1 Spin-orbital Formalism

The molecular Hamiltonian could be written as:

$$\hat{H} = -\frac{1}{2}\sum_{i}^{N_{\text{el}}}\nabla_i^2 + \sum_{K}^{N_{\text{nuc}}}\sum_{i}^{N_{\text{el}}}\frac{Z_K}{|\mathbf{R}_K - \mathbf{r}_i|} + \sum_{j>i}^{N_{\text{el}}}\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} + \sum_{K>L}^{N_{\text{nuc}}}\frac{Z_K Z_L}{|\mathbf{R}_K - \mathbf{R}_L|} \tag{1}$$

Alternatively, we could write the electronic part into second-quantized form:

$$\hat{H}_{\text{elec}} = \sum_{pq} h_{pq}\hat{p}^\dagger\hat{q} + \frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r} \tag{2}$$

where we denote the one-electron integral:

$$h_{pq} = \langle p|\hat{h}|q\rangle = \langle p|\Big(-\frac{1}{2}\nabla^2 + \sum_{K}^{N_{\text{nuc}}}\frac{Z_K}{|\mathbf{R}_K - \mathbf{r}|}\Big)|q\rangle \tag{3}$$

and the anti-symmetrized two-electron integrals:

$$\langle pq||rs\rangle = \langle pq|\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}|rs\rangle - \langle pq|\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}|sr\rangle \tag{4}$$

In these expressions the electron indices are implicitly carried.
Now to partition the Hamiltonian into reference and perturbation, we firstly expand the expression with Wick's theorm:

$$\hat{H}_{\text{elec}} = \sum_{pq} h_{pq}\{\hat{p}^\dagger\hat{q}\} + \sum_{i} h_{ii} + \frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} + \sum_{ipq}\langle pi||qi\rangle\{\hat{p}^\dagger\hat{q}\} + \frac{1}{2}\sum_{ij}\langle ij||ij\rangle \tag{5}$$

We can partition the Hamiltonian into:

$$\begin{aligned}
\hat{H}_{\text{elec}} =& \Big(\sum_{pq} h_{pq}\{\hat{p}^\dagger\hat{q}\} + \sum_{pqi}\langle pi||qi\rangle\{\hat{p}^\dagger\hat{q}\}\Big) + \Big(\sum_{i} h_{ii} + \frac{1}{2}\sum_{ij}\langle ij||ij\rangle\Big) + \frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} \\
=& \sum_{pq} f_{pq}\{\hat{p}^\dagger\hat{q}\} + \Big(\sum_{i} h_{ii} + \sum_{ij}\langle ij||ij\rangle\Big) - \frac{1}{2}\sum_{ij}\langle ij||ij\rangle + \frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} \\
=& \sum_{pq} f_{pq}\{\hat{p}^\dagger\hat{q}\} + \Big(\sum_{i} f_{ii} - \frac{1}{2}\sum_{ij}\langle ij||ij\rangle\Big) + \frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} \\
=& \sum_{pq} f_{pq}\{\hat{p}^\dagger\hat{q}\} + E_{\text{HF}} + \frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\}
\end{aligned} \tag{6}$$

In Møller–Plesset PT, the reference Hamiltonian is chosen to be the Fock operator:

$$\hat{H}^{(0)} = \hat{F} = \sum_{pq} f_{pq}\hat{p}^\dagger\hat{q} = \sum_{pq} f_{pq}\{\hat{p}^\dagger\hat{q}\} + \sum_{i} f_{ii} \tag{7}$$

The Fock matrix is defined as:

$$f_{pq} = h_{pq} + \sum_{i}\langle pi||qi\rangle \tag{8}$$

Hence, the electronic Hamiltonian could be partitioned into:

$$\hat{H}_{\text{elec}} = \hat{F} - \frac{1}{2}\sum_{ij}\langle ij||ij\rangle + \hat{V} = \hat{H}^{(0)} + \hat{V} \tag{9}$$

where the perturbation:

$$\hat{V} = \hat{H}_{\text{elec}} - \hat{F} = \frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} - \frac{1}{2}\sum_{ij}\langle ij||ij\rangle \tag{10}$$

