Linearized G_0W_0 Density Matrix

Patryk Kozlowski

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We have the equation for the density matrix:

$$\gamma^{\sigma}\left(\mathbf{r}_1,\mathbf{r}_2\right)=\gamma_0^{\sigma}\left(\mathbf{r}_1,\mathbf{r}_2\right)-\frac{\mathrm{i}}{2\pi}\int \mathrm{d}\mathbf{r}_3\ \mathrm{d}\mathbf{r}_4\ \mathrm{d}\omega \mathrm{e}^{\mathrm{i}\omega\eta} G_0^{\sigma}\left(\mathbf{r}_1,\mathbf{r}_3,\omega\right)\Sigma_c^{\sigma}\left(\mathbf{r}_3,\mathbf{r}_4,\omega\right)G_0^{\sigma}\left(\mathbf{r}_4,\mathbf{r}_2,\omega\right) \tag{1}$$

In order to simplify the integral, Let us consider

$$I=\int \mathrm{d}\mathbf{r}_3\ \mathrm{d}\mathbf{r}_4 G_0^{\sigma}\left(\mathbf{r}_1,\mathbf{r}_3\right)\Sigma_c^{\sigma}\left(\mathbf{r}_3,\mathbf{r}_4\right)G_0^{\sigma}\left(\mathbf{r}_4,\mathbf{r}_2\right) \tag{2}$$

The noninteracting Green's function is defined as:

$$G_0\left(\mathbf{r}_1,\mathbf{r}_2,\right)=\sum_{pq}\phi_p^*(\mathbf{r}_1)G_{pq}\phi_q(\mathbf{r}_2) \tag{3}$$

and likewise for the self-energy:

$$\Sigma_c\left(\mathbf{r}_1,\mathbf{r}_2\right)=\sum_{pq}\phi_p^*(\mathbf{r}_1)\Sigma_{pq}\phi_q(\mathbf{r}_2) \tag{4}$$

where G_{pq} and Σ_{pq} are the matrix elements of the noninteracting Green's function and the self-energy, respectively. We can rewrite the integral as:

$$I=\sum_{pq}\sum_{rs}\sum_{tu}\int \mathrm{d}\mathbf{r}_3\ \mathrm{d}\mathbf{r}_4\phi_p^*(\mathbf{r}_1)G_{pq}\phi_q(\mathbf{r}_3)\phi_r^*(\mathbf{r}_3)\Sigma_{rs}\phi_s(\mathbf{r}_4)\phi_t^*(\mathbf{r}_4)G_{tu}\phi_u(\mathbf{r}_2) \tag{5}$$

We can simplify this expression by using the orthonormality of the basis functions:

$$\int \mathrm{d}\mathbf{r}\phi_q^*(\mathbf{r})\phi_r(\mathbf{r})=\delta_{qr} \tag{6}$$

So we can simplify the expression to:

$$I = \sum_{pq} \sum_{r} \sum_{t} \phi_p^*(\mathbf{r}_1) G_{pr} \phi_r(\mathbf{r}) \phi_r^*(\mathbf{r}) \Sigma_{rt} \phi_t(\mathbf{r}') \phi_t^*(\mathbf{r}') G_{tq} \phi_q(\mathbf{r}_2) \tag{7}$$

We use this and then also rewrite equation 1 in terms of the matrix elements of the density matrix with the following definition:

$$D_{pq\sigma} = \langle p\sigma | \gamma^\sigma | q\sigma \rangle \tag{8}$$

By the derivation above, we can rewrite equation 1 as:

$$D_{pq\sigma} = \langle p\sigma | \gamma_0^\sigma | q\sigma \rangle - \frac{\mathrm{i}}{2\pi} \sum_r \sum_t \int_{-\infty}^{\infty} \mathrm{d}\omega \mathrm{e}^{\mathrm{i}\omega\eta} \langle p\sigma | G_0^\sigma(\omega) | r\sigma \rangle \langle r\sigma | \Sigma_c^\sigma(\omega) | t\sigma \rangle \langle t\sigma | G_0^\sigma(\omega) | q\sigma \rangle \tag{9}$$

Next, we plug in the following definitions into equation 9:

$$G_{0pq}^\sigma = \sum_i \frac{\delta_{pq}\delta_{pi}}{\omega - \epsilon_{i\sigma} - \mathrm{i}\eta} + \sum_a \frac{\delta_{pq}\delta_{pa}}{\omega - \epsilon_{a\sigma} + \mathrm{i}\eta} \tag{10}$$

and

$$\Sigma_{cpq}^\sigma(\omega) = \sum_{is} \frac{w_{pi\sigma}^s w_{qi\sigma}^s}{\omega - \epsilon_{i\sigma} + \Omega_s - \mathrm{i}\eta} + \sum_{as} \frac{w_{pa\sigma}^s w_{qa\sigma}^s}{\omega - \epsilon_{a\sigma} - \Omega_s + \mathrm{i}\eta} \tag{11}$$

Plugging in these definitions, we get:

$$D_{pq\sigma} = \langle p\sigma | \gamma_0^\sigma | q\sigma \rangle - \frac{\mathrm{i}}{2\pi} \sum_r \sum_t \int_{-\infty}^{\infty} \mathrm{d}\omega \mathrm{e}^{\mathrm{i}\omega\eta} \left(\sum_i \frac{\delta_{pr}\delta_{pi}}{\omega - \epsilon_{i\sigma} - \mathrm{i}\eta} + \sum_a \frac{\delta_{pr}\delta_{pa}}{\omega - \epsilon_{a\sigma} + \mathrm{i}\eta} \right) \left(\sum_{ks} \frac{w_{rk\sigma}^s w_{tk\sigma}^s}{\omega - \epsilon_{k\sigma} + \Omega_s - \mathrm{i}\eta} + \sum_{cs} \frac{w_{rc\sigma}^s w_{tc\sigma}^s}{\omega - \epsilon_{c\sigma} - \Omega_s + \mathrm{i}\eta} \right) \left(\sum_j \frac{\delta_{tq}\delta_{tj}}{\omega - \epsilon_{j\sigma} - \mathrm{i}\eta} + \sum_b \frac{\delta_{tq}\delta_{tb}}{\omega - \epsilon_{b\sigma} + \mathrm{i}\eta} \right) \tag{12}$$

