end{aligned}
$$

$$
\begin{aligned}
V_{ij}^{kl} &= \frac{1}{2}\mathcal{F}_{ij}^{\alpha\beta}\bar{g}_{kl}^{\alpha\beta} \\
&= \frac{1}{2}\langle ij|\hat{S}_{ij}f_{12}\hat{Q}_{12}|\alpha\beta\rangle\langle\alpha\beta|\frac{1}{r}|kl\rangle \\
&= \langle ij|\hat{S}_{ij}f_{12}\hat{Q}_{12}\frac{1}{r}|kl\rangle \\
&= \hat{S}_{ij}[\langle ij|f_{12}\frac{1}{r_{12}}|kl\rangle - \langle ij|f_{12}|ma'\rangle\langle ma'|\frac{1}{r_{12}}|kl\rangle - \frac{1}{2}\langle ij|f_{12}|pq\rangle\langle pq|\frac{1}{r_{12}}|kl\rangle \\
&= \hat{S}_{ij}[(\overline{rg})_{ij}^{kl} - \bar{r}_{ij}^{ma'}\bar{g}_{ma'}^{kl} - \frac{1}{2}\bar{r}_{ij}^{pq}\bar{g}_{pq}^{kl}]
\end{aligned}
$$

$$
\begin{aligned}
X_{mn}^{xy} &= \frac{1}{2}\mathcal{F}_{mn}^{\alpha\beta}\mathcal{F}_{\alpha\beta}^{xy} \\
&= \hat{S}_{mn}\hat{S}_{xy}[(\overline{r^2})_{mn}^{xy} - \bar{r}_{mn}^{ia'}\bar{r}_{ia'}^{xy} - \frac{1}{2}\bar{r}_{mn}^{pq}\bar{r}_{pq}^{xy}]
\end{aligned}
$$

3.2 C term

$$
\begin{aligned}
C_{ab}^{mn} &= \frac{1}{2}(\mathcal{F}_{\alpha b}^{mn}f_a^{\alpha} + \mathcal{F}_{a\beta}^{mn}f_b^{\beta}) \\
&= \hat{S}_{mn}\frac{1}{2}(\bar{r}_{a'b}^{mn}f_a^{a'} + \bar{r}_{ab'}^{mn}f_b^{b'})
\end{aligned}
$$

3.3 B term

Evaluate B term is most complex term. In this section we use different symbols for orbitals.

symbol	orbital	Capital letter
$\alpha\beta\gamma$	infinitly liary complementary orbital	A
$a'b'c'$	finitly approximation of cabs orbital	A'
$abcd$	virtual orbital in GBS	B
$ijkl$	occupied orbital in GBS	C
$pqrs$	total orbital sapce in GBS	D
$\kappa\lambda\mu\nu$	infinitly complete orbital	E
$p'q'r's'$	RI orbital	E'

The way to calculate B term is first convert into EEE part ,then use double commutator to calculate some term analytically. Others is calculated by RI approximation $A \approx A'$.

$$\begin{aligned}
B^{xy}_{mn} &= \mathcal{F}^{\kappa\lambda}_{mn} f^{\mu}_{\kappa} \mathcal{F}^{xy}_{\mu\lambda} \\
&= \hat{S}_{mn}\hat{S}_{xy}[\bar{r}^{\alpha\beta}_{mn} f^{\gamma}_{\alpha} \bar{r}^{xy}_{\gamma\beta} + \bar{r}^{a\beta}_{mn} f^{\gamma}_{a} \bar{r}^{xy}_{\gamma\beta} + \bar{r}^{\alpha b}_{mn} f^{\gamma}_{\alpha} \bar{r}^{xy}_{\gamma b} + \bar{r}^{\alpha\beta}_{mn} f^{c}_{\alpha} \bar{r}^{xy}_{c\beta} + \bar{r}^{a\beta}_{mn} f^{c}_{a} \bar{r}^{xy}_{c\beta}] \\
&= \hat{S}_{mn}\hat{S}_{xy}\mathbb{B}^{xy}_{mn}
\end{aligned}$$

$$\mathbb{B}^{xy}_{mn} = [\bar{r}^{\alpha\beta}_{mn} f^{\gamma}_{\alpha} \bar{r}^{xy}_{\gamma\beta} + \bar{r}^{a\beta}_{mn} f^{\gamma}_{a} \bar{r}^{xy}_{\gamma\beta} + \bar{r}^{\alpha b}_{mn} f^{\gamma}_{\alpha} \bar{r}^{xy}_{\gamma b} + \bar{r}^{\alpha\beta}_{mn} f^{c}_{\alpha} \bar{r}^{xy}_{c\beta} + \bar{r}^{a\beta}_{mn} f^{c}_{a} \bar{r}^{xy}_{c\beta}]$$