In summary: the zeroth-order Hamiltonian, perturbation, energy, and wavefunctions in spin-orbital basis:

$$\hat{H}^{(0)} = \sum_{i}^{N} f_{ii} + \sum_{pq}^{N} f_{pq}\{\hat{p}^\dagger\hat{q}\} \tag{11}$$

$$\hat{V} = \frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} - \frac{1}{2}\sum_{ij}\langle ij||ij\rangle \tag{12}$$

$$|\Psi^{(0)}\rangle = |\Phi_{\text{HF}}\rangle = |\Phi_0\rangle \tag{13}$$

$$E^{(0)} = \langle\Phi_0|\hat{H}^{(0)}|\Phi_0\rangle = \sum_{i}^{N} f_{ii} = \sum_{i}\varepsilon_i \tag{14}$$

$$E^{(1)} = \langle\Phi_0|\hat{V}|\Phi_0\rangle = -\frac{1}{2}\sum_{ij}\langle ij||ij\rangle \tag{15}$$

From Rayleigh-Schrödinger PT, we know that the second order energy correction is:

$$E^{(2)} = \langle\Phi_0|\hat{V}|\Psi^{(1)}\rangle \tag{16}$$

The first-order wavefunction is obtained by linear combination of zeroth-order wavefunctions.

$$|\Psi^{(1)}\rangle = \sum_{\eta\neq 0}\frac{\langle\Phi_\eta|\hat{V}|\Phi_0\rangle}{E^{(0)} - E_\eta^{(0)}}|\Phi_\eta\rangle = \sum_{i}\sum_{a}T_i^a|\Phi_i^a\rangle + \sum_{i<j}\sum_{a<b}T_{ij}^{ab}|\Phi_{ij}^{ab}\rangle + \dots \tag{17}$$

By Slater-Condon rule:

$$\langle\Phi_0|\hat{V}|\Phi_I\rangle = 0 \tag{18}$$

for any determinant $|\Phi_I\rangle$ with more than double excitation. By Brillouin theorem:

$$\begin{aligned}\langle\Phi_0|\hat{H}|\Phi_i^a\rangle &= 0 \Leftrightarrow \\ \langle\Phi_0|\hat{H}^{(0)}|\Phi_i^a\rangle + \langle\Phi_0|\hat{V}|\Phi_i^a\rangle &= 0 \Leftrightarrow \\ \langle\Phi_0|\hat{V}|\Phi_i^a\rangle &= 0\end{aligned} \tag{19}$$

Therefore, the only determinants contributing to second-order energy are the doubly excitated ones. Considering the permutation symmetry of $|\Phi_{ij}^{ab}\rangle$, i.e. $|\Phi_{ij}^{ab}\rangle = -|\Phi_{ij}^{ba}\rangle = -|\Phi_{ji}^{ab}\rangle = |\Phi_{ji}^{ba}\rangle$, the first-order wavefunction could be written as:

$$|\Psi^{(1)}\rangle = \frac{1}{4}\sum_{ijab}T_{ij}^{ab}|\Phi_{ij}^{ab}\rangle \tag{20}$$

To find the amplitude T_{ij}^{ab} , we solve the first-order RSPT equation by projecting $\langle\Phi_\eta| = \langle\Phi_{kl}^{cd}| \neq \langle\Phi_0|$ onto it:

$$(\hat{H}^{(0)} - E^{(0)})|\Psi^{(1)}\rangle + (\hat{V} - E^{(1)})|\Phi_0\rangle = 0 \tag{21}$$

$$\langle\Phi_{kl}^{cd}|\hat{H}^{(0)} - E^{(0)}|\Psi^{(1)}\rangle + \langle\Phi_{kl}^{cd}|\hat{V} - E^{(1)})|\Phi_0\rangle = 0 \Leftrightarrow$$

