Unitary Coupled Cluster Theory

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1 Derivation of Polarisation Propogator $G_{pr,rs}$ in the new unitary transformed excitation/deexcitation scheme

The Polarisation Propogator in superoperator representation is given by :

$$\begin{aligned} G_{pq,rs}(\omega) &= \left\langle \Psi_{gr} \right| \left[a_p a_q^\dagger, \left(\omega \hat{I} - \hat{H} \right)^{-1} a_r^\dagger a_s \right] \left| \Psi_{gr} \right\rangle \\ &= \left\langle \Psi_{gr} \right| \left[q_I, \left(\omega \hat{I} - \hat{H} \right)^{-1} q_J^\dagger \right] \left| \Psi_{gr} \right\rangle \end{aligned}$$

A Binary Product can be defined as follows :

$$(A|B) = \left\langle \Psi_{gr} \right| \left[A^\dagger, B \right] \left| \Psi \right\rangle$$

Another definition used in this derivation is :

$$(A|\hat{O}|B) \equiv (A|\hat{O}B)$$

Polarisation Propogator can be written in terms of binary product notation as :

$$G(\omega) = (q_i^\dagger|(\omega\hat{I} - \hat{H})^{-1} q_j^\dagger)$$

In our self consistant polarisation propogation theory, the unitary transformed excitation/deexcitation operators are defined as :

$$y_i^\dagger = \exp(\sigma) b_i^\dagger \exp(-\sigma)$$

Using the resolution of identity in G :

$$\begin{aligned} \hat{I} &= \sum_I \{ |y_I^\dagger)(y_I^\dagger| - |y_I)(y_I| \} \\ G(\omega) &= (q_I|y_I^\dagger)(y_I^\dagger|(\omega\hat{I} - \hat{H})^{-1} q_j^\dagger) - (q_I|y_I)(y_I|(\omega\hat{I} - \hat{H})^{-1} q_j^\dagger) \end{aligned}$$

Taking the second half of the expression and expanding through tailors expansion :

$$
\begin{aligned}
(y_I|(\omega\hat{I}-\hat{H})^{-1}q_j^\dagger) &= \big\langle\Psi_{gr}\big|\big[y_I,\big(\omega\hat{I}-\hat{H}\big)^{-1}q_j^\dagger\big]\big|\Psi_{gr}\big\rangle \\
&= \big\langle\Psi_{gr}\big|\big[y_I,\frac{1}{\omega}\Bigg(\big(\hat{I}-\hat{H}\big)\Bigg)^{-1}q_j^\dagger\big]\big|\Psi_{gr}\big\rangle \\
&= \big\langle\Psi_{gr}\big|\big[y_I,\frac{1}{\omega}\Bigg(\big(\hat{I}+\frac{1}{\omega}\hat{H}+\frac{1}{\omega^2}\hat{H}^2...\big)\Bigg)q_j^\dagger\big]\big|\Psi_{gr}\big\rangle \\
&= \frac{1}{\omega}\Bigg(\big\langle\Psi_{gr}\big|\big[y_I,\big(\hat{I}q_j^\dagger\big]\big|\Psi_{gr}\big\rangle+\big\langle\Psi_{gr}\big|\big[y_I,\frac{1}{\omega}\hat{H}q_j^\dagger\big]\big|\Psi_{gr}\big\rangle+\big\langle\Psi_{gr}\big|\big[y_I,\frac{1}{\omega^2}\hat{H}^2q_j^\dagger\big]\big|\Psi_{gr}\big\rangle\Bigg) \\
&= \frac{1}{\omega}\Bigg(\big(y_I\big|\big(\hat{I}q_j^\dagger\big)+\big(y_I\big|\frac{1}{\omega}\hat{H}q_j^\dagger\big)+\big(y_I\big|\frac{1}{\omega^2}\hat{H}^2q_j^\dagger\big) \\
&= \frac{1}{\omega}\Bigg(\big(y_I\big|\big(\hat{I}|q_j^\dagger\big)+\big(y_I\big|\frac{1}{\omega}\hat{H}|q_j^\dagger\big)+\big(y_I\big|\frac{1}{\omega^2}\hat{H}^2|q_j^\dagger\big)...\Bigg) \\
&= \frac{1}{\omega}\big(y_I\big|\big(\hat{I}+\frac{1}{\omega}\hat{H}+\frac{1}{\omega^2}\hat{H}^2...|q_j^\dagger\big) \\
&= \frac{1}{\omega}\big(y_I\big|\big(\hat{I}-\frac{\hat{H}}{\omega}\big)^{-1}|q_j^\dagger\big) \\
&= \big(y_I\big|\big(\omega\hat{I}-\hat{H}\big)^{-1}|q_j^\dagger\big)
\end{aligned}
$$