We project the summation range of $\kappa\lambda\mu$ out ,and do some manipulation of summation range:

$$\begin{aligned}
&AAA + BAA + ABA + AAB + BAB \\
&= (A+B)AA + ABA + (A+B)AB \\
&= (A+B)A(A+B) + ABA \\
&= (E-C)A(E-C) + ABA \\
&= (E-C)(E-D)(E-C) + ABA \\
&= (E-C)E(E-C) - (E-C)D(E-C) + ABA \\
&= EEE - EEC - CEE + CEC \\
&\quad - EDE + EDC + CED - CED + (E-D)B(E-D) \\
&= EEE - EEC - CEE + CEC \\
&\quad - EDE + EDC + CDE - CDC \\
&\quad + EBE - EBD - DBE + DBD) \\
&= EEE - EAC - CAE + CAC - ECE - ABD - DBA - DBD
\end{aligned}$$

3.3.1 RI approximation terms

CAC $\implies$ $CA'C$

$$\bar{r}^{ia'}_{mn} f^{j}_{i} \bar{r}^{xy}_{ja'}$$

ECE $\implies E'CE'$

$$\bar{r}^{p'i}_{mn} f^{q'}_{p'} \bar{r}^{xy}_{q'i}$$

DBD

$$\bar{r}^{pa}_{mn} f^{q}_{p} \bar{r}^{xy}_{qa}$$

DBA+ABD $\implies DBA' + A'BD$

$$\bar{r}^{pa}_{mn} f^{a'}_{p} \bar{r}^{xy}_{a'a} + \bar{r}^{a'a}_{mn} f^{p}_{a'} \bar{r}^{xy}_{pa}$$

EAC+CAE $\implies E'A'C + CA'E'$

$$\bar{r}^{p'a'}_{mn} f^{i}_{p'} \bar{r}^{xy}_{ia'} + \bar{r}^{ia'}_{mn} f^{p'}_{i} \bar{r}^{xy}_{p'a'}$$

We need to show DBA' and $A'BD$ are conjuate

$$\bar{r}^{aa'}_{mn} f^{p}_{a'} \bar{r}^{xy}_{pa} = \bar{r}^{pa}_{xy} f^{a'}_{p} \bar{r}^{mn}_{a'a}$$

Also $E'A'C$ and $CA'E'$ are conjugate

3.3.2 EEE term

First we calculate EEE using commutator trick
we can see the EEE part can convert into first quantization

$$\begin{aligned}
\langle mn|f_{12}\hat{F}f_{12}|xy\rangle &= \frac{1}{2}\langle mn|f_{12}|\alpha\beta\rangle\langle\alpha\beta|\hat{F}|\gamma\delta\rangle\langle\gamma\delta|f_{12}|xy\rangle\frac{1}{2} \\
&= \frac{1}{2}\bar{r}^{\alpha\beta}_{mn}\langle\alpha\beta|\hat{F}|\gamma\delta\rangle\bar{r}^{xy}_{\gamma\delta}\frac{1}{2} \\
&= \frac{1}{4}\bar{r}^{\alpha\beta}_{mn}(f^{\delta}_{\beta}\delta_{\alpha\gamma} - f^{\gamma}_{\beta}\delta_{\alpha\delta} + f^{\gamma}_{\alpha}\delta_{\beta\delta} - f^{\delta}_{\alpha}\delta_{\beta\gamma})\bar{r}^{xy}_{\gamma\delta} \\
&= \frac{1}{4}(\bar{r}^{\alpha\beta}_{mn}f^{\delta}_{\beta}\bar{r}^{xy}_{\alpha\delta} - r^{\alpha\beta}_{mn}f^{\gamma}_{\beta}\bar{r}^{xy}_{\gamma\alpha} + \bar{r}^{\alpha\beta}_{mn}f^{\gamma}_{\alpha}\bar{r}^{xy}_{\gamma\beta} - \bar{r}^{\alpha\beta}_{mn}f^{\delta}_{\alpha}\bar{r}^{xy}_{\beta\delta}) \\
&= \frac{1}{2}(\bar{r}^{\alpha\beta}_{mn}f^{\delta}_{\beta}\bar{r}^{xy}_{\alpha\delta} + \bar{r}^{\alpha\beta}_{mn}f^{\gamma}_{\alpha}\bar{r}^{xy}_{\gamma\beta}) \\
&= \bar{r}^{\alpha\beta}_{mn}f^{\delta}_{\beta}\bar{r}^{xy}_{\alpha\delta}
\end{aligned}$$

