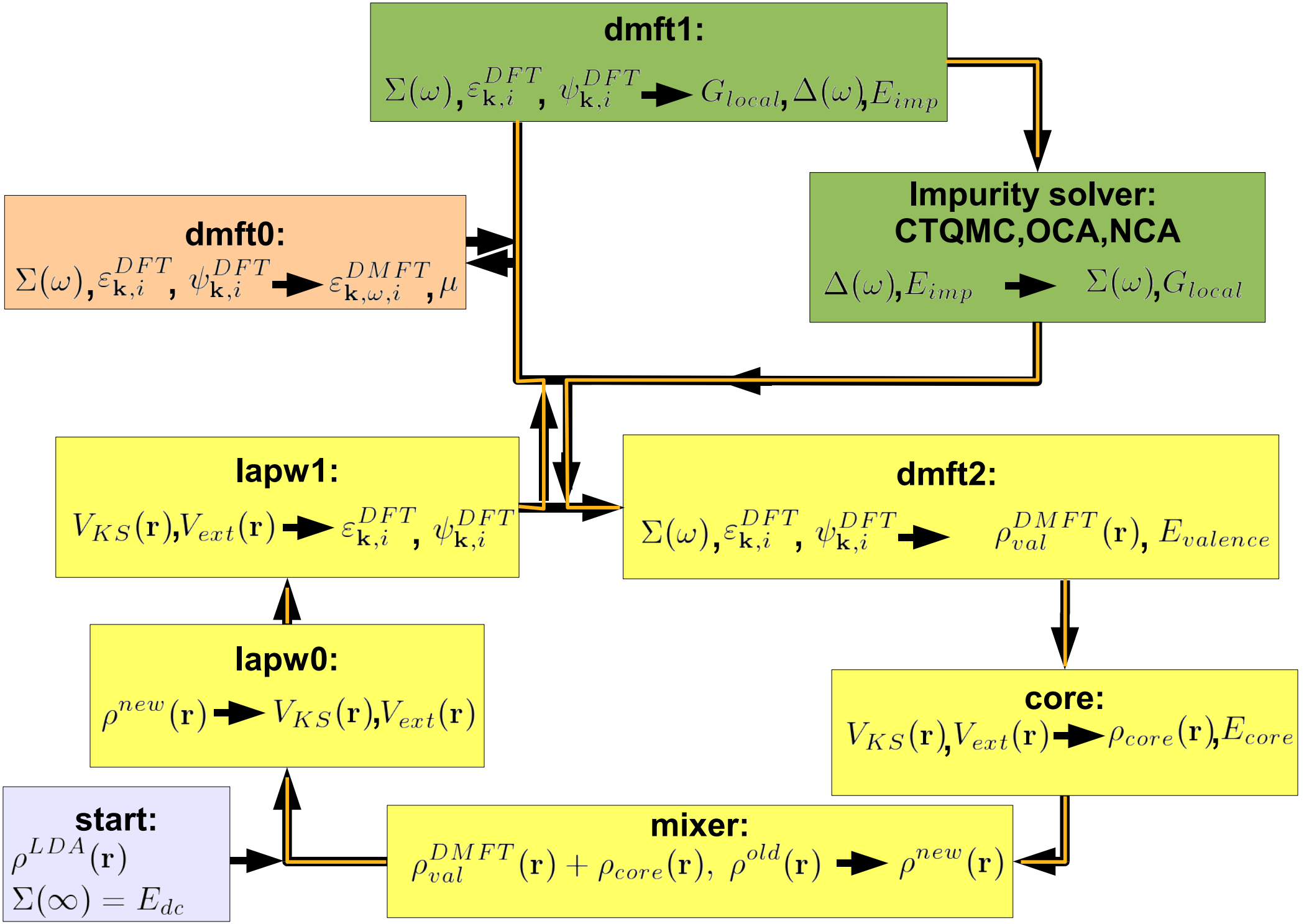
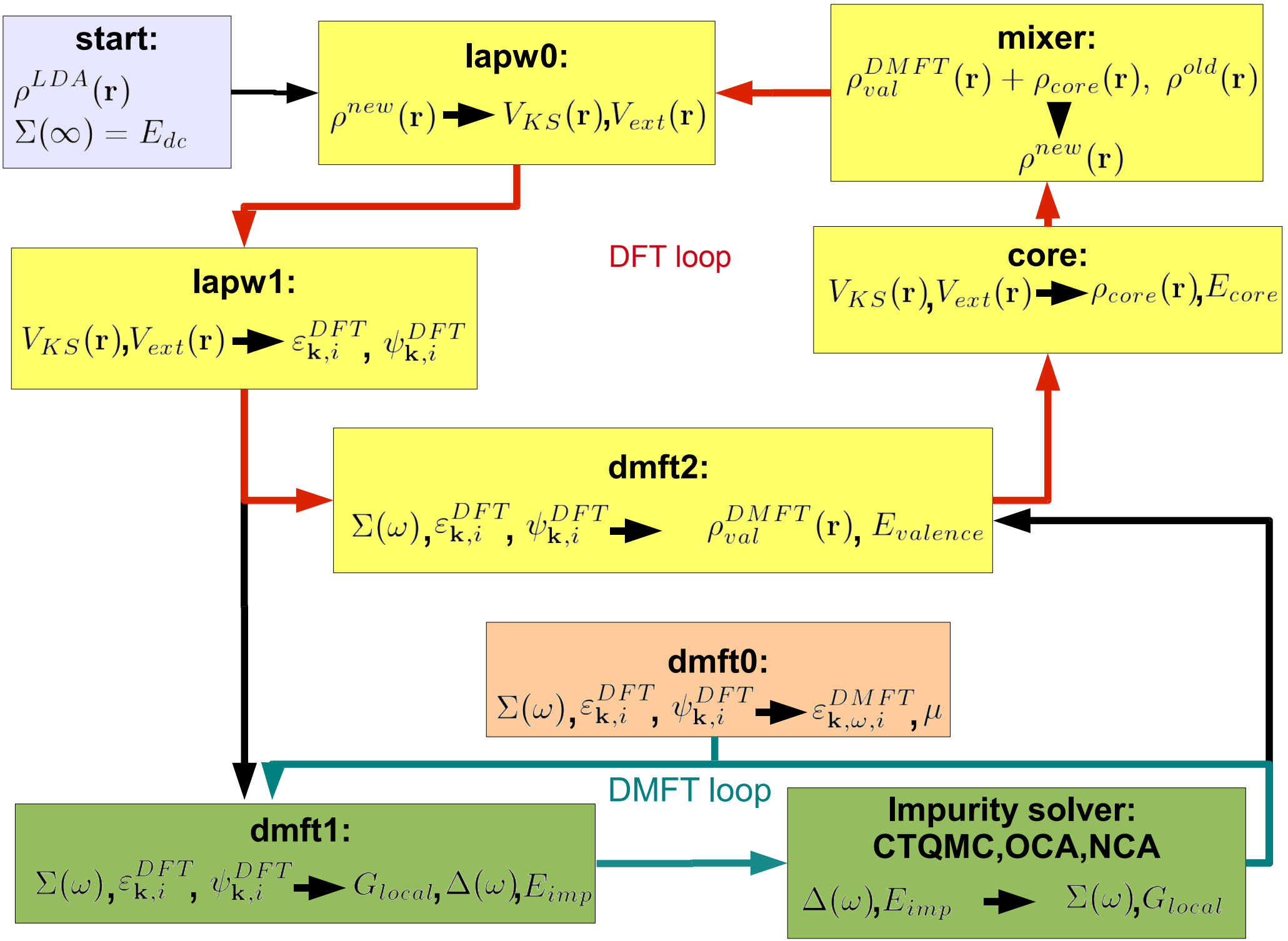

