Optics calculation in dmftopt

$$\sigma_{\alpha\beta}(\omega) = \frac{i}{\omega}\left[\Pi_{\alpha\beta}(q,\omega) + \frac{n_0 e^2}{m}\delta_{\alpha\beta}\right]_{q\to 0} \qquad \text{(From Mahan Eq. 3.8.9)}$$

$$\Pi_{\alpha\beta}(q,i\omega) = \int_0^\beta d\tau\, e^{i\omega\tau}\left(-\frac{1}{V}\right)\langle j^{\dagger}_{\alpha}(q,\tau)\, j_\beta(q,0)\rangle \qquad \text{(From Mahan Eq. 3.8.10)}$$

$$\vec{j}(\vec r) = \frac{e\hbar}{2mi}\sum_s \int\left[\hat\psi_s^\dagger(\vec r)\,\vec\nabla\hat\psi_s(\vec r) - \left(\vec\nabla\hat\psi_s^\dagger(\vec r)\right)\hat\psi_s(\vec r)\right]d^3r$$

Field operator $\hat\psi$ expanded in KS basis:

$$\hat\psi_s(\vec r) = \sum_i \psi_i(\vec r)\,\hat c_i$$

$$\vec{j}_q = \frac{e\hbar}{2mi}\int d^3r\, e^{i\vec q\vec r}\left[\psi_i^*(\vec r)\,\vec\nabla\psi_j(\vec r) - \left(\vec\nabla\psi_i^*(\vec r)\right)\psi_j(\vec r)\right] c_i^\dagger c_j$$

$$\vec v_{ij} \equiv \frac{e\hbar}{2mi}\int d^3r\left[\psi_{2i}^*(\vec r)\left(\vec\nabla\psi_{2j}(\vec r)\right) - \left(\nabla\psi_{2i}^*(\vec r)\right)\psi_{2j}(\vec r)\right] \underset{\text{by parts}}{=} \frac{e\hbar}{mi}\int d^3r\,\psi_{2i}^*(\vec r)\,\vec\nabla\psi_{2j}(\vec r)$$

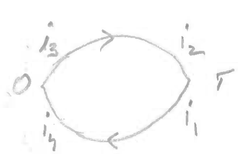
$$\vec v_{ij} = \underbrace{\left(\frac{e\hbar}{m a_0}\right)}_{\text{unit of velocity } [j\cdot V \Rightarrow Am]}\langle\psi_{2i}|-i a_0\vec\nabla|\psi_{2j}\rangle \qquad \text{Define } \tilde v_{ij} = \langle\psi_{2i}|-i a_0\vec\nabla|\psi_{2j}\rangle$$

has no units

$$\Pi_{\alpha\beta}(i\omega) = \int_0^\beta d\tau\, e^{i\omega\tau}\left(-\frac{1}{V}\right) v^\alpha_{i_1 i_2}\, v^\beta_{i_3 i_4}\langle c^\dagger_{i_1}(\tau)\, c_{i_2}(\tau)\, c^\dagger_{i_3}(0)\, c_{i_4}(0)\rangle$$

↓ Bubble approximation

$$\langle T_\tau c^\dagger_{i_1}(\tau)\, c_{i_4}(0)\rangle\langle T_\tau c_{i_2}(\tau)\, c^\dagger_{i_3}(0)\rangle$$



$$-\langle T_\tau c_{i_4}(-\tau)\, c^\dagger_{i_1}(0)\rangle\langle T_\tau c_{i_2}(\tau)\, c^\dagger_{i_3}(0)\rangle$$

$$G_{ij} = -\langle T_\tau c_i(\tau)\, c_j^\dagger(0)\rangle$$

$$-\mathcal{G}_{i_4 i_1}(-\tau)\,\mathcal{G}_{i_2 i_3}(\tau)$$

$$\Pi_{\alpha\beta}(i\Omega) = \int_0^\beta d\tau\, e^{i\Omega\tau}\,\frac{1}{V}\, v^\alpha_{i_1 i_2}\, v^\beta_{i_3 i_4}\,\mathcal{G}_{i_4 i_1}(-\tau)\,\mathcal{G}_{i_2 i_3}(\tau)\, d\tau =$$

$$= \frac{1}{V}\, v^\alpha_{i_1 i_2}\, v^\beta_{i_3 i_4}\int_0^\beta d\tau\, e^{i\Omega\tau}\,\mathcal{G}_{i_4 i_1}(-\tau)\,\mathcal{G}_{i_2 i_3}(\tau)\, d\tau$$