Double commutator

$$\hat{A}\hat{B}\hat{A} = \frac{1}{2}(\hat{A}\hat{A}\hat{B} + \hat{A}[\hat{B},\hat{A}] + \hat{B}\hat{A}\hat{A} + [\hat{A},\hat{B}]\hat{A}) = \frac{1}{2}(\hat{A}\hat{A}\hat{B} + \hat{B}\hat{A}\hat{A} + [[\hat{A},\hat{B}],\hat{A}]) \tag{3.3.1}$$

$$f_{12}\hat{F}f_{12} = f_{12}(\hat{F}+\hat{K})f_{12} - f_{12}(\hat{K})f_{12}$$

$$f_{12}(\hat{F}+\hat{K})f_{12} = \frac{1}{2}(f^2_{12}(\hat{F}+\hat{K}) + (\hat{F}+\hat{K})f^2_{12} + [[f_{12},\hat{T}],f_{12}])$$

Now we calculate matrix element of $f_{12}^2(\hat{F}+\hat{K})$

$$
\begin{aligned}
\langle mn|f_{12}^2(\hat{F}+\hat{K})|xy\rangle &= \frac{1}{2}\langle mn|f_{12}^2|\kappa\lambda\rangle\langle\kappa\lambda|(\hat{F}+\hat{K})|xy\rangle \\
&= \frac{1}{2}\langle mn|f_{12}^2|\kappa\lambda\rangle((f+k)_\lambda^y\delta_{\kappa x}+(f+k)_\kappa^x\delta_{\lambda y}-(f+k)_\lambda^x\delta_{\kappa y}-(f+k)_\kappa^y\delta_{\lambda x}) \\
&= \frac{1}{2}(\overline{r^2}_{mn}^{x\lambda}(f+k)_\lambda^y+\overline{r^2}_{mn}^{\kappa y}(f+k)_\kappa^x-\overline{r^2}_{mn}^{y\lambda}(f+k)_\lambda^x-\overline{r^2}_{mn}^{\kappa x}(f+k)_\kappa^y \\
&= \overline{r^2}_{mn}^{x\lambda}(f+k)_\lambda^y+\overline{r^2}_{mn}^{\kappa y}(f+k)_\kappa^x
\end{aligned}
$$

The EEE term is

$$
\frac{1}{2}(\overline{[[f_{12},T],f_{12}}_{mn}^{xy}+\overline{r^2}_{mn}^{x\lambda}(f+k)_\lambda^y+\overline{r^2}_{mn}^{\kappa y}(f+k)_\kappa^x+conj.)-\bar{r}_{mn}^{\alpha\beta}k_\beta^\delta\bar{r}_{\alpha\delta}^{xy}
$$

3.3.3 Result

$$
\begin{aligned}
\mathbb{B}_{mn}^{xy} &= \frac{1}{2}\overline{[[f_{12},T],f_{12}]}_{mn}^{xy} && (3.3.2)\\
&+\frac{1}{2}(\overline{r^2}_{mn}^{x\lambda}(f+k)_\lambda^y+\overline{r^2}_{mn}^{\kappa y}(f+k)_\kappa^x+conj.) && (3.3.3)\\
&-\bar{r}_{mn}^{p'q'}k_{p'}^{r'}\bar{r}_{r'q'}^{xy} && (3.3.4)\\
&+\bar{r}_{mn}^{ia'}f_i^j\bar{r}_{ja'}^{xy}-\bar{r}_{mn}^{p'i}f_{p'}^{q'}\bar{r}_{q'i}^{xy}-\bar{r}_{mn}^{pa}f_p^q\bar{r}_{qa}^{xy} && (3.3.5)\\
&+(\bar{r}_{mn}^{pa}f_p^{a'}\bar{r}_{a'a}^{xy}+\bar{r}_{mn}^{p'a'}f_{p'}^i\bar{r}_{ia'}^{xy}+conj.) && (3.3.6)
\end{aligned}
$$

4 Evaluate V ,X and C

4.1 V term

$$
V_{ij}^{kl}=\hat{S}_{ij}[(\overline{rg})_{ij}^{kl}-\bar{r}_{ij}^{ma'}\bar{g}_{ma'}^{kl}-\frac{1}{2}\bar{r}_{ij}^{pq}\bar{g}_{pq}^{kl}]
$$

