Introduction to LDA+DMFT

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CIFAR-PITP International Summer School on Numerical Methods for Correlated Systems in Condensed Matter
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Plan of the lectures

• Motivate the development of a mean field theory of correlated electron materials.
• General formulations of mean field theory: density functional theory, DMFT, spectral density functional, LDA+DMFT.
• Applications to the Mott transition.
• Some applications of LDA+DMFT
• More foundations, extensions, issues of implementation, applications.

Pressure Driven Mott Transition

FIG. 70. Phase diagram for doped V$_2$O$_3$ systems, (V$_{1-x}$Cr$_x$)$_2$O$_3$ and (V$_{1-x}$Ti$_x$)$_2$O$_3$. From McWhan et al., 1971, 1973.
Mott transition and transport crossovers in the organic compound \( \kappa=(\text{BEDT-TTF})_2\text{Cu}[\text{N(CN)}_2]\text{Cl} \)

P. Limelette et al., PRL 91 (2003) 016401

See also:

Kagawa et al. cond-mat/0307304


FIG. 6: Temperature-dependence of the resistivity at different pressures. The data (circles) are compared to a DMFT-NRG calculation (diamonds), with a pressure dependence of the bandwidth as indicated. The measured residual resistivity \( \rho_0 \) has been added to the theoretical curves.
Cerium

- Various phases:
  - Isostructural phase transition (T=298K, P=0.7GPa)
    - $\gamma$ (fcc) phase
      [magnetic moment (Curie-Wiess law)]
    - $\rightarrow \alpha$ (fcc) phase
      [loss of magnetic moment (Pauli-para)]
    - With large volume collapse
      $\Delta v/v \approx 15\%$
      ($\gamma$-phase $a \approx 5.16$ Å
      $\alpha$-phase $a \approx 4.8$ Å)

- $\gamma$-phase (localized):
  - High T phase
    - Curie-Weiss law (localized magnetic moment),
    - Large lattice constant
    - $T_k$ around 60-80K

- $\alpha$-phase (delocalized: Kondo-physics):
  - Low T phase
    - Loss of Magnetism (Fermi liquid Pauli susceptibility) - completely screened magnetic moment
    - Smaller lattice constant
    - $T_k$ around 1000-2000K

<table>
<thead>
<tr>
<th>Phases</th>
<th>Exp.</th>
<th>LDA</th>
<th>LDA+U</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\gamma$</td>
<td>34.4Å³</td>
<td>28Å³</td>
<td>24.7Å³</td>
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<tr>
<td>$\alpha$</td>
<td>35.2Å³</td>
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\[ LDA \]
Localization Delocalization in Actinides

Modern understanding of this phenomena using functional approach to DMFT. K Haule S. Savrasov J Shim
Strongly correlated materials do “big” things

Competition of localization and itineracy.

- Huge volume collapses in lanthanides and actindies, eg. Ce, Pu, .......
- Metal insulator transitions as a function of pressure and composition in transition metal oxides, VO2 V2O3
- Quasiparticles with large masses $m^* = 1000 \, m_e$ in Ce and U based heavy fermions.
- Colossal Magnetoresistance in La$_{1-x}$Sr$_x$MnO$_3$
- High Temperature Superconductivity 150 K Ca$_2$Ba$_2$Cu$_3$HgO$_8$
- Large thermoelectric response in Na$_x$Co$_2$O$_4$
- 50K superconductivity in SmO$_{1-x}$FxFeAs
- Many others......
CeMIn$_5$  M=Co, Ir, Rh

- CeRhIn$_5$: $T_N=3.8$ K; $\gamma \approx 450$ mJ/molK$^2$
- CeCoIn$_5$: $T_c=2.3$ K; $\gamma \approx 1000$ mJ/molK$^2$;  
- CeIrIn$_5$: $T_c=0.4$ K; $\gamma \approx 750$ mJ/molK$^2$
Iron based high-Tc superconductors

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<td>3.7</td>
<td>cm/0803.3978</td>
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x~5-20%

Fe, Ni, As, P
La, Sm, Ce
O

- 2D square lattice of Fe
- Fe - magnetic moment

- Y. Kamihara et.al., Tokyo, JACS
- X.H. Chen, et.al., Beijing, cm/0803.3790
- G.F. Chen et.al., Beijing, cm/0803.3603
- Z.A. Ren et.al, Beijing, unpublished
Two paths for ab-initio calculation of electronic structure of strongly correlated materials

- Crystal structure + Atomic positions
- Model Hamiltonian
- Correlation Functions Total Energies etc.

