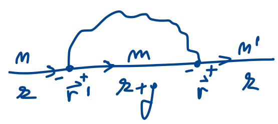
Some notes on PyGW implementation

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

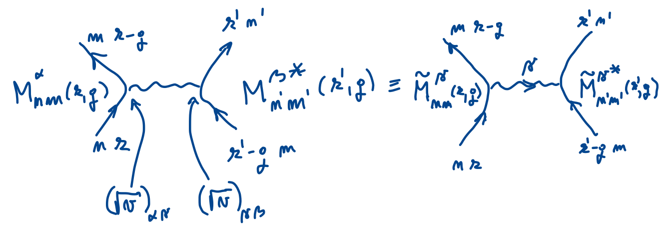


$\vec r' \longrightarrow \vec r$, $+$: $G(\vec r,\vec r')=-\langle T_\tau\,\psi(\vec r)\psi^\dagger(\vec r')\rangle=\psi_{mk}(\vec r)\,\frac{1}{\omega+\mu-\varepsilon_k}\,\psi^*_{mk}(\vec r')$

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

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

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



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

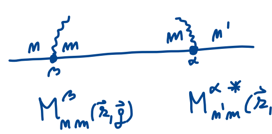
$$M^{\alpha*}_{m'm}(\vec k,\vec q)\,\chi^{\vec q*}_\alpha(\vec r)\,W_\Omega(\vec r,\vec r')\,M_{mm}(\vec k,\vec q)\,\chi^{\vec q}_\beta(\vec r')$$

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

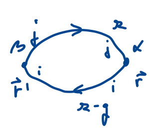
matrix form
$$v_{\alpha\beta}\equiv(\sqrt v)_{\alpha\gamma}\,(\sqrt v)_{\gamma\beta}$$

$$\Sigma_{mm'k}(i\omega)=-\frac1\beta\sum_{i\Omega}\sum_{\substack{mq\\ \alpha\beta}}M^{\alpha*}_{m'm}(\vec k,\vec q)\,W_{\alpha\beta}(q,\Omega)\,M^\beta_{mm}(\vec k,\vec q)\,\frac{1}{i\omega-i\Omega+\mu-\varepsilon^m_{k-q}}$$

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



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



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

$$P_{\alpha\beta}(\vec q,i\Omega)=\sum_{\substack{ij\\ \vec k}}M^\alpha_{ji}(\vec k,\vec q)\,M^{\beta*}_{ji}(\vec k,\vec q)\,\underbrace{\frac1\beta\sum_{i\omega}\frac{1}{i\omega-\varepsilon^j_k}\,\frac{1}{i\omega-i\Omega-\varepsilon^i_{k-q}}}_{F_{ji}(\vec k,\vec q;i\Omega)}$$

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

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

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

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

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 N.

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

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

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

Product basis :

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

LAPW basis

M.T.

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

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

$$A_{mk a\kappa_1 l_1 m_1} A^*_{m\,k-q\,a\kappa_2 l_2 m_2} \cdot \langle l_1 m_1 | LM\, l_2 m_2 \rangle^* \int dr_a r_a^2\, N_{aNLM}(r_a)\, u_{a\kappa_1 l_1}(r_a)\, u_{a\kappa_2 l_2}(r_a)$$

$$M_{mm}^{\alpha}(\vec{k},\vec{q}) = \sum_{\substack{\kappa_1 l_1 m_1 \\ \kappa_2 l_2 m_2 \\ NLM}} e^{-i\vec{q}\cdot\vec{R}_a} A_{mk a\kappa_1 l_1 m_1} A^*_{m\,k-q\,a\kappa_2 l_2 m_2} \cdot \langle l_1 m_1 | LM\, l_2 m_2 \rangle^* \int dr_a r_a^2\, N_{aNLM}(r_a)\, u_{a\kappa_1 l_1}(r_a)\, u_{a\kappa_2 l_2}(r_a)$$

Interstitial:

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

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

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

1) χ_α and χ_β in M.T.

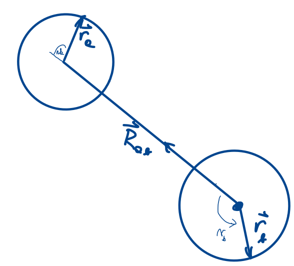
$$V_{\alpha\beta} = \iint Y^*_{L_1M_1}(\hat{r}_a)\,Y_{L_2M_2}(\hat{r}_b)\,\mathcal{N}_{aN_1L_1M_1}(r_a)\,\mathcal{N}_{bN_2L_2M_2}(r_b)\,\frac{e^{-i\vec{q}R_{ab}}}{|\vec{r}_a-\vec{r}_b+\vec{R}_{ab}|}\,d^3r_a\,d^3r_b$$

Same atom for a and b:

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

$$V_{\alpha\beta} = \delta_{L_1M_1=L_2M_2=lm}\sum_{N_1N_2}\frac{4\pi}{2l+1}\cdot\underbrace{\int dr_a\,r_a^2\int dr'\,r_a'^2\,\frac{r_<^l}{r_>^{l+1}}\Big|_{(r_a,r_a')}\,\mathcal{N}_{aN_1lm}(r_a)\,\mathcal{N}_{aN_2lm}(r_a')}_{\langle \mathcal{N}_{aN_1lm}|\frac{r_<^l}{r_>^{l+1}}|\mathcal{N}_{aN_2lm}\rangle}$$

Different atoms:



