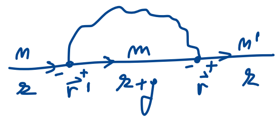
Some notes on PyGW implementation

$$\psi_{mk}(\vec r)\,\psi^*_{m\,k+q}(\vec r) = \sum_\alpha M^\alpha_{nm}(\vec k,\vec q)\,\chi^{\vec q}_\alpha(\vec r)$$

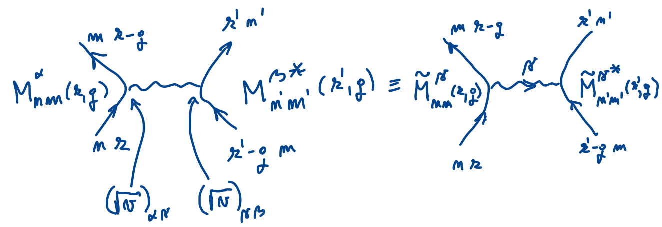


$$G(\vec r,\vec r\,') = -\langle T_\tau \psi(\vec r)\psi^+(\vec r\,')\rangle = \psi_{mk}(\vec r)\frac{1}{\omega+\mu-\varepsilon_k}\psi^*_{mk}(\vec r\,')$$

$$\Sigma(\vec r,\vec r\,') = \sum_{mm',k}\psi^*_{m'k}(\vec r)\,\Sigma_{m'mk}\,\psi_{mk}(\vec r\,')$$

$$\Sigma^x_{mm'k} = \iint \psi^*_{m'k}(\vec r)\,\overbrace{\Sigma(\vec r,\vec r\,')}^{-G^0(\vec r,\vec r\,')\,W(\vec r,\vec r\,')}\,\psi_{mk}(\vec r\,')\, d^3r\, d^3r'$$

$$G^0(\vec r,\vec r\,') = \psi_{m\,k-q}(\vec r)\frac{1}{i\omega-i\Omega+\mu-\varepsilon^m_{k-q}}\psi^*_{m\,k-q}(\vec r\,')$$



$$\Sigma_{mm'k} = -\iint d^3r\,d^3r'\,\underbrace{\psi^*_{m'k}(\vec r)\psi_{m\,k-q}(\vec r)}_{M^{\alpha *}_{m'm}(\vec k,\vec q)\,\chi^{\vec q *}_\alpha(\vec r)}\,W_\Omega(\vec r,\vec r\,')\,\underbrace{\psi^*_{m\,k-q}(\vec r\,')\psi_{mk}(\vec r\,')}_{M_{mm}(\vec k,\vec q)\,\chi^{\vec q}_\beta(\vec r\,')}\,\frac{1}{i\omega-i\Omega+\mu-\varepsilon^m_{k-q}}$$

$$W_{\alpha\beta}(q,\Omega) = \iint d^3r\,d^3r'\,\chi^{\vec q *}_\alpha(\vec r)\,W_\Omega(\vec r,\vec r\,')\,\chi^{\vec q}_\beta(\vec r\,')$$

matrix form

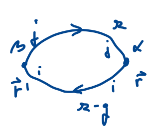
$$v_{\alpha\beta} \equiv (\sqrt{v})_{\alpha\nu}(\sqrt{v})_{\nu\beta}$$

$$\Sigma_{mm'k}(i\omega) = -\frac{1}{\beta}\sum_{i\Omega}\sum_{\substack{mq\\ \alpha\beta}} M^{\alpha *}_{m'm}(\vec k,\vec q)\,W_{\alpha\beta}(q,\Omega)\,M^\beta_{mm}(\vec k,\vec q)\,\frac{1}{i\omega-i\Omega+\mu-\varepsilon^m_{k-q}}$$

$$\Sigma^x_{mm'k} = \sum_{\substack{mq\\ \alpha\beta\nu}} \underbrace{M^{\alpha *}_{m'm}(\vec k,\vec q)(\sqrt{v})_{\alpha\nu}}_{\tilde M^{\nu *}_{m'm}(\vec k,\vec q)}\cdot\underbrace{(\sqrt{v})_{\nu\beta}M^\beta_{mm}(\vec k,\vec q)}_{\tilde M^\nu_{mm}(\vec k,\vec q)}\,f(\varepsilon^m_{k-q})$$

$M^\beta_{mm}(\vec k,\vec q)$ $\quad$ $M^{\alpha *}_{m'm}(\vec k,\vec q)$

$$P_{\alpha\beta}(q,\Omega) = \iint \chi^{\vec q *}_\alpha(\vec r)\,P_\Omega(\vec r,\vec r\,')\,\chi^{\vec q}_\beta(\vec r\,')\,d^3r\,d^3r'$$



$$\underbrace{\psi_{jk}(\vec r)\psi^*_{i\,k-q}(\vec r)}_{M^\alpha_{ji}(\vec k,\vec q)\,\chi^{\vec q}_\alpha(\vec r)}\frac{1}{i\omega-i\Omega-\varepsilon^i_{k-q}}\;\underbrace{\psi_{i\,k-q}(\vec r\,')\psi^*_{jk}(\vec r\,')}_{M^{\beta *}_{ji}(\vec k,\vec q)\,\chi^{\vec q}_\beta(\vec r\,')}\frac{1}{i\omega-\varepsilon^j_k}$$

$$P_{\alpha\beta}(\vec q,i\Omega) = \sum_{\substack{ij\\ \vec k}} M^\alpha_{ji}(\vec k,\vec q)\,M^{\beta *}_{ji}(\vec k,\vec q)\,\underbrace{\frac{1}{\beta}\sum_{i\omega}\frac{1}{i\omega-\varepsilon^j_k}\,\frac{1}{i\omega-i\Omega-\varepsilon^i_{k-q}}}_{F_{ji}(\vec k,\vec q;i\Omega)}$$

$$P_{\alpha\beta}(q,i\Omega) = \sum_{ij\vec k} M^\alpha_{ij}(\vec k,\vec q)\,M^{\beta *}_{ij}(\vec k,\vec q)\,F_{ij}(\vec k,\vec q;i\Omega)$$

$$W = \varepsilon^{-1}V = (V^{-1}-P)^{-1} \Rightarrow \varepsilon = 1-VP$$

$$\varepsilon_{\alpha\beta} = \delta_{\alpha\beta} - \sum_{\alpha'\beta'}(\sqrt{v_q})_{\alpha\alpha'}\,P_{\alpha'\beta'}(\vec q,i\Omega)\,(\sqrt{v_q})_{\beta'\beta} = \delta_{\alpha\beta} - \sum_{\alpha'\beta'}\underbrace{(\sqrt{v_q})_{\alpha\alpha'}M^{\alpha'}_{ij}(\vec k,\vec q)}_{\tilde M^\alpha_{ij}(\vec k,\vec q)}\,F_{ij}(\vec k,\vec q;i\Omega)\,\underbrace{M^{\beta' *}_{ij}(\vec k,\vec q)(\sqrt{v_q})_{\beta'\beta}}_{\tilde M^{\beta *}_{ij}(\vec k,\vec q)}$$

$$(W-V)_{\alpha\beta} = \sum_{\alpha'\beta'}(\sqrt{v_q})_{\alpha\alpha'}\,(\varepsilon^{-1}-1)_{\alpha'\beta'}\,(\sqrt{v_q})_{\beta'\beta}$$

product basis

$$\chi_\alpha^{\vec{q}} = \begin{cases} Y_{LM}(\hat{r}_a) N_{aNLM}(r_a) & \text{MT on atom } a \\ \frac{1}{\sqrt{\Omega}} e^{i(\vec{q}+\vec{G})\vec{r}} & \text{interstitial} \end{cases}$$

$\chi_\alpha^{q}(\vec{r})$ constructed from Φ.

Interstitial orthogonal functions: $\langle e^{-i(\vec{q}+\vec{G}_1)\vec{r}} | e^{i(\vec{q}+\vec{G}_2)\vec{r}} \rangle_{Int} = \int_{Int} d^3r \, e^{i(\vec{G}_2-\vec{G}_1)\vec{r}} = O_{G_1 G_2}$

rather use: $\sum_{G'} \left(\frac{1}{\sqrt{O}}\right)_{GG'} e^{i(\vec{q}+\vec{G}')\vec{r}}$

$$\chi_\alpha^{\vec{q}} = \begin{cases} Y_{LM}(\hat{r}_a) N_{aNLM}(r_a) \\ P_G(\vec{q}) = \frac{1}{\sqrt{\Omega}} \sum_{G'} \left(\frac{1}{\sqrt{O}}\right)_{GG'} e^{i(\vec{q}+\vec{G}')\vec{r}} \end{cases}$$

Definition of intermediate representation

$$W_{\vec{G}}^{\alpha}(\vec{q}) \equiv \frac{1}{\sqrt{\Omega}} \int_{\Omega} d^3r \, e^{i(\vec{q}+\vec{G})\vec{r}} \chi_\alpha^{\vec{q}*}(\vec{r}) = \begin{cases} 4\pi i^L \cdot Y_{LM}^*(\widehat{\vec{q}+\vec{G}}) e^{i\vec{G}\cdot\vec{R}_a} \frac{1}{\sqrt{\Omega}} \int dr_a r_a^2 N_{aNLM}(r_a) j_L(|\vec{q}+\vec{G}| r_a) \\ \left(\frac{1}{\sqrt{O}}\right)_{GG'} \int_{Inter} e^{i(\vec{G}-\vec{G}')\vec{r}} d^3r \end{cases}$$

$$e^{i(\vec{q}+\vec{G})\vec{r}} = 4\pi \sum_{lm} i^l j_l(|\vec{q}+\vec{G}|r) Y_{lm}(\widehat{\vec{q}+\vec{G}}) Y_{lm}^*(\hat{r})$$

Product basis:

K.S. $\psi_{mk}(\vec{r}) = \sum_G C_{mk,G} \phi_G^{k}(\vec{r}) = \begin{cases} \sum_{glm} A_{mkaglm} u_{agl}(r_a) Y_{lm}(\hat{r}_a) & \text{on atom } r_a \\ \frac{1}{\sqrt{\Omega}} \sum_G \Theta_G^{LO} C_{mk,G} e^{i(\vec{k}+\vec{G})\vec{r}} & \text{interstitial} \end{cases}$

(ϕ_G^{k}: LAPW basis)

M.T.

$$M_{mm}^{\alpha}(\vec{k},\vec{q}) = \int \chi_\alpha^{\vec{q}*}(\vec{r}) \psi_{mk}(\vec{r}) \psi_{m\,k-q}^*(\vec{r}) d^3r = \sum_{\substack{glm \\ g'l'm' \\ NLM}} \int_a d^3r \, Y_{LM}^*(\hat{r}_a) N_{aNLM}(r_a) A_{mkaglm} u_{agl}(r_a) Y_{lm}(\hat{r}_a) A^*_{m\,k-q\,ag'l'm'} u_{ag'l'}(r_a) Y^*_{l'm'}(\hat{r}_a)$$

$$\chi_\alpha^{\vec{q}*}(\vec{r}) = e^{-i\vec{q}\vec{R}_a} \chi_\alpha^{\vec{q}*}(\vec{r}-\vec{R}_a)$$

$$A_{mkag_1l_1m_1} A^*_{m\,k-q\,ag_2l_2m_2} \cdot \langle l_1m_1 | LM\, l_2m_2 \rangle^* \int dr_a r_a^2 N_{aNLM}(r_a) u_{ag_1l_1}(r_a) u_{ag_2l_2}(r_a)$$

$$M_{mm}^{\alpha}(\vec{k},\vec{q}) = \sum_{\substack{g_1 l_1 m_1 \\ g_2 l_2 m_2 \\ NLM}} e^{-i\vec{q}\cdot\vec{R}_a} A_{mkag_1l_1m_1} A^*_{m\,k-q\,ag_2l_2m_2} \cdot \langle l_1m_1 | LM\, l_2m_2 \rangle^* \int dr_a r_a^2 N_{aNLM}(r_a) u_{ag_1l_1}(r_a) u_{ag_2l_2}(r_a)$$

Interstitial:

$$\frac{1}{\Omega} \sum_{G_1 G_2} \Theta_{G_1}^{LO} \Theta_{G_2}^{LO} C_{mkG_1} C^*_{m\,k-q\,G_2} \int_{In} e^{i(\vec{q}+\vec{G}_1-\vec{G}_2)\vec{r}} \left(\frac{1}{\sqrt{O}}\right)_{\vec{G}\vec{G}'} e^{-i(\vec{q}+\vec{G}')\vec{r}} d^3r$$

$$M_{mm}^{\alpha\vec{G}}(\vec{k},\vec{q}) = \left(\frac{1}{\sqrt{O}}\right)_{GG'} \int_{In} e^{-i(\vec{G}'-\vec{G}_1+\vec{G}_2)\vec{r}} d^3r \, \frac{1}{\Omega^{3/2}} \sum_{G_1 G_2} \Theta_{G_1}^{LO} \Theta_{G_2}^{LO} C_{mkG_1} C^*_{m\,k-q\,G_2}$$

$$V_{\alpha\beta} = \iint d^3r\, d^3r'\, \chi_\alpha^{\vec q\,*}(\vec r)\, V(\vec r - \vec r')\, \chi_\beta^{\vec q}(\vec r') = \iint d^3r\, d^3r'\, \chi_\alpha^{\vec q\,*}(\vec r)\, V(\vec r - \vec r' + \vec R)\, e^{-i\vec q \vec R}\, \chi_\beta^{\vec q}(\vec r' - \vec R)$$

1) χ_α and χ_β in M.T.

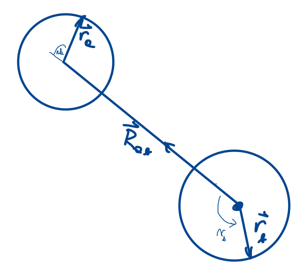
$$V_{\alpha\beta} = \iint Y^*_{L_1M_1}(\hat r_a)\, Y_{L_2M_2}(\hat r_b)\, \mathcal{N}_{aN_1L_1M_1}(r_a)\, \mathcal{N}_{bN_2L_2M_2}(r_b)\, \frac{e^{-i\vec q R_{ab}}}{|\vec r_a - \vec r_b + \vec R_{ab}|}\, d^3r_a\, d^3r_b$$

Same atom for a and b:

$$V_{\alpha\beta} = \iint Y^*_{L_1M_1}(\hat r_a)\, Y_{L_2M_2}(\hat r_b)\, \mathcal{N}_{aN_1L_1M_1}(r_a)\, \mathcal{N}_{bN_2L_2M_2}(r_b) \sum_{lm} \frac{4\pi}{2l+1} Y_{lm}(\hat r_a)\, Y^*_{lm}(\hat r_b)\, \frac{r_<^l}{r_>^{l+1}}\Big|_{(r_a, r_b)} d^3r_a\, d^3r_b$$

$$V_{\alpha\beta} = \delta_{L_1M_1 = L_2M_2 = lm} \sum_{N_1 N_2} \frac{4\pi}{2l+1} \cdot \underbrace{\int dr_a\, r_a^2 \int dr'\, r_a'^2\, \frac{r_<^l}{r_>^{l+1}}\Big|_{(r_a, r_a')} \mathcal{N}_{aN_1lm}(r_a)\, \mathcal{N}_{aN_2lm}(r_a')}_{\langle \mathcal{N}_{aN_1lm} | \frac{r_<^l}{r_>^{l+1}} | \mathcal{N}_{aN_2lm} \rangle}$$

Different atom:



$$V_{\alpha\beta} = \iint Y^*_{L_1M_1}(\hat r_a)\, Y_{L_2M_2}(\hat r_b)\, \mathcal{N}_{aN_1L_1M_1}(r_a)\, \mathcal{N}_{bN_2L_2M_2}(r_b)\, \frac{e^{-i\vec q R_{ab}}}{|\vec r_a - \vec r_b + \vec R_{ab}|}\, d^3r_a\, d^3r_b$$

$$V_{\alpha\beta} = \iint Y^*_{L_1M_1}(\hat r_a)\, \mathcal{N}_{aN_1L_1M_1}(r_a)\, \underbrace{\frac{1}{\left|1 + \frac{r_a}{R_{ab}}\cos\vartheta_a - \frac{r_b}{R_{ab}}\cos\vartheta_b\right|}}_{\text{lattice structure constant!}}\, Y_{L_2M_2}(\hat r_b)\, \mathcal{N}_{bN_2L_2M_2}(r_b)\, \frac{e^{-i\vec q \cdot \vec R_{ab}}}{|\vec R_{ab}|}$$

Ewald called $A_{lm}(lm, \vec R_i - \vec R_j)$

$\vec R_a = \Delta\vec R + \vec R$ ← lattice vector

$$\sum_{R_a} Y_{lm}(\hat R_a)\, e^{-i\vec q \vec R_a}\, \frac{1}{R_a^{l+1}} = \frac{1}{\sqrt\pi}\Bigg[\sum_{R_a = \Delta R + R} Y_{lm}(\hat R_a)\, e^{-i\vec q \vec R_a}\, \mathcal{N}_{R_a}(l) + \frac{4\pi^{3/2}}{V} \sum_{\vec G} Y_{lm}(\widehat{q+G})\, e^{i\vec G \Delta\vec R}\, e^{-(\eta|\vec q + \vec G|)^2/4}\, \frac{i^l}{|\vec q + \vec G|^2}\left(-\frac{|\vec q + \vec G|}{2}\right)^l\Bigg]$$

$$\mathcal{N}(l=0) = \sqrt\pi\, \mathrm{erfc}\left(\frac{R_a}{\eta}\right)\frac{1}{R_a}$$

$$\mathcal{N}(l=1) = \frac{(1-\frac{1}{2})}{R_a}\, \mathcal{N}(l=0) + \frac{R_a^{-1}}{\eta^2}\, e^{-\frac{R_a^2}{\eta^2}}$$

$$\mathcal{N}(l=2) = \frac{(2-\frac{1}{2})}{R_a}\, \mathcal{N}(l=1) + \frac{R_a^0}{\eta^3}\, e^{-R_a/\eta^2}$$

$$\mathcal{N}(l) = \frac{(l-\frac{1}{2})}{R_a}\, \mathcal{N}(l-1) + \frac{R_a^{l-2}}{\eta^{2l-1}}\, e^{-R_a^2/\eta^2}$$

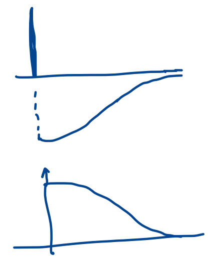
Ewald's summation

$$E = \sum_{\vec{m}} \sum_{ij} \frac{q_i q_j}{|\vec{r}_{ij} + \vec{m} L|}$$

$$\rho_i^S(\vec{r}) = q_i \delta(\vec{r} - \vec{r}_i) - q_i G(\vec{r} - \vec{r}_i)$$

$$\rho_i^L(\vec{r}) = q_i G(\vec{r} - \vec{r}_i)$$

$$G(r) = e^{-\frac{r^2}{\eta^2}} \frac{1}{(\eta^2 \cdot \pi)^{3/2}}$$



$$\nabla^2 \phi = -\frac{G}{\varepsilon_0} \Rightarrow \phi = -\frac{1}{4\pi\varepsilon r} \mathrm{Erfc}\left(\frac{r}{\eta}\right) \text{ or } \frac{1}{4\pi\varepsilon_0 r} \mathrm{Erf}\left(\frac{r}{\eta}\right)$$

$$\frac{1}{r} \frac{\partial^2}{\partial r^2}(r\phi) = -\frac{G}{\varepsilon_0}$$

$$\frac{\partial}{\partial r}(r\phi) = \int_r^\infty \frac{G r}{\varepsilon_0} dr = \frac{1}{\varepsilon (\eta^2 \pi)^{3/2}} \cdot \int_r^\infty e^{-\frac{r^2}{\eta^2}} r \, dr = \frac{\eta^2}{\varepsilon_0 \cdot 2 (\eta^2 \pi)^{3/2}} \int_{\frac{r^2}{\eta^2}}^\infty e^{-x} dx = \frac{\eta^2}{\varepsilon_0 \cdot 2 (\eta^2 \pi)^{3/2}} e^{-\frac{r^2}{\eta^2}}$$

$$r\phi = -\frac{\eta^2}{\varepsilon_0 \cdot 2 (\eta^2 \pi)^{3/2}} \int_r^\infty e^{-\frac{r^2}{\eta^2}} dr = -\frac{\eta^2 \sqrt{\pi}}{\varepsilon_0 \cdot 2 (\eta^2 \pi)^{3/2}} \frac{\eta}{2} \mathrm{Erfc}\left(\frac{r}{\eta}\right) = -\frac{1}{4\pi\varepsilon_0} \mathrm{Erfc}\left(\frac{r}{\eta}\right)$$

$$\phi = -\frac{1}{4\pi\varepsilon_0 r} \mathrm{Erfc}\left(\frac{r}{\eta}\right)$$

$$\left.\begin{array}{l} \rho_i^S(\vec{r}) = q_i \delta(\vec{r} - \vec{r}_i) - q_i G(\vec{r} - \vec{r}_i) \Rightarrow \phi_i^S = \frac{q_i}{4\pi\varepsilon_0 r} \mathrm{Erfc}\left(\frac{r}{\eta}\right) \\ \rho_i^L(\vec{r}) = q_i G(\vec{r} - \vec{r}_i) \Rightarrow \phi_i^L = \frac{q_i}{4\pi\varepsilon_0 r} \mathrm{Erf}\left(\frac{r}{\eta}\right) \end{array}\right\} \phi_i^S + \phi_i^L = \frac{q_i}{4\pi\varepsilon_0 r}$$

$$E = \sum_{\vec{m}} \sum_{ij} \frac{q_i q_j}{|\vec{r}_{ij} + \vec{m} L|} \left[\underbrace{\mathrm{Erf}\left(\frac{|\vec{r}_{ij} + \vec{m} L|}{\eta}\right)}_{\text{reciprocal}} + \underbrace{\mathrm{Erfc}\left(\frac{|\vec{r}_{ij} + \vec{m} L|}{\eta}\right)}_{\text{real space}} \right]$$

$$E = \sum_{\vec{m}} \sum_{ij} \frac{q_i q_j}{|\vec{r}_{ij} + \vec{m} L|} \mathrm{Erfc}\left(\frac{|\vec{r}_{ij} + \vec{m} L|}{\eta}\right) + \frac{4\pi}{V} \sum_{k \neq 0} \frac{e^{-\frac{\eta^2 k^2}{4}}}{k^2} \left| \sum_i q_i e^{i \vec{k} \cdot \vec{r}_i} \right|^2 - \frac{1}{\sqrt{\pi} \eta} \sum_{ij} q_i^2 \delta_{ij}$$

Singularity of the Coulomb repulsion

The implementation relays on the plane wave expansion (in Hartree units):

$$v_{GG'} = \frac{4\pi}{|q+G|^2}\delta_{GG'}$$

To calculate repulsion in product basis, we write:

$$v^{q}_{\alpha\beta} = \sum_{\vec G} \langle \chi^{\vec q}_{\alpha}|\vec G\rangle \frac{4\pi}{|q+G|^2}\langle \vec G|\chi^{\vec q}_{\beta}\rangle = \underbrace{\langle \chi^{\vec q}_{\alpha}|\vec G=0\rangle \frac{4\pi}{q^2}\langle \vec G=0|\chi^{\vec q}_{\beta}\rangle}_{\text{at } q=0 \text{ this term is dropped}} + \underbrace{\sum_{\vec G\neq 0}\langle \chi^{\vec q}_{\alpha}|\vec G\rangle\frac{4\pi}{|q+G|^2}\langle \vec G|\chi^{\vec q}_{\beta}\rangle}_{\tilde v^{q}_{\alpha\beta}}$$

Gives Drude. Added back later.

$$\tilde v^{q=0}_{\alpha\beta} = \sum_{\vec G\neq 0}\frac{4\pi}{G^2}\langle \chi^{\vec q=0}_{\alpha}|\vec G\rangle\langle \chi^{\vec q=0}_{\beta}|\vec G\rangle^*$$

$$\langle \chi^{\vec q=0}_{\alpha}|\vec G\rangle = \int_{MT} d^3r\,[\cos(\vec G\cdot\vec r)+i\sin(\vec G\cdot\vec r)]\, Y^*_{LM}(\hat r)\,\frac{u_{NLM}(r)}{r}$$

$$\langle \chi^{\vec q=0}_{\alpha}|\vec G\rangle = \int d\Omega\; e^{i(G_1\cos\varphi+G_2\sin\varphi)r\sin\vartheta+G_3 r\cos\vartheta}\cdot Y^*_{LM}(\hat r)\frac{u_{NLM}(r)}{r}r^2dr$$

In the atom is at high-enough symmetry, then only $L=0$ survives. This is what is implemented.

At $L=0$:

$$\langle \chi^{\vec q=0}_{L=0}|\vec G\rangle = \int_{-1}^{1} dx\, 2\pi\cos(G r x)\frac{1}{\sqrt{4\pi}}\frac{u_{N00}(r)}{r}r^2dr = \frac{2\pi}{\sqrt{4\pi}}\int_0 2\frac{\sin(Gr)}{Gr}\frac{u_{N00}}{r}r^2dr = \frac{\sqrt{4\pi}}{G}\int_0^{R_{MT}}\sin(Gr)\,u_{N00}(r)\,dr$$

$$\tilde v^{q=0}_{\alpha\beta} = \sum_{\vec G\neq 0}\frac{4\pi}{G^2}\left(\frac{\sqrt{4\pi}}{G}\right)^2\left[\int_0^{R_{MT}}\sin(Gr)\,u_{N_\alpha 00}(r)\,dr\right]\left[\int_0^{R_{MT}}\sin(Gr)\,u_{N_\beta 00}(r)\,dr\right]$$

$$\int e^{i(\vec q+\vec G)r}\, Y_{LM}(\hat r)\,d\Omega\,\frac{u_{NL}(r)}{r}r^2dr$$

$$\parallel$$

$$4\pi i^L Y_{LM}(\widehat{q+G})\underbrace{Y^*_{LM}(\hat r)Y_{LM}(\hat r)}_{1} j_L(|q+G|r)\frac{u_{NL}}{r}r^2dr$$

For generic case:

$$\langle \chi_\alpha^{\vec{q}} | \vec{G} \rangle = \int \underbrace{e^{i(\vec{q}+\vec{G})r}}_{4\pi i^L Y_{LM}(\widehat{q+G})\, Y^*_{LM}(\hat{r})\, j_L((q+G)r)} Y_{LM}(\hat{r})\, d\Omega\, \frac{u_{NL}(r)}{r}\, r^2 dr = 4\pi i^L Y_{LM}(\widehat{q+G}) \int_0^{R_{MT}} j_L((q+G)r)\, u_{NL}(r)\, r\, dr$$

$$\tilde{V}_{\alpha\beta}^{q=0} = \sum_{\vec{G}\neq 0} \frac{4\pi}{G^2} \langle \chi_\alpha^{\vec{q}=0} | \vec{G} \rangle \langle \chi_\beta^{\vec{q}=0} | \vec{G} \rangle^* =$$

$$= \sum_{\substack{\vec{G}\neq 0 \\ L L'}} \frac{4\pi}{G^2} (4\pi)^2 i^{L-L'} \sum_{M M'} Y_{LM}(\widehat{q+G})\, Y^*_{L'M'}(\widehat{q+G}) \left[\int_0^{R_{MT}} j_L((q+G)r)\, u_{NL}(r)\, r\, dr\right]\left[\int_0^{R_{MT}} j_{L'}((q+G)r)\, u_{N'L'}(r)\, r\, dr\right]$$

One form of Coulomb is $\sum_{\vec{K}} |\vec{K}+\vec{q}\rangle \frac{1}{|q+K|^2} \langle \vec{q}+\vec{K}|$ where $\vec{K}$ has a very large cutoff

- For the interstitial-interstitial part: $\langle \vec{G}+\vec{q} | \vec{K}+\vec{q}\rangle_I \frac{1}{|\vec{q}+\vec{K}|^2} \langle q+\vec{K} | \vec{G}'+\vec{q}\rangle_I$
- For the mixed interstitial-MT part: $\langle \vec{G}+\vec{q} | \vec{K}+\vec{q}\rangle_I \frac{1}{|\vec{q}+\vec{K}|^2} \langle q+\vec{K} | u^e_{NLM}(\vec{r})\rangle$
- For the MT part: $\langle u^{e'}_{N_1 L_1 M_1}(\vec{r}) | \vec{K}+\vec{G}\rangle_{MT} \frac{1}{|\vec{q}+\vec{K}|^2} \langle q+\vec{K} | u^e_{N_2 L_2 M_2}\rangle$

  The alternative for MT part is

$$\left\langle u^{e'}_{N_1 L_1 M_1}(\vec{r}) \right| \frac{e^{-i\vec{q}(\vec{R}'-\vec{R})}}{|\vec{r}'-\vec{r}+\vec{R}'-\vec{R}|} \left| u^e_{N_2 L_2 M_2}(\vec{r}) \right\rangle$$

Muffin-tin part

$$\left\langle u^{a}_{N_1 L_1 M_1}(\vec{r}') \left| \frac{e^{-i\vec{g}(\vec{R}'-\vec{R})}}{|\vec{r}'-\vec{r}|} \right| u^{b}_{N_2 L_2 M_2}(\vec{r}) \right\rangle$$

$$V_{\alpha\beta} = \iint Y^{*}_{L_1M_1}(\hat{r}_a)\, Y_{L_2M_2}(\hat{r}_b)\; u^{a}_{N_1L_1}(r_a)\; u^{b}_{N_2L_2}(r_b)\, \frac{e^{-i\vec{g}R_{ab}}}{|\vec{r}_a-\vec{r}_b+\vec{R}_{ab}|}\, d^3r_a\, d^3r_b$$

two center expansion exists: $\displaystyle \frac{1}{|\vec{R}+\vec{r}_1-\vec{r}_2|} = \sum_{\substack{l_1m_1\\l_2m_2}} \mathcal{Y}(l_1m_1, l_2m_2)\, r_1^{l_1} Y^{*}_{l_1m_1}(\hat{r}_1)\, r_2^{l_2} Y^{*}_{l_2m_2}(\hat{r}_2)\, \frac{1}{R^{l_1+l_2}}\, Y_{l_1+l_2,\, m_1+m_2}(\hat{R})$

with $\displaystyle \mathcal{Y}(l_1m_1, l_2m_2) = 4\pi^{\frac{3}{2}} (-1)^{l_1} \sqrt{\frac{\binom{l_1+m_1+l_2+m_2}{l_1+m_1}\binom{l_1-m_1+l_2-m_2}{l_1-m_1}}{(2l_2+1)(2l_1+1)(2l_1+2l_2+1)}}$

Hence

$$V_{\alpha\beta} = \sum_{\substack{l_1m_1\\l_2m_2}} \mathcal{Y}(l_1,-m_1,l_2,m_2)(-1)^{m_1} \sum_{R_{ab}} e^{-i\vec{g}\vec{R}_{ab}} \frac{Y_{l_1+l_2,\,m_2-m_1}(\hat{R}_{ab})}{R_{ab}^{l_1+l_2}} \langle r_a^{l_1} | u_{N_1l_1} \rangle \langle r_b^{l_2} | u_{N_2l_2} \rangle \quad \text{for } a \neq b$$

$$\sum_{R} e^{-i\vec{g}(\vec{R}+\vec{R}_{ab})} \cdot \frac{Y_{l_1+l_2,\,m_4+m_3}(\widehat{R+R_{ab}})}{|R+R_{ab}|^{l_1+l_2+1}} (-1)^{m_3}\, \mathcal{Y}(l_1,m_3,l_2,m_4)$$

If on the same atom then

$$V_{\alpha\beta} t = \sum_{L} \frac{4\pi}{2L+1} \left\langle \frac{r_<^L}{r_>^{L+1}} \middle| u_{N_1L}\, u_{N_2L} \right\rangle$$

Ewald: $\displaystyle \sum_{R} Y_{lm}(\widehat{R+R_{ab}})\, e^{-i\vec{g}\vec{R}+\vec{R}_{ab}} \frac{1}{|\vec{R}+\vec{R}_{ab}|^{l+1}} \equiv \mathrm{Sgm}(lm, R_{ab})$

$$V_{\alpha\beta} = \sum_{\substack{l_1m_1\\l_2m_2}} \mathcal{Y}(l_1,-m_1,l_2,m_2)(-1)^{m_1} R_{ab}\; \mathrm{Sgm}(l_1+l_2, m_2-m_1, \vec{R}_{ab}, \vec{g}) \langle r_a^{l_1} | u_{N_1l_1} \rangle \langle r_b^{l_2} | u_{N_2l_2} \rangle$$

Ewald called $\mathrm{Sgm}(lm, \vec{R}_i-\vec{R}_j)$

Note: $Y_{lm}(-\hat{R}) = (-1)^l\, Y_{lm}(\hat{R})$

$Y^{*}_{lm}(\hat{R}) = (-1)^m\, Y_{l-m}(\hat{R})$

$$\sum_{R_e} Y_{lm}(\hat{R}_e)\, e^{-i\vec{g}\vec{R}_e} \frac{1}{R_e^{l+1}} = \mathrm{Sgm}(lm, \vec{R}_i-\vec{R}_j)$$

$$\sum_{R} (-1)^l\, Y_{lm}(\hat{R}_e)\, e^{i\vec{g}\vec{R}_e} \frac{1}{R_e^{l+1}} = \mathrm{Sgm}(lm, -(\vec{R}_i-\vec{R}_j))$$

$$\sum_{R} (-1)^{l-m}\, Y^{*}_{l-m}(R_e)\left(e^{-i\vec{g}\vec{R}_e}\right)^{*} \frac{1}{R_e^{l+1}} = (-1)^{l-m}\, \mathrm{Sgm}(l,-m, \vec{R}_{ij})^{*} = \mathrm{Sgm}(l,m,-\vec{R}_{ij})$$

Muffin-tin part : Implementation

for - Coulomb.f90 :: MT- Coulomb
latest version is implemented!

$$\left\langle u^{a}_{N_1 L_1 M_1}(\vec{r}) \right| \frac{e^{-i\vec{g}(\vec{R}'-\vec{R})}}{|\vec{r}\,'-\vec{r}|} \left| u^{b}_{N_2 L_2 M_2}(\vec{r}) \right\rangle$$

$$V_{ab}(\vec{g}) = \sum_{\vec{R}} \iint Y^*_{L_1 M_1}(\hat{R}_a \hat{r}_a)\, Y_{L_2 M_2}(\hat{R}_b \hat{r}_b)\, u^{a}_{N_1 L_1}(r_a)\, u^{b}_{N_2 L_2}(r_b) \frac{e^{-i\vec{g}(\vec{R}_{ab}+\vec{R})}}{|\vec{r}_a - \vec{r}_b + \vec{R}_{ab} + \vec{R}\,|}\, d^3r_a\, d^3r_b$$

$\vec{R}$ lattice in real space

rotation matrix to global axis

$$D^*(l_1 m_1, -m_3)\, Y^*_{l_1 -m_3}(\hat{r}_a)\ D(l_2 m_2, m_4)\, Y_{l_2 m_4}(\hat{r}_b)$$

Here we concentrate on $\vec{R}_{ab}+\vec{R} \neq 0$
Case with $\vec{R}+\vec{R}_{ab}=0$ is elementary.

$D(j,m,m')$ Rotation matrices of spherical harmonics : $Y_{jm}(R\vec{r}) = \sum D(j,m',m)\, Y_{jm'}(\vec{r})$

two center expansion exists :

(M.E. Rose, J. Math. Phys 37, 215 (1958))

$$\frac{1}{|\vec{R}+\vec{r}_1-\vec{r}_2|} = \sum_{\substack{l_1 m_1\\ l_2 m_2}} \mathcal{M}(l_1 m_1\ l_2 m_2)\, r_1^{l_1}\, Y^*_{l_1 m_1}(\hat{r}_1)\, r_2^{l_2}\, Y^*_{l_2 m_2}(\hat{r}_2)\, \frac{1}{R^{l_1+l_2+1}}\, Y_{l_1+l_2,\, m_1+m_2}(\hat{R})$$

with $$\mathcal{M}(l_1 m_1\ l_2 m_2) = 4\pi^{3/2}(-1)^{l_1} \sqrt{\frac{\binom{l_1+m_1+l_2+m_2}{l_1+m_1}\binom{l_1-m_1+l_2-m_2}{l_1-m_1}}{(2l_2+1)(2l_1+1)(2l_1+2l_2+1)}}$$

Derivation

$$V_{ab}(\vec{g}) = \sum_{\substack{l_1 l_2 m_1 m_2\\ m_3 m_4}} D^*(l_1, -m_3, m_1)\, D(l_2, m_4, m_2) \iint d^3r_a\, d^3r_b\ Y^*_{l_1,-m_3}(\hat{r}_a)\, Y_{l_2 m_4}(\hat{r}_b)\, u^a_{N_1 l_1}(r_a)\, u^b_{N_2 l_2}(r_b) \sum_{\vec{R}} e^{-i\vec{g}(\vec{R}_{ab}+\vec{R})} \times$$

$$\times \sum_{\substack{l_1' m_3'\\ l_2' m_4'}} \mathcal{M}(l_1' m_3'\ l_2' m_4')\, r_a^{l_1'}\, \underbrace{Y^*_{l_1' m_3'}(\hat{r}_a)}_{=\,Y_{l_1',-m_3'}(\hat{r}_a)(-1)^{m_3'}}\, r_b^{l_2'}\, Y^*_{l_2' m_4'}(\hat{r}_b)\, \frac{1}{|\vec{R}_{ab}+\vec{R}|^{l_1'+l_2'+1}}\, Y_{l_1'+l_2',\, m_3'+m_4'}(\widehat{R+R_{ab}})$$

$$V_{ab}(\vec{g}) = \sum_{\substack{l_1 l_2 m_1 m_2\\ m_3 m_4}} D^*(l_1, -m_3, m_1)\, D(l_2, m_4, m_2) \iint dr_a r_a^2\, dr_b r_b^2\, (-1)^{m_3}\, u^a_{N_1 l_1}(r_a)\, u^b_{N_2 l_2}(r_b) \sum_{\vec{R}} e^{-i\vec{g}(\vec{R}_{ab}+\vec{R})}\, \mathcal{M}(l_1 m_3\ l_2 m_4)\, r_a^{l_1}\, r_b^{l_2}\, \frac{1}{|\vec{R}_{ab}+\vec{R}|^{l_1+l_2+1}}\, Y_{l_1+l_2,\, m_3+m_4}(\widehat{R+R_{ab}})$$

$$V_{ab}(\vec{g}) = \underbrace{\int dr_a r_a^2\, r_a^{l_1}\, u^a_{N_1 l_1}(r_a) \int dr_b r_b^2\, r_b^{l_2}\, u^b_{N_2 l_2}(r_b)}_{\text{rteij}}\ \underbrace{\sum_{\substack{l_1 l_2 m_1 m_2\\ m_3 m_4}} \underbrace{D^*(l_1, -m_3, m_1)}_{dj3}\, \underbrace{D(l_2, m_4, m_2)}_{dj4}\, \underbrace{\underbrace{\mathcal{M}(l_1 m_3\ l_2 m_4)}_{tp}\, \underbrace{(-1)^{m_3}}_{minn}\, \underbrace{\sum_{\vec{R}} e^{-i\vec{g}(\vec{R}_{ab}+\vec{R})}\, \frac{1}{|\vec{R}_{ab}+\vec{R}|^{l_1+l_2+1}}\, Y_{l_1+l_2,\, m_3+m_4}(\widehat{R+R_{ab}})}_{\text{Ewald sum } spm(l_1+l_2,\, m_3+m_4,\, \vec{R}_{ab},\, \vec{g})}}_{minn\cdot tp\cdot stc}}_{sum34}$$

MT_Coulomb

Debugging for $g=0$ and checking why is $V_{\alpha\beta}(g=0)$ complex is Si.

