Supporting Information for "An Algebraic-Diagrammatic Construction for Vertex Corrections to the GW Self-Energy"

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CONTENTS

I. PRELIMINARY

In this document, the indices $p,q,r,s,\dots$ are used for arbitrary orbitals, i,j,k,l label the occupied orbitals, a,b,c,d denote the virtual orbitals, and $\mu,\nu,\dots$ are used for combined occupied-virtual indices. All quantities are expressed in the spin-orbital basis.

The two-electron integrals, referred to as ERI in the following, are defined as

$$\langle pq|rs\rangle = \int \mathrm{d}(\boldsymbol{x}_1\boldsymbol{x}_2)\, \frac{\varphi_p^*(\boldsymbol{x}_1)\varphi_q^*(\boldsymbol{x}_2)\varphi_r(\boldsymbol{x}_1)\varphi_s(\boldsymbol{x}_2)}{|\boldsymbol{r}_1-\boldsymbol{r}_2|} \tag{1}$$

and the antisymmetrized integrals are $\langle pq||rs\rangle = \langle pq|rs\rangle - \langle pq|sr\rangle$. Here, $\varphi_p(\boldsymbol{x})$ is the pth spinorbital and $\boldsymbol{x}$ is a composite index gathering spin and spatial coordinates. The matrix elements of the one-body Green's function are given by

$$G_{pq}(\omega) = \sum_i \frac{\delta_{pqi}}{\omega-(\epsilon_i+\mathrm{i}\eta)} + \sum_a \frac{\delta_{pqa}}{\omega-(\epsilon_a-\mathrm{i}\eta)} \tag{2}$$

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while the screened Coulomb tensor elements read

$$W_{pqrs}(\omega) = \langle pq|rs\rangle + \sum_{\nu} \frac{M_{pr,\nu} M^*_{sq,\nu}}{\omega - (\Omega_\nu - \mathrm{i}\eta)} - \sum_{\nu} \frac{M^*_{rp,\nu} M_{qs,\nu}}{\omega - (-\Omega_\nu + \mathrm{i}\eta)} \tag{3}$$

where the Ω_ν's are direct RPA eigenvalues and the GW effective integrals are given by

$$M_{pq,\nu} = \sum_{ia} \left[\langle pa|qi\rangle\, X_{ia,\nu} + \langle pi|qa\rangle\, Y_{ai,\nu}\right] \tag{4}$$

where $X_{ia,\nu}$ and $Y_{ai,\nu}$ are the direct RPA eigenvectors. It was shown by Bruneval and co-workers that the Coulomb integrals and the GW effective integrals are related by[1]

$$-\langle iq|as\rangle = \sum_{\nu} \frac{M_{ia,\nu} M^*_{sq,\nu}}{(\epsilon_a - \epsilon_i - 2\mathrm{i}\eta) - (\Omega_\nu - \mathrm{i}\eta)} - \sum_{\nu} \frac{M^*_{ai,\nu} M_{qs,\nu}}{(\epsilon_a - \epsilon_i - 2\mathrm{i}\eta) - (-\Omega_\nu + \mathrm{i}\eta)} \tag{5a}$$

$$-\langle aq|is\rangle = \sum_{\nu} \frac{M_{ai,\nu} M^*_{sq,\nu}}{(\epsilon_i - \epsilon_a + 2\mathrm{i}\eta) - (\Omega_\nu - \mathrm{i}\eta)} - \sum_{\nu} \frac{M^*_{ia,\nu} M_{qs,\nu}}{(\epsilon_i - \epsilon_a + 2\mathrm{i}\eta) - (-\Omega_\nu + \mathrm{i}\eta)}. \tag{5b}$$

II. THE $G3W2$ SELF-ENERGY

The $G3W2$ self-energy is defined as[2]

$$\Sigma(11') = \Sigma^{GW}(11') + \mathrm{i}^2 G(33')W(12';32)W(3'4;4'1')G(4'2')G(24) \tag{6}$$

where the last term is the $G3W2$ contribution and the first term is the GW self-energy given by

$$\Sigma^{GW}(11') = \Sigma^{\mathrm{H}}(11') + \mathrm{i}G(2'2)W(12;2'1') \tag{7}$$

The expression of the GW self-energy matrix elements in a basis of spin-orbitals is well-known and reads[3]

$$\Sigma^{GW}_{pq}(\omega) = \sum_{i} \langle pi||qi\rangle + \sum_{i\nu} \frac{M_{pi,\nu} M^*_{qi,\nu}}{\omega - (\epsilon_i - \Omega_\nu + 2\mathrm{i}\eta)} + \sum_{a\nu} \frac{M^*_{ap,\nu} M_{aq,\nu}}{\omega - (\epsilon_a + \Omega_\nu - 2\mathrm{i}\eta)} \tag{8}$$

The aim of this section is to derive the expression of the matrix elements of the $G3W2$ contribution. The Fourier transform of this term yields

$$\begin{aligned} \Sigma^{G3W2}_{pq}(\omega) &= \sum_{rst} \frac{\mathrm{i}^2}{(2\pi)^2} \int \mathrm{d}\omega_4\, G_{rr}(\omega+\omega_4) W_{psrt}(\omega_4) \left[\int \mathrm{d}\omega_5\, G_{ss}(\omega+\omega_4+\omega_5) G_{tt}(\omega+\omega_5) W_{rtsq}(\omega_5)\right] \\ &= \sum_{rst} \frac{\mathrm{i}^2}{(2\pi)^2} \int \mathrm{d}\omega_4\, G_{rr}(\omega+\omega_4) W_{psrt}(\omega_4) I_{rtsq}(\omega,\omega_4) \end{aligned} \tag{9}$$

A. Intermediate integral

We start by computing the intermediate integral on ω_5

$$\begin{aligned} I_{rtsq}(\omega,\omega_4) = \int \mathrm{d}\omega_5 & \left[\sum_i \frac{\delta_{si}}{\omega_5 - (-\omega - \omega_4 + \epsilon_i + \mathrm{i}\eta)} + \sum_a \frac{\delta_{sa}}{\omega_5 - (-\omega - \omega_4 + \epsilon_a - \mathrm{i}\eta)}\right] \\ & \times \left[\sum_j \frac{\delta_{tj}}{\omega_5 - (-\omega + \epsilon_j + \mathrm{i}\eta)} + \sum_b \frac{\delta_{tb}}{\omega_5 - (-\omega + \epsilon_b - \mathrm{i}\eta)}\right] \\ & \times \left[\langle rt|sq\rangle + \sum_\nu \frac{M_{rs,\nu} M^*_{qt,\nu}}{\omega_5 - (\Omega_\nu - \mathrm{i}\eta)} - \sum_\nu \frac{M^*_{sr,\nu} M_{tq,\nu}}{\omega_5 - (-\Omega_\nu + \mathrm{i}\eta)}\right] \\ = \int \mathrm{d}\omega_5 \sum_{ib} \langle rt|sq\rangle & \frac{\delta_{si}}{\omega_5 - (-\omega - \omega_4 + \epsilon_i + \mathrm{i}\eta)} \frac{\delta_{tb}}{\omega_5 - (-\omega + \epsilon_b - \mathrm{i}\eta)} \end{aligned}$$

$$
\begin{aligned}
&+\int \mathrm{d}\omega_5 \sum_{aj} \langle rt|sq\rangle \frac{\delta_{sa}}{\omega_5-(-\omega-\omega_4+\epsilon_a-\mathrm{i}\eta)} \frac{\delta_{tj}}{\omega_5-(-\omega+\epsilon_j+\mathrm{i}\eta)} \\
&+\int \mathrm{d}\omega_5 \sum_{ib\nu} \frac{\delta_{si}}{\omega_5-(-\omega-\omega_4+\epsilon_i+\mathrm{i}\eta)} \frac{\delta_{tb}}{\omega_5-(-\omega+\epsilon_b-\mathrm{i}\eta)} \frac{M_{rs,\nu}M^*_{qt,\nu}}{\omega_5-(\Omega_\nu-\mathrm{i}\eta)} \\
&+\int \mathrm{d}\omega_5 \sum_{aj\nu} \frac{\delta_{sa}}{\omega_5-(-\omega-\omega_4+\epsilon_a-\mathrm{i}\eta)} \frac{\delta_{tj}}{\omega_5-(-\omega+\epsilon_j+\mathrm{i}\eta)} \frac{M_{rs,\nu}M^*_{qt,\nu}}{\omega_5-(\Omega_\nu-\mathrm{i}\eta)} \\
&-\int \mathrm{d}\omega_5 \sum_{ab\nu} \frac{\delta_{sa}}{\omega_5-(-\omega-\omega_4+\epsilon_a-\mathrm{i}\eta)} \frac{\delta_{tb}}{\omega_5-(-\omega+\epsilon_b-\mathrm{i}\eta)} \frac{M^*_{sr,\nu}M_{tq,\nu}}{\omega_5-(-\Omega_\nu+\mathrm{i}\eta)} \\
&-\int \mathrm{d}\omega_5 \sum_{aj\nu} \frac{\delta_{sa}}{\omega_5-(-\omega-\omega_4+\epsilon_a-\mathrm{i}\eta)} \frac{\delta_{tj}}{\omega_5-(-\omega+\epsilon_j+\mathrm{i}\eta)} \frac{M^*_{sr,\nu}M_{tq,\nu}}{\omega_5-(-\Omega_\nu+\mathrm{i}\eta)} \\
&-\int \mathrm{d}\omega_5 \sum_{ib\nu} \frac{\delta_{si}}{\omega_5-(-\omega-\omega_4+\epsilon_i+\mathrm{i}\eta)} \frac{\delta_{tb}}{\omega_5-(-\omega+\epsilon_b-\mathrm{i}\eta)} \frac{M^*_{sr,\nu}M_{tq,\nu}}{\omega_5-(-\Omega_\nu+\mathrm{i}\eta)} \\
&+\int \mathrm{d}\omega_5 \sum_{ij\nu} \frac{\delta_{si}}{\omega_5-(-\omega-\omega_4+\epsilon_i+\mathrm{i}\eta)} \frac{\delta_{tj}}{\omega_5-(-\omega+\epsilon_j+\mathrm{i}\eta)} \frac{M_{rs,\nu}M^*_{qt,\nu}}{\omega_5-(\Omega_\nu-\mathrm{i}\eta)} \\
&=(2\pi\mathrm{i})\sum_{ib} \frac{\langle rt|sq\rangle\,\delta_{si}\delta_{tb}}{(-\omega-\omega_4+\epsilon_i+\mathrm{i}\eta)-(-\omega+\epsilon_b-\mathrm{i}\eta)} +(2\pi\mathrm{i})\sum_{aj} \frac{\langle rt|sq\rangle\,\delta_{sa}\delta_{tj}}{(-\omega+\epsilon_j+\mathrm{i}\eta)-(-\omega-\omega_4+\epsilon_a-\mathrm{i}\eta)} \\
&+(2\pi\mathrm{i})\sum_{ib\nu} \frac{\delta_{si}\delta_{tb}}{(-\omega-\omega_4+\epsilon_i+\mathrm{i}\eta)-(-\omega+\epsilon_b-\mathrm{i}\eta)} \frac{M_{rs,\nu}M^*_{qt,\nu}}{(-\omega-\omega_4+\epsilon_i+\mathrm{i}\eta)-(\Omega_\nu-\mathrm{i}\eta)} \\
&+(2\pi\mathrm{i})\sum_{aj\nu} \frac{\delta_{sa}\delta_{tj}}{(-\omega+\epsilon_j+\mathrm{i}\eta)-(-\omega-\omega_4+\epsilon_a-\mathrm{i}\eta)} \frac{M_{rs,\nu}M^*_{qt,\nu}}{(-\omega+\epsilon_j+\mathrm{i}\eta)-(\Omega_\nu-\mathrm{i}\eta)} \\
&-(2\pi\mathrm{i})\sum_{ab\nu} \frac{\delta_{sa}\delta_{tb}}{(-\Omega_\nu+\mathrm{i}\eta)-(-\omega-\omega_4+\epsilon_a-\mathrm{i}\eta)} \frac{M^*_{sr,\nu}M_{tq,\nu}}{(-\Omega_\nu+\mathrm{i}\eta)-(-\omega+\epsilon_b-\mathrm{i}\eta)} \\
&+(2\pi\mathrm{i})\sum_{aj\nu} \frac{\delta_{sa}\delta_{tj}}{(-\omega-\omega_4+\epsilon_a-\mathrm{i}\eta)-(-\omega+\epsilon_j+\mathrm{i}\eta)} \frac{M^*_{sr,\nu}M_{tq,\nu}}{(-\omega-\omega_4+\epsilon_a-\mathrm{i}\eta)-(-\Omega_\nu+\mathrm{i}\eta)} \\
&+(2\pi\mathrm{i})\sum_{ib\nu} \frac{\delta_{si}\delta_{tb}}{(-\omega+\epsilon_b-\mathrm{i}\eta)-(-\omega-\omega_4+\epsilon_i+\mathrm{i}\eta)} \frac{M^*_{sr,\nu}M_{tq,\nu}}{(-\omega+\epsilon_b-\mathrm{i}\eta)-(-\Omega_\nu+\mathrm{i}\eta)} \\
&-(2\pi\mathrm{i})\sum_{ij\nu} \frac{\delta_{si}\delta_{tj}}{(\Omega_\nu-\mathrm{i}\eta)-(-\omega-\omega_4+\epsilon_i+\mathrm{i}\eta)} \frac{M_{rs,\nu}M^*_{qt,\nu}}{(\Omega_\nu-\mathrm{i}\eta)-(-\omega+\epsilon_j+\mathrm{i}\eta)}
\end{aligned}
$$

This yields

$$
\begin{aligned}
I_{rtsq}(\omega_4) = &-(2\pi\mathrm{i})\sum_{ia}\frac{\delta_{si}\delta_{ta}}{\omega_4-(\epsilon_i-\epsilon_a+2\mathrm{i}\eta)}\left(\langle rt|sq\rangle+\sum_{\nu}\frac{M^*_{sr,\nu}M_{tq,\nu}}{\omega-(\epsilon_a+\Omega_\nu-2\mathrm{i}\eta)}\right)\\
&+(2\pi\mathrm{i})\sum_{ia}\frac{\delta_{sa}\delta_{ti}}{\omega_4-(\epsilon_a-\epsilon_i-2\mathrm{i}\eta)}\left(\langle rt|sq\rangle-\sum_{\nu}\frac{M_{rs,\nu}M^*_{qt,\nu}}{\omega-(\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)}\right)\\
&-(2\pi\mathrm{i})\sum_{ij\nu}\frac{\delta_{si}\delta_{tj}}{\omega_4-(-\omega+\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)}\frac{M_{rs,\nu}M^*_{qt,\nu}}{\omega-(\epsilon_j-\Omega_\nu+2\mathrm{i}\eta)}\\
&-(2\pi\mathrm{i})\sum_{ab\nu}\frac{\delta_{sa}\delta_{tb}}{\omega_4-(-\omega+\epsilon_a+\Omega_\nu-2\mathrm{i}\eta)}\frac{M^*_{sr,\nu}M_{tq,\nu}}{\omega-(\epsilon_b+\Omega_\nu-2\mathrm{i}\eta)}\\
&+(2\pi\mathrm{i})\sum_{ia\nu}\frac{\delta_{si}\delta_{ta}}{\omega_4-(\epsilon_i-\epsilon_a+2\mathrm{i}\eta)}\frac{M_{rs,\nu}M^*_{qt,\nu}}{\omega_4-(-\omega+\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)}\\
&+(2\pi\mathrm{i})\sum_{ia\nu}\frac{\delta_{sa}\delta_{ti}}{\omega_4-(\epsilon_a-\epsilon_i-2\mathrm{i}\eta)}\frac{M^*_{sr,\nu}M_{tq,\nu}}{\omega_4-(-\omega+\epsilon_a+\Omega_\nu-2\mathrm{i}\eta)}\\
&=I^{\mathrm{I}}_{tpsr}(\omega_4)+I^{\mathrm{II}}_{tpsr}(\omega_4)+I^{\mathrm{III}}_{tpsr}(\omega_4)
\end{aligned}
\tag{10}
$$

where $I^{\mathrm{I}}_{tpsr}(\omega_4)$ corresponds to the first two terms, $I^{\mathrm{II}}_{tpsr}(\omega_4)$ the next two terms and $I^{\mathrm{III}}_{tpsr}(\omega_4)$ the last two terms.

B. Analytic expression of the self-energy

The self-energy contributions, see Eq. (9), associated with each of these terms will now be computed.