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

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

$\vec{R}_a = \Delta\vec{R}+\vec{R}$ ← lattice vector

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

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

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

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

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

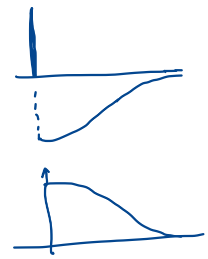
Ewald's summation

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

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

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

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



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

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

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

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

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

$$\rho_i^S(\vec{r}) = q_i \, \delta(\vec{r} - \vec{r}_i) - q_i \, G(\vec{r} - \vec{r}_i) \Rightarrow \phi_i^S = \frac{q_i}{4\pi\varepsilon_0 r} \mathrm{Erfc}\left(\frac{r}{\eta}\right)$$

$$\rho_i^L(\vec{r}) = q_i \, G(\vec{r} - \vec{r}_i) \Rightarrow \phi_i^L = \frac{q_i}{4\pi\varepsilon_0 r} \mathrm{Erf}\left(\frac{r}{\eta}\right)$$

$$\phi_i^S + \phi_i^L = \frac{q_i}{4\pi\varepsilon_0 r}$$

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

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

$$- \frac{1}{\sqrt{\pi} \eta} \sum_{ij} q_i^2 \delta_{ij}$$

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:

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

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

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

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

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

At $L=0$:

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

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

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

$$\parallel$$

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

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: $\langle u^{e'}_{N_1L_1M_1}(\vec{r}) | \vec{K}+\vec{G}\rangle_{MT} \frac{1}{|\vec{q}+\vec{K}|^2} \langle q+\vec{K} | u^e_{N_2L_2M_2}\rangle$

  The alternative for MT part is

$$\langle u^{e'}_{N_1L_1M_1}(\vec{r}) | \frac{e^{-i\vec{q}(\vec{R}'-\vec{R})}}{|\vec{r}'-\vec{r}|} | u^e_{N_2L_2M_2}(\vec{r}) \rangle$$

Muffin-tin part

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

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

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

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

Hence

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

If on the same atom then

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

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 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 $\langle r|\vec{K}\rangle = e^{i\vec{K}\cdot\vec{r}}$, 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]

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

ngq ngq-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]

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

ngq ngq-barc

- Next we compute

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

product basis on given atom a

- Finally we compute

$$\text{mpwipw} * \text{Vmatit} =$$

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

Laplace multicenter expansion

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

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

Alternative way to Calculate V from plane wave expression

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

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

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

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

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

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

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

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

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

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

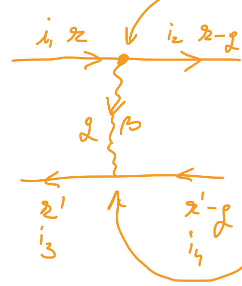
bvcvm $=$ self.Vmat $\cdot \sqrt{\mathcal{E}}$ so that $V_{mat} =$ bvcvm $\cdot$ bvcvm^{+}

bvcvm $= A_{\alpha i}\sqrt{\mathcal{E}_i}$ and $V_{mat} = A_{\alpha i}\sqrt{\mathcal{E}_i}\sqrt{\mathcal{E}_i}\, A^{*}_{\beta i}$

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

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

$minm\,(k, q, i_1, i_2, \beta)$



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

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

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

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

$$\Sigma^{x}_{i_1} = -\sum_{\beta, q, i_2} minm(i_1, i_2, k, q, \beta)\; minm(i_3, i_2, k, q, \beta)\, f(\mathcal{E}_2)\, w_q$$

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

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

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

<u>Interstitial</u>:

$$\langle e^{i\vec{G}_p\vec{r}} | e^{i\vec{G}_1\vec{r} - i\vec{G}_2\vec{r}} \rangle$$

from vector file

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

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

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

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

mpg ; mpg-barc

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

mpg ; mpg-barc

<u>Muffin-Tin</u>

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

nstart : nend

nstart : nend

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

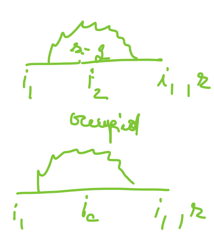
<u>Core states</u> :

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

core

cnst : cnend ; cst : cend

for exchange



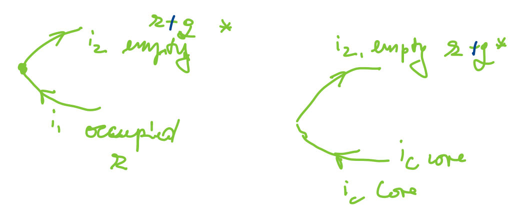
$$M_{i_c i_2}(\vec{k}+\vec{q}) = \langle N Y_{LM} | \psi_{i_c} \psi^*_{i_2 \vec{k}+\vec{q}} \rangle$$

core

$\vec{k}+\vec{q}$ instead of $\vec{k}$

empty

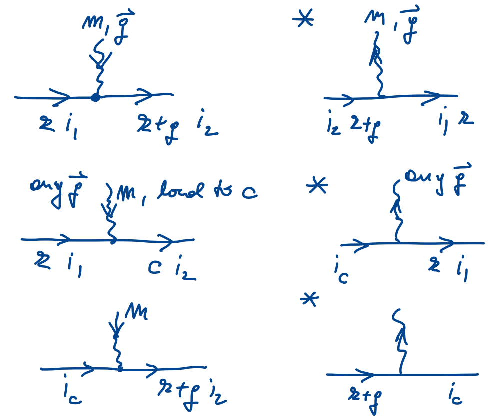
correlation:



