Local moment approach to the multi - orbital single impurity Anderson and Hubbard models

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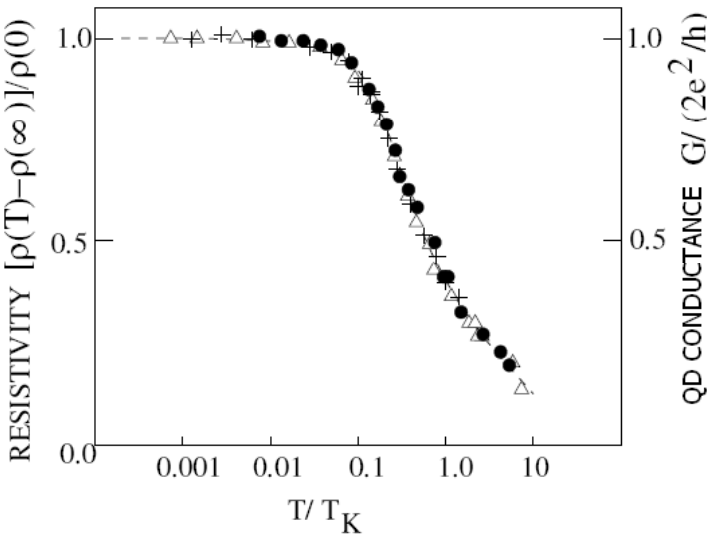
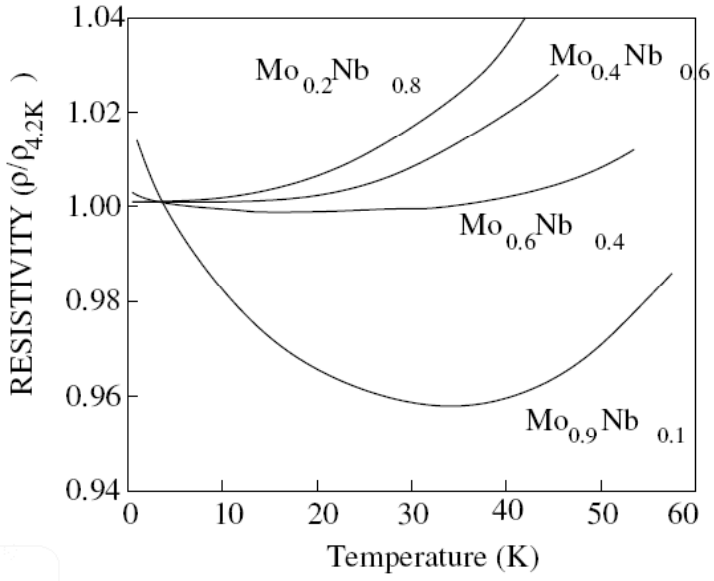
Outline

1. Kondo effect
2. Single impurity Anderson model
   - single orbital Anderson model
   - mean field
   - local moment approach (LMA)
   - multiorbital Anderson model and generalization of LMA
3. Hubbard model and DMFT
4. LMA + DMFT in multiorbital Hubbard model