Let us just distribute the integral, which technically spawns 8 terms. Also note that the delta functions will get rid of the sums over r and t:

$$
\begin{aligned}
I = \int_{-\infty}^{\infty} \mathrm{d}\omega \mathrm{e}^{\mathrm{i}\omega\eta} \Bigg(& \sum_{ijks} \left(\frac{w^s_{ik\sigma} w^s_{jk\sigma}}{(\omega - \epsilon_{k\sigma} + \Omega_s - \mathrm{i}\eta)(\omega - \epsilon_{i\sigma} - \mathrm{i}\eta)(\omega - \epsilon_{j\sigma} - \mathrm{i}\eta)} \right) \\
& + \sum_{ibks} \left(\frac{w^s_{ik\sigma} w^s_{bk\sigma}}{(\omega - \epsilon_{k\sigma} + \Omega_s - \mathrm{i}\eta)(\omega - \epsilon_{i\sigma} - \mathrm{i}\eta)(\omega - \epsilon_{b\sigma} + \mathrm{i}\eta)} \right) \\
& + \sum_{ijcs} \left(\frac{w^s_{ic\sigma} w^s_{jc\sigma}}{(\omega - \epsilon_{c\sigma} - \Omega_s + \mathrm{i}\eta)(\omega - \epsilon_{i\sigma} - \mathrm{i}\eta)(\omega - \epsilon_{j\sigma} - \mathrm{i}\eta)} \right) \\
& + \sum_{ibcs} \left(\frac{w^s_{ic\sigma} w^s_{bc\sigma}}{(\omega - \epsilon_{c\sigma} - \Omega_s + \mathrm{i}\eta)(\omega - \epsilon_{i\sigma} - \mathrm{i}\eta)(\omega - \epsilon_{b\sigma} + \mathrm{i}\eta)} \right) \\
& + \sum_{ajks} \left(\frac{w^s_{ak\sigma} w^s_{jk\sigma}}{(\omega - \epsilon_{k\sigma} + \Omega_s - \mathrm{i}\eta)(\omega - \epsilon_{a\sigma} + \mathrm{i}\eta)(\omega - \epsilon_{j\sigma} - \mathrm{i}\eta)} \right) \\
& + \sum_{abks} \left(\frac{w^s_{ak\sigma} w^s_{bk\sigma}}{(\omega - \epsilon_{k\sigma} + \Omega_s - \mathrm{i}\eta)(\omega - \epsilon_{a\sigma} + \mathrm{i}\eta)(\omega - \epsilon_{b\sigma} + \mathrm{i}\eta)} \right) \\
& + \sum_{ajcs} \left(\frac{w^s_{ac\sigma} w^s_{jc\sigma}}{(\omega - \epsilon_{c\sigma} - \Omega_s + \mathrm{i}\eta)(\omega - \epsilon_{a\sigma} + \mathrm{i}\eta)(\omega - \epsilon_{j\sigma} - \mathrm{i}\eta)} \right) \\
& + \sum_{abcs} \left(\frac{w^s_{ac\sigma} w^s_{bc\sigma}}{(\omega - \epsilon_{c\sigma} - \Omega_s + \mathrm{i}\eta)(\omega - \epsilon_{a\sigma} + \mathrm{i}\eta)(\omega - \epsilon_{b\sigma} + \mathrm{i}\eta)} \right) \Bigg)
\end{aligned} \tag{13}
$$

At this point, we note the following relation between integrals $\oint_{D_\pm} f(z) = \int_{-R}^{R} f(z) + \int_{C_{R\pm}} f(z)$. $D_\pm$ is a semicircular domain in either half of the complex plane, $C_{R\pm}$ is the semicircle in the upper or lower part of the complex plane, and R is the radius of the semicircle. We are able to take $R \to \infty$ and since $f(z) = e^{i\omega\eta} g(z)$, where $g(z)$ is analytic on D except for a finite number of poles, the integral over the semicircle will vanish by Jordan's lemma, leaving us with $\int_{-R=-\infty}^{R=\infty} f(z) = \oint_{D_\pm} f(z)$. The contribution over the fully occupied block will be given by the following two terms:

$$
\begin{aligned}
I_{ij} = & \sum_{ks} w^s_{ik\sigma} w^s_{jk\sigma} \oint_{D+} \mathrm{d}\omega \mathrm{e}^{\mathrm{i}\omega\eta} \frac{1}{(\omega - \epsilon_{k\sigma} + \Omega_s - \mathrm{i}\eta)(\omega - \epsilon_{i\sigma} - \mathrm{i}\eta)(\omega - \epsilon_{j\sigma} - \mathrm{i}\eta)} \\
& + \sum_{cs} w^s_{ic\sigma} w^s_{jc\sigma} \oint_{D+} \mathrm{d}\omega \mathrm{e}^{\mathrm{i}\omega\eta} \frac{1}{(\omega - \epsilon_{c\sigma} - \Omega_s + \mathrm{i}\eta)(\omega - \epsilon_{i\sigma} - \mathrm{i}\eta)(\omega - \epsilon_{j\sigma} - \mathrm{i}\eta)}
\end{aligned} \tag{14}
$$

Due to the contour that is chosen for this case, we have poles for the first term at $\omega_{11} = \epsilon_{k\sigma} - \Omega_s + \mathrm{i}\eta$, $\omega_{12} = \epsilon_{i\sigma} + \mathrm{i}\eta$, and $\omega_{13} = \epsilon_{j\sigma} + \mathrm{i}\eta$. For such simple poles, the Cauchy residue theorem simplifies to:

$$\mathrm{Res}_{\omega=\omega_0} f(\omega) = \phi(\omega_0) \tag{15}$$

where $\phi_{\omega_0}(\omega) = (\omega - \omega_0)f(\omega)$. For the first of these integrals in the occupied block, we have:

$$f_1(\omega) = \frac{e^{i\omega\eta}}{(\omega - \epsilon_{k\sigma} + \Omega_s - \mathrm{i}\eta)(\omega - \epsilon_{i\sigma} - \mathrm{i}\eta)(\omega - \epsilon_{j\sigma} - \mathrm{i}\eta)} \tag{16}$$