$g=0,\ L_1=0$

$$V_{\alpha\beta}(\vec{g}) = \sum_{\vec{R}} \iint Y^*_{L_1M_1}(\hat{R}_a \hat{r}_a)\, Y_{L_2M_2}(\hat{R}_b \hat{r}_b)\, \mathcal{U}^a_{N_1L_1}(r_a)\, \mathcal{U}^b_{N_2L_2}(r_b)\, \frac{e^{-i\vec{g}(\vec{R}_{ab}+\vec{R})}}{|\vec{r}_a - \vec{r}_b + \vec{R}_{ab} + \vec{R}|}\, d^3r_a\, d^3r_b$$

$\vec{R}$ lattice in real space

$\hat{R}$ rotation matrix to global axis

$$V_{\alpha\beta}(0) = \frac{1}{\sqrt{4\pi}} \iint d^3r_a\, d^3r_b\, Y_{L_2M_2}(\hat{R}_b\hat{r}_b)\, \mathcal{U}^a_{N_1L_1}(r_a)\, \mathcal{U}^b_{N_2L_2}(r_b) \sum_{\vec{R}} \frac{1}{|\vec{r}_a - \vec{r}_b + \vec{R}_{ab} + \vec{R}|}$$

$l_1 m_1 = 0$ $\quad l_2 m_2 = (3,-1)$
$\quad (3,3)$

$$\sum_{\substack{l_1 l_2 m_1 m_2 \\ m_3 m_4}} \underbrace{D^*(l_1, -m_3, m_1)}_{dj3}\, \underbrace{D(l_2, m_4, m_2)}_{dj4}\, \underbrace{\mathcal{Y}(l_1 m_3\ l_2 m_4)}_{tg}\, \underbrace{(-1)^{m_3}}_{minm} \sum_{\vec{R}} e^{-i\vec{g}(\vec{R}_{ab}+\vec{R})} \frac{1}{|\vec{R}_{ab}+\vec{R}|^{l_1+l_2+1}}\, Y_{l_1+l_2,\, m_3+m_4}(\widehat{R+R_{ab}})$$

$m_3 = 0$ because $l_1 = 0$

$$\sum_{l_2 m_2 m_4} D(l_2, m_4, m_2)\, \frac{4\pi^{3/2}}{(2l_2+1)} \sum_{\vec{R}} \frac{1}{|\vec{R}_{ab}+\vec{R}|^{l_2+1}}\, Y_{l_2, m_4}(\widehat{R+R_{ab}})$$

$m_4,\ -m_4$

$D(3, m_4, -1)$

$Y^*_{lm} = Y_{l,-m}(-1)^m$

$Y^*_{33} = -Y_{3,-3}$

$$\mathcal{Y}(0,0,l_2 m_2) = 4\pi^{3/2} \sqrt{\frac{\binom{l_2+m_2}{0}\binom{l_2-m_2}{0}}{(2l_2+1)^2}} = \frac{4\pi^{3/2}}{(2l_2+1)}$$

$djm(\overset{3}{l_2}, \overset{1}{m_1}, \overset{-1}{m_2})$

$l=3 \mid m\ m' = (-3,3)\quad i$
$(-2,2)\quad 1$
$(-1,1)\quad -i$
$(0,0)\quad -1$

$$\begin{matrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{matrix}$$

Product b.: Interstitial

$$\langle e^{i\vec{G}_1\vec{r}} | \frac{1}{|\vec{r}-\vec{r}'|} e^{-i\vec{q}(\vec{r}-\vec{r}')} | e^{i\vec{G}_2\vec{r}'}\rangle = \sum_{\vec{G}} \langle e^{i(\vec{G}_1+\vec{q})\vec{r}} | e^{i(\vec{K}+\vec{q})\vec{r}}\rangle_I \frac{4\pi}{|\vec{q}+K|^2} \langle e^{i(\vec{K}+\vec{q})\vec{r}} | e^{i(\vec{G}_2+\vec{q})\vec{r}}\rangle_I$$

- $|G_1\rangle$ Interstitial product basis cutoff mgg[ig]

- First orthogonalize this basis

$$\langle G_1|I|G_2\rangle = \int_{\text{Interstitials}} e^{i(\vec{G}_2-\vec{G}_1)\vec{r}} d^3r$$

$$\langle G_1|I|G_2\rangle A_{G_2 i} = A_{G_1 i}\,\varepsilon_i \Rightarrow \frac{1}{\sqrt{\varepsilon_i}}(A^+)_{iG_1}\langle G_1|I|G_2\rangle A_{G_2 j}\frac{1}{\sqrt{\varepsilon_j}} = \delta_{ij}$$

$$\text{Define: } \left(\frac{1}{\sqrt{O}}\right)_{Gi} = A_{Gi}\frac{1}{\sqrt{\varepsilon_i}} \Rightarrow \left(\frac{1}{\sqrt{O}}\right)^+ O \frac{1}{\sqrt{O}} = 1$$

where $O = \langle G_1|I|G_2\rangle$

- Next construct much larger (complete basis) of plane waves $\langle r|\vec{k}\rangle = e^{i\vec{k}\cdot\vec{r}}$, with cutoff K mgg-barc[ig], and compute the transformation

$$\frac{1}{\sqrt{O}}\langle G|I|K\rangle$$

cutoff for K is larger mgg-barc[ig]

$$\frac{1}{\sqrt{\varepsilon_i}}(A^T)_{iG}\langle G|I|K\rangle \equiv \text{mpwipw}[i, K_j]$$

mgg mgg-barc

- Next we compute $V_{ij} \equiv \text{mpwipw}[i,K_i]\frac{4\pi}{K_i^2}\text{mpwipw}[j,K_i]^* = \frac{1}{\sqrt{\varepsilon_i}}(A^T)_{iG}\langle G|I|K\rangle\frac{4\pi}{K^2}\langle K|I|G'\rangle A^*_{G'j}\frac{1}{\sqrt{\varepsilon_j}}$

$$Tr(V) = A_{Gi}\frac{1}{\varepsilon_i}(A^+)_{iG'}\langle G|I|K\rangle\frac{4\pi}{K^2}\langle K|I|G'\rangle$$

$$Tr(V) = (\langle G|I|G'\rangle)^{-1}\langle G|I|K\rangle\frac{4\pi}{K^2}\langle K|I|G'\rangle$$

Mixed Interstitial - MT

$$\langle e^{i\vec{G}\vec{r}} | \frac{1}{|\vec{r}-\vec{r}'|} e^{-i\vec{q}(\vec{r}-\vec{r}')} | u^{pb,a}_{NLM}(\vec{r}')\rangle = \sum_{\vec{k}} \langle e^{i(\vec{q}+\vec{G})\vec{r}} | e^{i(\vec{k}+\vec{q})\vec{r}}\rangle_I \frac{4\pi}{|\vec{k}+\vec{q}|^2} \langle e^{i(\vec{k}+\vec{q})\vec{r}} | u^{pb,a}_{NLM}(\vec{r})\rangle_{MT}$$

- $|G_1\rangle$ Interstitial product basis cutoff ngq[iq]

- First orthogonalize this basis

$$\langle G_1|I|G_2\rangle = \int_{\text{Interstitials}} e^{i(\vec{G}_2-\vec{G}_1)\vec{r}} d^3r$$

$$\langle G_1|I|G_2\rangle A_{G_2 i} = A_{G_1 i}\,\varepsilon_i \Rightarrow \frac{1}{\sqrt{\varepsilon_i}}(A^+)_{iG_1}\langle G_1|I|G_2\rangle A_{G_2 j}\frac{1}{\sqrt{\varepsilon_j}} = \delta_{ij}$$

$$\text{Define: } \left(\frac{1}{\sqrt{O}}\right)_{Gi} = A_{Gi}\frac{1}{\sqrt{\varepsilon_i}} \Rightarrow \left(\frac{1}{\sqrt{O}}\right)^+ O \frac{1}{\sqrt{O}} = 1$$

where $O = \langle G_1|I|G_2\rangle$

- Next construct much larger (complete basis) of plane waves with cutoff K ngq-barc[iq], and compute the transformation

$$\frac{1}{\sqrt{O}}\langle G|I|K\rangle$$

cutoff for K is larger ngq-barc[iq]

$$\frac{1}{\sqrt{\varepsilon_i}}(A^T)_{iG}\langle G|I|K\rangle \equiv mpwipw[i, K_j]$$

ngq ngq-barc

- Next we compute $V_{matit}[K,im] = \langle e^{i(\vec{q}+\vec{K})\vec{r}} | V_{coul} | u^{pb,a}_{im}\rangle = \sum_{R_a} e^{-i(\vec{q}+\vec{K})\vec{R}_a} \frac{4\pi}{|\vec{q}+\vec{K}|^2}\langle \vec{q}+\vec{K}| u^{pb,a}_{im}\rangle_{MT}$

product basis on given atom a

- Finally we compute mpwipw * Vmatit =

$$\frac{1}{\sqrt{\varepsilon_i}}(A^T)_{iG}\langle G|I|K\rangle\langle e^{i(\vec{q}+\vec{K})\vec{r}}|V_{coul}|u^{pb,a}_{im}\rangle \approx \frac{1}{\sqrt{O}}\langle G|V_{coul}|u^{pb,a}_{im}\rangle$$

Laplace multicenter expansion (M.E. Rose, J. Math. Phys 37, 215 (1958))

$$\frac{1}{|\vec{R}+\vec{r}_1-\vec{r}_2|} = (4\pi)^{3/2}\sum_{\substack{l_1 m_1\\ l_2 m_2}} (-1)^{l_1}\sqrt{\frac{\binom{l_1+m_1+l_2+m_2}{l_1+m_1}\binom{l_1-m_1+l_2-m_2}{l_1-m_1}}{(2l_2+1)(2l_1+1)(2l_1+2l_2+1)}}\; r_1^{l_1}\, Y^*_{l_1 m_1}(\hat{r}_1)\, r_2^{l_2}\, Y^*_{l_2 m_2}(\hat{r}_2)\,\frac{1}{R^{l_1+l_2}}\, Y_{l_1+l_2,\, m_1+m_2}(\hat{R})$$

Gap paper

$$\frac{4\pi}{(2L'+1)}\frac{1}{|\vec{r}-\vec{R}|^{L'+1}}\, Y_{L'M'}(\widehat{r-R}) = (-1)^{L'+M'}\sum_{l,m}\frac{r^l}{R^{L'+l+1}}\, Y_{lm}(\hat{r})\, Y^*_{L'+l,\, m-M'}(\hat{R})\; C_{L'M',lm}$$

Alternative way to Calculate V from plane wave expression

We want: $$\sum_{\vec{k}} \langle u_{product} | e^{i(\vec{k}+\vec{g})\vec{r}} \rangle_{all\,space} \frac{4\pi}{|\vec{g}+\vec{k}|^2} \langle e^{i(k+\vec{g})\vec{r}} | u_{product} \rangle$$

$$MPW[basis, \vec{k}] = \langle u_{product} | e^{i(\vec{k}+\vec{g})\vec{r}} \rangle_{all-space} = \begin{cases} MT: & \langle u^{a}_{NL} Y_{LM}(\hat{r}) | e^{i(\vec{k}+\vec{g})\vec{r}} \rangle_{MT} \\ Inter.: & \frac{1}{\sqrt{\Omega}} \langle G | K \rangle_{Int} \end{cases}$$

$$MPW[im, \vec{k}] = e^{i(\vec{k}+\vec{g})\vec{R}} \langle u^{a}_{NL}(r) Y_{LM}(\hat{r}) | e^{i(k+\vec{g})(\vec{r}-\vec{R})} \rangle_{MT} = \langle u^{a}_{NL} Y_{LM}(\hat{r}) | e^{i(\vec{k}+\vec{g})\vec{r}} \rangle_{MT}$$

$$e^{i(\vec{k}+\vec{g})\vec{R}} \langle u^{a}_{NL}(r) | 4\pi i^L j_L(|\vec{k}+\vec{g}| r) \rangle_{MT} Y^{*}_{LM}(\widehat{k+g})$$

$$MPW[\vec{G}, \vec{k}] = \frac{1}{\sqrt{\varepsilon_i}} (A^T)_{iG} \langle G | I | K \rangle \qquad \text{where} \quad \langle G_1 | I | G_2 \rangle A_{G_2 i} = A_{G_1 i}\, \varepsilon_i$$

$$V_{mat}[basis, basis] = MPW \times \frac{4\pi}{|\vec{g}+\vec{k}|^2} * MPW^{+}$$

When $g=0$ then: $$\langle u_{product} | e^{i\vec{k}\cdot\vec{r}} \rangle_{all-space} = \begin{cases} \int_{MT} u_{i}(r)\, r\, dr \\ \frac{1}{\sqrt{\Omega}} \int_{I} e^{i\vec{G}\cdot\vec{r}} \end{cases}$$

Once we have $V_{mat}(\alpha,\beta) = \langle \chi^{\alpha} | V_g | \chi^{\beta} \rangle$, we diagonalize it

V_{mat} = self.Vmat · $\mathcal{E}$ · self.Vmat† $\equiv \langle \chi^{\alpha} | V_g | \chi^{\beta} \rangle = A_{\alpha i}\, \varepsilon_i\, (A^{\dagger})_{i\beta}$

barcev = $\mathcal{E}$ when $|\mathcal{E}| >$ cutoff

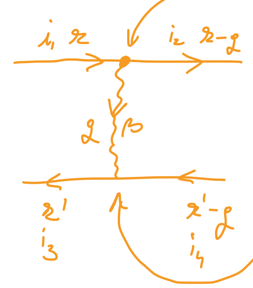
barcvm = self.Vmat · $\sqrt{\mathcal{E}}$ so that V_{mat} = barcvm · barcvm†

barcvm = $A_{\alpha i}\sqrt{\varepsilon_i}$ and $V_{mat} = A_{\alpha i}\sqrt{\varepsilon_i}\sqrt{\varepsilon_i}\, A^{*}_{\beta i}$

mmat$(i_1, i_2, \alpha) = \langle \chi^{\alpha} | \psi_{i_1 k}\, \psi^{*}_{i_2\, k-q} \rangle$

minm$(i_1, i_2, \beta) = \sqrt{\varepsilon_\beta}\, (A^{\dagger})_{\beta\alpha} \langle \chi^{\alpha} | \psi_{i_1 k}\, \psi^{*}_{i_2\, k-q} \rangle$

minm (k, q, i_1, i_2, β)



$\sqrt{\varepsilon_\beta} A^{\dagger}_{\beta\alpha} \langle \chi^{\alpha} | \psi_{i_1 k}\, \psi^{*}_{i_2\, k-q} \rangle$

$\langle \psi^{*}_{i_3 k'}\, \psi_{i_4\, k'-q} | \chi^{\alpha} \rangle A_{\alpha\beta} \sqrt{\varepsilon_\beta}$

minm$^{*}(k', q, i_3, i_4, \beta)$

$\langle \psi^{*}_{i_3 k'}\, \psi_{i_4\, k'-q} | \chi^{\gamma} \rangle V_{mat\, \gamma\alpha} \langle \chi^{\alpha} | \psi_{i_1 k}\, \psi^{*}_{i_2\, k-q} \rangle$

$\Sigma^{x}_{i_1 i_3} = - \sum_{\beta, q, i_2}$ minm(i_1, i_2, k, q, β) minm$(i_3, i_2, k, q, \beta)\, f(\varepsilon_2)\, w_q$

We need overlap between product basis and Kohn-Sham eigenvectors : $\langle \chi^\alpha | \psi_{i_1 k} \psi^*_{i_2\, k-q} \rangle$ which is

Note $\langle \chi^\alpha(\vec r) | \chi^\beta(\vec r) \rangle_{MT} = \delta_{\alpha\beta}$

$\langle \chi^\alpha_{MT}(\vec r) | \chi^\beta_{IN}(\vec r) \rangle = 0$

$\langle \chi^\alpha(\vec r) | \chi^\beta(\vec r) \rangle_{In} = \delta_{\alpha\beta}$

need to be orthogonalized

$$M^{aNLM}_{i_1 i_2}(\vec k, \vec q) \equiv \langle \chi_{NLM} | \psi_{i_1 k} \psi^*_{i_2\, k-q} \rangle_{MT} \quad \text{and}$$

$$M^{G_p}_{i_1 i_2}(\vec k, \vec q) \equiv \langle e^{i(\vec G_p + \vec q)\vec r} | \psi_{i_1 k} \psi^*_{i_2\, k-q} \rangle_{Int}$$

$$\langle e^{i G_p \vec r} | e^{i \vec G_1 \vec r - i \vec G_2 \vec r} \rangle$$

Interstitial:

from vector file

$$\frac{1}{\sqrt{\Omega}} \langle e^{i(\vec G_p + \vec q)\vec r} | \psi_{i_1 k} \psi^*_{i_2\, k-q} \rangle_{Int} = \frac{1}{\sqrt{2}} \sum_{G_1 G_2} \Theta^{LO}_{G_1} \Theta^{LO}_{G_2} C^{(k)}_{(i_1, G_1)} C^{(k-q)*}_{(i_2, G_2)} \int_{In} e^{i(\vec q + \vec G_1 - \vec G_2)\vec r} \left(\frac{1}{\sqrt{\Omega}}\right)_{\vec G \vec G'} e^{-i(\vec q + \vec G_p)\vec r} d^3 r$$

$$M^{G_p}_{i_1 i_2}(\vec k, \vec q) = \underbrace{\left(\frac{1}{\sqrt{\Omega}}\right) \int_{In} e^{-i(\vec G_p - \vec G_1 + \vec G_2)\vec r} d^3 r}_{mpwipw[G_p,\, G_1 - G_2]} \frac{1}{\sqrt{2}} \sum_{G_1 G_2} \Theta^{LO}_{G_1} \Theta^{LO}_{G_2} C^{(k)}_{(i_1, G_1)} C^{(k-q)*}_{(i_2, G_2)}$$

$$M^{G_p}_{i_1 i_2}(\vec k, \vec q) = \frac{1}{\sqrt{2}} \sum_{G_1 G_2} C^{(k)}(i_1, G_1) \cdot mpwipw[G_p, G_1 - G_2]\, C^{(k-q)*}(i_2, G_2)$$

$$\frac{1}{\sqrt{E_i}} (A^T)_{iG} \langle G | I | K \rangle \equiv mpwipw[i, K_j]$$

i: mgg; K_j: mgg-basc

Note $mpwipw[i, K_j] = \frac{1}{\sqrt{E_i}} (A^T)_{iG} \langle G | I | K \rangle = \frac{1}{\sqrt{\Omega}} \int_{In} e^{-i(G - \vec K)\vec r} d^3 r$

i: mgg; K_j: mgg-basc

Muffin-Tin

question, why is χ_{NLM} in the MT sphere not expressed as $e^{i\vec q \vec r} \tilde\chi_{NLM}(\vec r)$?

$$M^{aNLM}_{i_1 i_2}(\vec k, \vec q) = \langle N_{aNL} Y_{LM} | \psi_{i_1 k} \psi^*_{i_2\, k+q} \rangle_{MT} =$$

$$\sum_{\substack{q, \ell_1 m_1 \\ p, \ell_2 m_2}} e^{-i \vec q \cdot \vec R_a} A^{(k)}_{i_1\, a q_1 \ell_1 m_1} A^{(k-q)*}_{i_2\, a q_2 \ell_2 m_2} \langle \ell_1 m_1 | L M \ell_2 m_2 \rangle^* \underbrace{\int dr_a r_a^2 N_{aNLM}(r_a) u_{a q_1 \ell_1}(r_a) u_{a q_2 \ell_2}(r_a)}_{s3r}$$

nstart : nend

mstart : mend

Core states :

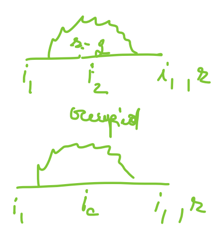
$$M_{i_1 i_c}(\vec k) = \langle N Y_{LM} | \psi_{i_1 k} \psi^*_{i_c} \rangle$$

i_1: cnst : cnend; i_c: cst : cend; i_c: core

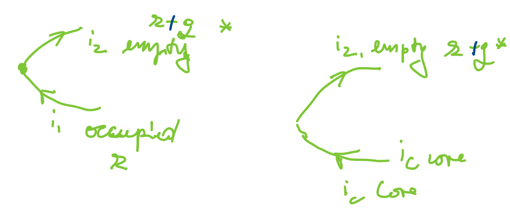
$$M_{i_c i_2}(\vec k + \vec q) = \langle N Y_{LM} | \psi_{i_c} \psi^*_{i_2\, k+q} \rangle$$

i_c: core; $\vec k + \vec q$ instead of $\vec k$; empty

for exchange



correlation:



$$N_{aNL} = j_l(br)\, Y^*_{LM}(\text{rotloc} \cdot \text{rotij} \cdot \text{z2cartes}(-\hat{b})) \cdot i^l\, 4\pi$$

$$M^{aNLM}_{i_1 i_2}(\vec{k},\vec{g}) = \langle N_{aNL} Y_{LM} | \psi_{i_1 k}\, \psi^*_{i_2\, k-g} \rangle_{MT} =$$

nstart : nend

nstart : nend

$$\sum_{\substack{q_1 l_1 m_1 \\ q_2 l_2 m_2}} e^{-i\vec{g}\cdot\vec{R}_a} A^{(k)}_{i_1\, a q_1 l_1 m_1} A^{(k-g)*}_{i_2\, a q_2 l_2 m_2} \langle l_1 m_1 | L M\, l_2 m_2 \rangle^* \underbrace{\int dr_a r_a^2\, N_{aNLM}(r_a)\, u_{a q_1 l_1}(r_a)\, u_{a q_2 l_2}(r_a)}_{s3r}$$

$$4\pi(-i)^l\, Y_{LM}(\text{rotloc}\cdot\text{rotij}\cdot\text{z2cartes}(-\hat{b})) \cdot \langle j_l(br)\, Y_{LM} | \psi_{i_1 k}\, \psi^*_{i_2\, k-g} \rangle_{MT}$$

$$\underbrace{[\text{rotloc}[iat,:,:] \cdot \text{rotij}[idf,:,:]\, \text{z2cartes} \cdot \vec{k}]}$$

$$\langle e^{i\vec{g}\vec{r}} | \psi^*_{m,\, k-g}(\vec{r})\, \psi_{m,k}(\vec{r}) \rangle = 4\pi(-i)^l\, Y_{lm}(\hat{g}) \langle j_l(gr) Y_{lm}(\hat{r}) | \psi^*_{m,\, k-g}(\vec{r})\, \psi_{m,k}(\vec{r}) \rangle$$

$$\begin{matrix} \| & & \| \\ i_{e_2} & & i_{e_1} \end{matrix}$$

$$\langle e^{-i\vec{b}\vec{r}} | \psi^*_{i_{e_2},\, \vec{k}+\vec{b}}(\vec{r})\, \psi_{i_{e_1} k}(\vec{r}) \rangle = 4\pi \underbrace{(-i)^l\, Y_{lm}(-\hat{b})}_{(i)^l Y_{lm}(\hat{b})} \langle j_l(br)\, Y_{lm}(\hat{r}) | \psi^*_{i_{e_2},\, \vec{k}+\vec{b}}\, \psi_{i_{e_1} k} \rangle$$

<u>Interstitial</u>:

from vector file

$$\langle e^{i(\cancel{\vec{G}_p}+\vec{g})\vec{r}} | \psi_{i_1 k}\, \psi^*_{i_2\, k-g} \rangle_{Int} = \frac{1}{\sqrt{\Omega}} \sum_{G_1 G_2} \Theta^{L0}_{G_1} \Theta^{L0}_{G_2}\, C^{(k)}_{(i_1,G_1)}\, C^{(k-g)*}_{(i_2,G_2)} \int_{Int} e^{i(\vec{g}+\vec{G}_1-\vec{G}_2)\vec{r}} \left(\cancel{\frac{1}{\sqrt{\Omega}}}\right)_{GG'} e^{-i(\vec{g}+\cancel{\vec{G}_p})\vec{r}}\, d^3r$$

$$M^{G_p''0}_{i_1 i_2}(\vec{k},\vec{g}) = \underbrace{\left(\cancel{\frac{1}{\sqrt{\Omega}}}\right) \int_{Int} e^{-i(\cancel{\vec{G}_p}-\vec{G}_1+\vec{G}_2)\vec{r}}\, d^3r}_{\text{mpwipw}[G_p,\, G_1-G_2]} \frac{1}{\sqrt{\Omega}} \sum_{G_1 G_2} \Theta^{L0}_{G_1} \Theta^{L0}_{G_2}\, C^{(k)}_{(i_1,G_1)}\, C^{(k-g)*}_{(i_2,G_2)}$$

$$M^{G_p''0}_{i_1 i_2}(\vec{k},\vec{g}) = \frac{1}{\sqrt{\Omega}} \sum_{G_1 G_2} C^{(k)}(i_1, G_1) \cdot \text{mpwipw}[G_p''0,\, G_1-G_2]\, C^{(k-g)*}(i_2, G_2)$$

$$\frac{1}{\sqrt{E_i}} (A^T)_{iG} \langle G | I | K \rangle \equiv \text{mpwipw}[i, K_j]$$

mgg   mgg-barc

Note $\text{mpwipw}[G, K_j] = \langle G | I | K \rangle = \int_{In} e^{-i(\vec{G}-\vec{K})\vec{r}}\, d^3r$

mgg   mgg-barc

$$\sum_{G_1 G_2} C^k_{i_1 G_1}\, C^{k*}_{i_2 G_2} \frac{1}{\sqrt{\Omega}} \int_{Int} e^{i(G_1-G_2)\vec{r}} = C_{i_2 G_1} \cdot \text{mpw}[G_1-G_2] \cdot C^*_{i_2 G_2}$$

$$\psi_{ik} = \sum_i A^k_{iG_1} a_{G_1 lm\alpha} u^\alpha_l(r) Y_{lm}(R_\alpha \hat{r})$$

$$\psi^*_{i_2 k} \psi_{i_1 k} = A^{k*}_{i_2 G_2} A_{i_1 G_1} a^*_{G_2 lm\alpha_2} a_{G_1 lm\alpha_1} \langle u^{\alpha_2}_l | u^{\alpha_1}_l \rangle$$

$$\langle \chi_{G_2} | \chi_{G_1} \rangle = a^*_{G_2 lm\alpha_2} a_{G_1 lm\alpha_1} \langle u^{\alpha_2}_l | u^{\alpha_1}_l \rangle$$

<u>here 6</u>

irk=4	irk=6
irk=5	irk=7
irk=6	irk=8
irk=7	irk=11
irk=8	irk=28

<u>mpwipw[G=0]</u> $\longrightarrow 1 - N_{at} \frac{V_{RMT}}{V}$

$$\longrightarrow -\frac{j_1(G R_{MT})}{G R_{MT}} \cdot 3 \frac{V_{RMT}}{V} \sum_{equiv} e^{i \vec{r}_\alpha \cdot \vec{G}}$$

(13) 134, 138,

$$\sum_G A^{k+q\,*}_{j\,G_1} A^k_{i\,G_2}$$

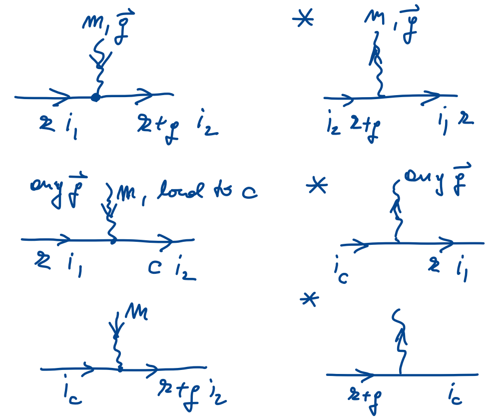
$$\langle G_1 | e^{i\vec{q}\vec{r}} | G_2 \rangle$$

$M^{m}_{i_1 i_2}(\vec{k},\vec{q}) \equiv \langle \chi^{\vec{q}}_{m} | \psi_{i_1 k}\, \psi^{*}_{i_2\, k+q} \rangle$

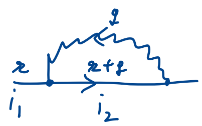
There core are q-independent:

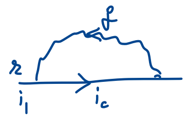
$M^{m}_{i_1 i_c}(\vec{k}) \equiv \langle \chi_m | \psi_{i_1 k}\, \psi^{*}_{i_2 c} \rangle$

$M^{m}_{i_c i_2}(\vec{k}+\vec{q}) \equiv \langle \chi_m | \psi_{i_c}\, \psi^{*}_{i_2\, k+q} \rangle = M^{*}_{i_2 i_c}(\vec{k}+\vec{q})$



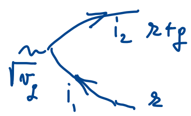
self-energy:



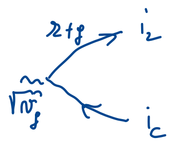


$M^{m}_{i_1 i_2}(\vec{k},\vec{q})\, M^{m' *}_{i_1 i_2}(\vec{k},\vec{q})$

polarization:



$+$



1) exchange self-energy

$M^{m}_{i_1 i_2}(\vec{k}_{irr}, \vec{q})$

external, occupied

2) correlation self-energy

$M^{m}_{i_1 i_2}(\vec{k}_{irr}, \vec{q})$

external, internal, mostly occupied + some empty

3) polarization

$M^{m}_{i_1 i_2}(\vec{k}, \vec{q})$ — all

occupied, empty

, $M^{*}_{i_2 i_c}(\vec{k}+\vec{q})$

SX:	k_{irr}	0:13 , 0:2	
SC:	k_{irr}	0:13 , 0:57	
polar:	k_{all}	0:2 , 1:57	

$\boxed{\begin{array}{lll} k_{all}: & 0:2\ ,\ 1:57 & \text{polar} \\ k_{irr}: & 0:13\ ,\ 0:57 & \text{SC} \end{array}}$

SX:	k_{irr}	0:14 , 0:4	0:14 , core
SC:	k_{irr}	0:14 , 0:225	0:14 , core
polar:	k_{all}	0:4 , 4:209	4:209 , core

core: k_{all} : 0:209 , core

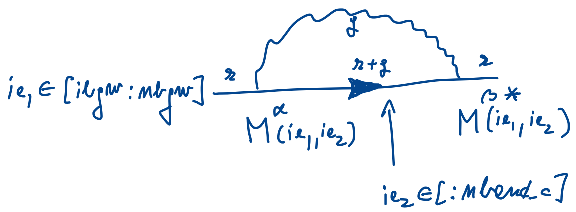
dot 2:10 , (9:49)

matmul 2:20 (10:9)

Convolution

Error

$(\sqrt{v}\,(\varepsilon^{-1}-1)\sqrt{v})(\cancel{q},\cancel{q})$



$$M^{aNLM}_{i_1 i_2}(\vec{k},\vec{q}) = \langle N_{aNL} Y_{LM} | \psi_{i_1 k} \psi^*_{i_2\, k+q} \rangle_{MT} =$$

$$\Sigma_k(i_1, i_3) = -\frac{1}{\beta} \sum_{i\Omega} \frac{M^{\alpha}(i_1,i_2)\, W_q^{\alpha\beta}(i\Omega)\, M^{\beta *}(i_3,i_2)}{i\omega - \varepsilon_{i_2}^{k+q} + i\Omega} = -\frac{1}{\beta}\sum_{i\Omega} \frac{\mathcal{W}^{q}_{i_1 i_3 i_2}(i\Omega)}{i\omega + i\Omega - \varepsilon_{i_2}^{k+q}}$$

where $\mathcal{W}^{q}_{i_1 i_3 i_2}(i\Omega) = \sum_{\alpha\beta} M^{\alpha}(i_1,i_2)\, W_q^{\alpha\beta}(i\Omega)\, M^{\beta *}(i_3,i_2)$

$$\mathcal{W}^{q}_{i_1 i_3, i_2 \Omega_m} = U_{i_1 i_3, p}\, s_p\, V_{p, i_2 \Omega_m}$$

$W_q(-i\Omega_m) = W_q(i\Omega_m) \in$ Hermitian

Interesting integral

$$\frac{1}{\beta}\sum_{i\Omega} \frac{W_q^{\alpha\beta}(i\Omega)\,[i\omega - \varepsilon_{i_2}^{k+q} - i\Omega]}{(i\omega - \varepsilon_{i_2}^{k+q})^2 + \Omega^2} = \frac{1}{\beta}\sum_{i\Omega} \frac{W_q^{\alpha\beta}(i\Omega)\,[i\omega - \varepsilon_{i_2}^{k+q}]}{\Omega^2 + (i\omega - \varepsilon_{i_2}^{k+q})^2} = \frac{1}{\pi}\int_0^{\infty} \frac{W_q^{\alpha\beta}(i\Omega)\,[i\omega - \varepsilon_{i_2}^{k+q}]}{\Omega^2 + (i\omega - \varepsilon_{i_2}^{k+q})^2}$$

$$\frac{1}{\beta}\sum_{\Omega_m} f\left(\frac{2m\pi}{\beta}\right) \xrightarrow[T\to 0]{} \frac{1}{2\pi}\int_{-\infty}^{\infty} f(x)\,dx$$

$$\Sigma(i\omega) = +\frac{1}{\pi}\int_0^{\infty} \frac{(\varepsilon - i\omega)\, W(i\Omega)}{(\varepsilon - i\omega)^2 + \Omega^2}\, d\Omega = \frac{(\varepsilon - i\omega)}{\pi}\int_0^{\infty} \frac{[W(\Omega) - W(\omega)]}{(\varepsilon - i\omega)^2 + \Omega^2}\, d\Omega + W(\omega)\frac{1}{2}\,\mathrm{sign}(\varepsilon)$$

because: $\displaystyle\int_0^{\infty} \frac{d\Omega}{(\varepsilon - i\omega)^2 + \Omega^2} = \frac{\pi}{2}\frac{1}{(\varepsilon - i\omega)}\,\mathrm{sign}(\varepsilon)$

$$\Sigma_{i_1}(i\omega) = \sum_{i_2 \ell} W_q^{i_1 i_2}(\ell)\, \underbrace{\frac{1}{\pi}\int_0^{\infty} \frac{U_\ell(i\Omega)\,[\varepsilon_{i_2}^{k+q} - i\omega]}{(i\omega - \varepsilon_{i_2}^{k+q})^2 + \Omega^2}\, d\Omega}_{C(i_2 \ell;\, i\omega)}$$

$$C(i_2\ell;\, i\omega) = \frac{(\varepsilon_{i_2} - i\omega)}{\pi}\int_0^{\infty} \frac{[U_\ell(i\Omega) - U_\ell(i\omega)]}{(\varepsilon_{i_2} - i\omega)^2 + \Omega^2}\, d\Omega + U_\ell(i\omega)\frac{1}{2}\,\mathrm{sign}(\varepsilon_{i_2})$$

$$\boxed{\Sigma(i_1\, i\omega) = \sum_{\ell, i_2} W_q(i_1; i_2\ell)\, C(i_2\ell; i\omega)}$$

$$\Sigma_{x}(i_1 i_3) = -\frac{1}{\beta}\sum_{i\Omega} \frac{W^{\ell}_{i_1 i_3 i_2}(i\Omega)}{i\omega + i\Omega - \varepsilon_{i_2}^{x+\ell}} \quad \text{where } W^{\ell}_{i_1 i_3 i_2}(i\Omega) = \sum_{\alpha\beta} M^{\alpha}(i_1, i_2)\, W_f^{\alpha\beta}(i\Omega)\, M^{\beta *}(i_3, i_2)$$