dmft1:
$\Sigma(\omega), \varepsilon^{DFT}_{\mathbf{k},i}, \psi^{DFT}_{\mathbf{k},i} \rightarrow G_{local}, \Delta(\omega), E_{imp}$
dmft0:
$\Sigma(\omega), \varepsilon^{DFT}_{\mathbf{k},i}, \psi^{DFT}_{\mathbf{k},i} \rightarrow \varepsilon^{DMFT}_{\mathbf{k},\omega,i}, \mu$
Impurity solver:
CTQMC,OCA,NCA
$\Delta(\omega), E_{imp} \rightarrow \Sigma(\omega), G_{local}$
lapw1:
$V_{KS}(\mathbf{r}), V_{ext}(\mathbf{r}) \rightarrow \varepsilon^{DFT}_{\mathbf{k},i}, \psi^{DFT}_{\mathbf{k},i}$
dmft2:
$\Sigma(\omega), \varepsilon^{DFT}_{\mathbf{k},i}, \psi^{DFT}_{\mathbf{k},i} \rightarrow \rho^{DMFT}_{val}(\mathbf{r}), E_{valence}$
lapw0:
$\rho^{new}(\mathbf{r}) \rightarrow V_{KS}(\mathbf{r}), V_{ext}(\mathbf{r})$
core:
$V_{KS}(\mathbf{r}), V_{ext}(\mathbf{r}) \rightarrow \rho_{core}(\mathbf{r}), E_{core}$
start:
$\rho^{LDA}(\mathbf{r})$
$\Sigma(\infty) = E_{dc}$
mixer:
$\rho^{DMFT}_{val}(\mathbf{r}) + \rho_{core}(\mathbf{r}), \rho^{old}(\mathbf{r}) \rightarrow \rho^{new}(\mathbf{r})$