$$\frac{1}{4}\sum_{ijab}\langle\Phi_{kl}^{cd}|\hat{H}^{(0)}|\Phi_{ij}^{ab}\rangle T_{ij}^{ab} - \frac{1}{4}E^{(0)}\sum_{ijab}\langle\Phi_{kl}^{cd}|\Phi_{ij}^{ab}\rangle T_{ij}^{ab} + \langle\Phi_{kl}^{cd}|\hat{V}|\Phi_0\rangle - E^{(1)}\langle\Phi_{kl}^{cd}|\Phi_0\rangle = 0 \Leftrightarrow$$

$$\frac{1}{4}\sum_{ijab} E^{(0)}_{ijab} T^{ab}_{ij}\langle\Phi^{cd}_{kl}|\Phi^{ab}_{ij}\rangle - \frac{1}{4}E^{(0)}\sum_{ijab} T^{ab}_{ij}\langle\Phi^{cd}_{kl}|\Phi^{ab}_{ij}\rangle + \langle\Phi^{cd}_{kl}|\hat{V}|\Phi_0\rangle = 0 \tag{22}$$

To work out the overlap integral:

$$|\Phi^{ab}_{ij}\rangle = \left(\{\hat{a}^\dagger\hat{b}^\dagger\hat{j}\hat{i}\} + \sum_{\substack{\text{all possible}\\\text{contractions}}} \{\overbrace{\hat{a}^\dagger\hat{b}^\dagger\hat{j}}\hat{i}\}\right)|\Phi_0\rangle \tag{23}$$

Noting that only fully contracted terms contribute to the vacuum expectation value:

$$\begin{aligned}\langle\Phi^{cd}_{kl}|\Phi^{ab}_{ij}\rangle = &\sum_{\substack{\text{fully}\\\text{contracted}}} \langle\Phi_0|\{\hat{c}^\dagger\hat{d}^\dagger\hat{l}\hat{k}\}\{\hat{a}^\dagger\hat{b}^\dagger\hat{j}\hat{i}\}|\Phi_0\rangle \\ =&\delta_{ca}\delta_{db}\delta_{ki}\delta_{lj} - \delta_{ca}\delta_{db}\delta_{kj}\delta_{li} - \delta_{cb}\delta_{ad}\delta_{ki}\delta_{lj} + \delta_{cb}\delta_{ad}\delta_{kj}\delta_{li}\end{aligned} \tag{24}$$

Therefore (exploiting the permutation symmetry $T^{ab}_{ij} = -T^{ab}_{ji} = -T^{ba}_{ij} = T^{ba}_{ji}$):

$$\sum_{ijab} T^{ab}_{ij}\langle\Phi^{cd}_{kl}|\Phi^{ab}_{ij}\rangle = T^{cd}_{kl} - T^{cd}_{lk} - T^{dc}_{kl} + T^{dc}_{lk} = 4T^{cd}_{kl} \tag{25}$$

hence we obtain the amplitude as:

$$T^{cd}_{kl} = \frac{\langle\Phi^{cd}_{kl}|\hat{V}|\Phi_0\rangle}{f_{kk} + f_{ll} - f_{cc} - f_{dd}} = \frac{\langle cd||kl\rangle}{\Delta^{kl}_{cd}} \tag{26}$$

and the second-order energy:

$$\begin{aligned}E^{(2)} =&\langle\Phi_0|\hat{V}|\Psi^{(1)}\rangle \\ =&\frac{1}{4}\sum_{ijab}\langle\Phi_0|\hat{V}|\Phi^{ab}_{ij}\rangle T^{ab}_{ij} \\ =&\frac{1}{4}\sum_{ijab}\frac{\langle\Phi_0|\hat{V}|\Phi^{ab}_{ij}\rangle\langle\Phi^{ab}_{ij}|\hat{V}|\Phi_0\rangle}{f_{ii} + f_{jj} - f_{aa} - f_{bb}} \\ =&\frac{1}{4}\sum_{ijab}\frac{\langle ij||ab\rangle\langle ab||ij\rangle}{f_{ii} + f_{jj} - f_{aa} - f_{bb}} \\ =&\frac{1}{4}\sum_{ijab} T^{ab}_{ij}\langle ij||ab\rangle = \frac{1}{4}\sum_{ijab}(T^{ab}_{ij})^*\langle ab||ij\rangle\end{aligned} \tag{27}$$