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

These core are q-independent:

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

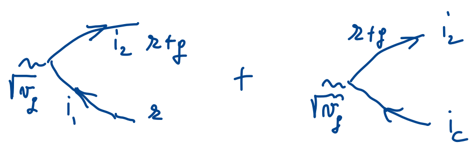


$M^{m}_{i_c i_2}(\vec{k}+\vec{q}) \equiv \langle \chi_{m} | \psi_{i_c}\, \psi^{*}_{i_2\, k+q} \rangle = M^{*}_{i_2 i_c}(\vec{k}+\vec{q})$

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

external $\quad$ occupied

2) correlation self-energy $\quad M^{m}_{i_1 i_2}(\vec{k}_{irr},\vec{q})$

external $\quad$ internal, mostly occupied + some empty

3) polarization $\quad M^{m}_{i_1 i_2}(\vec{k},\vec{q})$, $\quad M^{*}_{i_2 i_c}(\vec{k}+\vec{q})$

all

occupied $\quad$ empty

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

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

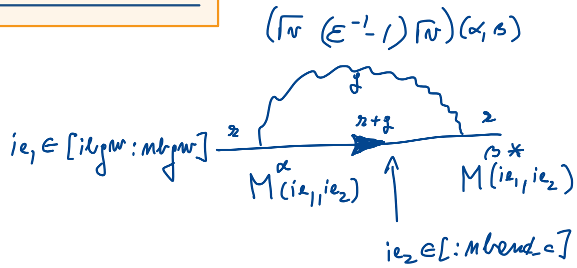
sx:	k_{irr}	0:14 , 0:4	0:14 , core
sc:	k_{irr}	0:14 , 0:225	0:14 , core
polar:	k_{all}	0:4 , 4:209	4:209 , core

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

dot $\quad$ 2:10 , (9:49)

matmul $\quad$ 2:20 $\quad$ (10:9)

$\boxed{\text{Convolution}}$



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

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

$\underline{W_q(-i\Omega_m) = W_q(i\Omega_m) \in \text{Hermitian}}$

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

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

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

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

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

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

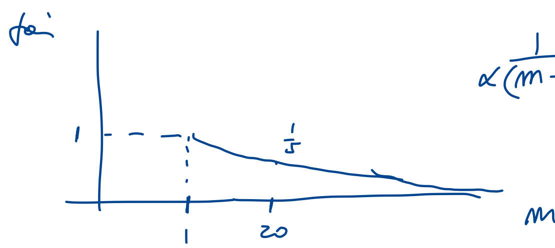
$$C(i_2 l; i\omega) = \frac{(\varepsilon_{i_2} - i\omega)}{\pi} \int_0^L \frac{[U_l(i\Omega) - U_l(i\omega)]}{(\varepsilon_{i_2} - i\omega)^2 + \Omega^2}\, d\Omega + U_l(i\omega)\, \underbrace{\frac{1}{\pi} \arctan\left(\frac{L}{(\varepsilon_2 - i\omega)}\right)}_{\text{instead of } \frac{1}{2}\,\mathrm{sign}(\varepsilon_2)}$$

Important change.

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

$m = 1 \Rightarrow 1$

$m = \infty \Rightarrow 0$



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

$19\alpha + 1 = 5$

$19\alpha = 4$

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

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

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

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

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

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

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

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

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

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

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

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

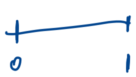
$$\omega = w\tan\left(x\cdot(\pi-2\delta)-\frac{\pi}{2}+\delta\right)$$

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

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

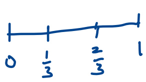
linspace [0, 1, 2N]

$N=1$



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

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

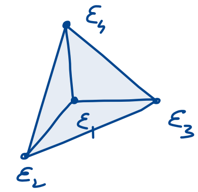
$$\Big(\sum_{\vec{R}} \langle \chi_i(\vec{r}') | V(\vec{r}-\vec{r}') | \chi_j(\vec{r}) \rangle e^{-i\vec{g}\vec{R}} - \lambda\delta_{ij} \Big)^{-1}$$

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

Tetrahedron integration:

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

where $\varepsilon(\vec r) = \varepsilon_1 + (\varepsilon_2 - \varepsilon_1)x + (\varepsilon_3 - \varepsilon_1)y + (\varepsilon_4 - \varepsilon_1)z$



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

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

Tetrahedron method:

$$\varepsilon(x,y,z) = \varepsilon_1 + (\varepsilon_2 - \varepsilon_1)x + (\varepsilon_3 - \varepsilon_1)y + (\varepsilon_4 - \varepsilon_1)z$$

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

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

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

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

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

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

$\varepsilon_k = \varepsilon_F$ and $\begin{aligned} \xi &= 0 \\ \eta &= 0 \\ \varphi &= 0 \end{aligned}$

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

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

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

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

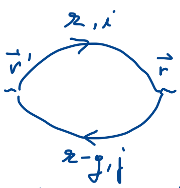
$$2\int \frac{d^3k}{(2\pi)^3}\left[\frac{f(\varepsilon_k)f(-\varepsilon_{k-q})}{i\Omega_m - (\varepsilon_{k-q} - \varepsilon_k)} + \frac{f(-\varepsilon_{k+q})f(\varepsilon_k)}{-i\Omega_m - (\varepsilon_{k+q} - \varepsilon_k)}\right]$$