Kondo effect

- Example: resistivity minimum in metals with rare earth impurities

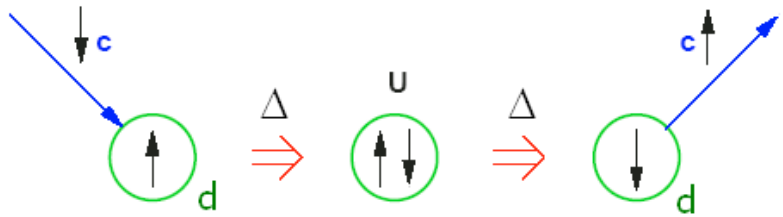




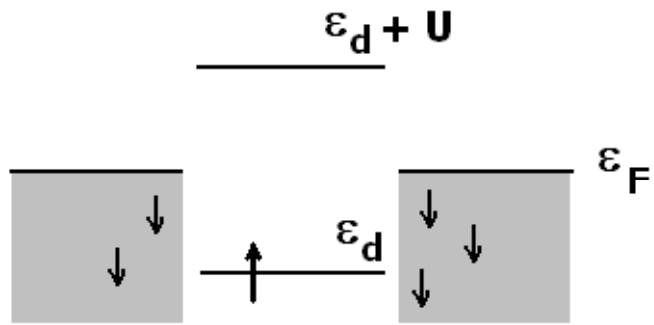
- Universal – in rare earth impurities, quantum dots, carbon nanotubes

Kondo effect

- below the temperature characteristic for a given material – Kondo temperature T_K – (crossover)
- spin fluctuations
  - spin-flip processes



  - screening of local moments

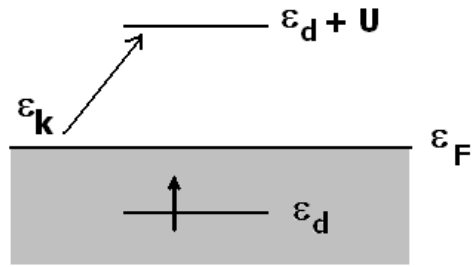


Single impurity Anderson model (SIAM)

$$H_{\mathrm{SIAM}} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\sigma} V_{\mathbf{k}} \left(d^{\dagger}_{\sigma} c_{\mathbf{k}\sigma} + c^{\dagger}_{\mathbf{k}\sigma} d_{\sigma} \right) + \sum_{\sigma} \left(\epsilon_d - U n_{d\bar{\sigma}} \right) n_{d\sigma}$$

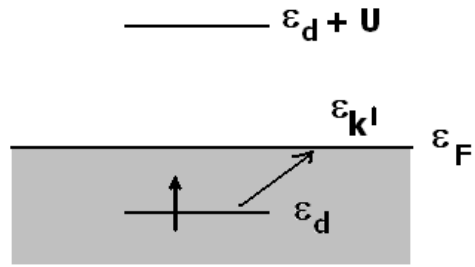
Hybridization function

$$\Delta(\omega) = \sum_{\mathbf{k}} \frac{|V_{\mathbf{k}}|^2}{\omega - \epsilon_{\mathbf{k}}} \approx \Delta$$



SIAM model describes

- charge fluctuations
- spin fluctuations
- screening of local magnetic moments



Mean field (Hartree-Fock) approximation

$$U n_{d\bar{\sigma}} n_{d\sigma} \approx U < n_{d\bar{\sigma}} > n_{d\sigma} + U n_{d\bar{\sigma}} < n_{d\sigma} > + U < n_{d\bar{\sigma}} >< n_{d\sigma} >$$

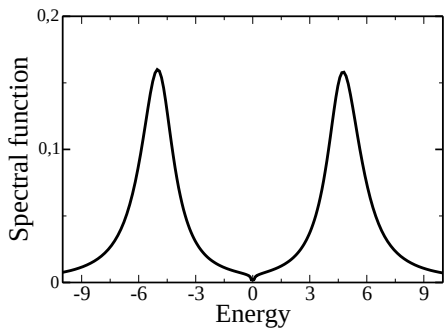
Energies depend on fillings $< n_\uparrow >$ and $< n_\downarrow >$