1. First term

The integral to compute for the first term is

$$
\begin{aligned}
\Sigma^{G3W2,\mathrm{I}}_{pq}(\omega) = &\sum_{rst}\frac{\mathrm{i}^3}{(2\pi)}\int \mathrm{d}\omega_4\left[\sum_k\frac{\delta_{rk}}{\omega_4-(-\omega+\epsilon_k+\mathrm{i}\eta)}+\sum_c\frac{\delta_{rc}}{\omega_4-(-\omega+\epsilon_c-\mathrm{i}\eta)}\right]\\
&\left[\langle ps|rt\rangle+\sum_\mu\frac{M_{pr,\mu}M^*_{ts,\mu}}{\omega_4-(\Omega_\mu-\mathrm{i}\eta)}-\sum_\mu\frac{M^*_{rp,\mu}M_{st,\mu}}{\omega_4-(-\Omega_\mu+\mathrm{i}\eta)}\right]\\
&\left[-\sum_{ia}\frac{\delta_{si}\delta_{ta}}{\omega_4-(\epsilon_i-\epsilon_a+2\mathrm{i}\eta)}\left(\langle rt|sq\rangle+\sum_\nu\frac{M^*_{sr,\nu}M_{tq,\nu}}{\omega-(\epsilon_a+\Omega_\nu-2\mathrm{i}\eta)}\right)\right.\\
&\left.+\sum_{ia}\frac{\delta_{sa}\delta_{ti}}{\omega_4-(\epsilon_a-\epsilon_i-2\mathrm{i}\eta)}\left(\langle rt|sq\rangle-\sum_\nu\frac{M_{rs,\nu}M^*_{qt,\nu}}{\omega-(\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)}\right)\right]
\end{aligned}
\tag{11}
$$

Applying the residue theorem gives

$$
\begin{aligned}
&\Sigma^{G3W2,\mathrm{I}}_{pq}(\omega)\\
&=\sum_{ika}\langle pa|ki\rangle\frac{1}{(-\omega+\epsilon_k+\mathrm{i}\eta)-(\epsilon_a-\epsilon_i-2\mathrm{i}\eta)}\left(\langle ki|aq\rangle-\sum_\nu\frac{M_{ka,\nu}M^*_{qi,\nu}}{\omega-(\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)}\right)\\
&-\sum_{iac}\langle pi|ca\rangle\frac{1}{(\epsilon_i-\epsilon_a+2\mathrm{i}\eta)-(-\omega+\epsilon_c-\mathrm{i}\eta)}\left(\langle ca|iq\rangle+\sum_\nu\frac{M^*_{ic,\nu}M_{aq,\nu}}{\omega-(\epsilon_a+\Omega_\nu-2\mathrm{i}\eta)}\right)\\
&+\sum_{ika\mu}\frac{M_{pk,\mu}M^*_{ia,\mu}}{(-\omega+\epsilon_k+\mathrm{i}\eta)-(\Omega_\mu-\mathrm{i}\eta)}\frac{1}{(-\omega+\epsilon_k+\mathrm{i}\eta)-(\epsilon_a-\epsilon_i-2\mathrm{i}\eta)}\left(\langle ki|aq\rangle-\sum_\nu\frac{M_{ka,\nu}M^*_{qi,\nu}}{\omega-(\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)}\right)
\end{aligned}
$$

$$
\begin{aligned}
&- \sum_{iac\mu} \frac{M^*_{cp,\mu} M_{ai,\mu}}{(-\Omega_\mu + \mathrm{i}\eta) - (-\omega + \epsilon_c - \mathrm{i}\eta)} \frac{1}{(-\Omega_\mu + \mathrm{i}\eta) - (\epsilon_a - \epsilon_i - 2\mathrm{i}\eta)} \left(\langle ci|aq \rangle - \sum_\nu \frac{M_{ca,\nu} M^*_{qi,\nu}}{\omega - (\epsilon_i - \Omega_\nu + 2\mathrm{i}\eta)} \right) \\
&- \sum_{iac\mu} \frac{M_{pc,\mu} M^*_{ai,\mu}}{(\epsilon_i - \epsilon_a + 2\mathrm{i}\eta) - (-\omega + \epsilon_c - \mathrm{i}\eta)} \frac{1}{(\epsilon_i - \epsilon_a + 2\mathrm{i}\eta) - (\Omega_\mu - \mathrm{i}\eta)} \left(\langle ca|iq \rangle + \sum_\nu \frac{M^*_{ic,\nu} M_{aq,\nu}}{\omega - (\epsilon_a + \Omega_\nu - 2\mathrm{i}\eta)} \right) \\
&- \sum_{iac\mu} \frac{M^*_{cp,\mu} M_{ia,\mu}}{(-\omega + \epsilon_c - \mathrm{i}\eta) - (-\Omega_\mu + \mathrm{i}\eta)} \frac{1}{(-\omega + \epsilon_c - \mathrm{i}\eta) - (\epsilon_i - \epsilon_a + 2\mathrm{i}\eta)} \left(\langle ca|iq \rangle + \sum_\nu \frac{M^*_{ic,\nu} M_{aq,\nu}}{\omega - (\epsilon_a + \Omega_\nu - 2\mathrm{i}\eta)} \right) \\
&+ \sum_{ika\mu} \frac{M_{pk,\mu} M^*_{ai,\mu}}{(\Omega_\mu - \mathrm{i}\eta) - (-\omega + \epsilon_k + \mathrm{i}\eta)} \frac{1}{(\Omega_\mu - \mathrm{i}\eta) - (\epsilon_i - \epsilon_a + 2\mathrm{i}\eta)} \left(\langle ka|iq \rangle + \sum_\nu \frac{M^*_{ik,\nu} M_{aq,\nu}}{\omega - (\epsilon_a + \Omega_\nu - 2\mathrm{i}\eta)} \right) \\
&+ \sum_{ika\mu} \frac{M^*_{kp,\mu} M_{ai,\mu}}{(\epsilon_a - \epsilon_i - 2\mathrm{i}\eta) - (-\omega + \epsilon_k + \mathrm{i}\eta)} \frac{1}{(\epsilon_a - \epsilon_i - 2\mathrm{i}\eta) - (-\Omega_\mu + \mathrm{i}\eta)} \left(\langle ki|aq \rangle - \sum_\nu \frac{M_{ka,\nu} M^*_{qi,\nu}}{\omega - (\epsilon_i - \Omega_\nu + 2\mathrm{i}\eta)} \right)
\end{aligned}
$$

and this yields

$$
\begin{aligned}
\Sigma^{G3W2,\mathrm{I}}_{pq}(\omega) = &\sum_{ika} \langle pa|ki \rangle \frac{1}{(\epsilon_i + \epsilon_k - \epsilon_a + 3\mathrm{i}\eta) - \omega} \left(\langle ki|aq \rangle - \sum_\nu \frac{M_{ka,\nu} M^*_{qi,\nu}}{\omega - (\epsilon_i - \Omega_\nu + 2\mathrm{i}\eta)} \right) \\
&- \sum_{iac} \langle pi|ca \rangle \frac{1}{\omega - (\epsilon_a + \epsilon_c - \epsilon_i - 3\mathrm{i}\eta)} \left(\langle ca|iq \rangle + \sum_\nu \frac{M^*_{ic,\nu} M_{aq,\nu}}{\omega - (\epsilon_a + \Omega_\nu - 2\mathrm{i}\eta)} \right) \\
&+ \sum_{ika\mu} \frac{M_{pk,\mu} M^*_{ia,\mu}}{(\epsilon_k - \Omega_\mu + 2\mathrm{i}\eta) - \omega} \frac{1}{(\epsilon_i + \epsilon_k - \epsilon_a + 3\mathrm{i}\eta) - \omega} \left(\langle ki|aq \rangle - \sum_\nu \frac{M_{ka,\nu} M^*_{qi,\nu}}{\omega - (\epsilon_i - \Omega_\nu + 2\mathrm{i}\eta)} \right) \\
&- \sum_{iac\mu} \frac{M^*_{cp,\mu} M_{ai,\mu}}{\omega - (\epsilon_c + \Omega_\mu - 2\mathrm{i}\eta)} \frac{1}{(\epsilon_i - \epsilon_a - \Omega_\mu + 3\mathrm{i}\eta)} \left(\langle ci|aq \rangle - \sum_\nu \frac{M_{ca,\nu} M^*_{qi,\nu}}{\omega - (\epsilon_i - \Omega_\nu + 2\mathrm{i}\eta)} \right) \\
&- \sum_{iac\mu} \frac{M_{pc,\mu} M^*_{ai,\mu}}{\omega - (\epsilon_a + \epsilon_c - \epsilon_i - 3\mathrm{i}\eta)} \frac{1}{(\epsilon_i - \epsilon_a - \Omega_\mu + 3\mathrm{i}\eta)} \left(\langle ca|iq \rangle + \sum_\nu \frac{M^*_{ic,\nu} M_{aq,\nu}}{\omega - (\epsilon_a + \Omega_\nu - 2\mathrm{i}\eta)} \right) \\
&- \sum_{iac\mu} \frac{M^*_{cp,\mu} M_{ia,\mu}}{(\epsilon_c + \Omega_\mu - 2\mathrm{i}\eta) - \omega} \frac{1}{(\epsilon_a + \epsilon_c - \epsilon_i - 3\mathrm{i}\eta) - \omega} \left(\langle ca|iq \rangle + \sum_\nu \frac{M^*_{ic,\nu} M_{aq,\nu}}{\omega - (\epsilon_a + \Omega_\nu - 2\mathrm{i}\eta)} \right) \\
&+ \sum_{ika\mu} \frac{M_{pk,\mu} M^*_{ai,\mu}}{\omega - (\epsilon_k - \Omega_\mu + 2\mathrm{i}\eta)} \frac{1}{(\epsilon_a - \epsilon_i + \Omega_\mu - 3\mathrm{i}\eta)} \left(\langle ka|iq \rangle + \sum_\nu \frac{M^*_{ik,\nu} M_{aq,\nu}}{\omega - (\epsilon_a + \Omega_\nu - 2\mathrm{i}\eta)} \right) \\
&+ \sum_{ika\mu} \frac{M^*_{kp,\mu} M_{ai,\mu}}{\omega - (\epsilon_i + \epsilon_k - \epsilon_a + 3\mathrm{i}\eta)} \frac{1}{(\epsilon_a - \epsilon_i + \Omega_\mu - 3\mathrm{i}\eta)} \left(\langle ki|aq \rangle - \sum_\nu \frac{M_{ka,\nu} M^*_{qi,\nu}}{\omega - (\epsilon_i - \Omega_\nu + 2\mathrm{i}\eta)} \right)
\end{aligned} \tag{12}
$$

2. Second term

The integral to compute for the second term is

$$
\begin{aligned}
\Sigma^{G3W2,\mathrm{II}}_{pq}(\omega) = \sum_{rst} \frac{\mathrm{i}^3}{(2\pi)} \int \mathrm{d}\omega_4 &\left[\sum_k \frac{\delta_{rk}}{\omega_4 - (-\omega + \epsilon_k + \mathrm{i}\eta)} + \sum_c \frac{\delta_{rc}}{\omega_4 - (-\omega + \epsilon_c - \mathrm{i}\eta)} \right] \\
&\left[\langle ps|rt \rangle + \sum_\mu \frac{M_{pr,\mu} M^*_{ts,\mu}}{\omega_4 - (\Omega_\mu - \mathrm{i}\eta)} - \sum_\mu \frac{M^*_{rp,\mu} M_{st,\mu}}{\omega_4 - (-\Omega_\mu + \mathrm{i}\eta)} \right] \\
\left[- \sum_{ij\nu} \frac{\delta_{si}\delta_{tj}}{\omega_4 - (-\omega + \epsilon_i - \Omega_\nu + 2\mathrm{i}\eta)} \frac{M_{rs,\nu} M^*_{qt,\nu}}{\omega - (\epsilon_j - \Omega_\nu + 2\mathrm{i}\eta)} \right. &\left. - \sum_{ab\nu} \frac{\delta_{sa}\delta_{tb}}{\omega_4 - (-\omega + \epsilon_a + \Omega_\nu - 2\mathrm{i}\eta)} \frac{M^*_{sr,\nu} M_{tq,\nu}}{\omega - (\epsilon_b + \Omega_\nu - 2\mathrm{i}\eta)} \right]
\end{aligned} \tag{13}
$$

Applying the residue theorem gives

$$\begin{aligned}
\Sigma^{G3W2,\mathrm{II}}_{pq}(\omega) = &-\sum_{kab\nu} \langle pa|kb\rangle \frac{1}{(-\omega+\epsilon_k+\mathrm{i}\eta)-(-\omega+\epsilon_a+\Omega_\nu-2\mathrm{i}\eta)} \frac{M^*_{ak,\nu}M_{bq,\nu}}{\omega-(\epsilon_b+\Omega_\nu-2\mathrm{i}\eta)} \\
&-\sum_{ijc\nu} \langle pi|cj\rangle \frac{1}{(-\omega+\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)-(-\omega+\epsilon_c-\mathrm{i}\eta)} \frac{M_{ci,\nu}M^*_{qj,\nu}}{\omega-(\epsilon_j-\Omega_\nu+2\mathrm{i}\eta)} \\
&-\sum_{kab\mu\nu} \frac{M_{pk,\mu}M^*_{ba,\mu}}{(-\omega+\epsilon_k+\mathrm{i}\eta)-(\Omega_\mu-\mathrm{i}\eta)} \frac{1}{(-\omega+\epsilon_k+\mathrm{i}\eta)-(-\omega+\epsilon_a+\Omega_\nu-2\mathrm{i}\eta)} \frac{M^*_{ak,\nu}M_{bq,\nu}}{\omega-(\epsilon_b+\Omega_\nu-2\mathrm{i}\eta)} \\
&+\sum_{abc\mu\nu} \frac{M^*_{cp,\mu}M_{ab,\mu}}{(-\Omega_\mu+\mathrm{i}\eta)-(-\omega+\epsilon_c-\mathrm{i}\eta)} \frac{1}{(-\Omega_\mu+\mathrm{i}\eta)-(-\omega+\epsilon_a+\Omega_\nu-2\mathrm{i}\eta)} \frac{M^*_{ac,\nu}M_{bq,\nu}}{\omega-(\epsilon_b+\Omega_\nu-2\mathrm{i}\eta)} \\
&-\sum_{ijc\mu\nu} \frac{M_{pc,\mu}M^*_{ji,\mu}}{(-\omega+\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)-(-\omega+\epsilon_c-\mathrm{i}\eta)} \frac{1}{(-\omega+\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)-(\Omega_\mu-\mathrm{i}\eta)} \frac{M_{ci,\nu}M^*_{qj,\nu}}{\omega-(\epsilon_j-\Omega_\nu+2\mathrm{i}\eta)} \\
&-\sum_{ijc\mu\nu} \frac{M^*_{cp,\mu}M_{ij,\mu}}{(-\omega+\epsilon_c-\mathrm{i}\eta)-(-\Omega_\mu+\mathrm{i}\eta)} \frac{1}{(-\omega+\epsilon_c-\mathrm{i}\eta)-(-\omega+\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)} \frac{M_{ci,\nu}M^*_{qj,\nu}}{\omega-(\epsilon_j-\Omega_\nu+2\mathrm{i}\eta)} \\
&+\sum_{ijk\mu\nu} \frac{M_{pk,\mu}M^*_{ji,\mu}}{(\Omega_\mu-\mathrm{i}\eta)-(-\omega+\epsilon_k+\mathrm{i}\eta)} \frac{1}{(\Omega_\mu-\mathrm{i}\eta)-(-\omega+\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)} \frac{M_{ki,\nu}M^*_{qj,\nu}}{\omega-(\epsilon_j-\Omega_\nu+2\mathrm{i}\eta)} \\
&-\sum_{kab\mu\nu} \frac{M^*_{kp,\mu}M_{ab,\mu}}{(-\omega+\epsilon_a+\Omega_\nu-2\mathrm{i}\eta)-(-\omega+\epsilon_k+\mathrm{i}\eta)} \frac{1}{(-\omega+\epsilon_a+\Omega_\nu-2\mathrm{i}\eta)-(-\Omega_\mu+\mathrm{i}\eta)} \frac{M^*_{ak,\nu}M_{bq,\nu}}{\omega-(\epsilon_b+\Omega_\nu-2\mathrm{i}\eta)}
\end{aligned}$$

This yields

$$\begin{aligned}
\Sigma^{G3W2,\mathrm{II}}_{pq}(\omega) = &-\sum_{kab\nu} \langle pa|kb\rangle \frac{1}{(\epsilon_k-\epsilon_a-\Omega_\nu+3\mathrm{i}\eta)} \frac{M^*_{ak,\nu}M_{bq,\nu}}{\omega-(\epsilon_b+\Omega_\nu-2\mathrm{i}\eta)} \\
&-\sum_{ijc\nu} \langle pi|cj\rangle \frac{1}{(\epsilon_i-\epsilon_c-\Omega_\nu+3\mathrm{i}\eta)} \frac{M_{ci,\nu}M^*_{qj,\nu}}{\omega-(\epsilon_j-\Omega_\nu+2\mathrm{i}\eta)} \\
&-\sum_{kab\mu\nu} \frac{M_{pk,\mu}M^*_{ba,\mu}}{(\epsilon_k-\Omega_\mu+2\mathrm{i}\eta)-\omega} \frac{1}{(\epsilon_k-\epsilon_a-\Omega_\nu+3\mathrm{i}\eta)} \frac{M^*_{ak,\nu}M_{bq,\nu}}{\omega-(\epsilon_b+\Omega_\nu-2\mathrm{i}\eta)} \\
&+\sum_{abc\mu\nu} \frac{M^*_{cp,\mu}M_{ab,\mu}}{\omega-(\epsilon_c+\Omega_\mu-2\mathrm{i}\eta)} \frac{1}{\omega-(\epsilon_a+\Omega_\nu+\Omega_\mu-3\mathrm{i}\eta)} \frac{M^*_{ac,\nu}M_{bq,\nu}}{\omega-(\epsilon_b+\Omega_\nu-2\mathrm{i}\eta)} \\
&-\sum_{ijc\mu\nu} \frac{M_{pc,\mu}M^*_{ji,\mu}}{(\epsilon_i-\epsilon_c-\Omega_\nu+3\mathrm{i}\eta)} \frac{1}{(\epsilon_i-\Omega_\nu-\Omega_\mu+3\mathrm{i}\eta)-\omega} \frac{M_{ci,\nu}M^*_{qj,\nu}}{\omega-(\epsilon_j-\Omega_\nu+2\mathrm{i}\eta)} \\
&-\sum_{ijc\mu\nu} \frac{M^*_{cp,\mu}M_{ij,\mu}}{(\epsilon_c+\Omega_\mu-2\mathrm{i}\eta)-\omega} \frac{1}{(\epsilon_c-\epsilon_i+\Omega_\nu-3\mathrm{i}\eta)} \frac{M_{ci,\nu}M^*_{qj,\nu}}{\omega-(\epsilon_j-\Omega_\nu+2\mathrm{i}\eta)} \\
&+\sum_{ijk\mu\nu} \frac{M_{pk,\mu}M^*_{ji,\mu}}{\omega-(\epsilon_k-\Omega_\mu+2\mathrm{i}\eta)} \frac{1}{\omega-(\epsilon_i-\Omega_\nu-\Omega_\mu+3\mathrm{i}\eta)} \frac{M_{ki,\nu}M^*_{qj,\nu}}{\omega-(\epsilon_j-\Omega_\nu+2\mathrm{i}\eta)} \\
&-\sum_{kab\mu\nu} \frac{M^*_{kp,\mu}M_{ab,\mu}}{(\epsilon_a-\epsilon_k+\Omega_\nu-3\mathrm{i}\eta)} \frac{1}{(\epsilon_a+\Omega_\nu+\Omega_\mu-3\mathrm{i}\eta)-\omega} \frac{M^*_{ak,\nu}M_{bq,\nu}}{\omega-(\epsilon_b+\Omega_\nu-2\mathrm{i}\eta)}
\end{aligned} \tag{14}$$

