Work in progress: Multi-orbital local 2-particle Green's functions from Exact Diagonalization

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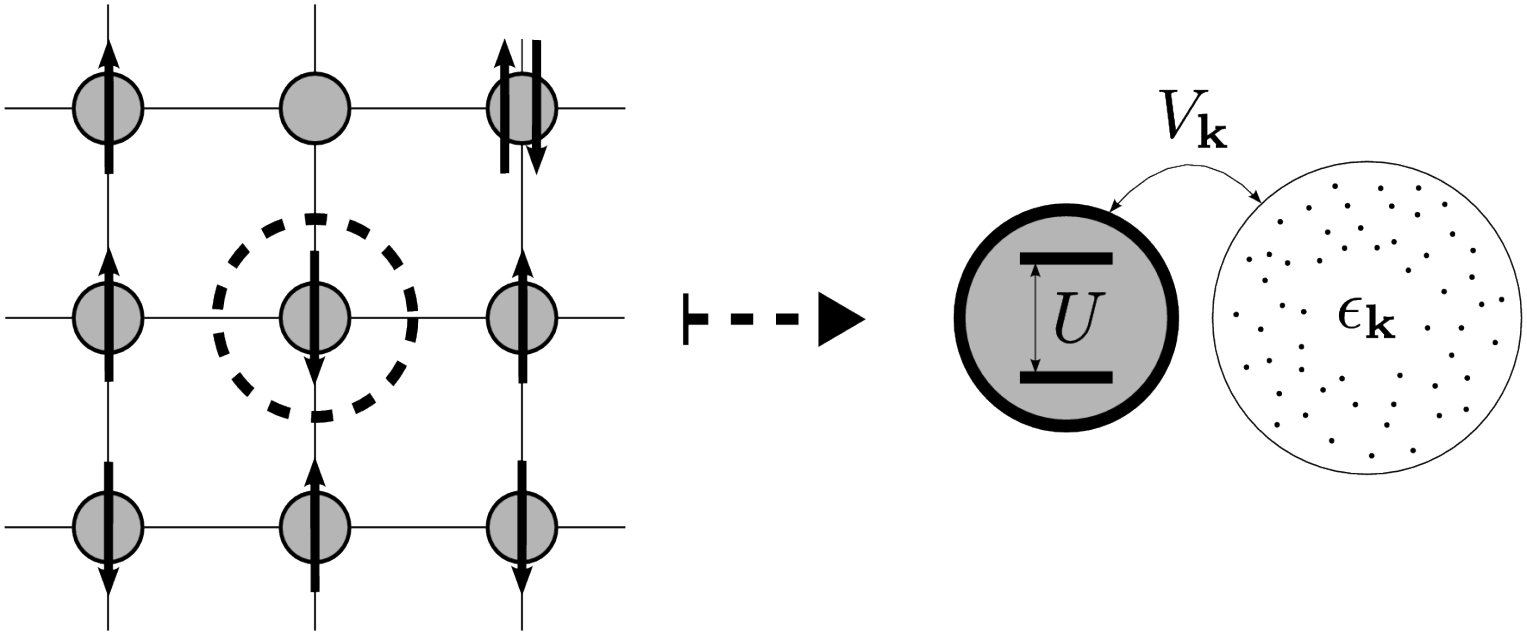
ERC workshop