$$E_\sigma = \epsilon_d + U < n_{\bar{\sigma}} >$$

Non-vanishing local magnetic moment

$$\mu = < n_\uparrow > - < n_\downarrow >$$

Total density of states $\longrightarrow$



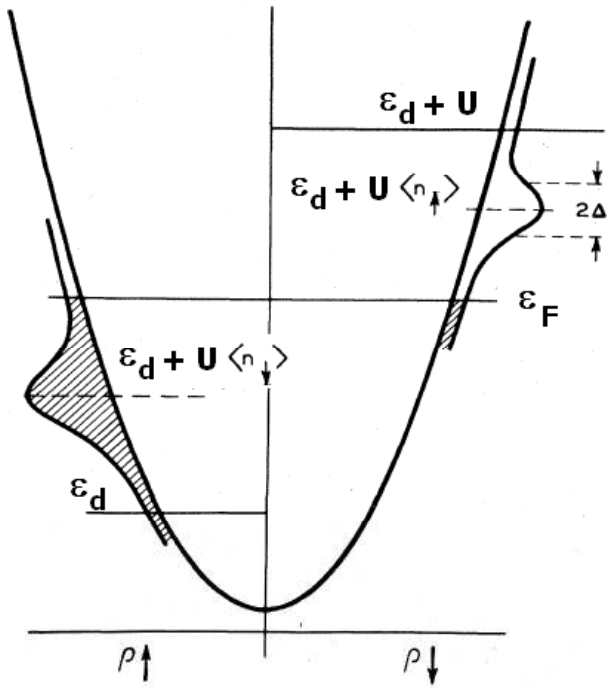
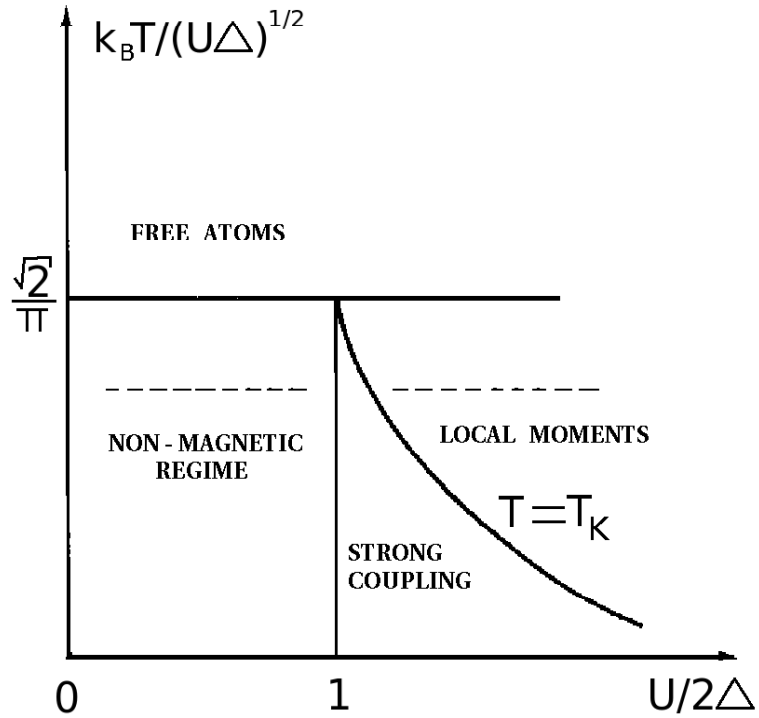


Figure: (*Anderson* 1961)

Energy scales

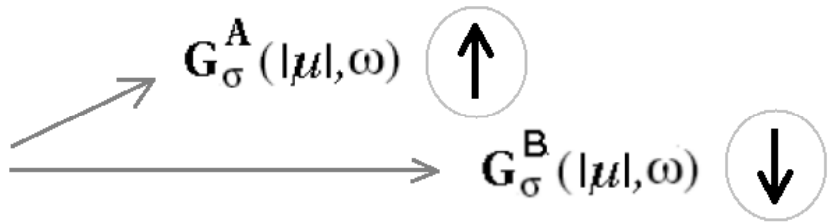
- $\epsilon_d, U \gg \Delta \gg T$ – atomic limit
- $U \ll \Delta$ – non-magnetic regime
- $\epsilon_d, U \gg \Delta,\ T > T_K$ – local moment regime
- $\epsilon_d, U \gg \Delta,\ T < T_K$ – strong coupling regime (Kondo effect)
- $\Delta \geq |\epsilon_d|$ – mixed valence regime