Let use some symbol to free from the rational generator $\hat{S}_{ij}$

$$
V_{ij}^{kl}=\hat{S}_{ij}\mathbb{V}_{ij}^{kl}\quad \mathbb{V}_{ij}^{kl}=[(\overline{rg})_{ij}^{kl}-\bar{r}_{ij}^{ma'}\bar{g}_{ma'}^{kl}-\frac{1}{2}\bar{r}_{ij}^{pq}\bar{g}_{pq}^{kl}]
$$

Now we use new symbol to seperate the bar parts

$$\begin{aligned}
\mathbb{V}_{ij}^{kl} &= [(\overline{rg})_{ij}^{kl} - \bar{r}_{ij}^{ma'}\bar{g}_{ma'}^{kl} - \frac{1}{2}\bar{r}_{ij}^{pq}\bar{g}_{pq}^{kl}] \\
&= (rg)_{ij}^{kl} - (rg)_{ij}^{lk} \\
&\quad - (r_{ij}^{ma'} - r_{ij}^{a'm})(g_{ma'}^{kl} - g_{ma'}^{lk}) \\
&\quad - \frac{1}{2}(r_{ij}^{pq} - r_{ij}^{qp})(g_{pq}^{kl} - g_{pq}^{lk}) \\
&= (rg)_{ij}^{kl} - (rg)_{ij}^{lk} \\
&\quad - (r_{ij}^{ma'}g_{ma'}^{kl} + r_{ij}^{a'm}g_{ma'}^{lk}) + (r_{ij}^{ma'}g_{ma'}^{lk} + r_{ij}^{a'm}g_{ma'}^{kl}) \\
&\quad - \frac{1}{2}(r_{ij}^{pq}g_{pq}^{kl} + r_{ij}^{qp}g_{pq}^{lk} - r_{ij}^{pq}g_{pq}^{lk} - r_{ij}^{qp}g_{pq}^{kl}) \\
&= (rg)_{ij}^{kl} - (rg)_{ij}^{lk} \\
&\quad - r_{ij}^{ma'}g_{ma'}^{kl} - r_{ji}^{ma'}g_{ma'}^{lk} + (r_{ij}^{ma'}g_{ma'}^{lk} + r_{ji}^{ma'}g_{ma'}^{kl}) \\
&\quad - r_{ij}^{pq}g_{pq}^{kl} + r_{ij}^{pq}g_{pq}^{lk} \\
&= \acute{\mathbb{V}}_{ij}^{kl} - \acute{\mathbb{V}}_{ij}^{lk}
\end{aligned}$$

$$\acute{\mathbb{V}}_{ij}^{kl} = (rg)_{ij}^{kl} - r_{ij}^{ma'}g_{ma'}^{kl} - r_{ji}^{ma'}g_{ma'}^{lk} - r_{ij}^{pq}g_{pq}^{kl}$$

4.2 X term

$$X_{mn}^{xy} = \hat{S}_{mn}\hat{S}_{xy}[(\overline{r^2})_{mn}^{xy} - \bar{r}_{mn}^{ma'}\bar{r}_{ma'}^{xy} - \frac{1}{2}\bar{r}_{mn}^{pq}\bar{r}_{pq}^{xy}]$$

$$X_{mn}^{xy} = \hat{S}_{mn}\hat{S}_{xy}\mathbb{X}_{mn}^{xy} \quad \mathbb{X}_{mn}^{xy} = (\overline{r^2})_{mn}^{xy} - \bar{r}_{mn}^{ia'}\bar{r}_{ia'}^{xy} - \frac{1}{2}\bar{r}_{mn}^{pq}\bar{r}_{pq}^{xy}$$

$$\mathbb{X}_{mn}^{xy} = \acute{\mathbb{X}}_{mn}^{xy} - \acute{\mathbb{X}}_{nm}^{xy}$$

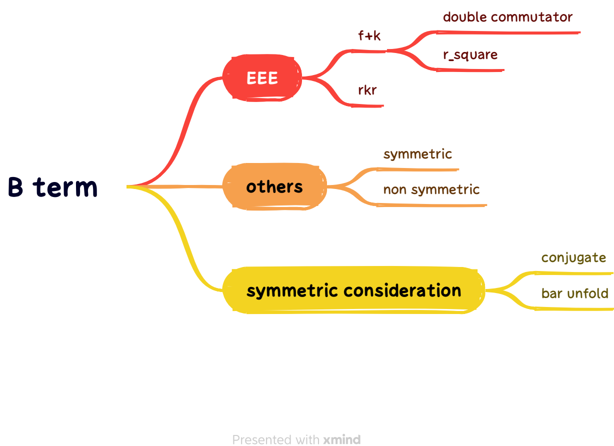
$$\acute{\mathbb{X}}_{mn}^{xy} = (r^2)_{mn}^{xy} - r_{mn}^{ia'}r_{ia'}^{xy} - r_{nm}^{ia'}r_{ia'}^{yx} - r_{mn}^{pq}r_{pq}^{xy}$$

