GW Approximation in ωk space

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1 Green function $G^{(0)}$

$$G^{(0)}(\zeta_1, \zeta_2; \omega) = \sum_i \frac{\phi_i^{(0)}(\zeta_1)\phi_i^{(0)*}(\zeta_2)}{\omega - \epsilon_i^{(0)} + i\eta \operatorname{sgn}\left(\epsilon_i^{(0)} - \mu\right)}$$

$$G^{(0)}(r_1, r_2; \omega) = \sum_i \frac{\phi_i^{(0)}(r_1)\phi_i^{(0)*}(r_2)}{\omega - \epsilon_i^{(0)} + i\eta \operatorname{sgn}\left(\epsilon_i^{(0)} - \mu\right)}$$

$$\begin{aligned}
G^{(0)}(r_1, r_2; \omega) &= \sum_{\xi_1\xi_2} G^{(0)}(\zeta_1, \zeta_2; \omega) \\
&= \sum_{\xi_1\xi_2} \sum_i \frac{\phi_i^{(0)}(\zeta_1)\phi_i^{(0)*}(\zeta_2)}{\omega - \epsilon_i^{(0)} + i\eta \operatorname{sgn}\left(\epsilon_i^{(0)} - \mu\right)} \\
&= \sum_{\xi_1} \sum_i \frac{\phi_i^{(0)}(\zeta_1)}{\omega - \epsilon_i^{(0)} + i\eta \operatorname{sgn}\left(\epsilon_i^{(0)} - \mu\right)} \left(\phi_i^{(0)*}(r_2, \xi_2 = -1/2) + \phi_i^{(0)*}(r_2, \xi_2 = +1/2)\right) \\
&= \sum_{\xi_1} \sum_i \frac{\phi_i^{(0)}(\zeta_1)}{\omega - \epsilon_i^{(0)} + i\eta \operatorname{sgn}\left(\epsilon_i^{(0)} - \mu\right)} \phi_i^{(0)*}(r_2) \\
&= \sum_i \left(\phi_i^{(0)}(r_1, \xi_1 = -1/2) + \phi_i^{(0)}(r_1, \xi_1 = +1/2)\right) \frac{\phi_i^{(0)*}(r_2)}{\omega - \epsilon_i^{(0)} + i\eta \operatorname{sgn}\left(\epsilon_i^{(0)} - \mu\right)}
\end{aligned}$$

2 Screened Interaction

$$W(\zeta_1, \zeta_2, \omega) = \int d\zeta_3\, \varepsilon^{-1}(\zeta_1, \zeta_3, \omega) w(\zeta_3, \zeta_2)$$

$$W(\zeta_1, \zeta_2, \omega) = W(r_1, r_2, \omega) = \int dr_3\, \varepsilon^{-1}(r_1, r_3, \omega) w(r_3, r_2) \qquad \text{spin independent (but it's not the case of } \varepsilon)$$

$$w(r_1, r_2) = \frac{1}{|r_1 - r_2|} \qquad \text{coulombian many body interaction}$$

$$w(q, G) = \frac{4\pi}{|q + G|^2} \qquad \text{fourier transform of the coulombian interaction}$$

$$\begin{aligned}
W(r_1, r_2, \omega) &= \int dr_3\, \varepsilon^{-1}(r_1, r_3, \omega) w(r_3, r_2) \\
W(r_1, r_2, \omega) &= \int dr_3\, \frac{1}{(2\pi)^3} \int_{\mathrm{BZ}} dq \sum_{G_1, G_3} e^{i(q+G_1)r_1} \varepsilon^{-1}(q, G_1, G_3, \omega) e^{-i(q+G_3)r_3}\,\cdot \\
&\quad \cdot \frac{1}{(2\pi)^3} \int_{\mathrm{BZ}} dq_1 \sum_{G_2} e^{i(q_1+G_2)r_3} \frac{4\pi}{(q_1 + G_2)^2} e^{-i(q_1+G_2)r_2} \\
&\quad \int dr_3\, e^{-i(q+G_3)r_3} e^{i(q_1+G_2)r_3} = (2\pi)^3 \delta(q - q_1) \delta(G_3 - G_2) \\
W(r_1, r_2, \omega) &= \frac{1}{(2\pi)^3} \int_{\mathrm{BZ}} dq \sum_{G_1, G_2} e^{i(q+G_1)r_1} \varepsilon^{-1}(q, G_1, G_2, \omega) \frac{4\pi}{(q + G_2)^2} e^{-i(q+G_2)r_2}
\end{aligned}$$

$$\begin{aligned}
W(r_1, r_2, \omega) &= \frac{1}{\Omega} \sum_{q, G_1, G_2} e^{i(q+G_1)r_1} W(q, G_1, G_2, \omega) e^{-i(q+G_2)r_2} \\
&= \frac{1}{\Omega} \sum_{q, G_1, G_2} e^{i(q+G_1)r_1} \varepsilon^{-1}(q, G_1, G_2, \omega) \frac{4\pi}{|q + G_2|^2} e^{-i(q+G_2)r_2}
\end{aligned}$$

$$W(q, G_1, G_2, \omega) = \varepsilon^{-1}(q, G_1, G_2, \omega) \frac{4\pi}{|q + G_2|^2} = \bar{\varepsilon}^{-1}(q, G_1, G_2, \omega) \frac{4\pi}{|q + G_1||q + G_2|}$$

$\bar{\varepsilon}$ = symmetrized epsilon.