$W_f(-i\Omega_m) = W_f(i\Omega_m) \in$ Hermitian

$$\langle \chi_f^{\alpha} | W_f(-i\Omega) | \chi_f^{\beta}\rangle = \langle \chi_f^{\alpha} | W_f^{*}(i\Omega) | \chi_f^{\beta}\rangle = \left(\langle \chi_f^{\beta} | W_f(i\Omega) | \chi_f^{\alpha}\rangle\right)^{*}$$

$$W^{\ell}_{i_1 i_3, i_2}(-i\Omega) = \sum_{\alpha\beta} M^{\alpha}(i_1 i_2)\langle \chi_f^{\alpha} | W_f(-i\Omega) | \chi_f^{\beta}\rangle M^{\beta *}(i_3, i_2) = \sum_{\alpha\beta} M^{*}_{\beta}(i_3 i_2)\left(\langle \chi_f^{\beta} | W_f(i\Omega) | \chi_f^{\alpha}\rangle\right)^{*} M^{\alpha}(i_1 i_2)$$

$$= \left(\sum_{\alpha\beta} M_{\beta}(i_3, i_2)\langle \chi_f^{\beta} | W_f(i\Omega) | \chi_f^{\alpha}\rangle M^{\alpha *}(i_1 i_2)\right)^{*}$$

$$= W^{\ell\,*}_{i_3 i_1, i_2}(i\Omega)$$

$$-\frac{1}{\beta}\sum_{\Omega_m} \frac{W^{\ell}_{i_1 i_3, i_2}(i\Omega)[i\omega - \varepsilon_{i_2}^{x+\ell} - i\Omega]}{(i\omega - \varepsilon_{i_2}^{x+\ell})^2 + \Omega^2} = -\frac{1}{\beta}\sum_{\Omega_m > 0} \frac{\left(W^{\ell}_{i_1 i_3, i_2}(i\Omega) + W^{\ell *}_{i_3 i_1, i_2}(i\Omega)\right)[i\omega - \varepsilon_{i_2}^{x+\ell}] - i\Omega\left[\left(W^{\ell}_{i_1 i_3, i_2}(i\Omega) - W^{\ell *}_{i_3 i_1, i_2}(i\Omega)\right)\right]}{(i\omega - \varepsilon_{i_2}^{x+\ell})^2 + \Omega^2}$$

$$\Sigma_{x}^{i_1 i_3}(i\omega) = -\frac{1}{\pi}\int_0^{\infty} \frac{\left(W^{\ell}_{i_1 i_3, i_2}(i\Omega) + W^{\ell *}_{i_3 i_1, i_2}(i\Omega)\right)[i\omega - \varepsilon_{i_2}^{x+\ell}]}{\Omega^2 + (i\omega - \varepsilon_{i_2}^{x+\ell})^2} d\Omega + \frac{1}{\pi}\int_0^{\infty} d\Omega \frac{\Omega \cdot i\left[\left(W^{\ell}_{i_1 i_3, i_2}(i\Omega) - W^{\ell *}_{i_3 i_1, i_2}(i\Omega)\right)\right]}{\Omega^2 + (i\omega - \varepsilon_{i_2}^{x+\ell})^2}$$

$$\Sigma_{x}^{i_1 i_3}(i\omega) = \left[\frac{\varepsilon_{i_2}^{x+\ell} - i\omega}{\pi}\right]\int_0^{\infty} \frac{\left(W^{\ell}_{i_1 i_3, i_2}(i\Omega) + W^{\ell *}_{i_3 i_1, i_2}(i\Omega)\right)}{\Omega^2 + (i\omega - \varepsilon_{i_2}^{x+\ell})^2} d\Omega + \frac{1}{\pi}\int_0^{\infty} d\Omega \frac{\Omega \cdot i\left[\left(W^{\ell}_{i_1 i_3, i_2}(i\Omega) - W^{\ell *}_{i_3 i_1, i_2}(i\Omega)\right)\right]}{\Omega^2 + (i\omega - \varepsilon_{i_2}^{x+\ell})^2}$$

$$S_{i_1 i_3}(i\Omega) = W^{\ell}_{i_1 i_3, i_2}(i\Omega) + W^{*}_{i_3 i_1, i_2}(i\Omega) \qquad R_{i_1 i_3}(i\Omega) = i\left(W^{\ell}_{i_1 i_3, i_2}(i\Omega) - W^{*}_{i_3 i_1, i_2}(i\Omega)\right)$$

$$S^{*}_{i_3 i_1}(i\Omega) = S_{i_1 i_3}(i\omega) \qquad R^{*}_{i_3 i_2}(i\Omega) = R_{i_1 i_3}(i\Omega)$$

$$\frac{z}{\pi}\int_0^{L} \frac{d\omega}{\Omega^2 + z^2} = \frac{1}{\pi}\arctan\left(\frac{L}{z}\right) \qquad \frac{1}{\pi}\int_0^{L} \frac{\Omega\, d\Omega}{\Omega^2 + z^2} = \frac{1}{2\pi}\left[\ln(L^2 + z^2) - \ln(z^2)\right]$$

$$= \frac{1}{2\pi}\cdot \ln\left(1 + \frac{L^2}{z^2}\right)$$

$$\left\{ \sum_i \frac{(m[i] - m[iw])\, w[i]}{w[i]^2 + (\varepsilon - i\, w[iw])^2} \right\} * \left(\frac{\varepsilon - i\, w[iw]}{\pi} \right) + m[iw] \frac{1}{\pi} \operatorname{atan}\left(\frac{w[-1]}{\varepsilon - i w[iw]} \right)$$

It seems that: $i\left[\left(W^{q}_{i_1 i_3, i_2}(i\Omega) - W^{q*}_{i_3 i_1, i_2}(i\Omega) \right) \right] = 0$

$$M^{m}_{i_1 i_2}(\vec{k}, \vec{q}) \equiv \langle \chi^{q}_{m} | \psi_{i_1 k} \psi^{*}_{i_2 k+q} \rangle$$

$$W^{q}_{i_1 i_3, i_2}(i\Omega) = \sum_{\alpha\beta} M^{\alpha}(i_1 i_2) \overbrace{\langle \chi^{\beta}_{q} | W_q(i\Omega) | \chi^{\alpha}_{q} \rangle}^{W(\beta,\alpha)} M^{\beta*}(i_3, i_2) = M^{\beta*}(i_3, i_2)\, W(\beta,\alpha)\, M^{\alpha}(i_1, i_2)$$

$$\langle \psi_{i_3 k} \psi^{*}_{i_2 k+q} | \chi^{\beta}_{q} \rangle \langle \chi^{\beta}_{q} | W_q(i\Omega) | \chi^{\alpha}_{q} \rangle \langle \chi^{\alpha}_{q} | \psi_{i_1 k} \psi^{*}_{i_2 k+q} \rangle$$

$$\sum_{\beta} M^{*}(i_3 i_2, \beta)\, W(\beta, \alpha) = \mathrm{mw}(i_3 i_2, \alpha)$$

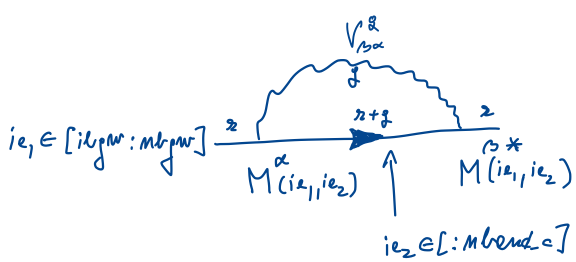
$$M(i_1, i_2, \alpha)\ \mathrm{mw.T}(\alpha, i_3 i_2)$$

$$W^{q}_{i_1 i_3, i_2}(i\Omega) = \sum_{\alpha\beta} \langle \psi_{i_3 k} \psi^{*}_{i_2 k+q} | W_q(i\Omega) | \psi_{i_1 k} \psi^{*}_{i_2 k+q} \rangle$$

$$W^{q*}_{i_3 i_1, i_2}(i\Omega) = \sum_{\alpha\beta} \langle \psi_{i_3 k} \psi^{*}_{i_2 k+q} | W^{*}_q(i\Omega) | \psi_{i_1 k} \psi^{*}_{i_2 k+q} \rangle$$

Notice that inversion symmetry makes

$P_q(i\Omega)$ is real $W_q(i\Omega)$ should be real!



$$\Sigma^{x}_{k}(i_1, i_3) = -\frac{1}{\beta} \sum_{\alpha\beta q} M^{\beta*}(i_3, i_2)\, V^{q}_{\beta\alpha} \cdot M^{\alpha}(i_1, i_2)\ f(\varepsilon^{k+q}_{i_2})$$

$$\Sigma^{x}_{k}(i_1 i_3) = \sum_{\alpha q} \tilde{M}^{*}(i_3 i_2; \alpha)\, \tilde{M}(i_1 i_2, \alpha)\, f(\varepsilon^{k+q}_{i_2})$$

for occupied: $\Sigma^{x}_{k}(i_1 i_3) = \sum_{i_2 \alpha} \tilde{M}(i_1; i_2 \alpha)\, \tilde{M}^{*}(i_3, i_2 \alpha)$

$\tilde{M} \cdot \tilde{M}^{*}$

all q-points

$$\sum_{q} W_{k+q}$$

$$C(i_2 l; i\omega) = \frac{\varepsilon_{i_2} - i\omega}{\pi} \int_0^L \frac{U_l(i\Omega)}{(\varepsilon_{i_2} - i\omega)^2 + \Omega^2}\, d\Omega$$ converges as $\frac{1}{\Omega^4}$, which is easy to integrate

We spline $U_l(i\Omega)(\Omega^2+1)$, and use second derivative $=0$ at $\Omega=0$ and first derivative $=0$ at $\Omega=L$, because we know $U_l \sim \frac{1}{\Omega^2}$ and $U_l(\Omega\sim 0)$ is constant.

For $|\varepsilon_{i_2}| \ll 1$, we do the following:

$$C(i_2 l; i\omega) = \frac{(\varepsilon_{i_2} - i\omega)}{\pi} \int_0^L \frac{[U_l(i\Omega) - U_l(i\omega)]}{(\varepsilon_{i_2} - i\omega)^2 + \Omega^2}\, d\Omega + U_l(i\omega)\, \frac{(\varepsilon_2 - i\omega)}{\pi} \int_0^L \frac{d\Omega}{(\varepsilon_2 - i\omega)^2 + \Omega^2}$$

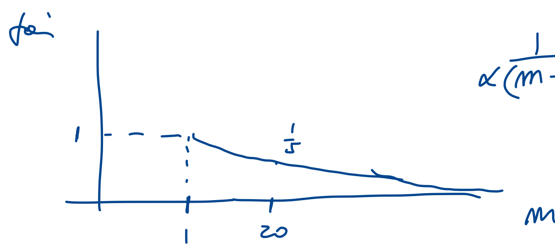
$$C(i_2 l; i\omega) = \frac{(\varepsilon_{i_2} - i\omega)}{\pi} \int_0^L \frac{[U_l(i\Omega) - U_l(i\omega)]}{(\varepsilon_{i_2} - i\omega)^2 + \Omega^2}\, d\Omega + U_l(i\omega)\, \underbrace{\frac{1}{\pi} \operatorname{atan}\left(\frac{L}{(\varepsilon_2 - i\omega)}\right)}_{\text{instead of } \frac{1}{2}\operatorname{sign}(\varepsilon_2)}$$

Important change.

$m = 20 \Rightarrow \frac{1}{5}$

$m = 1 \Rightarrow 1$

$m = \infty \Rightarrow 0$



$\frac{1}{\alpha(m-1)+1} \rightarrow \frac{1}{5} = \frac{1}{\alpha \cdot 19 + 1}$

$19\alpha + 1 = 5$

$19\alpha = 4$

$\alpha = \frac{4}{19} \sim 0.2$

$\frac{1}{1+0.2(m-1)}$

$x = \frac{i}{2N-1} \qquad i = 0 \dots 2N-1$

$$\omega = w \tan\left(x\cdot(\pi - 2\delta) - \frac{\pi}{2} + \delta\right) \qquad \frac{d\omega}{dx} = w\, \frac{(\pi - 2\delta)}{\cos^2\left(x(\pi-2\delta) - \frac{\pi}{2} + \delta\right)}\, dx$$

$\omega_0 = w \tan\left(-\frac{\pi}{2} + \delta\right)$

$\omega_1 = w \tan\left(\left(\frac{\pi}{2} - \delta\right)\frac{1}{2N-1}\right)$

$\omega_2 = w \tan\left(\frac{\pi}{2} - \delta\right)$

$$\int_{-\omega_0}^{\omega_2} f(\omega)\, d\omega = \int_0^1 f(\omega)\, \frac{d\omega}{dx}\, dx$$

$$\int_{\omega_0}^{\omega_2} \frac{d\omega}{\omega^2+\Gamma^2} = \int_0^1 \frac{d\omega}{dx}\,\frac{1}{\omega^2+\Gamma^2}\,dx = \frac{1}{\Gamma}\left[\operatorname{atg}\left(\frac{\omega_2}{\Gamma}\right)-\operatorname{atg}\left(\frac{\omega_0}{\Gamma}\right)\right] \longrightarrow \frac{2}{\Gamma}\left(\pi-2\delta-\frac{\pi}{2}+\delta\right) = \frac{2\left(\frac{\pi}{2}-\delta\right)}{\Gamma} = \frac{\pi-2\delta}{\Gamma}$$

$$\sum_{i=0}^{2N-1} \frac{1}{\omega^2+\Gamma^2}\left(\frac{d\omega}{dx}\right)\Delta x = \sum_{i=0}^{2N-1} \frac{1}{w^2\operatorname{tg}^2(g(x))+\Gamma^2}\;\frac{1}{2N}\;\frac{w\,(\pi-2\delta)}{\cos^2\left(x(\pi-2\delta)-\frac{\pi}{2}+\delta\right)}$$

$$\sum_{i=0}^{2N-1} \frac{w\,(\pi-2\delta)}{w^2\cdot 2N}\;\frac{1+\operatorname{tg}^2(g(x))}{\left(\frac{\Gamma}{w}\right)^2+\operatorname{tg}^2(g(x))}$$

If $\Gamma = w \Rightarrow \sum_{i=0}^{2N-1} \frac{(\pi-2\delta)}{w\cdot 2N} = \frac{2N}{w\cdot 2N}(\pi-2\delta) = \frac{\pi-2\delta}{w}$

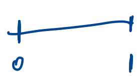
$$\omega = w\tan\left(x\cdot(\pi-2\delta)-\frac{\pi}{2}+\delta\right)$$

$$\frac{d\omega}{dx} = w\,\frac{(\pi-2\delta)}{\cos^2\left(x(\pi-2\delta)-\frac{\pi}{2}+\delta\right)} \qquad dx = \frac{1}{2N}$$

$x = \frac{i}{2N-1}$; $i \in [0, \dots 2N-1]$

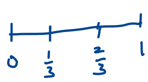
linspace $[0, 1, 2N]$

$N=1$



linspace $(0, 1, 2)$

$N=2$



Continuum space:

$$\frac{1}{V}\int \frac{e^{-\sqrt{\lambda}|\vec r-\vec r'|}}{|\vec r-\vec r'|} e^{-i\vec g(\vec r-\vec r')} d^3r\, d^3r' = 2\pi\int_{-1}^{1} dx \int_0^{\infty} dr\, r^2 \frac{e^{-\sqrt{\lambda}r - igrx}}{r} = 2\pi\int_0^{\infty} dr\, r\, e^{-\sqrt{\lambda}r} \frac{2\sin gr}{gr} = \frac{4\pi}{g}\mathrm{Im}\int_0^{\infty} dr\, e^{-\sqrt{\lambda}r+igr}$$

$$= \frac{4\pi}{g^2+\lambda}$$

$$V_g = \langle \vec G_1 | V(\vec r-\vec r') e^{i\vec g(\vec r-\vec r')} | \vec G_2\rangle = \frac{1}{V}\int d^3r\, d^3r'\, e^{-i(\vec G_1+\vec g)\vec r'} \frac{e^{-\sqrt{\lambda}|\vec r-\vec r'|}}{|\vec r-\vec r'|} e^{i(\vec G_2+\vec g)\vec r}$$

$$= \frac{1}{V}\int d^3r'\, e^{i(\vec G_2-\vec G_1)\vec r'} \int d^3(\vec r-\vec r') \frac{e^{i(\vec G_2+\vec g)(\vec r-\vec r')-\sqrt{\lambda}|\vec r-\vec r'|}}{|\vec r-\vec r'|} = \delta(\vec G_1-\vec G_2)\frac{4\pi}{|\vec g+\vec G_2|^2+\lambda}$$

$$\langle \chi_i(\vec r')| \frac{e^{-\sqrt{\lambda}|\vec r-\vec r'-\vec R|}}{|\vec r-\vec r'-\vec R|} e^{-i\vec g(\vec r-\vec r'-\vec R)} \cdot |\chi_j(\vec r-\vec R)\rangle$$

$\vec r'$ and $\vec r-\vec R$ in the same unit cell.
$\vec R$ distance between unit cells

$$\left(\langle \chi_i(\vec r')|\, V(\vec r-\vec r') e^{-i\vec g(\vec r-\vec r')} |\chi_j(\vec r)\rangle - \lambda\delta_{ij}\right)^{-1}$$

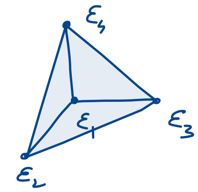
$$\left(\sum_{\vec R} \langle \chi_i(\vec r')|\, V(\vec r-\vec r') |\chi_j(\vec r)\rangle e^{-i\vec g\vec R} - \lambda\delta_{ij}\right)^{-1}$$

$\vec r, \vec r'$ the same unit cell

Tetrahedron integration:

$$\int_0^1 dz \int_0^{1-z} dy \int_0^{1-y-z} \frac{dx}{\omega - \mathcal{E}(\vec{r})}$$

where $\mathcal{E}(\vec{r}) = \varepsilon_1 + (\varepsilon_2 - \varepsilon_1)x + (\varepsilon_3 - \varepsilon_1)y + (\varepsilon_4 - \varepsilon_1)z$



$$\frac{1}{\beta}\sum_{i\omega} \frac{1}{i\omega - \varepsilon} = T\sum_{m=-\infty}^{\infty} \frac{-\varepsilon}{\varepsilon^2 + \omega_m^2}$$

$$\int_0^1 dz \int_0^{1-z} dy \int_0^{1-y-z} dx \begin{pmatrix} 1-x-y-z \\ x \\ y \\ z \end{pmatrix} = \frac{1}{24}$$

Tetrahedron method:

$$\mathcal{E}(x,y,z) = \varepsilon_1 + (\varepsilon_2 - \varepsilon_1)x + (\varepsilon_3 - \varepsilon_1)y + (\varepsilon_4 - \varepsilon_1)z$$

$$\iiint \begin{pmatrix} 1-x-y-z \\ x \\ y \\ z \end{pmatrix} \cdot \frac{\omega - \mathcal{E}(x,y,z)}{[\omega - \mathcal{E}(x,y,z)]^2 + \eta^2}\, dx\, dy\, dz = \iiint \begin{pmatrix} 1-x-y-z \\ x \\ y \\ z \end{pmatrix} \mathrm{Re}\left[\frac{1}{\omega - \mathcal{E}(x,y,z) + i\eta}\right] dx\, dy\, dz$$

$$\iiint \begin{pmatrix} 1-x-y-z \\ x \\ y \\ z \end{pmatrix} \left[\frac{1}{\omega - \varepsilon + i\eta} + \frac{1}{-\omega - \varepsilon + i\eta}\right] dx\, dy$$

$$\iiint \begin{pmatrix} 1-x-y-z \\ x \\ y \\ z \end{pmatrix} \frac{-2\mathcal{E}(x,y,z)}{\omega_m^2 + [\mathcal{E}(x,y,z)]^2} = \iiint \begin{pmatrix} 1-x-y-z \\ x \\ y \\ z \end{pmatrix} 2\mathrm{Re}\left(\frac{1}{i\omega_m - \varepsilon}\right) dx\, dy\, dz$$

$$\varepsilon_1 + (\varepsilon_2 - \varepsilon_1)\xi + (\varepsilon_3 - \varepsilon_1)\eta + (\varepsilon_4 - \varepsilon_1)\varphi = \varepsilon_k(\xi,\eta,\varphi)$$
$$\varepsilon_1' + (\varepsilon_2' - \varepsilon_1')\xi + (\varepsilon_3' - \varepsilon_1')\eta + (\varepsilon_4' - \varepsilon_1')\varphi = \varepsilon_{k-q}(\xi,\eta,\varphi)$$

$$\left.\begin{array}{l} \varepsilon_k(\xi,\eta,\varphi) = \varepsilon_F \\ \varepsilon_{k-q}(\xi,\eta,\varphi) = \varepsilon_F \end{array}\right\}$$

planes define tetrahedra: $\left.\begin{array}{l} \xi = 0 \\ \eta = 0 \\ \varphi = 0 \\ \xi + \eta + \varphi = 1 \end{array}\right\}$

$\varepsilon_k = \varepsilon_F$ and $\xi = 0$, $\eta = 0$, $\varphi = 0$

$$P(\omega) = \int \frac{f(\varepsilon_k) - f(\varepsilon_{k-q})}{\omega - \varepsilon_k + \varepsilon_{k-q}}\, d^3k = \int \frac{f(\varepsilon_k) f(-\varepsilon_{k-q}) - f(-\varepsilon_k) f(\varepsilon_{k-q})}{\omega - \varepsilon_k + \varepsilon_{k-q}}$$

$$f(x) - f(y) = f(x)f(-y) - f(-x)f(y)$$

$N_s = 2$

$$P^0_q(i\omega) = N_s \int \frac{d^3k}{(2\pi)^3} \frac{f(\varepsilon_k) - f(\varepsilon_{k+q})}{i\omega + \varepsilon_k - \varepsilon_{k+q}}$$

$$f(x) - f(y) = f(x)f(-y) - f(-x)f(y)$$

$$P^0_q(i\Omega_m) = N_s \int \frac{d^3k}{(2\pi)^3} \left[\frac{f(\varepsilon_k)f(-\varepsilon_{k-q})}{i\Omega_m - (\varepsilon_{k-q} - \varepsilon_k)} - \frac{f(-\varepsilon_k)f(\varepsilon_{k-q})}{i\Omega_m - (\varepsilon_{k-q} - \varepsilon_k)} \right]$$

$$+ \frac{f(-\varepsilon_{k+q})f(\varepsilon_k)}{-i\Omega_m + (\varepsilon_k - \varepsilon_{k+q})}$$

$$N_s \int \frac{d^3k}{(2\pi)^3} \left[\frac{f(\varepsilon_k)f(-\varepsilon_{k-q})}{i\Omega_m - (\varepsilon_{k-q} - \varepsilon_k)} + \frac{f(-\varepsilon_{k+q})f(\varepsilon_k)}{-i\Omega_m - (\varepsilon_{k+q} - \varepsilon_k)} \right]$$

$$\frac{1}{\Delta\varepsilon + i\Omega} = \frac{\Delta\varepsilon + i\Omega}{(\Delta\varepsilon)^2 + \Omega_m^2}$$

$$-N_s \int \frac{d^3k}{(2\pi)^3} \left[\frac{f(\varepsilon_k)f(-\varepsilon_{k-q})[(\varepsilon_{k-q} - \varepsilon_k) + \cancel{i\Omega_m}]}{(\varepsilon_{k-q} - \varepsilon_k)^2 + \Omega_m^2} + \frac{f(-\varepsilon_{k+q})f(\varepsilon_k)[(\varepsilon_{k+q} - \varepsilon_k) - \cancel{i\Omega_m}]}{(\varepsilon_{k+q} - \varepsilon_k)^2 + \Omega_m^2} \right]$$

inversion present!

$$N_s \int \frac{d^3k}{(2\pi)^3} \left[\frac{f(\varepsilon_k)f(-\varepsilon_{k-q})(-2\varepsilon_{\Delta,q})}{\Omega_m^2 + \varepsilon_{\Delta q}^2} \right]$$

Inversion present

Imaginary axis

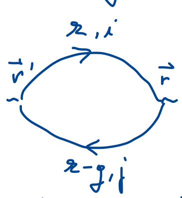
$$\varepsilon_{\Delta,q} = \varepsilon_{k-q} - \varepsilon_k > 0$$

k occupied

$k-q$ empty

$P_q(i\Omega)$ in band basis is real!

$$P^0_q(\Omega + i\delta) = 2 \int \frac{d^3k}{(2\pi)^3} \left[\frac{f(\varepsilon_k)f(-\varepsilon_{k-q})}{\Omega - (\varepsilon_{k-q} - \varepsilon_k) + i\delta} + \frac{f(\varepsilon_k)f(-\varepsilon_{k+q})}{-\Omega - (\varepsilon_{k+q} - \varepsilon_k) - i\delta} \right]$$



$$P_\Omega(\vec r, \vec r') = 2 \frac{1}{\beta} \sum_{i\omega, k ij} \psi^*_{ki}(\vec r') \frac{1}{i\omega + \mu - \varepsilon_{ki}} \psi_{ki}(\vec r) \psi^*_{k-qj}(\vec r) \frac{1}{i\omega - i\Omega + \mu - \varepsilon_{k-qj}} \psi_{k-qj}(\vec r')$$

$$\frac{1}{\beta} \sum_{i\omega} \frac{1}{i\omega + \mu - \varepsilon_{ki}} \frac{1}{i\omega - i\Omega + \mu - \varepsilon_{k-qj}} = -\oint \frac{dz}{2\pi i} f(z) \frac{1}{z + \mu - \varepsilon_{ki}} \frac{1}{z - i\Omega + \mu - \varepsilon_{k-qj}} = -\int \frac{d\epsilon}{\pi} f(x) \,\mathrm{Im}\left(\frac{1}{x + \mu - \varepsilon_i + i\delta} \right) \frac{1}{x - i\Omega + \mu - \varepsilon_{k-qj}}$$

$$-\int \frac{d\epsilon}{\pi} \underbrace{f(x + i\Omega)}_{f(x)} \frac{1}{x + i\Omega + \mu - \varepsilon_i} \,\mathrm{Im}\left(\frac{1}{x + \mu - \varepsilon_{k-qj} + i\delta} \right)$$

$$= f(\varepsilon_i - \mu) \frac{1}{\varepsilon_i - i\Omega - \varepsilon_{k-qj}} + f(\varepsilon_{k-qj} - \mu) \frac{1}{\varepsilon_{k-qj} + i\Omega - \varepsilon_i} = \frac{f(\varepsilon_{k-qj}) - f(\varepsilon_{ki})}{i\Omega - \varepsilon_{ki} + \varepsilon_{k-qj}}$$

$$P_{(q, i\Omega)}(\vec r, \vec r') = 2 \sum_{k ij} \psi^*_{ki}(\vec r') \psi_{k-qj}(\vec r') \psi_{ki}(\vec r) \psi^*_{k-qj}(\vec r) \frac{f(\varepsilon_{k-qj}) - f(\varepsilon_{ki})}{i\Omega - \varepsilon_{ki} + \varepsilon_{k-qj}}$$

$$= 2 \sum_{k ij} \psi^*_{ki}(\vec r') \psi_{k-qj}(\vec r') \psi_{ki}(\vec r) \psi^*_{k-qj}(\vec r) \frac{f(\varepsilon_{k-qj}) f(-\varepsilon_{ki}) - f(-\varepsilon_{k-qj}) f(\varepsilon_{ki})}{i\Omega - \varepsilon_{ki} + \varepsilon_{k-qj}}$$

$k \to k+q \quad i \leftrightarrow j \qquad \to *$

$$= \underbrace{\sum_{k ij} \psi^*_{k+qj}(\vec r') \psi_{ki}(\vec r') \psi_{k+qj}(\vec r) \psi^*_{ki}(\vec r) \frac{f(\varepsilon_{ki}) f(-\varepsilon_{k+qj})}{i\Omega + \varepsilon_{ki} - \varepsilon_{k+qj}}}_{R_{-q}(i\Omega)} + \left\{ \underbrace{\psi^*_{k-qj}(\vec r') \psi_{ki}(\vec r') \psi_{k-qj}(\vec r) \psi^*_{ki}(\vec r) \left[\frac{f(\varepsilon_{ki}) f(-\varepsilon_{k-qj})}{i\Omega + \varepsilon_{ki} - \varepsilon_{k-qj}} \right]}_{(R_q(i\Omega))^*} \right\}^*$$

i_o - occupied

i_e - empty

$$\sum_{i_o, i_e} \frac{f(\varepsilon_z^{i_o}) f(-\varepsilon_{z-q}^{i_e})(-2)(\varepsilon_{z-q}^{i_e} - \varepsilon_z^{i_o})}{\Omega_m^2 + (\varepsilon_{z-q}^{i_e} - \varepsilon_z^{i_o})^2} = \sum_{i_o, i_e} \frac{f(\varepsilon_z^{i_o})(1 - f(\varepsilon_{z-q}^{i_e})(-2)(\varepsilon_{z-q}^{i_e} - \varepsilon_z^{i_o})}{\Omega_m^2 + (\varepsilon_{z-q}^{i_e} - \varepsilon_z^{i_o})^2}$$

$$\sum_{i_o=1}^{N_{\text{occtual}}} \sum_{i_e} \frac{(1 - f(\varepsilon_{z-q}^{i_e}))(-2\Delta_{zq})}{\Omega_m^2 + (\Delta_{zq})^2}$$

Important: $r \leftrightarrow r'$ and $\vec{q} \to -\vec{q}$ and $\vec{k} \to -\vec{k}$

but k is dummy $\to$ $\vec{k} \to -\vec{k} \to \vec{k}$

$$P(-q, i\Omega) = \sum_{kij} \psi^*_{k-qj}(\vec r')\, \psi_{ki}(\vec r')\, \psi_{k-qj}(\vec r)\, \psi^*_{ki}(\vec r)\, \frac{f(\varepsilon_i) f(-\varepsilon_{k-qj})}{i\Omega + \varepsilon_{ki} - \varepsilon_{k-qj}} + \psi_{k+qj}(\vec r')\, \psi^*_{ki}(\vec r')\, \psi^*_{k+qj}(\vec r)\, \psi_{ki}(\vec r) \left[\frac{f(\varepsilon_i) f(-\varepsilon_{k+qj})}{-i\Omega + \varepsilon_i - \varepsilon_{k+qj}} \right]$$

$$\psi_{k-qj}(\vec r)\, \psi^*_{ki}(\vec r)\, \psi^*_{k-qj}(r')\, \psi_{ki}(\vec r)\, \frac{f(\varepsilon_i) f(-\varepsilon_{k-qj})}{-i\Omega + \varepsilon_i - \varepsilon_{k-qj}}$$

$$P(-q, i\Omega) = \sum_{k,ij} \psi^*_{k-qj}(\vec r')\, \psi_{ki}(\vec r')\, \psi_{k-qj}(\vec r)\, \psi^*_{ki}(\vec r)\, f(\varepsilon_i) f(-\varepsilon_{k-qj}) \left\{ \frac{1}{i\Omega + \varepsilon_{ki} - \varepsilon_{k-qj}} + \frac{1}{-i\Omega + \varepsilon_{ki} - \varepsilon_{k-qj}} \right\}$$

$$P(-q, i\Omega) = \sum_{k,ij} \psi^*_{k-qj}(\vec r')\, \psi_{ki}(\vec r')\, \psi_{k-qj}(\vec r)\, \psi^*_{ki}(\vec r)\, f(\varepsilon_i) f(-\varepsilon_{k-qj}) \left\{ \frac{2(\varepsilon_{ki} - \varepsilon_{k-qj})}{(\varepsilon_{ki} - \varepsilon_{k-qj})^2 + (\Omega_n)^2} \right\}$$

i - occupied
j - empty

$$P(-q, \Omega + i\delta) = \sum_{k,ij} \psi^*_{k-qj}(\vec r')\, \psi_{ki}(\vec r')\, \psi_{k-qj}(\vec r)\, \psi^*_{ki}(\vec r)\, f(\varepsilon_i) f(-\varepsilon_{k-qj}) \left\{ \underbrace{\frac{1}{\Omega + \varepsilon_{ki} - \varepsilon_{k-qj} + i\delta} - \frac{1}{\Omega - \varepsilon_{ki} + \varepsilon_{k-qj} \pm i\delta}}_{kcw} \right\}$$

for t ordered $T=0$ should be $-$!

this + still differs from GAP $-i\delta$!

$$\chi_\alpha(\vec r)\, \underbrace{\langle \chi_\alpha | \psi_{ki}\, \psi^*_{k-qj} \rangle}_{M^{\alpha}_{ij}(k,-q)}\, \underbrace{\langle \psi_{ki}\, \psi^*_{k-qj} | \chi_\beta \rangle}_{M^{\beta *}_{ij}(k,-q)}\, \chi^*_\beta(\vec r) \qquad kcw(ij, k, -q, \Omega)$$

Beware: This expression is for retarded $P(q,\omega)$. Gap2 code uses $T=0$ P_t formalism, hence poles are at $-i\delta$ for $\Omega > 0$ and at $+i\delta$ for $\Omega < 0$

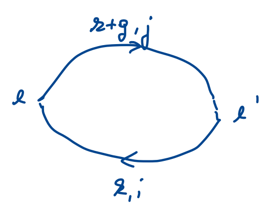
$$P_{\alpha\beta}(-q, \Omega) = \sum_{k,ij} M^{\alpha}_{ij}(k,-q)\; kcw(ij, k, -q, \Omega)\; M^{\beta *}_{ij}(k,-q)$$

$$\sum_{ij} M_k(\alpha, ij) \cdot kcw(ij; k\Omega) \cdot M^*_k(ij, \beta)$$

$$kcw(i\_occ, i\_emp, k, \Omega)$$

$\varepsilon_k < 0$
$\varepsilon_{k-q} > 0$ $\qquad \varepsilon_{k-q} - \varepsilon_k > 0$

$$\frac{f(z_1) - f(z_2)}{i\Omega + z_1 - z_2} = \frac{f(z_1) f(-z_2) - f(-z_1) f(z_2)}{i\Omega + z_1 - z_2}$$



$$P^{ll'}(q, i\Omega) = \sum_{kij} \psi^*_{k+qj}(r)\, \psi_{ki}(r)\, \psi^*_{ki}(r')\, \psi_{k+qj}(r')\, \frac{f(\varepsilon_i) f(-\varepsilon_{k+qj}) - f(-\varepsilon_i) f(\varepsilon_{k+qj})}{i\Omega + \varepsilon_i - \varepsilon_{k+qj}}$$

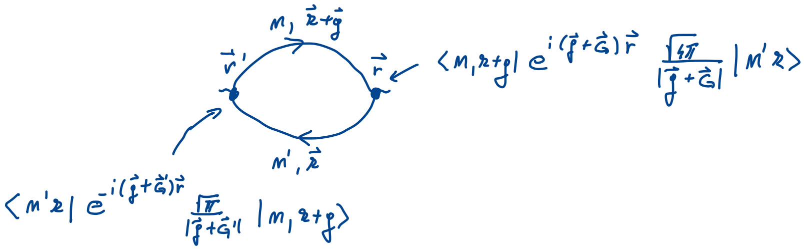
$k+q, j \to k'\, i'$
$k, i \to k'-q, j'$

$$\sum_{kij} \underbrace{\langle \chi_l(r) | \psi^*_{k+qj}(r)\, \psi_{ki}(r) \rangle}_{M_{l,ij}} \underbrace{\langle \psi_{ki}(r')\, \psi^*_{k+qj}(r') | \chi_{l'}(r') \rangle}_{M^*_{l',ij}} \frac{f(\varepsilon_i) f(-\varepsilon_{k+qj})}{i\Omega + \varepsilon_i - \varepsilon_{k+qj}}$$

$$+ \sum_{kij} \underbrace{\langle \chi_l(r) | \psi^*_{ki}(r)\, \psi_{k-qj}(r) \rangle} \langle \psi_{k-qj}(r')\, \psi^*_{ki}(r') | \chi_{l}(r') \rangle \left(- \frac{f(-\varepsilon_{k-qj}) f(\varepsilon_i)}{i\Omega + \varepsilon_{k-qj} - \varepsilon_{ki}} \right)$$

An alternative expression in plane-wave basis: $\vec{G}\vec{G}'$

$$\varepsilon_{GG'} = \delta_{GG'} + \frac{4\pi}{|\vec{q}+\vec{G}||\vec{q}+\vec{G}'|}\frac{1}{V_{cell}}\sum_{nn'k}\frac{f(\varepsilon_{n,k+q})-f(\varepsilon_{n',k})}{\omega-\varepsilon_{n,k+q}+\varepsilon_{n'k}}\langle\psi_{n,k+q}|e^{i(\vec{q}+\vec{G})\vec{r}}|\psi_{n'k}\rangle\langle\psi_{n'k}|e^{-i(\vec{q}+\vec{G}')\vec{r}}|\psi_{n,k+q}\rangle$$



<u>$k\cdot p$ perturbation theory for small q:</u> $\left(\frac{p^2}{2m}+V\right)\psi_{nk}(\vec{r}) = \varepsilon_{nk}\psi_{nk}(\vec{r})$ where $\psi_{nk}(\vec{r}) = e^{i\vec{k}\vec{r}}u_{nk}(\vec{r})$

$$\underbrace{e^{-i\vec{k}\vec{r}}\left(\frac{p^2}{2m}+V\right)e^{i\vec{k}\vec{r}}}_{H_k}u_{nk}(\vec{r}) = \varepsilon_{nk}u_{nk}(\vec{r})$$

$$\left(\frac{k^2+2\vec{k}\cdot\vec{p}+\vec{p}^2}{2m}+V\right) \quad \text{because} \quad e^{-i\vec{k}\vec{r}}(-i\vec{\nabla})^2\left[e^{i\vec{k}\vec{r}}u_{nk}\right] = \left[k^2u_{nk}+2\vec{k}(-i\vec{\nabla})u_{nk}+(-i\vec{\nabla})^2u_{nk}\right]$$

$$H_{k+q} = H_k + 2\vec{q}\frac{(\vec{k}+\vec{p})}{2m}+\frac{q^2}{2m}$$

$$H_{k+q}u_{n\,k+q}(\vec{r}) = \varepsilon_{n\,k+q}u_{n\,k+q}(\vec{r})$$

perturbation theory gives: $u_{n,k+q}(\vec{r}) = u_{nk}(\vec{r})+\sum_{n'\neq n}u_{n'k}(\vec{r})\frac{1}{\varepsilon_{nk}-\varepsilon_{n'k}}\frac{1}{V_{cell}}\int u^*_{n'k}(\vec{r})\,\Delta H\,u_n(\vec{r})d^3r$

$$\varepsilon_{n\,k+q} = \varepsilon_{nk}+\frac{1}{V_{cell}}\int u^*_{nk}(\vec{r})\,\Delta H\,u_{nk}(\vec{r})$$

small q: $\varepsilon_{n\,k+q} = \varepsilon_{nk}+\frac{1}{V_{cell}}\langle u_{nk}|\vec{k}+\vec{p}|u_{nk}\rangle\frac{\vec{q}}{m} = \varepsilon_{nk}+\frac{\vec{q}}{m}\left[\vec{k}+\vec{p}^{\,k}_{nn}\right] = \varepsilon_{nk}+\frac{\vec{q}}{m}\langle\psi_{nk}|-i\vec{\nabla}|\psi_{nk}\rangle$

$$u_{n\,k+q}(\vec{r}) = u_{nk}(\vec{r})+\sum_{n'\neq n}u_{n'k}(\vec{r})\frac{1}{\varepsilon_{nk}-\varepsilon_{n'k}}\frac{\vec{q}}{m}\left[\vec{k}+\vec{p}^{\,k}_{n'n}\right] \quad \text{where } \vec{p}^{\,k}_{n'n} = \frac{1}{V_{cell}}\int u^*_{n'k}(\vec{r})(-i\vec{\nabla})u_{nk}(\vec{r})$$

$$\langle\psi_{n\,k+q}|e^{i(\vec{q}+\vec{G})\vec{r}}|\psi_{n'k}\rangle = \langle u_{n\,k+q}|e^{i\vec{G}\vec{r}}|u_{n'k}\rangle = \langle u_{nk}|e^{i\vec{G}\vec{r}}|u_{n'k}\rangle+\sum_{n''\neq n}\frac{\vec{q}}{m}\left[\vec{k}+\vec{p}^{\,k}_{nn''}\right]\frac{1}{\varepsilon_{nk}-\varepsilon_{n''k}}\langle u_{n''k}e^{i\vec{G}\vec{r}}|u_{n'k}\rangle$$

for $\vec{G}=0$: $\langle\psi_{n\,k+q}|e^{i\vec{q}\vec{r}}|\psi_{n'k}\rangle = \delta_{nn'}+\frac{\vec{q}}{m}\frac{\left[\vec{k}+\vec{p}^{\,k}_{nn'}\right]}{\varepsilon_{nk}-\varepsilon_{n'k}}$

$$\varepsilon_{\substack{G=0\\G'=0}} = 1 + \frac{4\pi}{q^2}\frac{1}{V_{cell}}\sum_{nn'k}\frac{f(\varepsilon_{n,k+q})-f(\varepsilon_{n',k})}{\omega-\varepsilon_{n,k+q}+\varepsilon_{n'k}}\langle\psi_{n,k+q}|e^{i(\vec{q}+\vec{G})\vec{r}}|\psi_{n'k}\rangle\langle\psi_{n'k}|e^{-i(\vec{q}+\vec{G}')\vec{r}}|\psi_{n,k+q}\rangle$$

$$\varepsilon_{nk+q}-\varepsilon_{nk} = \frac{\vec{q}}{m}\vec{p}^{\,k}_{nn} \quad \text{where} \quad p^k_{nn} = \langle\psi_{nk}|-i\vec{\nabla}|\psi_{nk}\rangle$$

$$\langle\psi_{nk+q}|e^{i\vec{q}\vec{r}}|\psi_{n'k}\rangle = \delta_{nn'} + \frac{\vec{q}}{m}\frac{\vec{p}^{\,k}_{nn'}}{\varepsilon_{nk}-\varepsilon_{n'k}} \quad (n\neq n')$$