4.3 C term

$$C_{ab}^{mn} = \hat{S}_{mn}\frac{1}{2}(\bar{r}_{a'b}^{mn}f_a^{a'} + \bar{r}_{ab'}^{mn}f_b^{b'})$$

$$\begin{aligned}
\mathbb{C}_{ab}^{mn} &= \bar{r}_{a'b}^{mn}f_a^{a'} + \bar{r}_{ab'}^{mn}f_b^{b'} \\
&= (r_{a'b}^{mn} - r_{a'b}^{nm})f_a^{a'} + r_{ab'}^{mn}f_b^{b'} - r_{ab'}^{nm}f_b^{b'} \\
&= r_{a'b}^{mn}f_a^{a'} + r_{ab'}^{mn}f_b^{b'} - (r_{a'b}^{nm})f_a^{a'} + r_{ab'}^{nm}f_b^{b'}) \\
&= \acute{\mathbb{C}}_{ab}^{mn} - \acute{\mathbb{C}}_{ab}^{nm}
\end{aligned}$$

$$\acute{\mathbb{C}}_{ab}^{mn} = r_{a'b}^{mn}f_a^{a'} + r_{ab'}^{mn}f_b^{b'}$$



5 Evaluate B

5.1 EEE term

First we need to convert antisymmetrized part into no symmetric part

5.2 $f_{12}^2(\hat{F}+\hat{K})$

$$\frac{1}{2}((\overline{[[f_{12},T],f_{12}})^{xy}_{mn}+\overline{r2}^{x\lambda}_{mn}(f+k)^y_\lambda+\overline{r2}^{\kappa y}_{mn}(f+k)^x_\kappa+conj.)-\bar{r}^{\alpha\beta}_{mn}k^\delta_\beta\bar{r}^{xy}_{\alpha\delta}$$

We first unfold bar parts

$$\begin{aligned}
&\overline{r2}^{x\lambda}_{mn}(f+k)^y_\lambda+\overline{r2}^{\kappa y}_{mn}(f+k)^x_\kappa+conj.\\
&=((r^2)^{x\lambda}_{mn}-(r^2)^{\lambda x}_{mn})(f+k)^y_\lambda+((r^2)^{\kappa y}_{mn}-(r^2)^{y\kappa}_{mn})(f+k)^x_\kappa+conj.\\
&=(r^2)^{x\lambda}_{mn}(f+k)^y_\lambda+(r^2)^{\kappa y}_{mn}(f+k)^x_\kappa-(r^2)^{\lambda x}_{mn})(f+k)^y_\lambda-(r^2)^{y\kappa}_{mn})(f+k)^x_\kappa+conj.
\end{aligned}$$

Implement of plus two part

$$(r^2)^{x\lambda}_{mn}(f+k)^y_\lambda+(r^2)^{\kappa y}_{mn}(f+k)^x_\kappa=(r^2)^{x\lambda}_{mn}(f+k)^y_\lambda+(r^2)^{y\kappa}_{nm}(f+k)^x_\kappa$$

If the first result is temp

$$(tp)^{xy}_{mn}=(r^2)^{x\lambda}_{mn}(f+k)^y_\lambda$$

The second part is

$$(tp)^{yx}_{nm}=(r^2)^{y\lambda}_{nm}(f+k)^x_\lambda=(r^2)^{y\kappa}_{nm}(f+k)^x_\kappa$$

$$(temp)^{xy}_{mn}=(tp)^{xy}_{mn}+(tp)^{yx}_{nm}$$

5.2.1 Implement of minus two part

$$
\begin{aligned}
&-(r^2)^{\lambda x}_{mn})(f+k)^y_\lambda - (r^2)^{y\kappa}_{mn})(f+k)^x_\kappa \\
&= -(tp)^{xy}_{nm} - (tp)^{yx}_{mn} = -(temp)^{yx}_{mn}
\end{aligned}
$$

