Linearized G_0W_0 Density Matrix

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We have the equation for the density matrix:

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

with the following definitions:

$$D_{pq\sigma}=\langle p\sigma\left|\gamma^{\sigma}\right|q\sigma\rangle \tag{2}$$

Now we want to apply this bra-ket notation to the equation above. We can write the equation as, also redefining the integration over $\mathbf{r}_3$ and $\mathbf{r}_4$ as $\sum_r$ and $\sum_t$, respectively:

$$D_{pq\sigma}=\langle p\sigma|\,\gamma_0^{\sigma}\,|q\sigma\rangle-\frac{\mathrm{i}}{2\pi}\sum_r\sum_t\int \mathrm{d}\omega \mathrm{e}^{\mathrm{i}\omega\eta}\,\langle p\sigma|\,G_0^{\sigma}(\omega)\,|r\sigma\rangle\,\langle r\sigma|\,\Sigma_c^{\sigma}(\omega)\,|t\sigma\rangle\,\langle t\sigma|\,G_0^{\sigma}(\omega)\,|q\sigma\rangle \tag{3}$$

with the following definitions:

$$G_{0pq}^{\sigma}=\sum_i\frac{\delta_{pq}\delta_{pi}}{\omega-\epsilon_{i\sigma}-\mathrm{i}\eta}+\sum_a\frac{\delta_{pq}\delta_{pa}}{\omega-\epsilon_{a\sigma}+\mathrm{i}\eta} \tag{4}$$

and

$$\Sigma_{cpq}^{\sigma}(\omega)=\sum_{is}\frac{w_{pi\sigma}^{s}w_{qi\sigma}^{s}}{\omega-\epsilon_{i\sigma}+\Omega_s-\mathrm{i}\eta}+\sum_{as}\frac{w_{pa\sigma}^{s}w_{qa\sigma}^{s}}{\omega-\epsilon_{a\sigma}-\Omega_s+\mathrm{i}\eta} \tag{5}$$

Plugging in these definitions, we get:

$$D_{pq\sigma} = \langle p\sigma| \gamma_0^\sigma |q\sigma\rangle - \frac{\mathrm{i}}{2\pi}\sum_r\sum_t \int \mathrm{d}\omega e^{\mathrm{i}\omega\eta} \left(\sum_i \frac{\delta_{pr}\delta_{ri}}{\omega-\epsilon_{i\sigma}-\mathrm{i}\eta} + \sum_a \frac{\delta_{pr}\delta_{ra}}{\omega-\epsilon_{a\sigma}+\mathrm{i}\eta}\right) \left(\sum_{is} \frac{w^s_{ri\sigma}w^s_{ti\sigma}}{\omega-\epsilon_{i\sigma}+\Omega_s-\mathrm{i}\eta} + \sum_{as} \frac{w^s_{ra\sigma}w^s_{ta\sigma}}{\omega-\epsilon_{a\sigma}-\Omega_s+\mathrm{i}\eta}\right) \left(\sum_i \frac{\delta_{tq}\delta_{ti}}{\omega-\epsilon_{i\sigma}-\mathrm{i}\eta} + \sum_a \frac{\delta_{tq}\delta_{ta}}{\omega-\epsilon_{a\sigma}+\mathrm{i}\eta}\right) \tag{6}$$

Now we consider only the integral over ω:

$$I = \sum_r\sum_t \int \mathrm{d}\omega e^{\mathrm{i}\omega\eta} \left(\sum_i \frac{\delta_{pr}\delta_{ri}}{\omega-\epsilon_{i\sigma}-\mathrm{i}\eta} + \sum_a \frac{\delta_{pr}\delta_{ra}}{\omega-\epsilon_{a\sigma}+\mathrm{i}\eta}\right) \left(\sum_{is} \frac{w^s_{ri\sigma}w^s_{ti\sigma}}{\omega-\epsilon_{i\sigma}+\Omega_s-\mathrm{i}\eta} + \sum_{as} \frac{w^s_{ra\sigma}w^s_{ta\sigma}}{\omega-\epsilon_{a\sigma}-\Omega_s+\mathrm{i}\eta}\right) \left(\sum_i \frac{\delta_{tq}\delta_{ti}}{\omega-\epsilon_{i\sigma}-\mathrm{i}\eta} + \sum_a \frac{\delta_{tq}\delta_{ta}}{\omega-\epsilon_{a\sigma}+\mathrm{i}\eta}\right) \tag{7}$$