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

$$\int \frac{d^3k}{(2\pi)^3}\left[\underset{\substack{\uparrow\\ k \text{ occupied}\\ k-q \text{ empty}}}{\frac{f(\varepsilon_k)f(-\varepsilon_{k-q})(-2\varepsilon_{\Delta,q})}{\Omega_m^2 + \varepsilon_{\Delta q}^2}} + \underset{\substack{\uparrow\\ k \text{ occupied}\\ k+q \text{ empty}}}{\frac{f(\varepsilon_k)f(-\varepsilon_{k+q})(-2\varepsilon_{\Delta,-q})}{\Omega_m^2 + \varepsilon_{\Delta,-q}^2}}\right]$$

Imaginary axis

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



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

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

$$-\int\frac{dx}{\pi}\underset{f(x)}{\underset{\shortparallel}{f(x+i\Omega)}}\frac{1}{x + i\Omega + \mu - \varepsilon_{ki}}\,\mathrm{Im}\left(\frac{1}{x + \mu - \varepsilon_{k-qj} + i\delta}\right)$$

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

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

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

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

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

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

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

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

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

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

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

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

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

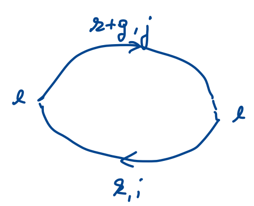
$$\chi_\alpha(\vec{r}) \underbrace{\langle \chi_\alpha | \psi_{ki} \psi^*_{k-qj} \rangle}_{M^\alpha_{ij}(k,-q)} \underbrace{\langle \psi_{ki} \psi^*_{k-qj} | \chi_\beta \rangle}_{M^{\beta *}_{ij}(k,-q)} \chi^*_\beta(\vec{r}) \qquad kcw(ij, k, -q, \Omega)$$

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

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

$kcw($i_occ, i_unp, $k, \Omega)$

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



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

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

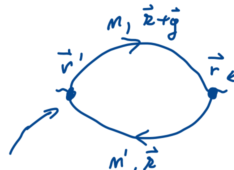
$k, i \to k' - q, j'$

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

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

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

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



$\langle n,k+q|e^{i(\vec{q}+\vec{G})\vec{r}}\frac{\sqrt{4\pi}}{|\vec{q}+\vec{G}|}|n'k\rangle$

$\langle n'k|e^{-i(\vec{q}+\vec{G}')\vec{r}}\frac{\sqrt{4\pi}}{|\vec{q}+\vec{G}'|}|n,k+q\rangle$

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

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

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

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

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

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

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

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

$n==n'$:

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

$n\neq n'$:

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

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

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

$n=n'$

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

$n\neq n'$

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

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

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

$$pm[i_1,i_2] = 2\sqrt{\frac{\pi}{V_{cell}}} \frac{\frac{1}{\sqrt{3}}\sum_\alpha p^{k,\alpha}_{i_1 i_2}}{\varepsilon_{k i_1} - \varepsilon_{k i_2}} \; ; \quad epsW1(\alpha,\omega) = \sum_{k, i_1 i_2} \sqrt{N_{core}} \langle X^\alpha | \psi^*_{k+q\, i_2} \psi_{k i_1} \rangle \frac{f(\varepsilon_{k i_1}) - f(\varepsilon_{k+q\, i_2})}{i\omega + \varepsilon_{k i_1} - \varepsilon_{k+q\, i_2}} 2\sqrt{\frac{\pi}{V_{cell}}} \frac{\frac{1}{\sqrt{3}}\sum_\alpha p^{k,\alpha}_{i_1 i_2}}{\varepsilon_{k i_1} - \varepsilon_{k i_2}} \equiv W_\mu(\omega)$$

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

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

$$w2b = \sum_\beta epsW1(\beta,\omega) [\varepsilon^{-1}_q(\omega)]^{\beta\alpha} \; ;$$

$$\varepsilon_{qwt} = bw1 \otimes \frac{1}{head - WW} \otimes w2b$$

gap paper:

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

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

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

gap-paper:

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

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

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

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

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

$$\langle \psi_{M_1 z}|\vec\nabla|\psi_{M_2 z}\rangle = a^{z*}_{M_1\ell_1m_1}\, a^{z}_{M_2\ell_2m_2}\, \langle u_{\ell_1} Y_{\ell_1m_1}\left(\vec e_r \frac{\partial}{\partial r} + \frac{1}{r}\nabla_{\theta\varphi}\right) Y_{\ell_2m_2} u_{\ell_2}\rangle =$$

$$= a^{z*}_{M_1\ell_1m_1}\, a^{z}_{M_2\ell_2m_2}\left\{\langle u_{\ell_1}|\frac{d}{dr}|u_{\ell_2}\rangle \underbrace{\langle Y_{\ell_1m_1}|\vec e_r|Y_{\ell_2m_2}\rangle}_{I^{(1)}_{\ell_1m_1\ell_2m_2}} + \langle u_{\ell_1}|\frac{1}{r}|u_{\ell_2}\rangle \underbrace{\langle Y_{\ell_1m_1}|r\vec\nabla|Y_{\ell_2m_2}\rangle}_{I^{(2)}_{\ell_1m_1\ell_2m_2}}\right\}$$