5.2.2 Implement of conj. part

$$
\begin{aligned}
&\langle mn|(\hat{F}+\hat{K})f_{12}^2|xy\rangle \\
&= \frac{1}{2}\langle mn(\hat{F}+\hat{K})|\kappa\lambda\rangle\langle\kappa\lambda|f_{12}^2|xy\rangle \\
&= \frac{1}{2}\langle\kappa\lambda|f_{12}^2|xy\rangle\langle mn(\hat{F}+\hat{K})|\kappa\lambda\rangle \\
&= \frac{1}{2}\langle xy|f_{12}^2|\kappa\lambda\rangle\langle\kappa\lambda(\hat{F}+\hat{K})|mn\rangle \\
&= \langle xy|f_{12}^2(\hat{F}+\hat{K})|mn\rangle
\end{aligned}
$$

5.3 fkf

$$
\langle mn|f_{12}\hat{K}f_{12}|xy\rangle = \bar{r}^{\alpha\beta}_{mn}k^\delta_\beta\bar{r}^{xy}_{\alpha\delta}
$$

unfold bar part

$$
\begin{aligned}
\bar{r}^{\alpha\beta}_{mn}k^\delta_\beta\bar{r}^{xy}_{\alpha\delta} &= (r^{\alpha\beta}_{mn} - r^{\beta\alpha}_{mn})k^\delta_\beta(r^{xy}_{\alpha\delta} - r^{yx}_{\alpha\delta}) \\
&= r^{\alpha\beta}_{mn}k^\delta_\beta r^{xy}_{\alpha\delta} + r^{\beta\alpha}_{mn}k^\delta_\beta r^{yx}_{\alpha\delta} - r^{\alpha\beta}_{mn}k^\delta_\beta r^{yx}_{\alpha\delta} - r^{\beta\alpha}_{mn}k^\delta_\beta r^{xy}_{\alpha\delta}
\end{aligned}
$$

5.3.1 plus two term

$$
\begin{aligned}
&r^{\alpha\beta}_{mn}k^\delta_\beta r^{xy}_{\alpha\delta} + r^{\beta\alpha}_{mn}k^\delta_\beta r^{yx}_{\alpha\delta} \\
&= r^{\alpha\beta}_{mn}k^\delta_\beta r^{xy}_{\alpha\delta} + r^{\alpha\beta}_{nm}k^\delta_\beta r^{yx}_{\alpha\delta}
\end{aligned}
$$

Define inter term

$$
\begin{aligned}
(tp)^{xy}_{mn} &= r^{\alpha\beta}_{mn}k^\delta_\beta r^{xy}_{\alpha\delta} \\
(temp)^{xy}_{mn} &= (tp)^{xy}_{mn} + (tp)^{yx}_{nm}
\end{aligned}
$$

5.3.2 minus two term

$$
-r^{\alpha\beta}_{mn}k^\delta_\beta r^{yx}_{\alpha\delta} - r^{\beta\alpha}_{mn}k^\delta_\beta r^{xy}_{\alpha\delta} = -(tp)^{yx}_{mn} - (tp)^{xy}_{nm} = -(temp)^{yx}_{mn}
$$

5.4 CAC -ECE -DBD

CAC as example

$$
\begin{aligned}
\bar{r}^{ia'}_{mn}f^j_i\bar{r}^{xy}_{ja'} &= (r^{ia'}_{mn} - r^{a'i}_{mn})f^j_i(r^{xy}_{ja'} - r^{yx}_{ja'}) \\
&= r^{ia'}_{mn}f^j_i r^{xy}_{ja'} + r^{a'i}_{mn}f^j_i r^{yx}_{ja'} - r^{ia'}_{mn}f^j_i r^{yx}_{ja'} - r^{a'i}_{mn}f^j_i r^{xy}_{ja'} \\
&= tp^{xy}_{mn} + tp^{yx}_{nm} - tp^{yx}_{mn} - tp^{xy}_{nm} \\
&= (temp)^{xy}_{mn} - (temp)^{yx}_{mn}
\end{aligned}
$$

5.5 -(DBA+ABD)-(EAC+CAE)

First of all, we need to unfold the bar .Secondly , the conj part is not calculated explicitly. Third we need to clarify the relationship between conj and bar

$$\begin{aligned}
\bar{T}_{ij}^{ab} + conj(\bar{T}_{ij}^{ab}) &= (T_{ij}^{ab} - T_{ij}^{ba}) + conj(T_{ij}^{ab} - T_{ij}^{ba}) \\
&= T_{ij}^{ab} + conj(T_{ij}^{ab}) - T_{ij}^{ba} - conj(T_{ij}^{ba}) \\
&= T_{ij}^{ab} + T_{ab}^{ij} - T_{ij}^{ba} - T_{ba}^{ij} \\
&= tp_{ij}^{ab} - T_{ij}^{ba} - T_{ba}^{ij} \\
&= tp_{ij}^{ab} - T_{ij}^{ba} - T_{ji}^{ab} \\
&= \overline{tp}_{ij}^{ab}
\end{aligned}$$