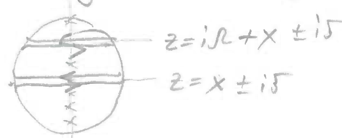
$$\Pi_{\alpha\beta}(i\Omega) = \frac{1}{V} v^{\alpha}_{i_1 i_2} v^{\beta}_{i_3 i_4} \frac{1}{\beta^2} \sum_{\substack{i\omega \\ i\omega'}} \int_0^\beta e^{i\Omega\tau}\, e^{i\omega\tau} \mathcal{G}_{i_4 i_1}(i\omega)\, \mathcal{G}_{i_2 i_3}(i\omega')\, e^{-i\omega'\tau}\, d\tau$$

because $\mathcal{G}(\tau) = \frac{1}{\beta}\sum_{i\omega} e^{-i\omega\tau}\mathcal{G}(i\omega)$

we know $\displaystyle\int_0^\beta e^{i(\Omega+\omega-\omega')\tau}\, d\tau = \frac{e^{i(\Omega+\omega-\omega')\tau}}{i(\Omega+\omega-\omega')}\Big|_0^\beta = \frac{e^{i2\pi m}-1}{i(\Omega+\omega-\omega')} = \beta\,\delta_{\Omega+\omega-\omega'}$

$$\Pi_{\alpha\beta}(i\Omega) = \frac{1}{V} v^{\alpha}_{i_1 i_2} v^{\beta}_{i_3 i_4} \frac{1}{\beta}\sum_{i\omega} \mathcal{G}_{i_4 i_1}(i\omega)\, \mathcal{G}_{i_2 i_3}(i\omega + i\Omega)$$

$$\Pi_{\alpha\beta}(i\Omega) = \frac{1}{V} v^{\alpha}_{i_1 i_2} v^{\beta}_{i_3 i_4} (-1)\oint \frac{dz}{2\pi i} f(z)\, \mathcal{G}_{i_4 i_1}(z)\, \mathcal{G}_{i_2 i_3}(z+i\Omega)$$



$$\Pi_{\alpha\beta}(i\Omega) = -\frac{1}{V} v^{\alpha}_{i_1 i_2} v^{\beta}_{i_3 i_4} \Big\{ \int \frac{dx}{\pi} f(x) \frac{1}{2i}\left[\mathcal{G}_{i_4 i_1}(x+i\delta) - \mathcal{G}_{i_4 i_1}(x-i\delta)\right] \mathcal{G}_{i_2 i_3}(x+i\Omega) +$$

$$+ \int \frac{dx}{\pi} f(x-i\Omega)\, \mathcal{G}_{i_4 i_1}(x-i\Omega) \frac{1}{2i}\left[\mathcal{G}_{i_2 i_3}(x+i\delta) - \mathcal{G}_{i_2 i_3}(x-i\delta)\right]$$

$\mathcal{G}(x-i\delta) = \mathcal{G}^{+}(x+i\delta)$ and $\mathcal{G}(x+i\delta) \equiv \mathcal{G}^{\text{retarded}}(x)$ hence

$$\Pi_{\alpha\beta}(i\Omega) = -\frac{1}{V} v^{\alpha}_{i_1 i_2} v^{\beta}_{i_3 i_4} \Big\{ \int \frac{dx}{\pi} f(x) \frac{1}{2i}\left[\mathcal{G}_{i_4 i_1}(x) - \mathcal{G}^{+}_{i_4 i_1}(x)\right] \mathcal{G}_{i_2 i_3}(x+i\Omega) +$$

$$+ \int \frac{dx}{\pi} f(x)\, \mathcal{G}_{i_4 i_1}(x-i\Omega) \frac{1}{2i}\left[\mathcal{G}_{i_2 i_3}(x) - \mathcal{G}^{+}_{i_2 i_3}(x)\right]\Big\}$$

$$\frac{1}{2i}\left[\Pi_{\alpha\beta}(\Omega+i\delta) - \Pi_{\alpha\beta}(\Omega-i\delta)\right] = -\frac{1}{V} v^{\alpha}_{i_1 i_2} v^{\beta}_{i_3 i_4} \Big\{ \int \frac{dx}{\pi} f(x) \frac{1}{2i}\left[\mathcal{G}_{i_4 i_1}(x) - \mathcal{G}^{+}_{i_4 i_1}(x)\right] \frac{1}{2i}\left[\mathcal{G}_{i_2 i_3}(x+\Omega) - \mathcal{G}^{+}_{i_2 i_3}(x+\Omega)\right]$$

$$+ \int \frac{dx}{\pi} f(x) \frac{1}{2i}\left[\mathcal{G}^{+}_{i_4 i_1}(x-\Omega) - \mathcal{G}_{i_4 i_1}(x-\Omega)\right] \frac{1}{2i}\left[\mathcal{G}_{i_2 i_3}(x) - \mathcal{G}^{+}_{i_2 i_3}(x)\right]$$

$$\underbrace{\frac{1}{2i}\left[\Pi_{\alpha\beta}(\Omega+i\delta) - \Pi_{\alpha\beta}(\Omega-i\delta)\right]}_{\text{Im}\, \Pi^{\text{ret}}(\Omega)} = \frac{1}{4}\frac{1}{V} v^{\alpha}_{i_1 i_2} v^{\beta}_{i_3 i_4} \int \frac{dx}{\pi}\left[f(x) - f(x+\Omega)\right]\left[\mathcal{G}_{i_4 i_1}(x) - \mathcal{G}^{+}_{i_4 i_1}(x)\right]\left[\mathcal{G}_{i_2 i_3}(x+\Omega) - \mathcal{G}^{+}_{i_2 i_3}(x+\Omega)\right]$$

$$\text{Re}\, \Sigma(\Omega) = -\frac{1}{4V} v^{\alpha}_{i_1 i_2} v^{\beta}_{i_3 i_4} \int \frac{dx}{\pi} \frac{f(x) - f(x+\Omega)}{\Omega}\left[\mathcal{G}_{i_4 i_1}(x) - \mathcal{G}^{+}_{i_4 i_1}(x)\right]\left[\mathcal{G}_{i_2 i_3}(x+\Omega) - \mathcal{G}^{+}_{i_2 i_3}(x+\Omega)\right]$$