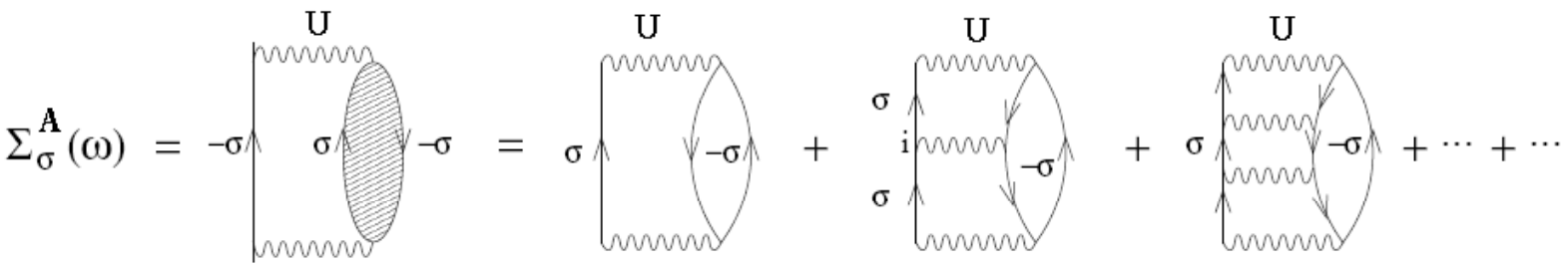
Local moment approach (*Logan*) – LMA

- Unrestricted Hartree-Fock solution dependent explicitly on local moment μ:

$$G_\sigma^{HF}(\mu,\omega)$$



- RPA perturbation series around the UHF solution: $G_\sigma^{A,B\,HF}$



Local moment approach (LMA)

- Using RPA we obtain two selfenergies Σ^A_σ and Σ^B_σ and two LMA Green functions:

$$G^A_\sigma(\Sigma^A)^{LMA}, \quad G^B_\sigma(\Sigma^B)^{LMA}$$

- Symmetry restoration

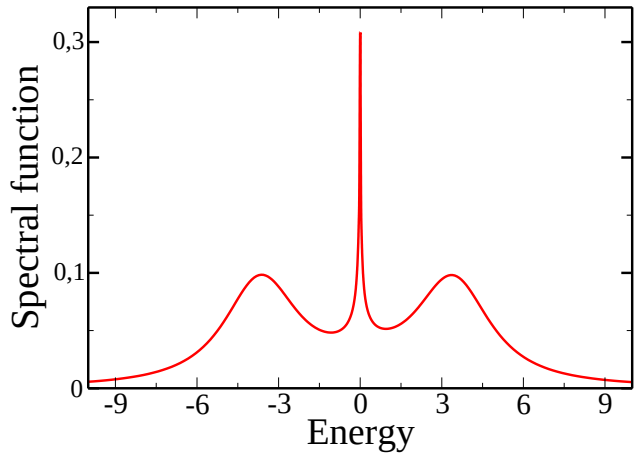
$$G_\sigma(\omega)^{LMA} = \frac{1}{2}\left(G^A_\sigma(\omega)^{LMA} + G^B_\sigma(\omega)^{LMA}\right)$$

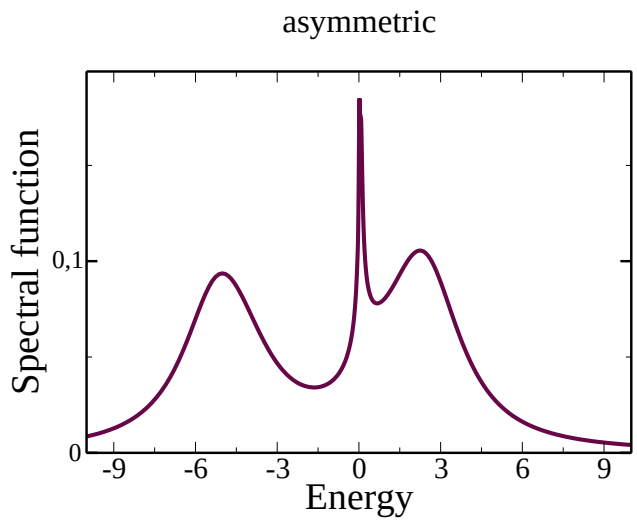
- Minimization of the ground state energy with respect to the local moment value $|\mu|$ and n

