Exact Diagonalization
Bath Fitting

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Single Impurity Anderson Model

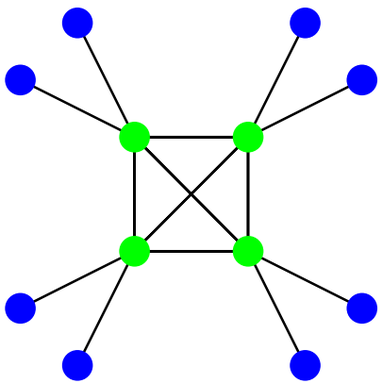
$$\mathcal{H} = \sum_{d,\sigma} \epsilon_d c^\dagger_{d\sigma} c_{d\sigma} + \frac{1}{2} \sum_{ijkl,\sigma\sigma'} U_{ijkl} c^\dagger_{i\sigma} c^\dagger_{j\sigma'} c_{l\sigma'} c_{k\sigma} +$$

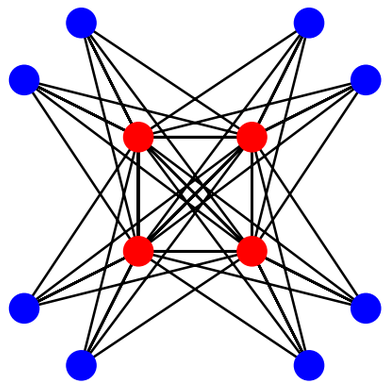
$$\sum_{k,\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{kd,\sigma} \left[V_{kd} c^\dagger_{k\sigma} c_{d\sigma} + h.c. \right]$$

Single Impurity Anderson Model

- Diagonal basis
  - Each bath orbital only hybridizes with single impurity orbital

- Off-diagonal basis
  - All bath orbitals are coupled to every impurity orbital





*A. Liebsch and H. Ishida 2012 *J. Phys.: Condens. Matter* **24** 053201

Real Frequency fitting

$$G_{ii}^{imp,0}(\omega) = \left[(\omega + i\delta) - H^0 - \Delta_{ii}(\omega)\right]^{-1}$$

$$\Delta_{ij}(\omega) = \sum_k \frac{V_{ki} V_{kj}^*}{\omega + i\delta - \epsilon_k}$$

- Suitable for diagonal basis
- Two possible fitting options:
  - Green's function fitting (Density of States)
  - Direct fitting of Hybridization function (if available)
- Broadening improves fitting

Real Frequency fitting

- Green's function fitting

$$\left| ImG_{ii}^{imp,0}(\omega) - Im\left\{ \frac{1}{\omega + i\delta - \epsilon_i - \sum_{k=1}^{N_s} \frac{V_{ki}^2}{\omega + i\delta - \epsilon_k^i}} \right\} \right| \rightarrow min$$

$$\{\epsilon_i, \epsilon_k^i, V_{ik}\}$$

- Hybridization function fitting

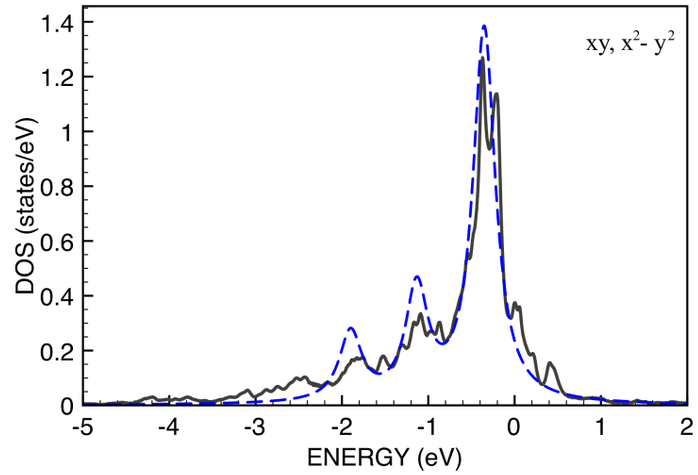
$$\left| Im\Delta_{ii}(\omega) - Im\left\{ \sum_{k=1}^{N_s} \frac{V_{ki}^2}{\omega + i\delta - \epsilon_k^i} \right\} \right| \rightarrow min$$