note that the $-\frac{1}{2}\sum_{ij}\langle ij||ij\rangle$ part in $\hat{V}$ does not contribute to the second-order energy, since $\langle\Phi_0|\Phi^{ab}_{ij}\rangle = 0$.
The total energy up to MP2-level correction is:

$$\begin{aligned}E_{\text{MP2}} =&E^{(0)} + E^{(1)} + E^{(2)} \\ =&\sum_i h_{ii} + \sum_{ij}\langle ij||ij\rangle - \frac{1}{2}\sum_{ij}\langle ij||ij\rangle + E^{(2)} \\ =&\underbrace{\sum_i h_{ii} + \frac{1}{2}\sum_{ij}\langle ij||ij\rangle}_{E_{\text{HF}} = E^{(0)} + E^{(1)}} + \frac{1}{4}\sum_{ijab}\frac{\langle ij||ab\rangle\langle ab||ij\rangle}{f_{ii} + f_{jj} - f_{aa} - f_{bb}}\end{aligned} \tag{28}$$

2 Spin-Adapted-Orbital Formalism

$$\hat{E}^p_q = \sum_\sigma \hat{p}^\dagger_\sigma \hat{q}_\sigma \tag{29}$$

$$\hat{e}^{pq}_{rs} = \sum_{\sigma\tau} \hat{p}^\dagger_\sigma \hat{q}^\dagger_\tau \hat{s}_\tau \hat{r}_\sigma \tag{30}$$

Noting that $[\hat{p}^\dagger, \hat{q}]_+ = \delta_{pq}$, we can get the relationship between one- and two-body operators:

$$\begin{aligned}
\hat{e}^{pr}_{qs} =& \sum_{\sigma\tau} \hat{p}^\dagger_\sigma \hat{r}^\dagger_\tau \hat{s}_\tau \hat{q}_\sigma \\
=& - \sum_{\sigma\tau} \hat{p}^\dagger_\sigma \hat{r}^\dagger_\tau \hat{q}_\sigma \hat{s}_\tau \\
=& - \sum_{\sigma\tau} \hat{p}^\dagger_\sigma (\delta_{rq}\delta_{\sigma\tau} - \hat{q}_\sigma \hat{r}^\dagger_\tau) \hat{s}_\tau \\
=& \sum_{\sigma\tau} \hat{p}^\dagger_\sigma \hat{q}_\sigma \hat{r}^\dagger_\tau \hat{s}_\tau - \sum_{\sigma\tau} \hat{p}^\dagger_\sigma \hat{s}_\tau \delta_{rq}\delta_{\sigma\tau} \\
=& \hat{E}^p_q \hat{E}^r_s - \delta_{rq} \sum_\sigma \hat{p}^\dagger_\sigma \hat{s}_\sigma \\
=& \hat{E}^p_q \hat{E}^r_s - \delta_{rq} \hat{E}^p_s
\end{aligned} \tag{31}$$

Consider the permutation symmetry of the two-body operator:

$$\begin{aligned}
\hat{e}^{rp}_{sq} =& \sum_{\sigma\tau} \hat{r}^\dagger_\sigma \hat{p}^\dagger_\tau \hat{q}_\tau \hat{s}_\sigma \\
=& - \sum_{\sigma\tau} \hat{p}^\dagger_\tau \hat{r}^\dagger_\sigma \hat{q}_\tau \hat{s}_\sigma \\
=& \sum_{\sigma\tau} \hat{p}^\dagger_\tau \hat{r}^\dagger_\sigma \hat{s}_\sigma \hat{q}_\tau \\
=& \hat{e}^{pr}_{qs}
\end{aligned} \tag{32}$$

we can evaluate the commutation relation between one-body operators:

$$\begin{aligned}
[\hat{E}^p_q, \hat{E}^r_s] =& \hat{E}^p_q \hat{E}^r_s - \hat{E}^r_s \hat{E}^p_q \\
=& e^{pr}_{qs} + \delta_{rq} \hat{E}^p_s - (\hat{e}^{rp}_{sq} + \delta_{ps} \hat{E}^r_q) \\
=& \delta_{rq} \hat{E}^p_s - \delta_{ps} \hat{E}^r_q
\end{aligned} \tag{33}$$