3 Single Plasmon Pole Model

$$\varepsilon^{-1}(\omega) = \delta + \frac{\Omega^2}{\omega^2 - \tilde{\omega}^2}$$

$$\varepsilon^{-1}(G, G', q, \omega) = \delta(G, G') + \frac{\Omega^2(G, G', q)}{\omega^2 - \tilde{\omega}^2(G, G', q)}$$

The poles are in $\omega = \pm\tilde{\omega}$.

$$A(G, G', q) = -\frac{\Omega^2(G, G', q)}{\tilde{\omega}^2(G, G', q)} = \varepsilon^{-1}(G, G', q, 0) - \delta(G, G')$$

$$\tilde{\omega}^2(G, G', q) = \left[\frac{A(G, G', q)}{\varepsilon^{-1}(G, G', q, 0) - \varepsilon^{-1}(G, G', q, iE_0)} - 1\right] E_0^2$$

$$\begin{aligned}
\varepsilon^{-1}(iE_0) &= \delta + \frac{\Omega^2}{-E_0^2 - \tilde{\omega}^2} \\
\varepsilon^{-1}(iE_0)[E_0^2 + \tilde{\omega}^2] &= \delta[E_0^2 + \tilde{\omega}^2] - \frac{\Omega^2}{\tilde{\omega}^2}\tilde{\omega}^2 = \delta E_0^2 + \varepsilon^{-1}(0)\tilde{\omega}^2 \\
\tilde{\omega}^2 &= \frac{\varepsilon^{-1}(iE_0) - \delta}{\varepsilon^{-1}(0) - \varepsilon^{-1}(iE_0)} E_0^2 \\
&= \left[\frac{\varepsilon^{-1}(iE_0) - \delta}{\varepsilon^{-1}(0) - \varepsilon^{-1}(iE_0)} + \frac{\varepsilon^{-1}(0) - \varepsilon^{-1}(iE_0)}{\varepsilon^{-1}(0) - \varepsilon^{-1}(iE_0)} - 1\right] E_0^2 \\
\tilde{\omega}^2 &= \left[\frac{\varepsilon^{-1}(0) - \delta}{\varepsilon^{-1}(0) - \varepsilon^{-1}(iE_0)} - 1\right] E_0^2 = \left[\frac{A}{\varepsilon^{-1}(0) - \varepsilon^{-1}(iE_0)} - 1\right] E_0^2
\end{aligned}$$

4 GW approximation for the Self-Energy

$$\tilde{\Sigma}_{\mathrm{M}}^{\mathrm{GW}}(x_1, x_2) = iG(x_1, x_2)W(x_1^+, x_2)$$

$$\tilde{\Sigma}_{\mathrm{M}}^{\mathrm{GW}}(\zeta_1, \zeta_2, \omega) = \frac{i}{2\pi}\int d\omega'\, e^{-i\omega'\eta} G(\zeta_1, \zeta_2, \omega - \omega')W(\zeta_1, \zeta_2, \omega')$$

W is spin-independent and G does not take factors 2 on spin sum:

$$\tilde{\Sigma}_{\mathrm{M}}^{\mathrm{GW}}(r_1, r_2, \omega) = \frac{i}{2\pi}\int d\omega'\, e^{-i\omega'\eta} G(r_1, r_2, \omega - \omega')W(r_1, r_2, \omega')$$

$$\begin{aligned}\tilde{\Sigma}_{\mathrm{M}}^{\mathrm{GW}}(r_1, r_2, \omega) \quad = \quad & \frac{i}{2\pi}\int d\omega'\, e^{-i\omega'\eta} \sum_i \frac{\phi_i^{(0)}(r_1)\phi_i^{(0)*}(r_2)}{\omega - \omega' - \epsilon_i^{(0)} + i\eta\, \mathrm{sgn}\left(\epsilon_i^{(0)} - \mu\right)} \cdot \\ & \cdot \frac{1}{\Omega}\sum_{q,G_1,G_2} e^{i(q+G_1)r_1}\bar{\varepsilon}^{-1}(q, G_1, G_2, \omega')\frac{4\pi}{|q+G_1||q+G_2|}e^{-i(q+G_2)r_2}\end{aligned}$$