start:
$\rho^{LDA}(\mathbf{r})$
$\Sigma(\infty) = E_{dc}$
lapw0:
$\rho^{new}(\mathbf{r}) \rightarrow V_{KS}(\mathbf{r}), V_{ext}(\mathbf{r})$
mixer:
$\rho_{val}^{DMFT}(\mathbf{r}) + \rho_{core}(\mathbf{r}),\ \rho^{old}(\mathbf{r})$
$\rho^{new}(\mathbf{r})$
lapw1:
$V_{KS}(\mathbf{r}), V_{ext}(\mathbf{r}) \rightarrow \varepsilon_{\mathbf{k},i}^{DFT},\ \psi_{\mathbf{k},i}^{DFT}$
DFT loop
core:
$V_{KS}(\mathbf{r}), V_{ext}(\mathbf{r}) \rightarrow \rho_{core}(\mathbf{r}), E_{core}$
dmft2:
$\Sigma(\omega), \varepsilon_{\mathbf{k},i}^{DFT},\ \psi_{\mathbf{k},i}^{DFT} \rightarrow \rho_{val}^{DMFT}(\mathbf{r}),\ E_{valence}$
dmft0:
$\Sigma(\omega), \varepsilon_{\mathbf{k},i}^{DFT},\ \psi_{\mathbf{k},i}^{DFT} \rightarrow \varepsilon_{\mathbf{k},\omega,i}^{DMFT}, \mu$
DMFT loop
dmft1:
$\Sigma(\omega), \varepsilon_{\mathbf{k},i}^{DFT},\ \psi_{\mathbf{k},i}^{DFT} \rightarrow G_{local}, \Delta(\omega), E_{imp}$
Impurity solver:
CTQMC,OCA,NCA
$\Delta(\omega), E_{imp} \rightarrow \Sigma(\omega), G_{local}$

dmft1

$$\Sigma(\omega), \varepsilon^{DFT}_{\mathbf{k},i}, \psi^{DFT}_{\mathbf{k},i} \rightarrow G_{local}, \Delta(\omega), E_{imp}$$

projector: $P(\mathbf{r}\mathbf{r}', \tau L L') \approx Y_L(\hat{\mathbf{r}}_\tau)\delta(r_\tau - r'_\tau)Y^*_{L'}(\hat{\mathbf{r}}'_\tau)$

self-energy in KS base: $\overline{\Sigma}_{\mathbf{k},ij}(\omega) = \sum_{\tau, L_1 L_2} P_{\mathbf{k}\tau}(ji, \tau L_2 L_1)(\Sigma^\tau_{L_1 L_2}(\omega) - E^\tau_{dc})$