Green's function $G_{ij}(\omega) = A^R_\omega \dfrac{1}{\omega+\mu-\varepsilon_{s\omega}} A^L_\omega$

$$\left[G_{i_4 i_1}(x) - G^+_{i_4 i_1}(x)\right]\left[G_{i_2 i_3}(x+\Omega) - G^+_{i_2 i_3}(x+\Omega)\right] = \left[\left(A^R_x\right)_{i_4 g} \frac{1}{x+\mu-\varepsilon^x_{sg}} \left(A^L_x\right)_{g i_1} - \left(A^{L+}_x\right)_{i_4 g} \frac{1}{x+\mu-\varepsilon^{x*}_{sg}} \left(A^{R+}_x\right)_{g i_1}\right] \times$$

$$\left[\left(A^R_{x+\Omega}\right)_{i_2 p} \frac{1}{x+\Omega+\mu-\varepsilon^{x+\Omega}_{sp}} \left(A^L_{x+\Omega}\right)_{p i_3} - \left(A^{L+}_{x+\Omega}\right)_{i_2 p} \frac{1}{x+\Omega+\mu-\varepsilon^{x+\Omega *}_{sp}} \left(A^{R+}_{x+\Omega}\right)_{p i_3}\right]$$

$$= \left(A^R_x\right)_{i_4 g}\left(A^L_x\right)_{g i_1}\left(A^R_{x+\Omega}\right)_{i_2 p}\left(A^L_{x+\Omega}\right)_{p i_3} \frac{1}{x+\mu-\varepsilon^x_{sg}} \frac{1}{x+\Omega+\mu-\varepsilon^{x+\Omega}_{sp}}$$

$$+ \left(A^{L+}_x\right)_{i_4 g}\left(A^{R+}_x\right)_{g i_1}\left(A^{L+}_{x+\Omega}\right)_{i_2 p}\left(A^{R+}_{x+\Omega}\right)_{p i_3} \left(\frac{1}{x+\mu-\varepsilon^x_{sg}} \frac{1}{x+\Omega+\mu-\varepsilon^{x+\Omega}_{sp}}\right)^*$$

$$- \left(A^R_x\right)_{i_4 g}\left(A^L_x\right)_{g i_1}\left(A^{L+}_{x+\Omega}\right)_{i_2 p}\left(A^{R+}_{x+\Omega}\right)_{p i_3} \frac{1}{x+\mu-\varepsilon^x_{sg}} \left(\frac{1}{x+\Omega+\mu-\varepsilon^{x+\Omega}_{sp}}\right)^*$$

$$- \left(A^{L+}_x\right)_{i_4 g}\left(A^{R+}_x\right)_{g i_1}\left(A^R_{x+\Omega}\right)_{i_2 p}\left(A^L_{x+\Omega}\right)_{p i_3} \left(\frac{1}{x+\mu-\varepsilon^x_{sg}}\right)^* \frac{1}{x+\Omega+\mu-\varepsilon^{x+\Omega}_{sp}}$$

$$\mathrm{Re}\,\Sigma(\Omega) = -\frac{1}{4\pi V}\int dx\, N^\alpha_{i_1 i_2} N^\beta_{i_3 i_4} \left(A^R_x\right)_{i_4 g}\left(A^L_x\right)_{g i_1}\left(A^R_{x+\Omega}\right)_{i_2 p}\left(A^L_{x+\Omega}\right)_{p i_3} \times \frac{f(x)-f(x+\Omega)}{\Omega} \frac{1}{(x+\mu-\varepsilon^x_{sg})(x+\Omega+\mu-\varepsilon^{x+\Omega}_{sp})}$$

$$-\frac{1}{4\pi V}\int dx\, N^\alpha_{i_1 i_2} N^\beta_{i_3 i_4} \left(A^{L+}_x\right)_{i_4 g}\left(A^{R+}_x\right)_{g i_1}\left(A^{L+}_{x+\Omega}\right)_{i_2 p}\left(A^{R+}_{x+\Omega}\right)_{p i_3} \times \frac{f(x)-f(x+\Omega)}{\Omega} \left(\frac{1}{(x+\mu-\varepsilon^x_{sg})(x+\Omega+\mu-\varepsilon^{x+\Omega}_{sp})}\right)^*$$

$$+\frac{1}{4\pi V}\int dx\, N^\alpha_{i_1 i_2} N^\beta_{i_3 i_4} \left(A^R_x\right)_{i_4 g}\left(A^L_x\right)_{g i_1}\left(A^{L+}_{x+\Omega}\right)_{i_2 p}\left(A^{R+}_{x+\Omega}\right)_{p i_3} \times \frac{f(x)-f(x+\Omega)}{\Omega} \frac{1}{x+\mu-\varepsilon^x_{sg}} \left(\frac{1}{x+\Omega+\mu-\varepsilon^{x+\Omega}_{sp}}\right)^*$$