5 Matrix elements of the Self-Energy operator

$$\begin{aligned}\langle\phi_j^{(0)}(r_1)|\tilde{\Sigma}_{\mathrm{M}}^{\mathrm{GW}}(r_1, r_2, \omega)|\phi_j^{(0)}(r_2)\rangle \quad = \quad & \frac{i}{2\pi}\frac{1}{\Omega}\sum_{q,G_1,G_2}\frac{4\pi}{|q+G_1||q+G_2|}\sum_i \cdot \\ & \cdot \int dr_1\, \phi_j^{(0)*}(r_1)e^{i(q+G_1)r_1}\phi_i^{(0)}(r_1)\int dr_2\, \phi_i^{(0)*}(r_2)e^{-i(q+G_2)r_2}\phi_j^{(0)}(r_2) \cdot \\ & \cdot \int_{-\infty}^{+\infty} d\omega'\, e^{-i\omega'\eta}\frac{1}{\omega - \omega' - \epsilon_i^{(0)} + i\eta\, \mathrm{sgn}\left(\epsilon_i^{(0)} - \mu\right)}\bar{\varepsilon}^{-1}(q, G_1, G_2, \omega')\end{aligned}$$

$$i = \{n_i, k_i\}$$

$$\rho_{ij}(G) = \int dr\, \phi_i^{(0)*}(r)e^{-i(q+G)r}\phi_j^{(0)}(r) \qquad \text{with} \qquad q = k_j - k_i - G_0, \quad q \in 1\mathrm{BZ}$$

$$\begin{aligned}\langle j|\tilde{\Sigma}_{\mathrm{M}}^{\mathrm{GW}}(\omega)|j\rangle \quad = \quad & \frac{i}{2\pi}\frac{1}{\Omega}\sum_i\sum_{G_1,G_2}\delta(q - (k_j - k_i - G_0))\frac{4\pi}{|q+G_1||q+G_2|}\rho_{ij}^*(G_1)\rho_{ij}(G_2) \cdot \\ & \cdot \int_{-\infty}^{+\infty} d\omega''\, e^{i\omega''\eta}\frac{1}{\omega'' + \omega - \epsilon_i^{(0)} + i\eta\, \mathrm{sgn}\left(\epsilon_i^{(0)} - \mu\right)}\bar{\varepsilon}^{-1}(q, G_1, G_2, \omega'')\end{aligned}$$

$$\varepsilon^{-1}(q, G, G', \omega) \quad \rightarrow \quad \delta(G, G') \qquad \rightarrow \Sigma_x \qquad \text{Sigma exchange}$$

$$\varepsilon^{-1}(q, G, G', \omega) \quad \rightarrow \quad \frac{\Omega^2(q, G, G')}{\omega^2 - \tilde{\omega}^2(q, G, G')} \qquad \rightarrow \Sigma_c \qquad \text{Sigma correlation}$$

6 Self-Energy: exchange term

$$\begin{aligned} \langle j|\tilde{\Sigma}_x^{\mathrm{GW}}(\omega)|j\rangle &= \frac{i}{2\pi}\frac{1}{\Omega}\sum_i\sum_{G_1}\delta(q-(k_j-k_i-G_0))\frac{4\pi}{|q+G_1|^2}|\rho_{ij}(G_1)|^2 \cdot \\ &\cdot \oint_{\circlearrowleft} d\omega''\, e^{i\omega''\eta}\frac{1}{\omega''+\omega-\epsilon_i^{(0)}+i\eta\,\mathrm{sgn}\left(\epsilon_i^{(0)}-\mu\right)} \end{aligned}$$

Only the the poles of G in the upper half imaginary ω-plane are included in the closed, anti-clockwise path. They correspond to the particle poles (excitation corresponding to occupied states). The integral yields ($f_i = 0, 1$ occupation number):

$$\oint d\omega''... = 2\pi i f_i \mathrm{Res}_i = 2\pi i f_i$$

$$\langle j|\tilde{\Sigma}_x^{\mathrm{GW}}|j\rangle = -\frac{4\pi}{\Omega}\sum_i f_i\sum_{G_1}\delta(q-(k_j-k_i-G_0))\frac{1}{|q+G_1|^2}|\rho_{ij}(G_1)|^2$$

it does not depend on ω because it constitutes only a shift term of the poles along the real axis which doesn't change the integral.

