Unitary Coupled Cluster Theory

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April 6, 2018

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 :

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

A Binary Product can be defined as follows :

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

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 :

$$\hat{I} = \sum_I \{ |y_I^\dagger)(y_I^\dagger| - |y_I)(y_I| \}$$

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

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 :

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

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