$$+\frac{1}{4\pi V}\int dx\, N^\alpha_{i_1 i_2} N^\beta_{i_3 i_4} \left(A^{L+}_x\right)_{i_4 g}\left(A^{R+}_x\right)_{g i_1}\left(A^R_{x+\Omega}\right)_{i_2 p}\left(A^L_{x+\Omega}\right)_{p i_3} \times \frac{f(x)-f(x+\Omega)}{\Omega} \left(\frac{1}{x+\mu-\varepsilon^x_{sp}}\right)^* \frac{1}{x+\Omega+\mu-\varepsilon^{x+\Omega}_{sp}}$$

$$\mathrm{Re}\,\Sigma(\Omega) = -\frac{1}{4\pi V}\int dx \left(A^L_x N^\alpha A^R_{x+\Omega}\right)_{gp}\left(A^L_{x+\Omega} N^\beta A^R_x\right)_{pg} \times \frac{f(x)-f(x+\Omega)}{\Omega} \frac{1}{x+\mu-\varepsilon^x_{sg}} \frac{1}{x+\Omega+\mu-\varepsilon^{x+\Omega}_{sp}}$$

$$-\frac{1}{4\pi V}\int dx \left(A^{R+}_x N^\alpha A^{L+}_{x+\Omega}\right)_{gp}\left(A^{R+}_{x+\Omega} N^\beta A^{L+}_x\right)_{pg} \times \frac{f(x)-f(x+\Omega)}{\Omega} \left[\frac{1}{x+\mu-\varepsilon^x_{sg}} \frac{1}{x+\Omega+\mu-\varepsilon^{x+\Omega}_{sp}}\right]^*$$

$$+\frac{1}{4\pi V}\int dx \left(A^L_x N^\alpha A^{L+}_{x+\Omega}\right)_{gp}\left(A^{R+}_{x+\Omega} N^\beta A^R_x\right)_{pg} \times \frac{f(x)-f(x+\Omega)}{\Omega} \frac{1}{x+\mu-\varepsilon^x_{sg}} \left(\frac{1}{x+\Omega+\mu-\varepsilon^{x+\Omega}_{sp}}\right)^*$$

$$+\frac{1}{4\pi V}\int dx \left(A^{R+}_x N^\alpha A^R_{x+\Omega}\right)_{gp}\left(A^L_{x+\Omega} N^\beta A^{L+}_x\right)_{pg} \times \frac{f(x)-f(x+\Omega)}{\Omega} \left(\frac{1}{x+\mu-\varepsilon^x_{sg}}\right)^* \frac{1}{x+\Omega+\mu-\varepsilon^{x+\Omega}_{sp}}$$

$$\mathrm{Re}\,\Sigma(\Omega) = -\frac{1}{4\pi V}\int dx \,(A^L_{x-\Omega} N^\alpha A^R_x)_{qp} (A^L_x N^\beta A^R_{x-\Omega})_{pq} \times \frac{f(x-\Omega)-f(x)}{\Omega} \times \frac{1}{x+\mu-\varepsilon_p^x}\,\frac{1}{x-\Omega+\mu-\varepsilon_q^{x-\Omega}}$$

$$-\frac{1}{4\pi V}\int dx \,(A^L_x N^{\alpha+} A^R_{x-\Omega})^*_{pq} (A^L_{x-\Omega} N^{\beta+} A^R_x)^*_{qp} \,\frac{f(x-\Omega)-f(x)}{\Omega} \times \left(\frac{1}{x+\mu-\varepsilon_p^x}\,\frac{1}{x-\Omega+\mu-\varepsilon_q^{x-\Omega}}\right)^*$$

$$+\frac{1}{4\pi V}\int dx \,(A^L_{x-\Omega} N^\alpha A^{L+}_x)_{qp} (A^{R+}_x N^\beta A^R_{x-\Omega})_{pq} \,\frac{f(x-\Omega)-f(x)}{\Omega} \times \left(\frac{1}{x+\mu-\varepsilon_p^x}\right)^*\frac{1}{x-\Omega+\mu-\varepsilon_q^{x-\Omega}}$$

$$+\frac{1}{4\pi V}\int dx \,(A^{R+}_x N^{\alpha+} A^R_{x-\Omega})^*_{pq} (A^L_{x-\Omega} N^{\beta+} A^{L+}_x)^*_{qp} \,\frac{f(x-\Omega)-f(x)}{\Omega}\,\frac{1}{x+\mu-\varepsilon_p^x}\left(\frac{1}{x-\Omega+\mu-\varepsilon_q^{x-\Omega}}\right)^*$$

$$C^{\alpha\beta}_{pq} \equiv (A^L_x \tilde N^\beta A^R_{x-\Omega})_{pq}\,(A^L_{x-\Omega}\tilde N^\alpha A^R_x)_{qp}$$

$$D^{\alpha\beta}_{pq} \equiv (A^{R+}_x \tilde N^\beta A^R_{x-\Omega})_{pq}\,(A^L_{x-\Omega}\tilde N^\alpha A^{L+}_x)_{qp}$$

$$\mathrm{Re}\,\Sigma(\Omega) = -\frac{\hbar}{4\pi V}\left(\frac{e\hbar}{m a_0}\right)^2 2\,\mathrm{Re}\int dx\left[C_{pq}\,\frac{1}{x+\mu-\varepsilon_p^x}\,\frac{1}{x-\Omega+\mu-\varepsilon_q^{x-\Omega}} - D_{pq}\left(\frac{1}{x+\mu-\varepsilon_p^x}\right)^*\frac{1}{x-\Omega+\mu-\varepsilon_q^{x-\Omega}}\right]\frac{f(x-\Omega)-f(x)}{\Omega}$$