DMFT self-consistency condition:

$$G_{local}{}^{\tau}_{LL'} = \sum_{\mathbf{k}ij} P_{\mathbf{k}\tau}(ij, LL') \left[\left(i\omega + \mu - \epsilon_{\mathbf{k}} - \overline{\Sigma}_{\mathbf{k}}(\omega) \right)^{-1} \right]_{ji}$$

$$= \left[\frac{1}{i\omega - E^\tau_{imp} - \Sigma^\tau(\omega) - \Delta^\tau(\omega)} \right]_{LL'}$$

dmft2

$$\Sigma(\omega), \varepsilon^{DFT}_{\mathbf{k},i}, \psi^{DFT}_{\mathbf{k},i} \rightarrow \rho^{DMFT}_{val}(\mathbf{r}), E_{valence}$$

projector: $$P(\mathbf{r}\mathbf{r}', \tau L L') \approx Y_L(\hat{\mathbf{r}}_\tau)\delta(r_\tau - r'_\tau)Y^*_{L'}(\hat{\mathbf{r}}'_\tau)$$

self-energy in KS base: $$\overline{\Sigma}_{\mathbf{k},ij}(\omega) = \sum_{\tau, L_1 L_2} P_{\mathbf{k}\tau}(ji, \tau L_2 L_1)(\Sigma^\tau_{L_1 L_2}(\omega) - E^\tau_{dc})$$

DMFT eigenvalues: $$\left(-\nabla^2 + V_{KS}(\mathbf{r}) + \overline{\Sigma}_{\mathbf{k}}(\omega)\right)\psi_{\mathbf{k}\omega_n i}(\mathbf{r}) = \varepsilon^{DMFT}_{\mathbf{k}\omega_n i}\psi_{\mathbf{k}\omega_n i}(\mathbf{r})$$

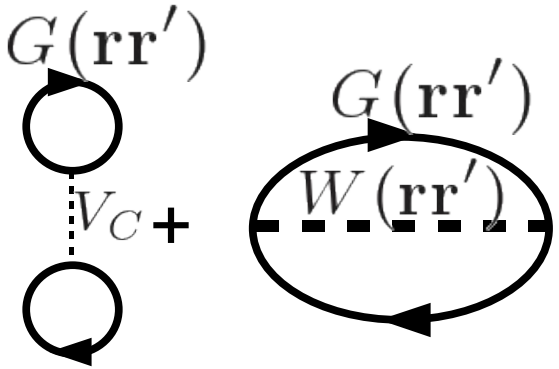
The chemical potential: $$N_{val} = T\sum_{\omega_n, i}\frac{1}{i\omega_n + \mu - \varepsilon_{\mathbf{k}\omega_n i}}$$

Valence charge density:

$$\rho^{DMFT}_{val} = \sum_{\mathbf{k},ij}\psi^{DFT}_{\mathbf{k}i}(\mathbf{r}) \times T\sum_{\omega_n}\left[\left(i\omega_n + \mu - \epsilon_{\mathbf{k}} - \overline{\Sigma}_{\mathbf{k}}(\omega)\right)^{-1}\right]_{ij} \times \psi^{DFT}_{\mathbf{k}j}(\mathbf{r})$$

total energy contribution: $$E_{valence} = \mathrm{Tr}((-\nabla^2 + V_{KS})\rho^{DMFT}_{val})$$

$\Phi_{GW}(G,W) =$



$\Phi_{DMFT}(G,W) =$