1 CC Density Matrix

1.1 Reduced Density Matrix

We have the one- and two-body RDM as:

$$\gamma(x,x') = \sum_{pq} \phi_q(x)\gamma_{qp}\phi_p^*(x') \tag{1}$$

$$\Gamma(x_1,x_2;x_1',x_2') = \sum_{pqrs} \phi_r(x_1)\phi_s(x_2)\Gamma_{rspq}\phi_p^*(x_1')\phi_q^*(x_2') \tag{2}$$

in which γ_{qp} and Γ_{rspq} are the elements of discrete representation of one- and two- body RDM $\gamma(x,x')$ and $\Gamma(x_1,x_2;x_1',x_2')$:

$$\gamma_{qp} = \frac{\langle\Psi|\hat{p}^\dagger\hat{q}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\langle 0|e^{\hat{T}^\dagger}\hat{p}^\dagger\hat{q}e^{\hat{T}}|0\rangle}{\langle 0|e^{\hat{T}^\dagger}e^{\hat{T}}|0\rangle} = \langle 0|e^{\hat{T}^\dagger}\hat{p}^\dagger\hat{q}e^{\hat{T}}|0\rangle_{\mathrm{C}} \tag{3}$$

$$\Gamma_{rspq} = \frac{\langle\Psi|\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\langle 0|e^{\hat{T}^\dagger}\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}e^{\hat{T}}|0\rangle}{\langle 0|e^{\hat{T}^\dagger}e^{\hat{T}}|0\rangle} = \langle 0|e^{\hat{T}^\dagger}\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}e^{\hat{T}}|0\rangle_{\mathrm{C}} \tag{4}$$

where we used the eqn(46(?)), i.e.:

$$\begin{aligned}\langle 0|e^{\hat{T}^\dagger}\hat{p}^\dagger\hat{q}e^{\hat{T}}|0\rangle =& \langle 0|e^{\hat{T}^\dagger}\{\hat{p}^\dagger\hat{q}\}e^{\hat{T}}|0\rangle + \langle 0|e^{\hat{T}^\dagger}\{\overline{\hat{p}^\dagger\hat{q}}\}e^{\hat{T}}|0\rangle \\ =& \langle 0|e^{\hat{T}^\dagger}e^{\hat{T}}|0\rangle\langle 0|e^{\hat{T}^\dagger}\{\hat{p}^\dagger\hat{q}\}e^{\hat{T}}|0\rangle_{\mathrm{C}} + \delta_{pq}\delta_{p\in\mathrm{occ}}\langle 0|e^{\hat{T}^\dagger}e^{\hat{T}}|0\rangle \end{aligned}\tag{5}$$

Therefore:

$$\begin{aligned}\gamma_{qp} =& \langle 0|e^{\hat{T}^\dagger}\{\hat{p}^\dagger\hat{q}\}e^{\hat{T}}|0\rangle_{\mathrm{C}} + \delta_{pq}\delta_{p\in\mathrm{occ}} \\ =& (\gamma_{\mathrm{N}})_{qp} + \delta_{pq}\delta_{p\in\mathrm{occ}}\end{aligned}\tag{6}$$

With these, we can evaluate the expected values operators. The one-body expression can be obtained as:

$$\begin{aligned}\bar{O} =& \frac{\langle\Psi|\hat{O}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \\ =& \frac{\sum_{pq} o_{pq}\langle 0|e^{\hat{T}^\dagger}\{\hat{p}^\dagger\hat{q}\}e^{\hat{T}}|0\rangle}{\langle 0|e^{\hat{T}^\dagger}e^{\hat{T}}|0\rangle} + \frac{\sum_{pq} o_{pq}\langle 0|e^{\hat{T}^\dagger}\{\overline{\hat{p}^\dagger\hat{q}}\}e^{\hat{T}}|0\rangle}{\langle 0|e^{\hat{T}^\dagger}e^{\hat{T}}|0\rangle} \\ =& \frac{\langle 0|e^{\hat{T}^\dagger}e^{\hat{T}}|0\rangle\sum_{pq} o_{pq}\langle 0|e^{\hat{T}^\dagger}\{\hat{p}^\dagger\hat{q}\}e^{\hat{T}}|0\rangle_{\mathrm{C}}}{\langle 0|e^{\hat{T}^\dagger}e^{\hat{T}}|0\rangle} + \frac{\sum_{pq} o_{pq}\langle 0|e^{\hat{T}^\dagger}e^{\hat{T}}|0\rangle\delta_{pq}\delta_{p\in\mathrm{occ}}}{\langle 0|e^{\hat{T}^\dagger}e^{\hat{T}}|0\rangle} \\ =& \sum_{pq} o_{pq}\langle 0|e^{\hat{T}^\dagger}\{\hat{p}^\dagger\hat{q}\}e^{\hat{T}}|0\rangle_{\mathrm{C}} + \sum_{pq} o_{pq}\delta_{pq}\delta_{p\in\mathrm{occ}} \\ =& \sum_{pq} o_{pq}(\gamma_{\mathrm{N}})_{qp} + \sum_{i} o_{ii} \\ =& \sum_{pq} o_{pq}\gamma_{qp}\end{aligned}\tag{7}$$

Similarly, for a general two-body operator $\hat{G} = \frac{1}{4}\sum_{pqrs}\langle pq|\hat{g}|rs\rangle_{\mathrm{A}}\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}$, where $\langle pq|\hat{g}|rs\rangle_{\mathrm{A}} = \langle pq|\hat{g}|rs\rangle - \langle pq|\hat{g}|sr\rangle$, the expectation value is:

$$\bar{G} = \frac{\langle\Psi|\hat{G}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{1}{4}\sum_{pqrs}\langle pq|\hat{g}|rs\rangle_{\mathrm{A}}\Gamma_{rspq} \tag{8}$$

The Γ_{rspq} tensor could be partitioned as:

1.2 Response Density Matrix

1.3 Relaxed/Effective Density Matrix