Plugging in $\omega_{11} = \epsilon_{k\sigma} - \Omega_s + \mathrm{i}\eta$, we get:

$$\phi_{\omega_{11}}(\omega) = (\omega - \epsilon_{k\sigma} + \Omega_s - \mathrm{i}\eta)f_1(\omega) = \frac{e^{i\omega\eta}}{(\omega - \epsilon_{i\sigma} - \mathrm{i}\eta)(\omega - \epsilon_{j\sigma} - \mathrm{i}\eta)} \tag{17}$$

Evaluating this at the pole, we get:

$$\phi_{\omega_{11}}(\epsilon_{k\sigma} - \Omega_s + \mathrm{i}\eta) = \frac{e^{i(\epsilon_{k\sigma} - \Omega_s + \mathrm{i}\eta)\eta}}{(\epsilon_{k\sigma} - \Omega_s + \mathrm{i}\eta - \epsilon_{i\sigma} - \mathrm{i}\eta)(\epsilon_{k\sigma} - \Omega_s + \mathrm{i}\eta - \epsilon_{j\sigma} - \mathrm{i}\eta)} \tag{18}$$

In the limit $\eta \to 0$, we get:

$$\boxed{\phi_{\omega_{11}}(\epsilon_{k\sigma} - \Omega_s + \mathrm{i}\eta) = \frac{1}{(\epsilon_{k\sigma} - \Omega_s - \epsilon_{i\sigma})(\epsilon_{k\sigma} - \Omega_s - \epsilon_{j\sigma})}} \tag{19}$$

For the other poles, the procedure is similar, so I will just summarise the results:

$$\boxed{\phi_{\omega_{12}}(\epsilon_{i\sigma} + \mathrm{i}\eta) = \frac{1}{(\epsilon_{i\sigma} - \epsilon_{k\sigma} + \Omega_s)(\epsilon_{i\sigma} - \epsilon_{j\sigma})}} \tag{20}$$

$$\boxed{\phi_{\omega_{13}}(\epsilon_{j\sigma} + \mathrm{i}\eta) = \frac{1}{(\epsilon_{j\sigma} - \epsilon_{k\sigma} + \Omega_s)(\epsilon_{j\sigma} - \epsilon_{i\sigma})}} \tag{21}$$

By Cauchy's residue theorem, the first term of the integral will be given by:

$$\begin{aligned} 2\pi i \sum_{ks} w^s_{ik\sigma} w^s_{jk\sigma} \Bigg(& \frac{1}{(\epsilon_{k\sigma} - \Omega_s - \epsilon_{i\sigma})(\epsilon_{k\sigma} - \Omega_s - \epsilon_{j\sigma})} \\ & + \frac{1}{(\epsilon_{i\sigma} - \epsilon_{k\sigma} + \Omega_s)(\epsilon_{i\sigma} - \epsilon_{j\sigma})} \\ & + \frac{1}{(\epsilon_{j\sigma} - \epsilon_{k\sigma} + \Omega_s)(\epsilon_{j\sigma} - \epsilon_{i\sigma})} \Bigg) \end{aligned} \tag{22}$$

We move on to the second integral in the occupied block. It only has two poles in the fully occupied contour: $\omega_{21} = \epsilon_{i\sigma} + \mathrm{i}\eta$ and $\omega_{22} = \epsilon_{j\sigma} + \mathrm{i}\eta$. We have $f_2(\omega)$ as:

$$f_2(\omega) = \frac{e^{i\omega\eta}}{(\omega - \epsilon_{c\sigma} - \Omega_s + \mathrm{i}\eta)(\omega - \epsilon_{i\sigma} - \mathrm{i}\eta)(\omega - \epsilon_{j\sigma} - \mathrm{i}\eta)} \tag{23}$$

So $\phi_{\omega_{21}}(\omega_{21})$ is:

$$\boxed{\phi_{\omega_{21}}(\epsilon_{i\sigma} + \mathrm{i}\eta) = \frac{1}{(\epsilon_{i\sigma} - \epsilon_{c\sigma} - \Omega_s)(\epsilon_{i\sigma} - \epsilon_{j\sigma})}} \tag{24}$$

Now we consider the second pole at $\omega_{22} = \epsilon_{j\sigma} + \mathrm{i}\eta$

$$\boxed{\phi_{\omega_{22}}(\epsilon_{j\sigma} + \mathrm{i}\eta) = \frac{1}{(\epsilon_{j\sigma} - \epsilon_{c\sigma} - \Omega_s)(\epsilon_{j\sigma} - \epsilon_{i\sigma})}} \tag{25}$$

So the second term of the integral will be given by:

$$\begin{aligned} 2\pi i \sum_{cs} w^s_{ic\sigma} w^s_{jc\sigma} \Bigg(& \frac{1}{(\epsilon_{i\sigma} - \epsilon_{c\sigma} - \Omega_s)(\epsilon_{i\sigma} - \epsilon_{j\sigma})} \\ & + \frac{1}{(\epsilon_{j\sigma} - \epsilon_{c\sigma} - \Omega_s)(\epsilon_{j\sigma} - \epsilon_{i\sigma})} \Bigg) \end{aligned} \tag{26}$$

Table 1: Summary of Poles and their Residues

Pole Notation	Position ω_0	Residue $\phi_{\omega_0}(\omega_0)$
	Series ω_1	
ω_{11}	$\epsilon_{k\sigma} - \Omega_s + \mathrm{i}\eta$	$\frac{1}{(\epsilon_{k\sigma}-\Omega_s-\epsilon_{i\sigma})(\epsilon_{k\sigma}-\Omega_s-\epsilon_{j\sigma})}$
ω_{12}	$\epsilon_{i\sigma} + \mathrm{i}\eta$	$\frac{1}{(\epsilon_{i\sigma}-\epsilon_{k\sigma}+\Omega_s)(\epsilon_{i\sigma}-\epsilon_{j\sigma})}$
ω_{13}	$\epsilon_{j\sigma} + \mathrm{i}\eta$	$\frac{1}{(\epsilon_{j\sigma}-\epsilon_{k\sigma}+\Omega_s)(\epsilon_{j\sigma}-\epsilon_{i\sigma})}$
	Series ω_2	
ω_{21}	$\epsilon_{i\sigma} + \mathrm{i}\eta$	$\frac{1}{(\epsilon_{i\sigma}-\epsilon_{c\sigma}-\Omega_s)(\epsilon_{i\sigma}-\epsilon_{j\sigma})}$
ω_{22}	$\epsilon_{j\sigma} + \mathrm{i}\eta$	$\frac{1}{(\epsilon_{j\sigma}-\epsilon_{c\sigma}-\Omega_s)(\epsilon_{j\sigma}-\epsilon_{i\sigma})}$