$$E_{\text{phys.}} = \min_{|\mu|,n} E(|\mu|, n).$$

Local moment approach in SIAM

- Reproduces Hubbard bands (charge fluctuations)
- Describes well Kondo resonance near the Fermi level (spin fluctuations), reproducing its exponential scale
- Conservative (there exists Luttinger - Ward functional for this theory)
- Numericaly efficient





Multiorbital Anderson model and LMA generalization

$$H_{\mathrm{SIAM}} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\sigma,\alpha} V_{\mathbf{k}\alpha} \left(d^{\dagger}_{\alpha\sigma} c_{\mathbf{k}\sigma} + c^{\dagger}_{\mathbf{k}\sigma} d_{\alpha\sigma} \right)$$

$$+ \sum_{\alpha,\sigma} \left(\epsilon_{\alpha} - U_{\alpha} n_{\alpha,\bar{\sigma}} \right) n_{\alpha,\sigma} + \sum_{\sigma,\sigma'} \sum_{\alpha \neq \beta} \left(U'_{\alpha\beta} - J\delta_{\sigma\sigma'} \right) n_{\alpha\sigma} n_{\beta\sigma'}$$

- RPA perturbation series around the UHF solutions, that are now dependent on local moments on the orbitals μ_{α}
- Symmetry restoration

$$G^{\alpha\beta}_{\sigma}(\omega) = \frac{1}{2N_{\mathrm{orb}}} \sum_{\pm|\mu_{\alpha}|,\pm|\mu_{\beta}|} G^{\alpha\beta}_{\sigma}(\mu_{\alpha}\mu_{\beta};\omega)$$

- Energy minimization with respect to μ_{α} and n_{α}

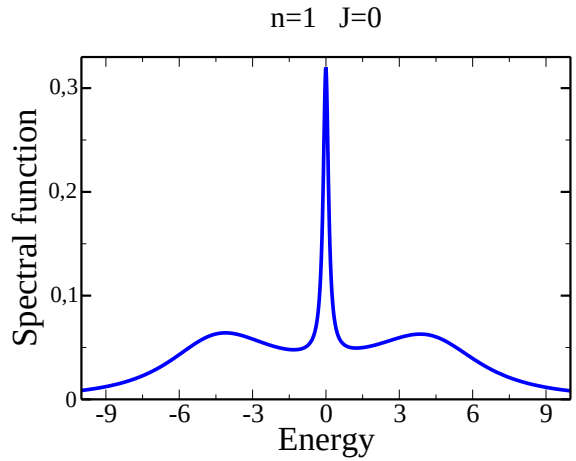
$$E_{\mathrm{phys.}} = \min_{\mu_{\alpha},n_{\alpha}} E(\mu_{\alpha}, n_{\alpha}).$$

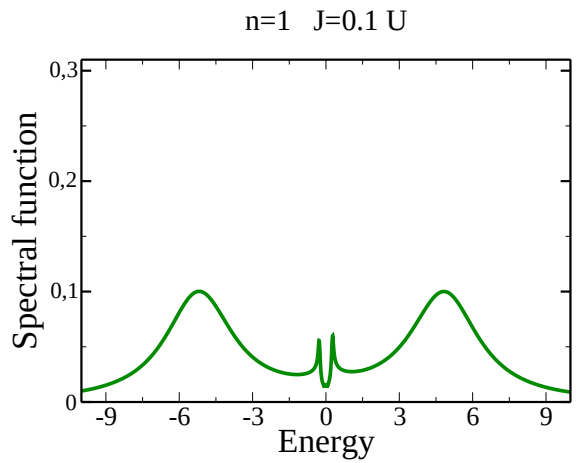
Multiorbital SIAM and LMA

- Spectral functions

$$A_{\sigma}^{\alpha\alpha}(\omega) = -\frac{1}{\pi} Im G_{\sigma}^{\alpha\alpha}$$