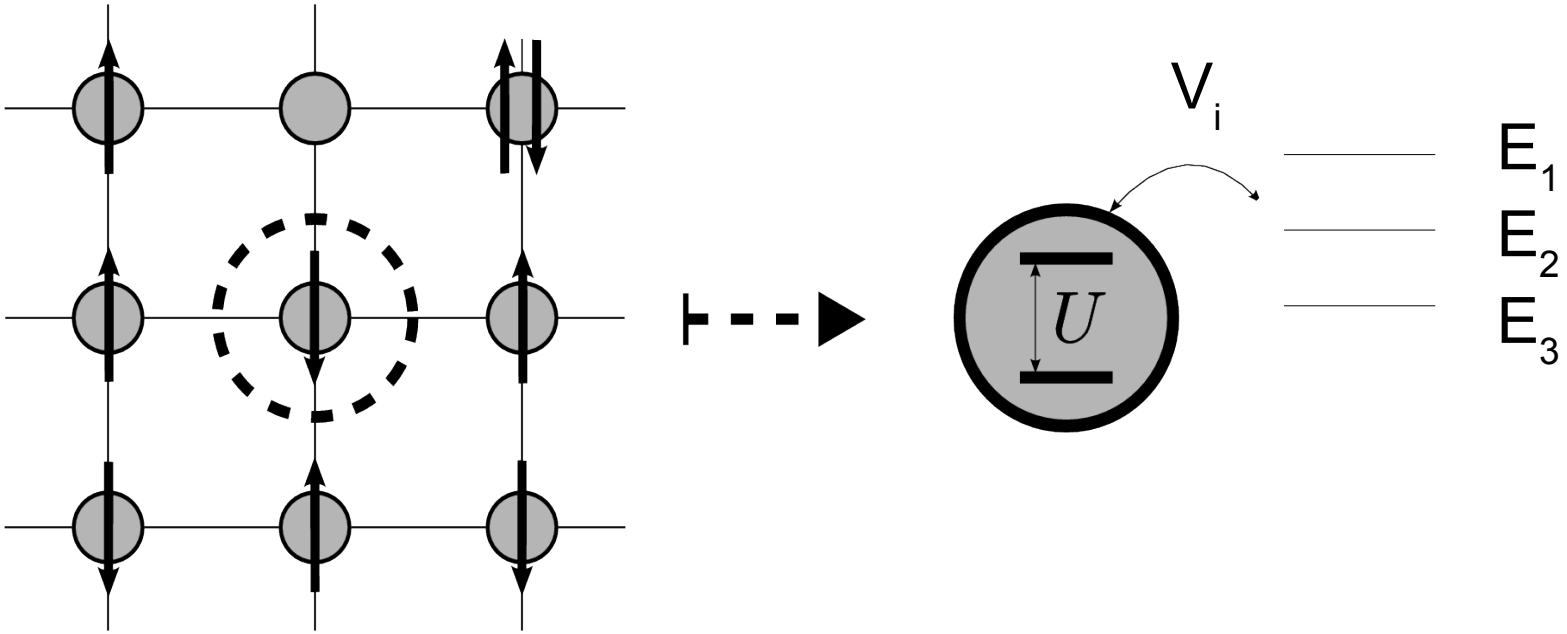
Outline

- DFT+DMFT
  - Exact Diagonalization solver
  - MnO, FeO, CoO, and NiO spectra
- Local 2-particle Green's function
  - Physical interpretation
  - Input to extensions of DMFT and ED
    - DGA, 1-particle, DF, Super-perturbation
- Numerical implementation
  - Lehmann representation
  - Scaling
- Preliminary test results (in progress)