$\varepsilon-1$: $n=n'$: $$-\frac{4\pi}{q^2}\frac{1}{V_{cell}}\sum_{nk}\frac{\left(-\frac{df}{d\varepsilon}\right)\frac{\vec{q}}{m}(\vec{p}^{\,k}_{nn})}{\omega-\frac{\vec{q}}{m}(\vec{p}^{\,k}_{nn})} \approx -\frac{4\pi}{q^2}\frac{1}{V_{cell}}\sum_{nk}\left(-\frac{df}{d\varepsilon}\right)\frac{\vec{q}}{m}\vec{p}^{\,k}_{nn}\frac{1}{\omega}\left[1+\frac{1}{\omega}\frac{\vec{q}}{m}\cdot\vec{p}^{\,k}_{nn}\right]$$

$$= -\frac{4\pi}{q^2}\frac{1}{V_{cell}}\sum_{nk}\left(-\frac{df}{d\varepsilon}\right)\frac{\vec{q}}{m}\vec{p}^{\,k}_{nn}\frac{1}{\omega} - \quad \leftarrow \text{diverging} \Rightarrow \text{remove}$$

$$-\frac{df}{d\varepsilon}(\varepsilon) = \delta(\varepsilon_{nk}-\varepsilon_F)$$

$$-\frac{4\pi}{q^2}\frac{1}{V_{cell}}\sum_{nk}\left(-\frac{df}{d\varepsilon}\right)\frac{1}{\omega^2}\left[\frac{\vec{q}}{m}\vec{p}^{\,k}_{nn}\right]^2 \quad \leftarrow \text{keep}$$

$n==n'$:

$$\varepsilon_{00} = 1 - \frac{4\pi N_{sp}}{V_{cell}}\sum_{nk}\left(-\frac{df}{d\varepsilon}(\varepsilon)\right)\frac{1}{\omega^2}\left[\frac{\vec{q}}{qm}\vec{p}^{\,k}_{nn}\right]^2 \quad \text{imaginary axis} \quad \varepsilon_{00} = 1 + \frac{4\pi}{V_{cell}}\sum_{nk}\left(-\frac{df}{d\varepsilon}(\varepsilon)\right)\frac{1}{\omega_m^2}\left[\frac{\vec{q}}{qm}\vec{p}^{\,k}_{nn}\right]^2$$

$n\neq n'$:

$$\varepsilon_{00} = -\frac{4\pi}{q^2}\frac{1}{V_{cell}}\sum_{\substack{n\neq n'\\k}}\frac{f(\varepsilon_n)-f(\varepsilon_{n'})}{\omega-\varepsilon_{nk}+\varepsilon_{n'k}}\frac{\left(\frac{\vec{q}}{m}\cdot\vec{p}^{\,k}_{nn'}\right)\left(\frac{\vec{q}}{m}\cdot\vec{p}^{\,k}_{n'n}\right)}{(\varepsilon_{nk}-\varepsilon_{n'k})^2} = -\frac{4\pi}{V_{cell}}\sum_{\substack{n\neq n'\\k}}\underbrace{\frac{f(\varepsilon_n)-f(\varepsilon_{n'})}{\omega-\varepsilon_{nk}+\varepsilon_{n'k}}}_{F_{n'n}(\omega,k,q=0)}\frac{\left(\frac{\vec{q}}{qm}\cdot\vec{p}^{\,k}_{nn'}\right)\left(\frac{\vec{q}}{qm}\cdot\vec{p}^{\,k}_{n'n}\right)}{(\varepsilon_{nk}-\varepsilon_{n'k})^2}$$

$G'=0$ and $G\neq 0$

$$\varepsilon_{G0} = \frac{4\pi}{|\vec{q}+\vec{G}|\cdot q}\frac{1}{V_{cell}}\sum_{nn'k}\frac{f(\varepsilon_{n,k+q})-f(\varepsilon_{n',k})}{\omega-\varepsilon_{n,k+q}+\varepsilon_{n'k}}\langle\psi_{n,k+q}|e^{i(\vec{q}+\vec{G})\vec{r}}|\psi_{n'k}\rangle\langle\psi_{n'k}|e^{-i\vec{q}\vec{r}}|\psi_{n,k+q}\rangle$$

$n=n'$

$$\varepsilon_{G0} = -\frac{4\pi}{|\vec{G}|}\frac{1}{V_{cell}}\sum_{nk}\frac{\left(-\frac{df}{d\varepsilon}\right)\vec{p}^{\,k}_{nn}\cdot\frac{\vec{q}}{m}/q}{\omega}\langle\psi_{nk}|e^{i\vec{G}\cdot\vec{r}}|\psi_{nk}\rangle$$

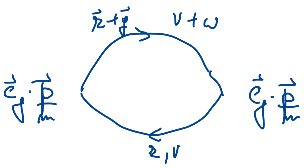
$n\neq n'$

$$\varepsilon_{G0} = \frac{4\pi}{|\vec{G}|}\frac{1}{V_{cell}}\sum_{\substack{n\neq n'\\k}}\underbrace{\frac{f(\varepsilon_{nk})-f(\varepsilon_{n'k})}{\omega-\varepsilon_{nk}+\varepsilon_{n'k}}}_{F_{n'n}(\omega,k,q=0)}\underbrace{\langle\psi_{nk}|e^{i\vec{G}\cdot\vec{r}}|\psi_{n'k}\rangle}_{\underbrace{\langle \text{Product}|\psi^*_{nk}\psi_{n'k}\rangle}_{M^G_{nn'}(k)}}\left(\frac{\vec{q}}{qm}\vec{p}^{\,k}_{n'n}\right)\frac{1}{\varepsilon_{n'k}-\varepsilon_{nk}}$$

From Vignale book

From gauge invariance it follows that $\tilde{\chi}_{nn}(q,\omega) = \frac{q^2}{\omega^2}\tilde{\chi}^{l}_{jj}(q,\omega)$ where

$\tilde{\chi}^{l}_{jj} = \langle \vec{e}_q \cdot j(t)\, \vec{e}_q \cdot \vec{j}(0) \rangle$ longitudinal component



$$\tilde{\chi}^{l}_{jj}(i\omega) = \frac{1}{\beta}\sum_{i\nu}\left(\vec{e}_q \cdot \frac{\vec{p}}{m}\right)^2 \frac{1}{i\nu - \varepsilon^{n}_{k}} \, \frac{1}{i\nu + i\omega - \varepsilon^{n'}_{k+q}} = \left(\vec{e}_q \cdot \frac{\vec{p}}{m}\right)^2 \frac{1}{V_{cell}} \sum_{nn'k} \frac{f(\varepsilon_{n,k+q}) - f(\varepsilon_{n',k})}{\omega - \varepsilon_{n,k+q} + \varepsilon_{n'k}}$$

$$\varepsilon = 1 - v_q \tilde{\chi}_{nn}(q,\omega) = 1 - \frac{4\pi}{q^2}\frac{q^2}{\omega^2}\tilde{\chi}^{l}_{jj} = 1 - \frac{4\pi}{\omega^2}\left(\vec{e}_q \cdot \frac{\vec{p}}{m}\right)^2 \frac{1}{V_{cell}} \sum_{nn'k} \frac{f(\varepsilon_{n,k+q}) - f(\varepsilon_{n',k})}{\omega - \varepsilon_{n,k+q} + \varepsilon_{n'k}}$$

$n = n'$

$$\varepsilon - 1 = -\frac{4\pi}{\omega^2}\frac{1}{V_{cell}}\sum_{nk} \frac{\frac{\partial f}{\partial \varepsilon}(\varepsilon_{nk})}{\omega} \cdot \overbrace{(\varepsilon_{n\,k+q} - \varepsilon_{nk})}^{\approx \omega} \left(\vec{e}_q \cdot \frac{\vec{p}_{nn}}{m}\right)^2 = -\frac{1}{\omega^2} \underbrace{\frac{4\pi}{V_{cell}}\sum_{nk} \frac{\partial f}{\partial \varepsilon}(\varepsilon_{nk}) \cdot \left(\vec{e}_q \cdot \frac{\vec{p}_{nn}}{m}\right)^2}_{\text{Co-head}}$$

$n \neq n'$

$$\varepsilon - 1 = -\frac{1}{\omega^2} \underbrace{\frac{4\pi}{V_{cell}} \sum_{nn'k} \frac{f(\varepsilon_{nk}) - f(\varepsilon_{n'k})}{\omega - \varepsilon_{nk} + \varepsilon_{n'k}} \left(\vec{e}_q \cdot \frac{\vec{p}_{nn'}}{m}\right)}_{\text{ohead}} \quad \checkmark$$

Drude term in GW

Eigenbasis of the Coulomb matrix, expressed in terms of LAPW product basis.

$$M_I^{\vec{q}}(\vec{r}) = \frac{1}{\sqrt{V}}\sum_{\vec{G}} C_{I\vec{G}}(\vec{q})\, e^{i(\vec{q}+\vec{G})\vec{r}}$$ formal Fourier expansion. $(M_I^{q} e^{-iqr})$ are periodic, hence expandable in terms of $\vec{G}$ vectors

Here $C_{I\vec{G}}(\vec{q}) = \frac{1}{\sqrt{V}}\int d^3r\, e^{-i(\vec{q}+\vec{G})\vec{r}} M_I^{\vec{q}}(\vec{r})$ Integral over the entire space.

Coulomb repulsion is $v_{IJ}(\vec{q}) = \iint \frac{M_I^{q*}(\vec{r}) M_J^{q}(\vec{r}')}{|\vec{r}-\vec{r}'|} d^3r d^3r'$

We can expand: $M_I^{\vec{q}}(\vec{r}) \approx \frac{1}{\sqrt{V}}\sum_{\vec{G}} e^{i(\vec{q}+\vec{G})\vec{r}}\left(C_{I\vec{G}} + \vec{q}\frac{\partial}{\partial\vec{q}}C_{I\vec{G}} + \frac{1}{2}\vec{q}\cdot\frac{\partial^2}{\partial\vec{q}^2}C_{I\vec{G}}\cdot\vec{q} + \cdots\right)$

Then we are interested in diverging terms at $q\to 0$

$$v_{IJ}(\vec{q}) \approx \sum_{\vec{G}_1,\vec{G}_2}\frac{1}{V}\iint d^3r\, d^3r'\, e^{-i(\vec{q}+\vec{G}_1)\vec{r}+i(\vec{q}+\vec{G}_2)\vec{r}'}\frac{1}{|\vec{r}-\vec{r}'|}\left(C^*_{I\vec{G}_1} + \vec{q}\frac{\partial}{\partial\vec{q}}C^*_{I\vec{G}_1} + \frac{1}{2}\vec{q}\cdot\frac{\partial^2}{\partial\vec{q}^2}C^*_{I\vec{G}}\cdot\vec{q}\right)\left(C_{J\vec{G}_2} + \vec{q}\frac{\partial}{\partial\vec{q}}C_{J\vec{G}_2} + \frac{1}{2}\vec{q}\frac{\partial^2}{\partial\vec{q}^2}C_{J\vec{G}_2}\cdot\vec{q}\right)$$

$$= \sum_{\vec{G}_1,\vec{G}_2}\frac{1}{V}\iint d^3r\, d^3r'\, e^{-i(\vec{q}+\vec{G}_1)\vec{r}+i(\vec{q}+\vec{G}_2)\vec{r}'}\frac{1}{|\vec{r}-\vec{r}'|}\Big(C^*_{I0}C_{J0} + C^*_{I\vec{G}_1}\vec{q}\frac{\partial}{\partial\vec{q}}C_{J\vec{G}_2} + C_{J\vec{G}_2}\vec{q}\frac{\partial}{\partial\vec{q}}C^*_{I\vec{G}_1} +$$
$$C^*_{I\vec{G}_1}\frac{1}{2}\vec{q}\frac{\partial^2}{\partial\vec{q}^2}C_{J\vec{G}_2}\cdot\vec{q} + C_{J\vec{G}_2}\frac{1}{2}\vec{q}\cdot\frac{\partial^2}{\partial\vec{q}^2}C^*_{I\vec{G}}\cdot\vec{q} + \vec{q}\frac{\partial}{\partial\vec{q}}C^*_{I\vec{G}_1}\,\vec{q}\frac{\partial}{\partial\vec{q}}C_{J\vec{G}_2}\Big)$$

The exact diverging eigenstate at $\vec{q}\to 0$ is $\frac{1}{\sqrt{V}}e^{i\vec{q}\vec{r}}$ in the basis which diagonalizes the coulomb matrix (expressed in LAPW product basis). Both the plane wave basis and this diagonal basis are eigenbasis of the Coulomb repulsion hamiltonian matrix. But eigenvectors are not unique, except in a non-degenerate subspace, like the limit $q\to 0$.

This eigen-function is particularly simple, i.e., constant at $q\to 0$.

Eigenvalue is $v_{11}(q) = \frac{8\pi}{q^2}$

MImm is $\langle \chi^\alpha | \psi_{i_2}\psi^*_{i_2\, k-q}\rangle = \int e^{-i\vec{q}\vec{r}}\psi_{i_2}(\vec{r})\psi^*_{i_2\, k-q}(\vec{r})\,d^3r \overset{q\to 0}{\approx} \langle \psi_{k i_2}|\psi_{k i_1}\rangle = \delta_{i_1 i_2}$

What is limit of the Lindhard formula in the $q\to 0$ limit? It has head $\frac{\varepsilon_{00}}{q^2}$ + wings $\frac{\varepsilon_{0q}}{q}$.

$v(q)_{\alpha\beta} = U_{\alpha e}\, v_e\, U^+_{e\beta}$

$(\sqrt{v}\, U^+ M)_{e\alpha} = \underbrace{\sqrt{v_e}\,(U^+)_{e\alpha}\, M^{\alpha}_{ij}}_{\tilde{M}^{e}_{ij} \leftarrow \text{eigenbasis}}$

$M^{\beta}_{i'j'}\, v_{\beta\alpha}\, M^{\alpha}_{ij}$

$M^{\beta}_{i'j'}\, U_{\beta e}\sqrt{v_e}\sqrt{v_e}\, U^+_{e\alpha}\, M^{\alpha}_{ij}$

Linhardt:

$$\varepsilon_{\substack{G=0\\G'=0}} = 1 + \frac{4\pi}{q^2}\frac{1}{V_{cell}}\sum_{nn'k}\frac{f(\varepsilon_{n,k+q}) - f(\varepsilon_{n',k})}{\omega - \varepsilon_{n,k+q} + \varepsilon_{n'k}} \langle\psi_{n,k+q}| e^{i(\vec{q}+\vec{G})\vec{r}} |\psi_{n'k}\rangle\langle\psi_{n'k}| e^{-i(\vec{q}+\vec{G}')\vec{r}} |\psi_{n,k+q}\rangle$$

$$\varepsilon_{nk+q} - \varepsilon_{nk} = \frac{\vec{q}}{m}\vec{p}^{\,k}_{nn} \quad \text{where} \quad \vec{p}^{\,k}_{nn} = \langle\psi_{nk}| -i\vec{\nabla} |\psi_{nk}\rangle$$

$$\langle\psi_{nk+q}| e^{i\vec{q}\vec{r}} |\psi_{n'k}\rangle = \delta_{nn'} + \frac{\vec{q}}{m}\frac{\vec{p}^{\,k}_{nn'}}{\varepsilon_{nk} - \varepsilon_{n'k}} \quad (n \neq n')$$

$\varepsilon - 1$: $n = n'$:

$$-\frac{4\pi}{q^2}\frac{1}{V_{cell}}\sum_{nk}\frac{\left(-\frac{df}{d\varepsilon}\right)\frac{\vec{q}}{m}(\vec{p}^{\,k}_{nn})}{\omega - \frac{\vec{q}}{m}(\vec{p}^{\,k}_{nn})} \approx -\frac{4\pi}{q^2}\frac{1}{V_{cell}}\sum_{nk}\left(-\frac{df}{d\varepsilon}\right)\frac{\vec{q}}{m}\vec{p}^{\,k}_{nn}\frac{1}{\omega}\left[1 + \frac{1}{\omega}\frac{\vec{q}}{m}\cdot\vec{p}^{\,k}_{nn}\right]$$

$$= -\frac{4\pi}{q^2}\frac{1}{V_{cell}}\sum_{nk}\left(-\frac{df}{d\varepsilon}\right)\frac{\vec{q}}{m}\vec{p}^{\,k}_{nn}\frac{1}{\omega} -$$

← diverging => remove

odd in q -> vanishes

$$-\frac{4\pi}{q^2}\frac{1}{V_{cell}}\sum_{nk}\left(-\frac{df}{d\varepsilon}\right)\frac{1}{\omega^2}\left[\frac{\vec{q}}{m}\vec{p}^{\,k}_{nn}\right]^2$$

← keep

$$-\frac{df}{d\varepsilon}(\varepsilon_k) = \delta(\varepsilon_{nk} - \varepsilon_F)$$

$n == n'$:

$$\varepsilon_{00} = 1 - \frac{4\pi N_{sp}}{V_{cell}}\sum_{nk}\left(-\frac{df}{d\varepsilon}(\varepsilon_k)\right)\frac{1}{\omega^2}\left[\frac{\vec{q}}{q\,m}\vec{p}^{\,k}_{nn}\right]^2$$

imaginary axis

$$\varepsilon_{00} = 1 + \frac{4\pi}{V_{cell}}\sum_{nk}\left(-\frac{df}{d\varepsilon}(\varepsilon_k)\right)\frac{1}{\omega_n^2}\left[\frac{\vec{q}}{q\,m}\vec{p}^{\,k}_{nn}\right]^2$$

Drude

$$P = V^{-1}(1-\varepsilon) = \frac{1}{V_{cell}}\sum_{nk}\frac{\left(-\frac{df}{d\varepsilon}\right)\frac{\vec{q}}{m}(\vec{p}^{\,k}_{nn})}{\omega - \frac{\vec{q}}{m}(\vec{p}^{\,k}_{nn})}$$

$$1 - \varepsilon_{00} = \frac{4\pi N_{sp}}{V_{cell}}\sum_{nk}\left(-\frac{df}{d\varepsilon}(\varepsilon_k)\right)\frac{1}{\omega^2 m^2}\left[\vec{e}_q\cdot\vec{p}^{\,k}_{nn}\right]^2 \; ; \quad \omega_p^2 = \frac{4\pi N_{sp}}{m^2}\frac{1}{V_{cell}}\sum_{nk}\left(-\frac{df_k}{d\varepsilon}\right)\left[\vec{e}_q\cdot\vec{p}^{\,k}_{nn}\right]^2$$

$$1 - \varepsilon_{00} = \frac{\omega_p^2}{\omega^2} = \frac{\omega_p^2}{(i\omega_n)^2}$$

$$H(\omega) += \frac{\omega_p^2}{\omega_m^2}$$

$$\varepsilon(\omega) = \begin{pmatrix} H(\omega) & \mathbf{W}^{+}(\omega) \\ \mathbf{W}(\omega) & \mathbf{B}(\omega) \end{pmatrix} \downarrow \text{basis}$$

$$H(\omega) += \frac{\omega_p^2}{\omega_m^2} \leftarrow \text{Matsubara}$$

$$(\varepsilon^{-1} - 1) \sim \left[\frac{1}{\left(1 + \frac{\omega_p^2}{\omega_m^2}\right)} - 1\right]$$

$$CO\_head = \frac{4\pi \cdot N_{sp}}{V_{cell}} \sum_{nk} \left(-\frac{df}{d\varepsilon_k}(\varepsilon')\right) \frac{1}{3}\sum_{\alpha=1..3} P^{k,\alpha}_{mm'} P^{k,\alpha}_{m'm} = \omega_p^2$$

$$head = 1 - \underbrace{\frac{4\pi N_{sp}}{V_{cell}} \sum_{nk} \left(\sum_\alpha \frac{1}{3} P^{k\alpha}_{mm'} P^{k\alpha}_{m'm}\right) \frac{1}{(\varepsilon_{nk} - \varepsilon_{m'k})^2} \frac{f(\varepsilon_n) - f(\varepsilon_{m'})}{i\omega_n - \varepsilon_{nk} + \varepsilon_{n'k}}}_{\Delta head} + \frac{Co\_head}{\omega_n^2} \rightarrow \varepsilon_{\infty}$$

See from previous page: $\varepsilon \equiv \frac{\varepsilon_{00}}{g^2}$

$$pm[i_1 i_2] = 2\sqrt{\frac{\pi}{V_{cell}}} \frac{\frac{1}{\sqrt{3}}\sum_\alpha P^{k\alpha}_{i_1 i_2}}{\varepsilon_{k i_1} - \varepsilon_{k i_2}} ;$$

$$epsW1(\alpha,\omega) = \sum_{k,i_1 i_2} \sqrt{N_{cell}} \langle X^\alpha | \varphi^*_{k+g\, i_2} \varphi_{k i_1} \rangle \frac{f(\varepsilon_{k i_1}) - f(\varepsilon_{k+g\, i_2})}{i\omega + \varepsilon_{k i_1} - \varepsilon_{k+g\, i_2}} \, 2\sqrt{\frac{\pi}{V_{cell}}} \frac{\frac{1}{\sqrt{3}}\sum_\alpha P^{k\alpha}_{i_1 i_2}}{\varepsilon_{k i_1} - \varepsilon_{k i_2}} \equiv W_\mu(\omega)$$

$$epsW2(\alpha,\omega) = epsW1^*(\alpha,\omega)$$

$$bw1 = \sum_\beta [\varepsilon^{-1}_g(\omega)]^{\alpha\beta} \cdot epsW1(\beta,\omega) ; \quad WW = \sum_{\alpha\beta} epsW1^*(\alpha, i\omega) [\varepsilon^{-1}_g(\omega)]^{\alpha\beta} \cdot epsW1(\beta, i\omega) = \sum_{\mu\nu} W_\mu^+ B^{-1}_{\mu\nu} W_\nu$$

$$W2b = \sum_\beta epsW1(\beta,\omega) [\varepsilon^{-1}_g(\omega)]^{\beta\alpha} ;$$

$$\varepsilon_{gwt} = bw1 \otimes \frac{1}{head - WW} \otimes W2b$$

gap paper:

$$\varepsilon^{-1} = B^{-1} + \varepsilon^{-1}_{\mu 0} \, \varepsilon^{-1}_{00} \, \varepsilon^{-1}_{0\nu}$$

$$epsW1(\alpha,\omega) = -\frac{1}{head - WW} \sum_\beta \varepsilon^{\alpha\beta}_g(\omega) \cdot epsW1(\beta,\omega) \, .$$

$$epsW2(\alpha,\omega) = -\frac{1}{head - WW} \sum_\beta epsW1(\beta,\omega) \, \varepsilon^{\beta\alpha}_g(\omega)$$

gap-paper:

$$(\varepsilon^{-1})_{00} = \frac{1}{head - WW} \equiv head(\omega)$$

$$(\varepsilon^{-1})_{\mu 0} = -\left(\sum_\nu B^{-1}_{\mu\nu} W_\nu\right) (\varepsilon^{-1})_{00} \equiv epsW1(\alpha,\omega)$$

$$(\varepsilon^{-1})_{0\mu} = -\left(\sum_\nu W_\nu B^{-1}_{\nu\mu}\right) (\varepsilon^{-1})_{00} \equiv epsW2(\alpha,\omega)$$

$$\left(M^+ (\varepsilon^{-1}_\omega - 1) M\right) + (\varepsilon^{-1})_{00} \cdot coef + M^+_{i_1 i_2 \mu} \varepsilon^{-1}_{\mu 0} + \varepsilon^{-1}_{0\nu} M_{i_1 i_2 \nu}$$

How we treat error due to finite q-point mesh around $q=0$

We have terms that diverge like $\frac{1}{q^2}$ and like $\frac{1}{q}$. Both are integrable!

$m = 1$ or 2

$$\mathrm{sfm} = \frac{1}{N_q}\left(\sum_{G\neq 0}\frac{e^{-\alpha G^2}}{G^m} + \sum_{q\neq 0}\sum_{G}\frac{e^{-\alpha|\vec{q}+\vec{G}|^2}}{|\vec{q}+\vec{G}|^m}\right),\text{ i.e., it is } \sum_{G,q}\frac{e^{-\alpha|\vec{q}+\vec{G}|}}{|\vec{q}+\vec{G}|^m}$$

but avoid $G=0$ and $q=0$, which is singular

$$\boxed{\begin{aligned}\mathrm{mingc1} &= \frac{V_{ol}}{4\pi^2\alpha} - \mathrm{sf1}\\ \mathrm{mingc2} &= \frac{V_{ol}}{4\pi^2}\sqrt{\frac{\pi}{\alpha}} - \mathrm{sf2}\end{aligned}}$$

$$\sum_{G} V\int\frac{d^3q}{(2\pi)^3}\frac{e^{-\alpha|\vec{q}+\vec{G}|^2}}{|\vec{q}+\vec{G}|^m} = \sum_{G} V\int\frac{d^3q}{(2\pi)^3}\frac{e^{-\alpha(q^2+2q\cdot G\cos\vartheta+G^2)}}{(q^2+G^2+2qG\cos\vartheta)^{m/2}}$$

Choose α such that $\alpha\cdot G_1 > 1$ so that the integral can be extended to infinity

$$\sum_{q}\frac{e^{-\alpha q^2}}{q^m} \overset{\text{exact}}{=} \frac{V}{(2\pi)^3}\int d^3q\,\frac{e^{-\alpha q^2}}{q^m} \underset{\alpha\cdot G^2 \gg 1}{\approx} \frac{V\,4\pi}{(2\pi)^3}\int_0^\infty dq\, q^{2-m}\, e^{-\alpha q^2} = \frac{V}{2\pi^2}\int_0^\infty \frac{dx}{2\alpha}\left(\frac{x}{\alpha}\right)^{\frac{1-m}{2}} e^{-x} = \frac{V}{2\pi^2}\begin{cases} m=1 & \frac{V}{2\pi^2}\frac{1}{2\alpha} = \frac{V}{4\pi^2\alpha} \rightarrow f_1\\ m=2 & \frac{V}{2\pi^2}\frac{1}{2\sqrt{\alpha}}\sqrt{\pi} = \frac{V}{4\pi^2}\sqrt{\frac{\pi}{\alpha}} \rightarrow f_2\end{cases}$$

$$= \sum_{q}^{\text{dense mesh}}\frac{e^{-\alpha q^2}}{q^m} - \frac{1}{N_q}\left(\sum_{G\neq 0}\frac{e^{-\alpha G^2}}{G^m} + \sum_{q\neq 0, G}\frac{e^{-\alpha|\vec{q}+\vec{G}|^2}}{|\vec{q}+\vec{G}|^m}\right)$$

$$\mathrm{coeff2} = \frac{4\pi}{V}\cdot\mathrm{mingc2} = \frac{4\pi}{V}\left(\frac{V_{ol}}{4\pi^2}\sqrt{\frac{\pi}{\alpha}} - \mathrm{sf2}\right)$$

$$\mathrm{Coeff1} = \sqrt{\frac{4\pi}{V}}\,\mathrm{mingc1} = \sqrt{\frac{4\pi}{V}}\left(\frac{V_{ol}}{4\pi^2\alpha} - \mathrm{sf1}\right)$$

$$\tilde{\Sigma}(\omega, ie_1, ie_2) = \underset{\uparrow\,\frac{1}{q^2}}{\mathrm{coeff2}}\cdot\mathrm{head}[\omega] + \underset{\uparrow\,\frac{1}{q}}{\mathrm{coeff1}}\left\{\sum_\alpha \mathrm{minm}[ie_1, ie_2, \alpha]\cdot \underset{\uparrow\,\mathrm{epsinv2}}{W_\alpha^2(\Omega)} + \sum_\alpha \mathrm{minm}[ie_1, ie_2, \alpha]^* \underset{\uparrow\,\mathrm{epsinv1}}{W_\alpha^1(\Omega)}\right]\Big]$$

$$\langle \psi_{ie_1}\psi^*_{ie_2}|\chi_q\rangle\frac{1}{\sqrt{N_q}}\left(\frac{1}{\varepsilon_q}-1\right)\frac{1}{\sqrt{N_q}}\langle\chi_q|\psi^*_{ie_2}\psi_{ie_3}\rangle$$

$$\frac{1}{q^2}\left(\frac{4\pi}{V}\frac{1}{\varepsilon_{00}}-1\right) = \mathrm{head}$$

see Eq 82, 83 in Gap paper.

gives contribution to only $ie_2 = ie_1$ and $ie_2 = ie_3$!!

When doing numerics, we just remove $q=0$ singular term $V_{00}^{q=0}=\infty$, and we need to correct for it. The idea is that the divergent term is the plane wave with $G=0$, hence when doing the sum $\sum_{G,q} \frac{1}{|\vec{q}+\vec{G}|^2}$ we just neglected $G=0$ when $q=0$.

We are interested of how large is the error.
We construct the following function $\frac{e^{-\alpha|\vec{q}+\vec{G}|^2}}{|\vec{q}+\vec{G}|^2}$, which has the same $q\to 0$ behaviour, but falls of quickly with q, i.e., screened interaction. We check how much we are supposed to get for infinitely precise mesh and integration extended to infinity!

$$V\int \frac{d^3q}{(2\pi)^3} \frac{e^{-\alpha q^2}}{q^2} = \frac{V}{4\pi^2}\sqrt{\frac{\pi}{\alpha}}$$

What we get with truncated sum is: $\frac{1}{N_q}\left(\sum_{G\neq 0} \frac{e^{-\alpha G^2}}{G^m} + \sum_{q\neq 0}\sum_{G} \frac{e^{-\alpha|\vec{q}+\vec{G}|^2}}{|\vec{q}+\vec{G}|^m}\right)$

The error for not treating $q=0$ point with fine mesh is

$$\frac{Vol}{4\pi^2}\sqrt{\frac{\pi}{\alpha}} - \frac{1}{N_q}\left(\sum_{G\neq 0} \frac{e^{-\alpha G^2}}{G^m} + \sum_{q\neq 0}\sum_{G} \frac{e^{-\alpha|\vec{q}+\vec{G}|^2}}{|\vec{q}+\vec{G}|^m}\right) \equiv \text{Minqc2}$$

This is if the function has $\frac{1}{q^2}$ form.

Example: $\Sigma^x_k(i_1,i_3) = -\sum_{\alpha\beta q} M^{\beta *}(i_3,i_2)\, V^{\alpha}_{\beta\alpha}\, M^{\alpha}(i_1,i_2)\; f(\varepsilon_{i_2}^{k+q})$

$$-\sum_{q\text{-precise}} \frac{\delta_{i_2 i_3}}{\sqrt{Vol}} \cdot \frac{4\pi}{q^2} f(\varepsilon_{i_2}^{k+q}) \cdot \frac{\delta_{i_1 i_2}}{\sqrt{Vol}}$$

because $M^{G=0}(i_1 i_2) = \frac{1}{\sqrt{V}}\delta_{i_1 i_2}$

$\langle \chi^{G=0}|\psi^*_{i_1 k}\psi_{i_2 k}\rangle = \frac{1}{\sqrt{V}}\delta_{i_1 i_2}$

Correction is $\Sigma^x = -\delta_{i_1 i_3}\delta_{i_1 i_2}\frac{4\pi}{Vol}\underbrace{f(\varepsilon_{i_2}^{k+q})\, W_{k+q}}_{1 \text{ for occupied}} \cdot N_q$.

$$\sum_{q} \frac{\mathcal{C}_m}{|\vec{q}+\vec{G}|^m} = \sum_{(q,G)\neq 0}{}^{'} \frac{\mathcal{C}_m}{|\vec{q}+\vec{G}|^m} + \Delta_c$$

$$\Delta_c = \mathcal{C}_m\left[\underbrace{\frac{V}{(2\pi)^3}\int d^3q\, \frac{e^{-\alpha q^2}}{q^m}}_{\text{all space}} - \sum_{(\vec{q},\vec{G})\neq 0}{}^{'} \frac{e^{-\alpha|\vec{q}+\vec{G}|^2}}{|\vec{q}+\vec{G}|^m}\right]$$

$$\parallel$$

$$\sum_{G}\frac{V}{(2\pi)^3}\int d^3q\, \frac{e^{-\alpha|\vec{q}+\vec{G}|^2}}{|\vec{q}+\vec{G}|^m} - \sum_{(\vec{q},\vec{G})\neq 0} \frac{e^{-\alpha|\vec{q}+\vec{G}|^2}}{|\vec{q}+\vec{G}|^m}$$

Matrix elements of $\vec{p} = -i\vec{\nabla}$

$$\langle \psi_{M_1 \mathfrak{r}} | \vec{\nabla} | \psi_{M_2 \mathfrak{r}} \rangle = a^{\mathfrak{r}*}_{M_1 \ell_1 m_1} a^{\mathfrak{r}}_{M_2 \ell_2 m_2} \langle u_{\ell_1} Y_{\ell_1 m_1} (\vec{e}_r \tfrac{\partial}{\partial r} + \tfrac{1}{r} \nabla_{\theta\varphi}) Y_{\ell_2 m_2} u_{\ell_2} \rangle =$$

$$= a^{\mathfrak{r}*}_{M_1 \ell_1 m_1} a^{\mathfrak{r}}_{M_2 \ell_2 m_2} \Big\{ \langle u_{\ell_1} | \tfrac{d}{dr} | u_{\ell_2} \rangle \underbrace{\langle Y_{\ell_1 m_1} | \vec{e}_r | Y_{\ell_2 m_2} \rangle}_{I^{(1)}_{\ell_1 m_1 \ell_2 m_2}} + \langle u_{\ell_1} | \tfrac{1}{r} | u_{\ell_2} \rangle \underbrace{\langle Y_{\ell_1 m_1} | r\vec{\nabla} | Y_{\ell_2 m_2} \rangle}_{I^{(2)}_{\ell_1 m_1 \ell_2 m_2}} \Big\}$$

$$= a^{\mathfrak{r}*}_{m'\ell'm'} a^{\mathfrak{r}}_{m\ell m} \Bigg\{ \langle u_{\ell'} | \tfrac{d}{dr} | u_\ell \rangle \begin{pmatrix} \frac{1}{2} Q(\ell,m) \delta_{\ell'=\ell+1} \delta_{m'=m+1} - \frac{1}{2} Q(\ell',-m') \delta_{\ell'=\ell-1} \delta_{m'=m+1} - \frac{1}{2} Q(\ell,-m) \delta_{\ell'=\ell+1} \delta_{m'=m-1} + \frac{1}{2} Q(\ell',m') \delta_{\ell'=\ell-1} \delta_{m'=m-1} \\ -\frac{i}{2} Q(\ell,m) \delta_{\ell'=\ell+1} \delta_{m'=m+1} + \frac{i}{2} Q(\ell',-m') \delta_{\ell'=\ell-1} \delta_{m'=m+1} - \frac{i}{2} Q(\ell,-m) \delta_{\ell'=\ell+1} \delta_{m'=m-1} + \frac{i}{2} Q(\ell',m') \delta_{\ell'=\ell-1} \delta_{m'=m-1} \\ f(\ell,m) \delta_{\ell'=\ell+1} \delta_{m'=m} + f(\ell'm') \delta_{\ell'=\ell-1} \delta_{m'=m} \end{pmatrix}$$

$$+ \langle u_{\ell'} | \tfrac{1}{r} u_\ell \rangle \begin{pmatrix} -\frac{\ell}{2} Q(\ell,m) \delta_{\ell'=\ell+1} \delta_{m'=m+1} - \frac{(\ell+1)}{2} Q(\ell',-m') \delta_{\ell'=\ell-1} \delta_{m'=m+1} + \frac{\ell}{2} Q(\ell,-m) \delta_{\ell'=\ell+1} \delta_{m'=m-1} + \frac{\ell+1}{2} Q(\ell',m') \delta_{\ell'=\ell-1} \delta_{m'=m-1} \\ i\frac{\ell}{2} Q(\ell,m) \delta_{\ell'=\ell+1} \delta_{m'=m+1} + i\frac{(\ell+1)}{2} Q(\ell',-m') \delta_{\ell'=\ell-1} \delta_{m'=m+1} + i\frac{\ell}{2} Q(\ell,-m) \delta_{\ell'=\ell+1} \delta_{m'=m-1} + i\frac{\ell+1}{2} Q(\ell'm') \delta_{\ell'=\ell-1} \delta_{m'=m-1} \\ -\ell f(\ell,m) \delta_{\ell'=\ell+1} \delta_{m'=m} + (\ell+1) f(\ell',m') \delta_{\ell'=\ell-1} \delta_{m'=m} \end{pmatrix} \Bigg\}$$

$$= a^{\mathfrak{r}*}_{m'\ell'm'} a^{\mathfrak{r}}_{m\ell m} \Bigg\{ \begin{pmatrix} \delta(\ell'=\ell+1 | m'=m+1) \frac{1}{2} Q(\ell,m) \langle u_{\ell'} | \frac{d}{dr} - \frac{\ell}{r} | u_\ell \rangle - \delta(\ell'=\ell-1 | m'=m+1) \frac{1}{2} Q(\ell',-m') \langle u_{\ell'} | \frac{d}{dr} + \frac{(\ell+1)}{r} | u_\ell \rangle \\ \delta(\ell'=\ell+1 | m'=m+1) (\frac{-i}{2}) Q(\ell,m) \langle u_{\ell'} | \frac{d}{dr} - \frac{\ell}{r} | u_\ell \rangle + \delta(\ell'=\ell-1 | m'=m+1) \frac{i}{2} Q(\ell',-m') \langle u_{\ell'} | \frac{d}{dr} + \frac{(\ell+1)}{r} | u_\ell \rangle \\ \delta(\ell'=\ell+1, m'=m) f(\ell,m) \langle u_{\ell'} | \frac{d}{dr} - \frac{\ell}{r} | u_\ell \rangle + \delta(\ell'=\ell-1 | m'=m) f(\ell'm') \langle u_{\ell'} | \frac{d}{dr} + \frac{(\ell+1)}{r} | u_\ell \rangle \end{pmatrix} +$$

$$+ \begin{pmatrix} -\delta(\ell'=\ell+1 | m'=m-1) \frac{1}{2} Q(\ell,-m) \langle u_{\ell'} | \frac{d}{dr} - \frac{\ell}{r} | u_\ell \rangle + \delta(\ell'=\ell-1 | m'=m-1) \frac{1}{2} Q(\ell'm') \langle u_{\ell'} | \frac{d}{dr} + \frac{\ell+1}{r} | u_\ell \rangle \\ -\delta(\ell'=\ell+1 | m'=m-1) \frac{i}{2} Q(\ell,-m) \langle u_{\ell'} | \frac{d}{dr} - \frac{\ell}{r} | u_\ell \rangle + \delta(\ell'=\ell-1 | m'=m-1) \frac{i}{2} Q(\ell',m') \langle u_{\ell'} | \frac{d}{dr} + \frac{\ell+1}{r} | u_\ell \rangle \\ 0 \end{pmatrix} \Bigg\}$$