3. Third term

The integral to compute for the third term is

$$\begin{aligned}\Sigma^{G3W2,\mathrm{III}}_{pq}(\omega) = \sum_{rst} \frac{\mathrm{i}^3}{(2\pi)} \int \mathrm{d}\omega_4 &\left[\sum_k \frac{\delta_{rk}}{\omega_4 - (-\omega + \epsilon_k + \mathrm{i}\eta)} + \sum_c \frac{\delta_{rc}}{\omega_4 - (-\omega + \epsilon_c - \mathrm{i}\eta)}\right] \\ &\left[\langle ps|rt\rangle + \sum_\mu \frac{M_{pr,\mu}M^*_{ts,\mu}}{\omega_4 - (\Omega_\mu - \mathrm{i}\eta)} - \sum_\mu \frac{M^*_{rp,\mu}M_{st,\mu}}{\omega_4 - (-\Omega_\mu + \mathrm{i}\eta)}\right] \\ \left[\sum_{ia\nu} \frac{\delta_{si}\delta_{ta}}{\omega_4 - (\epsilon_i - \epsilon_a + 2\mathrm{i}\eta)} \frac{M_{rs,\nu}M^*_{qt,\nu}}{\omega_4 - (-\omega + \epsilon_i - \Omega_\nu + 2\mathrm{i}\eta)}\right. &+ \left.\sum_{ia\nu} \frac{\delta_{sa}\delta_{ti}}{\omega_4 - (\epsilon_a - \epsilon_i - 2\mathrm{i}\eta)} \frac{M^*_{sr,\nu}M_{tq,\nu}}{\omega_4 - (-\omega + \epsilon_a + \Omega_\nu - 2\mathrm{i}\eta)}\right]\end{aligned} \tag{15}$$

Applying the residue theorem gives

$$\begin{aligned}\Sigma^{G3W2,\mathrm{III}}_{pq}(\omega) &= \sum_{rst} \frac{\mathrm{i}^3}{(2\pi)} \int \mathrm{d}\omega_4 \\ &\left[+ \sum_{ika\nu} \langle ps|rt\rangle \frac{\delta_{rk}}{\omega_4 - (-\omega + \epsilon_k + \mathrm{i}\eta)} \frac{\delta_{sa}\delta_{ti}}{\omega_4 - (\epsilon_a - \epsilon_i - 2\mathrm{i}\eta)} \frac{M^*_{sr,\nu}M_{tq,\nu}}{\omega_4 - (-\omega + \epsilon_a + \Omega_\nu - 2\mathrm{i}\eta)}\right. \\ &+ \sum_{iac\nu} \langle ps|rt\rangle \frac{\delta_{rc}}{\omega_4 - (-\omega + \epsilon_c - \mathrm{i}\eta)} \frac{\delta_{si}\delta_{ta}}{\omega_4 - (\epsilon_i - \epsilon_a + 2\mathrm{i}\eta)} \frac{M_{rs,\nu}M^*_{qt,\nu}}{\omega_4 - (-\omega + \epsilon_i - \Omega_\nu + 2\mathrm{i}\eta)} \\ &- \sum_{ika\mu\nu} \frac{\delta_{rk}}{\omega_4 - (-\omega + \epsilon_k + \mathrm{i}\eta)} \frac{M^*_{rp,\mu}M_{st,\mu}}{\omega_4 - (-\Omega_\mu + \mathrm{i}\eta)} \frac{\delta_{sa}\delta_{ti}}{\omega_4 - (\epsilon_a - \epsilon_i - 2\mathrm{i}\eta)} \frac{M^*_{sr,\nu}M_{tq,\nu}}{\omega_4 - (-\omega + \epsilon_a + \Omega_\nu - 2\mathrm{i}\eta)} \\ &+ \sum_{iac\mu\nu} \frac{\delta_{rc}}{\omega_4 - (-\omega + \epsilon_c - \mathrm{i}\eta)} \frac{M_{pr,\mu}M^*_{ts,\mu}}{\omega_4 - (\Omega_\mu - \mathrm{i}\eta)} \frac{\delta_{si}\delta_{ta}}{\omega_4 - (\epsilon_i - \epsilon_a + 2\mathrm{i}\eta)} \frac{M_{rs,\nu}M^*_{qt,\nu}}{\omega_4 - (-\omega + \epsilon_i - \Omega_\nu + 2\mathrm{i}\eta)} \\ &+ \sum_{ika\mu\nu} \frac{\delta_{rk}}{\omega_4 - (-\omega + \epsilon_k + \mathrm{i}\eta)} \frac{M_{pr,\mu}M^*_{ts,\mu}}{\omega_4 - (\Omega_\mu - \mathrm{i}\eta)} \frac{\delta_{si}\delta_{ta}}{\omega_4 - (\epsilon_i - \epsilon_a + 2\mathrm{i}\eta)} \frac{M_{rs,\nu}M^*_{qt,\nu}}{\omega_4 - (-\omega + \epsilon_i - \Omega_\nu + 2\mathrm{i}\eta)} \\ &+ \sum_{ika\mu\nu} \frac{\delta_{rk}}{\omega_4 - (-\omega + \epsilon_k + \mathrm{i}\eta)} \frac{M_{pr,\mu}M^*_{ts,\mu}}{\omega_4 - (\Omega_\mu - \mathrm{i}\eta)} \frac{\delta_{sa}\delta_{ti}}{\omega_4 - (\epsilon_a - \epsilon_i - 2\mathrm{i}\eta)} \frac{M^*_{sr,\nu}M_{tq,\nu}}{\omega_4 - (-\omega + \epsilon_a + \Omega_\nu - 2\mathrm{i}\eta)} \\ &- \sum_{iac\mu\nu} \frac{\delta_{rc}}{\omega_4 - (-\omega + \epsilon_c - \mathrm{i}\eta)} \frac{M^*_{rp,\mu}M_{st,\mu}}{\omega_4 - (-\Omega_\mu + \mathrm{i}\eta)} \frac{\delta_{si}\delta_{ta}}{\omega_4 - (\epsilon_i - \epsilon_a + 2\mathrm{i}\eta)} \frac{M_{rs,\nu}M^*_{qt,\nu}}{\omega_4 - (-\omega + \epsilon_i - \Omega_\nu + 2\mathrm{i}\eta)} \\ &\left.- \sum_{iac\mu\nu} \frac{\delta_{rc}}{\omega_4 - (-\omega + \epsilon_c - \mathrm{i}\eta)} \frac{M^*_{rp,\mu}M_{st,\mu}}{\omega_4 - (-\Omega_\mu + \mathrm{i}\eta)} \frac{\delta_{sa}\delta_{ti}}{\omega_4 - (\epsilon_a - \epsilon_i - 2\mathrm{i}\eta)} \frac{M^*_{sr,\nu}M_{tq,\nu}}{\omega_4 - (-\omega + \epsilon_a + \Omega_\nu - 2\mathrm{i}\eta)}\right] \\ &= \sum_{ika\nu} \langle pa|ki\rangle \frac{1}{(-\omega + \epsilon_k + \mathrm{i}\eta) - (\epsilon_a - \epsilon_i - 2\mathrm{i}\eta)} \frac{M^*_{ak,\nu}M_{iq,\nu}}{(-\omega + \epsilon_k + \mathrm{i}\eta) - (-\omega + \epsilon_a + \Omega_\nu - 2\mathrm{i}\eta)} \\ &- \sum_{iac\nu} \langle pi|ca\rangle \frac{1}{(-\omega + \epsilon_c - \mathrm{i}\eta) - (\epsilon_i - \epsilon_a + 2\mathrm{i}\eta)} \frac{M_{ci,\nu}M^*_{qa,\nu}}{(-\omega + \epsilon_c - \mathrm{i}\eta) - (-\omega + \epsilon_i - \Omega_\nu + 2\mathrm{i}\eta)} \\ &+ \sum_{ika\mu\nu} \frac{M^*_{kp,\mu}M_{ai,\mu}}{(-\omega + \epsilon_k + \mathrm{i}\eta) - (-\omega + \epsilon_a + \Omega_\nu - 2\mathrm{i}\eta)} \frac{1}{(-\Omega_\mu + \mathrm{i}\eta) - (\epsilon_a - \epsilon_i - 2\mathrm{i}\eta)} \frac{M^*_{ak,\nu}M_{iq,\nu}}{(-\Omega_\mu + \mathrm{i}\eta) - (-\omega + \epsilon_a + \Omega_\nu - 2\mathrm{i}\eta)} \\ &+ \sum_{ika\mu\nu} \frac{M^*_{kp,\mu}M_{ai,\mu}}{(-\omega + \epsilon_k + \mathrm{i}\eta) - (\epsilon_a - \epsilon_i - 2\mathrm{i}\eta)} \frac{1}{(-\omega + \epsilon_k + \mathrm{i}\eta) - (-\omega + \epsilon_a + \Omega_\nu - 2\mathrm{i}\eta)} \frac{M^*_{ak,\nu}M_{iq,\nu}}{(-\Omega_\mu + \mathrm{i}\eta) - (\epsilon_a - \epsilon_i - 2\mathrm{i}\eta)} \\ &- \sum_{iac\mu\nu} \frac{M_{pc,\mu}M^*_{ai,\mu}}{(\epsilon_i - \epsilon_a + 2\mathrm{i}\eta) - (\Omega_\mu - \mathrm{i}\eta)} \frac{1}{(-\omega + \epsilon_i - \Omega_\nu + 2\mathrm{i}\eta) - (-\omega + \epsilon_c - \mathrm{i}\eta)} \frac{M_{ci,\nu}M^*_{qa,\nu}}{(-\omega + \epsilon_i - \Omega_\nu + 2\mathrm{i}\eta) - (\Omega_\mu - \mathrm{i}\eta)} \\ &- \sum_{iac\mu\nu} \frac{M_{pc,\mu}M^*_{ai,\mu}}{(\epsilon_i - \epsilon_a + 2\mathrm{i}\eta) - (-\omega + \epsilon_c - \mathrm{i}\eta)} \frac{1}{(\epsilon_i - \epsilon_a + 2\mathrm{i}\eta) - (\Omega_\mu - \mathrm{i}\eta)} \frac{M_{ci,\nu}M^*_{qa,\nu}}{(-\omega + \epsilon_i - \Omega_\nu + 2\mathrm{i}\eta) - (-\omega + \epsilon_c - \mathrm{i}\eta)}\end{aligned}$$

$$
\begin{aligned}
&-\sum_{ika\mu\nu}\frac{M_{pk,\mu}M_{ai,\mu}^*}{(\Omega_\mu-\mathrm{i}\eta)-(-\omega+\epsilon_k+\mathrm{i}\eta)}\frac{1}{(\Omega_\mu-\mathrm{i}\eta)-(\epsilon_i-\epsilon_a+2\mathrm{i}\eta)}\frac{M_{ki,\nu}M_{qa,\nu}^*}{(\Omega_\mu-\mathrm{i}\eta)-(-\omega+\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)}\\
&+\sum_{ika\mu\nu}\frac{M_{pk,\mu}M_{ia,\mu}^*}{(-\omega+\epsilon_k+\mathrm{i}\eta)-(\Omega_\mu-\mathrm{i}\eta)}\frac{1}{(-\omega+\epsilon_k+\mathrm{i}\eta)-(\epsilon_a-\epsilon_i-2\mathrm{i}\eta)}\frac{M_{ak,\nu}^*M_{iq,\nu}}{(-\omega+\epsilon_k+\mathrm{i}\eta)-(-\omega+\epsilon_a+\Omega_\nu-2\mathrm{i}\eta)}\\
&+\sum_{iac\mu\nu}\frac{M_{cp,\mu}^*M_{ia,\mu}}{(-\omega+\epsilon_c-\mathrm{i}\eta)-(-\Omega_\mu+\mathrm{i}\eta)}\frac{1}{(-\omega+\epsilon_c-\mathrm{i}\eta)-(\epsilon_i-\epsilon_a+2\mathrm{i}\eta)}\frac{M_{ci,\nu}M_{qa,\nu}^*}{(-\omega+\epsilon_c-\mathrm{i}\eta)-(-\omega+\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)}\\
&-\sum_{iac\mu\nu}\frac{M_{cp,\mu}^*M_{ai,\mu}}{(-\Omega_\mu+\mathrm{i}\eta)-(-\omega+\epsilon_c-\mathrm{i}\eta)}\frac{1}{(-\Omega_\mu+\mathrm{i}\eta)-(\epsilon_a-\epsilon_i-2\mathrm{i}\eta)}\frac{M_{ac,\nu}^*M_{iq,\nu}}{(-\Omega_\mu+\mathrm{i}\eta)-(-\omega+\epsilon_a+\Omega_\nu-2\mathrm{i}\eta)}
\end{aligned}
$$

This yields

$$
\begin{aligned}
\Sigma_{pq}^{G3W2,\mathrm{III}}(\omega)=&\sum_{iac\nu}\langle pi|ca\rangle\frac{1}{\omega-(\epsilon_a+\epsilon_c-\epsilon_i-3\mathrm{i}\eta)}\frac{M_{ci,\nu}M_{qa,\nu}^*}{(\epsilon_c-\epsilon_i+\Omega_\nu-3\mathrm{i}\eta)}\\
&-\sum_{ika\nu}\langle pa|ki\rangle\frac{1}{\omega-(\epsilon_i+\epsilon_k-\epsilon_a+3\mathrm{i}\eta)}\frac{M_{ak,\nu}^*M_{iq,\nu}}{(\epsilon_k-\epsilon_a-\Omega_\nu+3\mathrm{i}\eta)}\\
&+\sum_{ika\mu\nu}\frac{M_{kp,\mu}^*M_{ai,\mu}}{(\epsilon_k-\epsilon_a-\Omega_\nu+3\mathrm{i}\eta)}\frac{1}{(\epsilon_i-\epsilon_a-\Omega_\mu+3\mathrm{i}\eta)}\frac{M_{ak,\nu}^*M_{iq,\nu}}{\omega-(\epsilon_a+\Omega_\nu+\Omega_\mu-3\mathrm{i}\eta)}\\
&-\sum_{ika\mu\nu}\frac{M_{kp,\mu}^*M_{ai,\mu}}{\omega-(\epsilon_i+\epsilon_k-\epsilon_a+3\mathrm{i}\eta)}\frac{1}{(\epsilon_k-\epsilon_a-\Omega_\nu+3\mathrm{i}\eta)}\frac{M_{ak,\nu}^*M_{iq,\nu}}{(\epsilon_i-\epsilon_a-\Omega_\mu+3\mathrm{i}\eta)}\\
&+\sum_{iac\mu\nu}\frac{M_{pc,\mu}M_{ai,\mu}^*}{(\epsilon_i-\epsilon_a-\Omega_\mu+3\mathrm{i}\eta)}\frac{1}{(\epsilon_i-\epsilon_c-\Omega_\nu+3\mathrm{i}\eta)}\frac{M_{ci,\nu}M_{qa,\nu}^*}{\omega-(\epsilon_i-\Omega_\nu-\Omega_\mu+3\mathrm{i}\eta)}\\
&-\sum_{iac\mu\nu}\frac{M_{pc,\mu}M_{ai,\mu}^*}{\omega-(\epsilon_a+\epsilon_c-\epsilon_i-3\mathrm{i}\eta)}\frac{1}{(\epsilon_i-\epsilon_a-\Omega_\mu+3\mathrm{i}\eta)}\frac{M_{ci,\nu}M_{qa,\nu}^*}{(\epsilon_i-\epsilon_c-\Omega_\nu+3\mathrm{i}\eta)}\\
&-\sum_{ika\mu\nu}\frac{M_{pk,\mu}M_{ai,\mu}^*}{\omega-(\epsilon_k-\Omega_\mu+2\mathrm{i}\eta)}\frac{1}{(\epsilon_a-\epsilon_i+\Omega_\mu-3\mathrm{i}\eta)}\frac{M_{ki,\nu}M_{qa,\nu}^*}{\omega-(\epsilon_i-\Omega_\nu-\Omega_\mu+3\mathrm{i}\eta)}\\
&+\sum_{ika\mu\nu}\frac{M_{pk,\mu}M_{ia,\mu}^*}{\omega-(\epsilon_k-\Omega_\mu+2\mathrm{i}\eta)}\frac{1}{\omega-(\epsilon_i+\epsilon_k-\epsilon_a+3\mathrm{i}\eta)}\frac{M_{ak,\nu}^*M_{iq,\nu}}{(\epsilon_k-\epsilon_a-\Omega_\nu+3\mathrm{i}\eta)}\\
&+\sum_{iac\mu\nu}\frac{M_{cp,\mu}^*M_{ia,\mu}}{\omega-(\epsilon_c+\Omega_\mu-2\mathrm{i}\eta)}\frac{1}{\omega-(\epsilon_a+\epsilon_c-\epsilon_i-3\mathrm{i}\eta)}\frac{M_{ci,\nu}M_{qa,\nu}^*}{(\epsilon_c-\epsilon_i+\Omega_\nu-3\mathrm{i}\eta)}\\
&-\sum_{iac\mu\nu}\frac{M_{cp,\mu}^*M_{ai,\mu}}{\omega-(\epsilon_c+\Omega_\mu-2\mathrm{i}\eta)}\frac{1}{(\epsilon_i-\epsilon_a-\Omega_\mu+3\mathrm{i}\eta)}\frac{M_{ac,\nu}^*M_{iq,\nu}}{\omega-(\epsilon_a+\Omega_\nu+\Omega_\mu-3\mathrm{i}\eta)}
\end{aligned}
\tag{16}
$$

C. Expression in terms of intermediates

The $G3W2$ self-energy derived in the previous subsection is now recast in terms of intermediate quantities, paving the way for the identification of the ADC blocks. To this end, it must be decomposed into contributions involving either single poles or products of poles located in the same half of the complex plane. The three self-energy contributions introduced previously are therefore reorganized as

$$
\Sigma_{pq}^{G3W2}(\omega)=\Sigma_{pq}^{G3W2,a}(\omega)+\Sigma_{pq}^{G3W2,b}(\omega)+\Sigma_{pq}^{G3W2,c}(\omega)+\Sigma_{pq}^{G3W2,d}(\omega)
$$

where $\Sigma^{G3W2,a}$ contains terms with two ERIs in the numerator, $\Sigma^{G3W2,b}$ those with a single ERI, and $\Sigma^{G3W2,c}$ and $\Sigma^{G3W2,d}$ the terms without ERIs. The latter are further separated into contributions containing only dressed poles, $\Sigma^{G3W2,c}$, and those involving undressed poles, $\Sigma^{G3W2,d}$.