Using this result in the previously derived expression :

$$
\begin{aligned}
\hat{I} &= \sum_I\{|y_I^\dagger)(y_I^\dagger|-|y_I)(y_I|\} \\
G(\omega) &= (q_I^\dagger|y_I^\dagger)(y_I^\dagger|(\omega\hat{I}-\hat{H})^{-1}q_j^\dagger)-(q_I^\dagger|y_I)(y_I|(\omega\hat{I}-\hat{H})^{-1}q_j^\dagger) \\
&= (q_I^\dagger|y_I^\dagger)(y_I^\dagger|(\omega\hat{I}-\hat{H})^{-1}|q_j^\dagger)-(q_I^\dagger|y_I)(y_I|(\omega\hat{I}-\hat{H})^{-1}|q_j^\dagger)
\end{aligned}
$$

Again using resolution of Identity Operator :

$$
\begin{aligned}
G(\omega) &= (q_I^\dagger|y_I^\dagger)(y_I^\dagger|(\omega\hat{I}-\hat{H})^{-1}|y_J^\dagger)(y_J^\dagger|q_j^\dagger)-(q_I^\dagger|y_I)(y_I|(\omega\hat{I}-\hat{H})^{-1}|y_J^\dagger)(y_J^\dagger|q_j^\dagger) \\
&\quad-(q_I^\dagger|y_I^\dagger)(y_I^\dagger|(\omega\hat{I}-\hat{H})^{-1}|y_J)(y_J|q_j^\dagger)+(q_I^\dagger|y_I)(y_I|(\omega\hat{I}-\hat{H})^{-1}|y_J)(y_J|q_j^\dagger) \\
&= ML^{-1}M^\dagger
\end{aligned}
$$

2 Resolution of Identity

2.1 Proof for the Identity for the notation

$$
\begin{aligned}
(A|B) &= \sum_I (A|y_I^\dagger)(y_I^\dagger|B) - (A|y_I)(y_I|B) \\
\sum_I (A|y_I^\dagger)(y_I^\dagger|B) &= \sum_I \left[\left\langle \Psi_{gr}|A^\dagger y_I^\dagger - y_I^\dagger A^\dagger|\Psi_{gr}\right\rangle + \left\langle \Psi_{gr}|y_I B - B y_I|\Psi_{gr}\right\rangle\right] \\
&= \left\langle \Psi_{gr}|A^\dagger y_I^\dagger|\Psi_{gr}\right\rangle \left\langle \Psi_{gr}|y_I B|\Psi_{gr}\right\rangle - \left\langle \Psi_{gr}|A^\dagger y_I^\dagger|\Psi_{gr}\right\rangle \left\langle \Psi_{gr}|iBy_I|\Psi_{gr}\right\rangle \\
&- \left\langle \Psi_{gr}|y_I^\dagger A^\dagger|\Psi_{gr}\right\rangle \left\langle \Psi_{gr}|y_I B|\Psi_{gr}\right\rangle + \left\langle \Psi_{gr}|y_I^\dagger A^\dagger|\Psi_{gr}\right\rangle \left\langle \Psi_{gr}|By_I|\Psi_{gr}\right\rangle \\
&= \left\langle \Psi_{gr}|A^\dagger B|\Psi_{gr}\right\rangle
\end{aligned}
$$

Similarly using Vaccume Anhilation Conditions :

$$
\sum_I (A|y_I)(y_I|B) = -\left\langle \Psi_{gr}|BA^\dagger|\Psi_{gr}\right\rangle
$$

Adding both terms, we prove our identity:

$$
\begin{aligned}
(A|B) &= \sum_I (A|y_I^\dagger)(y_I^\dagger|B) - (A|y_I)(y_I|B) \\
&= \left\langle \Psi_{gr}|A^\dagger B|\Psi_{gr}\right\rangle - \left\langle \Psi_{gr}|BA^\dagger|\Psi_{gr}\right\rangle \\
&= \left\langle \Psi_{gr}|\left[A^\dagger, B\right]|\Psi_{gr}\right\rangle \\
&= (A|B)
\end{aligned}
$$