$\delta(\ell'=\ell+1 | m'=m+1)$

$$\langle \psi_{m'\mathfrak{r}} | \vec{\nabla} | \psi_{m\mathfrak{r}} \rangle = \begin{pmatrix} \langle \psi^{m'}_{\ell+1,m+1} | \frac{1}{2} Q(\ell,m) (\frac{d}{dr} - \frac{\ell}{r}) \psi^m_{\ell m} \rangle - \langle \psi^{m'}_{\ell-1,m+1} | \frac{1}{2} Q(\ell-1,-m-1) (\frac{d}{dr} + \frac{\ell+1}{r}) | \psi^m_{\ell m} \rangle \\ -i \langle \psi^{m'}_{\ell+1,m+1} | \frac{1}{2} Q(\ell,m) (\frac{d}{dr} - \frac{\ell}{r}) \psi^m_{\ell m} \rangle + i \langle \psi^{m'}_{\ell-1,m+1} | \frac{1}{2} Q(\ell-1,-m-1) (\frac{d}{dr} + \frac{\ell+1}{r}) | \psi^m_{\ell m} \rangle \\ \langle \psi^{m'}_{\ell+1,m} | f(\ell,m) (\frac{d}{dr} - \frac{\ell}{r}) | \psi^m_{\ell m} \rangle + \langle \psi^{m'}_{\ell-1,m} | f(\ell-1,m) (\frac{d}{dr} + \frac{(\ell+1)}{r}) | \psi^m_{\ell m} \rangle \end{pmatrix}$$

$$+ \begin{pmatrix} -\langle \psi^{m'}_{\ell+1,m-1} | \frac{1}{2} Q(\ell,-m) (\frac{d}{dr} - \frac{\ell}{r}) | \psi^m_{\ell m} \rangle + \langle \psi^{m'}_{\ell-1,m-1} | \frac{1}{2} Q(\ell-1,m-1) (\frac{d}{dr} + \frac{\ell+1}{r}) | \psi^m_{\ell m} \rangle \\ -\frac{i}{2} \langle \psi^{m'}_{\ell+1,m-1} | Q(\ell,-m) (\frac{d}{dr} - \frac{\ell}{r}) | \psi^m_{\ell m} \rangle + \frac{i}{2} \langle \psi^{m'}_{\ell-1,m-1} | Q(\ell-1,m-1) (\frac{d}{dr} + \frac{\ell+1}{r}) | \psi^m_{\ell m} \rangle \\ 0 \end{pmatrix}$$

$$\langle \psi_{m'\mathfrak{r}} | i\vec{\nabla} | \psi_{m\mathfrak{r}} \rangle = \begin{pmatrix} -\frac{i}{2} \overbrace{\left(-\langle \psi^{m'}_{\ell+1,m+1} | Q(\ell,m) (\frac{d}{dr} - \frac{\ell}{r}) \psi^m_{\ell m} \rangle + \langle \psi^{m'}_{\ell,m} | Q(\ell,-m) (\frac{d}{dr} + \frac{\ell+2}{r}) | \psi^m_{\ell+1,m-1} \rangle \right)}^{p_x p_y} \\ -\frac{1}{2} \left(-\langle \psi^{m'}_{\ell+1,m+1} | Q(\ell,m) (\frac{d}{dr} - \frac{\ell}{r}) \psi^m_{\ell m} \rangle + \langle \psi^{m'}_{\ell,m} | Q(\ell,-m) (\frac{d}{dr} + \frac{\ell+2}{r}) | \psi^m_{\ell+1,m-1} \rangle \right) \\ i \underbrace{\left(\langle \psi^{m'}_{\ell+1,m} | f(\ell,m) (\frac{d}{dr} - \frac{\ell}{r}) | \psi^m_{\ell m} \rangle + \langle \psi^{m'}_{\ell,m} | f(\ell,m) (\frac{d}{dr} + \frac{\ell+2}{r}) | \psi^m_{\ell+1,m} \rangle \right)}_{p_z} \end{pmatrix}$$

$$\begin{pmatrix} -\frac{i}{2} \overbrace{\left(\langle \psi^{m'}_{\ell+1,m-1} | Q(\ell,-m) (\frac{d}{dr} - \frac{\ell}{r}) | \psi^m_{\ell m} \rangle - \langle \psi^{m'}_{\ell,m} | Q(\ell,m) (\frac{d}{dr} + \frac{\ell+2}{r}) | \psi^m_{\ell+1,m+1} \rangle \right)}^{p_x m p_y} \\ \frac{1}{2} \left(\langle \psi^{m'}_{\ell+1,m-1} | Q(\ell,-m) (\frac{d}{dr} - \frac{\ell}{r}) | \psi^m_{\ell m} \rangle - \langle \psi^{m'}_{\ell,m} | Q(\ell,m) (\frac{d}{dr} + \frac{\ell+1}{r}) | \psi^m_{\ell+1,m+1} \rangle \right) \\ 0 \end{pmatrix}$$

Matrix elements of $\vec{p} = -i\vec{\nabla}$

$$e(\ell,m) = \sqrt{\frac{(\ell+m+1)(\ell+m+2)}{(2\ell+1)(2\ell+3)}} \qquad f(\ell,m) = \sqrt{\frac{(\ell+m+1)(\ell-m+1)}{(2\ell+1)(2\ell+3)}}$$

$$I^{(1)}_{\ell' m' \ell m} = \frac{1}{2}\delta_{\ell'=\ell+1}\left[\left(-e(\ell,m)\begin{pmatrix}1\\-i\\0\end{pmatrix}\delta_{m'=m+1} - e(\ell,-m)\begin{pmatrix}-1\\-i\\0\end{pmatrix}\delta_{m'=m-1} + 2f(\ell,m)\begin{pmatrix}0\\0\\1\end{pmatrix}\delta_{m'=m}\right]$$
$$-\frac{1}{2}\delta_{\ell'=\ell-1}\left[-e(\ell',-m')\begin{pmatrix}1\\-i\\0\end{pmatrix}\delta_{m'=m+1} - e(\ell',m')\begin{pmatrix}-1\\-i\\0\end{pmatrix}\delta_{m'=m-1} - 2f(\ell',m')\begin{pmatrix}0\\0\\1\end{pmatrix}\delta_{m'=m}\right]$$

$$I^{(2)}_{\ell' m' \ell m} = -\frac{\ell}{2}\delta_{\ell'=\ell+1}\left[\left(-e(\ell,m)\begin{pmatrix}1\\-i\\0\end{pmatrix}\delta_{m'=m+1} - e(\ell,-m)\begin{pmatrix}-1\\-i\\0\end{pmatrix}\delta_{m'=m-1} + 2f(\ell,m)\begin{pmatrix}0\\0\\1\end{pmatrix}\delta_{m'=m}\right]$$
$$-\frac{(\ell+1)}{2}\delta_{\ell'=\ell-1}\left[-e(\ell',-m')\begin{pmatrix}1\\-i\\0\end{pmatrix}\delta_{m'=m+1} - e(\ell',m')\begin{pmatrix}-1\\-i\\0\end{pmatrix}\delta_{m'=m-1} - 2f(\ell',m')\begin{pmatrix}0\\0\\1\end{pmatrix}\delta_{m'=m}\right]$$

$$I^{(n)}_{\ell' m' \ell m} = C^n_\ell\,\delta_{\ell'=\ell+1}\,\vec{g}(\ell' m' \ell m) - d^n_\ell\,\delta_{\ell'=\ell-1}\,\vec{h}(\ell' m' \ell m) \quad \text{where } C^1_\ell = d^1_\ell = \frac{1}{2} \text{ and } C^2_\ell = -\frac{\ell}{2};\ d^2_\ell = \frac{\ell+1}{2}$$

$$g(\ell' m' \ell m) = \left[\left(-e(\ell,m)\begin{pmatrix}1\\-i\\0\end{pmatrix}\delta_{m'=m+1} - e(\ell,-m)\begin{pmatrix}-1\\-i\\0\end{pmatrix}\delta_{m'=m-1} + 2f(\ell,m)\begin{pmatrix}0\\0\\1\end{pmatrix}\delta_{m'=m}\right] \Rightarrow \begin{cases} g^x + i g^y = -2e(\ell,m)\,\delta_{m'=m+1} \\ g^x - i g^y = 2e(\ell,-m)\,\delta_{m'=m-1} \\ g^z = 2f(\ell,m)\,\delta_{m'=m} \end{cases}$$

$$h(\ell' m' \ell m) = \left[-e(\ell',-m')\begin{pmatrix}1\\-i\\0\end{pmatrix}\delta_{m'=m+1} - e(\ell',m')\begin{pmatrix}-1\\-i\\0\end{pmatrix}\delta_{m'=m-1} - 2f(\ell',m')\begin{pmatrix}0\\0\\1\end{pmatrix}\delta_{m'=m}\right] \Rightarrow \begin{cases} h^x + i h^y = -2e(\ell',-m')\,\delta_{m'=m+1} \\ h^x - i h^y = 2e(\ell',m')\,\delta_{m'=m-1} \\ h^z = -2f(\ell',m')\,\delta_{m'=m} \end{cases}$$

$$\vec{M}_{ji} = \langle \varphi^j | \vec{\nabla} | \varphi^i \rangle$$

$$\vec{M}_{ji} = \langle \varphi^j_{\ell' m'} | \tfrac{d}{dr} | \varphi^i_{\ell m} \rangle \left[C^1_\ell\,\delta_{\ell'=\ell+1}\,\vec{g}(\ell' m' \ell m) - d^1_\ell\,\delta_{\ell'=\ell-1}\,\vec{h}(\ell' m' \ell m)\right]$$
$$\langle \varphi^j_{\ell' m'} | \tfrac{1}{r} | \varphi^i_{\ell m} \rangle \left[C^2_\ell\,\delta_{\ell'=\ell+1}\,\vec{g}(\ell' m' \ell m) - d^2_\ell\,\delta_{\ell'=\ell-1}\,\vec{h}(\ell' m' \ell m)\right]$$

$$\vec{M}_{ji} = \left[\langle \varphi^j_{\ell' m'} | \tfrac{d}{dr} | \varphi^i_{\ell m} \rangle C^1_\ell + \langle \varphi^j_{\ell' m'} | \tfrac{1}{r} | \varphi^i_{\ell m} \rangle C^2_\ell\right]\delta_{\ell'=\ell+1}\,\vec{g}(\ell' m' \ell m)$$
$$-\left[\langle \varphi^j_{\ell' m'} | \tfrac{d}{dr} | \varphi^i_{\ell m} \rangle d^1_\ell + \langle \varphi^j_{\ell' m'} | \tfrac{1}{r} | \varphi^i_{\ell m} \rangle d^2_\ell\right]\delta_{\ell'=\ell-1}\,\vec{h}(\ell' m' \ell m)$$

$$\vec{M}_{ji} = \frac{1}{2}\langle \varphi^j_{\ell' m'} | \tfrac{d}{dr} - \tfrac{\ell}{r} | \varphi^i_{\ell m} \rangle\,\delta_{\ell'=\ell+1}\,\vec{g}(\ell' m' \ell m) - \frac{1}{2}\langle \varphi^j_{\ell' m'} | \tfrac{d}{dr} + \tfrac{(\ell+1)}{r} | \varphi^i_{\ell m} \rangle\,\delta_{\ell'=\ell-1}\,\vec{h}(\ell' m' \ell m)$$

$$M^x_{ji} + i M^y_{ji} = -\underbrace{\langle \varphi^j_{\ell+1,m+1} | \tfrac{d}{dr} - \tfrac{\ell}{r} | \varphi^i_{\ell m} \rangle}_{xpy1} e(\ell,m) + \underbrace{\langle \varphi^j_{\ell,m} | \tfrac{d}{dr} + \tfrac{(\ell+2)}{r} | \varphi^i_{\ell+1,m-1} \rangle}_{xpy2} e(\ell,-m) \equiv p\times py$$

$$M^x_{ji} - i M^y_{ji} = \underbrace{\langle \varphi^j_{\ell+1,m-1} | \tfrac{d}{dr} - \tfrac{\ell}{r} | \varphi^i_{\ell m} \rangle}_{xmy1} e(\ell,-m) - \underbrace{\langle \varphi^j_{\ell,m} | \tfrac{d}{dr} + \tfrac{(\ell+2)}{r} | \varphi^i_{\ell+1,m+1} \rangle}_{xmy2} e(\ell,m) \equiv p\times my$$

$$M^z_{ji} = \underbrace{\langle \varphi^j_{\ell+1,m} | \tfrac{d}{dr} - \tfrac{\ell}{r} | \varphi^i_{\ell m} \rangle}_{z1} f(\ell,m) + \underbrace{\langle \varphi^j_{\ell,m} | \tfrac{d}{dr} + \tfrac{(\ell+2)}{r} | \varphi^i_{\ell+1,m} \rangle}_{z2} f(\ell,m) \equiv p_z$$

$$\langle | -i\vec{\nabla} | \rangle^x = -\frac{i}{2}\left(p\times py + p\times my\right)$$
$$\langle | -i\vec{\nabla} | \rangle^y = -\frac{1}{2}\left(p\times py - p\times my\right)$$
$$\langle | -i\vec{\nabla} | \rangle^z = -i\,p_z$$

Alternative expansion for core states

$$\vec{M}_{ji} = \frac{1}{2}\langle \varphi^{j}_{l'm'} | \frac{d}{dr} - \frac{l}{r} | \varphi^{i}_{lm} \rangle \delta_{l'=l+1}\, \vec{g}(l'm'lm) - \frac{1}{2}\langle \varphi^{j}_{l'm'} | \frac{d}{dr} + \frac{(l+1)}{r} | \varphi^{i}_{lm} \rangle \delta_{l'=l-1}\, \vec{h}(l'm'lm)$$

$$g(l'm'lm) = \left[-a(l,m)\begin{pmatrix} 1 \\ -i \\ 0 \end{pmatrix}\delta_{m'=m+1} - a(l,-m)\begin{pmatrix} -1 \\ -i \\ 0 \end{pmatrix}\delta_{m'=m-1} + 2f(l,m)\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}\delta_{m'=m} \right] \Rightarrow \begin{cases} g^x + i g^y = -2a(l,m)\,\delta_{m'=m+1} \\ g^x - i g^y = 2a(l,-m)\,\delta_{m'=m-1} \\ g^z = 2f(l,m)\,\delta_{m'=m} \end{cases}$$

$$h(l'm'lm) = \left[-a(l',-m')\begin{pmatrix} 1 \\ -i \\ 0 \end{pmatrix}\delta_{m'=m+1} - a(l',m')\begin{pmatrix} -1 \\ -i \\ 0 \end{pmatrix}\delta_{m'=m-1} - 2f(l'm')\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}\delta_{m'=m} \right] \Rightarrow \begin{cases} h^x + i h^y = -2a(l',-m')\,\delta_{m'=m+1} \\ h^x - i h^y = 2a(l',m')\,\delta_{m'=m-1} \\ h^z = -2f(l'm')\,\delta_{m'=m} \end{cases}$$

$$M^x_{ji} + i M^y_{ji} = \frac{1}{2}\langle \varphi^c_{lm} | \frac{d}{dr} - \frac{l'}{r} | \varphi_{l'm'} \rangle \delta_{l=l'+1}\left(-2a(l',m')\,\delta_{m=m'+1}\right) - \frac{1}{2}\langle \varphi^c_{lm} | \frac{d}{dr} + \frac{(l'+1)}{r} | \varphi_{l'm'} \rangle \delta_{l=l'-1}\left(-2a(l,-m)\delta_{m=m'+1}\right)$$

$$- \langle \varphi^c_{lm} | \frac{d}{dr} - \frac{l-1}{r} | \varphi_{l-1,m-1} \rangle a(l-1,m-1) + \langle \varphi^c_{lm} | \frac{d}{dr} + \frac{l+2}{r} | \varphi_{l+1,m-1} \rangle a(l,-m)$$

$$M^x_{ji} - i M^y_{ji} = \frac{1}{2}\langle \varphi^c_{lm} | \frac{d}{dr} - \frac{l'}{r} | \varphi_{l'm'} \rangle \delta_{l=l'+1}\, 2a(l',-m')\,\delta_{m=m'-1} - \frac{1}{2}\langle \varphi^c_{lm} | \frac{d}{dr} + \frac{(l'+1)}{r} | \varphi_{l'm'} \rangle \delta_{l=l'-1}\, 2a(l,m)\,\delta_{m=m'-1}$$

$$\langle \varphi^c_{lm} | \frac{d}{dr} - \frac{l-1}{r} | \varphi_{l-1,m+1} \rangle a(l-1,-m-1) - \langle \varphi^c_{lm} | \frac{d}{dr} + \frac{l+2}{r} | \varphi_{l+1\,m+1} \rangle a(l,m)$$

$$M^z_{ji} = \frac{1}{2}\langle \varphi^c_{lm} | \frac{d}{dr} - \frac{l'}{r} | \varphi_{l'm'} \rangle \delta_{l=l'+1}\, 2f(l'm')\,\delta_{m'=m} + \frac{1}{2}\langle \varphi^c_{lm} | \frac{d}{dr} + \frac{(l'+1)}{r} | \varphi_{l'm'} \rangle \delta_{l=l'-1}\, 2f(l,m)\,\delta_{m'=m}$$

$$\langle \varphi^c_{lm} | \frac{d}{dr} - \frac{l-1}{r} | \varphi_{l-1,m} \rangle f(l-1,m) + \langle \varphi^c_{lm} | \frac{d}{dr} + \frac{l+2}{r} | \varphi_{l+1,m} \rangle f(l,m)$$

$$M^x_{ji} + i M^y_{ji} = \frac{1}{2}\langle \varphi_{l'm'} | \frac{d}{dr} - \frac{l}{r} | \varphi^c_{lm} \rangle \delta_{l'=l+1}\left(-2a(l,m)\,\delta_{m'=m+1}\right) - \frac{1}{2}\langle \varphi_{l'm'} | \frac{d}{dr} + \frac{(l+1)}{r} | \varphi^c_{lm} \rangle \left(-2a(l',-m')\,\delta_{m'=m+1}\,\delta_{l'=l-1}\right)$$

$$= -a(l,m)\langle \varphi_{l+1,m+1} | \frac{d}{dr} - \frac{l}{r} | \varphi^c_{lm} \rangle + a(l-1,-m-1)\cdot\langle \varphi_{l-1,m+1} | \frac{d}{dr} + \frac{(l+1)}{r} | \varphi^c_{lm} \rangle$$

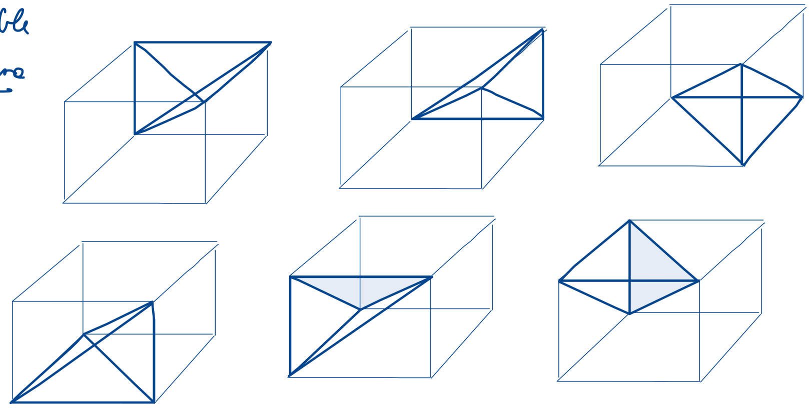
$$M^x_{ji} - i M^y_{ji} = \frac{1}{2}\langle \varphi_{l'm'} | \frac{d}{dr} - \frac{l}{r} | \varphi^c_{lm} \rangle \delta_{l'=l+1}\, 2a(l,-m)\,\delta_{m'=m-1} - \frac{1}{2}\langle \varphi_{l'm'} | \frac{d}{dr} + \frac{(l+1)}{r} | \varphi^c_{lm} \rangle \delta_{l'=l-1}\,\delta_{m'=m-1}\, 2a(l'm')$$

$$= a(l,-m)\langle \varphi_{l+1,m-1} | \frac{d}{dr} - \frac{l}{r} | \varphi^c_{lm} \rangle - a(l-1,m-1)\langle \varphi_{l-1,m-1} | \frac{d}{dr} + \frac{(l+1)}{r} | \varphi^c_{lm} \rangle$$

$$M^z_{ji} = \frac{1}{2}\langle \varphi_{l'm'} | \frac{d}{dr} - \frac{l}{r} | \varphi^c_{lm} \rangle \delta_{l'=l+1}\, 2f(l,m)\,\delta_{m'=m} - \frac{1}{2}\langle \varphi_{l'm'} | \frac{d}{dr} + \frac{(l+1)}{r} | \varphi^c_{lm} \rangle \delta_{l'=l-1}\left(-2f(l',m')\right)\delta_{m'=m}$$

$$= \langle \varphi_{l+1,m} | \frac{d}{dr} - \frac{l}{r} | \varphi^c_{lm} \rangle f(l,m) + \langle \varphi_{l-1,m} | \frac{d}{dr} + \frac{(l+1)}{r} | \varphi^c_{lm} \rangle f(l-1,m)$$

6 possible tetrahedra



from $r \to r + (1,0,0)$
$+ (0,1,0)$
$+ (0,0,1)$

Analytic continuation by PRL 74, 1827 (1996)

$$\Sigma^{m}(z) = \frac{\sum_{r=0}^{m} c_r z^r}{1+\sum_{r=1}^{m+1} c_{r+m} z^r} \quad ; \quad \left|\Sigma(i\omega) - \Sigma^{m}(z=i\omega)\right|^2 = \min$$

Wannier 90 $\qquad M_{mn} = \langle \psi_{k+g\,n} | e^{i\vec{g}\vec{r}} | \psi_{k\,m} \rangle$

α, atom, u, $\dot{u}$, u_{lo} ...

$$|\psi_{k i}\rangle = |\chi_{k+G}\rangle\, Q_{G i}$$

$$\langle r| e^{-i\vec{k}\vec{r}} |\psi_{k i}\rangle = e^{-i\vec{k}\vec{r}} \langle r|\chi_{k+G}\rangle\, Q_{G i}$$

$$\langle \psi_{k+g\,j}| e^{i\vec{g}\vec{r}} |\psi_{k i}\rangle = Q^{k+g\,*}_{G_1 j}\, Q^{k}_{G_2 i}\, \langle \chi_{k+g+G_1}| e^{i\vec{g}\vec{r}} |\chi_{k+G_2}\rangle$$

$$\langle \chi_{k+g+G_1}| e^{i\vec{g}\vec{r}} |\chi_{k+G_2}\rangle = \underbrace{\int_I \frac{d^3r}{V_{cell}}\, e^{i(\vec{G}_2-\vec{G}_1)\vec{r}}}_{\langle G_1|I|G_2\rangle_I} + \sum_a \underbrace{\int_{MT_a} d^3r\, \chi^*_{k+g\,G_1}(\vec{r})\, e^{i\vec{g}\vec{r}}\, \chi_{k+G_2}(\vec{r})}_{e^{i(\vec{G}_2-\vec{G}_1)\vec{r}_a}\cdot \langle \chi_{k+g\,G_1}| e^{i\vec{g}\vec{r}} | \chi_{k+G_2}\rangle_{MT_a}}$$

$$\langle G_1|I|G_2\rangle_I = \delta_{G_2 G_1} - \sum_a e^{i(\vec{G}_2-\vec{G}_1)\vec{r}_a} \int_{MT_a} \frac{d^3r}{V_{cell}}\, e^{i(\vec{G}_2-\vec{G}_1)\vec{r}} = \delta_{G_2 G_1} - \sum_a e^{i(\vec{G}_2-\vec{G}_1)\vec{r}_a} \frac{2}{(G_2-G_1)} \int_0^{R^a_{MT}} dr\, r \sin((G_2-G_1)r)$$

$$\chi_{k+G}(\vec{r}_a) = \sum_{lm\alpha a} Q^{k}_{G,lm\alpha}\, u^{\alpha}_{l}(r_a)\, Y_{lm}(\hat{r}_a)$$

$$\langle \chi_{k+g\,G_1}| e^{i\vec{g}\vec{r}} |\chi_{k+G_2}\rangle_{MT_a} = Q^{k+g\,*}_{G_1\, l_1 m_1 \alpha_1}\, Q^{k}_{G_2\, l_2 m_2 \alpha_2} \langle u^{\alpha_1}_{l_1} Y_{l_1 m_1} | \underset{\displaystyle 4\pi i^l Y^*_{lm}(\hat{g})\, j_l(gr)\, Y_{lm}(\hat{r})}{\underset{\|}{e^{i\vec{g}\vec{r}}}} | u^{\alpha_2}_{l_2} Y_{l_2 m_2}\rangle_{MT_a}$$

$$= Q^{k+g\,*}_{G_1\, l_1 m_1 \alpha_1}\, Q^{k}_{G_2\, l_2 m_2 \alpha_2} \langle u^{\alpha_1}_{l_1} | j_l(gr) | u^{\alpha_2}_{l_2}\rangle_{MT_a} \langle Y_{l_1 m_1} | Y_{lm} | Y_{l_2 m_2}\rangle\, 4\pi i^l\, Y^*_{lm}(\hat{g})$$

$$\langle \chi_{k+g+G_1}| e^{i\vec{g}\vec{r}} |\chi_{k+G_2}\rangle = \langle G_1|I|G_2\rangle_I + \sum_a e^{i(\vec{G}_2-\vec{G}_1)\vec{r}_a}\, Q^{k+g\,*}_{G_1\, l_1 m_1 \alpha_1}\, Q^{k}_{G_2\, l_2 m_2 \alpha_2} \langle u^{\alpha_1}_{l_1} | j_l(gr) | u^{\alpha_2}_{l_2}\rangle_{MT_a} \langle Y_{l_1 m_1} | Y_{lm} | Y_{l_2 m_2}\rangle\, 4\pi i^l\, Y^*_{lm}(\hat{g})$$

$$\langle \psi_{k+g\,j}| e^{i\vec{g}\vec{r}} |\psi_{k i}\rangle = Q^{k+g\,*}_{G_1 j}\, \langle G_1|I|G_2\rangle_I\, Q^{k}_{G_2 i} +$$

$$+ \sum_a e^{i(\vec{G}_2-\vec{G}_1)\vec{r}_a}\, A^{k+g\,*}_{j,\, l_1 m_1 \alpha_1}\, A^{k}_{i,\, l_2 m_2 \alpha_2} \cdot \langle u^{\alpha_1}_{l_1} | j_l(gr) | u^{\alpha_2}_{l_2}\rangle_{MT_a} \langle Y_{l_1 m_1} | Y_{lm} | Y_{l_2 m_2}\rangle\, 4\pi i^l\, Y^*_{lm}(\hat{g})$$

Interpolation of energy on denser k-mesh:

Pickett
PRB 38, 2721 (1988)

E_k is a scalar, therefore it can be expanded in terms of the star of the lattice

$$S_m(\vec{k}) = \frac{1}{N_{sym}} \sum_r e^{i \vec{k} \Gamma_r \vec{R}_m} \qquad S_{m=0} = 1$$

Let's assume that there exist a smooth interpolation $\mathcal{E}(\vec{k})$ on dense k grid for each band. This is in general not the case because of band crossings.

The simplest possibility : $\mathcal{E}(\vec{k}_i) = \sum_m S_m(\vec{k}_i)\, Q_m$ and $Q_m = \sum_{\vec{k}_i} S_m^*(\vec{k}_i)\, \mathcal{E}(\vec{k}_i)$

with the same number of $\vec{k}_i$ and m. This is just inverse Fourier.

Mathematically, we can also write: $\mathcal{E}(\vec{k}_i) = \sum_m S_m(\vec{k}_i)\, Q_m = \sum_m S_{im}\, Q_m$

$$Q_m = \sum_{k_i} (S^{-1})_{mi}\, \mathcal{E}(\vec{k}_i)$$

But we know $\sum_{k_i} S_m(\vec{k}_i)\, S_{m'}^*(\vec{k}_i) = \delta_{mm'}$

$$\sum_i (S^+)_{m'i}\, S_{im} = 1 \quad \text{and} \quad (S^{-1})_{mi} = (S^+)_{mi}$$

hence $Q_m = \sum_{k_i} S_m^*(\vec{k}_i)\, \mathcal{E}(\vec{k}_i)$ This is just inverse fourier

It has a problem with cutoff $\#m = \#k_i$ with small number of $\vec{k}_i$ and introduces oscilations. How to remove oscilations?

Pickett has an improvement of such naive approach.

We define the star function

$$S_m(\vec{k}) = \frac{1}{N_\sigma}\sum_{\sigma} e^{i\vec{k}\cdot\sigma\vec{R}_m}$$

$\uparrow$ all group operation $\vec{R}_m$ vectors on the lattice.

$S_m(\vec{k})$ has full symmetry of the crystal and is a scalar in the space group, therefore we expect Fourier expansion of any scalar to have a form:

$$\tilde{\varepsilon}(\vec{k}) = \sum_{m=1}^{M} a_m S_m(\vec{k}) \quad \text{with } M \gg \#\vec{k}_i \text{ being calculated}$$

But our data exist on limited number of momentum points and we want to interpolate it smoothly by requiring:

$$R = \frac{1}{N_k}\sum_{k_i}\left(|\tilde{\varepsilon}(\vec{k}_i)|^2 + c_1|\vec{\nabla}_k\tilde{\varepsilon}(\vec{k}_i)|^2 + c_2|\vec{\nabla}^2\tilde{\varepsilon}(\vec{k}_i)|^4 + \cdots\right) = \min$$

and $\tilde{\varepsilon}(\vec{k}_i) = \varepsilon(\vec{k}_i)$ on data $\varepsilon(\vec{k}_i)$ being known.

Note $\frac{1}{N_k}\sum_{k_i}|\tilde{\varepsilon}(\vec{k}_i)|^2 = \sum_{m,m'} a_m a^*_{m'} \underbrace{\frac{1}{N}\sum_{k_i} S_m(\vec{k}_i) S^*_{m'}(\vec{k}_i)}_{\delta_{mm'}} = |a_m|^2$

Similarly $\frac{1}{N_k}\sum_{k_i}|\vec{\nabla}\tilde{\varepsilon}(\vec{k}_i)|^2 = \sum_{m m'} a_m a_{m'} \underbrace{\frac{1}{N_\sigma}\sum_{\sigma\sigma'}\sigma\vec{R}_m\,\sigma'\vec{R}_{m'}}_{\delta_{mm'} R_m^2} \underbrace{\sum_{k_i} e^{i\vec{k}\sigma\vec{R}_m} e^{-i\vec{k}\sigma\vec{R}_{m'}}}_{\delta_{mm'}} = \sum_m |a_m|^2 R_m^2$

Hence $R = \sum_m |a_m|^2 (1 + c_1|R_m|^2 + c_2|R_m|^4 + \cdots)$

We can rewrite $R = \sum_{m>0}^{N} |a_m|^2 (1 + c_1|R_m|^2 + c_2|R_m|^4 + \cdots) + |a_{m=0}|^2$

because at $m=0$ $R_m=0$ since the first is origin

Pickett argues that this first term is harmfull, because tries to force average close to 0, rather than $\langle\varepsilon\rangle$. Hence he proposes to drop $m=0$ term. Hence

$$R = \sum_{m>0}^{N} |a_m|^2 (1 + c_1|R_m|^2 + c_2|R_m|^4 + \cdots) \quad \text{and fix } a_0 = \sum_{k_i}\varepsilon(\vec{k}_i)$$

We have a constraint $\tilde{\varepsilon}(\vec{k}_i) = \varepsilon(\vec{k}_i)$ hence we use Lagrange multipliers λ_i

$$\sum_i \lambda_i[\tilde{\varepsilon}(\vec{k}_i) - \varepsilon(\vec{k}_i)]$$

The functional to minimize with constraint is

$$R = \sum_{m>0}^{N} |Q_m|^2 (1 + C_1 R_m^2 + C_2 R_m^4) - \sum_{\vec{z}_i} 2\lambda_i \left(\sum_{m=0}^{N} Q_m S_m(\vec{z}_i) - \mathcal{E}(\vec{z}_i) \right)$$

$$0 = \frac{1}{2} \frac{\delta R}{\delta Q_m} = Q_m^* \left(1 + C_1 R_m^2 + C_2 R_m^4 + \cdots\right) - \sum_i \lambda_i S_m(\vec{z}_i) \qquad m \geq 1$$

$$\sum_i \lambda_i S_0(\vec{z}_i) = 0 \qquad m = 0 \qquad \text{note } \underline{S_0(\vec{z}) = 1}$$

Define: $\rho(\vec{R}_m) \equiv \left(1 + C_1 R_m^2 + C_2 R_m^4 + \cdots\right)$

Then:

$$\boxed{\begin{array}{ll} Q_m^* \rho(\vec{R}_m) = \sum_i \lambda_i S_m(\vec{z}_i) & \text{for } m > 0 \\ \text{and } \sum_i \lambda_i = 0 & \text{for } m = 0 \end{array}}$$

$$Q_0 = \sum_i \lambda_i$$

Solution: $\lambda_{i=N} = -\sum_{i<N} \lambda_i$ and $Q_m^* \rho(\vec{R}_m) = \sum_{i<N} \lambda_i \left[S_m(\vec{z}_i) - S_m(\vec{z}_N) \right]$

hence

$$\left[S_m^*(\vec{z}_j) - S_m^*(\vec{z}_N) \right] Q_m^* = \sum_{i<N} \lambda_i \frac{\left[S_m(\vec{z}_i) - S_m(\vec{z}_N) \right] \left[S_m^*(\vec{z}_j) - S_m^*(\vec{z}_N) \right]}{\rho(\vec{R}_m)}$$

$$\tilde{\mathcal{E}}^*(\vec{z}_j) - \tilde{\mathcal{E}}^*(\vec{z}_N)$$

$$\left(\tilde{\mathcal{E}}^*(\vec{z}_j) - \tilde{\mathcal{E}}^*(\vec{z}_N) \right) = \sum_{i<N} \lambda_i \underbrace{\frac{\left[S_m(\vec{z}_i) - S_m(\vec{z}_N) \right] \left[S_m^*(\vec{z}_j) - S_m^*(\vec{z}_N) \right]}{\rho(\vec{R}_m)}}_{H_{ij}}$$

Solution:

$$\tilde{\mathcal{E}}(\vec{z}_j) - \tilde{\mathcal{E}}(\vec{z}_N) = \sum_{i<N} \lambda_i^* \underbrace{\frac{\left[S_m^*(\vec{z}_i) - S_m^*(\vec{z}_N) \right] \left[S_m(\vec{z}_j) - S_m(\vec{z}_N) \right]}{\rho(\vec{R}_m)}}_{H_{ji}}$$

and

$$\lambda_i^* = \left(H^{-1} (\tilde{\mathcal{E}} - \tilde{\mathcal{E}}_N) \right)_i$$

and

$$Q_m = \sum_{z_i} \frac{\lambda_i^* \left[S_m^*(\vec{z}_i) - S_m^*(\vec{z}_N) \right]}{\rho(\vec{R}_m)} \qquad m > 0$$

What is coded?