1. Gathering terms: Two ERIs

There are two terms contributing to $\Sigma^{G3W2,a}$ and they are both in $\Sigma^{G3W2,\mathrm{I}}$ [see Eq. (12)]

$$\Sigma^{G3W2,a}_{pq}(\omega) = -\sum_{ika} \langle pa|ki\rangle \frac{1}{\omega - (\epsilon_i + \epsilon_k - \epsilon_a + 3\mathrm{i}\eta)} \langle ki|aq\rangle - \sum_{iac} \langle pi|ca\rangle \frac{1}{\omega - (\epsilon_a + \epsilon_c - \epsilon_i - 3\mathrm{i}\eta)} \langle ca|iq\rangle \tag{17}$$

Hence, the $\Sigma^{G3W2,a}$ is identified with the SOX self-energy $\Sigma^{\mathrm{SOX}}_{pq}(\omega)$.

2. Gathering terms: One ERI

In the first term [see Eq. (12)], there is (after decomposition of some product of poles)

$$\begin{aligned}
&+\sum_{ika\nu} \langle pa|ki\rangle M_{ka,\nu} M^*_{qi,\nu} \frac{1}{(\epsilon_i + \epsilon_k - \epsilon_a + 3\mathrm{i}\eta) - (\epsilon_i - \Omega_\nu + 2\mathrm{i}\eta)} \left[\frac{1}{\omega - (\epsilon_i + \epsilon_k - \epsilon_a + 3\mathrm{i}\eta)} - \frac{1}{\omega - (\epsilon_i - \Omega_\nu + 2\mathrm{i}\eta)} \right] \\
&-\sum_{iac\nu} \langle pi|ca\rangle M^*_{ic,\nu} M_{aq,\nu} \frac{1}{(\epsilon_a + \epsilon_c - \epsilon_i - 3\mathrm{i}\eta) - (\epsilon_a + \Omega_\nu - 2\mathrm{i}\eta)} \left[\frac{1}{\omega - (\epsilon_a + \epsilon_c - \epsilon_i - 3\mathrm{i}\eta)} - \frac{1}{\omega - (\epsilon_a + \Omega_\nu - 2\mathrm{i}\eta)} \right] \\
&+\sum_{ika\mu} M_{pk,\mu} M^*_{ia,\mu} \langle ki|aq\rangle \frac{1}{(\epsilon_k - \Omega_\mu + 2\mathrm{i}\eta) - (\epsilon_i + \epsilon_k - \epsilon_a + 3\mathrm{i}\eta)} \left[\frac{1}{\omega - (\epsilon_k - \Omega_\mu + 2\mathrm{i}\eta)} - \frac{1}{\omega - (\epsilon_i + \epsilon_k - \epsilon_a + 3\mathrm{i}\eta)} \right] \\
&-\sum_{c\mu} M^*_{cp,\mu} \frac{1}{\omega - (\epsilon_c + \Omega_\mu - 2\mathrm{i}\eta)} \left[\sum_{ia} \frac{M_{ai,\mu} \langle ci|aq\rangle}{(\epsilon_i - \epsilon_a - \Omega_\mu + 3\mathrm{i}\eta)} \right] \\
&-\sum_{iac\mu} \left[\sum_{\mu} \frac{M_{pc,\mu} M^*_{ai,\mu}}{(\epsilon_i - \epsilon_a - \Omega_\mu + 3\mathrm{i}\eta)} \right] \frac{1}{\omega - (\epsilon_a + \epsilon_c - \epsilon_i - 3\mathrm{i}\eta)} \langle ca|iq\rangle \\
&-\sum_{iac\mu} M^*_{cp,\mu} M_{ia,\mu} \langle ca|iq\rangle \frac{1}{(\epsilon_c + \Omega_\mu - 2\mathrm{i}\eta) - (\epsilon_a + \epsilon_c - \epsilon_i - 3\mathrm{i}\eta)} \left[\frac{1}{\omega - (\epsilon_c + \Omega_\mu - 2\mathrm{i}\eta)} - \frac{1}{\omega - (\epsilon_a + \epsilon_c - \epsilon_i - 3\mathrm{i}\eta)} \right] \\
&+\sum_{k\mu} M_{pk,\mu} \frac{1}{\omega - (\epsilon_k - \Omega_\mu + 2\mathrm{i}\eta)} \left[\sum_{ia} \frac{M^*_{ai,\mu} \langle ka|iq\rangle}{(\epsilon_a - \epsilon_i + \Omega_\mu - 3\mathrm{i}\eta)} \right] \\
&+\sum_{ika} \left[\sum_{\mu} \frac{M^*_{kp,\mu} M_{ai,\mu}}{(\epsilon_a - \epsilon_i + \Omega_\mu - 3\mathrm{i}\eta)} \right] \frac{1}{\omega - (\epsilon_i + \epsilon_k - \epsilon_a + 3\mathrm{i}\eta)} \langle ki|aq\rangle
\end{aligned} \tag{18}$$

in the second [see Eq. (14)]

$$-\sum_{b\nu} \left[\sum_{ka} \frac{\langle pa|kb\rangle M^*_{ak,\nu}}{(\epsilon_k - \epsilon_a - \Omega_\nu + 3\mathrm{i}\eta)} \right] \frac{1}{\omega - (\epsilon_b + \Omega_\nu - 2\mathrm{i}\eta)} M_{bq,\nu} - \sum_{j\nu} \left[\sum_{ic} \frac{\langle pi|cj\rangle M_{ci,\nu}}{(\epsilon_i - \epsilon_c - \Omega_\nu + 3\mathrm{i}\eta)} \right] \frac{1}{\omega - (\epsilon_j - \Omega_\nu + 2\mathrm{i}\eta)} M^*_{qj,\nu}$$

and in the third [see Eq. (16)]

$$\begin{aligned}
&-\sum_{ika} \langle pa|ki\rangle \frac{1}{\omega - (\epsilon_i + \epsilon_k - \epsilon_a + 3\mathrm{i}\eta)} \left[\sum_{\nu} \frac{M^*_{ak,\nu} M_{iq,\nu}}{(\epsilon_k - \epsilon_a - \Omega_\nu + 3\mathrm{i}\eta)} \right] \\
&+\sum_{iac} \langle pi|ca\rangle \frac{1}{\omega - (\epsilon_a + \epsilon_c - \epsilon_i - 3\mathrm{i}\eta)} \left[\sum_{\nu} \frac{M_{ci,\nu} M^*_{qa,\nu}}{(\epsilon_c - \epsilon_i + \Omega_\nu - 3\mathrm{i}\eta)} \right]
\end{aligned}$$

These terms are gathered as

$$\begin{aligned}\Sigma_{pq}^{G3W2,b}(\omega) = &\sum_{ika} \langle pa|ki\rangle \frac{1}{\omega-(\epsilon_i+\epsilon_k-\epsilon_a+3\mathrm{i}\eta)}\left[\sum_{\nu}\frac{M_{ka,\nu}M_{qi,\nu}^*}{(\epsilon_k-\epsilon_a+\Omega_\nu+\mathrm{i}\eta)}-\sum_{\nu}\frac{M_{ak,\nu}^*M_{iq,\nu}}{(\epsilon_k-\epsilon_a-\Omega_\nu+3\mathrm{i}\eta)}\right]\\
&+\sum_{iac}\langle pi|ca\rangle\frac{1}{\omega-(\epsilon_a+\epsilon_c-\epsilon_i-3\mathrm{i}\eta)}\left[\sum_{\nu}\frac{M_{ci,\nu}M_{qa,\nu}^*}{(\epsilon_c-\epsilon_i+\Omega_\nu-3\mathrm{i}\eta)}-\sum_{\nu}\frac{M_{ic,\nu}^*M_{aq,\nu}}{(\epsilon_c-\epsilon_i-\Omega_\nu-\mathrm{i}\eta)}\right]\\
&+\sum_{ika}\left[\sum_{\mu}\frac{M_{kp,\mu}^*M_{ai,\mu}}{(\epsilon_a-\epsilon_i+\Omega_\mu-3\mathrm{i}\eta)}-\sum_{\mu}\frac{M_{pk,\mu}M_{ia,\mu}^*}{(\epsilon_a-\epsilon_i-\Omega_\mu-\mathrm{i}\eta)}\right]\frac{1}{\omega-(\epsilon_i+\epsilon_k-\epsilon_a+3\mathrm{i}\eta)}\langle ki|aq\rangle\\
&+\sum_{iac}\left[\sum_{\mu}\frac{M_{cp,\mu}^*M_{ia,\mu}}{(\epsilon_i-\epsilon_a+\Omega_\mu+\mathrm{i}\eta)}-\sum_{\mu}\frac{M_{pc,\mu}M_{ai,\mu}^*}{(\epsilon_i-\epsilon_a-\Omega_\mu+3\mathrm{i}\eta)}\right]\frac{1}{\omega-(\epsilon_a+\epsilon_c-\epsilon_i-3\mathrm{i}\eta)}\langle ca|iq\rangle\\
&+\sum_{k\mu}M_{pk,\mu}\frac{1}{\omega-(\epsilon_k-\Omega_\mu+2\mathrm{i}\eta)}\left[\sum_{ia}\frac{M_{ia,\mu}^*\langle ki|aq\rangle}{(\epsilon_a-\epsilon_i-\Omega_\mu-\mathrm{i}\eta)}+\sum_{ia}\frac{M_{ai,\mu}^*\langle ka|iq\rangle}{(\epsilon_a-\epsilon_i+\Omega_\mu-3\mathrm{i}\eta)}\right]\\
&+\sum_{c\mu}M_{cp,\mu}^*\frac{1}{\omega-(\epsilon_c+\Omega_\mu-2\mathrm{i}\eta)}\left[\sum_{ia}\frac{M_{ia,\mu}\langle ca|iq\rangle}{(\epsilon_a-\epsilon_i-\Omega_\mu-\mathrm{i}\eta)}+\sum_{ia}\frac{M_{ai,\mu}\langle ci|aq\rangle}{(\epsilon_a-\epsilon_i+\Omega_\mu-3\mathrm{i}\eta)}\right]\\
&+\sum_{a\nu}\left[\sum_{ic}\frac{\langle pi|ca\rangle M_{ic,\nu}^*}{(\epsilon_c-\epsilon_i-\Omega_\nu-\mathrm{i}\eta)}-\sum_{ic}\frac{\langle pc|ia\rangle M_{ci,\nu}^*}{(\epsilon_i-\epsilon_c-\Omega_\nu+3\mathrm{i}\eta)}\right]\frac{1}{\omega-(\epsilon_a+\Omega_\nu-2\mathrm{i}\eta)}M_{aq,\nu}\\
&+\sum_{i\nu}\left[\sum_{ka}\frac{\langle pa|ki\rangle M_{ka,\nu}}{(\epsilon_a-\epsilon_k-\Omega_\nu-\mathrm{i}\eta)}-\sum_{ka}\frac{\langle pk|ai\rangle M_{ak,\nu}}{(\epsilon_k-\epsilon_a-\Omega_\nu+3\mathrm{i}\eta)}\right]\frac{1}{\omega-(\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)}M_{qi,\nu}^*\end{aligned}$$

Using Bruneval's relation [see Eq. (5)], we can simplify this as

$$\begin{aligned}\Sigma_{pq}^{G3W2,b}(\omega) = &-2\Sigma_{pq}^{\mathrm{SOX}}(\omega)\\
&+\sum_{k\mu}M_{pk,\mu}\frac{1}{\omega-(\epsilon_k-\Omega_\mu+2\mathrm{i}\eta)}\left[\sum_{ia}\frac{M_{ia,\mu}^*\langle ki|aq\rangle}{(\epsilon_a-\epsilon_i-\Omega_\mu-\mathrm{i}\eta)}+\sum_{ia}\frac{M_{ai,\mu}^*\langle ka|iq\rangle}{(\epsilon_a-\epsilon_i+\Omega_\mu-3\mathrm{i}\eta)}\right]\\
&+\sum_{c\mu}M_{cp,\mu}^*\frac{1}{\omega-(\epsilon_c+\Omega_\mu-2\mathrm{i}\eta)}\left[\sum_{ia}\frac{M_{ia,\mu}\langle ca|iq\rangle}{(\epsilon_a-\epsilon_i-\Omega_\mu-\mathrm{i}\eta)}+\sum_{ia}\frac{M_{ai,\mu}\langle ci|aq\rangle}{(\epsilon_a-\epsilon_i+\Omega_\mu-3\mathrm{i}\eta)}\right]\\
&+\sum_{a\nu}\left[\sum_{ic}\frac{\langle pi|ca\rangle M_{ic,\nu}^*}{(\epsilon_c-\epsilon_i-\Omega_\nu-\mathrm{i}\eta)}+\sum_{ic}\frac{\langle pc|ia\rangle M_{ci,\nu}^*}{(\epsilon_c-\epsilon_i+\Omega_\nu-3\mathrm{i}\eta)}\right]\frac{1}{\omega-(\epsilon_a+\Omega_\nu-2\mathrm{i}\eta)}M_{aq,\nu}\\
&+\sum_{i\nu}\left[\sum_{ka}\frac{\langle pa|ki\rangle M_{ka,\nu}}{(\epsilon_a-\epsilon_k-\Omega_\nu-\mathrm{i}\eta)}+\sum_{ka}\frac{\langle pk|ai\rangle M_{ak,\nu}}{(\epsilon_a-\epsilon_k+\Omega_\nu-3\mathrm{i}\eta)}\right]\frac{1}{\omega-(\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)}M_{qi,\nu}^*\end{aligned} \tag{19}$$

3. Gathering terms: Zero ERI and only dressed poles

In the first term [see Eq. (12)], there is

$$\begin{aligned}&+\sum_{ic\mu\nu}M_{cp,\mu}^*\frac{1}{\omega-(\epsilon_c+\Omega_\mu-2\mathrm{i}\eta)}\left[\sum_{a}\frac{M_{ca,\nu}M_{ai,\mu}}{(\epsilon_i-\epsilon_a-\Omega_\mu+3\mathrm{i}\eta)}\right]\frac{1}{\omega-(\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)}M_{qi,\nu}^*\\
&+\sum_{ka\mu\nu}M_{pk,\mu}\frac{1}{\omega-(\epsilon_k-\Omega_\mu+2\mathrm{i}\eta)}\left[\sum_{i}\frac{M_{ai,\mu}^*M_{ik,\nu}^*}{(\epsilon_a-\epsilon_i+\Omega_\mu-3\mathrm{i}\eta)}\right]\frac{1}{\omega-(\epsilon_a+\Omega_\nu-2\mathrm{i}\eta)}M_{aq,\nu}\end{aligned}$$

in the second [see Eq. (14)]

$$+\sum_{ic\mu\nu}M_{cp,\mu}^*\frac{1}{\omega-(\epsilon_c+\Omega_\mu-2\mathrm{i}\eta)}\left[\sum_{j}\frac{M_{cj,\nu}M_{ji,\mu}}{(\epsilon_c-\epsilon_j+\Omega_\nu-3\mathrm{i}\eta)}\right]\frac{1}{\omega-(\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)}M_{qi,\nu}^*$$

$$
\begin{aligned}
&+\sum_{kb\mu\nu} M_{pk,\mu}\frac{1}{\omega-(\epsilon_k-\Omega_\mu+2\mathrm{i}\eta)}\left[\sum_a \frac{M^*_{ba,\mu}M^*_{ak,\nu}}{(\epsilon_k-\epsilon_a-\Omega_\nu+3\mathrm{i}\eta)}\right]\frac{1}{\omega-(\epsilon_b+\Omega_\nu-2\mathrm{i}\eta)}M_{bq,\nu}\\
&+\sum_{ijk\mu\nu} M_{pk,\mu}\frac{1}{\omega-(\epsilon_k-\Omega_\mu+2\mathrm{i}\eta)}\frac{M^*_{ji,\mu}M_{ki,\nu}}{\omega-(\epsilon_i-\Omega_\nu-\Omega_\mu+3\mathrm{i}\eta)}\frac{1}{\omega-(\epsilon_j-\Omega_\nu+2\mathrm{i}\eta)}M^*_{qj,\nu}\\
&+\sum_{ijc\mu\nu}\frac{M_{pc,\mu}M_{ci,\nu}M^*_{ji,\mu}M^*_{qj,\nu}}{(\epsilon_i-\epsilon_c-\Omega_\nu+3\mathrm{i}\eta)}\frac{1}{\omega-(\epsilon_i-\Omega_\nu-\Omega_\mu+3\mathrm{i}\eta)}\frac{1}{\omega-(\epsilon_j-\Omega_\nu+2\mathrm{i}\eta)}\\
&+\sum_{abc\mu\nu} M^*_{cp,\mu}\frac{1}{\omega-(\epsilon_c+\Omega_\mu-2\mathrm{i}\eta)}\frac{M^*_{ac,\nu}M_{ab,\mu}}{\omega-(\epsilon_a+\Omega_\nu+\Omega_\mu-3\mathrm{i}\eta)}\frac{1}{\omega-(\epsilon_b+\Omega_\nu-2\mathrm{i}\eta)}M_{bq,\nu}\\
&+\sum_{kab\mu\nu}\frac{M^*_{kp,\mu}M_{ab,\mu}M^*_{ak,\nu}M_{bq,\nu}}{(\epsilon_a-\epsilon_k+\Omega_\nu-3\mathrm{i}\eta)}\frac{1}{\omega-(\epsilon_a+\Omega_\nu+\Omega_\mu-3\mathrm{i}\eta)}\frac{1}{\omega-(\epsilon_b+\Omega_\nu-2\mathrm{i}\eta)}
\end{aligned}
$$

and in the third [see Eq. (16)]

$$
\begin{aligned}
&-\sum_{ika\mu\nu}\frac{M_{pk,\mu}M_{ki,\nu}M^*_{ai,\mu}M^*_{qa,\nu}}{(\epsilon_a-\epsilon_i+\Omega_\mu-3\mathrm{i}\eta)}\frac{1}{\omega-(\epsilon_i-\Omega_\nu-\Omega_\mu+3\mathrm{i}\eta)}\frac{1}{\omega-(\epsilon_k-\Omega_\mu+2\mathrm{i}\eta)}\\
&+\sum_{i\mu\nu}\left[\sum_c\frac{M_{pc,\mu}M_{ci,\nu}}{(\epsilon_i-\epsilon_c-\Omega_\nu+3\mathrm{i}\eta)}\right]\frac{1}{\omega-(\epsilon_i-\Omega_\nu-\Omega_\mu+3\mathrm{i}\eta)}\left[\sum_a\frac{M^*_{ai,\mu}M^*_{qa,\nu}}{(\epsilon_i-\epsilon_a-\Omega_\mu+3\mathrm{i}\eta)}\right]\\
&-\sum_{iac\mu\nu}\frac{M^*_{cp,\mu}M_{ai,\mu}M^*_{ac,\nu}M_{iq,\nu}}{(\epsilon_i-\epsilon_a-\Omega_\mu+3\mathrm{i}\eta)}\frac{1}{\omega-(\epsilon_a+\Omega_\nu+\Omega_\mu-3\mathrm{i}\eta)}\frac{1}{\omega-(\epsilon_c+\Omega_\mu-2\mathrm{i}\eta)}\\
&+\sum_{a\mu\nu}\left[\sum_k\frac{M^*_{kp,\mu}M^*_{ak,\nu}}{(\epsilon_k-\epsilon_a-\Omega_\nu+3\mathrm{i}\eta)}\right]\frac{1}{\omega-(\epsilon_a+\Omega_\nu+\Omega_\mu-3\mathrm{i}\eta)}\left[\sum_i\frac{M_{ai,\mu}M_{iq,\nu}}{(\epsilon_i-\epsilon_a-\Omega_\mu+3\mathrm{i}\eta)}\right]
\end{aligned}
$$

Of these twelve terms, four consist of products of 2h1p and 2p1h poles, four involve a 3h2p pole, and the remaining four a 3p2h pole. The former must be further decomposed, while the latter can be written directly in terms of intermediate quantities.