- The influence of Hund's rule – $J \neq 0$ suppresses Kondo peak
- Differences in spectral functions between different orbials
- Possible investigation of transport in multiorbital quantum dots



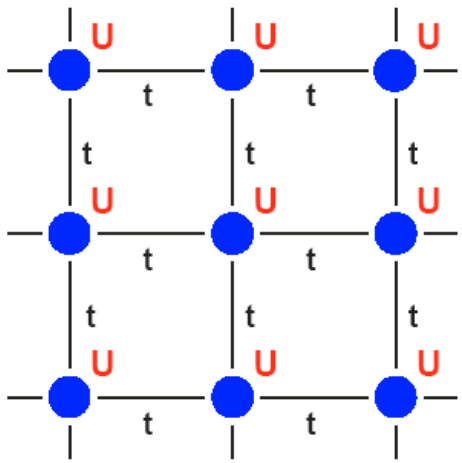


Hubbard model

- interaction U (repulsion) between electrons on each site

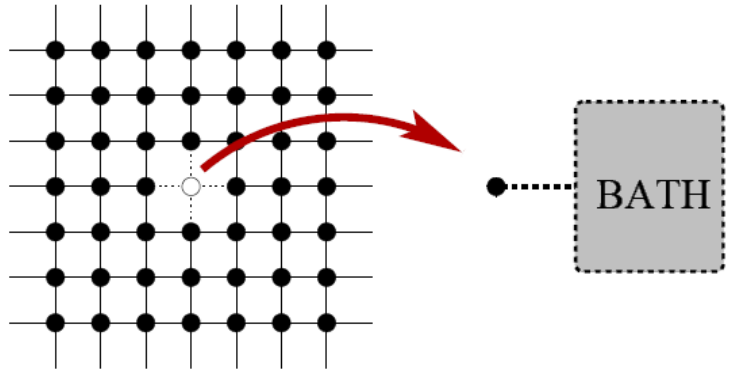
$$H_{\mathrm{Hubbard}} = \sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

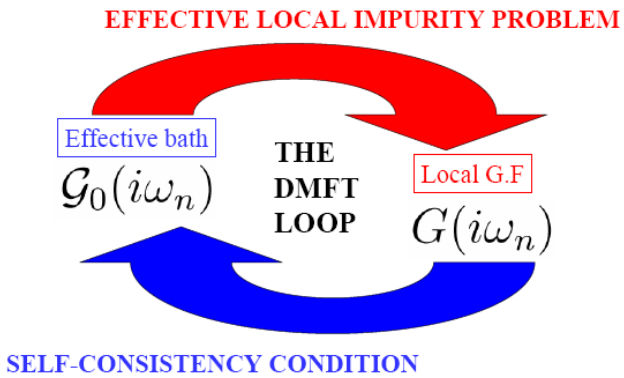
- solution (approx.) within the scheme of dynamical mean field theory



Dynamical mean field theory (DMFT)

- Hubbard model is mapped onto a model of a single impurity in mean field $\mathcal{G}_0(i\omega_n)$
- this mean field is frequency dependent (dynamical)





- DMFT Green function

$$G(\mathbf{k}, i\omega_n)^{-1} = i\omega_n + \mu - \epsilon_{\mathbf{k}} - \Sigma^{LOC}(i\omega_n)$$