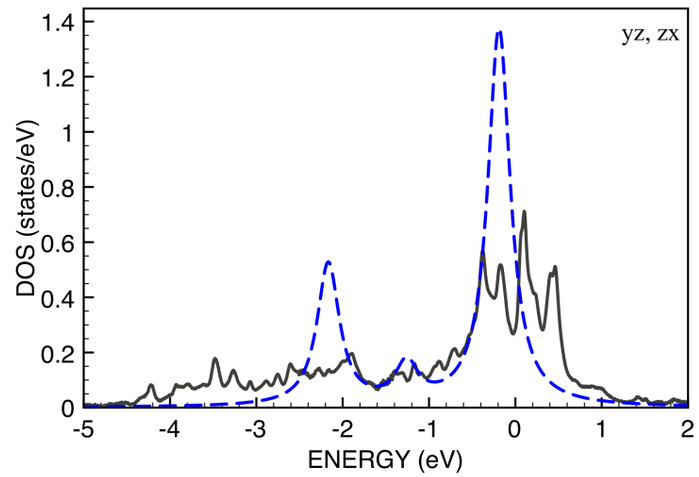
$$\{\epsilon_k^i, V_{ik}\}$$

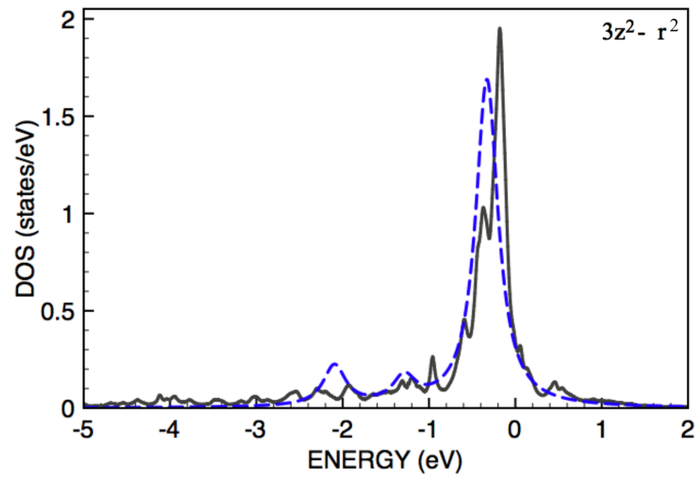
  - ε_i are chosen to preserve target density

Real Frequency fitting

- Green's function fitting
  - Can capture main features of non-interacting density of states
  - Can reproduce main features of interacting spectra