$V = a_0^3\,\tilde V$; x and Ω in units of Ry

$$\mathrm{Re}\,\Sigma(\Omega) = \underbrace{\left(\frac{e_0\hbar}{m a_0}\right)^2\frac{\hbar}{a_0^3}\,\frac{1}{2\pi}\,\frac{1}{(R_y)^2}}\left(-\frac{1}{\tilde V}\right)\mathrm{Re}\int dx\,\frac{f(x-\Omega)-f(x)}{\Omega}\left[\frac{C_{pq}}{(x+\mu-\varepsilon_p^x)(x-\Omega+\mu-\varepsilon_q^{x-\Omega})} - \frac{D_{pq}}{(x+\mu-\varepsilon_p^x)^*(x-\Omega+\mu-\varepsilon_q^{x-\Omega})}\right]$$

$$\left(\frac{e_0^2}{a_0\hbar}\right)\left[\frac{\hbar^2}{m a_0^2 R_y}\right]^2\frac{1}{2\pi}\quad\left(-\frac{1}{\tilde V}\right)\mathrm{Re}\int dx\;\cdots$$

$$\frac{\hbar^2}{m a_0^2 R_y} = 2$$

$$\mathrm{Re}\,\Sigma(\Omega) = \left(\frac{e_0^2}{a_0\hbar}\right)\left(\frac{4}{2\pi}\right)\left(-\frac{1}{\tilde V}\right)\mathrm{Re}\int dx\,\frac{f(x-\Omega)-f(x)}{\Omega}\left[\frac{C_{pq}}{(x+\mu-\varepsilon_p^x)(x-\Omega+\mu-\varepsilon_q^{x-\Omega})} - \frac{D_{pq}}{(x+\mu-\varepsilon_p^x)^*(x-\Omega+\mu-\varepsilon_q^{x-\Omega})}\right]$$

$\left(\frac{e_0^2}{a_0\hbar}\right) = \frac{1}{2.17326\times10^{-5}\,\Omega\mathrm{cm}}$; $\left(\frac{4}{2\pi}\right) = \left(\frac{2}{\pi}\right)$

Exactly what is implemented in <u>optmain.f90</u>

The correct $\tilde N^\alpha_{ij} = \langle \psi_{ki}| -i a_0 \frac{\partial}{\partial x_\alpha} |\psi_{kj}\rangle$ is taken from x_lapw optic!

Non interacting limit $\quad A^2 = A'^2 = I \ , \ C_{pg} = D_{pg} = \tilde{v}^{\alpha}_{gp} \tilde{v}^{\beta}_{pg}$

$$\sigma' = -\left(\frac{e\hbar}{m c_0}\right)^2 \frac{\hbar}{2\pi V} \, Re \int dx \, \frac{f(x-\Omega) - f(x)}{\Omega} \underbrace{\frac{1}{x-\Omega+\mu-\varepsilon_{g}}}_{-\pi i \delta(x-\Omega+\mu-\varepsilon_{g})} \underbrace{\left[\frac{1}{x+\mu-\varepsilon_p+i\delta} - \frac{1}{x+\mu-\varepsilon_p - i\delta}\right]}_{-2\pi i \delta(x+\mu-\varepsilon_p)} \tilde{v}^{\beta}_{pg} \tilde{v}^{\alpha}_{gp}$$

$$\sigma' = +\left(\frac{e\hbar}{m c_0}\right)^2 \frac{\hbar}{2\pi V} \quad \frac{f(\varepsilon_g-\mu) - f(\varepsilon_p-\mu)}{\varepsilon_p - \varepsilon_g} \, 2\pi^2 \, \delta(\varepsilon_p - \varepsilon_g - \Omega) \, \tilde{v}^{\beta}_{pg} \tilde{v}^{\alpha}_{gp}$$

$x = \varepsilon_p - \mu$
$x - \Omega = \varepsilon_g - \mu$
$\Omega = \varepsilon_p - \varepsilon_g$

$$\sigma' = \left(\frac{e\hbar}{m c_0}\right)^2 \frac{\pi\hbar}{V} \quad \frac{f(\varepsilon_g-\mu) - f(\varepsilon_p-\mu)}{\varepsilon_p - \varepsilon_g} \, \tilde{v}^{\beta}_{pg} \tilde{v}^{\alpha}_{gp} \, \delta(\varepsilon_p - \varepsilon_g - \Omega)$$

$$\text{Im}\, \varepsilon(\Omega) = \frac{1}{\Omega}\sigma'(\Omega) = \left(\frac{e\hbar}{m c_0}\right)^2 \frac{\pi\hbar}{V} \quad \frac{f(\varepsilon_g-\mu) - f(\varepsilon_p-\mu)}{(\varepsilon_p - \varepsilon_g)^2} \, \tilde{v}^{\beta}_{pg} \tilde{v}^{\alpha}_{gp} \, \delta(\varepsilon_p - \varepsilon_g - \Omega)$$

$\downarrow$ analytic continuation

$$\varepsilon(\Omega) = \text{const} \; \underbrace{- \left(\frac{e\hbar}{m c_0}\right)^2 \frac{\hbar}{V} \quad \frac{f(\varepsilon_g-\mu) - f(\varepsilon_p-\mu)}{(\varepsilon_p - \varepsilon_g)^2} \, \tilde{v}^{\beta}_{pg} \tilde{v}^{\alpha}_{gp} \, \frac{1}{\varepsilon_p - \varepsilon_g - \Omega}}$$

4π difference with Claudia's Eq. 19 in Claudia's paper!
This is likely due to gaussian units!