7 Self-Energy: correlation term

$$\begin{aligned}\langle j|\tilde{\Sigma}_c^{\mathrm{GW}}(\omega)|j\rangle &= \frac{i}{2\pi}\frac{1}{\Omega}\sum_i\sum_{G_1,G_2}\delta(q-(k_j-k_i-G_0))\frac{4\pi}{|q+G_1||q+G_2|}\rho_{ij}^*(G_1)\rho_{ij}(G_2)\cdot \\ &\cdot\oint d\omega''\,e^{i\omega''\eta}\frac{1}{\omega''+\omega-\epsilon_i^{(0)}+i\eta\,\mathrm{sgn}\left(\epsilon_i^{(0)}-\mu\right)}\frac{\Omega^2(q,G_1,G_2)}{\omega''^2-(\tilde{\omega}(q,G_1,G_2)-i\eta)^2}\end{aligned}$$

The plasmon pole model presents a pole in the upper half plane for ω'' negative at $-\tilde{\omega}+i\eta$ and a pole in the bottom half plane for ω'' positive at $\tilde{\omega}-i\eta$

$$\oint d\omega''\,e^{i\omega''\eta}\frac{1}{\omega''+\omega-\epsilon_i^{(0)}+i\eta\,\mathrm{sgn}\left(\epsilon_i^{(0)}-\mu\right)}\frac{1}{(\omega''-\tilde{\omega}+i\eta)(\omega''+\tilde{\omega}-i\eta)}$$

The included poles are in $\omega''=-\tilde{\omega}+i\eta$ and if $f_i=1$ in $\omega''=\epsilon_i^{(0)}-\omega+i\eta$.

$$\begin{aligned}\oint d\omega''\ldots &= 2\pi i\left(\frac{f_i}{(\epsilon_i^{(0)}-\omega)^2-\tilde{\omega}^2}+\frac{1}{\omega-\tilde{\omega}-\epsilon_i^{(0)}}\frac{1}{-2\tilde{\omega}}\right) \\ &= -i\pi\left(\frac{1}{\tilde{\omega}(\omega-\tilde{\omega}-\epsilon_i^{(0)})}-\frac{2f_i}{(\omega-\epsilon_i^{(0)})^2-\tilde{\omega}^2}\right) \\ &= -i\pi\left(\frac{\omega-\epsilon_i^{(0)}+\tilde{\omega}}{\tilde{\omega}(\omega-\epsilon_i^{(0)}+\tilde{\omega})(\omega-\epsilon_i^{(0)}-\tilde{\omega})}-\frac{\tilde{\omega}2f_i}{\tilde{\omega}(\omega-\epsilon_i^{(0)}+\tilde{\omega})(\omega-\epsilon_i^{(0)}-\tilde{\omega})}\right) \\ &= -i\pi\frac{\omega-\epsilon_i^{(0)}-\tilde{\omega}(2f_i-1)}{\tilde{\omega}(\omega-\epsilon_i^{(0)}+\tilde{\omega})(\omega-\epsilon_i^{(0)}-\tilde{\omega})}\frac{\omega-\epsilon_i^{(0)}+\tilde{\omega}(2f_i-1)}{\omega-\epsilon_i^{(0)}+\tilde{\omega}(2f_i-1)} \\ &= -i\pi\frac{(\omega-\epsilon_i^{(0)})^2-\tilde{\omega}^2(2f_i-1)^2}{(\omega-\epsilon_i^{(0)})^2-\tilde{\omega}^2}\frac{1}{\tilde{\omega}(\omega-\epsilon_i^{(0)}+\tilde{\omega}(2f_i-1))} \\ &= -i\pi\frac{1}{\tilde{\omega}(\omega-\epsilon_i^{(0)}+\tilde{\omega}(2f_i-1))}\end{aligned}$$

Here we mean that we should replace $\tilde{\omega}\to\tilde{\omega}-i\eta$ and $\epsilon_i^{(0)}\to\epsilon_i^{(0)}-i\eta\,\mathrm{sgn}(\epsilon_i^{(0)}-\mu)$
As $(2f_i-1)^2$ is always 1.

$$\begin{aligned}\langle j|\tilde{\Sigma}_c^{\mathrm{GW}}(\omega)|j\rangle &= \frac{2\pi}{\Omega}\sum_i\sum_{G_1,G_2}\delta(q-(k_j-k_i-G_0))\frac{\rho_{ij}^*(G_1)\rho_{ij}(G_2)}{|q+G_1||q+G_2|}\cdot \\ &\cdot\frac{\Omega^2(q,G_1,G_2)}{\tilde{\omega}(q,G_1,G_2)(\omega-\epsilon_i^{(0)}+\tilde{\omega}(q,G_1,G_2)(2f_i-1))}\end{aligned}$$