Using this relation, we can evaluate the overlap integral of doubly-excited determinants:

$$\begin{aligned}
\langle \Phi^{ab}_{ij} | \Phi^{cd}_{kl} \rangle =& \delta_{ac}\delta_{bd} \langle \Phi_0 | \hat{e}^{ij}_{kl} | \Phi_0 \rangle + \delta_{ad}\delta_{bc} \langle \Phi_0 | \hat{e}^{ij}_{lk} | \Phi_0 \rangle \\
=& \delta_{ad}\delta_{bc} (4\delta_{jk}\delta_{il} - 2\delta_{ik}\delta_{jl}) + \delta_{ac}\delta_{bd} (4\delta_{jl}\delta_{ik} - 2\delta_{il}\delta_{jk})
\end{aligned} \tag{34}$$

3 Spin-Adapted-Contravariant-Configuration Formalism

The Hamiltonian in spin-adapted form:

$$\hat{H}_{\text{elec}} = \sum_{pq} h_{pq} \hat{E}^p_q + \frac{1}{2} \sum_{pqrs} \langle pq|rs \rangle \hat{e}^{pq}_{rs} \tag{35}$$

$$\begin{aligned}
\hat{H}_{\text{elec}} &= \sum_{pq} h_{pq} \hat{E}^p_q + \frac{1}{2} \sum_{pqrs} \langle pq|rs \rangle (\hat{E}^p_r \hat{E}^q_s - \delta_{qr} \hat{E}^p_s) \\
&= \sum_{pq} h_{pq} \hat{E}^p_q + \frac{1}{2} \sum_{pqs} \langle pq|sq \rangle \hat{E}^p_s + \frac{1}{2} \sum_{pqrs} \langle pq|rs \rangle \hat{E}^p_r \hat{E}^q_s
\end{aligned} \tag{36}$$

The contravariant configurations:

$$|\tilde{\Phi}^a_i\rangle = \frac{1}{2} |\Phi^a_i\rangle = \frac{1}{2} \hat{E}^a_i |\Phi_0\rangle \tag{37}$$

$$|\tilde{\Phi}^{ab}_{ij}\rangle = \frac{1}{6} (2|\Phi^{ab}_{ij}\rangle + |\Phi^{ab}_{ji}\rangle) = \frac{1}{6} (2\hat{E}^a_i \hat{E}^b_j + \hat{E}^a_j \hat{E}^b_i) |\Phi_0\rangle \tag{38}$$

Now:

$$\begin{aligned}
\langle \tilde{\Phi}^{ab}_{ij} | \Phi^{cd}_{kl} \rangle =& \frac{1}{3} \langle \Phi^{ab}_{ij} | \Phi^{cd}_{kl} \rangle + \frac{1}{6} \langle \Phi^{ab}_{ji} | \Phi^{cd}_{kl} \rangle \\
=& \frac{1}{3} (\delta_{ad}\delta_{bc}(4\delta_{jk}\delta_{il} - 2\cancel{\delta_{ik}\delta_{jl}}) + \delta_{ac}\delta_{bd}(4\delta_{jl}\delta_{ik} - 2\cancel{\delta_{jk}\delta_{il}})) \\
&+ \frac{1}{6} (\delta_{ad}\delta_{bc}(4\cancel{\delta_{ik}\delta_{jl}} - 2\delta_{jk}\delta_{il}) + \delta_{ac}\delta_{bd}(4\cancel{\delta_{il}\delta_{jk}} - 2\delta_{ik}\delta_{jl})) \\
=& \delta_{ad}\delta_{bc}\delta_{jk}\delta_{il} + \delta_{ac}\delta_{bd}\delta_{jl}\delta_{ik}
\end{aligned} \tag{39}$$

