Some notes on the Free Energy in DFT+DMFT

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(Dated: January 29, 2017)

I. HOW IS FREE ENERGY IMPLEMENTED?

The details of the algorithm are published in Phys. Rev. Lett. 115, 256402 (2015). Here we just mention some implementation details, which are not completely detailed there.

The total energy is printed in column six of *info.iterate*. We compute it by

$$E_6 = E^H[\rho] + E^{XC}[\rho] + E_{nuc} - \text{Tr}((V_H + V_{XC})\rho) + \text{Tr}(\varepsilon_{\mathbf{k}}^{DFT}\rho) + E_{imp}^{pot} - \Phi^{DC}[n_{imp}] \tag{1}$$

The blue terms are computed from the impurity quantities, and the black and red are computed from the lattice quantities. The black are evaluated in *lapw0* and *lapwc*. The red terms are evaluated in *dmft2*.

The free energy is printed in column seven and eight of *info.iterate*. The seventh column is computed by

$$F_7 = E^H[\rho] + E^{XC}[\rho] + E_{nuc} - \text{Tr}((V_H + V_{XC})\rho) + \text{Tr}\log(G) + \mu N - \text{Tr}\log(G_{loc}) + \text{Tr}((\varepsilon_{imp} + V_{DC})n_{loc}) \tag{2}$$

$$+ E_{imp}^{pot} + \text{Tr}\left((\Delta - \omega_n \frac{d\Delta}{d\omega_n})G_{imp}\right) - \Phi^{DC}[n_{imp}] - TS_{imp} \tag{3}$$

The blue terms are computed from the impurity quantities, and the black and red are computed from the lattice quantities. The black are evaluated in *lapw0* and *lapwc*. The red terms are evaluated in *dmft2*. The green term is missing in *info.iterate* and needs to be computed at postprocessing as explained in the above PRL.

The eight column is computed by

$$F_8 = E^H[\rho] + E^{XC}[\rho] + E_{nuc} - \text{Tr}((V_H + V_{XC})\rho) + \text{Tr}\log(G) + \mu N - \text{Tr}((\Sigma - V_{DC})G_{loc}) \tag{4}$$

$$+ E_{imp}^{pot} + \text{Tr}\left((\Delta - \omega_n \frac{d\Delta}{d\omega_n})G_{imp}\right) - \text{Tr}\log(G_{imp}) + \text{Tr}(\varepsilon_{imp}n_{imp}) + \text{Tr}(\Sigma_{imp}G_{imp}) - \Phi^{DC}[n_{imp}] - TS_{imp} \tag{5}$$

The difference between the seventh and eight column is then

$$F_8 - F_7 = \text{Tr}\log(G_{loc}) - \text{Tr}(\Sigma G_{loc}) - \text{Tr}(\varepsilon_{imp}n_{loc}) - \text{Tr}\log(G_{imp}) + \text{Tr}(\Sigma G_{imp}) + \text{Tr}(\varepsilon_{imp}n_{imp}) \tag{6}$$