DFT+DMFT

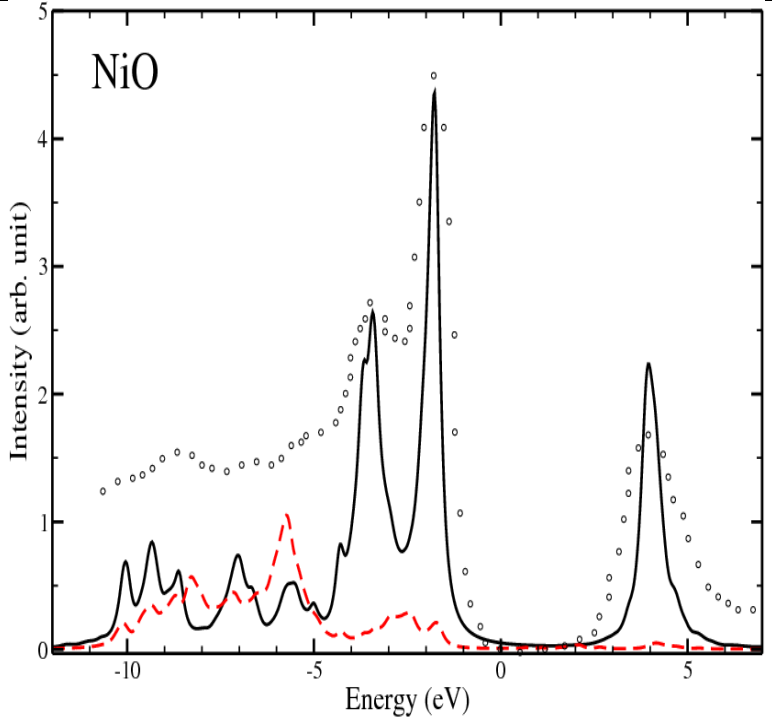


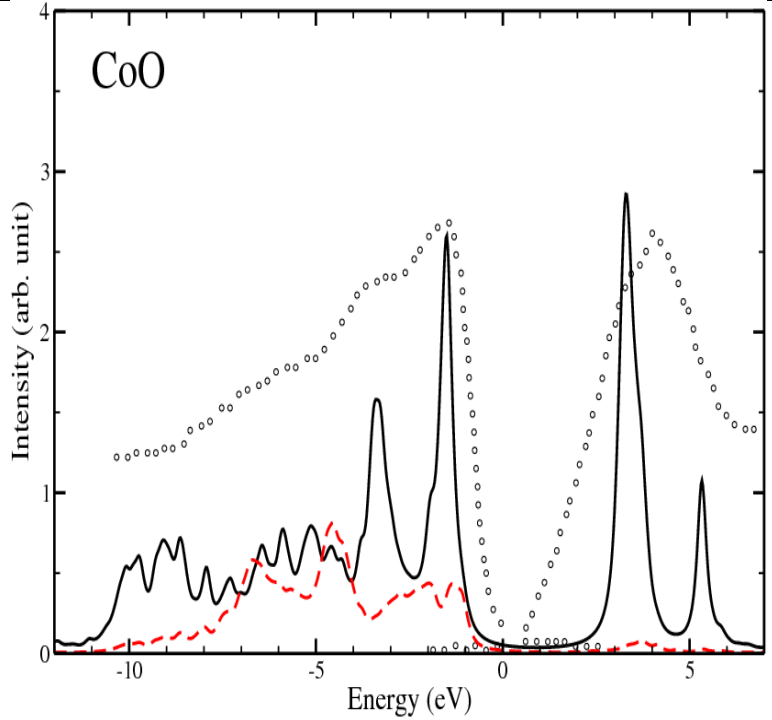
DFT+DMFT

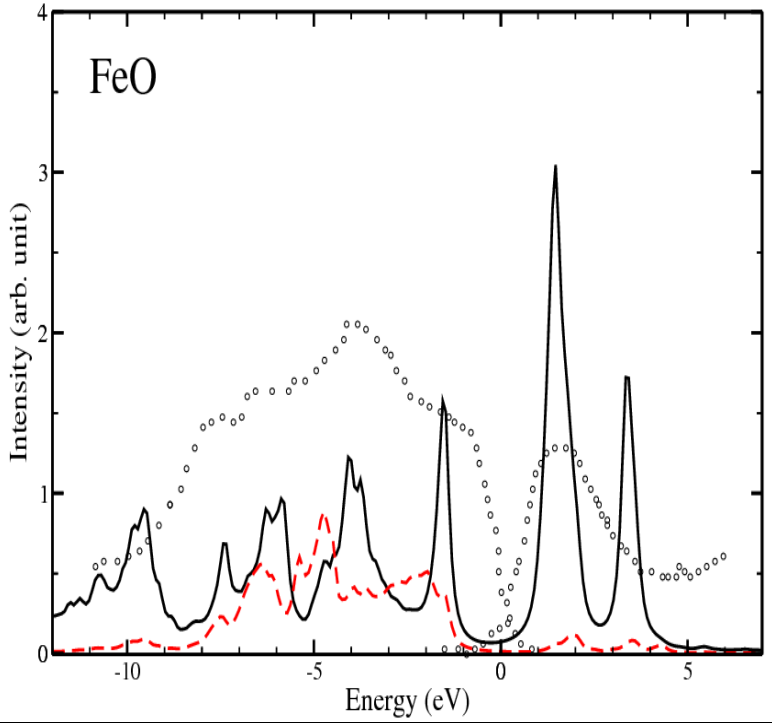


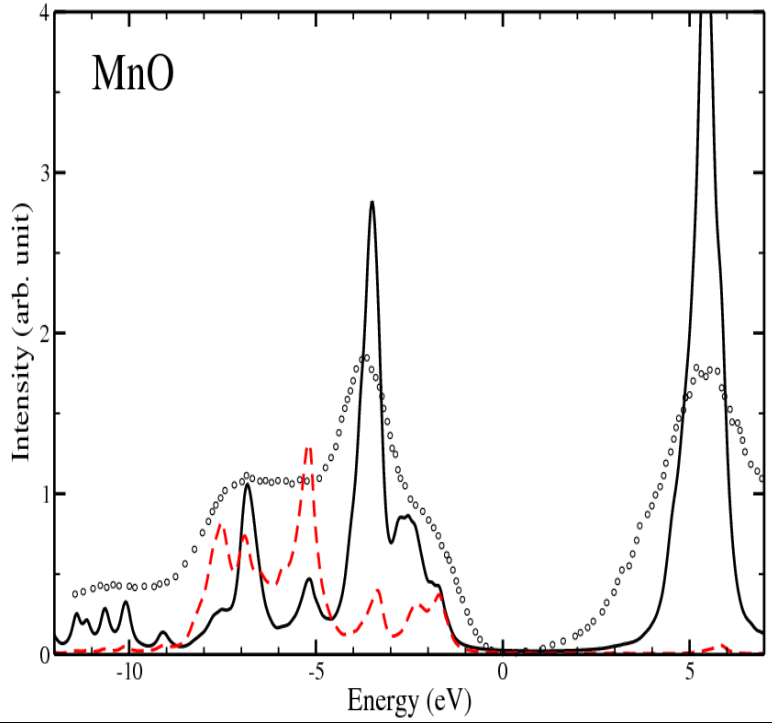
- Exact Diagonalization
  - A few auxiliary bath states mimic the hybridization to the bath
  - E_i and V_i obtained from fitting the hybridization function

[Review: A. Liebsch, H. Ishida 2012 J. Phys.: Condens. Matter 24 053201]


NiO
Intensity (arb. unit)
Energy (eV)


CoO
Intensity (arb. unit)
Energy (eV)


FeO
Intensity (arb. unit)
Energy (eV)


MnO
Intensity (arb. unit)
Energy (eV)

Local 2-particle Green's function

- Local 2-particle Green's function

$$\chi^{mnop}_{\omega_1\omega_2\omega_3} = \frac{1}{\beta^2}\int_0^\beta \tau_1 \int_0^\beta \tau_2 \int_0^\beta \tau_3 \, e^{i(\omega_1\tau_1+\omega_2\tau_2+\omega_3\tau_3)} \times \left\langle T_\tau c_m(\tau_1) c_n(\tau_2) c_p^\dagger(\tau_3) c_o^\dagger(0) \right\rangle$$

- Local 1-particle Green's function

$$G(\omega)_{mn} = \frac{1}{\beta}\int_0^\beta \tau \, e^{i\omega\tau} \times \left\langle T_\tau c_m(\tau_1) c_n^\dagger(0) \right\rangle$$

Local 2-particle Green's function

- Input to extensions