Adding the two terms together, we get:

$$I_{ij} = 2\pi i \left(\sum_{ks} w^s_{ik\sigma} w^s_{jk\sigma} \left(\frac{1}{(\epsilon_{k\sigma} - \Omega_s - \epsilon_{i\sigma})(\epsilon_{k\sigma} - \Omega_s - \epsilon_{j\sigma})} + \frac{1}{(\epsilon_{i\sigma} - \epsilon_{k\sigma} + \Omega_s)(\epsilon_{i\sigma} - \epsilon_{j\sigma})} \right.\right.$$
$$\left. + \frac{1}{(\epsilon_{j\sigma} - \epsilon_{k\sigma} + \Omega_s)(\epsilon_{j\sigma} - \epsilon_{i\sigma})} \right)$$
$$\left. + \sum_{cs} w^s_{ic\sigma} w^s_{jc\sigma} \left(\frac{1}{(\epsilon_{i\sigma} - \epsilon_{c\sigma} - \Omega_s)(\epsilon_{i\sigma} - \epsilon_{j\sigma})} + \frac{1}{(\epsilon_{j\sigma} - \epsilon_{c\sigma} - \Omega_s)(\epsilon_{j\sigma} - \epsilon_{i\sigma})} \right) \right) \tag{27}$$

Let as first just consider the first term:

$$\sum_{ks} w^s_{ik\sigma} w^s_{jk\sigma} \left(\frac{1}{(\epsilon_{k\sigma} - \Omega_s - \epsilon_{i\sigma})(\epsilon_{k\sigma} - \Omega_s - \epsilon_{j\sigma})} + \frac{1}{(\epsilon_{i\sigma} - \epsilon_{k\sigma} + \Omega_s)(\epsilon_{i\sigma} - \epsilon_{j\sigma})} + \frac{1}{(\epsilon_{j\sigma} - \epsilon_{k\sigma} + \Omega_s)(\epsilon_{j\sigma}} \right. \tag{28}$$

Getting a common denominator for all of the terms:

$$\begin{aligned}
&\frac{1}{(\epsilon_{k\sigma} - \Omega_s - \epsilon_{i\sigma})(\epsilon_{k\sigma} - \Omega_s - \epsilon_{j\sigma})} + \frac{1}{(\epsilon_{i\sigma} - \epsilon_{k\sigma} + \Omega_s)(\epsilon_{i\sigma} - \epsilon_{j\sigma})} + \frac{1}{(\epsilon_{j\sigma} - \epsilon_{k\sigma} + \Omega_s)(\epsilon_{j\sigma} - \epsilon_{i\sigma})} \\
&= \frac{(\epsilon_{i\sigma} - \epsilon_{j\sigma})}{(\epsilon_{k\sigma} - \Omega_s - \epsilon_{i\sigma})(\epsilon_{k\sigma} - \Omega_s - \epsilon_{j\sigma})(\epsilon_{i\sigma} - \epsilon_{j\sigma})} - \frac{(\epsilon_{k\sigma} - \Omega_s - \epsilon_{j\sigma})}{(\epsilon_{k\sigma} - \Omega_s - \epsilon_{i\sigma})(\epsilon_{k\sigma} - \Omega_s - \epsilon_{j\sigma})(\epsilon_{i\sigma} - \epsilon_{j\sigma})} \\
&+ \frac{(\epsilon_{k\sigma} - \Omega_s - \epsilon_{i\sigma})}{(\epsilon_{k\sigma} - \Omega_s - \epsilon_{i\sigma})(\epsilon_{k\sigma} - \Omega_s - \epsilon_{j\sigma})(\epsilon_{i\sigma} - \epsilon_{j\sigma})} \\
&= 0
\end{aligned} \tag{29}$$

So the first term simplifies to zero. The second term is:

$$\sum_{cs} w^s_{ic\sigma} w^s_{jc\sigma} \left(\frac{1}{(\epsilon_{i\sigma} - \epsilon_{c\sigma} - \Omega_s)(\epsilon_{i\sigma} - \epsilon_{j\sigma})} + \frac{1}{(\epsilon_{j\sigma} - \epsilon_{c\sigma} - \Omega_s)(\epsilon_{j\sigma} - \epsilon_{i\sigma})} \right) \tag{30}$$

Getting a common denominator for all of the terms:

$$
\begin{aligned}
&\frac{1}{(\epsilon_{i\sigma}-\epsilon_{c\sigma}-\Omega_s)(\epsilon_{i\sigma}-\epsilon_{j\sigma})}+\frac{1}{(\epsilon_{j\sigma}-\epsilon_{c\sigma}-\Omega_s)(\epsilon_{j\sigma}-\epsilon_{i\sigma})} \\
&=\frac{(\epsilon_{j\sigma}-\epsilon_{c\sigma}-\Omega_s)}{(\epsilon_{i\sigma}-\epsilon_{c\sigma}-\Omega_s)\left(\epsilon_{i\sigma}-\epsilon_{j\sigma}\right)\left(\epsilon_{j\sigma}-\epsilon_{c\sigma}-\Omega_s\right)}-\frac{(\epsilon_{i\sigma}-\epsilon_{c\sigma}-\Omega_s)}{(\epsilon_{i\sigma}-\epsilon_{c\sigma}-\Omega_s)\left(\epsilon_{i\sigma}-\epsilon_{j\sigma}\right)\left(\epsilon_{j\sigma}-\epsilon_{c\sigma}-\Omega_s\right)} \\
&=\frac{(\epsilon_{j\sigma}-\epsilon_{i\sigma})}{(\epsilon_{i\sigma}-\epsilon_{c\sigma}-\Omega_s)\left(\epsilon_{j\sigma}-\epsilon_{c\sigma}-\Omega_s\right)\left(\epsilon_{i\sigma}-\epsilon_{j\sigma}\right)} \\
&=-\frac{1}{(\epsilon_{i\sigma}-\epsilon_{c\sigma}-\Omega_s)\left(\epsilon_{j\sigma}-\epsilon_{c\sigma}-\Omega_s\right)}=-\frac{1}{(\Omega_s+\epsilon_{c\sigma}-\epsilon_{i\sigma})\left(\Omega_s+\epsilon_{c\sigma}-\epsilon_{j\sigma}\right)}
\end{aligned}
\tag{31}
$$