Considering the first two parenthesis, we notice that the latter delta functions for the first and second expression in the first term will only be non-zero when they multiply the first and second expression in the second term, respectively. This means that we can simplify the expression to:

$$I = \sum_r\sum_t \Bigg(\int \mathrm{d}\omega e^{\mathrm{i}\omega\eta} \sum_i \frac{\delta_{pr}\delta_{ri}}{\omega-\epsilon_{i\sigma}-\mathrm{i}\eta} \sum_{is} \frac{w^s_{ri\sigma}w^s_{ti\sigma}}{\omega-\epsilon_{i\sigma}+\Omega_s-\mathrm{i}\eta} \sum_i \frac{\delta_{tq}\delta_{ti}}{\omega-\epsilon_{i\sigma}-\mathrm{i}\eta} + \int \mathrm{d}\omega e^{\mathrm{i}\omega\eta} \sum_a \frac{\delta_{pr}\delta_{ra}}{\omega-\epsilon_{a\sigma}+\mathrm{i}\eta} \sum_{as} \frac{w^s_{ra\sigma}w^s_{ta\sigma}}{\omega-\epsilon_{a\sigma}-\Omega_s+\mathrm{i}\eta} \sum_a \frac{\delta_{tq}\delta_{ta}}{\omega-\epsilon_{a\sigma}+\mathrm{i}\eta}\Bigg) \tag{8}$$

The delta function terms will pick out a single term in the sum over excitation vector, so we can relabel the indices to:

$$I = \left(\int \mathrm{d}\omega e^{\mathrm{i}\omega\eta} \sum_{is} \frac{w^s_{pi\sigma}w^s_{qi\sigma}}{\omega-\epsilon_{i\sigma}+\Omega_s-\mathrm{i}\eta} \left(\frac{1}{\omega-\epsilon_{i\sigma}-\mathrm{i}\eta}\right)^2\right) + \left(\int \mathrm{d}\omega e^{\mathrm{i}\omega\eta} \sum_{as} \frac{w^s_{pa\sigma}w^s_{qa\sigma}}{\omega-\epsilon_{a\sigma}-\Omega_s+\mathrm{i}\eta} \left(\frac{1}{\omega-\epsilon_{a\sigma}+\mathrm{i}\eta}\right)^2\right) \tag{9}$$

Considering only the first term we can swab the summation with the integral:

$$I_1 = \sum_{is} \left(w^s_{pi\sigma}w^s_{qi\sigma}\right) \int \mathrm{d}\omega e^{\mathrm{i}\omega\eta} \frac{1}{\omega-\epsilon_{i\sigma}+\Omega_s-\mathrm{i}\eta} \left(\frac{1}{\omega-\epsilon_{i\sigma}-\mathrm{i}\eta}\right)^2 \tag{10}$$

This suggests a simple pole at $\omega = \epsilon_{i\sigma} - \Omega_s + \mathrm{i}\eta$ and a pole of the second order at $\omega = \epsilon_{i\sigma} + \mathrm{i}\eta$. We have:

$$f(\omega) = \frac{\mathrm{e}^{\mathrm{i}\omega\eta}}{\omega - \epsilon_{i\sigma} + \Omega_s - \mathrm{i}\eta} \left(\frac{1}{\omega - \epsilon_{i\sigma} - \mathrm{i}\eta} \right)^2 \tag{11}$$

We start by considering the first pole at $\omega = \epsilon_{i\sigma} - \Omega_s + \mathrm{i}\eta$. We consider:

$$g_0(\omega) = (\omega - \epsilon_{i\sigma} + \Omega_s - \mathrm{i}\eta)\, f(\omega) = e^{i\omega\eta} \left(\frac{1}{\omega - \epsilon_{i\sigma} - i\eta} \right)^2 \tag{12}$$

Evaluating this at the pole, we get:

$$g_0(\epsilon_{i\sigma} - \Omega_s + \mathrm{i}\eta) = e^{i(\epsilon_{i\sigma} - \Omega_s + \mathrm{i}\eta)\eta} \left(-\frac{1}{\Omega_s} \right)^2 \tag{13}$$

Now we consider the second pole at $\omega = \epsilon_{i\sigma} + \mathrm{i}\eta$. We consider:

$$g_1(\omega) = (\omega - \epsilon_{i\sigma} - \mathrm{i}\eta)^2\, f(\omega) = \frac{e^{i\omega\eta}}{\omega - \epsilon_{i\sigma} + \Omega_s - \mathrm{i}\eta} \tag{14}$$