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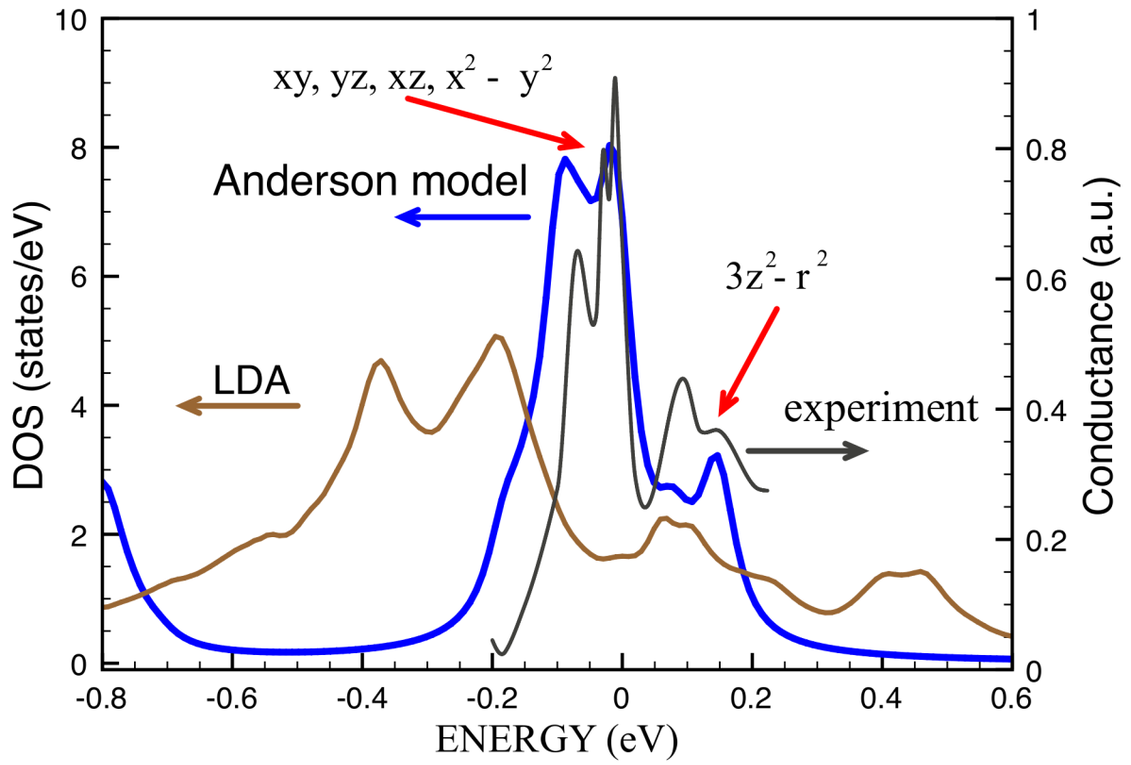
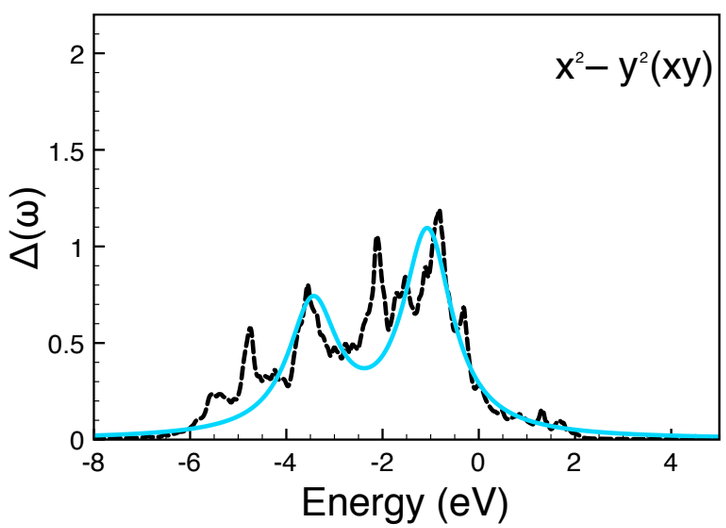
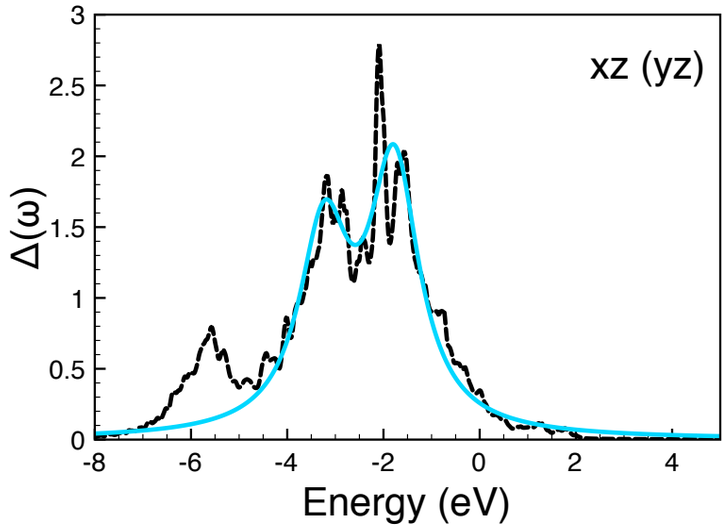
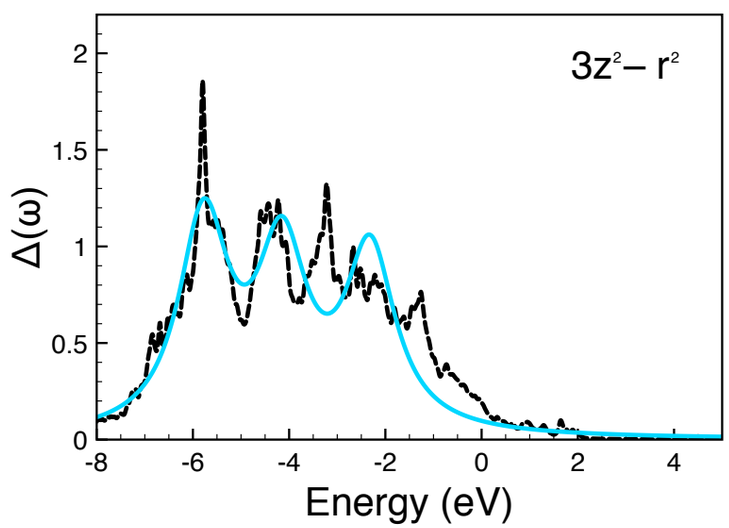