Mean field ideas can be used in both cases.
Mean Field Theory: general construction principles
Spectral density functional. Effective action construction. e.g. Fukuda et al.

\[ Z = e^{-F[J]} = \int d\psi d\psi^+ e^{-[S(\psi^+\psi)+JA]} \]

\[ \frac{\delta F}{\delta J}[J] = \langle A \rangle = a \]

\[ \Gamma[a] = F[J[a]] - aJ[a] \]
\[ S = S_0 + \lambda S_{\text{int}} \]

\[ J = J_0 + \lambda J_1 + \cdots \]

\[ \Gamma[\alpha] = F_0[\psi_0] - a J_0 + \lambda \Delta \Gamma \Gamma[\alpha] \cdots \]

\[ \Delta \Gamma = \Gamma_{\text{hartree}} + \Gamma_{xc} \]
\[ \Delta \Gamma [a] = \int_{0}^{1} d\lambda < S_{\text{int}} > (\lambda, J(\lambda, a)) \]

In practice we need good approximations to the exchange correlation, in DFT LDA. In spectral density functional theory, DMFT. Review: Kotliar et.al. Rev. Mod. Phys. 78, 865 (2006)

\[ \frac{\delta F}{\delta J_0} [J_0] = a \quad \frac{\delta \Delta \Gamma}{\delta a} = J_0[a] \]

Kohn Sham equations
Remarks:

• Exact functionals of an observable $A$, $\Gamma_{\text{exact}}[a]$
• In practice approx are needed $\Gamma_{\text{mft}}[a] \sim \Gamma_{\text{exact}}[a]$
• Many a’s many theories.

• Introduction of a reference system. Separation into “free part” and exchange+ correlation.
• Formal expression for the correlation part of the exact functional as a coupling constant integration.
• Good approximate functionals obtained by approximating the xc part. [ small parameter $d$ helps!]
• While the construction aims to calculate $\langle A \rangle = a$, other quantities, e.g. correlation functions, emerge as a byproduct.
Crucial Role of the constraining field

\[ J_0[a] \]

Different reference systems [ e.g. band limit or atomic limit ] define different constraining fields.

- Different functionals (self energy functional, BK functional, Harris Foulkes functional, etc )

\[ \Gamma[a], \Gamma[a,J], \Gamma[a,J_0], \Gamma[J_0] \]
Analogy with spin systems.
Density functional and Kohn Sham reference system

$$-\nabla^2 / 2 + V_{KS}(r) \psi_{kj} = \varepsilon_{kj} \psi_{kj}$$

$$\rho(r) = \sum_{kj} f(\varepsilon_{kj}) |\psi_{kj}(r)|^2$$

$$V_{KS}(r)[\rho(r)] = V_{ext}(r) + \int \frac{\rho(r')}{|r - r'|} dr' + \frac{\delta E_{xc}}{\delta \rho(r)} \rho$$

• Kohn Sham spectra, proved to be an excellent starting point for doing perturbation theory in screened Coulomb interactions GW.
Kohn Sham Eigenvalues and Eigensates: Excellent starting point for perturbation theory in the screened interactions (Hedin 1965)

Self Energy

VanShilfgaarde (2005)
Model Hamiltonians and DMFT
Dynamical Mean Field Theory. Cavity Construction.


\[-\sum_{i,j} J_{ij} S_i S_j - \hbar \sum_i S_i \]

\[-\sum_{<i,j>,\sigma} (t_{ij} + \mu \delta_{ij})(c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma}) = \sum_{a,\sigma} (V_a^{\dagger} A_{a\sigma}^{\dagger} + c.c.) + \sum_{a,\sigma} \epsilon_{a\alpha} A_{a\alpha}^{\dagger} A_{a\alpha} + \sum_{a,\sigma} \mu c_{0\sigma}^{\dagger} c_{0\sigma} + U c_{0\uparrow}^{\dagger} c_{0\uparrow}^{\dagger} c_{0\downarrow}^{\dagger} c_{0\downarrow}^{\dagger} \]