So we see that the whole integral just evaluate to the second term, giving:

$$
I_{ij}=-2\pi i\sum_{cs}\frac{w^s_{ic\sigma}w^s_{jc\sigma}}{(\Omega_s+\epsilon_{c\sigma}-\epsilon_{i\sigma})(\Omega_s+\epsilon_{c\sigma}-\epsilon_{j\sigma})} \tag{32}
$$

So, the expression for D_{ij} is:

$$
D_{ij}=\langle i\sigma|\,\gamma^\sigma_0\,|j\sigma\rangle+\frac{2\pi i^2}{2\pi}\sum_{cs}\frac{w_{ic}w_{jc}}{(\Omega_s+\epsilon_{c\sigma}-\epsilon_{i\sigma})(\Omega_s+\epsilon_{c\sigma}-\epsilon_{j\sigma})} \tag{33}
$$

The first term is the matrix element of the noninteracting part of the density matrix, so this just simplifies to δ_{ij} and then we relabel the virtual index $c \to a$:

$$
D_{ij}=\delta_{ij}-\sum_{as}\frac{w_{ia}w_{ja}}{(\Omega_s+\epsilon_{a\sigma}-\epsilon_{i\sigma})(\Omega_s+\epsilon_{a\sigma}-\epsilon_{j\sigma})} \tag{34}
$$

1 Fully Virtual Block

For the fully virtual block, we need to consider third to last and last terms of the integral in equation 13:

$$
\begin{aligned}
I_{ab}=&\sum_{ks}w^s_{ak\sigma}w^s_{bk\sigma}\int \mathrm{d}\omega \mathrm{e}^{\mathrm{i}\omega\eta}\frac{1}{(\omega-\epsilon_{k\sigma}+\Omega_s-\mathrm{i}\eta)(\omega-\epsilon_{a\sigma}+\mathrm{i}\eta)(\omega-\epsilon_{b\sigma}+\mathrm{i}\eta)} \\
&+\sum_{cs}w^s_{ac\sigma}w^s_{bc\sigma}\int \mathrm{d}\omega \mathrm{e}^{\mathrm{i}\omega\eta}\frac{1}{(\omega-\epsilon_{c\sigma}-\Omega_s+\mathrm{i}\eta)(\omega-\epsilon_{a\sigma}+\mathrm{i}\eta)(\omega-\epsilon_{b\sigma}+\mathrm{i}\eta)}
\end{aligned}
\tag{35}
$$

Due to the contour that is chosen for this case, we have poles for the first term at just $\omega_{11} = \epsilon_{a\sigma} - \mathrm{i}\eta$ and $\omega_{12} = \epsilon_{b\sigma} - \mathrm{i}\eta$. Using the Cauchy residue theorem from equation 15:

$$f_1(\omega) = \frac{e^{i\omega\eta}}{(\omega - \epsilon_{k\sigma} + \Omega_s - \mathrm{i}\eta)(\omega - \epsilon_{a\sigma} + \mathrm{i}\eta)(\omega - \epsilon_{b\sigma} + \mathrm{i}\eta)} \tag{36}$$

Plugging in $\omega_{11} = \epsilon_{a\sigma} - \mathrm{i}\eta$, we get:

$$\boxed{\phi_{\omega_{11}}(\epsilon_{a\sigma} - \mathrm{i}\eta) = \frac{1}{(\epsilon_{a\sigma} - \epsilon_{k\sigma} + \Omega_s)(\epsilon_{a\sigma} - \epsilon_{b\sigma})}} \tag{37}$$

$$\boxed{\phi_{\omega_{12}}(\epsilon_{b\sigma} - \mathrm{i}\eta) = \frac{1}{(\epsilon_{b\sigma} - \epsilon_{k\sigma} + \Omega_s)(\epsilon_{b\sigma} - \epsilon_{a\sigma})}} \tag{38}$$

So the first term of the integral will be given by:

$$2\pi i \sum_{ks} w^s_{ak\sigma} w^s_{bk\sigma} \left(\frac{1}{(\epsilon_{a\sigma} - \epsilon_{k\sigma} + \Omega_s)(\epsilon_{a\sigma} - \epsilon_{b\sigma})} + \frac{1}{(\epsilon_{b\sigma} - \epsilon_{k\sigma} + \Omega_s)(\epsilon_{b\sigma} - \epsilon_{a\sigma})} \right) \tag{39}$$

We move on to the second integral in the virtual block. It has now three poles in the fully virtual contour: $\omega_{21} = \epsilon_{c\sigma} + \Omega_s - \mathrm{i}\eta$, $\omega_{22} = \epsilon_{a\sigma} - \mathrm{i}\eta$, and $\omega_{23} = \epsilon_{b\sigma} - \mathrm{i}\eta$. We have $f_2(\omega)$ as:

$$f_2(\omega) = \frac{e^{i\omega\eta}}{(\omega - \epsilon_{c\sigma} - \Omega_s + \mathrm{i}\eta)(\omega - \epsilon_{a\sigma} + \mathrm{i}\eta)(\omega - \epsilon_{b\sigma} + \mathrm{i}\eta)} \tag{40}$$

So $\phi_{\omega_{21}}(\omega_{21})$ is:

$$\boxed{\phi_{\omega_{21}}(\epsilon_{c\sigma} + \Omega_s - \mathrm{i}\eta) = \frac{1}{(\epsilon_{c\sigma} + \Omega_s - \epsilon_{a\sigma})(\epsilon_{c\sigma} + \Omega_s - \epsilon_{b\sigma})}} \tag{41}$$

Now we consider the second pole at $\omega_{22} = \epsilon_{a\sigma} - \mathrm{i}\eta$.

$$\boxed{\phi_{\omega_{22}}(\epsilon_{a\sigma} - \mathrm{i}\eta) = \frac{1}{(\epsilon_{a\sigma} - \epsilon_{c\sigma} - \Omega_s)(\epsilon_{a\sigma} - \epsilon_{b\sigma})}} \tag{42}$$

Now we consider the third pole at $\omega_{23} = \epsilon_{b\sigma} - \mathrm{i}\eta$.