$$= a^{z*}_{M'\ell'm'}\, a^{z}_{M\ell m}\left\{\langle u_{\ell'}|\frac{d}{dr}|u_\ell\rangle \begin{pmatrix} \frac12 a(\ell,m)\delta_{\ell'=\ell+1}\delta_{m'=m+1} - \frac12 a(\ell',-m')\delta_{\ell'=\ell-1}\delta_{m'=m+1} - \frac12 a(\ell,-m)\delta_{\ell'=\ell+1}\delta_{m'=m-1} + \frac12 a(\ell',m')\delta_{\ell'=\ell-1}\delta_{m'=m-1} \\ -\frac{i}{2} a(\ell,m)\delta_{\ell'=\ell+1}\delta_{m'=m+1} + \frac{i}{2} a(\ell',-m')\delta_{\ell'=\ell-1}\delta_{m'=m+1} - \frac{i}{2} a(\ell,-m)\delta_{\ell'=\ell+1}\delta_{m'=m-1} + \frac{i}{2} a(\ell',m')\delta_{\ell'=\ell-1}\delta_{m'=m-1} \\ f(\ell,m)\delta_{\ell'=\ell+1}\delta_{m'=m} + f(\ell'm')\delta_{\ell'=\ell-1}\delta_{m'=m} \end{pmatrix}\right.$$

$$\left. + \langle u_{\ell'}|\frac{1}{r}|u_\ell\rangle \begin{pmatrix} -\frac{\ell}{2} a(\ell,m)\delta_{\ell'=\ell+1}\delta_{m'=m+1} - \frac{(\ell+1)}{2} a(\ell',-m')\delta_{\ell'=\ell-1}\delta_{m'=m+1} + \frac{\ell}{2} a(\ell,-m)\delta_{\ell'=\ell+1}\delta_{m'=m-1} + \frac{\ell+1}{2} a(\ell',m')\delta_{\ell'=\ell-1}\delta_{m'=m-1} \\ i\frac{\ell}{2} a(\ell,m)\delta_{\ell'=\ell+1}\delta_{m'=m+1} + i\frac{(\ell+1)}{2} a(\ell',-m')\delta_{\ell'=\ell-1}\delta_{m'=m+1} + i\frac{\ell}{2} a(\ell,-m)\delta_{\ell'=\ell+1}\delta_{m'=m-1} + i\frac{\ell+1}{2} a(\ell'm')\delta_{\ell'=\ell-1}\delta_{m'=m-1} \\ -\ell f(\ell,m)\delta_{\ell'=\ell+1}\delta_{m'=m} + (\ell+1) f(\ell'm')\delta_{\ell'=\ell-1}\delta_{m'=m} \end{pmatrix}\right\}$$

$$= a^{z*}_{M'\ell'm'}\, a^{z}_{M\ell m}\left\{\begin{pmatrix} \delta(\ell'=\ell+1|m'=m+1)\frac12 a(\ell,m)\langle u_{\ell'}|\frac{d}{dr}-\frac{\ell}{r}|u_\ell\rangle - \delta(\ell'=\ell-1|m'=m+1)\frac12 a(\ell',-m')\langle u_{\ell'}|\frac{d}{dr}+\frac{(\ell+1)}{r}|u_\ell\rangle \\ \delta(\ell'=\ell+1|m'=m+1)\left(-\frac{i}{2}\right) a(\ell,m)\langle u_{\ell'}|\frac{d}{dr}-\frac{\ell}{r}|u_\ell\rangle + \delta(\ell'=\ell-1|m'=m+1)\frac{i}{2} a(\ell',-m')\langle u_{\ell'}|\frac{d}{dr}+\frac{(\ell+1)}{r}|u_\ell\rangle \\ \delta(\ell'=\ell+1, m'=m) f(\ell,m)\langle u_{\ell'}|\frac{d}{dr}-\frac{\ell}{r}|u_\ell\rangle + \delta(\ell'=\ell-1|m'=m) f(\ell'm')\langle u_{\ell'}|\frac{d}{dr}+\frac{(\ell+1)}{r}|u_\ell\rangle \end{pmatrix} + \begin{pmatrix} -\delta(\ell'=\ell+1|m'=m-1)\frac12 a(\ell,-m)\langle u_{\ell'}|\frac{d}{dr}-\frac{\ell}{r}|u_\ell\rangle + \delta(\ell'=\ell-1|m'=m-1)\frac12 a(\ell'm')\langle u_{\ell'}|\frac{d}{dr}+\frac{\ell+1}{r}|u_\ell\rangle \\ -\delta(\ell'=\ell+1|m'=m-1)\frac{i}{2} a(\ell,-m)\langle u_{\ell'}|\frac{d}{dr}-\frac{\ell}{r}|u_\ell\rangle + \delta(\ell'=\ell-1|m'=m-1)\frac{i}{2} a(\ell',m')\langle u_{\ell'}|\frac{d}{dr}+\frac{\ell+1}{r}|u_\ell\rangle \\ 0 \end{pmatrix}\right\}$$

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

$$\langle\psi_{m'z}|\vec\nabla|\psi_{mz}\rangle = \begin{pmatrix} \langle\psi^{m'}_{\ell+1,m+1}|\frac12 a(\ell,m)\left(\frac{d}{dr}-\frac{\ell}{r}\right)\psi^m_{\ell m}\rangle - \langle\psi^{m'}_{\ell-1,m+1}|\frac12 a(\ell-1,-m-1)\left(\frac{d}{dr}+\frac{\ell+1}{r}\right)|\psi^m_{\ell m}\rangle \\ -i\langle\psi^{m'}_{\ell+1,m+1}|\frac12 a(\ell,m)\left(\frac{d}{dr}-\frac{\ell}{r}\right)\psi^m_{\ell m}\rangle + i\langle\psi^{m'}_{\ell-1,m+1}|\frac12 a(\ell-1,-m-1)\left(\frac{d}{dr}+\frac{\ell+1}{r}\right)|\psi^m_{\ell m}\rangle \\ \langle\psi^{m'}_{\ell+1,m}|f(\ell,m)\left(\frac{d}{dr}-\frac{\ell}{r}\right)|\psi^m_{\ell m}\rangle + \langle\psi^{m'}_{\ell-1,m}|f(\ell-1,m)\left(\frac{d}{dr}+\frac{(\ell+1)}{r}\right)|\psi^m_{\ell m}\rangle \end{pmatrix}$$