First construct:

$$S_m(\vec{k}) = \frac{1}{N_{sym}} \sum_{r} e^{i \vec{k} \Gamma_r \vec{R}_m} \qquad S_{m=0} = 1$$

$$\rho_m \equiv \rho(R_m) = \left(1 - c_1 \left(\frac{R_m}{R_1}\right)^2\right)^2 + c_2 \left(\frac{R_m}{R_1}\right)^6$$

$$\left(1 - c_1 \left(\frac{R_m}{R_1}\right)^2\right)^2 + c_2 \left(\frac{R_m}{R_1}\right)^6$$

$$1 - 2c_1 \left(\frac{R_m}{R_1}\right)^2 + c_1^2 \left(\frac{R_m}{R_1}\right)^4 + c_2 \left(\frac{R_m}{R_1}\right)^6$$

Next construct:

$$\tilde{S}_m(\vec{k}_i) = S_m(\vec{k}_i) - S_m(\vec{k}_N) \quad \text{where now: } \tilde{S}_{m=0} = 0$$

$$\Delta\mathcal{E}(k_i) \equiv \mathcal{E}(\vec{k}_i) - \mathcal{E}(\vec{k}_N)$$

$$\frac{-2(0.25)}{R_1^2} = c_1$$

$$c_1 R_m^2 = -0.5$$

$$\frac{(0.25)^2}{R_1^4} = c_2$$

$$h_{ij} = \sum_m \frac{\tilde{S}_m(\vec{k}_i)\, \tilde{S}_m^*(\vec{k}_j)}{\rho_m}$$

$$H_f^m(\vec{k}_j) = \frac{1}{\rho_m} \sum_i \tilde{S}_m^*(k_i)(h^{-1})_{ij}$$

$$Q_m = \sum_{k_j} H_f^m(\vec{k}_j) \cdot \Delta\mathcal{E}(k_j) \qquad \text{for } m > 0$$

$$Q_0 = \mathcal{E}(\vec{k}_N) - \sum_{m>0} S_m(\vec{k}_N)\, Q_m \quad \text{which is equivalent to } \mathcal{E}(\vec{k}_N) = \sum_{m=0}^{N} S_m(\vec{k}_N)\, Q_m = \tilde{\mathcal{E}}(\vec{k}_N)$$

$$\mathcal{E}_{final}(\vec{k}) = \sum_m Q_m S_m(\vec{k})$$

$$\mathcal{E}_{final}(\vec{k}) = \left[\mathcal{E}(\vec{k}_N) - \sum_{m>0} S_m(\vec{k}_N) \sum_j H_f^m(k_j)\, \Delta\mathcal{E}(k_j)\right] + \sum_{m>0} S_m(\vec{k}) \sum_j H_f^m(k_j)\, \Delta\mathcal{E}(k_j)$$

$$\mathcal{E}_{final}(\vec{k}) = \mathcal{E}(\vec{k}_N) + \sum_{m>0} \left[S_m(\vec{k}) - S_m(\vec{k}_N)\right] \sum_j H_f^m(k_j) \left[\mathcal{E}(k_j) - \mathcal{E}(k_N)\right]$$

$$\mathcal{E}_{final}(\vec{k}) = \mathcal{E}(\vec{k}_N) + \underbrace{\sum_{m>0} \left[S_m(\vec{k}) - S_m(\vec{k}_N)\right] \sum_j \frac{1}{\rho_m} \sum_i \left[S_m^*(\vec{k}_i) - S_m^*(\vec{k}_N)\right] (h^{-1})_{ij}}_{K(\vec{k}, \vec{k}_j) \sim \text{ should have eigenvalues } \lesssim 1} \left[\mathcal{E}(k_j) - \mathcal{E}(k_N)\right]$$

$$A_{i\alpha}(k) = \langle \psi_{k_i} | \phi_\alpha \rangle \qquad N_i \geq N_\alpha$$

$$(A^+(k)\, A(k))_{\alpha\beta}$$

$A_{i\alpha} = \mathcal{U}\, \Delta\, V$ and the best unitary trans is $\mathcal{U}_{i\alpha} = (\mathcal{U}\cdot V)_{i\alpha}$

$$H_{\alpha\beta} = \langle \phi_\alpha | \psi_{k_i} \rangle\, \varepsilon_i \langle \psi_{k_i} | \phi_\beta \rangle = (A^+(k)\, \varepsilon_k\, A(k))_{\alpha\beta}$$

But unitary transf: $H_{\alpha\beta}(k) = \left(\mathcal{U}^+(k)\, \varepsilon_k\, \mathcal{U}(k)\right)_{\alpha\beta}$

We want to have $\mathcal{H}_{\alpha\beta}(\vec{k}) = \sum_m e^{+i\vec{k}\vec{R}_m} \mathcal{H}_{\alpha\beta}(\vec{R}_m)$ and we want to determine $\mathcal{H}_{\alpha\beta}(\vec{R}_m)$

The naive choice is $\mathcal{H}_{\alpha\beta}(\vec{R}_m) = \sum_{\vec{k}_i \in mesh} H_{\alpha\beta}(\vec{k}_i)\, e^{-i\vec{k}_i\vec{R}_m}$

But this might not be the best choice. We will instead also optimize smothness

$$R = min = Tr\left(\mathcal{H}^+\mathcal{H} + c_1 \vec{\nabla}_k \mathcal{H}^+ \vec{\nabla}_k \mathcal{H} + c_2 \vec{\nabla}_k^2 \mathcal{H}^+ \nabla_k^2 \mathcal{H} + \cdots\right)$$ with some coefficients $c_1 c_2$

This can be written as $R = Tr\left(\mathcal{H}^+(R_m)\mathcal{H}(\vec{R}_m)(1 + c_1 R_m^2 + c_2 R_m^4 + \cdots)\right)$

and we also want $\mathcal{H}_{\alpha\beta}(\vec{k}_i) \approx H_{\alpha\beta}(\vec{k}_i)$, which can be constrained by Lagrange multipliers:

$$R = \sum_{m>0} Tr\left(\mathcal{H}^+(R_m)\mathcal{H}(\vec{R}_m)(1 + c_1 R_m^2 + c_2 R_m^4 + \cdots)\right) - 2\sum_{i\alpha\beta} \lambda_i^{\alpha\beta}\left(\sum_{R_m} e^{i\vec{k}_i\vec{R}_m}\mathcal{H}_{\beta\alpha}(\vec{R}_m) - H_{\beta\alpha}(k)\right)$$

$$\boxed{\begin{aligned} \frac{1}{2}\frac{\delta R}{\delta \mathcal{H}_{\beta\alpha}(R_m)} &= \mathcal{H}^*_{\beta\alpha}(R_m)\,\rho_m - \sum_i \lambda_i^{\alpha\beta}\, e^{i\vec{k}_i\vec{R}_m} = 0\,; \quad m>0 \\ \sum_i \lambda_i^{\alpha\beta} &= 0 \qquad ; \quad m=0 \end{aligned}}$$

$$\Rightarrow \lambda_0^{\alpha\beta} = -\sum_{i>0} \lambda_i^{\alpha\beta}$$

$$\mathcal{H}_{\alpha\beta}(\vec{R}_m) = \frac{1}{\rho_m}\left(\sum_{i>0} \lambda_i^{\beta\alpha *} e^{-i\vec{k}_i\vec{R}_m} - \lambda_i^{\beta\alpha *} e^{-i\vec{k}_0\vec{R}_m}\right) = \sum_{i>0} \lambda_i^{\beta\alpha *} \frac{[e^{-i\vec{k}_i\vec{R}_m} - e^{-i\vec{k}_0\vec{R}_m}]}{\rho_m}$$

$$H_{\alpha\beta}(k_j) - H_{\alpha\beta}(k_0) = \sum_{R_m}\left(e^{i k_j R_m} - e^{i k_0 R_m}\right)\mathcal{H}_{\alpha\beta}(\vec{R}_m) = \sum_{i>0} \lambda_i^{\beta\alpha *} \sum_{R_m} \frac{[e^{-i\vec{k}_i\vec{R}_m} - e^{-i\vec{k}_0\vec{R}_m}][e^{i k_j R_m} - e^{i k_0 R_m}]}{\rho_m}$$

Define $\boxed{h_{ij} \equiv \sum_{R_m} \frac{[e^{i\vec{k}_i\vec{R}_m} - e^{i\vec{k}_0\vec{R}_m}][e^{-i k_j R_m} - e^{-i k_0 R_m}]}{\rho_m}}$ and $h^+ = h$

Then: $\underbrace{H_{\alpha\beta}(q_j) - H_{\alpha\beta}(q_0)}_{\Delta H_{\alpha\beta}(q_j)} = \sum_{i>0} \lambda_i^{\beta\alpha *} h_{ji}$ and $[h^{-1} \Delta H_{\alpha\beta}]_i = \lambda_i^{\beta\alpha *}$

From: $\mathcal{H}_{\alpha\beta}(R_m)\, \rho_m = \sum_i \lambda_i^{\beta\alpha *} e^{-i \vec{q}_i \vec{R}_m} = \sum_i [h^{-1} \Delta H_{\alpha\beta}]_i \, e^{-i \vec{q}_i \cdot \vec{R}_m}$

Hence:
$$\boxed{\begin{aligned} \mathcal{H}_{\alpha\beta}(R_m) &= \sum_{ij} e^{-i\vec{q}_i \vec{R}_m} \cdot \frac{1}{\rho_m} (h^{-1})_{ij} \cdot \Delta H_{\alpha\beta}(q_j) \\ \mathcal{H}_{\alpha\beta}(R_0 = 0) &= \mathcal{H}_{\alpha\beta}(\vec{q}_0) - \sum_{m>0} \mathcal{H}_{\alpha\beta}(R_m)\, e^{i\vec{q}_0 \vec{R}_m} \end{aligned}}$$

for $m > 0$

which comes from the fact that

$\mathcal{H}_{\alpha\beta}(\vec{q}_0) = \sum_{m=0}^{N} \mathcal{H}_{\alpha\beta}(R_m)\, e^{i\vec{q}_0 \vec{R}_m}$ is the correct average

Here $h_{ij} \equiv \sum_{R_m} \frac{[e^{i\vec{q}_i \cdot \vec{R}_m} - e^{i\vec{q}_0 \vec{R}_m}][e^{-i\vec{q}_j \cdot \vec{R}_m} - e^{-i\vec{q}_0 \vec{R}_m}]}{\rho_m}$

only # irreducible q-points

Recall Wannierization.

1) Find localized projection functions $\varphi_m(\vec{r})$ and compute

$$\langle \psi_{ki} | \varphi_m(\vec{r}) \rangle \equiv \mathcal{U}_{im}$$ Note ψ_{ki} should be u_{ki}

2) Minimize the spread

$$\min = \langle \varphi_n | \psi_{jk} \rangle \langle \psi_{jk} | i \frac{\partial}{\partial k} | \psi_{ik} \rangle \langle \psi_{ik} | \varphi_m(\vec{r}) \rangle$$

3) Find the closest unitary transformation to $\langle \psi_{ki} | \varphi_m(\vec{r}) \rangle = \mathcal{U} s V$

The unitary transformation is $\mathcal{U} \cdot V$

then rewrite

$$H_{mn}(\vec{R}) \approx \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{R}} \langle \varphi_m | \psi_{ki} \rangle \varepsilon_{ik} \langle \psi_{ki} | \varphi_n \rangle$$

$$H_{mn}(\vec{R}) = \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} (\mathcal{U}\cdot V)^{\dagger}_{mi} \, \varepsilon_{ik} \, (\mathcal{U}\cdot V)_{in}$$

unitary hence identical eigenvalues

4) Evaluate $\varepsilon(\vec{k})$ at any point by diagonalizing: $\sum_{\vec{R}} e^{i\vec{k}\vec{R}} H_{mn}(\vec{R})$

We could use the same unitary transformation to produce $\Sigma_{mn}(\vec{R})$ and

evaluate $\Sigma_k(\vec{R})$ by F.T.

The slowest part of the code

$$P_{ij}^{k}(q,\Omega) = N_s \frac{d^3k}{(2\pi)^3} \frac{f(\varepsilon_{k+q\,i}) - f(\varepsilon_{kj})}{i\Omega - \varepsilon_{k+q\,i} + \varepsilon_{kj}} \rightarrow \frac{f(\varepsilon_k) f(-\varepsilon_{k-q})(-2(\varepsilon_{k-q} - \varepsilon_k))}{\Omega_n^2 + (\varepsilon_{k-q} - \varepsilon_k)^2} N_s \frac{d^3k}{(2\pi)^3}$$

To calculate Σ_x we only need $\Sigma_{ki} = \sum_{j,q,\alpha} |M_{kq}(\alpha,ij)|^2 f(\varepsilon_{kj})\, v_{q\alpha}$

To calculate ε we need the off-diagonal matrix elements in α,β product basis, i.e.,

$$\sqrt{v}\, P_{q\omega} \sqrt{v} = \sum_{k,ij} M_{kq}^*(\alpha,ij)\, P_{ij}^{k}(q,\omega)\, M_{kq}(\beta,ij)$$

We now use tetrahedra only for the low energy bands, and for high energy band we use the discrete sum:

$$\sqrt{v}\, P_{q\omega} \sqrt{v} = \sum_{\substack{k,ij \\ k \text{ occupied} \\ k-q \text{ empty}}} M_{kq}^*(\alpha,ij) \frac{(-2(\varepsilon_{k-q} - \varepsilon_k)) N_s}{\Omega_n^2 + (\varepsilon_{k-q} - \varepsilon_k)^2} M_{kq}(\beta,ij)$$

At low energy we have to properly integrate $\int \frac{f(\varepsilon_k) f(-\varepsilon_{k-q})(-2(\varepsilon_{k-q} - \varepsilon_k))}{\Omega_n^2 + (\varepsilon_{k-q} - \varepsilon_k)^2} N_s \frac{d^3k}{(2\pi)^3}$ over tetrahedra.

We first calculate $M_{kq}^*(\alpha,ij)\, P_{ij}^{k}(q,\omega) \equiv R_k^{q\omega}(\alpha,ij)$ and then we matrix multiply

$$\sum_k \sum_{ij} R_k^{q\omega}(\alpha,ij) \cdot M_{kq}^T(ij,\beta) = \sqrt{v}\, P_{q\omega} \sqrt{v}$$

even after a lot of optimization, this matrix product is still the slowest part of the code, because α,β are large basis $\sim 10^3$ and ij is similarly 10^3 or more.

The slowest part of the code

1) Obtain Lindhard formula in band basis using tetrahedron integration. Has been sufficiently optimized now

$$P_{ij}^{k}(q,i\Omega) = \frac{f(\varepsilon_{k+q\,i}) - f(\varepsilon_{kj})}{i\Omega - \varepsilon_{k+q\,i} + \varepsilon_{kj}} \Rightarrow$$

transform to svd

$$\boxed{P_{ij}^{k}(q,l) = \int P_{ij}^{k}(q,i\Omega)\, U_l(i\Omega)\, d\Omega}$$

2) Transformed into product basis

$$(V_q P_q)_{\alpha\beta}(q,i\Omega) = \frac{1}{V_{cell}} \sum_{ij,k} M_{kq}^{*}(\alpha,ij)\, P_{ij}^{k}(q,i\Omega) \cdot M_{kq}(\beta,ij) \Rightarrow \boxed{(V_q P_q)_{\alpha\beta}(q,l) = \frac{1}{V_{cell}} \sum_{ij,k} M_{kq}^{*}(\alpha,ij) \cdot P_{ij}^{k}(q,l) \cdot M_{kq}(\beta,ij)}$$

$$(V_q P_q)_{\alpha\beta}(q,i\Omega) = \sum_l (V_q P_q)_{\alpha\beta}(q,l)\, U_l(i\Omega)$$

$$W_\Omega = V_q (1 - V_q P_{q\Omega})^{-1}$$

This is for the slowest part since number of bands $i \otimes j$ is of the order 4000

α index is of the order 300

$\underbrace{M^{*} \cdot \chi^{\Omega}}_{} \cdot M$ Estimate time

for Li : $i \otimes j \sim 86$

$\alpha \sim 160$

$$N_\Omega (N_\alpha N_{ij} + N_\alpha^2 N_{ij}) \sim N_\Omega \cdot C \times (300)^2 \times (4000) = N_\Omega \cdot C \cdot 3.6 \times 10^8$$

Alternative: $K_{l\Omega} \chi^{\Omega} = \chi_l$ only $N_l \sim 20$ values

$M^{*} \cdot \chi_l \cdot M = (VP)_l$ $\quad (VP)_l \cdot K_{l\Omega}$

$C \cdot N_l \cdot (N_\alpha^2 N_{ij})$ $\quad C \cdot N_\alpha^2 N_l N_\Omega$

example: $N_\Omega = 100$; $N_l = 20$

original: $C\, N_\Omega N_\alpha^2 N_{ij}$ $\quad 3.6 \times 10^{10}$

alternative: $C\, N_l N_\alpha^2 N_{ij} + C\, N_\alpha^2 N_l N_\Omega$ $\quad 0.72 \cdot 10^{10} + 0.018 \times 10^{10} = 0.74 \times 10^{10}$

3)

$$\varepsilon(q,i\Omega) = (1 - V_q P_q)^{-1}$$

SVD

What we have in svdwrap:

Inverse Fourier: $G(\tau)=\frac{1}{\beta}\sum_{i\omega} e^{-i\omega\tau} G(i\omega)$ subtract tail and sum:

Fourier Fermion: $G(i\omega)=\int_0^\beta e^{i\omega\tau} G(\tau)\, d\tau$ using spline

Tan mesh ω: Tan(ω-dh, x_0, L, $N\omega$)

$$G(\tau)=\int \frac{dx}{\pi} f(-x)\, e^{-x\tau}\, \mathrm{Im}\, G(x)$$

$$K(\tau,x)=\frac{e^{-x\tau}}{e^{-\beta x}+1}=\frac{e^{\beta\frac{x}{2}-x\tau}}{2\,\mathrm{ch}\frac{\beta x}{2}}=\frac{e^{-\frac{\beta x}{2}\left(\frac{2\tau}{\beta}-1\right)}}{2\,\mathrm{ch}\frac{\beta x}{2}}\;;\quad K(\tau_j,x_i)\,\Delta x_i\,\sqrt{\Delta\tau_j}$$

$$\sqrt{\Delta\tau_j}\,(\Delta x_i)\cdot K(\tau_j,x_i)=\mathcal{U}(\tau_j)\,S_\ell\,V(x_i)\;;\quad \mathcal{U}(\tau_j)\to\mathcal{U}(\tau_j)\frac{1}{\sqrt{\Delta\tau_j}}$$

Spline $\mathcal{U}_\ell(\tau_j)\to\tilde{\mathcal{U}}_\ell(\tau)$ $\qquad \int\tilde{\mathcal{U}}_\ell(\tau)\,\tilde{\mathcal{U}}_{\ell'}(\tau)\,d\tau=O_{\ell\ell'}=T_{\ell m}\,O_m\,T_{\ell' m}$

$$\sum_\ell \tilde{\mathcal{U}}_\ell(\tau)\underbrace{\left(T\frac{1}{\sqrt{O}}T^{+}\right)_{\ell m}}_{\mathrm{Soul}(m,\ell)}=\tilde{\mathcal{U}}_m^{\,new}(\tau)$$

$$G(\tau)=-\int\frac{dx}{\pi}\, n(-x)\, e^{-x\tau}\,\mathrm{Im}\, G(x)$$

$$K(\tau,x)=-\frac{e^{-x\tau}}{e^{-\beta x}-1}=\frac{e^{-x\tau+\frac{\beta x}{2}}}{2\,\mathrm{sh}\frac{\beta x}{2}}=\frac{e^{-\frac{\beta x}{2}\left(\frac{2\tau}{\beta}-1\right)}}{2\,\mathrm{sh}\frac{\beta x}{2}}$$

$$G(i\omega)=\int\frac{A(x)\,dx}{i\omega-x}\;;\quad K(i\omega,x)=\frac{1}{i\omega-x}\;;\quad K(i\omega_j,x_i)=\frac{\Delta x_i\sqrt{\Delta\omega_j}}{i\omega_j-x_i}$$

$$\sqrt{\Delta\omega_j}\,G(i\omega_j)=\sum_i K(i\omega_j,x_i)\,A(x_i)=\tilde{\mathcal{U}}_\ell(i\omega_j)\,S_\ell\,V_\ell(x_i)\;;\quad \mathcal{U}_\ell(i\omega_j)=\tilde{\mathcal{U}}_\ell(i\omega_j)/\sqrt{\Delta\omega_j}$$

$$\sum_j\tilde{\mathcal{U}}^*_\ell(i\omega_j)\,\tilde{\mathcal{U}}_{\ell'}(i\omega_j)=\delta_{\ell\ell'}\;\Rightarrow\;\sum_j\mathcal{U}_\ell(i\omega_j)\,\mathcal{U}_{\ell'}(i\omega_j)\,\Delta\omega_j=\delta_{\ell\ell'}\;\Rightarrow\;\int d\omega_j\,\mathcal{U}_\ell(i\omega_j)\,\mathcal{U}_{\ell'}(i\omega_j)=\delta_{\ell\ell'}$$

$$\underline{\chi'}+i\chi''=+\frac{1}{\pi}\int\frac{\mathrm{Im}\,\chi''(x)\,(x+i\omega)}{(x-i\omega)(x+i\omega)}=\underline{\frac{1}{\pi}\int\frac{\mathrm{Im}\,\chi(x)\,x}{x^2+\omega_m^2}}+\frac{i\omega_m}{\pi}\int\frac{\mathrm{Im}\,\chi(x)}{x^2+\omega_m^2}$$

$$K(i\omega_m,x)=\frac{1}{\pi}\frac{x}{x^2+\omega_m^2}\,\Delta x\,\sqrt{\Delta\omega_m}=\underset{\uparrow}{\tilde{\mathcal{U}}_\ell(\omega_m)}\,S_\ell\,V_\ell(x)$$

$$\sum_m\tilde{\mathcal{U}}_\ell(\omega_m)\,\tilde{\mathcal{U}}^*_\ell(\omega_m)=1\qquad\qquad \frac{\tilde{\mathcal{U}}_\ell(\omega_m)}{\sqrt{\Delta\omega_m}}=\mathcal{U}_\ell(\omega_m)$$

$$\mathrm{Rcw}(ij, z, i\Omega_m) = \sum_{\ell} \mathcal{U}_\ell(i\Omega_m)\, \overline{\mathrm{Rcw}}(ij, z, \ell) \quad \Big/ \sum_{m} \mathcal{U}_\ell(i\Omega_m)\, \Delta\Omega_m$$

$$\sum_{m} \mathrm{Rcw}(ij, z, i\Omega_m)\, \mathcal{U}_\ell(i\Omega_m)\, \Delta\Omega_m = \overline{\mathrm{Rcw}}(ij, z, \ell)$$

$$\chi_{\alpha\beta}(\ell) = \sum_{ij} m(\alpha, ij) \cdot \overline{\mathrm{Rcw}}(ij, \ell) \cdot m(ij, \beta)$$

$$\chi_{\alpha\beta}(i\Omega_m) = \sum_{\ell} \chi_{\alpha\beta}(\ell)\, \mathcal{U}_\ell(i\Omega_m)$$

$$\chi(\alpha\beta, \ell)\, \mathcal{U}_\ell(i\Omega_m)$$

$$\uparrow$$

$$N_\alpha^2 \cdot N_\ell \cdot N_\Omega$$

$$\langle \vec r | \Gamma \vec G\rangle = \langle \vec R^{-1}\vec r + \vec T | \vec G\rangle = e^{i\vec G \vec T} \langle \vec r | R\vec G\rangle$$

$$\langle \vec r | \Gamma^{-1}\vec G\rangle = \langle R(\vec r - \vec T) | \vec G\rangle = e^{-(R\vec T)\cdot G}\langle \vec r | R^{-1}\vec G\rangle = e^{T\cdot(R^{-1}G)}\langle \vec r | R^{-1}\vec G\rangle$$

$$\langle lm | i k\rangle = \int Y^*_{lm}(\hat r)\, u_l(r)\, \chi_{ik}(\vec r)\, d^3r$$

$$\langle lm | R_0 T_{T_1} \Gamma_n \Gamma_\alpha | i k_{IBZ}\rangle$$

final local rotation. Not needed here

shift the origin from the first to the current atom

rotij tauij

tmat, tau from IBZ to RBZ

tmat = 1, tau = 0

phase: G·tauij(:, latom) + rotij(:,:, latom)·$\vec G$·pos(:, lfirst)

rotation: crotloc(:,:)·rotij(:,:, latom)·$\vec G$

$$\langle \vec G | \Gamma_\alpha | \vec k_{ir}\rangle = \qquad e^{i(\vec k + \vec G)\cdot T_{isym}}$$

$$\Gamma_\alpha \vec r = R^{-1}\vec r + \vec t$$

$$\vec k\, \Gamma_\alpha \vec r = \vec k(R^{-1}\vec r + \vec t) = (R\cdot\vec k)\vec r + \vec k\cdot\vec t$$

$\Gamma_\alpha \vec k =$ $R\cdot\vec k$, phase $\vec k\cdot\vec t$

tmat(:,:,N) tau(:,N)

Currently we have: $e^{-2\pi i(\vec{k}+\vec{G})\cdot\vec{\tau}_{isym}}$

$\uparrow$ tau

kcar: $\begin{pmatrix}\frac{2\pi}{a} & \frac{2\pi}{b} & \frac{2\pi}{c}\end{pmatrix}\cdot\vec{k}$

kpg: $\begin{pmatrix}\frac{2\pi}{a} & \frac{2\pi}{b} & \frac{2\pi}{c}\end{pmatrix}(\vec{k}+\vec{G}) = (\vec{k}_c+\vec{G}_c)$

r2: $|kpg|^2$

$rotloc(iat,:,:)\cdot\left[(\vec{k}_c+\vec{G}_c)\cdot trotij(idf,:,:)\right]$

timat[isym] + tau[isym]

kcar timat[isym]

$$i^l \frac{4\pi}{\sqrt{V_{ol}}} R_{MT}^2 \times e^{i2\pi(\vec{k}+\vec{G})\cdot pos(idf)}\; Y_{lm}\left(rotloc(iat)\cdot rotij(idf,)(\vec{k}_c+\vec{G}_c)\right)\cdot\begin{pmatrix}a_l\\ b_l\\ c_l\end{pmatrix}$$

$\uparrow$

$j_{lm}\left((\vec{k}_c+\vec{G}_c)R_{MT}\right)$

?

$$A_{iG}\, e^{-2\pi i(\vec{k}+\vec{G})\cdot tau(isim,:)}\cdot Q_{lm\,G,\,alm}$$

---

dmft1: $K_n = BR1\cdot(\vec{k}+\vec{G}) \to \vec{k}_c+\vec{G}_c$

$aK_n = |K_n|^2 \to j_{lm}\left(|\vec{k}_c+\vec{G}_c| R_{MT}\right)$

$gind(ig)=ig$

isym: symmetry operation index

$\frac{4\pi R_{MT}^2}{\sqrt{V_{ol}}}$

$crotloc(:,:,lcore,icore)\cdot BR1$

in semicartesian

$$Y_{lm}\left(crotloc[l,iat]\cdot BR1\cdot rotij[latom]\cdot timat[isym]\cdot(\vec{k}+\vec{G})\right)\times$$

$j_{lm}\left(|\vec{k}_c+\vec{G}_c| R_{MT}\right)$

$\downarrow$

$$\times e^{2\pi i\left(\underbrace{(pos[latom]\cdot rotij[idf]+tauij[latom])\cdot timat[isym]}_{pos[idf]+\tilde{R}_{latt}}\cdot(\vec{k}+\vec{G}) + tau[isym]\cdot(\vec{k}+\vec{G})\right)}\begin{pmatrix}a_l\\ b_l\\ c_l\end{pmatrix}$$

dmft: $timat[isym]\cdot pos[latom] + tau[isym] = pos[idf]$

gw: $\begin{pmatrix}timat[isym]\\ \parallel\\ trotij[latom]\end{pmatrix} pos[latom] + \begin{pmatrix}tau[isym]\\ \parallel\\ tauij[latom]\end{pmatrix} = pos[latom]$

$$\text{tizmat}^T = \text{rbas} * \text{timat}^T * \text{gbas} = BR2^{-1} \cdot \text{timat}^T \cdot BR2$$

$$(i_0', i_1', i_2') = \text{izmat} \cdot (i_0, i_1, i_2)$$

$$r_{in} = \text{r2icartes}(i_0, i_1, i_2)$$
$$r2 = \text{r2icartesian}(i_0', i_1', i_2')$$

$$\text{r2icartesian} = \begin{cases} \text{ortho or CxZ} : & BR2 \cdot \frac{a_i}{2\pi} \\ \text{else} : & Id \end{cases}$$

$$\text{izmat} = \begin{cases} \text{ortho}: & BR2^{-1} \cdot \text{imat} \cdot BR2 \\ \text{else} & \text{imat} \end{cases}$$

ORTHO:

$$BR2(i_0', i_1', i_2') = \text{imat} \cdot BR2\,(i_0, i_1, i_2)$$

$$\frac{a_i}{2\pi} BR2(i_0', i_1', i_2') = \frac{a_i}{2\pi} \cdot \text{imat} \cdot BR2\,(i_0, i_1, i_2)$$
$$r \qquad \approx \qquad r_{in}$$

GW: $$BR2 \equiv \begin{pmatrix} 0 & \frac{2\pi}{a} & \frac{2\pi}{a} \\ \frac{2\pi}{b} & 0 & \frac{2\pi}{b} \\ \frac{2\pi}{c} & \frac{2\pi}{c} & 0 \end{pmatrix}$$

$\boxed{\text{BR2 in GW and DMFT is the same}}$

$$gbas = \frac{1}{2\pi} \cdot BR2$$

k-point generated by : $\underbrace{rbas\ timat^T \cdot gbas}_{izmat} \cdot (i_1\ i_2\ i_3)$

$$rbas = gbas^{-1}$$

trotij , tauij

$$tizmat = rbas \cdot timat \cdot gbas$$

DMFT: $$BR2 \equiv \begin{pmatrix} 0 & \frac{2\pi}{a} & \frac{2\pi}{a} \\ \frac{2\pi}{b} & 0 & \frac{2\pi}{b} \\ \frac{2\pi}{c} & \frac{2\pi}{c} & 0 \end{pmatrix} = \begin{pmatrix} \frac{2\pi}{a} & 0 & 0 \\ 0 & \frac{2\pi}{b} & 0 \\ 0 & 0 & \frac{2\pi}{c} \end{pmatrix} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

$$BR1 \equiv \begin{pmatrix} \frac{2\pi}{a} & 0 & 0 \\ 0 & \frac{2\pi}{b} & 0 \\ 0 & 0 & \frac{2\pi}{c} \end{pmatrix}$$

If ortho = true then $BR1 \approx \text{Identy} \cdot \frac{2\pi}{a}$

$rbas\ (i_1 i_2 i_3) \cdot gbas\ \frac{1}{2\pi}$

$tizmat = (rbas \cdot timat^T \cdot gbas)^T$

$izmat^T \cdot (i_1, i_2, i_3) = rbas \cdot imat \cdot gbas\ (i_1\ i_2\ i_3)$

$$Sk\_ = \begin{cases} \text{ortho:} & \left(\frac{2\pi}{a} k_x,\ \frac{2\pi}{b} k_y,\ \frac{2\pi}{c} k_z\right) \\ \text{else:} & BR2 \cdot (k_x, k_y, k_z) \end{cases}$$

$$Sb = BR2 \cdot (i_1, i_2, i_3) + Sk\_$$

$$RK(i) = |\ BR2 \cdot (i_1 i_2 i_3) + Sk\_\ |$$

$$KN(3,i) = BR2 \cdot (i_1 i_2 i_3) + Sk\_$$

$$KZZ(3,i) = \begin{cases} \text{ortho :} & \left(BR2 \cdot (i_1, i_2, i_3) + Sk\_\right) / \left(\frac{2\pi}{a_i}\right) - (k_x, k_y, k_z) \equiv \frac{2\pi}{a_i} \cdot BR2 \cdot (i_1\ i_2\ i_3) \\ \text{else :} & \begin{cases} CXZ: & (i_1 + i_3,\ i_2,\ i_1 - i_3) \\ \text{else:} & (i_1,\ i_2\ \ i_3) \end{cases} \end{cases}$$

Pade

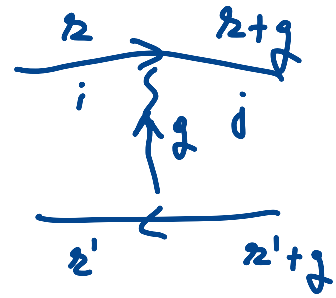
$$P(z) = \frac{\sum_{i=1}^{r} a_i z^{i-1}}{\sum_{i=1}^{r} b_i z^{i-1} + z^r} = \frac{(a_1, a_2, \dots a_r)\cdot(1, z, z_1^2 \dots z^{r-1})}{(b_1, b_2, \dots b_r)\cdot(1, z_1 z^2 \dots z^{r-1}) + z^r} \sim \frac{a_r}{z} + \frac{1}{z^2}\left(a_{r-1} - a_r b_r\right)$$

$$\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_r \\ b_1 \\ b_2 \\ \vdots \\ b_r \end{bmatrix} \qquad \tilde{\mathcal{G}} = \begin{bmatrix} \mathcal{G}_1 & (i\omega_1)^r \\ \mathcal{G}_2 & (i\omega_2)^r \\ \vdots & \\ \mathcal{G}_{2r} & (i\omega_{2r})^r \end{bmatrix}$$

$$X = \begin{bmatrix} 1 & i\omega_1 & \cdots & (i\omega_1)^{r-1} & -\mathcal{G}_1 & \cdots & -\mathcal{G}_1^{r-1} \\ 1 & i\omega_2 & & (i\omega_2)^{r-1} & -\mathcal{G}_2 & & -\mathcal{G}_2^{r-1} \\ 1 & \vdots & & \vdots & & & \vdots \\ 1 & i\omega_{2r} & & (i\omega_{2r})^{r-1} & -\mathcal{G}_{2r} & & -\mathcal{G}_{2r}^{r-1} \end{bmatrix}$$

$$\begin{bmatrix} a \\ b \end{bmatrix} = X^{-1}\cdot \mathcal{G}$$

$\frac{a_1}{b_1 + z}$ 2 frequencies $\rightarrow N = 2$



$$V_{\alpha\beta}(q)\cdot U_{\beta\ell} = U_{\alpha\ell}\, v_\ell \Rightarrow U^{\dagger}_{\ell\alpha} V_{\alpha\beta}(q)\, U_{\beta\ell} = v_\ell$$

$$V_{\alpha\beta} = U\, v_\ell\, U^{\dagger}$$

$$\left(U\sqrt{V}\,U^{\dagger}\right)_{\alpha\beta} \langle \chi_\beta | \psi_{ki}\, \psi^{*}_{k+q\,j}\rangle$$

$$\sqrt{v_\ell}\left(U^{\dagger}\right)_{\ell\beta} \langle \chi_\beta | \psi_{ki}\, \psi^{*}_{k+q\,j}\rangle$$

Γ − X gap. Real gap is smaller

$a = 10.23543$

4x4x4 No LO: 1.131 eV

2 LO: 1.162 eV (1 LO in product)

5 LO: 1.183 eV (1 LO in product)

GW⁰: 1.166 eV with 5LO

RKmax=7

$a = 10.262536$

No LO: 1.141 eV

2 LO: 1.072 eV

5 LO: 1.094 eV (1.081 eV)

larger mixed basis: 1.093 eV

5LO, RKmax=8, 1.123 eV

5LO, RKmax=8, Lmax=5; 1.126 eV

4x4x4: No LO: 1.141 eV

6x6x6: No LO: 1.107 eV

8x8x8: No LO: 1.01 eV

$a = 10.262536$

K = 4x4x4; 5 Local orbitals

	X − Γ G⁰W⁰	Gap G⁰W⁰	X−Γ GW⁰	Gap GW⁰	mbsize P.B. size
5LO, RKmax=7, Lmax=3, MB_emax=20:	1.094 eV	0.947 eV	1.143 eV	0.978 eV	545
5LO, RKmax=7, Lmax=3:	1.093 eV	0.953 eV	1.166 eV	1.02 eV	1377
5LO, RKmax=8, Lmax=3:	1.123 eV	0.983 eV	1.2 eV	1.06 eV	1407
5LO, RKmax=8, Lmax=5:	1.126 eV	0.99 eV	1.203 eV	1.06 eV	2019

0.578

0.579 0.612 eV

$a = 10.262536$

K=4x4x4; No local orbitals

RKmax = 7, MB_emax=20:

RKmax = 9, MB_emax=150: 0.44 eV

min 1.48 X: 1.57539

	LDA Gap	LDA X−Γ	GGA Gap	X−Γ
KS: Default W2k:	0.472 eV	0.609 eV	0.572	0.712
5LO, RKmax=8:	0.444 eV	0.579 eV	0.573	0.712
Default RKmax=9:			0.573	
RKmax=9 RMT=2.1			0.574	

Silicon

$a = 10.262536\, a_B$; GGA

$K = 4\times4\times4$;

	X−Γ G^0W^0	Gap G^0W^0	X−Γ GW^0	Gap GW^0	GGA	Mbsize P.B. size	#evals > 0.1H
No LO's, RKmax = 9, Lmax = 3, Mb_emax = 20	1.201 eV	1.063 eV	1.267 eV	1.128 eV	0.573 eV	437	405
SLO, RKmax = 8, Lmax = 3, Mb_emax = 20	1.224 eV	1.090 eV	1.292 eV	1.158 eV	–//–	575	466
SLO, RKmax = 8, Lmax = 3, Mb_emax = ∞	1.224 eV	1.090 eV	1.292 eV	1.158 eV	–//–	1407	544
SLO, RKmax = 8, Lmax = 5, Mb_emax = 20	1.227 eV	1.094 eV	1.295 eV	1.162 eV	–//–	1013	820
SLO, RKmax = 8, Lmax = 5, Mb_emax = ∞	1.227 eV	1.094 eV	1.295 eV	1.162 eV	–//–	2019	958
Blaha, $a = 10.235430\, a_B$		1.12 eV		1.19 eV			
Bluegel		1.11 eV					
Experiment	1.25 eV	1.17 eV	1.25 eV	1.17 eV			