- **The 2h1p-2p1h poles**

These four terms are gathered as

$$
\begin{aligned}
&+\sum_{ic\mu\nu}M^*_{cp,\mu}\frac{1}{\omega-(\epsilon_c+\Omega_\mu-2\mathrm{i}\eta)}\left[\sum_j\frac{M_{cj,\nu}M_{ji,\mu}}{(\epsilon_c-\epsilon_j+\Omega_\nu-3\mathrm{i}\eta)}+\sum_a\frac{M_{ca,\nu}M_{ai,\mu}}{(\epsilon_i-\epsilon_a-\Omega_\mu+3\mathrm{i}\eta)}\right]\frac{1}{\omega-(\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)}M^*_{qi,\nu}\\
&+\sum_{kb\mu\nu}M_{pk,\mu}\frac{1}{\omega-(\epsilon_k-\Omega_\mu+2\mathrm{i}\eta)}\left[\sum_i\frac{M^*_{bi,\mu}M^*_{ik,\nu}}{(\epsilon_b-\epsilon_i+\Omega_\mu-3\mathrm{i}\eta)}+\sum_a\frac{M^*_{ba,\mu}M^*_{ak,\nu}}{(\epsilon_k-\epsilon_a-\Omega_\nu+3\mathrm{i}\eta)}\right]\frac{1}{\omega-(\epsilon_b+\Omega_\nu-2\mathrm{i}\eta)}M_{bq,\nu}
\end{aligned}
$$

Upon decomposition of the poles, this yields

$$
\begin{aligned}
&+\sum_{ic\mu\nu}M^*_{cp,\mu}M^*_{qi,\nu}\left[\sum_j\frac{M_{cj,\nu}M_{ji,\mu}}{(\epsilon_c-\epsilon_j+\Omega_\nu-3\mathrm{i}\eta)}+\sum_a\frac{M_{ca,\nu}M_{ai,\mu}}{(\epsilon_i-\epsilon_a-\Omega_\mu+3\mathrm{i}\eta)}\right]\\
&\qquad\qquad\frac{1}{(\epsilon_c+\Omega_\mu-2\mathrm{i}\eta)-(\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)}\left[\frac{1}{\omega-(\epsilon_c+\Omega_\mu-2\mathrm{i}\eta)}-\frac{1}{\omega-(\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)}\right]\\
&+\sum_{kb\mu\nu}M_{pk,\mu}M_{bq,\nu}\left[\sum_i\frac{M^*_{bi,\mu}M^*_{ik,\nu}}{(\epsilon_b-\epsilon_i+\Omega_\mu-3\mathrm{i}\eta)}+\sum_a\frac{M^*_{ba,\mu}M^*_{ak,\nu}}{(\epsilon_k-\epsilon_a-\Omega_\nu+3\mathrm{i}\eta)}\right]\\
&\qquad\qquad\frac{1}{(\epsilon_k-\Omega_\mu+2\mathrm{i}\eta)-(\epsilon_b+\Omega_\nu-2\mathrm{i}\eta)}\left[\frac{1}{\omega-(\epsilon_k-\Omega_\mu+2\mathrm{i}\eta)}-\frac{1}{\omega-(\epsilon_b+\Omega_\nu-2\mathrm{i}\eta)}\right]
\end{aligned}
$$

This finally gives

$$
\begin{aligned}
&+\sum_{c\mu} M^*_{cp,\mu} \frac{1}{\omega-(\epsilon_c+\Omega_\mu-2\mathrm{i}\eta)} \\
&\qquad \left[\sum_{i\nu}\left(\sum_j \frac{M_{cj,\nu}M_{ji,\mu}}{(\epsilon_c-\epsilon_j+\Omega_\nu-3\mathrm{i}\eta)}+\sum_a \frac{M_{ca,\nu}M_{ai,\mu}}{(\epsilon_i-\epsilon_a-\Omega_\mu+3\mathrm{i}\eta)}\right)\frac{M^*_{qi,\nu}}{(\epsilon_c-\epsilon_i+\Omega_\nu+\Omega_\mu-4\mathrm{i}\eta)}\right] \\
&+\sum_{k\mu} M_{pk,\mu} \frac{1}{\omega-(\epsilon_k-\Omega_\mu+2\mathrm{i}\eta)} \\
&\qquad \left[\sum_{b\nu}\frac{M_{bq,\nu}}{(\epsilon_k-\epsilon_b-\Omega_\nu-\Omega_\mu+4\mathrm{i}\eta)}\left(\sum_i \frac{M^*_{bi,\mu}M^*_{ik,\nu}}{(\epsilon_b-\epsilon_i+\Omega_\mu-3\mathrm{i}\eta)}+\sum_a \frac{M^*_{ba,\mu}M^*_{ak,\nu}}{(\epsilon_k-\epsilon_a-\Omega_\nu+3\mathrm{i}\eta)}\right)\right] \\
&+\sum_{i\nu}\left[-\sum_{c\mu}\frac{M^*_{cp,\mu}}{(\epsilon_c-\epsilon_i+\Omega_\nu+\Omega_\mu-4\mathrm{i}\eta)}\left(\sum_j \frac{M_{cj,\nu}M_{ji,\mu}}{(\epsilon_c-\epsilon_j+\Omega_\nu-3\mathrm{i}\eta)}+\sum_a \frac{M_{ca,\nu}M_{ai,\mu}}{(\epsilon_i-\epsilon_a-\Omega_\mu+3\mathrm{i}\eta)}\right)\right] \\
&\qquad \frac{1}{\omega-(\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)} M^*_{qi,\nu} \\
&+\sum_{b\nu}\left[-\sum_{k\mu}\frac{M_{pk,\mu}}{(\epsilon_k-\epsilon_b-\Omega_\nu-\Omega_\mu+4\mathrm{i}\eta)}\left(\sum_i \frac{M^*_{bi,\mu}M^*_{ik,\nu}}{(\epsilon_b-\epsilon_i+\Omega_\mu-3\mathrm{i}\eta)}+\sum_a \frac{M^*_{ba,\mu}M^*_{ak,\nu}}{(\epsilon_k-\epsilon_a-\Omega_\nu+3\mathrm{i}\eta)}\right)\right] \\
&\qquad \frac{1}{\omega-(\epsilon_b+\Omega_\nu-2\mathrm{i}\eta)} M_{bq,\nu}
\end{aligned} \tag{20}
$$

- **The 3h2p poles**

The 3h2p terms can be rearranged as

$$
\begin{aligned}
&+\sum_{ijk\mu\nu\mu'\nu'} M_{pk,\mu'} \frac{1}{\omega-(\epsilon_k-\Omega_{\mu'}+2\mathrm{i}\eta)}\left[M_{ki,\nu}\delta_{\mu\mu'}\right]\frac{1}{\omega-(\epsilon_i-\Omega_\nu-\Omega_\mu+3\mathrm{i}\eta)}\left[M^*_{ji,\mu}\delta_{\nu\nu'}\right]\frac{1}{\omega-(\epsilon_j-\Omega_{\nu'}+2\mathrm{i}\eta)} M^*_{qj,\nu'} \\
&+\sum_{ij\mu\nu\nu'}\left[\sum_c \frac{M_{pc,\mu}M_{ci,\nu}}{(\epsilon_i-\epsilon_c-\Omega_\nu+3\mathrm{i}\eta)}\right]\frac{1}{\omega-(\epsilon_i-\Omega_\nu-\Omega_\mu+3\mathrm{i}\eta)}\left[M^*_{ji,\mu}\delta_{\nu\nu'}\right]\frac{1}{\omega-(\epsilon_j-\Omega_{\nu'}+2\mathrm{i}\eta)} M^*_{qj,\nu'} \\
&+\sum_{ik\mu\nu\mu'} M_{pk,\mu'} \frac{1}{\omega-(\epsilon_k-\Omega_{\mu'}+2\mathrm{i}\eta)}\left[M_{ki,\nu}\delta_{\mu\mu'}\right]\frac{1}{\omega-(\epsilon_i-\Omega_\nu-\Omega_\mu+3\mathrm{i}\eta)}\left[\sum_a \frac{M^*_{ai,\mu}M^*_{qa,\nu}}{(\epsilon_i-\epsilon_a-\Omega_\mu+3\mathrm{i}\eta)}\right] \\
&+\sum_{i\mu\nu}\left[\sum_c \frac{M_{pc,\mu}M_{ci,\nu}}{(\epsilon_i-\epsilon_c-\Omega_\nu+3\mathrm{i}\eta)}\right]\frac{1}{\omega-(\epsilon_i-\Omega_\nu-\Omega_\mu+3\mathrm{i}\eta)}\left[\sum_a \frac{M^*_{ai,\mu}M^*_{qa,\nu}}{(\epsilon_i-\epsilon_a-\Omega_\mu+3\mathrm{i}\eta)}\right]
\end{aligned} \tag{21}
$$

- **The 3p2h poles**

The 3p2h poles can be rearranged as

$$
\begin{aligned}
&+\sum_{abc\mu\nu\mu'\nu'} M^*_{cp,\mu'} \frac{1}{\omega-(\epsilon_c+\Omega_{\mu'}-2i\eta)} \left[M^*_{ac,\nu}\delta_{\mu\mu'}\right] \frac{1}{\omega-(\epsilon_a+\Omega_\nu+\Omega_\mu-3i\eta)} \left[M_{ab,\mu}\delta_{\nu\nu'}\right] \frac{1}{\omega-(\epsilon_b+\Omega_{\nu'}-2i\eta)} M_{bq,\nu'} \\
&+\sum_{ab\mu\nu\nu'} \left[\sum_k \frac{M^*_{kp,\mu}M^*_{ak,\nu}}{(\epsilon_a-\epsilon_k+\Omega_\nu-3i\eta)}\right] \frac{1}{\omega-(\epsilon_a+\Omega_\nu+\Omega_\mu-3i\eta)} \left[M_{ab,\mu}\delta_{\nu\nu'}\right] \frac{1}{\omega-(\epsilon_b+\Omega_{\nu'}-2i\eta)} M_{bq,\nu'} \\
&+\sum_{ac\mu\nu\mu'} M^*_{cp,\mu'} \frac{1}{\omega-(\epsilon_c+\Omega_{\mu'}-2i\eta)} \left[M^*_{ac,\nu}\delta_{\mu\mu'}\right] \frac{1}{\omega-(\epsilon_a+\Omega_\nu+\Omega_\mu-3i\eta)} \left[\sum_i \frac{M_{ai,\mu}M_{iq,\nu}}{(\epsilon_a-\epsilon_i+\Omega_\mu-3i\eta)}\right] \\
&+\sum_{a\mu\nu} \left[\sum_k \frac{M^*_{kp,\mu}M^*_{ak,\nu}}{(\epsilon_a-\epsilon_k+\Omega_\nu-3i\eta)}\right] \frac{1}{\omega-(\epsilon_a+\Omega_\nu+\Omega_\mu-3i\eta)} \left[\sum_i \frac{M_{ai,\mu}M_{iq,\nu}}{(\epsilon_a-\epsilon_i+\Omega_\mu-3i\eta)}\right]
\end{aligned} \tag{22}
$$

4. *Gathering terms: Zero ERI and undressed poles*

In the first term [see Eq. (12)], there is

$$
\begin{aligned}
&-\sum_{ika\mu\nu} \frac{M_{pk,\mu}M^*_{ia,\mu}}{\omega-(\epsilon_k-\Omega_\mu+2i\eta)} \frac{1}{\omega-(\epsilon_i+\epsilon_k-\epsilon_a+3i\eta)} \frac{M_{ka,\nu}M^*_{qi,\nu}}{\omega-(\epsilon_i-\Omega_\nu+2i\eta)} \\
&-\sum_{iac\mu\nu} \frac{M_{pc,\mu}M^*_{ai,\mu}}{\omega-(\epsilon_a+\epsilon_c-\epsilon_i-3i\eta)} \frac{1}{(\epsilon_i-\epsilon_a-\Omega_\mu+3i\eta)} \frac{M^*_{ic,\nu}M_{aq,\nu}}{\omega-(\epsilon_a+\Omega_\nu-2i\eta)} \\
&-\sum_{iac\mu\nu} \frac{M^*_{cp,\mu}M_{ia,\mu}}{\omega-(\epsilon_c+\Omega_\mu-2i\eta)} \frac{1}{\omega-(\epsilon_a+\epsilon_c-\epsilon_i-3i\eta)} \frac{M^*_{ic,\nu}M_{aq,\nu}}{\omega-(\epsilon_a+\Omega_\nu-2i\eta)} \\
&-\sum_{ika\mu\nu} \frac{M^*_{kp,\mu}M_{ai,\mu}}{\omega-(\epsilon_i+\epsilon_k-\epsilon_a+3i\eta)} \frac{1}{(\epsilon_a-\epsilon_i+\Omega_\mu-3i\eta)} \frac{M_{ka,\nu}M^*_{qi,\nu}}{\omega-(\epsilon_i-\Omega_\nu+2i\eta)}
\end{aligned}
$$

and in the third [see Eq. (16)]

$$
\begin{aligned}
&+\sum_{ika\mu\nu} \frac{M_{pk,\mu}M^*_{ia,\mu}}{(\epsilon_k-\Omega_\mu+2i\eta)-\omega} \frac{1}{(\epsilon_i+\epsilon_k-\epsilon_a+3i\eta)-\omega} \frac{M^*_{ak,\nu}M_{iq,\nu}}{(\epsilon_k-\epsilon_a-\Omega_\nu+3i\eta)} \\
&+\sum_{iac\mu\nu} \frac{M^*_{cp,\mu}M_{ia,\mu}}{(\epsilon_c+\Omega_\mu-2i\eta)-\omega} \frac{1}{(\epsilon_a+\epsilon_c-\epsilon_i-3i\eta)-\omega} \frac{M_{ci,\nu}M^*_{qa,\nu}}{(\epsilon_c-\epsilon_i+\Omega_\nu-3i\eta)} \\
&-\sum_{ika} \left[\sum_\mu \frac{M^*_{kp,\mu}M_{ai,\mu}}{(\epsilon_i-\epsilon_a-\Omega_\mu+3i\eta)}\right] \frac{1}{\omega-(\epsilon_i+\epsilon_k-\epsilon_a+3i\eta)} \left[\sum_\nu \frac{M^*_{ak,\nu}M_{iq,\nu}}{(\epsilon_k-\epsilon_a-\Omega_\nu+3i\eta)}\right] \\
&-\sum_{iac} \left[\sum_\mu \frac{M_{pc,\mu}M^*_{ai,\mu}}{(\epsilon_i-\epsilon_a-\Omega_\mu+3i\eta)}\right] \frac{1}{\omega-(\epsilon_a+\epsilon_c-\epsilon_i-3i\eta)} \left[\sum_\nu \frac{M_{ci,\nu}M^*_{qa,\nu}}{(\epsilon_i-\epsilon_c-\Omega_\nu+3i\eta)}\right]
\end{aligned}
$$

The last two terms, corresponding to one 2h1p and one 2p1h contribution, are already expressed in terms of intermediate quantities. The remaining six terms are partitioned into three 2h1p and three 2p1h contributions.