\[\Delta(\omega) = \sum_{\alpha} \frac{V_{\alpha}^{\dagger} V_{\alpha}}{\omega - \epsilon_{\alpha}} \]

\[\int_0^\beta \int_0^\beta c_{\alpha\sigma}^{\dagger}(\tau)[(\frac{\partial}{\partial \tau} + \mu)\delta(\tau - \tau') - \Delta(\tau - \tau')] c_{\alpha\sigma}(\tau') + U \int_0^\beta n_{0\uparrow} n_{0\downarrow} \]

\[\text{DMFT} \Rightarrow \text{A}(\omega) \]

\[|0\rangle \rightarrow |\uparrow\rangle \rightarrow |\uparrow\downarrow\rangle \rightarrow |0\rangle \]

\[V_{\text{electron}}: + \rightarrow \uparrow \rightarrow - \rightarrow + \]

\[V_{\text{electron}}: e_{\uparrow} \rightarrow e_{\downarrow} \rightarrow e_{\downarrow} \rightarrow e_{\uparrow} \]

\[V_{\text{electron}}: \text{electron reservoir} \]
A(ω)  \quad \Delta(\omega)

\[ m_i = th[\beta \sum_j J_{ij} m_j + h] \]

Solving A for given bath, is not easy Impurity solvers; See P. Werner and M Jarrell’s talks.

\[ i\omega_n - \sum (i\omega_n)[\Delta] \overset{=}{\approx} -\Delta(i\omega_n) + \frac{1}{G_{imp}(i\omega_n)[\Delta]} \]

\[ i\omega_n - \sum (i\omega_n)[\Delta] - t(k) + \mu = G_{latt}(i\omega_n,k)^{-1} \]

\[ G_{imp}(i\omega_n)[\Delta] = \sum_k G_{latt}(i\omega_n,k)[\Delta] \]
DMFT

\[ H = - \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U n_{i\uparrow} n_{i\downarrow} \]

\[ G_c(\tau) = - \langle T c(\tau) c^\dagger(0) \rangle_{S_{\text{eff}}} \]

\[ S_{\text{eff}} = - \int_0^\beta c_{\sigma}^\dagger(\tau) G_0^{-1}(\tau - \tau') c_\sigma(\tau') + \int_0^\beta d\tau U n_{\uparrow}(\tau) n_{\downarrow}(\tau) \]

\[ \Sigma = G_0^{-1} - G_c^{-1} \]

\[ G_0^{-1}(i\omega_n) = \left( \sum_k \frac{1}{i\omega_n + \mu - t(k) - \Sigma(i\omega_n)} \right)^{-1} + \Sigma(i\omega_n) \]

IMPURITY PROBLEM

SELF CONSISTENCY

\[ G_0 \quad \rightarrow \quad G_0, \Sigma \quad \rightarrow \quad G_c, \Sigma \]
Evolution of the DOS. Theory and experiments

\[ A(\omega) \]
Qualitative Phase diagram: frustrated Hubbard model, integer filling *M. Rozenberg et.al. 75, 105 (1995)*
Interaction with Experiments. V2O3: Anomalous transfer of spectral weight

Spinodals and Ising critical endpoint.

Observation in $V_2O_3$: *P. Limelette et.al. Science 302, 89 (2003)*
LDA+DMFT

- The light, SP (or SPD) electrons are extended, well described by LDA. The heavy, D (or F) electrons are localized treat by DMFT.

- LDA Kohn Sham Hamiltonian already contains an average interaction of the heavy electrons, subtract this out by shifting the heavy level (double counting term)

- Kinetic energy is provided by the Kohn Sham Hamiltonian (sometimes after downfolding). The U matrix can be estimated from first principles of viewed as parameters. Solve resulting model using DMFT.

\[
G(k, i\omega) = \frac{1}{i\omega - t(k) - \Sigma(i\omega)}
\]

$U \rightarrow U_{abcd}$

$\Sigma \rightarrow \begin{pmatrix} 0 & 0 \\ 0 & \Sigma_{ff} \end{pmatrix}$

$t(k) \rightarrow \begin{pmatrix} H[k]_{spd,sps} & H[k]_{spd,f} \\ H[k]_{f,spd} & H[k]_{ff} \end{pmatrix}$

$|0>, |\uparrow>, |\downarrow>, |\uparrow\downarrow> \rightarrow |LSJM\gamma...>$