Real Frequency fitting

- Hybridization function fitting
  - Allow better control of low-energy features
  - Orbital energies are chosen to maintain target density







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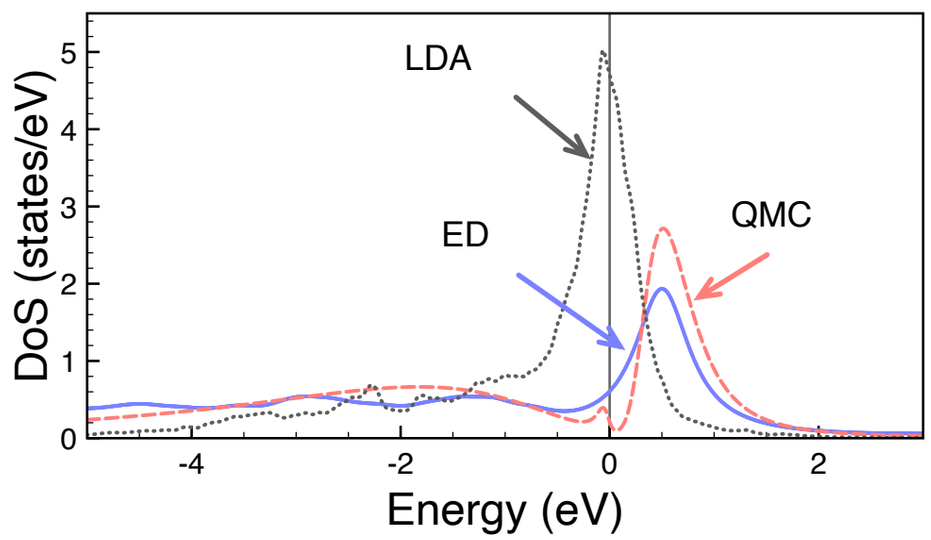

Real Frequency fitting

- Pros
  - Provides control to features that need to be captured
  - Allows to work directly with DFT data

- Cons
  - Fitting result strongly depends on initial parameters
  - Extremely hard for automatic fitting

Matsubara frequency fitting

- Data is available on Matsubara axis (DMFT or SEET)

$$\mathbf{G}(i\omega_n) = \left[(i\omega_n) - H^0 - \mathbf{\Delta}(i\omega_n)\right]^{-1}$$

$$\Delta_{ij}(i\omega_n) = \sum_k \frac{V_{ik}V_{jk}^*}{i\omega_n - \epsilon_k} \approx \sum_{k=1}^{N_s} \frac{V_{ik}V_{jk}^*}{i\omega_n - \epsilon_k}$$

- Minimization of G
- Minimization of 1/G
- Minimization of hybridization function
- High frequency data suppression

Matsubara frequency fitting. Minimization of G

$$Diff_i = \sum_{n=0}^{M} W_n \left| G_{ii}^{0}(\omega_n) - G_{ii}^{0,exact}(\omega_n) \right|^2$$

- Provide better fitting for small Matsubara frequencies
- Additional weight functions could improve convergence

Matsubara frequency fitting. Minimization of 1/G

$$Diff_i = \sum_{n=0}^{M} W_n \left| \frac{1}{G_{ii}^{0}(\omega_n)} - \frac{1}{G_{ii}^{0,exact}(\omega_n)} \right|^2$$

- That corresponds to minimization of Hybridization function.

- And for large n

$$\left| G_{ii}^{0}(\omega_n) - G_{ii}^{0,exact}(\omega_n) \right| \rightarrow \frac{1}{\omega_n^2} \left| \Delta_{ii}(\omega_n) - \Delta_{ii}^{exact}(\omega_n) \right|$$

- Improves asymptotic behavior

Matsubara frequency fitting. Weight function

$$Diff_i = \sum_{n=0}^{M} W_n \left| G_{ii}^{0}(\omega_n) - G_{ii}^{0,exact}(\omega_n) \right|^2$$

- Small Matsubara frequencies if Δ has insulating behavior (min_type=2 in SEET code)

$$W_n = \omega_n$$

- Larger Matsubara frequencies if Δ shows metalic behavior (min_type=1 in SEET code)

$$W_n = 1$$

Matsubara frequency fitting. Off-diagonal Δ

- Need to perform full optimization for matrix-valued functions
- For small number of bath sites this procedure is unstable
- Better to find diagonal basis