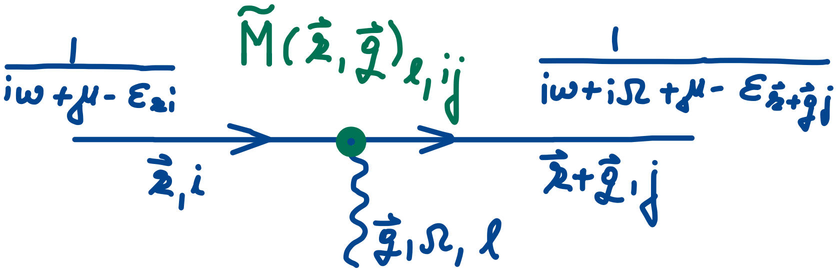
Ne

KS: 3.192 eV

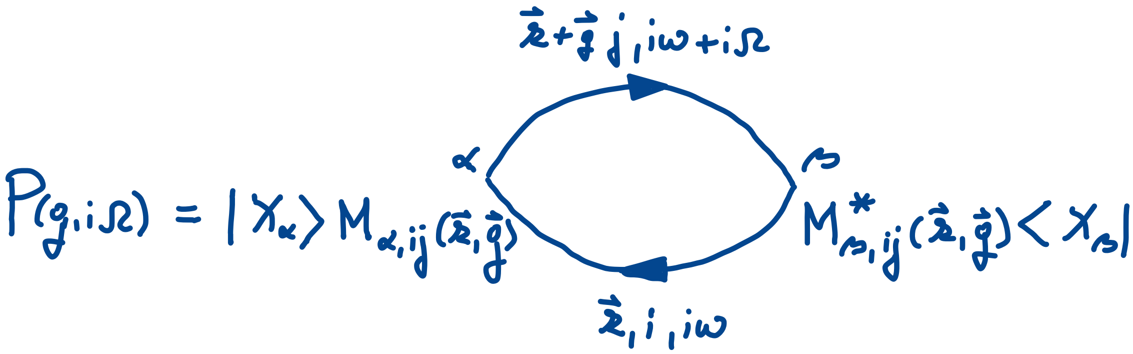
10×10×10 : 3.085 eV

12×12×12 : 3.146 eV

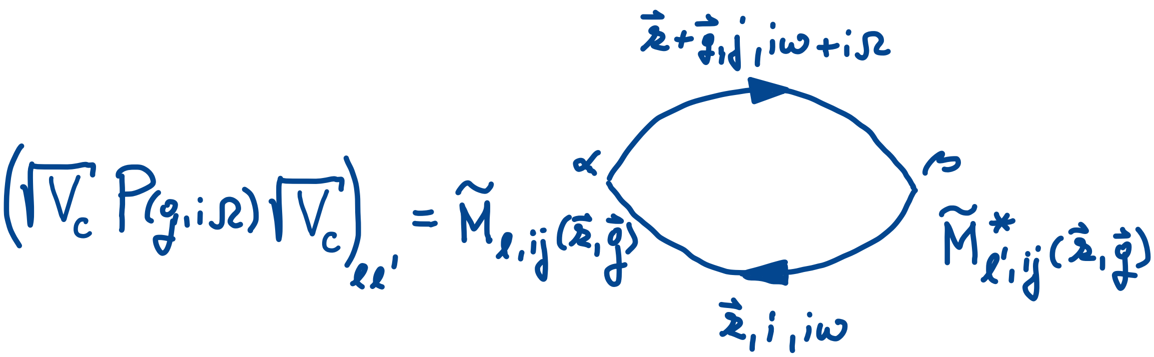
$\sim$ 3.10 eV



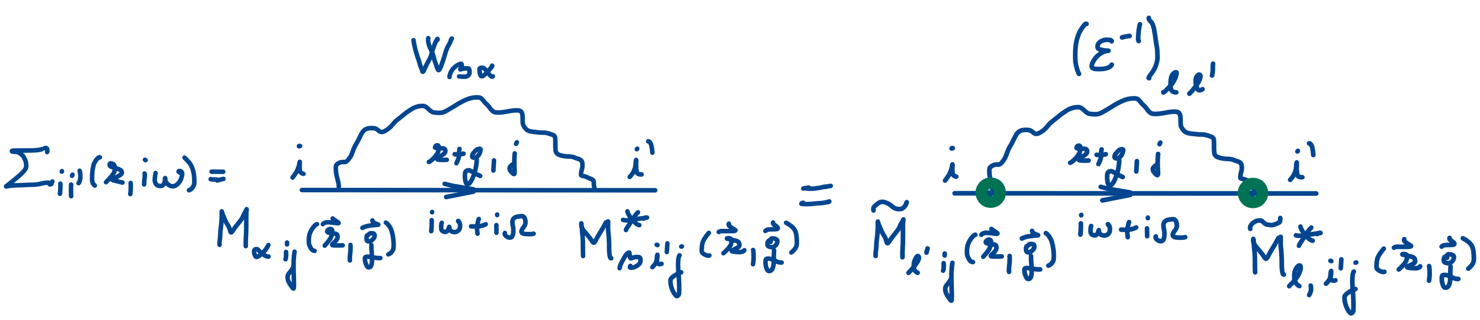
$\frac{1}{i\omega+\mu-\varepsilon_{ki}}$
$\tilde{M}(\vec{k},\vec{q})_{l,ij}$
$\frac{1}{i\omega+i\Omega+\mu-\varepsilon_{\vec{k}+\vec{q}j}}$
$\vec{k},i$
$\vec{k}+\vec{q},j$
$\vec{q},\Omega,l$



$\vec{k}+\vec{q}\,j,i\omega+i\Omega$
$P(q,i\Omega) = |\chi_\alpha\rangle M_{\alpha,ij}(\vec{k},\vec{q})$
α
β
$M^*_{\beta,ij}(\vec{k},\vec{q})\langle\chi_\beta|$
$\vec{k},i,i\omega$



$\vec{k}+\vec{q},j,i\omega+i\Omega$
$\left(\sqrt{V_c}\,P(q,i\Omega)\sqrt{V_c}\right)_{ll'} = \tilde{M}_{l,ij}(\vec{k},\vec{q})$
α
β
$\tilde{M}^*_{l',ij}(\vec{k},\vec{q})$
$\vec{k},i,i\omega$



$W_{\beta\alpha}$
$\Sigma_{ii'}(k,i\omega) =$
i
$k+q,j$
i'
$M_{\alpha ij}(\vec{k},\vec{q})$
$i\omega+i\Omega$
$M^*_{\beta i'j}(\vec{k},\vec{q})$
$=$
$(\varepsilon^{-1})_{ll'}$
i
$k+q,j$
i'
$\tilde{M}_{l' ij}(\vec{k},\vec{q})$
$i\omega+i\Omega$
$\tilde{M}^*_{l,i'j}(\vec{k},\vec{q})$

- Write something about speedup.
- Self energy at the fermi level.

$$G = \frac{1}{\omega + \mu - \varepsilon_k^0 - \Sigma(\omega) - V_{xc}} = \frac{1}{\omega + \mu - \varepsilon_k - \Sigma(\varepsilon_k) - V_{xc} - \frac{d\Sigma}{d\omega}(\varepsilon_k - \mu)(\omega - \varepsilon_k + \mu)}$$

$$\frac{1}{(\omega + \mu - \varepsilon_k)\left(1 - \frac{d\Sigma}{d\omega}(\varepsilon_k - \mu)\right) - \Sigma(\varepsilon_k - \mu)} \approx \boxed{\frac{1}{\omega - \varepsilon_k^0 - Z_k(\Sigma(\varepsilon_k) - V_{xc})}}$$

$$Z_k = \frac{1}{1 - \frac{d\Sigma}{d\omega}(\varepsilon_k)}$$

$$\varepsilon_k = \varepsilon_k^0 + Z_k(\Sigma(\varepsilon_k) - V_{xc})$$

$$\delta = \Sigma(\varepsilon_k) - V_{xc} + \varepsilon_k^0 - \varepsilon_k$$

$$\delta = Z_k(\Sigma(\varepsilon_k) - V_{xc}) + \varepsilon_k^0 - \varepsilon_k$$

$$\varepsilon_k^{new} = \begin{cases} \varepsilon_k^0 + \Sigma(\varepsilon_k) - V_{xc} \\ \varepsilon_k^0 + Z_k(\Sigma(\varepsilon_k) - V_{xc}) \end{cases}$$

$$\frac{1}{\underline{\omega} - \varepsilon_k^0 - \Sigma(k_F, 0) - \underline{\frac{d\Sigma}{d\omega}\omega} - \frac{d\Sigma}{dk}(k - k_F)}$$

$$\omega\left(1 - \frac{d\Sigma}{d\omega}\right) - \frac{(k - k_F)k_F}{m} - \frac{d\Sigma}{dk}(k - k_F) - \Sigma(k_F, 0)$$

$$\frac{\omega}{z} - \frac{(k - k_F)k_F}{m}\left[1 + \frac{m}{k_F}\frac{d\Sigma}{dk}\right]$$

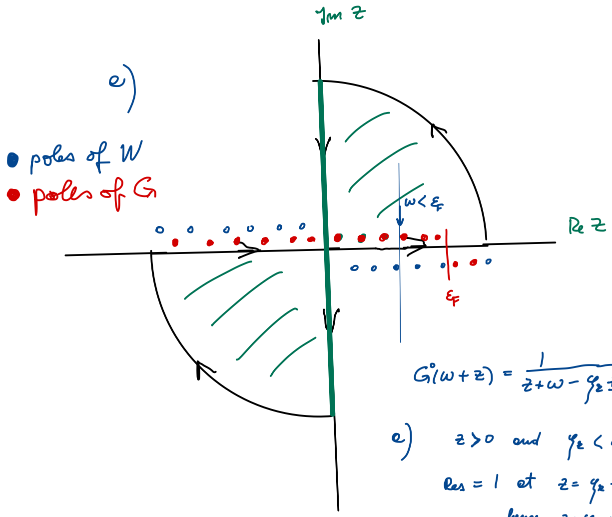
$$\omega - \underbrace{\frac{(k - k_F)k_F}{m} z\left[1 + \frac{m}{k_F}\frac{d\Sigma}{dk}\right]}$$

$$(k - k_F)\frac{k_F}{m^*} = (k - k_F)\frac{k_F}{m} z\left[1 + \frac{m}{k_F}\frac{d\Sigma}{dk}\right]$$

$$\frac{1}{m^*} = \frac{1}{m} z\left[1 + \frac{m}{k_F}\frac{d\Sigma}{dk}\right]$$

$$\frac{m^*}{m} = \frac{1}{z\left[1 + \frac{m}{k_F}\frac{d\Sigma}{dk}\right]}$$

The contour deformation technique



$G^0(\omega+z) = \dfrac{1}{z+\omega-\varepsilon_k \pm i\delta_k}$

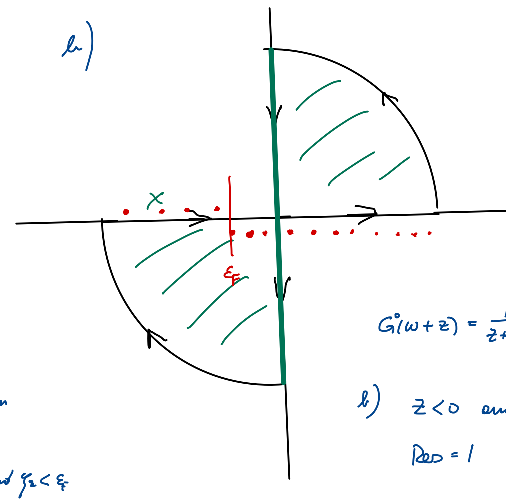
a) $z>0$ and $\varepsilon_k < \varepsilon_F$ then

Res $=1$ at $z=\varepsilon_k-\omega$

hence $z=\varepsilon_k-\omega>0$ and $\varepsilon_k<\varepsilon_F$

hence $\omega<\varepsilon_k<\varepsilon_F$

Integral orientation adds $+1$



$G^0(\omega+z) = \dfrac{1}{z+\omega-\varepsilon_k \pm i\delta_k}$

b) $z<0$ and $\varepsilon_k > \varepsilon_F$ then

Res $=1$ at $z=\varepsilon_k-\omega$

hence $\varepsilon_k-\omega<0$ and $\varepsilon_k>\varepsilon_F$

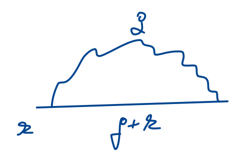
hence $\varepsilon_F<\varepsilon_k<\omega$

Integral orientation adds -1

$$\Sigma_k(\omega) = -\int_{-\infty}^{\infty}\frac{dx}{2\pi i} W_q(x)\, G^0_{k+q}(x+\omega) = \underbrace{-\oint \frac{dz}{2\pi i} W_q(z)\, G^0_{k+q}(z+\omega)}_{-\sum \text{Res}\{W(z)G^0(z+\omega),\, z\}} + \underbrace{\int \frac{dz}{2\pi i} W(z)\, G^0(z+\omega)}_{\text{Imaginary axis}}$$

$$-\sum \text{Res}\{W(z)G^0(z+\omega),\, z\} \;\to\; -\sum_{\omega<\varepsilon_k<\varepsilon_F} W(\varepsilon_k-\omega) \qquad + \sum_{\varepsilon_F<\varepsilon_k<\omega} W(\varepsilon_k-\omega)$$

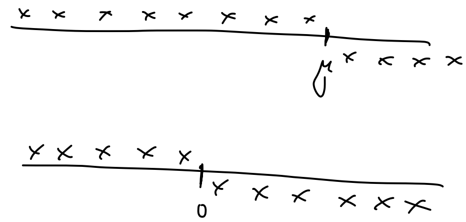
$$\underbrace{+\int_{\infty}^{-\infty} \frac{d\omega' i}{2\pi i} W(i\omega')\, G^0(\omega+i\omega')}_{-\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi} W(i\omega')\, G^0(\omega+i\omega')}$$



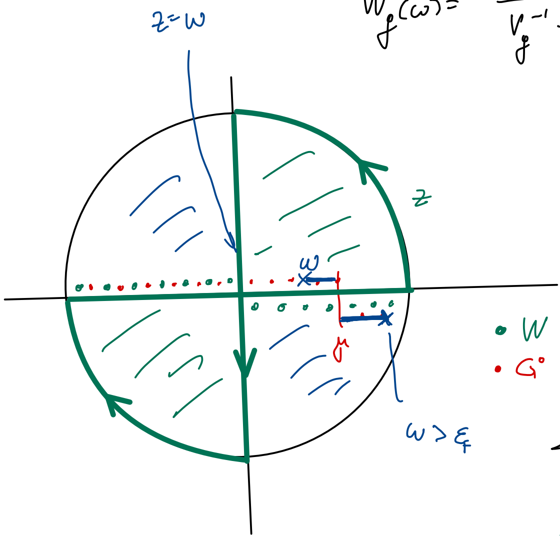
$$\Sigma_k(\omega) = -\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi} W_q(i\omega')\, G^0_{k+q}(\omega+i\omega') - \sum_{\omega<\varepsilon_{k+q}<\varepsilon_F} W(\varepsilon_{k+q}-\omega) + \sum_{\varepsilon_F<\varepsilon_{k+q}<\omega} W(\varepsilon_{k+q}-\omega)$$

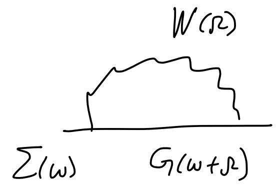
$$\Sigma(i\omega) = -\frac{1}{\beta}\sum_{i\Omega} W(i\Omega)\frac{1}{i\omega-i\Omega-\varepsilon_{k-p}} = -\int_{-\infty}^{\infty}\frac{d\Omega}{2\pi} W(i\Omega)\frac{1}{i\omega-i\Omega-\varepsilon_{k-q}} = -\int_{-\infty}^{\infty}\frac{d\Omega}{2\pi} W(i\Omega)\frac{1}{i\Omega+i\omega-\varepsilon_{k-q}}$$

Time ordered $\quad G^0_{\varepsilon}(\omega) = \dfrac{1}{\omega + \mu - \varepsilon_{\varepsilon} + i\delta\, \mathrm{sgn}(\varepsilon_{\varepsilon} - \mu)}$



$W_g(\omega) = \dfrac{1}{V_g^{-1} - P_g(\omega)}$





$z + \omega - \varepsilon_{\varepsilon} = 0 \Rightarrow z = \varepsilon_{\varepsilon} - \omega$

$$\Sigma(\omega) = -\oint \frac{dz}{2\pi i} W(z) G^0(z+\omega)$$

$$\Sigma(\omega) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} W(i\omega') G^0(\omega + i\omega') + \underset{\text{direction}}{(-1)} \sum_{Res} W(\varepsilon_{\varepsilon} - \omega)\, \mathrm{Re}(G^0(\varepsilon))$$

$0 < \varepsilon_{\varepsilon} - \omega < \mu \qquad 1$

$$-\sum_{\omega < \varepsilon_{\varepsilon} < \mu + \omega} W(\varepsilon_{\varepsilon} - \omega)$$

$$\Sigma(i\omega) = \frac{1}{\beta} \sum_{i\Omega} G(i\omega + i\Omega) W(i\Omega) = \int_{-\infty}^{\infty} \frac{di\Omega}{2\pi i} G(i\omega + i\Omega) W(i\Omega)$$

$$\Sigma(\omega) = \int_{-\infty}^{\infty} \frac{d\Omega}{2\pi i} G(\omega + \Omega + i\delta) W(\Omega)$$

$$\Sigma(\omega) = +\int_{-\infty}^{\infty} \frac{dz}{2\pi i} W(z) G^0(z+\omega) \rightarrow -\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} W(i\omega') G^0(\omega + i\omega') - \sum_{\varepsilon_i < \varepsilon_F} W(\varepsilon_{\varepsilon_i} - \omega)\, \Theta(\varepsilon_{\varepsilon_i} - \omega)$$

$$+ \sum_{\varepsilon_a > \varepsilon_F} W(\omega - \varepsilon_{\varepsilon_a})\, \Theta(\omega - \varepsilon_{\varepsilon_a})$$

occupied $\omega < \varepsilon_{\varepsilon} < \varepsilon_F$

empty $\varepsilon_F < \varepsilon_{\varepsilon} < \omega$

$\dfrac{1}{\underbrace{z + \omega - \varepsilon_{\varepsilon}}}$ $\quad > 0$ $\quad < 0$

$0 < z$ and $\varepsilon_{\varepsilon} < \varepsilon_F$

$z = \varepsilon_{\varepsilon} - \omega$

$\Downarrow$

$0 < \varepsilon_{\varepsilon} - \omega$

$\omega + z - \varepsilon_{\varepsilon} = 0$

$z = \varepsilon_{\varepsilon} - \omega - i\delta$	$\varepsilon_{\varepsilon} > \varepsilon_F$
$z = \varepsilon_{\varepsilon} - \omega + i\delta$	$\varepsilon_{\varepsilon} < \varepsilon_F$

$z > 0$

$z = \varepsilon_{\varepsilon} - \omega > 0$

$\varepsilon_{\varepsilon} > \omega$

$\omega < \varepsilon_{\varepsilon} < \varepsilon_F$

4, 14, 51–54

I modified Bessel functions of the first kind $I(x) \sim$

K — // — second kind $K(x) \sim \sqrt{\frac{\pi}{2x}}\, e^{-x}$

$$\frac{e^{-\lambda|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|} = 4\pi\lambda \cdot \sum_{\ell m} I_\ell(\lambda r_<)\, K_\ell(\lambda r_>)\, Y^*_{\ell m}(\hat{r}')\, Y_{\ell m}(\hat{r})$$

Multicenter integral of Coulomb repulsion

product functions in Bloch form: Following Com. Phys. Commun 180, 347 (2009)

$$M^{q}_{a\kappa\ell m}(\vec r)=\frac{1}{\sqrt N}\sum_{\vec T}\underbrace{e^{i\vec q(\vec T+\vec R_a)}}_{\text{Bloch phase}}\underbrace{M_{a\kappa\ell}(|\vec r-\vec T-\vec R_a|)Y_{\ell m}(\vec r-\vec T-\vec R_a)}_{\text{product function on atom}}$$

interstitials: $M^{k}_{\vec G}(\vec r)=\frac{1}{\sqrt V}e^{i(\vec k+\vec G)\vec r}\Theta(\vec r)=\frac{1}{\sqrt V}\sum_{\vec G'}e^{i(\vec k+\vec G+\vec G')\vec r}\Theta_{\vec G'}$ where

easy to evaluate $\langle V_c\rangle$ for this form

$$\Theta_{\vec G}=\frac{1}{V}\int e^{-i\vec G\cdot\vec r}\Theta(\vec r)d^3r=\begin{cases}1-\frac{4\pi}{3V_c}\sum_a R_a^3 & G=0\\ \dots\end{cases}$$

can use either one of the two

Can also write $M^{k}_{\vec G}(\vec r)=\frac{1}{\sqrt V}\left[e^{i\vec g\cdot\vec r}-\sum_{\vec T,a}e^{i\vec g(\vec T+\vec R_a)}\Theta(r'-S_a)e^{i\vec g\vec r'}\right]=\lim_{\ell\to\infty}\frac{1}{\sqrt V}\left[e^{i\vec g\cdot\vec r}-\sum_{\vec T,a}e^{i\vec g(\vec T+\vec R_a)}4\pi\sum_{\ell=0,m}^{\infty}i^\ell j_\ell(gr')Y_{\ell m}(\hat r')Y^*_{\ell m}(\hat g)\right]$

where $\vec g=\vec k+\vec G$ and $\vec r'=\vec r-\vec T-\vec R_a$

Coulomb repulsion: $V_{a\kappa\ell m,a'\kappa'\ell'm'}(\vec k)=\iint\frac{M^{\vec k\,*}_{a\kappa\ell m}(\vec r)\,M^{\vec k}_{a'\kappa'\ell'm'}(\vec r')\,d^3r'd^3r}{|\vec r-\vec r'|}$

MT - MT:

take: $\vec r_s'=\vec r'-\vec T-\vec R_{a'}$ so that $\vec r_s'$ is inside MT at home unit cell
$\vec r_s=\vec r-\vec R_a$ is inside MT at home unit cell.

$$V_{a\kappa\ell m,a'\kappa'\ell'm'}(\vec k)=\sum_{\vec T}\iint\frac{d^3r_s d^3r_s'}{|\vec r-\vec r'|}M_{a\kappa\ell}(r_s)Y^*_{\ell m}(\vec r_s)M_{a'\kappa'\ell'}(\vec r_s')Y_{\ell'm'}(\vec r_s')e^{i\vec k(\vec T+\vec R_{a'}-\vec R_a)}$$ or equivalently

$$V_{a\kappa\ell m,a'\kappa'\ell'm'}(\vec k)=\sum_{\vec T}\iint\frac{d^3r_s d^3r'}{|\vec r-\vec r'|}M_{a\kappa\ell}(r_s)Y^*_{\ell m}(\hat r_s)M_{a'\kappa'\ell'}(\vec r'-\vec T-\vec R_{a'}+\vec R_a)Y_{\ell'm'}(\vec r'-\vec T-\vec R_{a'}+\vec R_a)e^{i\vec k(\vec T+\vec R_{a'}-\vec R_a)}$$

$\vec r-\vec r'=\vec r_s+\vec R_a-\vec r_s'-\vec T-\vec R_{a'}$

If $\vec T+\vec R_{a'}-\vec R_a=0$ it is very simple as both are inside the same MT. When this vector is nonzero, it is more involved.

Continue MT-MT part

$$V_{a\kappa\ell m,a'\kappa'\ell'm'}(\vec{k})=\sum_{\vec{T}}\iint\frac{d^3r_s\,d^3r_s'}{|\vec{r}_s-\vec{r}_s'-\vec{T}-\vec{R}_{a'}+\vec{R}_a|}\,M_{a\kappa\ell}(r_s)Y^*_{\ell m}(\vec{r}_s)\,M_{a'\kappa'\ell'}(r_s')Y_{\ell'm'}(\vec{r}_s')\,e^{i\vec{k}(\vec{T}+\vec{R}_{a'}-\vec{R}_a)}$$

Define $\vec{R}\equiv\vec{T}+\vec{R}_{a'}-\vec{R}_a$

If $\vec{R}=0$ (same M.T.) we have $V_{a\kappa\ell m,a'\kappa'\ell'm'}(\vec{k})=\iint M_{a\kappa\ell}(r_s)M_{a'\kappa'\ell'}(r_s')\,Y_{\ell'm'}(\vec{r}_s')Y^*_{\ell m}(\vec{r}_s)\frac{4\pi}{2\ell+1}\frac{r_<^\ell}{r_>^{\ell+1}}Y_{\ell m}(\vec{r}_s)Y^*_{\ell m}(\vec{r}_s')$

$$=\delta_{\ell\ell'}\delta_{mm'}\frac{4\pi}{2\ell+1}\iint M_{a\kappa\ell}(r_s)M_{a'\kappa'\ell}(r_s')\frac{r_<^\ell}{r_>^{\ell+1}}\,r_s^2r_s'^2\,dr_s\,dr_s'$$

Next $\vec{R}\neq 0$

$$V_{a\kappa\ell m,a'\kappa'\ell'm'}(\vec{k})=\sum_{\vec{T}}\iint\frac{d^3r_s\,d^3r_s'}{|\vec{r}_s-\vec{r}_s'-\vec{R}|}\,M_{a\kappa\ell}(r_s)Y^*_{\ell m}(\vec{r}_s)\,M_{a'\kappa'\ell'}(r_s')Y_{\ell'm'}(\vec{r}_s')\,e^{i\vec{k}\vec{R}}$$

$$=\sum_{\vec{T}}\iint d^3r_s\,d^3r_s'\,M_{a\kappa\ell}(r_s)M_{a'\kappa'\ell'}(r_s')\,Y^*_{\ell m}(\vec{r}_s)Y_{\ell'm'}(\vec{r}_s')\,e^{i\vec{k}\vec{R}}\sum_{\ell''}\frac{4\pi}{(2\ell''+1)}\frac{r_s'^{\ell''}}{|\vec{r}_s-\vec{R}|^{\ell''+1}}Y_{\ell''m''}(\vec{r}_s-\vec{R})Y^*_{\ell''m''}(\vec{r}_s')$$

$$=\sum_{\vec{T}}\int dr_s'\,r_s'^2M_{a'\kappa'\ell'}(r_s')\,r_s'^{\ell'}\cdot\frac{4\pi}{(2\ell'+1)}\int d^3r_s\,M_{a\kappa\ell}(r_s)\,Y^*_{\ell m}(\vec{r}_s)\,e^{i\vec{k}\vec{R}}\frac{1}{|\vec{r}_s-\vec{R}|^{\ell'+1}}Y_{\ell'm'}(\vec{r}_s-\vec{R})$$

Expansion from Skriver (LMTO method):

$$\frac{4\pi}{2L+1}\frac{1}{|\vec{r}-\vec{R}|^{L+1}}Y_{LM}(\vec{r}-\vec{R})=(-1)^{L+M}\sum_{\substack{\ell=0\\m}}^{\infty}C_{LM,\ell m}\frac{r^\ell}{R^{L+\ell+1}}Y_{\ell m}(\hat{r})Y^*_{L+\ell,m-M}(\vec{R})$$

$$C_{LM,\ell m}=(4\pi)^{\frac{3}{2}}\frac{1}{\sqrt{(2L+1)(2\ell+1)(2(\ell+L)+1)}}\sqrt{\frac{(\ell+L+m-M)!(\ell+L-m+M)!}{(L+M)!(L-M)!(\ell+m)!(\ell-m)!}}$$

or $C_{LM,\ell m}=(-1)^M(4\pi)^2\frac{(2(L+\ell)-1)!!}{(2L+1)!!(2\ell+1)!!}\,g(LM,\ell m,L+\ell,m-M)$

where gaunt: $g_{LL'L''}=\int Y_L(\hat{r})Y^*_{L'}(\hat{r})Y_{L''}(\hat{r})\,d\Omega$

$$V_{a\kappa\ell m,a'\kappa'\ell'm'}(\vec{k})=\sum_{\vec{T}}\int dr_s'\,r_s'^2M_{a'\kappa'\ell'}(r_s')\,r_s'^{\ell'}\cdot\frac{4\pi}{(2\ell'+1)}\int d^3r_s\,M_{a\kappa\ell}(r_s)\,Y^*_{\ell m}(\vec{r}_s)\,e^{i\vec{k}\vec{R}}\times$$

$$\times\frac{2\ell'+1}{4\pi}(-1)^{\ell'+m'}\sum_{\ell''m''}C_{\ell'm',\ell''m''}\frac{r_s^{\ell''}}{R^{\ell''+\ell'+1}}Y_{\ell''m''}(\vec{r}_s)Y^*_{\ell''+\ell',m''-m'}(\vec{R})$$

$$=(-1)^{\ell'+m'}C_{\ell'm',\ell m}\int dr_s'\,r_s'^2M_{a'\kappa'\ell'}(r_s')\,r_s'^{\ell'}\int dr_s\,r_s^2M_{a\kappa\ell}(r_s)\,r_s^\ell\cdot\sum_{\vec{T}}\frac{e^{i\vec{k}\vec{R}}}{R^{\ell+\ell'+1}}Y^*_{\ell+\ell',m-m'}(\vec{R})$$

$$=(-1)^{\ell'+m'}C_{\ell'm',\ell m}\underbrace{\int dr_s'\,r_s'^2M_{a'\kappa'\ell'}(r_s')\,r_s'^{\ell'}}_{Q_{a'\kappa'\ell'}}\underbrace{\int dr_s\,r_s^2M_{a\kappa\ell}(r_s)\,r_s^\ell}_{Q_{a\kappa\ell}}\cdot\underbrace{\sum_{\vec{T}}\frac{e^{i\vec{k}\cdot(\vec{T}+\vec{R}_{a'}-\vec{R}_a)}}{|\vec{T}+\vec{R}_{a'}-\vec{R}_a|^{\ell+\ell'+1}}Y^*_{\ell+\ell',m-m'}(\vec{T}+\vec{R}_{a'}-\vec{R}_a)}_{\text{Ewald sum}}$$

We derived:

$$V_{a\kappa l m, a'\kappa' l' m'}(\vec{k}) = (-1)^{l'+m'} \times \underbrace{(4\pi)^{\frac{3}{2}} \frac{1}{\sqrt{(2l'+1)(2l+1)(2(l+l')+1)}} \sqrt{\frac{(l+l'+m-m')!\,(l+l'-m+m')!}{(l'+m')!\,(l'-m')!\,(l+m)!\,(l-m)!}}}^{C_{l'm'lm}} \times$$

$$\times \underbrace{\int dr_s' \, r_s'^2 \, M_{a'\kappa' l'}(r_s') \, r_s'^{l'}}_{Q_{a'\kappa' l'}} \underbrace{\int dr_s \, r_s^2 \, M_{a\kappa l}(r_s) \, r_s^{l}}_{Q_{a\kappa l}} \cdot \underbrace{\sum_{\vec{T}} \frac{e^{i\vec{k}\cdot(\vec{T}+\vec{R}_{a'}-\vec{R}_a)}}{|\vec{T}+\vec{R}_{a'}-\vec{R}_a|^{l+l'+1}} Y^*_{l+l', m-m'}(\vec{T}+\vec{R}_{a'}-\vec{R}_a)}_{\text{Ewald sum}}$$

$C_{l'm', lm} =$

What is implemented in PyGW?

$$V_{\alpha\beta} = \iint Y^*_{l_1 m_1}(\hat{r}_a) \, Y_{l_2 m_2}(\hat{r}_b) \, u^{a}_{N_1 l_1}(r_a) \, u^{b}_{N_2 l_2}(r_b) \frac{e^{-i\vec{q}\vec{R}_{ab}}}{|\vec{r}_a - \vec{r}_b + \vec{R}_{ab}|} d^3 r_a \, d^3 r_b$$

two center expansion exists: $$\frac{1}{|\vec{R}+\vec{r}_1-\vec{r}_2|} = \sum_{\substack{l_1 m_1 \\ l_2 m_2}} \mathcal{Y}(l_1 m_1, l_2 m_2) \, r_1^{l_1} Y^*_{l_1 m_1}(\hat{r}_1) \, r_2^{l_2} Y^*_{l_2 m_2}(\hat{r}_2) \frac{1}{R^{l_1+l_2}} Y_{l_1+l_2, m_1+m_2}(\hat{R})$$

with $$\mathcal{Y}(l_1 m_1, l_2 m_2) = 4\pi^{\frac{3}{2}} (-1)^{l_1} \sqrt{\frac{\binom{l_1+m_1+l_2+m_2}{l_1+m_1} \binom{l_1-m_1+l_2-m_2}{l_1-m_1}}{(2l_2+1)(2l_1+1)(2l_1+2l_2+1)}}$$

Hence

$$V_{\alpha\beta} = \sum_{\substack{l_1 m_1 \\ l_2 m_2}} \underbrace{\sqrt{\frac{\binom{l_1-m_1+l_2+m_2}{l_1-m_1} \binom{l_1+m_1+l_2-m_2}{l_1+m_1}}{(2l_2+1)(2l_1+1)(2l_1+2l_2+1)}} \, 4\pi^{\frac{3}{2}}}_{C_{l_1 m_1, l_2 m_2}} \underbrace{(-1)^{l_1}(-1)^{m_1}} \sum_{R_{ab}} e^{-i\vec{q}\vec{R}_{ab}} \frac{Y_{l_1+l_2, -m_1+m_2}(\hat{R}_{ab})}{R_{ab}^{l_1+l_2+1}} \underbrace{\langle r_a^{l_1} | u_{N_1 l_1} \rangle}_{Q_{a N_1 l_1}} \underbrace{\langle r_b^{l_2} | u_{N_2 l_2} \rangle}_{Q_{b N_2 l_2}}$$

should be −

is this missing?

When you debug should check there!!

PW - PW part:

$$V_{\vec{G}\vec{G}'}(\vec{k}) = \frac{1}{V}\iint \frac{e^{-i(\vec{k}+\vec{G})\vec{r}} \quad e^{i(\vec{k}+\vec{G}')\vec{r}'}}{|\vec{r}-\vec{r}'|} \Theta(\vec{r}) \Theta(\vec{r}') d^3r\, d^3r'$$

$$V_{\vec{G}\vec{G}'}(\vec{k}) = \frac{1}{V}\iint \frac{e^{-i(\vec{k}+\vec{G})\vec{r}} \quad e^{i(\vec{k}+\vec{G}')\vec{r}'}}{|\vec{r}-\vec{r}'|} \Theta(\vec{r}) \Theta(\vec{r}') d^3r\, d^3r'$$

$\boxed{\text{Variant a}}$

$$\frac{1}{|\vec{r}-\vec{r}'|} = \sum_{\vec{G},\vec{q}} \frac{8\pi}{|\vec{G}+\vec{q}|^2} e^{+i(\vec{q}+\vec{G})\cdot(\vec{r}-\vec{r}')}$$

$$V_{\vec{G}\vec{G}'}(\vec{k}) = \frac{1}{V}\iint d^3r\, d^3r'\, e^{-i(\vec{k}+\vec{G})\vec{r}} e^{i(\vec{k}+\vec{G}')\vec{r}'} \Theta(\vec{r}) \Theta(\vec{r}') \sum_{\vec{G}'',\vec{q}} \frac{8\pi}{|\vec{G}''+\vec{q}|^2} e^{+i(\vec{q}+\vec{G}'')\cdot(\vec{r}-\vec{r}')}$$

$$= \sum_{\vec{G}'',\vec{q}} \frac{8\pi}{|\vec{G}''+\vec{q}|^2} \frac{1}{V}\iint d^3r\, d^3r'\, e^{i(\vec{q}+\vec{G}''-\vec{k}-\vec{G})\vec{r}} \quad e^{i(\vec{k}+\vec{G}'-\vec{q}-\vec{G}'')\vec{r}''}$$

$$= \sum_{\vec{G}'',\vec{q}} \frac{8\pi}{|\vec{G}''+\vec{q}|^2} \frac{1}{N_{cell}}\sum_{T} \frac{1}{V_{cell}}\int_{V_{cell}} d^3r\, e^{i(\vec{q}-\vec{k}+\vec{G}''-\vec{G})(\vec{r}+\vec{T})} \int e^{i(\vec{k}+\vec{G}'-\vec{q}-\vec{G}'')\vec{r}''} d^3r'$$

$$= \sum_{\vec{G}'',\vec{q}} \frac{8\pi}{|\vec{G}''+\vec{q}|^2} \cdot \underbrace{\frac{1}{N_{cell}}\sum_{\vec{T}} e^{i(\vec{q}-\vec{k})\vec{T}}}_{\delta_{\vec{q}-\vec{k}}} \cdot \frac{1}{V_{cell}}\int_{V_{cell}} e^{i(\vec{G}''-\vec{G})\vec{r}} d^3r \int_{V} e^{i(\vec{G}'-\vec{G}'')\vec{r}''} d^3r'$$

$$= \sum_{\vec{G}'',\vec{q}} \frac{8\pi}{|\vec{G}''+\vec{k}|^2} \tilde{\Theta}(\vec{G}''-\vec{G}) \cdot \tilde{\Theta}(\vec{G}'-\vec{G}'')$$

We could just write: $V^{\vec{k}}_{coulomb} = \sum_{\vec{G}''} |\vec{k}+\vec{G}''\rangle \frac{1}{|\vec{k}+\vec{G}''|^2} \langle \vec{k}+\vec{G}''|$ and evaluate

$$V_{\vec{G}\vec{G}'}(\vec{k}) = \sum_{\vec{G}''} \langle \vec{k}+\vec{G} | \vec{k}+\vec{G}''\rangle_I \frac{1}{|\vec{k}+\vec{G}''|^2} \langle \vec{k}+\vec{G}'' | \vec{k}+\vec{G}'\rangle_I = \sum_{\vec{G}''} \frac{8\pi}{|\vec{G}''+\vec{k}|^2} \Theta(\vec{G}''-\vec{G}) \Theta(\vec{G}'-\vec{G}'')$$

This is actually implemented.

