Introduction to LDA + DMFT (II) [Kotliar]

- Example: Building Kohn-Sham Eqs.
  \[ S_0 + \int \frac{d^3 r}{2\pi^3} V_{\text{ext}} = \int \frac{d^3 r}{2\pi^3} V_{\text{ext}} + V^2 + J_0 \frac{\partial}{\partial r} \]
  \[ \rightarrow I_0 \left[ \rho \right] = -\text{Tr} \ln \left( \frac{\mathcal{H}}{\mathcal{H}_0} \right) - \int J_0(x) \rho(x) \]
  \[ \Delta I \left[ \rho \right] = \frac{g^2}{2} \int \int \rho(r) \rho(r') \frac{4}{1} \left< \psi^* (r') \psi^* (r) \psi (r') \psi (r) \right> \mathcal{I} (\rho, \lambda) \ dr dr' \ d\lambda \]
  \[ \Delta \text{Now define } V_{ks} \text{ via } V_{ks} = V_{\text{ext}} + J_0 \]
  \[ \Delta \text{By factorization, } \Delta I (\rho) = \frac{g^2}{2} \int \int \rho(r) \rho(r') \frac{4}{1} \left< \psi^* (r') \psi^* (r) \psi (r') \psi (r) \right> \mathcal{I} (\rho, \lambda) \ dr dr' \ d\lambda \]
  \[ \Delta \text{In LDA, } \Delta I_x (\rho) \approx \int \mathcal{I} (\rho, \lambda) \ dr \]

Technically, we may solve numerically the interesting \( \epsilon \) problem and extract \( \mathcal{I} (\rho, \lambda) \), & use it for all problems.

- Example: Building DMFT for Hubbard
  \[ H = \sum (t_{ij} - \mu \delta_{ij}) (c_i \cdot c_j + h.c.) + U \sum_n n_i n_{-i} \]
  \[ I_0 [G_{ii}, M_{ii}] = -\text{Tr} \ln \left( i\omega_n + \mu - t_{ij} - M_{ii} \right) - \text{Tr} \left[ M \mathcal{I} \right] \]
  \[ \Delta I_{xc} \approx \sum_i \Delta I_{xc-atom} [G_{ii}] \]
  \[ G_{ii} = \sum_{k} \frac{1}{i\omega_n + \mu - E(k) - M_{ii}} \]
  \[ M_{ii} = \delta_{\text{Gii}} \Delta \Gamma \text{atom} [G_{ii}] \]

We start with atomic problem as \( S_0 \). Thus diagrammatically the above corresponds to summing diagrams to all order.

- Self-consistency:
  \[ G_0 \leftrightarrow \text{impurity problem} \rightarrow G_0, M \]
  \[ \text{self-consistency} \]

where
\[
\begin{align*}
S_{\text{eff}} &= -\int_0^\beta \psi^* (\tau) G_{\text{eff}} (\tau, \tau') \psi (\tau') + \int_0^\beta d\tau \ \text{On} \ \mathcal{M} (\tau) \ n_\tau (\tau) \\
M &= G_0 \rightarrow G_0^{-1} \quad G_0^{-1} (i\omega) &= \left( \sum_k i\omega_n + \mu - t(k) - M(i\omega_n) \right)^{-1} + M(i\omega_n)
\end{align*}
\]
In doing so, we need efficient numerical method to solve the one-site interacting problem, i.e., a "black box":

\[ \Delta(r) \rightarrow \mathcal{G}[\Delta](r) \rightarrow \mathcal{V} \rightarrow \mu = \mathcal{G}^{-1} - \mathcal{G}_0^{-1} \]

where \( \mathcal{G}_0^{-1} = i\omega_n + \mu - \Delta \).

- The Weiss field \( \Delta(\omega) \) quantifies degree of localization.
  - \( \Delta(\omega) \) small \( \Rightarrow \) localized, \( \Delta(\omega) \) large \( \Rightarrow \) delocalize.
  - Note that localization is not is freq. dependent.

\[ \Delta(\omega)^{ab} \sim \sum_x \frac{\mathcal{V}^* x^a \mathcal{V}^b}{\omega - \varepsilon_x} \]

- From the calculation we can also extract valence histogram.

- Phase diagram — frustrated Hubbard.
  - Pozenberg, PRL, 75, 105 (1995)

- Example: \( V_2O_3 \)
  - DMFT suggests transfer of spectral weight, which is observed in experiment.

\[ T/W \]

- The (Ising) critical point & hysteresis are also observed.

- To solve for strip order, etc., need multi-impurity model.
  - But each impurity
- The hunt for strip pattern, need multi-impurity model
  ▶ each impurity interacts with each other only through self-consistency.

- For 5f, Pu is close to Mott transition. Traditional (~DFT) methods have problem getting good results, but LDA+DMFT get reasonable results.
  ▶ e.g. total energy as function of volume for Pu
  ▶ Allowing coupling to lattice, rich phase diagram can be obtained (lattice structure, etc.)
  ▶ DMFT also match well to phonon spectrum of Pu
    ▶ Phonon spectrum of Pu is hard to measure by neutron, since single crystal is hard to get & Pu absorb neutron. Problem can be circumvent by X-ray.
  ▶ The high temperature (S-phase) phase is more localized than the low temperature (α-phase) phase for 5f electrons.
    ➞ transfer of spectral weight in (e.g.) photoemission
  ▶ Pu also shows very different valence diagram than usual (many valence states are important, particular between $5^+$ & $6^+$)
    ➞ The "conjugate" element Cm in Cm does not show the same mixed valence.

- Idea of LDA+DMFT — treat delocalized $e^-$ (s,p, sometimes d) by DFT & localized $e^-(f$, sometimes d) by DMFT.
- LDA+U amounts to  beating the localized problem by Hartree-Fock.
- LDA+U & LDA+DMFT are "2nd principle" calculations, since some parameters ("J", "U") have to be put in.
  (LDA itself is parameter free)