Non-collinear Koopmans potential $\mathcal{V}_i^{KI(2)}(\mathbf{r}) = -\frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\boldsymbol{n}_i(\mathbf{r})\mathbb{F}_{Hxc}(\mathbf{r},\mathbf{r}')\boldsymbol{n}_i(\mathbf{r}')\sigma_0 + (1-f_i)\sum\int d\mathbf{r}'\left[\mathbb{F}_{Hxc}(\mathbf{r},\mathbf{r}')\boldsymbol{n}_i(\mathbf{r}')\right]_\alpha \sigma_\alpha$

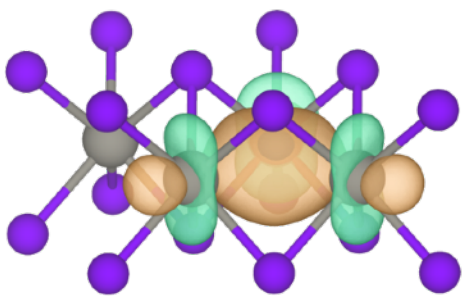
Wannier function charge density / Wannier function spin density

$$\left(n_\rho(\mathbf{r}), n_{m_x}(\mathbf{r}), n_{m_y}(\mathbf{r}), n_{m_z}(\mathbf{r})\right) \cdot \begin{pmatrix} \mathbb{F}_{Hxc}^{\rho,\rho} & \mathbb{F}_{xc}^{\rho,m_x} & \mathbb{F}_{xc}^{\rho,m_y} & \mathbb{F}_{xc}^{\rho,m_z} \\ \mathbb{F}_{xc}^{m_x,\rho} & \mathbb{F}_{xc}^{m_x,m_x} & \mathbb{F}_{xc}^{m_x,m_y} & \mathbb{F}_{xc}^{m_x,m_z} \\ \mathbb{F}_{xc}^{m_y,\rho} & \mathbb{F}_{xc}^{m_y,m_x} & \mathbb{F}_{xc}^{m_y,m_y} & \mathbb{F}_{xc}^{m_y,m_z} \\ \mathbb{F}_{xc}^{m_z,\rho} & \mathbb{F}_{xc}^{m_z,m_x} & \mathbb{F}_{xc}^{m_z,m_y} & \mathbb{F}_{xc}^{m_z,m_z} \end{pmatrix} \cdot \begin{pmatrix} n_\rho(\mathbf{r}) \\ n_{m_x}(\mathbf{r}) \\ n_{m_y}(\mathbf{r}) \\ n_{m_z}(\mathbf{r}) \end{pmatrix}$$

charge-charge interaction; charge-spin interaction; spin-spin interaction

screened interaction = un-screened interaction + interacting response function

$$\mathbb{F}_{Hxc}(\mathbf{r},\mathbf{r}') = \mathbf{F}_{Hxc}(\mathbf{r},\mathbf{r}') + \int d\mathbf{r}''\mathbf{F}_{Hxc}(\mathbf{r},\mathbf{r}'')\int d\mathbf{r}'''\boldsymbol{\chi}(\mathbf{r}'',\mathbf{r}''')\mathbf{F}_{Hxc}(\mathbf{r}''',\mathbf{r}')$$



$$\begin{pmatrix} \chi^{\rho,\rho} & \chi^{\rho,m_x} & \chi^{\rho,m_y} & \chi^{\rho,m_z} \\ \chi^{m_x,\rho} & \chi^{m_x,m_x} & \chi^{m_x,m_y} & \chi^{m_x,m_z} \\ \chi^{m_y,\rho} & \chi^{m_y,m_x} & \chi^{m_y,m_y} & \chi^{m_y,m_z} \\ \chi^{m_z,\rho} & \chi^{m_z,m_x} & \chi^{m_z,m_y} & \chi^{m_z,m_z} \end{pmatrix} \cdot \begin{pmatrix} F_{Hxc}^{\rho,\rho} & F_{xc}^{\rho,m_x} & F_{xc}^{\rho,m_y} & F_{xc}^{\rho,m_z} \\ F_{xc}^{m_x,\rho} & F_{xc}^{m_x,m_x} & F_{xc}^{m_x,m_y} & F_{xc}^{m_x,m_z} \\ F_{xc}^{m_y,\rho} & F_{xc}^{m_y,m_x} & F_{xc}^{m_y,m_y} & F_{xc}^{m_y,m_z} \\ F_{xc}^{m_z,\rho} & F_{xc}^{m_z,m_x} & F_{xc}^{m_z,m_y} & F_{xc}^{m_z,m_z} \end{pmatrix}$$

charge-charge; charge-spin; spin-spin