$$+ \begin{pmatrix} -\langle\psi^{m'}_{\ell+1,m-1}|\frac12 a(\ell,-m)\left(\frac{d}{dr}-\frac{\ell}{r}\right)|\psi^m_{\ell m}\rangle + \langle\psi^{m'}_{\ell-1,m-1}|\frac12 a(\ell-1,m-1)\left(\frac{d}{dr}+\frac{\ell+1}{r}\right)|\psi^m_{\ell m}\rangle \\ -\frac{i}{2}\langle\psi^{m'}_{\ell+1,m-1}|a(\ell,-m)\left(\frac{d}{dr}-\frac{\ell}{r}\right)|\psi^m_{\ell m}\rangle + \frac{i}{2}\langle\psi^{m'}_{\ell-1,m-1}|a(\ell-1,m-1)\left(\frac{d}{dr}+\frac{\ell+1}{r}\right)|\psi^m_{\ell m}\rangle \\ 0 \end{pmatrix}$$

$$\langle\psi_{m'z}|i\vec\nabla|\psi_{mz}\rangle = \begin{pmatrix} -\frac{i}{2}\overbrace{\left(-\langle\psi^{m'}_{\ell+1,m+1}|a(\ell,m)\left(\frac{d}{dr}-\frac{\ell}{r}\right)\psi^m_{\ell m}\rangle + \langle\psi^{m'}_{\ell,m}|a(\ell,-m)\left(\frac{d}{dr}+\frac{\ell+2}{r}\right)|\psi^m_{\ell+1,m-1}\rangle\right)}^{\text{pxpy}} \\ -\frac{1}{2}\left(-\langle\psi^{m'}_{\ell+1,m+1}|a(\ell,m)\left(\frac{d}{dr}-\frac{\ell}{r}\right)\psi^m_{\ell m}\rangle + \langle\psi^{m'}_{\ell,m}|a(\ell,-m)\left(\frac{d}{dr}+\frac{\ell+2}{r}\right)|\psi^m_{\ell+1,m-1}\rangle\right) \\ i\underbrace{\left(\langle\psi^{m'}_{\ell+1,m}|f(\ell,m)\left(\frac{d}{dr}-\frac{\ell}{r}\right)|\psi^m_{\ell m}\rangle + \langle\psi^{m'}_{\ell,m}|f(\ell,m)\left(\frac{d}{dr}+\frac{\ell+2}{r}\right)|\psi^m_{\ell+1,m}\rangle\right)}_{\text{pz}} \end{pmatrix}$$

$$\begin{pmatrix} -\frac{i}{2}\overbrace{\left(\langle\psi^{m'}_{\ell+1,m-1}|a(\ell,-m)\left(\frac{d}{dr}-\frac{\ell}{r}\right)|\psi^m_{\ell m}\rangle - \langle\psi^{m'}_{\ell,m}|a(\ell,m)\left(\frac{d}{dr}+\frac{\ell+2}{r}\right)|\psi^m_{\ell+1,m+1}\rangle\right)}^{\text{pxmpy}} \\ \frac12\left(\langle\psi^{m'}_{\ell+1,m-1}|a(\ell,-m)\left(\frac{d}{dr}-\frac{\ell}{r}\right)|\psi^m_{\ell m}\rangle - \langle\psi^{m'}_{\ell,m}|a(\ell,m)\left(\frac{d}{dr}+\frac{\ell+1}{r}\right)|\psi^m_{\ell+1,m+1}\rangle\right) \\ 0 \end{pmatrix}$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\langle | -i\vec{\nabla} | \rangle^x = -\frac{i}{2}\left(pxpy + pxmy\right)$$
$$\langle | -i\vec{\nabla} | \rangle^y = -\frac{1}{2}\left(pxpy - pxmy\right)$$
$$\langle | -i\vec{\nabla} | \rangle^z = -i\,pz$$

Alternative expansion for core states

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

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

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

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

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

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

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

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

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

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

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

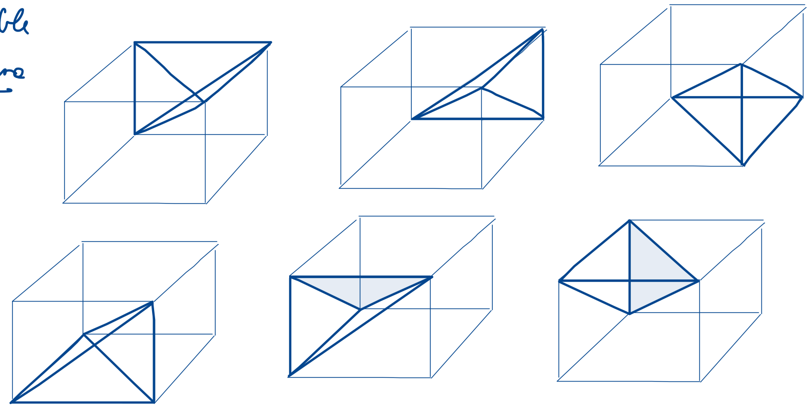
$$M^x_{ji} - i M^y_{ji} = \frac{1}{2}\langle \varphi_{l'm'} | \frac{d}{dr} - \frac{l}{r} | \varphi^c_{lm}\rangle \delta_{l'=l+1}\, 2a(l,-m)\,\delta_{m'=m-1} - \frac{1}{2}\langle \varphi_{l'm'} | \frac{d}{dr} + \frac{(l+1)}{r} | \varphi^c_{lm}\rangle \delta_{l'=l-1}\,\delta_{m'=m-1}\, 2a(l'm')$$