$$\boxed{\phi_{\omega_{23}}(\epsilon_{b\sigma} - \mathrm{i}\eta) = \frac{1}{(\epsilon_{b\sigma} - \epsilon_{c\sigma} - \Omega_s)(\epsilon_{b\sigma} - \epsilon_{a\sigma})}} \tag{43}$$

So the second term of the integral will be given by:

$$2\pi i\sum_{cs} w^s_{ac\sigma}w^s_{bc\sigma}\left(\frac{1}{(\epsilon_{c\sigma}+\Omega_s-\epsilon_{a\sigma})(\epsilon_{c\sigma}+\Omega_s-\epsilon_{b\sigma})}\right.$$
$$+\frac{1}{(\epsilon_{a\sigma}-\epsilon_{c\sigma}-\Omega_s)(\epsilon_{a\sigma}-\epsilon_{b\sigma})} \tag{44}$$
$$\left.+\frac{1}{(\epsilon_{b\sigma}-\epsilon_{c\sigma}-\Omega_s)(\epsilon_{b\sigma}-\epsilon_{a\sigma})}\right)$$

The results we got are summarized in the table: Adding the two terms

Table 2: Summary of Poles and their Residues

Pole Notation	Position ω_0	Residue $\phi_{\omega_0}(\omega_0)$
Series ω_1		
ω_{11}	$\epsilon_{a\sigma}-\mathrm{i}\eta$	$\frac{1}{(\epsilon_{a\sigma}-\epsilon_{k\sigma}+\Omega_s)(\epsilon_{a\sigma}-\epsilon_{b\sigma})}$
ω_{12}	$\epsilon_{b\sigma}-\mathrm{i}\eta$	$\frac{1}{(\epsilon_{b\sigma}-\epsilon_{k\sigma}+\Omega_s)(\epsilon_{b\sigma}-\epsilon_{a\sigma})}$
Series ω_2		
ω_{21}	$\epsilon_{c\sigma}+\Omega_s-\mathrm{i}\eta$	$\frac{1}{(\epsilon_{c\sigma}+\Omega_s-\epsilon_{a\sigma})(\epsilon_{c\sigma}+\Omega_s-\epsilon_{b\sigma})}$
ω_{22}	$\epsilon_{a\sigma}-\mathrm{i}\eta$	$\frac{1}{(\epsilon_{a\sigma}-\epsilon_{c\sigma}-\Omega_s)(\epsilon_{a\sigma}-\epsilon_{b\sigma})}$
ω_{23}	$\epsilon_{b\sigma}-\mathrm{i}\eta$	$\frac{1}{(\epsilon_{b\sigma}-\epsilon_{c\sigma}-\Omega_s)(\epsilon_{b\sigma}-\epsilon_{a\sigma})}$

together, we get:

$$I_{ab}=2\pi i\left(\sum_{ks} w^s_{ak\sigma}w^s_{bk\sigma}\left(\frac{1}{(\epsilon_{a\sigma}-\epsilon_{k\sigma}+\Omega_s)(\epsilon_{a\sigma}-\epsilon_{b\sigma})}+\frac{1}{(\epsilon_{b\sigma}-\epsilon_{k\sigma}+\Omega_s)(\epsilon_{b\sigma}-\epsilon_{a\sigma})}\right)\right.$$
$$+\sum_{cs} w^s_{ac\sigma}w^s_{bc\sigma}\left(\frac{1}{(\epsilon_{c\sigma}+\Omega_s-\epsilon_{a\sigma})(\epsilon_{c\sigma}+\Omega_s-\epsilon_{b\sigma})}\right.$$
$$+\frac{1}{(\epsilon_{a\sigma}-\epsilon_{c\sigma}-\Omega_s)(\epsilon_{a\sigma}-\epsilon_{b\sigma})}$$
$$\left.\left.+\frac{1}{(\epsilon_{b\sigma}-\epsilon_{c\sigma}-\Omega_s)(\epsilon_{b\sigma}-\epsilon_{a\sigma})}\right)\right) \tag{45}$$

A similar simplification as the one done before gives:

$$I_{ab}=-2\pi i\sum_{ks}\frac{w_{ak}w_{bk}}{(\Omega_s+\epsilon_{k\sigma}-\epsilon_{a\sigma})(\Omega_s+\epsilon_{k\sigma}-\epsilon_{b\sigma})} \tag{46}$$

So, the expression for D_{ab} is:

$$D_{ab} = \langle a\sigma | \gamma_0^\sigma | b\sigma \rangle + \frac{2\pi i^2}{2\pi} \sum_{ks} \frac{w_{ak} w_{bk}}{(\Omega_s + \epsilon_{k\sigma} - \epsilon_{a\sigma})(\Omega_s + \epsilon_{k\sigma} - \epsilon_{b\sigma})} \tag{47}$$

The matrix element of the noninteracting density matrix does not mix virtual states and we relabel the occupied index $k \to i$:

$$D_{ab} = -\sum_{is} \frac{w_{ai} w_{bi}}{(\Omega_s + \epsilon_{i\sigma} - \epsilon_{a\sigma})(\Omega_s + \epsilon_{i\sigma} - \epsilon_{b\sigma})} \tag{48}$$

Now, we want to consider the mixed block i.e. the second and fourth terms of the integral in equation 13:

$$\begin{aligned} I_{ib} = &\sum_{ks} w_{ik\sigma}^s w_{bk\sigma}^s \int \mathrm{d}\omega \mathrm{e}^{\mathrm{i}\omega\eta} \frac{1}{(\omega - \epsilon_{k\sigma} + \Omega_s - \mathrm{i}\eta)(\omega - \epsilon_{i\sigma} - \mathrm{i}\eta)(\omega - \epsilon_{b\sigma} + \mathrm{i}\eta)} \\ &+ \sum_{cs} w_{ic\sigma}^s w_{bc\sigma}^s \int \mathrm{d}\omega \mathrm{e}^{\mathrm{i}\omega\eta} \frac{1}{(\omega - \epsilon_{c\sigma} - \Omega_s + \mathrm{i}\eta)(\omega - \epsilon_{i\sigma} - \mathrm{i}\eta)(\omega - \epsilon_{b\sigma} + \mathrm{i}\eta)} \end{aligned} \tag{49}$$