$\Gamma_{dft}[\rho] \rightarrow \Gamma_{lda} + dmf\Gamma[G_{loc}, \rho, U]$
LDA+DMFT Self-Consistency loop

\[ \langle \chi_{k\alpha} | -\nabla^2 + V_{xc}(\rho) | \chi_{k\alpha} \rangle = H_{LMTO}(k) \]

\[ \rho(r) = T \sum_{i\omega} G(r, r, i\omega) e^{i\omega 0^+} \]

\[ n_{HH} = T \sum_{i\omega} G_{HH}(r, r, i\omega) e^{i\omega 0^+} \]
LDA+DMFT functional

\[ \Gamma_{LDA + DMFT} \left[ \rho(r) G_{ab} V_{KS}(r) \Sigma_{ab} \right] \]

\[ - \text{Tr} \log \left[ i \omega_n + \nabla^2 / 2 - V_{KS} - \chi^{*}_{\alpha R}(r) \Sigma_{\alpha \beta R} \chi^{*}_{\beta R}(r) \right] - \]

\[ \int V_{KS}(r) \rho(r) \, dr - \sum_{i \omega_n} \text{Tr} \Sigma(i \omega_n) G(i \omega_n) + \]

\[ \int V_{ext}(r) \rho(r) \, dr + \frac{1}{2} \int \frac{\rho(r) \rho(r')}{|r - r'|} \, dr \, dr' + E^{LDA}_{xc}[\rho] + \]

\[ \sum_R \Phi \left[ G_{\alpha \beta R} \right] - \Phi_{DC} \]

\[ \Phi \text{ Sum of local 2PI graphs with local U matrix and local G} \]

\[ \Phi_{DC}[G] = Un(n-1) \frac{1}{2} \]

\[ n = T \sum_{\omega \epsilon \omega} \left( G_{ab}(i\omega) e^{i\omega} \right) \]
Embedding

\[ \Sigma_{HH} = \begin{bmatrix} \Sigma_{22} & 0 \\ 0 & \Sigma_{11} \end{bmatrix} \rightarrow \hat{\Sigma} = \begin{bmatrix} 0 & 0 \\ 0 & \Sigma_{HH} \end{bmatrix} \]

\[ \hat{H} = \begin{bmatrix} H_{LL} & H_{LH} \\ H_{HL} & H_{HH} \end{bmatrix} \]

Inversion

\[ i\omega_n \hat{O}_k - \hat{H}(k) - \hat{E} - \hat{\Sigma}(i\omega_n) \rightarrow \frac{1}{i\omega_n \hat{O}_k - \hat{H}(k) - \hat{E} - \hat{\Sigma}(i\omega_n)} \]

Integrating over BZ

\[ \hat{G}_{loc}(i\omega_n) = \sum_k \frac{1}{i\omega_n \hat{O}_k - \hat{H}(k) - \hat{E} - \hat{\Sigma}(i\omega_n)} \]

Truncation

\[ \hat{G}_{loc} = \begin{bmatrix} 0 & 0 \\ 0 & G_{HH} \end{bmatrix} \rightarrow G_{HH} \]

\[ G_0^{-1}(i\omega_n) = G_{HH}^{-1} + \Sigma_{HH}(i\omega_n) \]
Inversion in realistic DMFT

\[
[(i \omega + \mu) \hat{O}(\mathbf{k}) - \hat{h}^{(0)}(\mathbf{k}) - M_{\text{int}}(i \omega)]^{-1}.
\]

\[
[h^{(0)}_{\alpha \beta}(\mathbf{k}) + M_{\text{int}, \alpha \beta}(i \omega) - \epsilon_{kj \omega} O_{\alpha \beta}(\mathbf{k})] \psi_{kj \omega, \beta}^R = 0
\]

\[
G_{\alpha \beta}(\mathbf{k}, i \omega) = \sum_j \frac{\psi_{kj \omega, \alpha}^R \psi_{kj \omega, \beta}^L}{i \omega + \mu - \epsilon_{kj \omega}}.
\]

\[
\rho(\mathbf{r}) = T \sum_{i \omega} \sum_{kj} \frac{\psi_{kj \omega}^R(\mathbf{r}) \psi_{kj \omega}^L(\mathbf{r})}{i \omega + \mu - \epsilon_{kj \omega}} e^{i \omega 0^+}.
\]
Generalized Kohn Sham eigenstates

