Chapter 1

GWA in ωk space

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

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

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

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

1.2 Screened Interaction

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

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

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

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

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

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

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

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

1.3 Single Plasmon Pole Model

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

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

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

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

$$\varepsilon^{-1}(iE_0) = \delta + \frac{\Omega^2}{-E_0^2 - \tilde{\omega}^2}$$

$$\varepsilon^{-1}(iE_0)[E_0^2 + \tilde{\omega}^2] = \delta[E_0^2 + \tilde{\omega}^2] - \frac{\Omega^2}{\tilde{\omega}^2}\tilde{\omega}^2 = \delta E_0^2 + \varepsilon^{-1}(0)\tilde{\omega}^2$$

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

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

1.4 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:

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

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

1.5 Matrix elements of the Self-Energy operator

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

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

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

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

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

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

1.6 Self-Energy: exchange term

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

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.

1.7 Self-Energy: correlation term

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

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

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

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

as $(2f_i-1)^2$ is always 1.

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

Appendix A

Definitions, Fourier transforms

A.1 Definitions, notations

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

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

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

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

A.2 Fourier transform definition

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

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

A.3 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:

$$f(Q_1,Q_2) = \frac{1}{(2\pi)^3}\int dr_1 dr_2\, e^{-iQ_1r_1} f(r_1.r_2) e^{iQ_2r_2} \qquad \text{definition fourier transform}$$
$$f(r_1,r_2) = \frac{1}{(2\pi)^3}\int dQ_1 dQ_2\, e^{iQ_1r_1} f(Q_1.Q_2) e^{-iQ_2r_2} \qquad \text{definition inverse fourier transform}$$
$$f(r_1+R,r_2+R) = f(r_1,r_2) \qquad \text{lattice periodicity}$$
$$\frac{1}{(2\pi)^3}\int dQ_1 dQ_2\, e^{iQ_1(r_1+R)} f(Q_1.Q_2) e^{-iQ_2(r_2+R)} = \frac{1}{(2\pi)^3}\int dQ_1 dQ_2\, e^{iQ_1r_1} f(Q_1.Q_2) e^{-iQ_2r_2}$$
$$\frac{1}{(2\pi)^3}\int dq_1 dq_2 \sum_{G_1,G_2} e^{i(q_1+G_1)(r_1+R)} f(q_1.q_2,G_1,G_2) e^{-i(q_2+G_2)(r_2+R)}$$
$$= \frac{1}{(2\pi)^3}\int dq_1 dq_2 \sum_{G_1,G_2} e^{i(q_1+G_1)r_1} f(q_1.q_2,G_1,G_2) e^{-i(q_2+G_2)r_2}$$
$$e^{iG_1R} = e^{-iG_2R} = 1$$
$$e^{i(q_1-q_2)R} = 1 \quad\Rightarrow\quad q_1 = q_2 \quad\Rightarrow\quad f(q_1.q_2,G_1,G_2) = f(q_1,G_1,G_2)\delta(q_1-q_2)$$

A.4 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:

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