- **The 2h1p poles**

We start with the 2h1p terms. After a first pole decomposition, this gives

$$
\begin{aligned}
&-\frac{1}{2}\sum_{ika\mu\nu} \frac{M_{pk,\mu}M^*_{ia,\mu}M_{ka,\nu}M^*_{qi,\nu}}{\omega-(\epsilon_k-\Omega_\mu+2i\eta)} \frac{1}{(\epsilon_i+\epsilon_k-\epsilon_a+3i\eta)-(\epsilon_i-\Omega_\nu+2i\eta)} \left[\frac{1}{\omega-(\epsilon_i+\epsilon_k-\epsilon_a+3i\eta)} - \frac{1}{\omega-(\epsilon_i-\Omega_\nu+2i\eta)}\right] \\
&-\frac{1}{2}\sum_{ika\mu\nu} \frac{M_{pk,\mu}M^*_{ia,\mu}M_{ka,\nu}M^*_{qi,\nu}}{\omega-(\epsilon_i-\Omega_\nu+2i\eta)} \frac{1}{(\epsilon_i+\epsilon_k-\epsilon_a+3i\eta)-(\epsilon_k-\Omega_\mu+2i\eta)} \left[\frac{1}{\omega-(\epsilon_i+\epsilon_k-\epsilon_a+3i\eta)} - \frac{1}{\omega-(\epsilon_k-\Omega_\mu+2i\eta)}\right]
\end{aligned}
$$

$$
+\sum_{ika\mu\nu}\frac{M^*_{kp,\mu}M_{ai,\mu}M_{ka,\nu}M^*_{qi,\nu}}{(\epsilon_i-\epsilon_a-\Omega_\mu+3\mathrm{i}\eta)}\frac{1}{(\epsilon_i+\epsilon_k-\epsilon_a+3\mathrm{i}\eta)-(\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)}\left[\frac{1}{\omega-(\epsilon_i+\epsilon_k-\epsilon_a+3\mathrm{i}\eta)}-\frac{1}{\omega-(\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)}\right]
$$

$$
+\sum_{ika\mu\nu}\frac{M_{pk,\mu}M^*_{ia,\mu}M^*_{ak,\nu}M_{iq,\nu}}{(\epsilon_k-\epsilon_a-\Omega_\nu+3\mathrm{i}\eta)}\frac{1}{(\epsilon_i+\epsilon_k-\epsilon_a+3\mathrm{i}\eta)-(\epsilon_k-\Omega_\mu+2\mathrm{i}\eta)}\left[\frac{1}{\omega-(\epsilon_i+\epsilon_k-\epsilon_a+3\mathrm{i}\eta)}-\frac{1}{\omega-(\epsilon_k-\Omega_\mu+2\mathrm{i}\eta)}\right]
$$

$$
-\sum_{ika}\left[\sum_\mu\frac{M^*_{kp,\mu}M_{ai,\mu}}{(\epsilon_i-\epsilon_a-\Omega_\mu+3\mathrm{i}\eta)}\right]\frac{1}{\omega-(\epsilon_i+\epsilon_k-\epsilon_a+3\mathrm{i}\eta)}\left[\sum_\nu\frac{M^*_{ak,\nu}M_{iq,\nu}}{(\epsilon_k-\epsilon_a-\Omega_\nu+3\mathrm{i}\eta)}\right]
$$

and this can be rewritten as

$$
+\sum_{ika\mu\nu}M_{pk,\mu}\frac{1}{\omega-(\epsilon_k-\Omega_\mu+2\mathrm{i}\eta)}\left[\frac{1}{2}\sum_a\frac{M^*_{ia,\mu}M_{ka,\nu}}{(\epsilon_k-\epsilon_a+\Omega_\nu+\mathrm{i}\eta)}+\frac{1}{2}\sum_a\frac{M^*_{ia,\mu}M_{ka,\nu}}{(\epsilon_i-\epsilon_a+\Omega_\mu+\mathrm{i}\eta)}\right]\frac{1}{\omega-(\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)}M^*_{qi,\nu}
$$

$$
-\frac{1}{2}\sum_{ika\mu\nu}\frac{M_{pk,\mu}M^*_{ia,\mu}M_{ka,\nu}M^*_{qi,\nu}}{(\epsilon_k-\epsilon_a+\Omega_\nu+\mathrm{i}\eta)}\frac{1}{\omega-(\epsilon_i+\epsilon_k-\epsilon_a+3\mathrm{i}\eta)}\frac{1}{\omega-(\epsilon_k-\Omega_\mu+2\mathrm{i}\eta)}
$$

$$
-\frac{1}{2}\sum_{ika\mu\nu}\frac{M_{pk,\mu}M^*_{ia,\mu}M_{ka,\nu}M^*_{qi,\nu}}{(\epsilon_i-\epsilon_a+\Omega_\mu+\mathrm{i}\eta)}\frac{1}{\omega-(\epsilon_i+\epsilon_k-\epsilon_a+3\mathrm{i}\eta)}\frac{1}{\omega-(\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)}
$$

$$
+\sum_{i\nu}\left[-\sum_{ka\mu}\frac{M^*_{kp,\mu}M_{ai,\mu}M_{ka,\nu}}{(\epsilon_i-\epsilon_a-\Omega_\mu+3\mathrm{i}\eta)(\epsilon_k-\epsilon_a+\Omega_\nu+\mathrm{i}\eta)}\right]\frac{1}{\omega-(\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)}M^*_{qi,\nu}
$$

$$
+\sum_{k\mu}M_{pk,\mu}\frac{1}{\omega-(\epsilon_k-\Omega_\mu+2\mathrm{i}\eta)}\left[-\sum_{ia\nu}\frac{M^*_{ia,\mu}M^*_{ak,\nu}M_{iq,\nu}}{(\epsilon_k-\epsilon_a-\Omega_\nu+3\mathrm{i}\eta)(\epsilon_i-\epsilon_a+\Omega_\mu+\mathrm{i}\eta)}\right]
$$

$$
+\sum_{ika}\left[\sum_\mu\frac{M^*_{kp,\mu}M_{ai,\mu}}{(\epsilon_i-\epsilon_a-\Omega_\mu+3\mathrm{i}\eta)}\right]\frac{1}{\omega-(\epsilon_i+\epsilon_k-\epsilon_a+3\mathrm{i}\eta)}\left[\sum_\nu\frac{M_{ka,\nu}M^*_{qi,\nu}}{(\epsilon_k-\epsilon_a+\Omega_\nu+\mathrm{i}\eta)}\right]
$$

$$
+\sum_{ika}\left[\sum_\mu\frac{M_{pk,\mu}M^*_{ia,\mu}}{(\epsilon_i-\epsilon_a+\Omega_\mu+\mathrm{i}\eta)}\right]\frac{1}{\omega-(\epsilon_i+\epsilon_k-\epsilon_a+3\mathrm{i}\eta)}\left[\sum_\nu\frac{M^*_{ak,\nu}M_{iq,\nu}}{(\epsilon_k-\epsilon_a-\Omega_\nu+3\mathrm{i}\eta)}\right]
$$

$$
-\sum_{ika}\left[\sum_\mu\frac{M^*_{kp,\mu}M_{ai,\mu}}{(\epsilon_i-\epsilon_a-\Omega_\mu+3\mathrm{i}\eta)}\right]\frac{1}{\omega-(\epsilon_i+\epsilon_k-\epsilon_a+3\mathrm{i}\eta)}\left[\sum_\nu\frac{M^*_{ak,\nu}M_{iq,\nu}}{(\epsilon_k-\epsilon_a-\Omega_\nu+3\mathrm{i}\eta)}\right]
$$

There are two terms that needs to be further decomposed and this finally yields

$$
\begin{aligned}
&+\sum_{ika\mu\nu} M_{pk,\mu}\frac{1}{\omega-(\epsilon_k-\Omega_\mu+2\mathrm{i}\eta)}\left[\frac{1}{2}\sum_a\frac{M^*_{ia,\mu}M_{ka,\nu}}{(\epsilon_k-\epsilon_a+\Omega_\nu+\mathrm{i}\eta)}+\frac{1}{2}\sum_a\frac{M^*_{ia,\mu}M_{ka,\nu}}{(\epsilon_i-\epsilon_a+\Omega_\mu+\mathrm{i}\eta)}\right]\frac{1}{\omega-(\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)}M^*_{qi,\nu}\\
&+\sum_{k\mu} M_{pk,\mu}\frac{1}{\omega-(\epsilon_k-\Omega_\mu+2\mathrm{i}\eta)}\left[-\sum_{ia\nu}\frac{M^*_{ia,\mu}M^*_{ak,\nu}M_{iq,\nu}}{(\epsilon_k-\epsilon_a-\Omega_\nu+3\mathrm{i}\eta)(\epsilon_i-\epsilon_a+\Omega_\mu+\mathrm{i}\eta)}\right]\\
&\qquad+\sum_{i\nu}\left[-\sum_{ka\mu}\frac{M^*_{kp,\mu}M_{ai,\mu}M_{ka,\nu}}{(\epsilon_i-\epsilon_a-\Omega_\mu+3\mathrm{i}\eta)(\epsilon_k-\epsilon_a+\Omega_\nu+\mathrm{i}\eta)}\right]\frac{1}{\omega-(\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)}M^*_{qi,\nu}\\
&+\sum_{k\mu} M_{pk,\mu}\frac{1}{\omega-(\epsilon_k-\Omega_\mu+2\mathrm{i}\eta)}\left[\frac{1}{2}\sum_{ia\nu}\frac{M^*_{ia,\mu}M_{ka,\nu}M^*_{qi,\nu}}{(\epsilon_k-\epsilon_a+\Omega_\nu+\mathrm{i}\eta)}\frac{1}{(\epsilon_i-\epsilon_a+\Omega_\mu+\mathrm{i}\eta)}\right]\\
&\qquad+\sum_{i\nu}\left[\frac{1}{2}\sum_{ka\mu}\frac{M_{pk,\mu}M^*_{ia,\mu}M_{ka,\nu}}{(\epsilon_i-\epsilon_a+\Omega_\mu+\mathrm{i}\eta)(\epsilon_k-\epsilon_a+\Omega_\nu+\mathrm{i}\eta)}\right]\frac{1}{\omega-(\epsilon_i-\Omega_\nu+2\mathrm{i}\eta)}M^*_{qi,\nu}\\
&+\sum_{ika}\left[\sum_\mu\frac{M_{pk,\mu}M^*_{ia,\mu}}{(\epsilon_i-\epsilon_a+\Omega_\mu+\mathrm{i}\eta)}-\sum_\mu\frac{M^*_{kp,\mu}M_{ai,\mu}}{(\epsilon_i-\epsilon_a-\Omega_\mu+3\mathrm{i}\eta)}\right]\\
&\qquad\frac{1}{\omega-(\epsilon_i+\epsilon_k-\epsilon_a+3\mathrm{i}\eta)}\left[\sum_\nu\frac{M^*_{ak,\nu}M_{iq,\nu}}{(\epsilon_k-\epsilon_a-\Omega_\nu+3\mathrm{i}\eta)}-\sum_\nu\frac{M_{ka,\nu}M^*_{qi,\nu}}{(\epsilon_k-\epsilon_a+\Omega_\nu+\mathrm{i}\eta)}\right]
\end{aligned}
\tag{23}
$$

- **The 2p1h poles**

The 2h1p terms are dealt with similarly. The first pole decomposition yields

$$
\begin{aligned}
&-\frac{1}{2}\sum_{iac\mu\nu}\frac{M^*_{cp,\mu}M_{ia,\mu}M^*_{ic,\nu}M_{aq,\nu}}{\omega-(\epsilon_c+\Omega_\mu-2\mathrm{i}\eta)}\frac{1}{(\epsilon_a+\epsilon_c-\epsilon_i-3\mathrm{i}\eta)-(\epsilon_a+\Omega_\nu-2\mathrm{i}\eta)}\left[\frac{1}{\omega-(\epsilon_a+\epsilon_c-\epsilon_i-3\mathrm{i}\eta)}-\frac{1}{\omega-(\epsilon_a+\Omega_\nu-2\mathrm{i}\eta)}\right]\\
&-\frac{1}{2}\sum_{iac\mu\nu}\frac{M^*_{cp,\mu}M_{ia,\mu}M^*_{ic,\nu}M_{aq,\nu}}{\omega-(\epsilon_a+\Omega_\nu-2\mathrm{i}\eta)}\frac{1}{(\epsilon_a+\epsilon_c-\epsilon_i-3\mathrm{i}\eta)-(\epsilon_c+\Omega_\mu-2\mathrm{i}\eta)}\left[\frac{1}{\omega-(\epsilon_a+\epsilon_c-\epsilon_i-3\mathrm{i}\eta)}-\frac{1}{\omega-(\epsilon_c+\Omega_\mu-2\mathrm{i}\eta)}\right]\\
&-\sum_{iac\mu\nu}\frac{M_{pc,\mu}M^*_{ai,\mu}M^*_{ic,\nu}M_{aq,\nu}}{(\epsilon_i-\epsilon_a-\Omega_\mu+3\mathrm{i}\eta)}\frac{1}{(\epsilon_a+\epsilon_c-\epsilon_i-3\mathrm{i}\eta)-(\epsilon_a+\Omega_\nu-2\mathrm{i}\eta)}\left[\frac{1}{\omega-(\epsilon_a+\epsilon_c-\epsilon_i-3\mathrm{i}\eta)}-\frac{1}{\omega-(\epsilon_a+\Omega_\nu-2\mathrm{i}\eta)}\right]\\
&+\sum_{iac\mu\nu}\frac{M^*_{cp,\mu}M_{ia,\mu}M_{ci,\nu}M^*_{qa,\nu}}{(\epsilon_c-\epsilon_i+\Omega_\nu-3\mathrm{i}\eta)}\frac{1}{(\epsilon_a+\epsilon_c-\epsilon_i-3\mathrm{i}\eta)-(\epsilon_c+\Omega_\mu-2\mathrm{i}\eta)}\left[\frac{1}{\omega-(\epsilon_a+\epsilon_c-\epsilon_i-3\mathrm{i}\eta)}-\frac{1}{\omega-(\epsilon_c+\Omega_\mu-2\mathrm{i}\eta)}\right]\\
&-\sum_{iac}\left[\sum_\mu\frac{M_{pc,\mu}M^*_{ai,\mu}}{(\epsilon_i-\epsilon_a-\Omega_\mu+3\mathrm{i}\eta)}\right]\frac{1}{\omega-(\epsilon_a+\epsilon_c-\epsilon_i-3\mathrm{i}\eta)}\left[\sum_\nu\frac{M_{ci,\nu}M^*_{qa,\nu}}{(\epsilon_i-\epsilon_c-\Omega_\nu+3\mathrm{i}\eta)}\right]
\end{aligned}
$$

and this can be rewritten as

$$
\begin{aligned}
&+\sum_{ac\mu\nu}M^*_{cp,\mu}\frac{1}{\omega-(\epsilon_c+\Omega_\mu-2\mathrm{i}\eta)}\left[\frac{1}{2}\sum_i\frac{M_{ia,\mu}M^*_{ic,\nu}}{(\epsilon_c-\epsilon_i-\Omega_\nu-\mathrm{i}\eta)}+\frac{1}{2}\sum_i\frac{M_{ia,\mu}M^*_{ic,\nu}}{(\epsilon_a-\epsilon_i-\Omega_\mu-\mathrm{i}\eta)}\right]\frac{1}{\omega-(\epsilon_a+\Omega_\nu-2\mathrm{i}\eta)}M_{aq,\nu}\\
&-\frac{1}{2}\sum_{iac\mu\nu}\frac{M^*_{cp,\mu}M_{ia,\mu}M^*_{ic,\nu}M_{aq,\nu}}{(\epsilon_c-\epsilon_i-\Omega_\nu-\mathrm{i}\eta)}\frac{1}{\omega-(\epsilon_a+\epsilon_c-\epsilon_i-3\mathrm{i}\eta)}\frac{1}{\omega-(\epsilon_c+\Omega_\mu-2\mathrm{i}\eta)}\\
&-\frac{1}{2}\sum_{iac\mu\nu}\frac{M^*_{cp,\mu}M_{ia,\mu}M^*_{ic,\nu}M_{aq,\nu}}{(\epsilon_a-\epsilon_i-\Omega_\mu-\mathrm{i}\eta)}\frac{1}{\omega-(\epsilon_a+\epsilon_c-\epsilon_i-3\mathrm{i}\eta)}\frac{1}{\omega-(\epsilon_a+\Omega_\nu-2\mathrm{i}\eta)}\\
&+\sum_{a\nu}\left[\sum_{ic\mu}\frac{M_{pc,\mu}M^*_{ai,\mu}M^*_{ic,\nu}}{(\epsilon_i-\epsilon_a-\Omega_\mu+3\mathrm{i}\eta)(\epsilon_c-\epsilon_i-\Omega_\nu-\mathrm{i}\eta)}\right]\frac{1}{\omega-(\epsilon_a+\Omega_\nu-2\mathrm{i}\eta)}M_{aq,\nu}
\end{aligned}
$$

$$+\sum_{c\mu} M^*_{cp,\mu} \frac{1}{\omega - (\epsilon_c + \Omega_\mu - 2\mathrm{i}\eta)} \left[\sum_{ia\nu} \frac{M_{ia,\mu} M_{ci,\nu} M^*_{qa,\nu}}{(\epsilon_i - \epsilon_c - \Omega_\nu + 3\mathrm{i}\eta)(\epsilon_a - \epsilon_i - \Omega_\mu - \mathrm{i}\eta)} \right]$$
$$+\sum_{iac\mu\nu} \left[\sum_{\mu} \frac{M_{pc,\mu} M^*_{ai,\mu}}{(\epsilon_i - \epsilon_a - \Omega_\mu + 3\mathrm{i}\eta)} \right] \frac{1}{\omega - (\epsilon_a + \epsilon_c - \epsilon_i - 3\mathrm{i}\eta)} \left[\sum_{\nu} \frac{M^*_{ic,\nu} M_{aq,\nu}}{(\epsilon_i - \epsilon_c + \Omega_\nu + \mathrm{i}\eta)} \right]$$
$$+\sum_{iac\mu\nu} \left[\sum_{\mu} \frac{M^*_{cp,\mu} M_{ia,\mu}}{(\epsilon_i - \epsilon_a + \Omega_\mu + \mathrm{i}\eta)} \right] \frac{1}{\omega - (\epsilon_a + \epsilon_c - \epsilon_i - 3\mathrm{i}\eta)} \left[\sum_{\nu} \frac{M_{ci,\nu} M^*_{qa,\nu}}{(\epsilon_i - \epsilon_c - \Omega_\nu + 3\mathrm{i}\eta)} \right]$$
$$-\sum_{iac} \left[\sum_{\mu} \frac{M_{pc,\mu} M^*_{ai,\mu}}{(\epsilon_i - \epsilon_a - \Omega_\mu + 3\mathrm{i}\eta)} \right] \frac{1}{\omega - (\epsilon_a + \epsilon_c - \epsilon_i - 3\mathrm{i}\eta)} \left[\sum_{\nu} \frac{M_{ci,\nu} M^*_{qa,\nu}}{(\epsilon_i - \epsilon_c - \Omega_\nu + 3\mathrm{i}\eta)} \right]$$