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*Derivation

Spin-orbital Formalism

Some expansions using Wick's theorem:
Expanding the electronic Hamiltonian using Wick's theorem:

$$\hat{p}^\dagger\hat{q} = \{\hat{p}^\dagger\hat{q}\} + \{\hat{p}^\dagger\hat{q}\} = \{\hat{p}^\dagger\hat{q}\} + \delta_{pq}\delta_{pi} \tag{40}$$

$$\begin{aligned}\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r} =& \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} + \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} + \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} + \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} + \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} + \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} + \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\}\\ =& \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} - \delta_{ps}\delta_{pi}\{\hat{q}^\dagger\hat{r}\} + \delta_{pr}\delta_{pi}\{\hat{q}^\dagger\hat{s}\} + \delta_{qs}\delta_{qi}\{\hat{p}^\dagger\hat{r}\} - \delta_{qr}\delta_{qi}\{\hat{p}^\dagger\hat{s}\}\\ &+ \delta_{pr}\delta_{pi}\delta_{qs}\delta_{qj} - \delta_{ps}\delta_{pi}\delta_{qr}\delta_{qj}\end{aligned} \tag{41}$$

hence:

$$\begin{aligned}\sum_{pq} h_{pq}\hat{p}^\dagger\hat{q} &= \sum_{pq} h_{pq}\{\hat{p}^\dagger\hat{q}\} + \sum_{pq} h_{pq}\delta_{pq}\delta_{pi}\\ &= \sum_{pq} h_{pq}\{\hat{p}^\dagger\hat{q}\} + \sum_{i} h_{ii}\end{aligned} \tag{42}$$

$$\begin{aligned}\frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r} =& \frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} - \frac{1}{4}\sum_{iqr}\langle iq||ri\rangle\{\hat{q}^\dagger\hat{r}\} + \frac{1}{4}\sum_{iqs}\langle iq||is\rangle\{\hat{q}^\dagger\hat{s}\}\\ &+ \frac{1}{4}\sum_{ipr}\langle pi||ri\rangle\{\hat{p}^\dagger\hat{r}\} - \frac{1}{4}\sum_{ips}\langle pi||is\rangle\{\hat{p}^\dagger\hat{s}\}\\ &+ \frac{1}{4}\sum_{ij}\langle ij||ijab\rangle - \frac{1}{4}\sum_{ij}\langle ij||ji\rangle\\ =& \frac{1}{4}\sum_{pqrs}\langle pq||rs\rangle\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} + \sum_{pqi}\langle pi||qi\rangle\{\hat{p}^\dagger\hat{q}\} + \frac{1}{2}\sum_{ij}\langle ij||ij\rangle\end{aligned} \tag{43}$$

The perturbation integral:

$$\begin{aligned}\langle\Phi_0|\hat{V}|\Phi_{ij}^{ab}\rangle =& \frac{1}{4}\sum_{pqrs}\langle\Phi_0|\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\}\{\hat{a}^\dagger\hat{b}^\dagger\hat{j}\hat{i}\}|\Phi_0\rangle\langle pq||rs\rangle\\ =& \frac{1}{4}\sum_{pqrs}\langle\Phi_0|\Big(\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{b}^\dagger\hat{j}\hat{i}\} + \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{b}^\dagger\hat{j}\hat{i}\}\\ &+ \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{b}^\dagger\hat{j}\hat{i}\} + \{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\hat{a}^\dagger\hat{b}^\dagger\hat{j}\hat{i}\}\Big)|\Phi_0\rangle\langle pq||rs\rangle\\ =& \frac{1}{4}\sum_{pqrs}(\delta_{pi}\delta_{qj}\delta_{sb}\delta_{ra} - \delta_{pj}\delta_{qi}\delta_{sb}\delta_{ra} - \delta_{pi}\delta_{qj}\delta_{sa}\delta_{rb} + \delta_{pj}\delta_{qi}\delta_{sa}\delta_{rb})\langle pq||rs\rangle\\ =& \frac{1}{4}(\langle ij||ab\rangle - \langle ji||ab\rangle - \langle ij||ba\rangle + \langle ji||ba\rangle)\\ =& \langle ij||ab\rangle\end{aligned} \tag{44}$$