Multicenter integral of Yukawa repulsion

$$V_{\alpha\kappa\ell m,\alpha'\kappa'\ell'm'}(\vec{k}) = \sum_{\vec{T}} \iint d^3r\, d^3r'\; M_{\alpha\kappa\ell}(r)\, Y^*_{\ell m}(\hat{r})\, M_{\alpha'\kappa'\ell'}(|\vec{r}'-\vec{R}|)\, Y_{\ell'm'}(\vec{r}'-\vec{R})\, e^{i\vec{k}\cdot\vec{R}}\; \underbrace{\frac{e^{-\lambda|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}}_{=\,4\pi\lambda \sum_{LM} i_L(\lambda|\vec{r}'-\vec{R}|)\, k_L(\lambda|\vec{r}-\vec{R}|)\, Y^*_{LM}(\vec{r}'-\vec{R})\, Y_{LM}(\vec{r}-\vec{R})}$$

where: $\vec{R} = \vec{T} + \vec{R}_{\alpha'} - \vec{R}_{\alpha}$

use: $\dfrac{e^{-\lambda|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} = 4\pi\lambda \cdot \sum_{\ell m} i_\ell(\lambda r_<)\, k_\ell(\lambda r_>)\, Y^*_{\ell m}(\hat{r}')\, Y_{\ell m}(\hat{r})$

$$V_{\alpha\kappa\ell m,\alpha'\kappa'\ell'm'}(\vec{k}) = \sum_{\vec{T}} \int d^3r\, M_{\alpha\kappa\ell}(r)\, Y^*_{\ell m}(\hat{r})\, e^{i\vec{k}\cdot\vec{R}}\; 4\pi\lambda \cdot k_{\ell'}(\lambda|\vec{r}-\vec{R}|)\, Y_{\ell'm'}(\vec{r}-\vec{R}) \cdot \underbrace{\int dr' r'^2\, M_{\alpha'\kappa'\ell'}(|\vec{r}'-\vec{R}|)\, i_{\ell'}(\lambda|\vec{r}'-\vec{R}|)}_{Q_{\alpha'\kappa'\ell'} \,\equiv\, \int dr' r'^2\, M_{\alpha'\kappa'\ell'}(r')\, i_{\ell'}(\lambda r')}$$

$$= \sum_{\vec{T}} \int d^3r\, M_{\alpha\kappa\ell}(r)\, Y^*_{\ell m}(\hat{r})\, e^{i\vec{k}\cdot\vec{R}} \cdot Q_{\alpha'\kappa'\ell'} \cdot \underbrace{4\pi\lambda \cdot k_{\ell'}(\lambda|\vec{r}-\vec{R}|)\, Y_{\ell'm'}(\vec{r}-\vec{R})}$$

$$k_\ell(\lambda|\vec{r}-\vec{R}|)\, Y_{\ell m}(\vec{r}-\vec{R}) = 4\pi(-1)^\ell \sum_{\substack{\ell'm'\\ \ell''m''}} \underbrace{g(\ell m, \ell'm', \ell''m'')}_{\int Y_{\ell m} Y^*_{\ell'm'} Y_{\ell''m''}} \cdot i^{(1)}_{\ell'}(\lambda r) \cdot k_{\ell''}(\lambda R) \cdot Y_{\ell'm'}(\vec{r})\, Y^*_{\ell''m''}(\vec{R}) \cdot i^{\ell'-\ell''+\ell}$$

Crucial Eq. which should be checked!

$$= \sum_{\vec{T}} \underbrace{\int dr\, r^2 M_{\alpha\kappa\ell}(r) \cdot i^{(1)}_\ell(\lambda r)}_{Q_{\alpha\kappa\ell}}\; e^{i\vec{k}\cdot\vec{R}} \cdot Q_{\alpha'\kappa'\ell'} \cdot 4\pi\lambda\, 4\pi \sum_{\ell''m''} g(\ell'm', \ell m, \ell''m'')\, Y^*_{\ell''m''}(\vec{R})\, i^{\ell-\ell''+\ell'}\, k_{\ell''}(\lambda R)\, (-1)^{\ell'}$$

$$= (-1)^{\ell'} Q_{\alpha\kappa\ell}\, Q_{\alpha'\kappa'\ell'}\, (4\pi)^2 \lambda \sum_{\ell''m''} g(\ell'm', \ell m, \ell''m'') \cdot i^{\ell+\ell'-\ell''} \sum_{\vec{T}} e^{i\vec{k}(\vec{T}+\vec{R}_{\alpha'}-\vec{R}_\alpha)}\, Y^*_{\ell''m''}(\vec{T}+\vec{R}_{\alpha'}-\vec{R}_\alpha)\, k_{\ell''}(\lambda|\vec{T}+\vec{R}_{\alpha'}-\vec{R}_\alpha|)$$

Deriving multicenter expansion from Steiner and Danos & Maximon

$$\frac{4\pi}{2L+1}\frac{1}{|\vec r-\vec R|^{L+1}}\mathcal{Y}_{LM}(\hat r-\hat R)=(-1)^{L+M}\sum_{\substack{\ell=0\\ m}}^{\infty}C_{LM,\ell m}\frac{r^\ell}{R^{L+\ell+1}}\mathcal{Y}_{\ell m}(\hat r)\mathcal{Y}^*_{L+\ell,m-M}(\vec R)$$

$$C_{LM,\ell m}=(-1)^M(4\pi)^2\frac{(2(L+\ell)-1)!!}{(2L+1)!!\,(2\ell+1)!!}\,g(LM,\ell m,L+\ell\,m-M)$$

$$g_{LL'L''}=\int \mathcal{Y}_L(\hat r)\mathcal{Y}^*_{L'}(\hat r)\mathcal{Y}_{L''}(\hat r)\,d\Omega=\sqrt{\frac{2\ell''+1}{4\pi}}\,C^{\ell''}(\ell'm';\ell m)$$

$m''=m'-m$

Condon & Shortley

differs in this $(-1)^L$

$$\frac{1}{2L+1}\frac{1}{|\vec r-\vec R|^{L+1}}\mathcal{Y}_{LM}(\vec r-\vec R)=(4\pi)(-1)^L\sum_{\substack{\ell=0\\ m}}^{\infty}\frac{(2(L+\ell)-1)!!}{(2L+1)!!(2\ell+1)!!}g(LM,\ell m,L+\ell,m-M)\frac{r^\ell}{R^{L+\ell+1}}\mathcal{Y}_{\ell m}(\hat r)\mathcal{Y}^*_{L+\ell,m-M}(\vec R)$$

can be hankel or neumann!

$$n_\ell(\varkappa|\vec r-\vec R|)\mathcal{Y}_{\ell m}(\vec r-\vec R)=4\pi\sum_{\ell'm'\ell''m''}g(\ell m,\ell'm',\ell''m'')\,j_{\ell'}(\varkappa r)\,n_{\ell''}(\varkappa R)\,\mathcal{Y}_{\ell'm'}(\hat r)\,\mathcal{Y}^*_{\ell''m''}(\hat R)$$

$m''=m'-m$

[from Steiner page 82]

$|\vec r-\vec R|<|\vec R|$

$$\boxed{\begin{aligned}&\varkappa=i\lambda\\ &n_\ell(ix)=i^{\ell+1}\,i_\ell^{(2)}(x)\\ &j_\ell(ix)=i^\ell\,i_\ell^{(1)}(x)\end{aligned}}\qquad \boxed{\begin{aligned}&\text{theorem also valid for hankel}\\ &h_\ell^{(1)}(ix)=-(i)^{-\ell}\,k_\ell(x)\end{aligned}}$$

$$i^{\ell+1}\,i_\ell^{(2)}(\lambda|\vec r-\vec R|)\mathcal{Y}_{\ell m}(\vec r-\vec R)=4\pi\sum_{\substack{\ell'm'\\ \ell''m''}}g(\ell m,\ell'm',\ell''m'')\,i^{\ell'}\,i_{\ell'}^{(1)}(\lambda r)\,i^{\ell''+1}\,i_{\ell''}^{(2)}(\lambda R)\,\mathcal{Y}_{\ell'm'}(\vec r)\,\mathcal{Y}^*_{\ell''m''}(\vec R)$$

$$k_\ell(\lambda|\vec r-\vec R|)\mathcal{Y}_{\ell m}(\vec r-\vec R)=(-1)^\ell 4\pi\sum_{\substack{\ell'm'\\ \ell''m''}}\underbrace{g(\ell m,\ell'm',\ell''m'')}_{\int \mathcal{Y}_{\ell m}\mathcal{Y}^*_{\ell'm'}\mathcal{Y}_{\ell''m''}}\cdot i_{\ell'}^{(1)}(\lambda r)\cdot k_{\ell''}(\lambda R)\cdot\mathcal{Y}_{\ell'm'}(\vec r)\,\mathcal{Y}^*_{\ell''m''}(\vec R)\cdot i^{\ell'-\ell''+\ell}$$

Spherical Bessel and Neumann

$$\left(-\frac{d^2}{dr^2}+\frac{\ell(\ell+1)}{r^2}-\varkappa^2\right)r\,y_\ell(\varkappa r)=0$$

$$\left.\begin{aligned}&j_\ell(\varkappa r)\sim\frac{(\varkappa r)^\ell}{(2\ell+1)!!}\\ &n_\ell(\varkappa r)=-\frac{(2\ell-1)!!}{(\varkappa r)^{\ell+1}}\end{aligned}\right\}\ \varkappa r\to 0$$

$(-1)!!=1$

$$\left.\begin{aligned}&j_\ell(\varkappa r)=\frac{\sin(\varkappa r-\ell\pi/2)}{\varkappa r}\\ &n_\ell(\varkappa r)=-\frac{\cos(\varkappa r-\ell\pi/2)}{\varkappa r}\end{aligned}\right\}\ r\to\infty$$

$\varkappa\to 0$

$$\frac{1}{(2L+1)|\vec r-\vec R|^{L+1}}\mathcal{Y}_{LM}(\vec r-\vec R)=4\pi\sum_{\substack{\ell m\\ \ell''m''}}\frac{(2\ell''-1)!!}{(2L+1)!!\,(2\ell+1)!!}g(LM,\ell m,\ell''m'')\,\varkappa^{L+\ell-\ell''}\cdot\left(\frac{r^\ell}{r^{\ell''+1}}\right)\cdot\mathcal{Y}_{\ell m}(\hat r)\mathcal{Y}^*_{\ell''m''}(\hat R)$$

finite only for $\ell''=L+\ell$, $m''=m-M$

$i_0=\frac{\sinh x}{x}$ $\quad k_0=\frac{e^{-x}}{x}$

$i_1=\frac{x\cosh x-\sinh x}{x^2}$ $\quad k_1=\frac{e^{-x}(x+1)}{x^2}$

$i_m(x)=i^{-m}j_m(ix)$

$i_m^{(2)}(x)=i^{-m-1}n_m(ix)$

$k_m(x)=-i^m h_m^{(1)}(ix)=-i^m\frac{\pi}{2}\left[j_m(ix)+i n_m(ix)\right]$

hankel

$k_m(x)=(-1)^{m+1}\frac{\pi}{2}\left[i_m(x)-i_m^{(2)}(x)\right]$

Helmholtz Eq: solution is modified bessel

$$r/\left(\frac{d^2}{dr^2}-\frac{2}{r}\frac{d}{dr}+\frac{\ell(\ell+1)}{r^2}+\chi^2\right)u_\ell=0$$

$$\Big(\underbrace{-r\frac{d^2}{dr^2}-2\frac{d}{dr}}_{-\frac{d^2}{dr^2}(r u_\ell)}+\frac{\ell(\ell+1)}{r}+\chi^2 r\Big)u_\ell=0$$

$$\left(-\frac{d^2}{dr^2}+\frac{\ell(\ell+1)}{r^2}+\lambda^2\right)(r u_\ell)=0$$ The only difference $\lambda=i\varkappa$

$z=\lambda r$

$$i_\ell(z)=(z)^\ell\sum_{k=0}^{\infty}\frac{(\frac{1}{2}z^2)^k}{k!\,(2\ell+2k+1)!!}\approx\frac{(z)^\ell}{(2\ell+1)!!}$$

$$k_\ell(z)=(-1)^{\ell+1}\frac{\pi}{2}\left[z^\ell\sum_{k=0}^{\infty}\frac{(\frac{1}{2}z^2)^k}{k!\,(2\ell+2k+1)!!}-\frac{(-1)^\ell}{z^{\ell+1}}\sum_{k=0}^{\ell}\frac{(2\ell-2k-1)!!(-\frac{1}{2}z^2)^k}{k!}-\frac{1}{z^{\ell+1}}\sum_{k=\ell+1}^{\infty}\frac{(\frac{1}{2}z^2)^k}{k!\,(2k-2\ell-1)!!}\right]$$

Note $k_\ell(z)=(-1)^{\ell+1}\frac{\pi}{2}\left[i_\ell(z)-i_\ell^{(2)}(z)\right]$

Checking multi center expansion in different limits

$$i_\ell^{(1)}(x) = z^\ell \sum_{k=0}^{\infty} \frac{\left(\frac{1}{2}z^2\right)^k}{k!\,(2\ell+2k+1)!!}$$

$$i_\ell^{(2)}(x) = \frac{(-1)^\ell}{z^{\ell+1}} \sum_{k=0}^{\ell} \frac{(2\ell-2k-1)!!}{k!} \left(-\tfrac{1}{2}z^2\right)^k + \frac{1}{z^{\ell+1}} \sum_{k=\ell+1}^{\infty} \frac{1}{k!\,(2k-2\ell-1)!!} \left(\tfrac{1}{2}z^2\right)^k$$

$$k_\ell(\lambda|\vec r-\vec R|)\, Y_{\ell m}(\vec r-\vec R) = 4\pi(-1)^\ell \sum_{\substack{\ell' m'\\ \ell'' m''}} \underbrace{g(\ell m, \ell' m', \ell'' m'')}_{\int Y_{\ell m} Y^*_{\ell' m'} Y_{\ell'' m''}} \cdot i_{\ell'}^{(1)}(\lambda r) \cdot k_{\ell''}(\lambda R) \cdot Y_{\ell' m'}(\vec r)\, Y^*_{\ell'' m''}(\vec R) \cdot i^{\ell'-\ell''+\ell}$$

limit $r \to 0$

$$k_\ell(\lambda R)\, Y_{\ell m}(-\vec R) = 4\pi(-1)^\ell \sum_{\substack{\ell' m'\\ \ell'' m''}} \underbrace{g(\ell m, \ell' m', \ell'' m'')}_{\ell'=0} k_{\ell''}(\lambda R) \frac{1}{\sqrt{4\pi}} Y^*_{\ell'' m''}(\vec R)\, i^{-\ell''+\ell} = (-1)^\ell 4\pi\, k_\ell(\lambda R) \frac{1}{\sqrt{4\pi}} \frac{1}{\sqrt{4\pi}} Y^*_{\ell\,-m}(\vec R)\,(-1)^m$$

$$= (-1)^\ell k_\ell(\lambda R)\, Y_{\ell m}(\vec R)$$

$$\frac{1}{\sqrt{4\pi}} \delta_{m''=-m} \cdot (-1)^m \delta_{\ell''=\ell}$$

$$\| \qquad (-1)^\ell Y_{\ell m}(\vec R)$$

✓

limit $\lambda \to 0$

$$k_\ell(\lambda x) \sim \frac{\pi}{2} \frac{(2\ell-1)!!}{(\lambda x)^{\ell+1}}$$

$$i_\ell^{(1)}(\lambda x) \sim \frac{(\lambda x)^\ell}{(2\ell+1)!!}$$

$$\frac{\pi}{2} \frac{(2\ell-1)!!}{|\vec r-\vec R|^{\ell+1}} Y_{\ell m}(\vec r-\vec R) = 4\pi(-1)^\ell \sum_{\substack{\ell' m'\\ \ell'' m''}} g(\ell m\, \ell' m'\, \ell'' m'') \frac{r^{\ell'}}{(2\ell'+1)!!} \delta_{\ell''=\ell+\ell'} \frac{\pi}{2} \frac{(2\ell''-1)!!}{R^{\ell''+1}} Y_{\ell' m'}(\vec r)\, Y^*_{\ell'' m''}(\vec R)\, i^{\ell'-\ell''+\ell}$$

$$\frac{1}{(2\ell+1)} \frac{1}{|\vec r-\vec R|^{\ell+1}} Y_{\ell m}(\vec r-\vec R) = 4\pi(-1)^\ell \sum_{\ell' m'} g(\ell m, \ell' m', \ell+\ell', m'-m) \frac{(2(\ell'+\ell)-1)!!}{(2\ell'+1)!!\,(2\ell+1)!!} \cdot r^{\ell'} \cdot Y_{\ell' m'}(\vec r)\, Y^*_{\ell+\ell', m'-m}(\vec R)$$

✓

Coulomb Repulsion in Wannier basis

First generic way of calculating Coulomb in solids

Let $\varphi_\alpha^{\vec{q}}(\vec{r})$ form a complete product basis, and satisfy Bloch's theorem, i.e.,

$$\varphi_\alpha^{\vec{q}}(\vec{r}+\vec{R}) = e^{i\vec{q}\cdot\vec{R}}\,\varphi_\alpha^{\vec{q}}(\vec{r}),$$ because $\varphi_\alpha^{\vec{q}}(\vec{r}) = e^{i\vec{q}\cdot\vec{r}}\,\tilde{\varphi}_\alpha^{\vec{q}}(\vec{r})$ with $\tilde{\varphi}$ periodic.

Then we write

$$V_{\alpha\beta} = \iint_{V\,V} \varphi_\alpha^*(\vec{r}\,')\frac{1}{|\vec{r}\,'-\vec{r}|}\varphi_\beta(\vec{r})\,d^3r\,d^3r'$$ and choose $\vec{r} = \vec{r}_0 + \vec{R}$, $\vec{r}\,' = \vec{r}_0\,' + \vec{R}'$ where $\vec{r}_0$ and $\vec{r}_0\,'$ are in the first U.C.

$$\iint_{V\,V} \varphi_\alpha^*(\vec{r}_0\,'+\vec{R}')\frac{1}{|\vec{r}_0\,'-\vec{r}_0+\vec{R}'-\vec{R}|}\varphi_\beta(\vec{r}_0+\vec{R})\,d^3r\,d^3r' = \sum_{RR'}\iint_{\Omega\,\Omega} e^{-i\vec{q}\vec{R}'}\varphi_\alpha^{\vec{q}*}(\vec{r}_0\,')\frac{1}{|\vec{r}_0\,'-\vec{r}_0+\vec{R}'-\vec{R}|}\varphi_\beta^{\vec{q}}(\vec{r}_0)\,e^{i\vec{q}\vec{R}}\,d^3r_0\,d^3r_0$$

$$\boxed{V_{\alpha\beta}^{\vec{q}} = \iint_{\Omega\,\Omega} d^3r\,d^3r'\;\varphi_\alpha^{\vec{q}*}(\vec{r}\,')\left(\sum_{\vec{R}}\frac{e^{-i\vec{q}\vec{R}}}{|\vec{r}\,'-\vec{r}+\vec{R}|}\right)\varphi_\beta^{\vec{q}}(\vec{r})}$$

The problem is that we need a lot of product function $\varphi_\alpha^{\vec{q}}(\vec{r})$, and we need to also calculate the proper matrix elements

$$V_{ijlm} = \int \psi_{k_i}^*(\vec{r})\,\psi_{k+q j}(\vec{r})\frac{1}{|\vec{r}-\vec{r}\,'|}\psi_{k' l}(\vec{r}\,')\,\psi_{k'+q m}^*(\vec{r}\,') = \underbrace{\langle \psi_{k_i}\psi_{k+qj}^*|\varphi_\alpha^{\vec{q}}\rangle}_{M_{ij}^\alpha(\vec{k},\vec{q})}\underbrace{\langle\varphi_\alpha^{q}|V_c|\varphi_\beta^{\vec{q}}\rangle}_{V_{\alpha\beta}(\vec{q})}\underbrace{\langle\varphi_\beta^{\vec{q}}|\psi_{k'l}\,\psi_{k'+qm}^*\rangle}_{M_{lm}^\beta(\vec{k}',\vec{q})}$$

Now the alternative Wannier basis!

$$W_{\alpha R}(\vec{r}) = \frac{\Omega}{(2\pi)^3}\int d^3k\; e^{-i\vec{k}\vec{R}}\sum_i U_{i\alpha}\,\psi_{ik}(\vec{r})$$

$W_{\alpha R}(\vec{r}) = W_{\alpha 0}(\vec{r}-\vec{R})$ where $W_{\alpha 0}$ is peaked in the home unit cell.

$$\psi_{ik}(\vec{r}) = \sum_{\vec{R},\alpha} e^{i\vec{k}\vec{R}}\,U_{i\alpha}^*\,W_{\alpha 0}(\vec{r}-\vec{R})$$ The idea: there are only a few Wanniers α and are localized.

$$V_{c\,ijlm} = \int \psi_{k_i}^*(\vec{r})\,\psi_{k+qj}(\vec{r})\frac{1}{|\vec{r}-\vec{r}\,'|}\psi_{k'l}(\vec{r}\,')\,\psi_{k'+qm}^*(\vec{r}\,') = \int d^3r\,d^3r'\sum_{\substack{R_1..R_4\\ \alpha\beta\kappa\delta}} e^{-i\vec{k}\vec{R}_1}U_{i\alpha}\,W_{\alpha 0}^*(\vec{r}-\vec{R}_1)\,e^{i(\vec{k}+\vec{q})\vec{R}_2}U_{j\beta}^*\,W_{\beta 0}(\vec{r}-\vec{R}_2)\frac{1}{|\vec{r}-\vec{r}\,'|}e^{i\vec{k}'R_4}U_{l\kappa}^*\,W_{\kappa 0}(\vec{r}\,'-\vec{R}_4)\,e^{-i(\vec{k}'+\vec{q})\vec{R}_3}U_{m\delta}\,W_{\delta 0}^*(\vec{r}\,'-\vec{R}_3)$$

$\vec{r}\to\vec{r}+\vec{R}_2$ and $\vec{r}\,'\to\vec{r}\,'+\vec{R}_3$

$$\sum_{\substack{R_1..R_4\\ \alpha\beta\kappa\delta}} U_{i\alpha}U_{j\beta}^*U_{l\kappa}^*U_{m\delta}\;e^{i\vec{k}(\vec{R}_2-\vec{R}_1)+i\vec{q}(\vec{R}_2-\vec{R}_3)+i\vec{k}'(\vec{R}_4-\vec{R}_3)}\int d^3r\,d^3r'\;W_{\alpha 0}^*(\vec{r}+\vec{R}_2-\vec{R}_1)\,W_{\beta 0}(\vec{r})\frac{1}{|\vec{r}-\vec{r}\,'+\vec{R}_2-\vec{R}_3|}W_{\kappa 0}(\vec{r}\,'+\vec{R}_3-\vec{R}_4)\,W_{\delta 0}^*(\vec{r}\,')$$

$R_1\to R_1+R_2$ and $\vec{R}_4\to\vec{R}_4+\vec{R}_3$

$$=\sum_{\substack{R_1..R_4\\ \alpha\beta\kappa\delta}} U_{i\alpha}U_{j\beta}^*U_{l\kappa}^*U_{m\delta}\;e^{-i\vec{k}R_1+i\vec{q}(\vec{R}_2-\vec{R}_3)+i\vec{k}'\vec{R}_4}\cdot\int d^3r\,d^3r'\;W_{\alpha 0}^*(\vec{r}-\vec{R}_1)\,W_{\beta 0}(\vec{r})\frac{1}{|\vec{r}-\vec{r}\,'+\vec{R}_2-\vec{R}_3|}W_{\kappa 0}(\vec{r}\,'-\vec{R}_4)\,W_{\delta 0}^*(\vec{r}\,')$$

$$=\sum_{\substack{\alpha\beta\kappa\delta\\ R_1R_2R_3}} U_{i\alpha}U_{j\beta}^*U_{l\kappa}^*U_{m\delta}\;e^{-i\vec{k}\vec{R}_1}\left\{\int d^3r\,d^3r'\,W_{\alpha 0}^*(\vec{r}-\vec{R}_1)\,W_{\beta 0}(\vec{r})\frac{e^{-i\vec{q}\vec{R}_2}}{|\vec{r}-\vec{r}\,'-\vec{R}_2|}W_{\kappa 0}(\vec{r}\,'-\vec{R}_3)\,W_{\delta 0}^*(\vec{r}\,')\right\}e^{i\vec{k}'R_3}$$

product basis $W_{\alpha 0}^*(\vec{r}-\vec{R})\,W_{\beta 0}(\vec{r}) = \varphi_{\alpha\beta}^{\vec{R}}(\vec{r})$ use SVD to find only necessary

$\vec{R}$ nearest neighbour and next nearest neighbour

What we already have in terms of product functions $\chi_g(\vec{r})$

$$V_{ijkl} = \langle \psi_{i_1 k} \psi^*_{i_2 k+g} | \chi^g_\alpha \rangle \langle \chi^g_\alpha | V_g | \chi^g_\beta \rangle \langle \chi^g_\beta | \psi_{i_3 k'} \psi^*_{i_4 k'+g} \rangle \qquad M^m_{i_1 i_2}(\vec{k},\vec{g}) \equiv \langle \chi^g_m | \psi_{i_1 k} \psi^*_{i_2 k+g} \rangle$$

$$V_{ijkl} = M^*_{i_1 i_2}(\vec{k},\vec{g}) \langle \chi^g_\alpha | V_g | \chi^g_\beta \rangle M_{i_3 i_4}(\vec{k},\vec{g})$$

$$\sum_{\substack{\alpha\beta\gamma\delta \\ R_1 R_2 R_3}} U^k_{i\alpha} U^*_{j\beta} U^*_{l\gamma} U_{m\delta} \; e^{-i\vec{k}\vec{R}_1} \left\{ \int d\vec{r} d\vec{r}' w^*_{\alpha 0}(\vec{r}-\vec{R}_1) w_{\beta 0}(\vec{r}) \frac{e^{-i\vec{g}\vec{R}_2}}{|\vec{r}-\vec{r}'-\vec{R}_2|} w_{\gamma 0}(\vec{r}'-\vec{R}_3) w^*_{\delta 0}(\vec{r}') \right\} e^{i\vec{k}' R_3} = M^{*\alpha}_{ij}(\vec{k},\vec{g}) \, V^g_{\alpha\beta} \, M^\beta_{lm}(\vec{k}',\vec{g})$$

$$e^{-i\vec{k}\vec{R}_1} \left\{ \int d\vec{r} d\vec{r}' w^*_{\alpha 0}(\vec{r}-\vec{R}_1) w_{\beta 0}(\vec{r}) \frac{e^{-i\vec{g}\vec{R}_2}}{|\vec{r}-\vec{r}'-\vec{R}_2|} w_{\gamma 0}(\vec{r}'-\vec{R}_3) w^*_{\delta 0}(\vec{r}') \right\} e^{i\vec{k}' R_3} = \sum_{ijlm} \underline{U^{k*}_{i\alpha}} \, \underline{U^{k+g}_{j\beta}} \, U^{k'}_{l\gamma} \, U^{k'+g\,*}_{m\delta} \, M^*_{ij}(\vec{k},\underline{\vec{g}}) \, V^g_{\alpha\beta} \, M_{lm}(\vec{k}',\vec{g})$$

$$\int d\vec{r} d\vec{r}' w^*_{\alpha 0}(\vec{r}-\vec{R}_1) w_{\beta 0}(\vec{r}) \frac{e^{-i\vec{g}\vec{R}_2}}{|\vec{r}-\vec{r}'-\vec{R}_2|} w_{\gamma 0}(\vec{r}'-\vec{R}_3) w^*_{\delta 0}(\vec{r}') = \sum_k \left\{ e^{i\vec{k}\vec{R}_1} \left(U^{k\dagger} M^{*m}(\vec{k},\vec{g}) U^{k+g} \right)_{\alpha\beta} \right\} V^g_{mm'} \sum_{k'} \left\{ \left(U^{k'T} M^{m'}(\vec{k}',\vec{g}) U^{k'+g\,*} \right)_{\gamma\delta} e^{-i\vec{k}'\vec{R}_3} \right\}$$

$$M^m_{ij}(k,g) = \langle \chi^g_m | \psi_{ik} \psi^*_{jk+g} \rangle = \int \chi^{g*}_m(\vec{r}) \, w_{\alpha 0}(\vec{r}-\vec{R}_1) \, w^*_{\beta 0}(\vec{r}-\vec{R}_2) \, U^{k*}_{i\alpha} U^{k+g}_{j\beta} \, e^{+i\vec{k}\vec{R}_1 - i(k+g)\vec{R}_2}$$

$$= \int \chi^{g*}_m(\vec{r}+\vec{R}_2) \, w_{\alpha 0}(\vec{r}+\vec{R}_2-\vec{R}_1) \, w^*_{\beta 0}(\vec{r}) \, U^{k*}_{i\alpha} U^{k+g}_{j\beta} \, e^{i\vec{k}(\vec{R}_1-\vec{R}_2) - i\vec{g}\vec{R}_2}$$

$$\chi_g(\vec{r}+\vec{R}) = \chi_g(\vec{r}) e^{-i\vec{g}\cdot\vec{R}}$$

$$\chi^{g*}_m(\vec{r}+\vec{R}_2) = e^{+i\vec{g}\vec{R}_2} \chi^{g*}_m(\vec{r})$$

$$= \int \chi^{g*}_m(\vec{r}) \, w_{\alpha 0}(\vec{r}-\vec{R}_1) \, w^*_{\beta 0}(\vec{r}) \, U^{k*}_{i\alpha} U^{k+g}_{j\beta} \, e^{i\vec{k}\vec{R}_1} = \langle \chi^g_m | w_{\alpha R_1} w^*_{\beta 0} \rangle \, U^{k*}_{i\alpha} U^{k+g}_{j\beta} \, e^{i\vec{k}\vec{R}_1}$$

$$\sum_k \left(U^{kT} M^m_{(k,g)} U^{k+g*} \right)_{\alpha\beta} e^{-i\vec{k}\vec{R}_1} = \langle \chi^g_m | w_{\alpha R_1} w^*_{\beta 0} \rangle$$

$$\boxed{\sum_k \left(U^{k\dagger} M^{m*}_{(k,g)} U^{k+g} \right)_{\alpha\beta} e^{i\vec{k}\vec{R}_1} = \langle w_{\alpha R_1} w^*_{\beta 0} | \chi^g_m \rangle} \equiv W^{mg}_{\alpha\beta R_1}$$

$$\langle w_{\alpha R_1} w^*_{\beta 0} | w_{\alpha' R_2} w^*_{\beta' 0} \rangle = O_{\alpha\beta R_1, \alpha'\beta' R_2} = v^+ o \, v$$

$N_\alpha \sim 4$

$N_\alpha^2 \cdot N_R \sim 4 \cdot 4 \cdot 8 =$

$$\mathcal{E}_{qp} = \mathcal{E}^0 + Z(\Sigma - V_{xc})$$

$$Z = \frac{1}{1 - \frac{d\Sigma}{d\omega}(\mathcal{E}^0)} \qquad \Sigma = \Sigma_x + \Sigma_c(\mathcal{E}^0)$$

$$\omega - \mathcal{E}^0 - \Sigma_{xc}(\omega) + V_{xc} = 0$$

$$\Sigma_{xc}(\omega) \approx \Sigma_{xc}(\mathcal{E}^0) + \frac{d\Sigma_c}{d\omega}(\omega - \mathcal{E}^0)$$

$$\omega\left(1 - \frac{d\Sigma_c}{d\omega}\right) - \mathcal{E}^0\left(1 - \frac{d\Sigma_c}{d\omega}\right) - \Sigma_{xc}(\mathcal{E}^0) + \mathcal{E}^0 + V_{xc} = 0$$

$$\frac{\omega}{Z} = \frac{\mathcal{E}^0}{Z} + \Sigma_{xc}(\mathcal{E}^0) - V_{xc}$$

$$\omega = \mathcal{E}^0 + Z(\Sigma_{xc}(\mathcal{E}^0) - V_{xo})$$

$$\omega - \mathcal{E}^0 I - \hat{\Sigma}_{xc}(\omega) + V_{xc} = 0$$

$$\omega - \mathcal{E}^0 I - \hat{\Sigma}_{xc}(\mathcal{E}^0) - \frac{d\hat{\Sigma}_{xc}}{d\omega}(\mathcal{E}^0)(\omega - \mathcal{E}_0) + V_{xc} = 0$$

$$\omega - \varepsilon_2 - \Sigma_{22}(\varepsilon_1) - \frac{d\Sigma_{12}}{d\omega}(\omega - \varepsilon_1)$$

$$(\omega - \varepsilon_1)\left(1 - \frac{d\Sigma_{22}}{d\omega}\right) + \varepsilon_1 - \varepsilon_2 - \Sigma_{22}(\varepsilon_1)$$

$$\begin{matrix} \Sigma_{11}(\varepsilon_1), & \Sigma_{12}(\quad) \\ \Sigma_{21}(\quad), & \Sigma_{22}(\varepsilon_2) \end{matrix}$$

$$\begin{pmatrix} \omega - \varepsilon_1 - \Sigma_{11}(\omega) & -\Sigma_{12}(\omega) \\ -\Sigma_{12}(\omega) & \omega - \varepsilon_2 - \Sigma_{22}(\omega) \end{pmatrix} = \begin{pmatrix} (\omega - \varepsilon_1)\left(1 - \frac{d\Sigma_{11}}{d\omega}(\varepsilon_1)\right) - \Sigma_{11}(\varepsilon_1) & -\Sigma_{12}(x_1) \\ -\Sigma_{12}(x_1) & (\omega - \varepsilon_2)\left(1 - \frac{d\Sigma_{22}}{d\omega}(\varepsilon_2)\right) - \Sigma_{22}(\varepsilon_2) \end{pmatrix}$$

$$\underline{x_1 = \varepsilon_1, \varepsilon_2}$$

$$\left[\frac{(\omega - \varepsilon_1)}{z_1} - \Sigma_{11}(\varepsilon_1)\right]\left[\frac{\omega - \varepsilon_2}{z_2} - \Sigma_{22}(\varepsilon_2)\right] = \left[\Sigma_{12}(x_1)\right]^2$$

$$\left[\omega - (\varepsilon_1 + z_1\Sigma_{11}(\varepsilon_1))\right]\left[\omega - (\varepsilon_2 + z_2\Sigma_{22}(\varepsilon_2))\right] - z_1 z_2 \cdot \Sigma_{12}^2 = 0$$

$$\omega = \tfrac{1}{2}(a_1 + a_2) \pm \tfrac{1}{2}\sqrt{(a_1 - a_2)^2 + 4b}$$

$$\omega = \tfrac{1}{2}\left(\varepsilon_1 + z_1\Sigma_{11}(\varepsilon_1) + \varepsilon_2 + z_2\Sigma_{22}(\varepsilon_2)\right) \pm \tfrac{1}{2}\sqrt{\left(\varepsilon_1 + z_1\Sigma_{11}(\varepsilon_1) - \varepsilon_2 - z_2\Sigma_{22}(\varepsilon_2)\right)^2 + 4 z_1 z_1 \Sigma_{12}^2}$$

$$(\omega - \varepsilon_1)I = \begin{pmatrix} z_1\Sigma_{11}(\varepsilon_1), & z_1\Sigma_{12}(\varepsilon_1) \\ z_1\Sigma_{12}(\varepsilon_1), & z_1[\Sigma_{22}(\varepsilon_1) + \varepsilon_2 - \varepsilon_1] \end{pmatrix}$$

$$Ax - \lambda x = 0$$

$$\mathrm{Det}(A - \lambda I) = 0$$

$$\mathrm{eigval}\begin{pmatrix} \varepsilon_1 + z_1\Sigma_{11}(\varepsilon_1), & z_1\Sigma_{12}(\varepsilon_1) \\ z_1\Sigma_{12}(\varepsilon_1) & \varepsilon_1 + z_1(\Sigma_{22}(\varepsilon_1) + \varepsilon_2 - \varepsilon_1) \end{pmatrix}$$

Quasiparticle equation with off-diagonal sigma

$$\omega - \hat{\varepsilon} - \hat{\Sigma}_{xc}(\omega) + V_{xc} = 0$$

$$\omega - \varepsilon_i + \varepsilon_i \cdot I - \hat{\varepsilon} - \hat{\Sigma}_{xc}(\varepsilon_i) - \frac{\partial \Sigma_{xc}}{\partial \omega}(\varepsilon_i)(\omega - \varepsilon_i) + \hat{V}_{xc} = 0$$

$$I - \frac{\partial \Sigma_{xc}}{\partial \omega}(\varepsilon_i) = \hat{Z}_i^{-1}$$

$$\hat{Z}_i^{-\frac{1}{2}}(\omega - \varepsilon_i)\hat{Z}_i^{-\frac{1}{2}} = \hat{\varepsilon} - \varepsilon_i I + \hat{\Sigma}_{xc}(\varepsilon_i) - \hat{V}_{xc}$$

$$\underbrace{\hat{Z}_i^{\frac{1}{2}}\left(\hat{\varepsilon} - \varepsilon_i I + \hat{\Sigma}_{xc}(\varepsilon_i) - \hat{V}_{xc}\right)\hat{Z}_i^{\frac{1}{2}}}_{\Delta\hat{H}} - (\omega - \varepsilon_i) I = 0$$

$(\Delta\hat{H} - \lambda I)\vec{x} = 0$ $\quad \vec{x}$ closest to $\begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ 0 \\ 0 \end{pmatrix} \leftarrow i$ is correct eigenvalue λ_i

so that $\underline{\underline{\omega = \varepsilon_i + \lambda_i}}$

<u>S.C.</u>

$$\omega - \hat{\varepsilon}_0 - \Sigma_{xc}(\omega) + V_{xc} = 0 \qquad \omega \approx \varepsilon_i$$

$$\omega - \hat{\varepsilon}_0 - \hat{\Sigma}_{xc}(\varepsilon_i) - \frac{d\hat{\Sigma}_{xc}}{d\omega}(\omega - \varepsilon_i) + V_{xc} = 0$$

$$Z_i^{-\frac{1}{2}}(\omega - \varepsilon_i) I \, Z_i^{-\frac{1}{2}} + (\varepsilon_i I - \hat{\varepsilon}_0) - \hat{\Sigma}_{xc}(\varepsilon_i) + V_{xc} = 0$$

$$\left(1 - \frac{d\Sigma}{d\omega}\right)^{-1} = Z$$

$$\left(1 - \frac{1}{Z}\right) = \frac{d\Sigma}{d\omega}$$

$$(\omega - \varepsilon_i) = \underbrace{Z_i^{1/2}\left(\hat{\varepsilon}_0 - \varepsilon_i I + \Sigma_{xc}(\varepsilon_i) - V_{xc}\right) Z_i^{\frac{1}{2}}}_{\Delta\hat{H}}$$

$$(\Delta\hat{H} - \lambda I)\vec{x} = 0 \qquad \omega = \varepsilon_i + \lambda_i$$

$$\varepsilon_i + \left(\Sigma_{xc}(\varepsilon_i) - V_{xc}\right) + \varepsilon_i^0 - \varepsilon_i$$

Z ? $\quad \varepsilon^{LDA} \quad \varepsilon^{sc}$

$$\omega - \varepsilon^0 + V_{xc} - (I - Z_2^{-1})(\omega - \varepsilon_2^i) = 0$$

$$(\omega - \varepsilon_{2i}^{q})I + (\varepsilon_{2i} I - \varepsilon_0) + V_{xc} - (I - Z_2^{-1})(\omega - \varepsilon_2^i)$$

$$Z_2^{-1}(\omega - \varepsilon_2^i)$$

- We added wannier90 interpolation
- We added off-diagonal self-energy capability.
- We added contour deformation technique.

$$Q_m^2 \left(1 - 2\,0.25 \frac{R_m^2}{R_{mm}^2} + (0.25)^2 \frac{R_m^4}{R_{mn}^4} + 0.25 \frac{R_m^6}{R_{mn}^6}\right)$$

$$Q_m^2 \left(\left[1 - 0.25\left(\frac{R_m}{R_{mm}}\right)^2\right]^2 + 0.25\left(\frac{R_m}{R_{m.m}}\right)^6\right)$$