DBA as an example

$$\begin{aligned}
\bar{r}_{mn}^{pa} f_p^{a'} \bar{r}_{a'a}^{xy} &= (r_{mn}^{pa} - r_{mn}^{ap}) f_p^{a'} (r_{a'a}^{xy} - r_{a'a}^{yx}) \\
&= r_{mn}^{pa} f_p^{a'} r_{a'a}^{xy} + r_{mn}^{ap} f_p^{a'} r_{a'a}^{yx} - r_{mn}^{pa} f_p^{a'} r_{a'a}^{yx} - r_{mn}^{ap} f_p^{a'} r_{a'a}^{xy} \\
&= tp_{mn}^{xy} + tp_{nm}^{yx} - tp_{mn}^{yx} - tp_{nm}^{xy} \\
&= temp_{mn}^{xy} - temp_{mn}^{yx}
\end{aligned}$$

5.6 Result

$$B_{mn}^{xy} =$$

6 Evaluate $\tilde{V}$ and $\tilde{B}$

6.1 terms in $\tilde{B}$

$$2\frac{1}{\Delta_{ij}^{ab}} C_{ab}^{xy} C_{kl}^{ab} = 2\hat{S}_{xy}\hat{S}_{kl}\frac{1}{2}\mathbb{C}_{ab}^{xy}\frac{1}{2}\mathbb{C}_{kl}^{ab} = \frac{1}{2}\hat{S}_{xy}\hat{S}_{kl}\mathbb{C}_{ab}^{xy}\mathbb{C}_{kl}^{ab}$$

$$\begin{aligned}
\frac{1}{2}\mathbb{C}_{ab}^{xy}\mathbb{C}_{kl}^{ab} &= \frac{1}{2}(\acute{\mathbb{C}}_{ab}^{xy} - \acute{\mathbb{C}}_{ab}^{yx})(\acute{\mathbb{C}}_{ab}^{kl} - \acute{\mathbb{C}}_{ab}^{lk}) \\
&= \acute{\mathbb{C}}_{ab}^{xy}\acute{\mathbb{C}}_{ab}^{kl} - \acute{\mathbb{C}}_{ab}^{xy}\acute{\mathbb{C}}_{ab}^{lk}
\end{aligned}$$

6.2 terms in $\tilde{V}$

$$\frac{1}{\Delta_{ij}^{ab}} C_{kl}^{ab}\bar{g}_{ij}^{ab} = \frac{1}{\Delta_{ij}^{ab}}\hat{S}_{kl}\frac{1}{2}\mathbb{C}_{ab}^{kl}\bar{g}_{ij}^{ab}$$

$$\begin{aligned}
\frac{1}{2}\mathbb{C}_{ab}^{kl}\bar{g}_{ij}^{ab} &= \frac{1}{2}(\acute{\mathbb{C}}_{ab}^{kl} - \acute{\mathbb{C}}_{ab}^{lk})(g_{ij}^{ab} - g_{ji}^{ab}) \\
&= \acute{\mathbb{C}}_{ab}^{kl} g_{ij}^{ab} - \acute{\mathbb{C}}_{ab}^{kl} g_{ji}^{ab}
\end{aligned}$$