- Beyond DMFT
  - DΓA
    - Bethe-Salpeter equations + Parquet equation
  - 1-particle irreducible diagrams approach
  - Dual Fermion approach
    - Taylor expansion of V after dual fermion transformation
- Beyond ED
  - Super-perturbation impurity solver
    - Dual fermion-like treatment of the local problem starting from ED
  - What about local DGA?

Numerical implementation

- Lehmann representation
  - 6 different time-orderings of the operators
  - Chain of eigenstates
    - Evaluate a function of the three frequencies for each eigenvalue chain!

$$\chi^{mnop}_{\omega_1\omega_2\omega_3} = \frac{1}{Z}\sum_{ijkl}\sum_{\Pi}\theta\left(E_i, E_j, E_k, E_l, \omega_{\Pi_1}, \omega_{\Pi_2}, \omega_{\Pi_3}\right)$$
$$\times sgn(\Pi)\langle i|C_{\Pi_1}|j\rangle\langle j|C_{\Pi_2}|k\rangle\langle k|C_{\Pi_3}|l\rangle\langle l|c_o^{\dagger}(0)|i\rangle$$

Numerical implementation

- Lehmann representation
  - 6 different time-orderings of the operators
  - Chain of eigenstates
    - Evaluate a function of the three frequencies for each eigenvalue chain!
- Scaling
  - Naively spin-orbitals^4*Eigenstates^4*freq^3
  - Depends strongly on the conserved quantum number