\[ \rho(r) = T \sum_{i\omega} \sum_{kj} \frac{\psi_{kj\omega}^R(r) \psi_{kj\omega}^L(r)}{i\omega + \mu - \epsilon_{kj\omega}} e^{i\omega t}. \]

\[ g_{kj\omega} = \frac{1}{i\omega + \mu - \epsilon_{kj\omega}} \]

\[ \rho(r) = \sum_{kj} f(\epsilon_{kj}) |\psi_{kj}(r)|^2 \]
Comments on LDA+DMFT

- Static limit of the LDA+DMFT functional, with $\Phi = \Phi_{HF}$ reduces to LDA+U
- Removes inconsistencies and shortcomings of this approach. **DMFT retain correlations effects in the absence of orbital ordering.**
- Only in the orbitally ordered Hartree Fock limit, the Greens function of the heavy electrons is fully coherent
- **Gives the local spectra and the total energy simultaneously, treating QP and H bands on the same footing.**
Localization Delocalization in Actinides

Modern understanding of this phenomena using functional approach to DMFT. K Haule S.Savrasov J Shim
Volume Collapse Transitions: relaxing the lattice positions. Savrasov et. al.
DMFT Phonons in fcc $\delta$-Pu

\begin{table}
\centering
\begin{tabular}{|c|c|c|c|c|}
\hline
 & $C_{11}$ (GPa) & $C_{44}$ (GPa) & $C_{12}$ (GPa) & $C'(GPa)$ \\
\hline
Theory & 34.56 & 33.03 & 26.81 & 3.88 \\
\hline
Experiment & 36.28 & 33.59 & 26.73 & 4.78 \\
\hline
\end{tabular}
\end{table}

(Dai, Savrasov, Kotliar, Ledbetter, Migliori, Abrahams, Science, 9 May 2003)
(experiments from Wong et.al, Science, 22 August 2003)
Curium has large magnetic moment and orders antif Pu does is non magnetic.
Volume and Spectra

alpha->delta volume collapse transition

Gouder
Havela
Lander

The “DMFT-valence” in the late actinides.

Time scale of the fluctuations. $E_f^*$
Iron based high-Tc superconductors

- 2D square lattice of Fe
- Fe - magnetic moment

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Fe, Ni, As, P, La, Sm, Ce

x ~ 5-20%
LDA+DMFT: LaOFeAs is at the verge of the metal-insulator transition (for realistic $U=4eV$, $J=0.7eV$) For a larger ($U=4.5$, $J=0.7eV$) Mott-Slater insulator

Not a one band model: all 5 bands important (for $J>0.3$)

K. Haule J. Shim G. Kotliar
arXiv:0803.1279
Iron Pnictides vs Cuprates

- Both are strongly correlated high temperature superconductors.
- In both cases the superconductor is proximate to a Mott insulator and is not well described by Fermi Liquid at high t.

### DIFFERENCES

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<td>• $U &lt; U_{c2}$</td>
<td>• $U &gt; U_{c2}$, doped Mott insulator</td>
</tr>
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<td>• One band model</td>
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<tr>
<td>• Important role of Jhunds</td>
<td>• Importance of Superexchange</td>
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<tr>
<td>• Single Site DMFT</td>
<td>• Cluster DMFT</td>
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Coherence-incoherence crossover in DMFT: crucial role played by J
Coherence-incoherence crossover in DMFT: crucial role played by J
Experimental predictions

\[ \gamma \text{ (mJ/molK}^2) \]

\[ J(\text{eV}) \]

\[
S = \int dx \psi^+(x) \left[ \partial_\tau - \nabla^2 + V_{\text{ext}}(x) \right] \psi(x) + \frac{1}{2} \int dx dx' \psi^+(x) \psi^+(x') \psi(x) \psi(x')
\]

\[
\Gamma[G,W] = Tr LnG - Tr[G_{0}^{-1} - G^{-1}]G - \frac{1}{2} Tr LnW + \frac{1}{2} Tr[V_{c}^{-1} - W^{-1}]W + E_{\text{hartree}} + \Phi[G,W]
\]

\[
\Phi[G,W] \square \Phi_{\text{EDMFT}}[G_{\text{loc}},W_{\text{loc}},G_{\text{nonloc}} = 0,W_{\text{nonloc}} = 0] \quad \text{Double loop in Gloc and Wloc}
\]

![Diagram](image)

**Input:** \( M, P \)

**Output:** Self-Consistent Solution


THE END
Thanks for your attention!!!!!