Derivation of the f-sumrule

polarization $\vec{P} = \int \Psi^+(\vec r)\, e\vec r\, \Psi(\vec r)\, d^3r$

$$\frac{dP_\alpha}{dt} = j_\alpha \quad \text{and} \quad P_\alpha = \int_{-\infty}^{t} j_\alpha(t')dt' = \int_{-\infty}^{t} e^{iHt'} j_\alpha\, e^{-iHt'} dt'$$

We will show that $\langle [P_\alpha, j_\alpha] \rangle$ is proportional to $\int_{-\infty}^{\infty} \sigma_{\alpha\alpha}(\omega)\, d\omega$.

We see that:

$$\langle [P_\alpha, j_\alpha] \rangle = \sum_i \langle [e x_{i\alpha}, \tfrac{e}{m} p_{i\alpha}] \rangle = \frac{e^2}{m} i\hbar N$$

Next we use exact eigenstates $|m\rangle$ to prove:

$$\langle [P_\alpha, j_\alpha] \rangle = \sum_m \langle m| \frac{e^{-\beta H}}{Z} \big(P_\alpha(0) j_\alpha(0) - j_\alpha(0) P_\alpha(0)\big)|m\rangle = \sum_{mn} \langle m| \frac{e^{-\beta H}}{Z} \int_{-\infty}^{0} e^{iHt} j_\alpha e^{-iHt} dt |n\rangle \langle n| j_\alpha |m\rangle$$

$$- \langle m| \frac{e^{-\beta H}}{Z} j_\alpha |n\rangle \langle n| \int_{-\infty}^{0} e^{iHt} j_\alpha e^{-iHt} dt |m\rangle$$

$$= \sum_{mn} \frac{e^{-\beta E_m}}{Z} \int_{-\infty}^{0} e^{i(E_m - E_n)t} dt\, \langle m| j_\alpha |n\rangle \langle n| j_\alpha |m\rangle - \frac{e^{-\beta E_m}}{Z} \langle m| j_\alpha |n\rangle \langle n| j_\alpha |m\rangle \int_{-\infty}^{0} e^{i(E_n - E_m)t} =$$

$$= \sum_{mn} \frac{e^{-\beta E_m}}{Z} \frac{2}{i(E_m - E_n)} \langle m| j_\alpha |n\rangle \langle n| j_\alpha |m\rangle$$

For optics we have: $\sigma'(\omega) = -\frac{1}{\omega} \Pi''(\omega)$ where $\Pi(\omega) = +\frac{i}{V}\int_0^{\infty} dt\, e^{i\omega t} \langle [j_\alpha(0), j_\alpha(t)] \rangle$

$$\Pi(\omega) = +\frac{i}{V}\int_0^{\infty} dt\, e^{i\omega t} \sum_{mn} \frac{e^{-\beta E_m}}{Z} \big(\langle m| j_\alpha |n\rangle \langle n| e^{iHt} j_\alpha e^{-iHt} |m\rangle - \langle m| e^{iHt} j_\alpha e^{-iHt} |n\rangle \langle n| j_\alpha |m\rangle \big)$$

$$= +\frac{i}{V} \sum_{mn} \frac{e^{-\beta E_m}}{Z} |\langle m| j_\alpha |n\rangle|^2 \int_0^{\infty} \Big(e^{i(\omega + E_n - E_m + i\delta)t} - e^{i(\omega + E_m - E_n + i\delta)t} \Big) dt$$

$$= +\frac{i}{V} \sum_{mn} \frac{e^{-\beta E_m}}{Z} |\langle m| j_\alpha |n\rangle|^2 \left[\frac{(-1)}{i(\omega + E_n - E_m + i\delta)} - \frac{(-1)}{i(\omega + E_m - E_n + i\delta)} \right] = -\frac{1}{V} \sum_{mn} \frac{e^{-\beta E_m}}{Z} |\langle m| j_\alpha |n\rangle|^2 \left(\frac{1}{\omega + E_n - E_m + i\delta} - \frac{1}{\omega + E_m - E_n + i\delta} \right)$$

$$\mathrm{Im}\, \Pi(\omega) = +\frac{\pi}{V} \sum_{mn} \frac{e^{-\beta E_m}}{Z} |\langle m| j_\alpha |n\rangle|^2 \big[\delta(\omega + E_n - E_m) - \delta(\omega + E_m - E_n) \big]$$

$$= +\frac{\pi}{V} \sum_{mn} |\langle m| j_\alpha |n\rangle|^2 \frac{1}{Z} \big(e^{-\beta E_m} - e^{-\beta E_n} \big) \delta(\omega + E_n - E_m)$$

