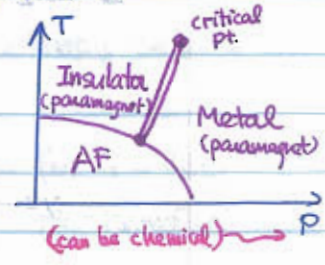
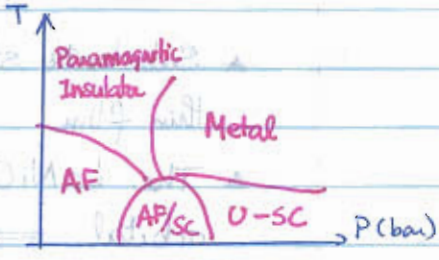
Introduction to LDA + DMFT (I) [Kotliar]

- Rev. Mod. Phys, 78, 000865 (2006) for review

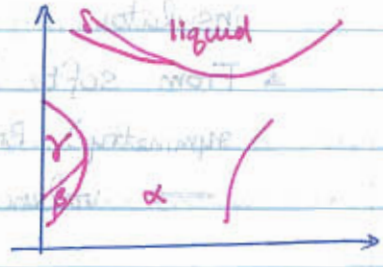
- Motivation: Mott transition in V_2O_3 (driven by pressure)
  - ▲ Metal side well described by Fermi liquid insulator side well described by atomic theory. Challenge is to connect the two. (e.g., in intermediate region the resistance is not low)



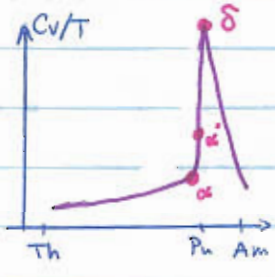
- Another example: kappa organics
  - ▲ Does not require very high pressure to tune

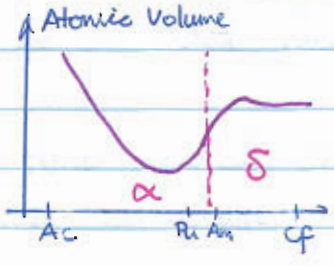


- Third example: Cerium
  - ▲ γ-phase (localized)
  - ▲ α-phase (delocalized Kondo)



- Fauth example: Actinides





- Problem: understand localization – delocalization effect at FINITE temperature.

- Fifth Example: CeM (M = Rh, Co, Ir)
  - At low temperature these behave differently

- "Big" effects arise from itinacy – localization competition
  - Huge volume collapse in lanthanides & actindies
  - metal – insulator transition
  - quasiparticle with large m^*
  - colossal magnetoresistance
  - large thermoelectric response
  - high-Tc superconductivity

- We want a "good enough" reference system for understanding strongly correlated system.
  - simple enough to solve, complex enough to be useful
  - predecessor: Weiss mean-field theory for Stat. mech.

- Definition of strongly/weakly correlated system
  - Weakly correlated if Fermi liquid theory & Kohn-Sham theory works.
  - DMFT describes an atom in medium that obey self-consistency, which gives reference point for strongly correlated system.

- Density Functional Theory
  - Description of weakly correlated system well described by Kohn-Sham eqns. i.e. there is a frictitous free-electron system that together with Kohn-Sham potential gives good description of electron density

▲ Kohn-Sham eqn:

$$\begin{cases} \left[-\nabla^2 + V_{KS}[\rho](\vec{r})\right]\psi_{kj}(\vec{r}) = \varepsilon_{kj}\psi_{kj}(\vec{r}) \\ \rho(\vec{r}) = \sum_{kj} |\psi_{kj}(\vec{r})|^2 f(\varepsilon_{kj}) \\ V_{KS}[\rho] = V_{crystal}(\vec{r}) + \underbrace{\mathcal{N}[\rho(\vec{r})]}_{\text{nonlinear universal functional, to be approximated in practice}} \end{cases}$$

▲ In Hartree-Fock, $V_{KS}[\rho]$ is replaced by some non-local potential

▲ Hartree-Fock performs poorly for metal, DFT performs reasonable for metal.

▲ HF & DFT are both examples of static mean-field theory.

▲ Can thought of HF as picking $\langle\psi^\dagger(\vec{r})\psi(\vec{r}')\rangle$ as central observable, & DFT as picking $\langle\psi^\dagger(\vec{r})\psi(\vec{r})\rangle$ as central observable.