Hope it raised your interest and you want to contribute so that we can have a predictive theory of correlated materials in the very near future........

kotliar@physics.rutgers.edu
CeMIn$_5$  M=Co, Ir, Rh

- CeRhIn$_5$: $TN=3.8$ K; $\gamma \approx 450$ mJ/molK$^2$
- CeCoIn$_5$: $Tc=2.3$ K; $\gamma \approx 1000$ mJ/molK$^2$; CeIrIn$_5$: $Tc=0.4$ K; $\gamma \approx 750$ mJ/molK$^2$
Phase diagram of 115’s

Why CeIrIn$_5$?

- Ir atom is less correlated than Co or Rh (5d / 3d or 4d)
- CeIrIn$_5$ is more itinerant (coherent) than Co (further away from QCP)
Generalized Anderson Lattice Model

\[
\sum_{i,\sigma} \varepsilon_f f_{i\sigma}^\dagger f_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \sum_{<i,j>,\sigma} (t_{ij} + \mu \delta_{ij})(c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}) \\
+ \sum_{<i,j>,\sigma} V_{ij} f_{i\sigma}^\dagger c_{j\sigma} + c.c. = H_{ALM}
\]

- High temperature
  - Ce-4f local moments
  - $v_F \sim 10^6$ m/s

- Low temperature – Itinerant heavy bands
Angle integrated photoemission


Experimental resolution ~30meV
Surface sensitivity at 122 eV, theory predicts 3meV broad band

Theory: LDA+DMFT, impurity solvers SUNCA and CTQMC Shim Haule and GK (2007)
Buildup of coherence in single impurity case

Slow crossover pointed out by NPF 2004

Crossover around 50K

Very slow crossover!
DMFT is not a single impurity calculation

Auxiliary impurity problem:

Weiss field $\Delta(\omega)$ temperature dependent:

High-temperature $\Delta$ given mostly by LDA

low T: Impurity hybridization affected by the emerging coherence of the lattice (collective phenomena)

DMFT SCC:

$$\Delta(\omega) = \omega - E_{imp} - \Sigma_\omega - \left( \sum_k \frac{1}{\omega + \mu - H_k^{\text{imp}} - \Sigma_\omega} \right)^{-1} (\omega + \mu - H_k^{\text{imp}} - \Sigma_\omega)^{-1}$$

Feedback effect on $\Delta$ makes the crossover from incoherent to coherent state very slow!
At 300K very broad Drude peak (e-e scattering, spd lifetime~0.1eV)

At 10K:
• very narrow Drude peak
• First MI peak at 0.03eV~250cm⁻¹
• Second MI peak at 0.07eV~600cm⁻¹

Multiple hybridization gaps

- Larger gap due to hybridization with out of plane In
- Smaller gap due to hybridization with in-plane In
DMFT - Momentum resolved Ce-4f spectra $\rho_f(\omega,k)$

- Hybridization gap
- Fingerprint of spd’s due to hybridization
- q.p. band
- SO
- Scattering rate $\sim 100\text{meV}$
- Not much weight

$q.p.$ band

SO

Hybridization gap

Fingerprint of spd’s due to hybridization

Scattering rate $\sim 100\text{meV}$

Not much weight
Momentum resolved total spectra $\text{tr}A(\omega, k)$

- Most of weight transferred into the UHB
- LDA $f$-bands [-0.5eV, 0.8eV] almost disappear, only In-p bands remain
- Very heavy qp at $E_f$, hard to see in total spectra
- Below -0.5eV: almost rigid downshift
- Unlike in LDA+U, no new band at -2.5eV

Short lifetime of HBs $\rightarrow$ similar to LDA(f-core) rather than LDA or LDA+U
Quasiparticle bands

\[ \omega = \epsilon_{k,n}^{(0)} + \Sigma(\omega) \]

LDA bands

DMFT qp bands

\( W_{LDA} \sim 0.6\text{eV} \)

tails due to \( V_{\text{spd-f}} \)

three bands, \( Z_j=5/2 \sim 1/200 \)