8 Self-Energy: correlation term without plasmon pole model

$$\begin{aligned}\langle j|\tilde{\Sigma}_c^{\mathrm{GW}}(\omega)|j\rangle &= \frac{i}{2\pi}\frac{1}{\Omega}\sum_i \sum_{q,G_1,G_2} \delta(q-(k_j-k_i-G_0))\frac{4\pi}{|q+G_1||q+G_2|}\rho_{ij}^*(G_1)\rho_{ij}(G_2)\cdot \\ &\quad \cdot \int_{-\infty}^{+\infty} d\omega''\, e^{i\omega''\eta}\frac{1}{\omega''+\omega-\epsilon_i^{(0)}+i\eta\,\mathrm{sgn}\left(\epsilon_i^{(0)}-\mu\right)}\bar{\varepsilon}_c^{-1}(q,G_1,G_2,\omega'')\end{aligned}$$

where the correlation part of the inverse dielectric matrix is

$$\bar{\varepsilon}_c^{-1}(q,G_1,G_2,\omega) = \bar{\varepsilon}^{-1}(q,G_1,G_2,\omega) - \delta(G_1,G_2)$$

the dielectric function is symmetric in ω

$$\bar{\varepsilon}^{-1}(q,G_1,G_2,-\omega) = \bar{\varepsilon}^{-1}(q,G_1,G_2,\omega)$$

$$\begin{aligned}\langle j|\tilde{\Sigma}_c^{\mathrm{GW}}(\omega)|j\rangle &= \frac{1}{\Omega}\sum_i \sum_{q,G_1,G_2} \delta(q-(k_j-k_i-G_0))\frac{4\pi}{|q+G_1||q+G_2|}\rho_{ij}^*(G_1)\rho_{ij}(G_2)\cdot \\ &\quad \cdot\Big\{ -\frac{1}{\pi}\int_0^{\infty} d\omega'\, \bar{\varepsilon}_c^{-1}(q,G_1,G_2,i\omega')\frac{\omega-\epsilon_i^{(0)}}{(\omega-\epsilon_i^{(0)})^2+\omega'^2} + \\ &\quad +\bar{\varepsilon}_c^{-1}(q,G_1,G_2,\epsilon_i^{(0)}-\omega)\left(\theta(\omega-\epsilon_i^{(0)})-\theta(\mu-\epsilon_i^{(0)})\right)\Big\}\end{aligned}$$

The second term comes into paly only in two cases: when i is conduction with $+$ sign (many cases at high energies):

$$\mu < \epsilon_i^{(0)} < \omega$$

and when i is valence with $-$ sign (few cases):

$$\omega < \epsilon_i^{(0)} < \mu$$

For the dielectric function we must use the tetraedral method to integrate or otherwise use a small imaginary part in ω to account for finite k-point sampling.

9 Imaginary part of the Self-Energy

$$\tilde{\Sigma}_c^{\rm GW}(r_1, r_2, \omega) = \frac{i}{2\pi} \int d\omega' \, e^{-i\omega'\eta} G(r_1, r_2, \omega - \omega') W_c(r_1, r_2, \omega')$$

$$G(r_1, r_2, \omega) = \int d\omega' \, \frac{A(\omega')}{\omega - \omega' + i\eta \, \mathrm{sgn}(\omega' - \mu)}$$

$$W_c(r_1, r_2, \omega) = W(r_1, r_2, \omega) - v(r_1, r_2)$$

$$W_c(r_1, r_2, \omega) = \int d\omega' \, \frac{D(\omega')}{\omega - \omega' + i\eta \, \mathrm{sgn}(\omega')}$$

$$W_c(r_1, r_2, \omega) = \mathrm{vp} \int d\omega' \, \frac{D(\omega')}{\omega - \omega'} - i\pi \mathrm{sgn}(\omega') \delta(\omega - \omega') D(\omega') = \mathrm{vp} \int d\omega' \, \frac{D(\omega')}{\omega - \omega'} - i\pi \mathrm{sgn}(\omega) D(\omega)$$

$$D(r_1, r_2, \omega) = -\frac{1}{\pi} \Im W_c(r_1, r_2, \omega) \, \mathrm{sgn}(\omega)$$

$$D(r_1, r_2, -\omega) = -D(r_1, r_2, \omega)$$

$$W_c(r_1, r_2, \omega) = W_c(r_1, r_2, -\omega)$$

$$\Rightarrow \Re W_c(-\omega) = \mathrm{vp} \int d\omega' \, \frac{D(\omega')}{-\omega - \omega'} = \mathrm{vp} \int d\omega' \, \frac{D(-\omega')}{\omega + \omega'} = \Re W_c(\omega)$$

$$\tilde{\Sigma}_c^{\rm GW}(r_1, r_2, \omega) = \frac{i}{2\pi} \int d\omega' \, e^{i\omega'\eta} G(r_1, r_2, \omega + \omega') W_c(r_1, r_2, \omega')$$

$$\begin{aligned} \tilde{\Sigma}_c^{\rm GW}(r_1, r_2, \omega) = \frac{i}{2\pi} \int d\omega' \quad e^{i\omega'\eta} \quad & \left(\int_{-\infty}^{\mu} d\omega_1 \, \frac{A(\omega_1)}{\omega + \omega' - \omega_1 - i\eta} + \int_{\mu}^{\infty} d\omega_1 \, \frac{A(\omega_1)}{\omega + \omega' - \omega_1 + i\eta} \right) \cdot \\ & \left(\int_{-\infty}^{0} d\omega_2 \, \frac{D(\omega_2)}{\omega' - \omega_2 - i\eta} + \int_{o}^{\infty} d\omega_2 \, \frac{D(\omega_2)}{\omega' - \omega_2 + i\eta} \right) \end{aligned}$$