Spin-Adapted Formalism

(Blue indicates the operator pairs being swapped)

$$
\begin{aligned}
\langle\Phi_{ij}^{ab}|\Phi_{kl}^{cd}\rangle =& \langle\Phi_0|\hat{E}_b^j\hat{E}_a^i\hat{E}_k^c\hat{E}_l^d|\Phi_0\rangle \\
=& \langle\Phi_0|\hat{E}_b^j\hat{E}_k^c\hat{E}_a^i\hat{E}_l^d|\Phi_0\rangle + \delta_{ac}\langle\Phi_0|\hat{E}_b^j\hat{E}_k^i\hat{E}_l^d|\Phi_0\rangle - \delta_{ik}\langle\Phi_0|\hat{E}_b^j\hat{E}_a^c\hat{E}_l^d|\Phi_0\rangle \\
=& \langle\Phi_0|\hat{E}_b^j\hat{E}_k^c\hat{E}_l^d\cancel{\hat{E}_a^i|\Phi_0\rangle} + \delta_{ad}\langle\Phi_0|\hat{E}_b^j\hat{E}_k^c\hat{E}_l^i|\Phi_0\rangle - \delta_{il}\langle\Phi_0|\hat{E}_b^j\hat{E}_k^c\hat{E}_a^d|\Phi_0\rangle \\
&+ \delta_{ac}\langle\Phi_0|\hat{E}_b^j\hat{E}_k^i\hat{E}_l^d|\Phi_0\rangle - \delta_{ik}\langle\Phi_0|\hat{E}_b^j\hat{E}_a^c\hat{E}_l^d|\Phi_0\rangle \\
=& \delta_{ad}\langle\Phi_0|\hat{E}_b^j\hat{E}_k^c\hat{E}_l^i|\Phi_0\rangle - \delta_{il}\langle\Phi_0|\hat{E}_b^j\hat{E}_k^c\hat{E}_a^d|\Phi_0\rangle \\
&+ \delta_{ac}\langle\Phi_0|\hat{E}_b^j\hat{E}_k^i\hat{E}_l^d|\Phi_0\rangle - \delta_{ik}\langle\Phi_0|\hat{E}_b^j\hat{E}_a^c\hat{E}_l^d|\Phi_0\rangle
\end{aligned} \tag{45}
$$

Evaluating term by term (noting that $\hat{E}_b^a|\Phi_0\rangle = 0$):

$$
\begin{aligned}
\langle\Phi_0|\hat{E}_b^j\hat{E}_k^c\hat{E}_l^i|\Phi_0\rangle =& \cancel{\langle\Phi_0|\hat{E}_k^c}\hat{E}_b^j\hat{E}_l^i|\Phi_0\rangle + \delta_{bc}\langle\Phi_0|\hat{E}_k^j\hat{E}_l^i|\Phi_0\rangle - \delta_{jk}\langle\Phi_0|\hat{E}_b^c\hat{E}_l^i|\Phi_0\rangle \\
=& \delta_{bc}\langle\Phi_0|\hat{E}_k^j\hat{E}_l^i|\Phi_0\rangle - \delta_{jk}\cancel{\langle\Phi_0|\hat{E}_b^c}\hat{E}_l^i|\Phi_0\rangle
\end{aligned} \tag{46}
$$

$$
\langle\Phi_0|\hat{E}_b^j\hat{E}_k^c\cancel{\hat{E}_a^d|\Phi_0\rangle} = 0 \tag{47}
$$