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

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

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

6 possible tetrahedra



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

Analytic continuation by PRL 74, 1827 (1996)

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

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:

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

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

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

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

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

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

Hence $\mathcal{R} = \sum_m |a_m|^2(1 + c_1|R_m|^2 + c_2|R_m|^4 + \ldots)$

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

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

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

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

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

The functional to minimize with constraint is

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

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

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

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

then:

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

$$Q_0 = \sum_i \lambda_i$$

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

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

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

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

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:

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

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

Next construct:

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

$$\Delta\mathcal{E}(z_i) \equiv \mathcal{E}(\vec{z}_i) - \mathcal{E}(\vec{z}_N)$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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 smoothness

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

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

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:

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

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

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

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

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

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

only # irreducible q-points

Recall Wannierization.

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

$$\langle \psi_{\vec{k}i} | \varphi_n(\vec{r}) \rangle \equiv U_{in}$$

2) Minimize the spread

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

3) Find the closest unitary transformation to $\langle \psi_{\vec{k}i} | \varphi_n(\vec{r}) \rangle = U s V$

The unitary transformation is $U \cdot V$

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

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

unitary hence identical eigenvalues

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

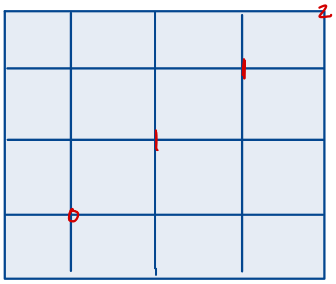
We could use the same unitary transformation to produce $\Sigma_{mn}(\vec{R})$ and evaluate $\Sigma_k(\vec{R})$ by F.T.

$\varepsilon > 0$: ω, $\Sigma_{z_i}(\omega)$

$\varepsilon < 0$: $-\omega$, $\Sigma^{*}_{z_i}(\omega)$

$\frac{0.16}{2} \sim 0.08$

$Z = \frac{1}{1+0.08} \sim 0.92$



$\vec{b}_1 = (0, 1, 1)$

$\vec{b}_2 = (1, 0, 1)$

$\vec{b}_3 = (1, 1, 0)$

$z = 0.25$

0: $(0.25, 0.25)$
1: $(0.5, 0.5)$
2: $(0.75, 0.75)$
3: $(1, 1)$

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

$N_\Omega(N_\alpha N_{ij} + N_\alpha^2 N_{ij}) \sim N_\Omega\cdot C\times(300)^2\times(4000) = N_\Omega\cdot C\cdot 3.6\times10^8$

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

$\alpha \sim 160$

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

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

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

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

original: $C\,N_\Omega\,N_\alpha^2 N_{ij}$ $\qquad 3.6\times10^{10}$

alternative: $C\,N_l\,N_\alpha^2 N_{ij} + C\,N_\alpha^2 N_l\,N_\Omega$ $\qquad 0.72\cdot10^{10} + 0.018\times10^{10} = 0.74\times10^{10}$

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$(\omega$-dl$, x_0, L, N\omega)$

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\mathrm{rcnr}(ij, r, i\Omega_n) = \sum_l U_l(i\Omega_n)\, \overline{\mathrm{rcnr}}(ij, r, l) \Big/ \sum_n U_l(i\Omega_n)\, \Delta\Omega_n$$

$$\sum_n \mathrm{rcnr}(ij, r, i\Omega_n)\, U_l(i\Omega_n)\, \Delta\Omega_n = \overline{\mathrm{rcnr}}(ij, r, l)$$

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

$$\chi_{\alpha\beta}(i\Omega_n) = \sum_l \chi_{\alpha\beta}(l)\, U_l(i\Omega_n)$$

$$\chi(\alpha\beta, l)\, U_l(i\Omega_n)$$

$$\uparrow$$

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

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

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

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

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

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: $G \cdot tauij(:, latom) + rotij(:,:, latom) \cdot \vec{G} \cdot pos(:, lfirst)$

rotation: $crotloc(:,:) \cdot rotij(:,:, latom) \cdot \vec{G}$

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

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

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

$$\Gamma_\alpha \vec{k} = R \cdot \vec{k}, \quad \text{phase } \vec{k} \cdot \vec{t}$$

$R \cdot \vec{k}$ ← tmat(:,:,N) ; $\vec{k} \cdot \vec{t}$ ← tau(:,N)

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

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

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

r2: $|rpg|^2$

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

timat[isym] + tau[isym]

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

rcar, timat[isym]

$\begin{pmatrix}a_l\\ b_l\\ c_l\end{pmatrix}$ ← $j_{lm}((\vec{q}_c+\vec{G}_c)R_{MT})$

?