There are two terms that needs to be further decomposed and this finally yields

$$\begin{aligned}
&+\sum_{ac\mu\nu} M^*_{cp,\mu} \frac{1}{\omega - (\epsilon_c + \Omega_\mu - 2\mathrm{i}\eta)} \left[\frac{1}{2} \sum_{i} \frac{M_{ia,\mu} M^*_{ic,\nu}}{(\epsilon_c - \epsilon_i - \Omega_\nu - \mathrm{i}\eta)} + \frac{1}{2} \sum_{i} \frac{M_{ia,\mu} M^*_{ic,\nu}}{(\epsilon_a - \epsilon_i - \Omega_\mu - \mathrm{i}\eta)} \right] \frac{1}{\omega - (\epsilon_a + \Omega_\nu - 2\mathrm{i}\eta)} M_{aq,\nu} \\
&+\sum_{c\mu} M^*_{cp,\mu} \frac{1}{\omega - (\epsilon_c + \Omega_\mu - 2\mathrm{i}\eta)} \left[\sum_{ia\nu} \frac{M_{ia,\mu} M_{ci,\nu} M^*_{qa,\nu}}{(\epsilon_i - \epsilon_c - \Omega_\nu + 3\mathrm{i}\eta)(\epsilon_a - \epsilon_i - \Omega_\mu - \mathrm{i}\eta)} \right] \\
&\qquad + \sum_{a\nu} \left[\sum_{ic\mu} \frac{M_{pc,\mu} M^*_{ai,\mu} M^*_{ic,\nu}}{(\epsilon_i - \epsilon_a - \Omega_\mu + 3\mathrm{i}\eta)(\epsilon_c - \epsilon_i - \Omega_\nu - \mathrm{i}\eta)} \right] \frac{1}{\omega - (\epsilon_a + \Omega_\nu - 2\mathrm{i}\eta)} M_{aq,\nu} \\
&+\sum_{c\mu} M^*_{cp,\mu} \frac{1}{\omega - (\epsilon_c + \Omega_\mu - 2\mathrm{i}\eta)} \left[\frac{1}{2} \sum_{ia\nu} \frac{M_{ia,\mu} M^*_{ic,\nu} M_{aq,\nu}}{(\epsilon_c - \epsilon_i - \Omega_\nu - \mathrm{i}\eta)} \frac{1}{(\epsilon_a - \epsilon_i - \Omega_\mu - \mathrm{i}\eta)} \right] \\
&\qquad + \sum_{a\nu} \left[\frac{1}{2} \sum_{ic\mu} \frac{M^*_{cp,\mu} M_{ia,\mu} M^*_{ic,\nu}}{(\epsilon_a - \epsilon_i - \Omega_\mu - \mathrm{i}\eta)(\epsilon_c - \epsilon_i - \Omega_\nu - \mathrm{i}\eta)} \right] \frac{1}{\omega - (\epsilon_a + \Omega_\nu - 2\mathrm{i}\eta)} M_{aq,\nu} \\
&-\sum_{iac} \left[\sum_{\mu} \frac{M_{pc,\mu} M^*_{ai,\mu}}{(\epsilon_i - \epsilon_a - \Omega_\mu + 3\mathrm{i}\eta)} - \sum_{\mu} \frac{M^*_{cp,\mu} M_{ia,\mu}}{(\epsilon_i - \epsilon_a + \Omega_\mu + \mathrm{i}\eta)} \right] \\
&\qquad \frac{1}{\omega - (\epsilon_a + \epsilon_c - \epsilon_i - 3\mathrm{i}\eta)} \left[\sum_{\nu} \frac{M_{ci,\nu} M^*_{qa,\nu}}{(\epsilon_i - \epsilon_c - \Omega_\nu + 3\mathrm{i}\eta)} - \sum_{\nu} \frac{M^*_{ic,\nu} M_{aq,\nu}}{(\epsilon_i - \epsilon_c + \Omega_\nu + \mathrm{i}\eta)} \right]
\end{aligned} \tag{24}$$

This last term, and its 2h1p analog of the previous subsection, can also be simplified using Bruneval's relation [see Eq. (5)].

III. THE ADC-$G3W2$ ELEMENTS

The lesser and greater (correlation part of the) $G3W2$ self-energy [see Eq. (6)] can each be written as

$$\begin{aligned}
\boldsymbol{\Sigma}^{\pm}(\omega) = &\left[\boldsymbol{U}_1^{\pm,(1)}\right]^\dagger \cdot \left(\boldsymbol{\omega} - \boldsymbol{K}_1^{\pm}\right)^{-1} \cdot \boldsymbol{U}_1^{\pm,(1)} \\
&+ \left[\boldsymbol{U}_1^{\pm,(2)}\right]^\dagger \cdot \left(\boldsymbol{\omega} - \boldsymbol{K}_1^{\pm}\right)^{-1} \cdot \boldsymbol{U}_1^{\pm,(1)} + \left[\boldsymbol{U}_1^{\pm,(1)}\right]^\dagger \cdot \left(\boldsymbol{\omega} - \boldsymbol{K}_1^{\pm}\right)^{-1} \cdot \boldsymbol{U}_1^{\pm,(2)} \\
&+ \left[\boldsymbol{U}_1^{\pm,(3)}\right]^\dagger \cdot \left(\boldsymbol{\omega} - \boldsymbol{K}_1^{\pm}\right)^{-1} \cdot \boldsymbol{U}_1^{\pm,(1)} + \left[\boldsymbol{U}_1^{\pm,(1)}\right]^\dagger \cdot \left(\boldsymbol{\omega} - \boldsymbol{K}_1^{\pm}\right)^{-1} \cdot \boldsymbol{U}_1^{\pm,(3)} \\
&+ \left[\boldsymbol{U}_1^{\pm,(1)}\right]^\dagger \cdot \left(\boldsymbol{\omega} - \boldsymbol{K}_1^{\pm}\right)^{-1} \cdot \boldsymbol{C}_1^{\pm} \cdot \left(\boldsymbol{\omega} - \boldsymbol{K}_1^{\pm}\right)^{-1} \cdot \boldsymbol{U}_1^{\pm,(1)} \\
&+ \left[\boldsymbol{U}_2^{\pm,(1)} + \boldsymbol{C}_{2/1}^{\pm} \cdot \left(\boldsymbol{\omega} - \boldsymbol{K}_1^{\pm}\right)^{-1} \cdot \boldsymbol{U}_1^{\pm,(1)}\right]^\dagger \cdot \left(\boldsymbol{\omega} - \boldsymbol{K}_2^{\pm}\right)^{-1} \cdot \left[\boldsymbol{U}_2^{\pm,(1)} + \boldsymbol{C}_{2/1}^{\pm} \cdot \left(\boldsymbol{\omega} - \boldsymbol{K}_1^{\pm}\right)^{-1} \cdot \boldsymbol{U}_1^{\pm,(1)}\right]
\end{aligned} \tag{25}$$

The definition of each intermediate quantity will be given in the following subsections.

A. 2h1p and 2p1h diagonal matrices

$$\left(\boldsymbol{K}_1^{-}\right)_{i\nu,j\mu} = (\epsilon_i - \Omega_\nu)\delta_{ij}\delta_{\nu\mu} \tag{26a}$$
$$\left(\boldsymbol{K}_1^{+}\right)_{a\nu,b\mu} = (\epsilon_a + \Omega_\nu)\delta_{ab}\delta_{\nu\mu} \tag{26b}$$

B. First contribution to the 2h1p and 2p1h coupling block

$$\left(\boldsymbol{U}_1^{-,(1)}\right)_{i\nu,q} = M^*_{qi,\nu} \tag{27a}$$
$$\left(\boldsymbol{U}_1^{+,(1)}\right)_{a\nu,q} = M_{aq,\nu} \tag{27b}$$

C. Second contribution to the 2h1p and 2p1h coupling block

$$\left(\boldsymbol{U}_1^{-,(2)}\right)_{i\nu,q} = \sum_{jb} \frac{M^*_{bj,\nu}\,\langle ib|jq\rangle}{(\epsilon_b-\epsilon_j)+\Omega_\nu} + \sum_{jb} \frac{M^*_{jb,\nu}\,\langle ij|bq\rangle}{(\epsilon_b-\epsilon_j)-\Omega_\nu} \tag{28a}$$
$$\left(\boldsymbol{U}_1^{+,(2)}\right)_{a\nu,q} = \sum_{jb} \frac{M_{bj,\nu}\,\langle aj|bq\rangle}{(\epsilon_b-\epsilon_j)+\Omega_\nu} + \sum_{jb} \frac{M_{jb,\nu}\,\langle ab|jq\rangle}{(\epsilon_b-\epsilon_j)-\Omega_\nu} \tag{28b}$$

D. Third contribution to the 2h1p and 2p1h coupling block

$$\begin{aligned}\left(\boldsymbol{U}_1^{-,(3)}\right)_{i\nu,q} = &-\sum_{ja\mu} \frac{M^*_{ja,\nu}M^*_{ai,\mu}M_{jq,\mu}}{[(\epsilon_a-\epsilon_j)-\Omega_\nu][(\epsilon_a-\epsilon_i)+\Omega_\mu]} + \frac{1}{2}\sum_{ja\mu} \frac{M^*_{ja,\nu}M_{ia,\mu}M^*_{qj,\mu}}{[(\epsilon_a-\epsilon_j)-\Omega_\nu][(\epsilon_a-\epsilon_i)-\Omega_\mu]} \\ &-\sum_{ja\mu} \frac{M^*_{ji,\mu}M^*_{aj,\nu}M_{aq,\mu}}{[(\epsilon_a-\epsilon_i)+\Omega_\nu+\Omega_\mu][(\epsilon_a-\epsilon_j)+\Omega_\nu]} + \sum_{ab\mu} \frac{M^*_{ai,\mu}M^*_{ba,\nu}M_{bq,\mu}}{[(\epsilon_b-\epsilon_i)+\Omega_\nu+\Omega_\mu][(\epsilon_a-\epsilon_i)+\Omega_\mu]}\end{aligned} \tag{29a}$$
$$\begin{aligned}\left(\boldsymbol{U}_1^{+,(3)}\right)_{a\nu,q} = &-\sum_{ib\mu} \frac{M_{ib,\nu}M_{ai,\mu}M^*_{qb,\mu}}{[(\epsilon_b-\epsilon_i)-\Omega_\nu][(\epsilon_a-\epsilon_i)+\Omega_\mu]} + \frac{1}{2}\sum_{ib\mu} \frac{M_{ib,\nu}M^*_{ia,\mu}M_{bq,\mu}}{[(\epsilon_b-\epsilon_i)-\Omega_\nu][(\epsilon_a-\epsilon_i)-\Omega_\mu]} \\ &-\sum_{ib\mu} \frac{M_{ab,\mu}M_{bi,\nu}M^*_{qi,\mu}}{[(\epsilon_a-\epsilon_i)+\Omega_\nu+\Omega_\mu][(\epsilon_b-\epsilon_i)+\Omega_\nu]} + \sum_{ij\mu} \frac{M_{aj,\mu}M_{ji,\nu}M^*_{qi,\mu}}{[(\epsilon_a-\epsilon_i)+\Omega_\nu+\Omega_\mu][(\epsilon_a-\epsilon_j)+\Omega_\mu]}\end{aligned} \tag{29b}$$

E. First contribution to the diagonal 2h1p and 2p1h C block

$$\left(\boldsymbol{C}_1^{-,(1)}\right)_{i\nu,j\mu} = \frac{1}{2}\sum_{c} \frac{M_{ic,\mu}M^*_{jc,\nu}}{\epsilon_i-(\epsilon_c-\Omega_\mu)} + \frac{1}{2}\sum_{c} \frac{M_{ic,\mu}M^*_{jc,\nu}}{\epsilon_j-(\epsilon_c-\Omega_\nu)} \tag{30a}$$
$$\left(\boldsymbol{C}_1^{+,(1)}\right)_{a\nu,b\mu} = \frac{1}{2}\sum_{k} \frac{M^*_{ka,\mu}M_{kb,\nu}}{\epsilon_a-(\epsilon_k+\Omega_\mu)} + \frac{1}{2}\sum_{k} \frac{M^*_{ka,\mu}M_{kb,\nu}}{\epsilon_b-(\epsilon_k+\Omega_\nu)} \tag{30b}$$

F. 3h2p and 3p2h diagonal matrices

$$\left(\boldsymbol{K}_2^{-}\right)_{i\nu\mu,j\lambda\sigma} = (\epsilon_i - \Omega_\nu - \Omega_\mu)\delta_{ij}\delta_{\nu\lambda}\delta_{\mu\sigma} \tag{31a}$$

$$\left(\boldsymbol{K}_2^{+}\right)_{a\nu\mu,b\lambda\sigma} = (\epsilon_a + \Omega_\nu + \Omega_\mu)\delta_{ab}\delta_{\nu\lambda}\delta_{\mu\sigma} \tag{31b}$$

G. First contribution to the 3h2p and 3p2h coupling block

$$\left(\boldsymbol{U}_2^{-,(1)}\right)_{i\nu\mu,q} = -\sum_a \frac{M_{ai,\mu}^* M_{qa,\nu}^*}{(\epsilon_a - \epsilon_i) + \Omega_\mu} \tag{32a}$$

$$\left(\boldsymbol{U}_2^{+,(1)}\right)_{a\nu\mu,q} = +\sum_i \frac{M_{ai,\mu} M_{iq,\nu}}{(\epsilon_a - \epsilon_i) + \Omega_\mu} \tag{32b}$$

H. First contribution to the off-diagonal 2h1p-3h2p and 2p1h-3p2h C coupling blocks

$$\left(\boldsymbol{C}_{2/1}^{-,(1)}\right)_{i\nu\mu,j\lambda} = M_{ji,\mu}^* \delta_{\nu\nu'} \tag{33a}$$

$$\left(\boldsymbol{C}_{2/1}^{+,(1)}\right)_{a\nu\mu,b\lambda} = M_{ab,\mu} \delta_{\nu\nu'} \tag{33b}$$

IV. RESULTS

Figure 1 compares the error distributions of the Dyson and non-Dyson ADC(2) and ADC(3) schemes relative to the TBEs, highlighting the effect of the Dyson treatment. Table I presents the IPs computed within the diagonal approximation for the various GW-based approaches, while Table II reports the corresponding results obtained without the diagonal approximation together with Dyson ADC(2) and ADC(3) reference calculations. Mean absolute errors (MAEs) and mean signed errors (MSEs) are provided at the bottom of each table to facilitate the comparison of the different methods.

[1] F. Bruneval, A. Förster, and Y. Pavlyukh, "GW+2SOSEX self-energy made positive semidefinite," J. Chem. Theory Comput. **21**, 10223–10240 (2025).

[2] F. Bruneval and A. Förster, "Fully dynamic $G3W2$ self-energy for finite systems: Formulas and benchmark," J. Chem. Theory Comput. **20**, 3218–3230 (2024).

[3] A. Marie, A. Ammar, and P.-F. Loos, "The GW approximation: A quantum chemistry perspective," in *Advances in Quantum Chemistry*, Novel Treatments of Strong Correlations, Vol. 90 (2024) pp. 157–184.

TABLE I. Inner- and outer-valence IPs (in eV) in the aug-cc-pVDZ basis set computed at various levels of theory. All calculations are performed within the diagonal approximation.