$$
\begin{aligned}
\langle\Phi_0|\hat{E}_b^j\hat{E}_k^i\hat{E}_l^d|\Phi_0\rangle =& \langle\Phi_0|\hat{E}_b^j\hat{E}_l^d\hat{E}_k^i|\Phi_0\rangle + \cancel{\delta_{dk}}\langle\Phi_0|\hat{E}_b^j\hat{E}_l^i|\Phi_0\rangle - \delta_{il}\langle\Phi_0|\hat{E}_b^j\hat{E}_k^d|\Phi_0\rangle \\
=& \cancel{\langle\Phi_0|\hat{E}_l^d}\hat{E}_b^j\hat{E}_k^i|\Phi_0\rangle + \delta_{bd}\langle\Phi_0|\hat{E}_l^j\hat{E}_k^i|\Phi_0\rangle - \delta_{jl}\langle\Phi_0|\hat{E}_b^d\hat{E}_k^i|\Phi_0\rangle \\
&- \delta_{il}\langle\Phi_0|\hat{E}_b^j\hat{E}_k^d|\Phi_0\rangle \\
=& \delta_{bd}\langle\Phi_0|\hat{E}_l^j\hat{E}_k^i|\Phi_0\rangle - \delta_{jl}\cancel{\langle\Phi_0|\hat{E}_b^d}\hat{E}_k^i|\Phi_0\rangle - \delta_{il}\langle\Phi_0|\hat{E}_b^j\hat{E}_k^d|\Phi_0\rangle
\end{aligned} \tag{48}
$$

$$
\begin{aligned}
\langle\Phi_0|\hat{E}_b^j\hat{E}_a^c\hat{E}_l^d|\Phi_0\rangle =& \langle\Phi_0|\hat{E}_b^j\hat{E}_l^d\cancel{\hat{E}_a^c|\Phi_0\rangle} + \delta_{ad}\langle\Phi_0|\hat{E}_b^j\hat{E}_l^c|\Phi_0\rangle - \cancel{\delta_{cl}}\langle\Phi_0|\hat{E}_b^j\hat{E}_a^d|\Phi_0\rangle \\
=& \delta_{ad}\langle\Phi_0|\hat{E}_b^j\hat{E}_l^c|\Phi_0\rangle
\end{aligned} \tag{49}
$$

The violet terms (using $\hat{E}_j^i|\Phi_0\rangle = (\hat{i}_\alpha^\dagger\hat{j}_\alpha + \hat{i}_\beta^\dagger\hat{j}_\beta)|\Phi_0\rangle = 2\delta_{ij}|\Phi_0\rangle$):

$$
\begin{aligned}
\langle\Phi_0|\hat{E}_b^j\hat{E}_l^c|\Phi_0\rangle =& \langle\Phi_0|\hat{E}_l^c\cancel{\hat{E}_b^j|\Phi_0\rangle} + \delta_{bc}\langle\Phi_0|\hat{E}_l^j|\Phi_0\rangle - \delta_{jl}\langle\Phi_0|\cancel{\hat{E}_b^c|\Phi_0\rangle} \\
=& 2\delta_{bc}\delta_{jl}
\end{aligned} \tag{50}
$$

$$
\langle\Phi_0|\hat{E}_b^j\hat{E}_k^d|\Phi_0\rangle = 2\delta_{bd}\delta_{jk} \tag{51}
$$

Putting them together :

$$
\begin{aligned}
\langle\Phi_{ij}^{ab}|\Phi_{kl}^{cd}\rangle =& \delta_{ad}\delta_{bc}\langle\Phi_0|\hat{E}_k^j\hat{E}_l^i|\Phi_0\rangle + \delta_{ac}\delta_{bd}\langle\Phi_0|\hat{E}_l^j\hat{E}_k^i|\Phi_0\rangle \\
&- 2\delta_{ac}\delta_{il}\delta_{bd}\delta_{jk} - 2\delta_{ik}\delta_{ad}\delta_{bc}\delta_{jl} \\
=& 4\delta_{ad}\delta_{bc}\delta_{jk}\delta_{il} + 4\delta_{ac}\delta_{bd}\delta_{jl}\delta_{ik} - 2\delta_{ac}\delta_{bd}\delta_{il}\delta_{jk} - 2\delta_{ad}\delta_{bc}\delta_{ik}\delta_{jl} \\
=& \delta_{ad}\delta_{bc}(4\delta_{jk}\delta_{il} - 2\delta_{ik}\delta_{jl}) + \delta_{ac}\delta_{bd}(4\delta_{jl}\delta_{ik} - 2\delta_{il}\delta_{jk})
\end{aligned} \tag{52}
$$