Due to the contour that is chosen for this case, we have poles for the first term which lies in the upper half of the complex plane at $\omega_{11} = \epsilon_{k\sigma} - \Omega_s + \mathrm{i}\eta$ and $\omega_{12} = \epsilon_{i\sigma} + \mathrm{i}\eta$. Using the Cauchy residue theorem from equation 15:

$$f_1(\omega) = \frac{e^{i\omega\eta}}{(\omega - \epsilon_{k\sigma} + \Omega_s - \mathrm{i}\eta)(\omega - \epsilon_{i\sigma} + \mathrm{i}\eta)(\omega - \epsilon_{b\sigma} + \mathrm{i}\eta)} \tag{50}$$

Plugging in $\omega_{11} = \epsilon_{k\sigma} - \Omega_s + \mathrm{i}\eta$, we get:

$$\boxed{\phi_{\omega_{11}}(\epsilon_{k\sigma} - \Omega_s + \mathrm{i}\eta) = \frac{1}{(\epsilon_{k\sigma} - \epsilon_{i\sigma} - \Omega_s)(\epsilon_{k\sigma} - \epsilon_{b\sigma} - \Omega_s)}} \tag{51}$$

Now we consider the second pole at $\omega_{12} = \epsilon_{i\sigma} + \mathrm{i}\eta$.

$$\boxed{\phi_{\omega_{12}}(\epsilon_{i\sigma} + \mathrm{i}\eta) = \frac{1}{(\epsilon_{i\sigma} - \epsilon_{k\sigma} + \Omega_s)(\epsilon_{i\sigma} - \epsilon_{b\sigma})}} \tag{52}$$

So the first term of the integral will be given by:

$$\begin{aligned} 2\pi i \sum_{ks} w_{ik\sigma}^s w_{bk\sigma}^s \Bigg(&\frac{1}{(\epsilon_{k\sigma} - \epsilon_{i\sigma} - \Omega_s)(\epsilon_{k\sigma} - \epsilon_{b\sigma} - \Omega_s)} \\ &+ \frac{1}{(\epsilon_{i\sigma} - \epsilon_{k\sigma} + \Omega_s)(\epsilon_{i\sigma} - \epsilon_{b\sigma})} \Bigg) \end{aligned} \tag{53}$$

We move on to the second integral in the mixed block. It has two poles in D_-: $\omega_{21} = \epsilon_{c\sigma} + \Omega_s - \mathrm{i}\eta$ and $\omega_{22} = \epsilon_{b\sigma} - \mathrm{i}\eta$. We have $f_2(\omega)$ as:

$$f_2(\omega) = \frac{e^{i\omega\eta}}{(\omega - \epsilon_{c\sigma} - \Omega_s + \mathrm{i}\eta)(\omega - \epsilon_{i\sigma} - \mathrm{i}\eta)(\omega - \epsilon_{b\sigma} + \mathrm{i}\eta)} \tag{54}$$

So $\phi_{\omega_{21}}(\omega_{21})$ is:

$$\boxed{\phi_{\omega_{21}}(\epsilon_{c\sigma} + \Omega_s - \mathrm{i}\eta) = \frac{1}{(\epsilon_{c\sigma} + \Omega_s - \epsilon_{i\sigma})(\epsilon_{c\sigma} + \Omega_s - \epsilon_{b\sigma})}} \tag{55}$$

Now we consider the second pole at $\omega_{22} = \epsilon_{b\sigma} - \mathrm{i}\eta$.

$$\boxed{\phi_{\omega_{22}}(\epsilon_{b\sigma} - \mathrm{i}\eta) = \frac{1}{(\epsilon_{b\sigma} - \epsilon_{c\sigma} - \Omega_s)(\epsilon_{b\sigma} - \epsilon_{i\sigma})}} \tag{56}$$

So the second term of the integral will be given by:

$$\begin{aligned} 2\pi i \sum_{cs} w^s_{ic\sigma} w^s_{bc\sigma} \Bigg(& \frac{1}{(\epsilon_{c\sigma} + \Omega_s - \epsilon_{i\sigma})(\epsilon_{c\sigma} + \Omega_s - \epsilon_{b\sigma})} \\ & + \frac{1}{(\epsilon_{b\sigma} - \epsilon_{c\sigma} - \Omega_s)(\epsilon_{b\sigma} - \epsilon_{i\sigma})} \Bigg) \end{aligned} \tag{57}$$

The results we got are summarized in the table: Adding the two terms

Table 3: Summary of Poles and their Residues

Pole Notation	Position ω_0	Residue $\phi_{\omega_0}(\omega_0)$
Series ω_1		
ω_{11}	$\epsilon_{k\sigma} - \Omega_s + \mathrm{i}\eta$	$\frac{1}{(\epsilon_{k\sigma} - \epsilon_{i\sigma} - \Omega_s)(\epsilon_{k\sigma} - \epsilon_{b\sigma} - \Omega_s)}$
ω_{12}	$\epsilon_{i\sigma} + \mathrm{i}\eta$	$\frac{1}{(\epsilon_{i\sigma} - \epsilon_{k\sigma} + \Omega_s)(\epsilon_{i\sigma} - \epsilon_{b\sigma})}$
Series ω_2		
ω_{21}	$\epsilon_{c\sigma} + \Omega_s - \mathrm{i}\eta$	$\frac{1}{(\epsilon_{c\sigma} + \Omega_s - \epsilon_{i\sigma})(\epsilon_{c\sigma} + \Omega_s - \epsilon_{b\sigma})}$
ω_{22}	$\epsilon_{b\sigma} - \mathrm{i}\eta$	$\frac{1}{(\epsilon_{b\sigma} - \epsilon_{c\sigma} - \Omega_s)(\epsilon_{b\sigma} - \epsilon_{i\sigma})}$

together, we get:

$$
\begin{aligned}
I_{ib} = 2\pi i \Bigg(\sum_{ks} w^s_{ik\sigma} w^s_{bk\sigma} \Bigg(& \frac{1}{(\epsilon_{k\sigma} - \epsilon_{i\sigma} - \Omega_s)(\epsilon_{k\sigma} - \epsilon_{b\sigma} - \Omega_s)} \\
& + \frac{1}{(\epsilon_{i\sigma} - \epsilon_{k\sigma} + \Omega_s)(\epsilon_{i\sigma} - \epsilon_{b\sigma})} \Bigg) \\
& + \sum_{cs} w^s_{ic\sigma} w^s_{bc\sigma} \Bigg(\frac{1}{(\epsilon_{c\sigma} + \Omega_s - \epsilon_{i\sigma})(\epsilon_{c\sigma} + \Omega_s - \epsilon_{b\sigma})} \\
& + \frac{1}{(\epsilon_{b\sigma} - \epsilon_{c\sigma} - \Omega_s)(\epsilon_{b\sigma} - \epsilon_{i\sigma})} \Bigg) \Bigg)
\end{aligned}
\tag{58}
$$