- self-consistency condition

$$\Sigma^{LOC}(i\omega_n) = \mathcal{G}_0(i\omega_n)^{-1} + G^{LOC}(i\omega_n)^{-1}$$

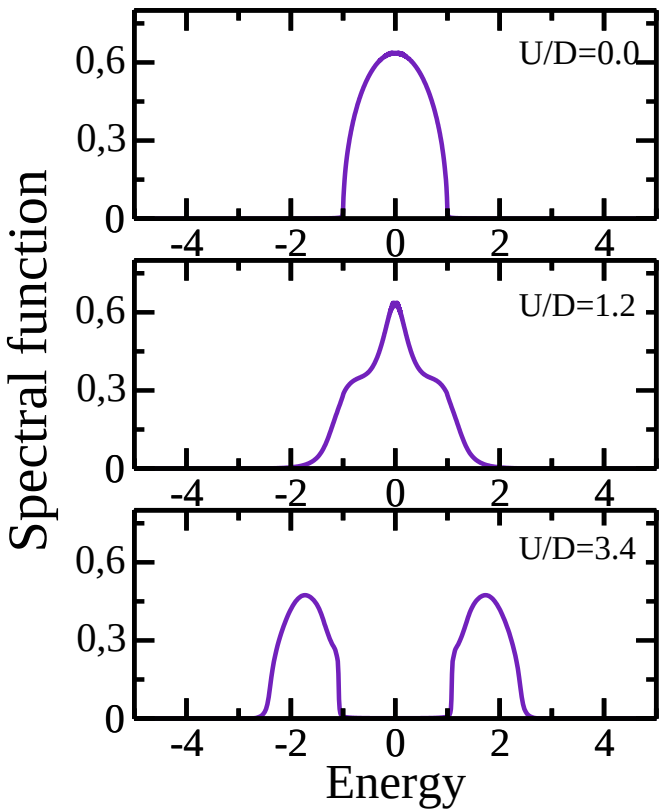
oraz $\mathcal{G}_0 = \mathcal{G}_0[G^{LOC}]$

Dynamical mean field theory (DMFT)

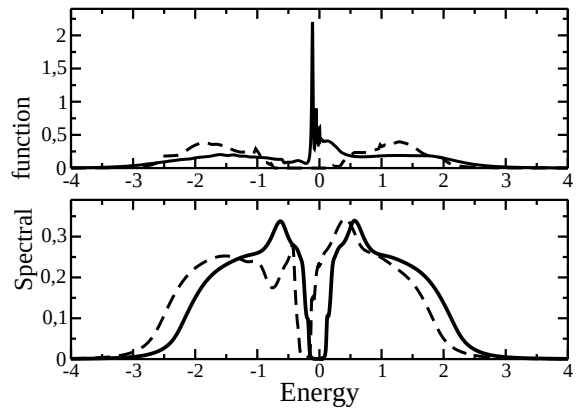
- Thermodynamicaly consistent and conservative
- Exact in the non-trivial limit of $d = \infty$
- Frequency dependent mean field (Weiss field $\mathcal{G}_0(i\omega_n)$) describes spin and charge fluctuations on sites
- Exact in the atomic ($t_{i,j} = 0$) and non-interacting ($U = 0$) limits
- Requires an impurity solver to solve self-consistent equations – the solver must work for arbitrary hybridization function (e.g. NRG, QMC, IPT, NCA) – LMA can serve as an impurity solver

DMFT + LMA

- Mott-Hubbard metal - insulator transition



- Suppression of Kondo peak when $J \neq 0$ (Hund's rule)
- Orbital selective metal - insulator transition



(Bethe lattice at half-filling)

Summary

Local moment approach (LMA):

- Conservative, numericaly efficient method to treat multiorbital Anderson and Hubbard models
- Can be used to invesigate:
  - Mott- Hubbard metal - insulator transition in multiorbital Hubbard model
  - transport in multilevel quantum dots that are described by Anderson impurity model