$$\mathrm{Re}\, \sigma(\omega) = -\frac{\pi}{V} \sum_{mn} |\langle m| j_\alpha |n\rangle|^2 \frac{1}{Z} \frac{\big(e^{-\beta E_m} - e^{-\beta E_n} \big)}{E_m - E_n} \delta(\omega + E_n - E_m)$$

$$\int_{-\infty}^{\infty} \mathrm{Re}\, \sigma(\omega) = -\frac{\pi}{V} \sum_{mn} |\langle m| j_\alpha |n\rangle|^2 \frac{1}{Z} \frac{e^{-\beta E_m} - e^{-\beta E_n}}{E_m - E_n} = -\frac{2\pi}{V} \sum_{mn} |\langle m| j_\alpha |n\rangle|^2 \frac{e^{-\beta E_m}}{E_m - E_n} \frac{1}{Z}$$

$$\int_{-\infty}^{\infty} \mathrm{Re}\,\Sigma(\omega) = -\frac{2\pi}{V\hbar}\sum_{nm} |\langle n| j_\alpha |m\rangle|^2 \frac{e^{-\beta E_m}}{E_n - E_m}\frac{1}{Z} = -\frac{\pi}{V}\frac{i}{\hbar}\langle [P_\alpha, j_\alpha]\rangle = \frac{\pi}{V}\frac{\hbar e^2}{\hbar m} N = \frac{\pi e^2 n}{m}$$

To prove the f-sumrule in LDA, we need to construct operator r_α, so that $p_\alpha = \int^t r_\alpha$, then we can write $\frac{\langle \psi_p | p_\alpha | \psi_q \rangle \langle \psi_q | p_\alpha | \psi_p \rangle}{\varepsilon_p - \varepsilon_q}$ as

$$\sum_q \langle \psi_p | r_\alpha | \psi_q \rangle \langle \psi_q | p_\alpha | \psi_p \rangle \cdots \Rightarrow \langle \psi_p | [r_\alpha, p_\alpha] | \psi_p \rangle$$

The important question is: would K.S. basis satisfy

$$\sum_q \langle \psi_p | x | \psi_q \rangle \langle \psi_q | p_x | \psi_p \rangle \stackrel{?}{=} \langle \psi_p | x p_x | \psi_p \rangle$$

need complete basis set!

Matrix elements of $\vec\nabla$ $\quad (-i\vec\nabla)$

$$\Psi_{ik} = \left[a_{ilm}\, u_l(r) + b_{ilm}\, \dot u_l(r) + c_{ilm}\, u^{LO}(r)\right] Y_{lm}(\hat r) \equiv \varphi^i_{lm}(r)\, Y_{lm}(\hat r)$$

$$\vec M_{ji} \equiv \langle \Psi_{jk} | \vec\nabla | \Psi_{ik}\rangle = \langle \varphi^j_{l'm'}(r)\, Y_{l'm'}(\hat r) | \vec\nabla | \varphi^i_{lm}(r)\, Y_{lm}(\hat r)\rangle =$$

$$= \langle \varphi^j_{l'm'}(r) | \tfrac{d}{dr} | \varphi^i_{lm}(r)\rangle \langle Y_{l'm'} | \vec e_r | Y_{lm}\rangle +$$

$$\langle \varphi^j_{l'm'}(r) | \tfrac{1}{r} | \varphi^i_{lm}(r)\rangle \langle Y_{l'm'} | (r\vec\nabla) | Y_{lm}\rangle$$

$$I^{(1)}_{l'm'lm} \equiv \int d\Omega\, Y^*_{l'm'}(\hat r)\, \vec e_r\, Y_{lm}$$

$$I^{(2)}_{l'm'lm} \equiv \int d\Omega\, Y^*_{l'm'}(\hat r)\, (r\vec\nabla)\, Y_{lm}$$

$$I^{(m)}_{l'm'lm} = c^m_l\, \delta_{l'=l+1}\, \vec g(l'm', lm) - d^m_l\, \delta_{l'=l-1}\, \vec h(l'm', lm)$$ [Due to Wigner-Eckart theor.

here
$$\vec g(l'm', lm) = -a(l,m)\begin{pmatrix}1\\-i\\0\end{pmatrix}\delta_{m'=m+1} - a(l,-m)\begin{pmatrix}-1\\-i\\0\end{pmatrix}\delta_{m'=m-1} + 2f(l,m)\begin{pmatrix}0\\0\\1\end{pmatrix}\delta_{m'=m}$$

$$\vec h(l'm', lm) = -a(l',-m')\begin{pmatrix}1\\-i\\0\end{pmatrix}\delta_{m'=m+1} - a(l',m')\begin{pmatrix}-1\\-i\\0\end{pmatrix}\delta_{m'=m-1} - 2f(l'm')\begin{pmatrix}0\\0\\1\end{pmatrix}\delta_{m'=m}$$