Evaluating this at the pole, we get:

$$g_1(\epsilon_{i\sigma} + \mathrm{i}\eta) = \frac{e^{i(\epsilon_{i\sigma} + \mathrm{i}\eta)\eta}}{\Omega_s} \tag{15}$$

So,

$$I_1 = 2\pi i \sum_{is} \left(w^s_{pi\sigma} w^s_{qi\sigma} \right) \left(e^{i(\epsilon_{i\sigma} - \Omega_s + \mathrm{i}\eta)\eta} \left(-\frac{1}{\Omega_s} \right)^2 + \frac{e^{i(\epsilon_{i\sigma} + \mathrm{i}\eta)\eta}}{\Omega_s} \right) \tag{16}$$

Now we consider the second term:

$$I_2 = \sum_{as} \left(w^s_{pa\sigma} w^s_{qa\sigma} \right) \int \mathrm{d}\omega \mathrm{e}^{\mathrm{i}\omega\eta} \frac{1}{\omega - \epsilon_{a\sigma} - \Omega_s + \mathrm{i}\eta} \left(\frac{1}{\omega - \epsilon_{a\sigma} + \mathrm{i}\eta} \right)^2 \tag{17}$$

This suggests a simple pole at $\omega = \epsilon_{a\sigma} + \Omega_s - \mathrm{i}\eta$ and a pole of the second order at $\omega = \epsilon_{a\sigma} - \mathrm{i}\eta$. We have:

$$f(\omega) = \frac{\mathrm{e}^{\mathrm{i}\omega\eta}}{\omega - \epsilon_{a\sigma} - \Omega_s + \mathrm{i}\eta} \left(\frac{1}{\omega - \epsilon_{a\sigma} + \mathrm{i}\eta} \right)^2 \tag{18}$$

We start by considering the first pole at $\omega = \epsilon_{a\sigma} + \Omega_s - \mathrm{i}\eta$. We consider:

$$g_0(\omega) = (\omega - \epsilon_{a\sigma} - \Omega_s + \mathrm{i}\eta)\, f(\omega) = e^{i\omega\eta} \left(\frac{1}{\omega - \epsilon_{a\sigma} + i\eta} \right)^2 \tag{19}$$

Evaluating this at the pole, we get:

$$g_0(\epsilon_{a\sigma} + \Omega_s - \mathrm{i}\eta) = e^{i(\epsilon_{a\sigma} + \Omega_s - \mathrm{i}\eta)\eta} \left(\frac{1}{\Omega_s} \right)^2 \tag{20}$$

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

$$g_1(\omega) = (\omega - \epsilon_{a\sigma} - \mathrm{i}\eta)^2\, f(\omega) = \frac{e^{i\omega\eta}}{\omega - \epsilon_{a\sigma} - \Omega_s + \mathrm{i}\eta} \tag{21}$$

Evaluating this at the pole, we get:

$$g_1(\epsilon_{a\sigma} - \mathrm{i}\eta) = -\frac{e^{i(\epsilon_{a\sigma} - \mathrm{i}\eta)\eta}}{\Omega_s} \tag{22}$$

So,

$$I_2 = 2\pi i \sum_{as} \left(w^s_{pa\sigma} w^s_{qa\sigma} \right) \left(e^{i(\epsilon_{a\sigma} + \Omega_s - \mathrm{i}\eta)\eta} \left(\frac{1}{\Omega_s} \right)^2 - \frac{e^{i(\epsilon_{a\sigma} - \mathrm{i}\eta)\eta}}{\Omega_s} \right) \tag{23}$$

So,

$$\begin{aligned} I =& I_1 + I_2 \\ =& 2\pi i \sum_{is} \left(w^s_{pi\sigma} w^s_{qi\sigma} \right) \left(e^{i(\epsilon_{i\sigma} - \Omega_s + \mathrm{i}\eta)\eta} \left(-\frac{1}{\Omega_s} \right)^2 + \frac{e^{i(\epsilon_{i\sigma} + \mathrm{i}\eta)\eta}}{\Omega_s} \right) \\ &+ 2\pi i \sum_{as} \left(w^s_{pa\sigma} w^s_{qa\sigma} \right) \left(e^{i(\epsilon_{a\sigma} + \Omega_s - \mathrm{i}\eta)\eta} \left(\frac{1}{\Omega_s} \right)^2 - \frac{e^{i(\epsilon_{a\sigma} - \mathrm{i}\eta)\eta}}{\Omega_s} \right) \end{aligned} \tag{24}$$