Let us make some simplifications on the first term:

$$
\begin{aligned}
& \Bigg(\frac{1}{(\epsilon_{k\sigma} - \epsilon_{i\sigma} - \Omega_s)(\epsilon_{k\sigma} - \epsilon_{b\sigma} - \Omega_s)} \\
& + \frac{1}{(\epsilon_{i\sigma} - \epsilon_{k\sigma} + \Omega_s)(\epsilon_{i\sigma} - \epsilon_{b\sigma})} \Bigg) \\
& = \frac{(\epsilon_{i\sigma} - \epsilon_{b\sigma})}{(\epsilon_{k\sigma} - \epsilon_{i\sigma} - \Omega_s)(\epsilon_{k\sigma} - \epsilon_{b\sigma} - \Omega_s)(\epsilon_{i\sigma} - \epsilon_{b\sigma})} - \frac{(\epsilon_{k\sigma} - \epsilon_{b\sigma} + \Omega_s)}{(\epsilon_{k\sigma} - \epsilon_{i\sigma} + \Omega_s)(\epsilon_{k\sigma} - \epsilon_{b\sigma} - \Omega_s)(\epsilon_{i\sigma} - \epsilon_{b\sigma})} \\
& = - \frac{(\epsilon_{k\sigma} - \epsilon_{i\sigma} - \Omega_s)}{(\epsilon_{k\sigma} - \epsilon_{i\sigma} - \Omega_s)(\epsilon_{k\sigma} - \epsilon_{b\sigma} - \Omega_s)(\epsilon_{i\sigma} - \epsilon_{b\sigma})} = - \frac{1}{(\epsilon_{k\sigma} - \epsilon_{b\sigma} - \Omega_s)(\epsilon_{i\sigma} - \epsilon_{b\sigma})}
\end{aligned}
\tag{59}
$$

Doing the same for the second term will give:

$$
\begin{aligned}
& \Bigg(\frac{1}{(\epsilon_{c\sigma} + \Omega_s - \epsilon_{i\sigma})(\epsilon_{c\sigma} + \Omega_s - \epsilon_{b\sigma})} \\
& + \frac{1}{(\epsilon_{b\sigma} - \epsilon_{c\sigma} - \Omega_s)(\epsilon_{b\sigma} - \epsilon_{i\sigma})} \Bigg) \\
& = \frac{(\epsilon_{b\sigma} - \epsilon_{i\sigma})}{(\epsilon_{c\sigma} + \Omega_s - \epsilon_{i\sigma})(\epsilon_{c\sigma} + \Omega_s - \epsilon_{b\sigma})(\epsilon_{b\sigma} - \epsilon_{i\sigma})} - \frac{(\epsilon_{c\sigma} + \Omega_s - \epsilon_{i\sigma})}{(\epsilon_{c\sigma} + \Omega_s - \epsilon_{i\sigma})(\epsilon_{c\sigma} + \Omega_s - \epsilon_{b\sigma})(\epsilon_{b\sigma} - \epsilon_{i\sigma})} \\
& = \frac{\epsilon_{b\sigma} - \epsilon_{c\sigma} - \Omega_s}{(\epsilon_{c\sigma} + \Omega_s - \epsilon_{i\sigma})(\epsilon_{c\sigma} + \Omega_s - \epsilon_{b\sigma})(\epsilon_{b\sigma} - \epsilon_{i\sigma})} = - \frac{1}{(\epsilon_{c\sigma} + \Omega_s - \epsilon_{i\sigma})(\epsilon_{b\sigma} - \epsilon_{i\sigma})}
\end{aligned}
\tag{60}
$$

So, the expression for D_{ib} is:

$$D_{ib} = \langle i\sigma | \gamma_0^\sigma | b\sigma \rangle + \frac{2\pi i^2}{2\pi\left(\epsilon_{i\sigma} - \epsilon_{b\sigma}\right)} \left[\sum_{ks} \frac{w_{ik}^s w_{bk}^s}{\epsilon_{k\sigma} - \epsilon_{b\sigma} - \Omega_s} - \sum_{cs} \frac{w_{ic}^s w_{bc}^s}{\epsilon_{c\sigma} + \Omega_s - \epsilon_{i\sigma}} \right] \tag{61}$$

The matrix element of the noninteracting density matrix does not mix copied wait virtual states and we relabel the occupied index $k \to j$ and the virtual index $c \to a$:

$$D_{ib} = \frac{1}{\epsilon_{i\sigma} - \epsilon_{b\sigma}} \left[\sum_{as} \frac{w_{ia}^s w_{ba}^s}{\epsilon_{i\sigma} - \epsilon_{a\sigma} - \Omega_s} - \sum_{js} \frac{w_{ij}^s w_{bj}^s}{\epsilon_{j\sigma} - \epsilon_{b\sigma} - \Omega_s} \right] \tag{62}$$

I am just curious what would happen if we chose the opposite contour for the previous integrations. We would just have one pole in D_- at $\omega_{11} = \epsilon_{b\sigma} - \mathrm{i}\eta$ for the first term and $\omega_{21} = \epsilon_{i\sigma} + \mathrm{i}\eta$ for the second term. The residues would be:

$$\begin{aligned} \phi_{\omega_{11}}(\epsilon_{b\sigma} - \mathrm{i}\eta) &= \frac{1}{(\epsilon_{b\sigma} - \epsilon_{k\sigma} + \Omega_s)(\epsilon_{b\sigma} - \epsilon_{i\sigma})} \\ \phi_{\omega_{21}}(\epsilon_{i\sigma} + \mathrm{i}\eta) &= \frac{1}{(\epsilon_{i\sigma} - \epsilon_{c\sigma} - \Omega_s)(\epsilon_{i\sigma} - \epsilon_{b\sigma})} \end{aligned} \tag{63}$$