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

$$c^1_l = d^1_l = \tfrac12 \qquad c^2_l = -\tfrac{l}{2} \quad d^2_l = \tfrac{l+1}{2}$$

$$\vec M_{ji} = \langle \varphi^j_{l'm'} | \tfrac{d}{dr} | \varphi^i_{lm}\rangle \left[c^1_l\, \delta_{l'=l+1}\, \vec g(l'm' lm) - d^1_l\, \delta_{l'=l-1}\, \vec h(l'm' lm)\right]$$
$$+ \langle \varphi^j_{l'm'} | \tfrac{1}{r} | \varphi^i_{lm}\rangle \left[c^2_l\, \delta_{l'=l+1}\, \vec g(l'm' lm) - d^2_l\, \delta_{l'=l-1}\, \vec h(l'm' lm)\right]$$

$$\vec M_{ji} = \langle \varphi^j_{l'm'} | \underbrace{c^1_l}_{=\frac12} \tfrac{d}{dr} + \underbrace{c^2_l}_{=-\frac{l}{2}} \tfrac{1}{r} | \varphi^i_{lm}\rangle\, \delta_{l'=l+1}\, \vec g(l'm' lm) +$$

$$- \langle \varphi^j_{l'm'} | \underbrace{d^1_l}_{=\frac12} \tfrac{d}{dr} + \underbrace{d^2_l}_{=\frac{l+1}{2}} \tfrac{1}{r} | \varphi^i_{lm}\rangle\, \delta_{l'=l-1}\, \vec h(l'm' lm)$$

$$g^x(l'm'lm) + i\,g^y(l'm'lm) = -2\,Q(l,m)\,\delta_{m'=m+1}$$

$$g^x(l'm'lm) - i\,g^y(l'm'lm) = +2\,Q(l,-m)\,\delta_{m'=m-1}$$

$$g^z(l'm'lm) = 2f(l,m)\,\delta_{m'=m}$$

$$h^x(l'm'lm) + i\,h^y(l'm'lm) = -2\,Q(l',-m')\,\delta_{m'=m+1}$$

$$h^x(l'm'lm) - i\,h^y(l'm'lm) = +2\,Q(l'm')\,\delta_{m'=m-1}$$

$$h^z(l'm'lm) = -2f(l'm')\,\delta_{m'=m}$$

$$M^x_{ji} + i\,M^y_{ji} = -\langle \varphi^j_{l'm'} | \tfrac{1}{2}\tfrac{d}{dr} - \tfrac{l}{2}\tfrac{1}{r} | \varphi^i_{lm}\rangle\, \delta_{l'=l+1}\, 2Q(l,m)\,\delta_{m'=m+1}$$

$$+ \langle \varphi^j_{l'm'} | \tfrac{1}{2}\tfrac{d}{dr} + \tfrac{l+1}{2}\tfrac{1}{r} | \varphi^i_{lm}\rangle\, \delta_{l'=l-1}\, 2Q(l',-m')\,\delta_{m'=m+1}$$

$$= -\langle \varphi^j_{l+1,m+1} | \tfrac{d}{dr} - \tfrac{l}{r} | \varphi^i_{lm}\rangle\, Q(l,m) + \langle \varphi^j_{l'm'} | \tfrac{d}{dr} + \tfrac{l'+2}{r} | \varphi^i_{l'+1,m'-1}\rangle\, Q(l',-m')$$

l', m' is dummy index $\Rightarrow$ could be replaced by lm

$$\boxed{M^x_{ji} + i\,M^y_{ji} = -\langle \varphi^j_{l+1\,m+1} | \tfrac{d}{dr} - \tfrac{l}{r} | \varphi^i_{lm}\rangle \sqrt{\frac{(l+m+1)(l+m+2)}{(2l+1)(2l+3)}} + \langle \varphi^j_{lm} | \tfrac{d}{dr} + \tfrac{l+2}{r} | \varphi^i_{l+1\,m-1}\rangle \sqrt{\frac{(l-m+1)(l-m+2)}{(2l+1)(2l+3)}}}$$

$$M^x_{ji} - i\,M^y_{ji} = \langle \varphi^j_{l'm'} | \tfrac{d}{dr} - \tfrac{l}{r} | \varphi^i_{lm}\rangle\, \delta_{l'=l+1}\,(+1)\,Q(l,-m)\,\delta_{m'=m-1}$$

$$- \langle \varphi^j_{l'm'} | \tfrac{d}{dr} + \tfrac{l+1}{r} | \varphi^i_{lm}\rangle\, \delta_{l'=l-1}\,(+1)\,Q(l'm')\,\delta_{m'=m-1}$$

$$\boxed{M^x_{ji} - i\,M^y_{ji} = \langle \varphi^j_{l+1\,m-1} | \tfrac{d}{dr} - \tfrac{l}{r} | \varphi^i_{lm}\rangle \sqrt{\frac{(l-m+1)(l-m+2)}{(2l+1)(2l+3)}} - \langle \varphi^j_{lm} | \tfrac{d}{dr} + \tfrac{l+2}{r} | \varphi^i_{l+1,m+1}\rangle \sqrt{\frac{(l+m+1)(l+m+2)}{(2l+1)(2l+3)}}}$$

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

$$\boxed{M^z_{ji} = \langle \varphi^j_{l+1,m} | \tfrac{d}{dr} - \tfrac{l}{r} | \varphi^i_{lm}\rangle + \langle \varphi^j_{lm} | \tfrac{d}{dr} + \tfrac{l+2}{r} | \varphi^i_{l+1\,m}\rangle\, f(l,m)}$$