The terms contributing to the integral in ω' are only those who present poles both up and down the real axis, as for those presenting poles only up or only down, you can close the contour integration path in the upper or in the bottom half plane resulting in zero.

$$\begin{aligned} \tilde{\Sigma}_c^{\rm GW}(r_1, r_2, \omega) = \frac{i}{2\pi} \int d\omega' \quad e^{i\omega'\eta} \quad & \left(\int_{\mu}^{\infty} d\omega_1 \, \frac{A(\omega_1)}{\omega + \omega' - \omega_1 + i\eta} \int_{-\infty}^{0} d\omega_2 \, \frac{D(\omega_2)}{\omega' - \omega_2 - i\eta} \right) \\ + \quad & \left(\int_{-\infty}^{\mu} d\omega_1 \, \frac{A(\omega_1)}{\omega + \omega' - \omega_1 - i\eta} \cdot \int_{0}^{\infty} d\omega_2 \, \frac{D(\omega_2)}{\omega' - \omega_2 + i\eta} \right) \end{aligned}$$

Then, closing the contour integration up ($e^{i\omega'\eta}$) and considering the residual of the poles which are in $\omega' = \omega_2 + i\eta$ for the first term and in $\omega' = \omega_1 - \omega + i\eta$ for the second term, in the upper plane ($2\pi i$Res)

$$\begin{aligned} \tilde{\Sigma}_c^{\rm GW}(r_1, r_2, \omega) &= \frac{i}{2\pi} 2\pi i \left\{ \int_{\mu}^{\infty} d\omega_1 \int_{-\infty}^{0} d\omega_2 \, \frac{A(\omega_1) D(\omega_2)}{\omega + \omega_2 - \omega_1 + i\eta} + \int_{-\infty}^{\mu} d\omega_1 \int_{0}^{\infty} d\omega_2 \, \frac{A(\omega_1) D(\omega_2)}{-\omega + \omega_1 - \omega_2 + i\eta} \right\} \\ &= -\left\{ \int_{\mu}^{\infty} d\omega_1 \int_{-\infty}^{\infty} d\omega_2 \, \theta(-\omega_2) \frac{A(\omega_1) D(\omega_2)}{\omega + \omega_2 - \omega_1 + i\eta} + \int_{-\infty}^{\mu} d\omega_1 \int_{-\infty}^{\infty} d\omega_2 \, \theta(\omega_2) \frac{A(\omega_1) D(\omega_2)}{-\omega + \omega_1 - \omega_2 + i\eta} \right\} \end{aligned}$$

$$\int d\omega \, \frac{1}{\omega \pm i\eta} = \mathrm{vp} \int d\omega \frac{1}{\omega} \mp i\pi\delta\omega$$

$$i\Im\tilde{\Sigma}_c^{\mathrm{GW}}(r_1, r_2, \omega) = -\Big\{ \int_\mu^\infty d\omega_1 \, (-i\pi) A(\omega_1) D(-\omega + \omega_1) \theta(-\omega_1 + \omega) + \int_{-\infty}^\mu d\omega_1 \, (-i\pi) A(\omega_1) D(-\omega + \omega_1) \theta(-\omega + \omega_1)$$

$$\begin{aligned}
\Im\tilde{\Sigma}_c^{\mathrm{GW}}(r_1, r_2, \omega) &= -\int_{-\infty}^\infty d\omega_1 \, \pi A(\omega_1) D(-\omega + \omega_1) \big(-\theta(\omega_1 - \omega)\theta(\mu - \omega_1) - \theta(\omega - \omega_1)\theta(\omega_1 - \mu) \big) \\
&= -\int_{-\infty}^\infty d\omega_1 \, \pi A(\omega_1) D(\omega - \omega_1) \big(\theta(\omega_1 - \omega)\theta(\mu - \omega_1) + \theta(\omega - \omega_1)\theta(\omega_1 - \mu) \big) \\
&= -\int_{-\infty}^\infty d\omega_1 \, \pi A(\omega_1) \frac{-1}{\pi} \Im W_c(\omega - \omega_1) \, \mathrm{sgn}(\omega - \omega_1) \big(\theta(\omega_1 - \omega)\theta(\mu - \omega_1) + \theta(\omega - \omega_1)\theta(\omega_1 - \mu) \big) \\
&= -\int_{-\infty}^\infty d\omega_1 \, A(\omega_1) \Im W_c(\omega - \omega_1) \big(\theta(\omega_1 - \omega)\theta(\mu - \omega_1) - \theta(\omega - \omega_1)\theta(\omega_1 - \mu) \big)
\end{aligned}$$