System	State	TBE	GW	2SOSEX	2SOSEX-psd	$G3W2$	ADC-$G3W2$
Ar	$1\ ^2\mathrm{P}/(3p)^{-1}$	15.529	15.458	15.788	15.841	15.785	15.767
	$1\ ^2\mathrm{S}/(3s)^{-1}$	29.449	30.759	31.048	33.280	31.513	31.433
BeO	$1\ ^2\Pi/(1\pi)^{-1}$	9.962	9.489	9.630	9.723	9.786	9.754
	$1\ ^2\Sigma^+/(4\sigma)^{-1}$	11.103	10.798	10.987	10.709	11.076	10.990
BF	$1\ ^2\Sigma^+/(5\sigma)^{-1}$	11.054	11.117	11.450	11.218	11.414	11.427
	$2\ ^2\Pi/(1\pi)^{-1}$	18.581	18.456	18.730	18.856	18.821	18.746
	$2\ ^2\Sigma^+/(4\sigma)^{-1}$	20.913	21.402	21.697	21.464	21.739	21.639
BH_3	$1\ ^2\mathrm{E}'/(1e')^{-1}$	13.194	13.395	13.625	13.381	13.588	13.578
	$1\ ^2\mathrm{A}_1'/(2a_1')^{-1}$	18.238	18.470	18.870	18.999	18.861	18.839
BN	$1\ ^2\Pi/(1\pi)^{-1}$	11.875	11.447	11.814	11.453	11.783	11.811
	$1\ ^2\Sigma^+/(4\sigma)^{-1}$	13.660	13.171	13.449	13.239	13.555	13.578
C_2	$1\ ^2\Pi_u/(2\pi_u)^{-1}$	12.323	12.613	13.127	12.737	13.013	13.031
CH_2O	$1\ ^2\mathrm{B}_2/(2b_2)^{-1}$	10.739	10.996	11.183	10.863	11.172	11.158
	$1\ ^2\mathrm{B}_1/(1b_1)^{-1}$	14.502	14.283	14.640	14.402	14.626	14.624
	$1\ ^2\mathrm{A}_1/(5a_1)^{-1}$	16.032	16.292	16.589	16.258	16.538	16.513
	$2\ ^2\mathrm{B}_2/(1b_2)^{-1}$	17.002	17.714	17.979	17.763	17.964	17.935
CH_4	$1\ ^2\mathrm{T}_2/(1t_2)^{-1}$	14.285	14.466	14.724	14.432	14.666	14.670
	$1\ ^2\mathrm{A}_1/(2a_1)^{-1}$	23.056	23.626	24.098	24.874	24.165	24.150
CO	$1\ ^2\Sigma^+/(5\sigma)^{-1}$	13.752	14.467	14.763	14.662	14.757	14.759
	$1\ ^2\Pi/(1\pi)^{-1}$	16.845	16.762	17.087	17.073	17.123	17.114
	$2\ ^2\Sigma^+/(4\sigma)^{-1}$	19.550	20.045	20.347	20.245	20.364	20.331
CO_2	$1\ ^2\Pi_g/(1\pi_g)^{-1}$	13.567	13.837	14.077	14.040	14.130	14.122
	$1\ ^2\Pi_u/(1\pi_u)^{-1}$	17.391	18.209	18.464	18.597	18.555	18.526
	$1\ ^2\Sigma_u^+/(3\sigma_u)^{-1}$	17.889	18.474	18.774	18.577	18.757	18.733
	$1\ ^2\Sigma_g^+/(4\sigma_g)^{-1}$	19.137	19.856	20.182	20.061	20.181	20.147
CS	$1\ ^2\Sigma^+/(7\sigma)^{-1}$	11.151	12.119	12.393	12.171	12.368	12.367
	$1\ ^2\Pi/(2\pi)^{-1}$	12.768	12.679	13.043	12.904	13.016	13.018
	$2\ ^2\Sigma^+/(6\sigma)^{-1}$	17.844	17.713	17.959	18.263	18.061	18.029
F_2	$1\ ^2\Pi_g/(1\pi_g)^{-1}$	15.628	15.964	16.266	16.046	16.259	16.234
	$1\ ^2\Pi_u/(1\pi_u)^{-1}$	18.807	19.589	19.857	19.601	19.864	19.820
	$1\ ^2\Sigma_g^+/(3\sigma_g)^{-1}$	21.132	20.625	21.283	20.396	21.056	21.068
H_2O	$1\ ^2\mathrm{B}_1/(1b_1)^{-1}$	12.540	12.485	12.745	12.732	12.798	12.780
	$1\ ^2\mathrm{A}_1/(3a_1)^{-1}$	14.829	14.781	15.049	14.911	15.072	15.057
	$1\ ^2\mathrm{B}_2/(1b_2)^{-1}$	18.995	18.865	19.151	18.774	19.111	19.101
H_2S	$1\ ^2\mathrm{B}_1/(2b_1)^{-1}$	10.199	10.172	10.461	10.413	10.449	10.448
	$1\ ^2\mathrm{A}_1/(5a_1)^{-1}$	13.268	13.339	13.625	13.465	13.592	13.590
	$1\ ^2\mathrm{B}_2/(2b_2)^{-1}$	15.562	15.698	15.979	15.767	15.927	15.924
HCl	$1\ ^2\Pi/(1\pi)^{-1}$	12.539	12.488	12.797	12.799	12.783	12.779
	$1\ ^2\Sigma^+/(5\sigma)^{-1}$	16.579	16.635	16.935	16.767	16.898	16.891
HF	$1\ ^2\Pi/(1\pi)^{-1}$	16.059	15.868	16.161	16.212	16.205	16.180
	$1\ ^2\Sigma^+/(3\sigma)^{-1}$	20.043	19.812	20.103	19.897	20.116	20.099
LiCl	$1\ ^2\Pi/(2\pi)^{-1}$	9.810	9.734	10.029	10.061	10.023	10.011
	$1\ ^2\Sigma^+/(6\sigma)^{-1}$	10.545	10.500	10.789	10.738	10.772	10.758
LiF	$1\ ^2\Pi/(1\pi)^{-1}$	11.328	10.979	11.225	11.388	11.309	11.262
	$1\ ^2\Sigma^+/(4\sigma)^{-1}$	11.833	11.549	11.797	11.646	11.831	11.779
N_2	$1\ ^2\Sigma_g^+/(3\sigma_g)^{-1}$	15.308	15.984	16.255	16.162	16.263	16.255
	$1\ ^2\Pi_u/(1\pi_u)^{-1}$	16.811	16.790	17.269	16.969	17.179	17.183
	$1\ ^2\Sigma_u^+/(2\sigma_u)^{-1}$	18.516	19.558	19.824	20.019	19.922	19.898
Ne	$1\ ^2\mathrm{P}/(2p)^{-1}$	21.426	21.104	21.458	21.672	21.490	21.466
	$1\ ^2\mathrm{S}/(2s)^{-1}$	48.417	47.785	48.712	49.908	48.750	48.522
NH_3	$1\ ^2\mathrm{A}_1/(3a_1)^{-1}$	10.762	10.837	11.081	11.093	11.126	11.120
	$1\ ^2\mathrm{E}/(1e_g)^{-1}$	16.534	16.578	16.855	16.505	16.798	16.794
	$3\ ^2\mathrm{A}_1/(2a_1)^{-1}$	26.659	28.118	28.885	29.764	28.563	28.674
PH_3	$1\ ^2\mathrm{A}_1/(5a_1)^{-1}$	10.436	10.497	10.762	10.572	10.731	10.736
	$1\ ^2\mathrm{E}/(2e_g)^{-1}$	13.615	13.831	14.085	13.885	14.037	14.038
	$2\ ^2\mathrm{A}_1/(4a_1)^{-1}$	19.445	21.378	21.620	22.800	21.846	21.793
SiH_4	$1\ ^2\mathrm{T}_2/(2t_2)^{-1}$	12.676	12.960	13.184	12.976	13.135	13.141
	$1\ ^2\mathrm{A}_1/(3a_1)^{-1}$	18.173	18.824	19.246	19.725	19.260	19.259
MAE			0.385	0.549	0.615	0.546	0.532
MSE			0.200	0.520	0.515	0.529	0.510

TABLE II. Inner- and outer-valence IPs (in eV) in the aug-cc-pVDZ basis set computed at various levels of theory. All calculations are performed without diagonal approximation. The ADC(2) and ADC(3) calculations are performed within the Dyson scheme.

System	State	TBE	ADC-GW	ADC-2SOSEX	ADC(3)-$G3W2$	ADC-$G3W2$	ADC(2)	ADC(3)
Ar	$1\ ^2\mathrm{P}/(3p)^{-1}$	15.529	15.465	15.844	15.855	15.772	15.206	15.651
	$1\ ^2\mathrm{S}/(3s)^{-1}$	29.449	30.761	33.280	33.137	31.434	30.400	29.853
BeO	$1\ ^2\Pi/(1\pi)^{-1}$	9.962	9.530	9.749	9.832	9.808	8.223	9.992
	$1\ ^2\Sigma^+/(4\sigma)^{-1}$	11.103	10.820	10.741	10.936	11.024	8.755	11.500
BF	$1\ ^2\Sigma^+/(5\sigma)^{-1}$	11.054	11.114	11.212	11.233	11.423	10.904	11.348
	$2\ ^2\Pi/(1\pi)^{-1}$	18.581	18.485	18.880	18.950	18.777	17.215	18.797
	$2\ ^2\Sigma^+/(4\sigma)^{-1}$	20.913	21.412	21.492	21.628	21.657	19.933	21.273
BH_3	$1\ ^2\mathrm{E}'/(1e')^{-1}$	13.194	13.398	13.383	13.408	13.580	13.097	13.328
	$1\ ^2\mathrm{A}_1'/(2a_1')^{-1}$	18.238	18.476	18.999	18.997	18.844	18.347	18.356
BN	$1\ ^2\Pi/(1\pi)^{-1}$	11.875	11.469	11.468	11.545	11.839	10.972	11.931
	$1\ ^2\Sigma^+/(4\sigma)^{-1}$	13.660	13.230	13.283	13.388	13.659	12.421	13.291
C_2	$1\ ^2\Pi_u/(2\pi_u)^{-1}$	12.323	12.622	12.742	12.765	13.040	12.897	13.027
CH_2O	$1\ ^2\mathrm{B}_2/(2b_2)^{-1}$	10.739	10.928	10.837	10.952	11.108	9.581	11.026
	$1\ ^2\mathrm{B}_1/(1b_1)^{-1}$	14.502	14.306	14.416	14.478	14.651	13.832	14.539
	$1\ ^2\mathrm{A}_1/(5a_1)^{-1}$	16.032	16.236	16.236	16.382	16.469	14.727	16.406
	$2\ ^2\mathrm{B}_2/(1b_2)^{-1}$	17.002	17.845	17.858	17.960	18.063	16.866	17.422
CH_4	$1\ ^2\mathrm{T}_2/(1t_2)^{-1}$	14.285	14.470	14.437	14.491	14.674	13.923	14.522
	$1\ ^2\mathrm{A}_1/(2a_1)^{-1}$	23.056	23.630	24.875	24.859	24.154	23.262	23.406
CO	$1\ ^2\Sigma^+/(5\sigma)^{-1}$	13.752	14.460	14.647	14.697	14.750	13.821	14.493
	$1\ ^2\Pi/(1\pi)^{-1}$	16.845	16.785	17.090	17.126	17.140	16.287	16.977
	$2\ ^2\Sigma^+/(4\sigma)^{-1}$	19.550	20.050	20.287	20.433	20.347	18.382	20.024
CO_2	$1\ ^2\Pi_g/(1\pi_g)^{-1}$	13.567	13.841	14.044	14.110	14.127	12.866	13.952
	$1\ ^2\Pi_u/(1\pi_u)^{-1}$	17.391	18.264	18.580	18.692	18.588	17.187	18.183
	$1\ ^2\Sigma_u^+/(3\sigma_u)^{-1}$	17.889	18.446	18.635	18.733	18.714	16.802	18.700
	$1\ ^2\Sigma_g^+/(4\sigma_g)^{-1}$	19.137	19.841	20.080	20.238	20.143	18.090	20.063
CS	$1\ ^2\Sigma^+/(7\sigma)^{-1}$	11.151	12.116	12.171	12.264	12.366	11.111	12.178
	$1\ ^2\Pi/(2\pi)^{-1}$	12.768	12.694	12.915	12.921	13.034	12.815	12.899
	$2\ ^2\Sigma^+/(6\sigma)^{-1}$	17.844	17.735	18.289	18.343	18.055	16.940	18.181
F_2	$1\ ^2\Pi_g/(1\pi_g)^{-1}$	15.628	15.982	16.059	16.216	16.253	14.006	15.944
	$1\ ^2\Pi_u/(1\pi_u)^{-1}$	18.807	19.624	19.640	19.846	19.861	17.210	19.163
	$1\ ^2\Sigma_g^+/(3\sigma_g)^{-1}$	21.132	20.617	20.389	20.509	21.056	20.277	21.197
H_2O	$1\ ^2\mathrm{B}_1/(1b_1)^{-1}$	12.540	12.507	12.750	12.842	12.804	11.340	12.795
	$1\ ^2\mathrm{A}_1/(3a_1)^{-1}$	14.829	14.772	14.919	15.018	15.056	13.632	15.064
	$1\ ^2\mathrm{B}_2/(1b_2)^{-1}$	18.995	18.876	18.782	18.876	19.112	18.006	19.129
H_2S	$1\ ^2\mathrm{B}_1/(2b_1)^{-1}$	10.199	10.176	10.416	10.435	10.453	9.950	10.362
	$1\ ^2\mathrm{A}_1/(5a_1)^{-1}$	13.268	13.338	13.470	13.505	13.592	13.009	13.464
	$1\ ^2\mathrm{B}_2/(2b_2)^{-1}$	15.562	15.704	15.772	15.808	15.929	15.375	15.754
HCl	$1\ ^2\Pi/(1\pi)^{-1}$	12.539	12.494	12.803	12.820	12.784	12.212	12.679
	$1\ ^2\Sigma^+/(5\sigma)^{-1}$	16.579	16.629	16.770	16.806	16.888	16.321	16.766
HF	$1\ ^2\Pi/(1\pi)^{-1}$	16.059	15.893	16.231	16.319	16.207	14.504	16.201
	$1\ ^2\Sigma^+/(3\sigma)^{-1}$	20.043	19.804	19.901	20.000	20.097	18.742	20.105
LiCl	$1\ ^2\Pi/(2\pi)^{-1}$	9.810	9.743	10.065	10.086	10.020	9.381	9.959
	$1\ ^2\Sigma^+/(6\sigma)^{-1}$	10.545	10.507	10.743	10.779	10.765	10.097	10.706
LiF	$1\ ^2\Pi/(1\pi)^{-1}$	11.328	11.011	11.410	11.493	11.299	9.535	11.469
	$1\ ^2\Sigma^+/(4\sigma)^{-1}$	11.833	11.574	11.671	11.813	11.810	9.890	12.028
N_2	$1\ ^2\Sigma_g^+/(3\sigma_g)^{-1}$	15.308	15.986	16.169	16.265	16.259	14.847	16.130
	$1\ ^2\Pi_u/(1\pi_u)^{-1}$	16.811	16.794	16.973	16.995	17.186	16.964	17.183
	$1\ ^2\Sigma_u^+/(2\sigma_u)^{-1}$	18.516	19.571	20.033	20.144	19.911	18.068	19.373
Ne	$1\ ^2\mathrm{P}/(2p)^{-1}$	21.426	21.128	21.686	21.730	21.489	19.901	21.403
	$1\ ^2\mathrm{S}/(2s)^{-1}$	48.417	47.805	49.918	49.955	48.548	47.112	48.656
NH_3	$1\ ^2\mathrm{A}_1/(3a_1)^{-1}$	10.762	10.841	11.101	11.160	11.127	10.017	11.061
	$1\ ^2\mathrm{E}/(1e_g)^{-1}$	16.534	16.585	16.511	16.589	16.801	15.831	16.753
	$3\ ^2\mathrm{A}_1/(2a_1)^{-1}$	26.659	28.125	29.765	29.742	28.687	27.390	27.474
PH_3	$1\ ^2\mathrm{A}_1/(5a_1)^{-1}$	10.436	10.500	10.576	10.603	10.740	10.231	10.624
	$1\ ^2\mathrm{E}/(2e_g)^{-1}$	13.615	13.836	13.891	13.922	14.043	13.513	13.794
	$2\ ^2\mathrm{A}_1/(4a_1)^{-1}$	19.445	21.389	22.801	22.720	21.807	21.081	19.595
SiH_4	$1\ ^2\mathrm{T}_2/(2t_2)^{-1}$	12.676	12.963	12.980	13.006	13.145	12.668	12.821
	$1\ ^2\mathrm{A}_1/(3a_1)^{-1}$	18.173	18.830	19.726	19.696	19.264	18.773	18.303
MAE			0.381	0.620	0.649	0.537	0.781	0.314
MSE			0.210	0.526	0.589	0.524	-0.605	0.300

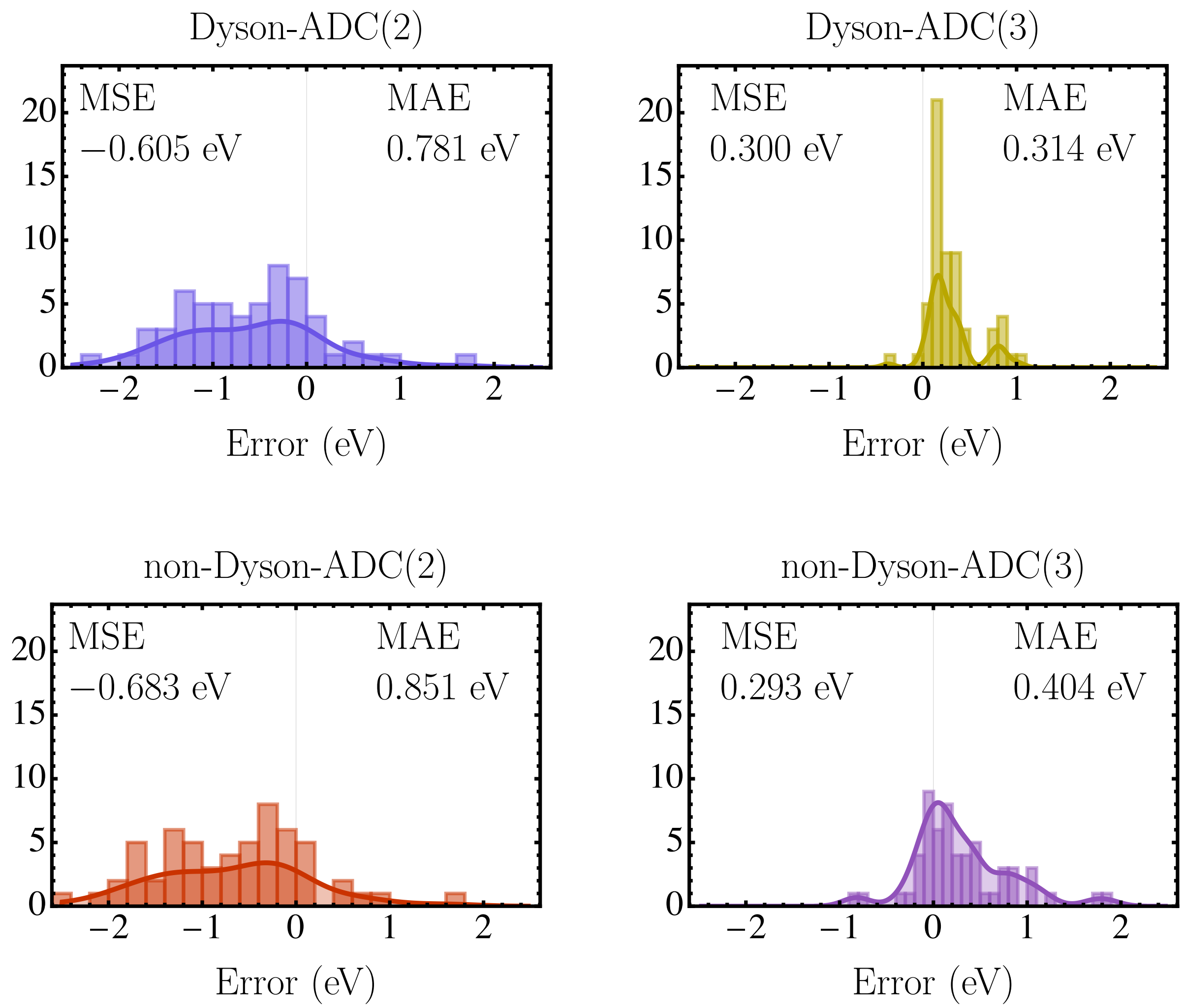

FIG. 1. Histogram of the errors (with respect to the TBEs) for the inner- and outer-valence IPs computed with the Dyson and non-Dyson ADC(2) and ADC(3) schemes in the aug-cc-pVDZ basis set. All calculations are performed without diagonal approximation.