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

---

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

$aK_n = |K_n|^2 \rightarrow j_{lm}(|\vec{q}_c+\vec{G}_c|R_{MT})$

gind(ig) = ig

isym: symmetry operation index

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

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

in semicartesian

$j_{lm}(|\vec{q}_c+\vec{G}_c|R_{MT})$

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

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

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

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

$$tizmat^T = rbas * timat^T * gbas = BRZ^{-1} \cdot timat^T \cdot BZZ$$

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

$$r_{ir} = rzicartes(i_0, i_1, i_2)$$
$$r = rzicartesian(i_0', i_1', i_2')$$

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

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

ORTHO : $BRZ(i_0', i_1', i_2') = imat \cdot BRZ\,(i_0, i_1, i_2)$

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

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

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

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

$rbas = gbas^{-1}$

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

$trotij$, $tauij$

$tizmat = rbas \cdot timat \cdot gbas$

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 $BR1 \approx \text{Identy} \cdot \frac{2\pi}{a}$

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

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

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

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

$Sb = BR2 \cdot (i_1, i_2, i_3) + Sk_-$

$RK(i) = |\, BR2 \cdot (i_1\, i_2\, i_3) + Sk_- |$

$KN(3,i) = BR2 \cdot (i_1\, i_2\, i_3) + Sk_-$

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

Pade

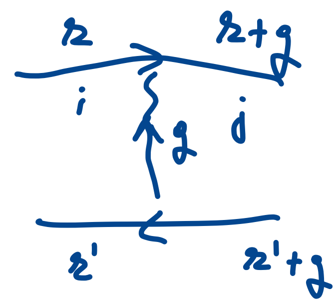
$$P(z) = \frac{\sum_{i=1}^{r} a_i z^{i-1}}{\sum_{i=1}^{r} b_i z^{i-1} + z^r} = \frac{(a_1, a_2, \dots a_r)\cdot(1, z, z^2, \dots z^{r-1})}{(b_1, b_2, \dots b_r)\cdot(1, z, z^2, \dots z^{r-1}) + z^r} \sim \frac{a_r}{z} + \frac{1}{z^2}\left(a_{r-1} - a_r b_r\right)$$

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

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

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

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



$$V_{\alpha\beta}(q)\cdot U_{\beta l} = U_{\alpha l} v_l \Rightarrow U^{+}_{l\alpha} V_{\alpha\beta}(q) U_{\beta l} = v_l$$

$$V_{\alpha\beta} = U v_l U^{+}$$

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

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

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)

GW^0 : 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 G^0W^0	Gap G^0W^0	X−Γ GW^0	Gap GW^0	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

$K = 4\times4\times4$;

$a = 10.262536\, a_B$; GGA, $K = 4\times4\times4$	$X-\Gamma$ G^0W^0	Gap G^0W^0	$X-\Gamma$ 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
5LO, RKmax = 8, Lmax = 3, Mb_emax = 20	1.224 eV	1.090 eV	1.292 eV	1.158 eV	–//–	575	466
5LO, RKmax = 8, Lmax = 3, Mb_emax = ∞	1.224 eV	1.090 eV	1.292 eV	1.158 eV	–//–	1407	544
5LO, RKmax = 8, Lmax = 5, Mb_emax = 20	1.227 eV	1.094 eV	1.295 eV	1.162 eV	–//–	1013	820
5LO, 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			

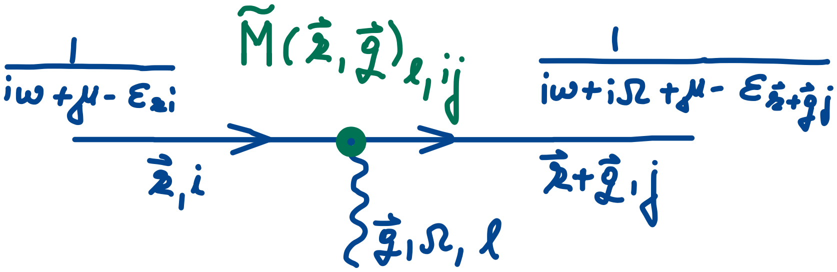
Ne

KS: 3.192 eV

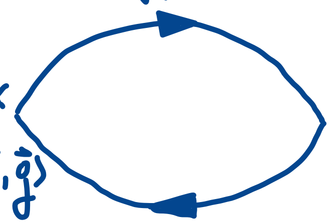
$10\times10\times10$: 3.085 eV

$12\times12\times12$: 3.146 eV

$\sim$ 3.10 eV

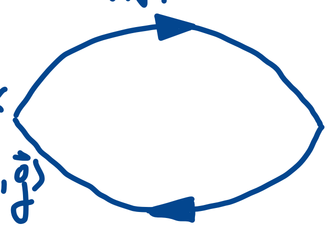


$P(q, i\Omega) = |\chi_\alpha\rangle M_{\alpha,ij}(\vec{k},\vec{q})$



$M^*_{\beta,ij}(\vec{k},\vec{q})\langle\chi_\beta|$

$\left(\sqrt{V_c}\, P(q, i\Omega)\sqrt{V_c}\right)_{\ell\ell'} = \tilde{M}_{\ell,ij}(\vec{k},\vec{q})$



$\tilde{M}^*_{\ell',ij}(\vec{k},\vec{q})$

$\Sigma_{ii'}(k, i\omega) =$

$M_{\alpha\, ij}(\vec{k},\vec{q})$ $M^*_{\beta i'j}(\vec{k},\vec{q})$ $=$ $\tilde{M}_{\ell' ij}(\vec{k},\vec{q})$

$\tilde{M}^*_{\ell, i'j}(\vec{k},\vec{q})$