7 Spin Adaptation

7.1 $\tilde{V}$

$$
\begin{aligned}
E_1 &= \frac{1}{4}c^{ij}_{kl}(2\tilde{V}^{kl}_{ij}) \\
&= \frac{1}{4}(\delta^{kl}_{ij} - \delta^{lk}_{ij})2\hat{S}_{kl}(\acute{\hat{\mathbb{V}}}^{kl}_{ij} - \acute{\hat{\mathbb{V}}}^{lk}_{ij}) \\
&= \frac{1}{2}2\hat{S}_{ij}(\acute{\hat{\mathbb{V}}}^{ij}_{ij} - \acute{\hat{\mathbb{V}}}^{ji}_{ij}) \\
&= \frac{1}{2}2\hat{S}_{IJ}(\acute{\hat{\mathbb{V}}}^{IJ}_{IJ} - \acute{\hat{\mathbb{V}}}^{JI}_{IJ} + \acute{\hat{\mathbb{V}}}^{\bar{I}\bar{J}}_{\bar{I}\bar{J}} - \acute{\hat{\mathbb{V}}}^{\bar{J}\bar{I}}_{\bar{I}\bar{J}} + \acute{\hat{\mathbb{V}}}^{\bar{I}J}_{\bar{I}J} - \acute{\hat{\mathbb{V}}}^{J\bar{I}}_{\bar{I}J} + \acute{\hat{\mathbb{V}}}^{I\bar{J}}_{I\bar{J}} - \acute{\hat{\mathbb{V}}}^{\bar{J}I}_{I\bar{J}}) \\
&= \frac{1}{2}2(\frac{3}{8} + \frac{1}{8}\hat{P}_{IJ})(\acute{\hat{\mathbb{V}}}^{IJ}_{IJ} - \acute{\hat{\mathbb{V}}}^{JI}_{IJ} \\
&\quad + \acute{\hat{\mathbb{V}}}^{IJ}_{IJ} - \acute{\hat{\mathbb{V}}}^{JI}_{IJ} + \acute{\hat{\mathbb{V}}}^{IJ}_{IJ} + \acute{\hat{\mathbb{V}}}^{IJ}_{IJ}) \\
&= \frac{1}{2}2(\frac{3}{8} + \frac{1}{8}\hat{P}_{IJ})[3(\acute{\hat{\mathbb{V}}}^{IJ}_{IJ} - \acute{\hat{\mathbb{V}}}^{JI}_{IJ}) + (\acute{\hat{\mathbb{V}}}^{IJ}_{IJ} + \acute{\hat{\mathbb{V}}}^{JI}_{IJ})] \\
&= \frac{1}{2}2(\frac{3}{8} - \frac{1}{8})3(\acute{\hat{\mathbb{V}}}^{IJ}_{IJ} - \acute{\hat{\mathbb{V}}}^{JI}_{IJ}) + \frac{1}{2}2(\frac{3}{8} + \frac{1}{8})(\acute{\hat{\mathbb{V}}}^{IJ}_{IJ} + \acute{\hat{\mathbb{V}}}^{JI}_{IJ})
\end{aligned}
$$

7.2 $\tilde{B}$

$$
\begin{aligned}
E_2 &= \frac{1}{4}c^{ij}_{kl}\tilde{B}^{xy}_{kl}(i,j)\frac{1}{2}c^{ij}_{xy} \\
&= \frac{1}{4}(\delta^{kl}_{ij} - \delta^{lk}_{ij})\hat{S}_{xy}\hat{S}_{kl}[\acute{\hat{\mathbb{B}}}^{xy}_{kl}(i,j) - \acute{\hat{\mathbb{B}}}^{yx}_{kl}(i,j)]\frac{1}{2}(\delta^{xy}_{ij} - \delta^{yx}_{ij}) \\
&= \frac{1}{2}\hat{S}_{xy}\hat{S}_{ij}[\acute{\hat{\mathbb{B}}}^{xy}_{ij}(i,j) - \acute{\hat{\mathbb{B}}}^{yx}_{ij}(i,j)]\frac{1}{2}(\delta^{xy}_{ij} - \delta^{yx}_{ij}) \\
&= \frac{1}{2}\hat{S}_{ij}\hat{S}_{ij}[\acute{\hat{\mathbb{B}}}^{ij}_{ij}(i,j) - \acute{\hat{\mathbb{B}}}^{ji}_{ij}(i,j)] \\
&= \frac{1}{2}\hat{S}_{IJ}\hat{S}_{IJ}[3(\acute{\hat{\mathbb{B}}}^{IJ}_{IJ}(I,J) - \acute{\hat{\mathbb{B}}}^{JI}_{IJ}(I,J)) + (\acute{\hat{\mathbb{B}}}^{IJ}_{IJ}(I,J) + \acute{\hat{\mathbb{B}}}^{JI}_{IJ}(I,J)] \\
&= \frac{1}{2}3[(\frac{3}{8} - \frac{1}{8})(\acute{\hat{\mathbb{B}}}^{IJ}_{IJ}(I,J) - \acute{\hat{\mathbb{B}}}^{JI}_{IJ}(I,J))(\frac{3}{8} - \frac{1}{8})] + \frac{1}{2}[(\frac{3}{8} + \frac{1}{8})(\acute{\hat{\mathbb{B}}}^{IJ}_{IJ}(I,J) - \acute{\hat{\mathbb{B}}}^{JI}_{IJ}(I,J))(\frac{3}{8} + \frac{1}{8})]
\end{aligned}
$$