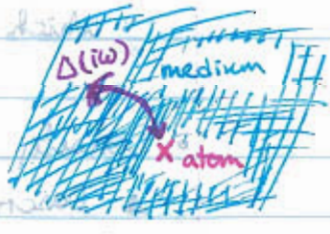
▲ DMFT, instead, pick $\langle\psi_i^\dagger(t)\psi_i(0)\rangle$ as central observable.

▲ In DFT, we approx. $[i\omega - \nabla^2 - V_x - V_H - \underbrace{\Sigma}_{\text{self-energy}}]^{-1}$ with $[i\omega - \nabla^2 - V_{KS}]^{-1}$. This works if these two are not differ much, and in such case perturbation theory can be used to improve the results.

◦ DMFT on one-band Hubbard model

▲ Concentrate on local Green function:

$$G_L(i\omega) = -\langle c_i(i\omega)\, c_i^\dagger(i\omega)\rangle$$



▲ We assume a "magic" $\mathcal{M}(i\omega)$ s.t.

$$G_L(i\omega) = \sum_k \frac{i}{i\omega + \mu - t(k) - \mathcal{M}(i\omega)}$$

▲ We shall assume $\mathcal{M}$ to be functional of hybridization $\Delta(i\omega)$ (which describe atom-environment interaction), and that $\mathcal{M}[\Delta](i\omega)$ is "universal" (independent of $t(k)$)

▲ The result will be exact in atomic limit (i.e. $t \to 0$), band limit (i.e. $U \to 0$), & high coordination limit.

▲ Unlike DFT, there is no general theorem to show that a universal $M[\Delta](i\omega)$ exists.
(But note that from a full function $\Gamma[\rho]$ to a local potential $V_{KS}[\rho]$ in DFT is still a jump in rigid logic).

• Construction of DMFT (& other related methods)

1., choose some observable A_i, $a_i = \langle A_i \rangle$
(e.g. $\rho(\vec{r})$ & $\langle d_\alpha^\dagger d_\beta \rangle$ in LDA+U ; $\rho(\vec{r})$ in DFT)

2., write down souced partition function:

$$Z_J[J_i] = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi\, e^{-(S + J_i A_i)} \quad (= e^{-F[J_i]})$$

observe that $\frac{\delta F}{\delta J_i} = \langle A_i \rangle = a_i$ ——— (*)

inverting (*) gives $J_i = J_i(a)$

Now apply Legendre transformation to get:

$$\Gamma[a] = F[J(a)] - J(a)\cdot a$$

then $\frac{\delta \Gamma}{\delta a_i} = -J_i(a)$

define a^* via $\frac{\delta \Gamma}{\delta a}(a^*) = 0$, then $\Gamma(a^*) = F[J=0]$

3., Split S into two parts:

$$S = S_0 + \lambda S_1$$

S_0: problem w/ known answer, reference state; λS_1: $\lambda = 1$ in real problem

Expanding Γ & J:

$$\begin{cases} \Gamma(a) = \Gamma_0(a) + \lambda \Gamma_1(a) + \ldots = \Gamma_0(a) + \Delta\Gamma(a) \\ J(a) = J_0(a) + \lambda J_1(a) + \ldots \end{cases}$$

Then J_0 satisfies

$$\begin{cases} Z_0 = e^{-F_0} = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi\, e^{-(S + J_0 A)} \\ \Gamma_0(a) = F(J_0(a)) - J_0(a)\cdot a \end{cases}$$

(Turns out that Γ converges better than F)

Exercise: Consider classical Ising model, $a_i = \langle s_i \rangle$.

Take $\lambda = 1/T$, Γ is then $\Gamma(m_i)$

1st-order gives Weiss' mean-field theory

2nd-order gives Onsager's correction.

Now we want to approximate $\Delta\Gamma(a)$. Take $\Delta\Gamma_{approx}$ to be $\Delta\Gamma$ of atom-environment system. Then:

$$\Gamma_{approx}[a] = \Gamma_0[a] + \Delta\Gamma_{approx}[a]$$

Self-consistency: $\frac{\delta \Gamma_{approx}}{\delta a} = 0$

(Formally, $\Delta\Gamma(a) = \int_0^1 d\lambda \, \langle s_i \rangle (\lambda, J(\lambda, a))$

In DMFT, we'll take S_0 to be the full "atom in medium" Hamiltonian