In the $G^0 W^{\mathrm{RPA}}$ approximation

$$A(r_1, r_2, \omega) = \sum_i \phi_i^{(0)}(r_1) \phi_i^{(0)*}(r_2) \delta(\omega - \epsilon_i^{(0)})$$

$$\Im\tilde{\Sigma}_c^{\mathrm{GW}}(r_1, r_2, \omega) = -\sum_i \phi_i^{(0)}(r_1) \phi_i^{(0)*}(r_2) \Im W_c(r_1, r_2, \omega - \epsilon_i^{(0)}) \big(\theta(\epsilon_i^{(0)} - \omega)\theta(\mu - \epsilon_i^{(0)}) - \theta(\omega - \epsilon_i^{(0)})\theta(\epsilon_i^{(0)} - \mu) \big)$$

$$\Im\tilde{\Sigma}_c^{\mathrm{GW}}(r_1, r_2, \omega) = \begin{cases} -\sum_i^{\mathrm{occ}} \phi_i^{(0)}(r_1) \phi_i^{(0)*}(r_2) \Im W_c(r_1, r_2, \omega - \epsilon_i^{(0)}) \theta(\epsilon_i^{(0)} - \omega) & \omega \le \mu \\ +\sum_i^{\mathrm{unocc}} \phi_i^{(0)}(r_1) \phi_i^{(0)*}(r_2) \Im W_c(r_1, r_2, \omega - \epsilon_i^{(0)}) \theta(\omega - \epsilon_i^{(0)}) & \omega > \mu \end{cases}$$

$$\begin{aligned}
\langle j | \Im\tilde{\Sigma}_c^{\mathrm{GW}}(\omega) | j \rangle &= \int dr_1 dr_2 \, \phi_j^{(0)*}(r_1) \phi_j^{(0)}(r_2) \\
&\quad (-) \sum_i \phi_i^{(0)}(r_1) \phi_i^{(0)*}(r_2) \big(\theta(\epsilon_i^{(0)} - \omega)\theta(\mu - \epsilon_i^{(0)}) - \theta(\omega - \epsilon_i^{(0)})\theta(\epsilon_i^{(0)} - \mu) \big) \\
&\quad \frac{1}{\Omega} \sum_{q, G_1, G_2} e^{i(q+G_1)r_1} \Im\bar{\varepsilon}_c^{-1}(q, G_1, G_2, \omega - \epsilon_i^{(0)}) e^{-i(q+G_2)r_2} \frac{4\pi}{|q + G_1||q + G_2|}
\end{aligned}$$

So that the final result is

$$\begin{aligned}
\langle j | \Im\tilde{\Sigma}_c^{\mathrm{GW}}(\omega) | j \rangle &= -\frac{1}{\Omega} \sum_i \big(\theta(\epsilon_i^{(0)} - \omega)\theta(\mu - \epsilon_i^{(0)}) - \theta(\omega - \epsilon_i^{(0)})\theta(\epsilon_i^{(0)} - \mu) \big) \\
&\quad \sum_{q, G_1, G_2} \delta(q - (k_j - k_i - G_0)) \rho_{ij}^*(G_1) \rho_{ij}(G_2) \frac{4\pi}{|q + G_1||q + G_2|} \Im\bar{\varepsilon}_c^{-1}(q, G_1, G_2, \omega - \epsilon_i^{(0)})
\end{aligned}$$

$$\theta(\epsilon_i^{(0)} - \omega)\theta(\mu - \epsilon_i^{(0)}) - \theta(\omega - \epsilon_i^{(0)})\theta(\epsilon_i^{(0)} - \mu) = \theta(\mu - \epsilon_i^{(0)}) - \theta(\omega - \epsilon_i^{(0)}) = \theta(\epsilon_i^{(0)} - \omega) f_i - \theta(\omega - \epsilon_i^{(0)})(1 - f_i)$$

$$-\Im\varepsilon_c^{-1}(\omega) = -\Im\varepsilon_c^{-1}(-\omega) \qquad \text{even function}$$

A Definitions, notations

$\Omega = N_k \Omega_{\text{cell}}$ Crystal Volume

$$\Omega_{\text{BZ}} = \frac{(2\pi)^3}{\Omega_{\text{cell}}}$$

$$\frac{1}{(2\pi)^3} \int_{\text{BZ}} dk = \frac{1}{\Omega} \sum_k^{\text{BZ}}$$

$$\frac{1}{\Omega_{\text{BZ}}} \int_{\text{BZ}} dk = \frac{1}{N_k} \sum_k^{\text{BZ}}$$

B Fourier transform definition

$f(\omega) = \int dt\, e^{-i\omega t} f(t)$ direct fourier transform

$f(t) = \frac{1}{2\pi} \int d\omega\, f(\omega) e^{i\omega t}$ inverse fourier transform

C Fourier transform of a two lattice indices quantity

$$f(q,G_1,G_2) = \frac{1}{(2\pi)^3}\int dr_1 dr_2\, e^{-i(q+G_1)r_1} f(r_1.r_2) e^{i(q+G_2)r_2}$$
$$f(r_1,r_2) = \frac{1}{(2\pi)^3}\int_{\mathrm{BZ}} dq \sum_{G_1,G_2} e^{i(q+G_1)r_1} f(q,G_1.G_2) e^{-i(q+G_2)r_2}$$
$$f(r_1,r_2) = \frac{1}{\Omega}\sum_{q,G_1,G_2} e^{i(q+G_1)r_1} f(q,G_1.G_2) e^{-i(q+G_2)r_2}$$

Demonstration:

$$f(Q_1,Q_2) = \frac{1}{(2\pi)^3}\int dr_1 dr_2\, e^{-iQ_1 r_1} f(r_1.r_2) e^{iQ_2 r_2} \qquad \text{definition fourier transform}$$
$$f(r_1,r_2) = \frac{1}{(2\pi)^3}\int dQ_1 dQ_2\, e^{iQ_1 r_1} f(Q_1.Q_2) e^{-iQ_2 r_2} \qquad \text{definition inverse fourier transform}$$
$$f(r_1+R,r_2+R) = f(r_1,r_2) \qquad \text{lattice periodicity}$$
$$\frac{1}{(2\pi)^3}\int dQ_1 dQ_2\, e^{iQ_1(r_1+R)} f(Q_1.Q_2) e^{-iQ_2(r_2+R)} = \frac{1}{(2\pi)^3}\int dQ_1 dQ_2\, e^{iQ_1 r_1} f(Q_1.Q_2) e^{-iQ_2 r_2}$$
$$\frac{1}{(2\pi)^3}\int dq_1 dq_2 \sum_{G_1,G_2} e^{i(q_1+G_1)(r_1+R)} f(q_1.q_2,G_1,G_2) e^{-i(q_2+G_2)(r_2+R)}$$
$$= \frac{1}{(2\pi)^3}\int dq_1 dq_2 \sum_{G_1,G_2} e^{i(q_1+G_1)r_1} f(q_1.q_2,G_1,G_2) e^{-i(q_2+G_2)r_2}$$
$$e^{iG_1R} = e^{-iG_2R} = 1$$
$$e^{i(q_1-q_2)R} = 1 \quad\Rightarrow\quad q_1 = q_2 \quad\Rightarrow\quad f(q_1.q_2,G_1,G_2) = f(q_1,G_1,G_2)\delta(q_1-q_2)$$

D Case $q \to 0, G = 0$ for $\rho^2(q, G = 0)/q^2$

$$F = \frac{1}{\Omega} \sum_{q}^{\mathrm{BZ}} \frac{f(q)}{q^2} = \frac{1}{\Omega} f(q = 0) I_{\mathrm{SZ}} + \frac{1}{\Omega} \sum_{q \neq 0}^{\mathrm{BZ}} \frac{f(q)}{q^2}$$

$$I_{\mathrm{SZ}} = \frac{\Omega}{(2\pi)^3} \int_{\Omega_{\mathrm{BZ}}/N_k} d\mathbf{q} \frac{1}{q^2} = \frac{N_k}{\Omega_{\mathrm{BZ}}} \int_{\Omega_{\mathrm{BZ}}/N_k} d\mathbf{q} \frac{1}{q^2}$$

If we assume a spheric Brillouin zone of volume V and radius $(3V/4\pi)^{1/3}$:

$$\frac{1}{V} \int_V d\mathbf{q} \frac{1}{q^2} = \frac{4\pi}{V} \int_0^{(3V/4\pi)^{1/3}} dq = 3^{1/3} (4\pi)^{2/3} V^{-2/3}$$

$$I_{\mathrm{SZ}} = 7.79 \left(\frac{\Omega_{\mathrm{BZ}}}{N_k} \right)^{-2/3}$$

In the case of a Brillouin Zone shape such for an fcc material:

$$I_{\mathrm{SZ}} = 7.44 \left(\frac{\Omega_{\mathrm{BZ}}}{N_k} \right)^{-2/3}$$

For other materials:
sc: 6.188
fcc: 7.431
bcc: 6.946
wz: 5.255 (hcp for ideal u=3/8 wurzite)