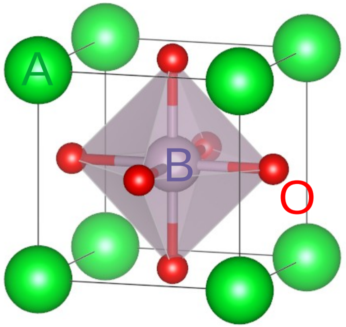
Correlated materials modelling:
The example of magnetism in Ba_2YIrO_6

Hermann Schnait

arXiv:2202.10794

Transition Metal Oxides



- Periovskites ABO_3
  - A: (mostly) alkaline earth metal (Sr, Ba)
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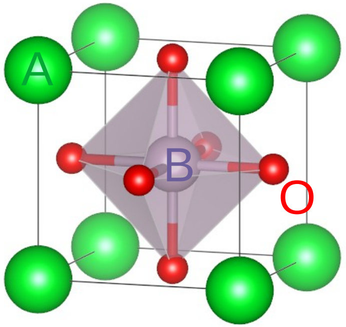

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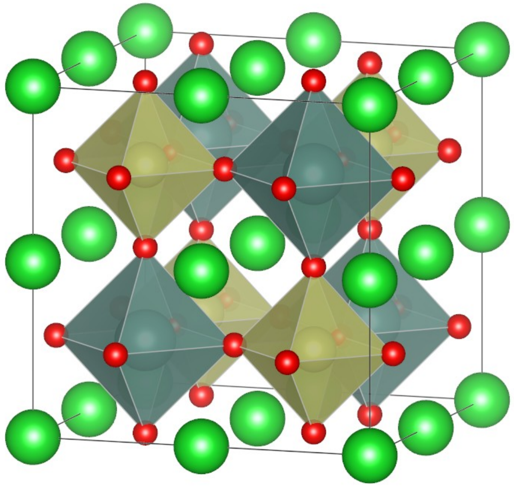

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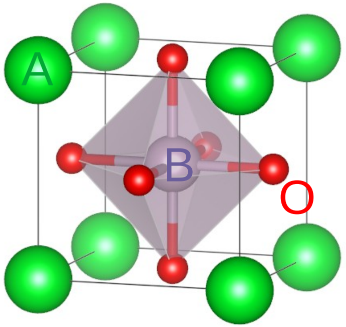

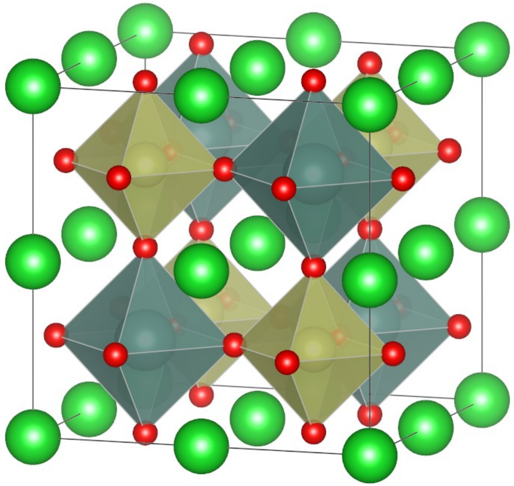

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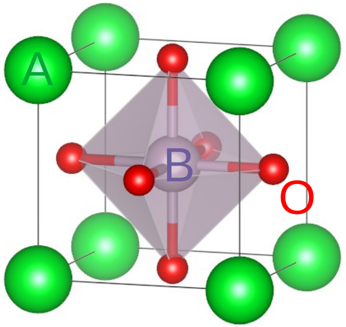
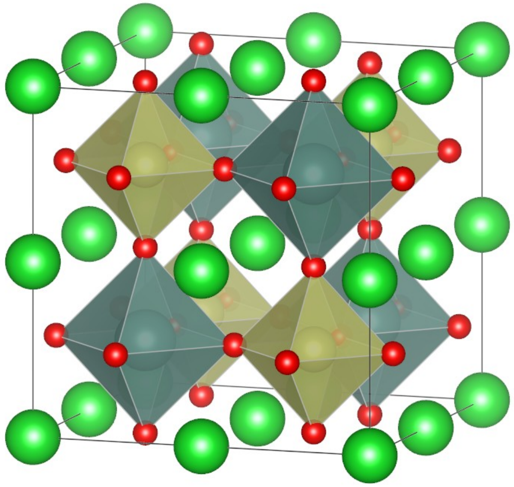
- **Ba$_2$YIrO$_6$** → 4 electrons in Ir d-shell
- Two effects at play:
  - Crystal Field splitting
  - Spin-Orbit coupling





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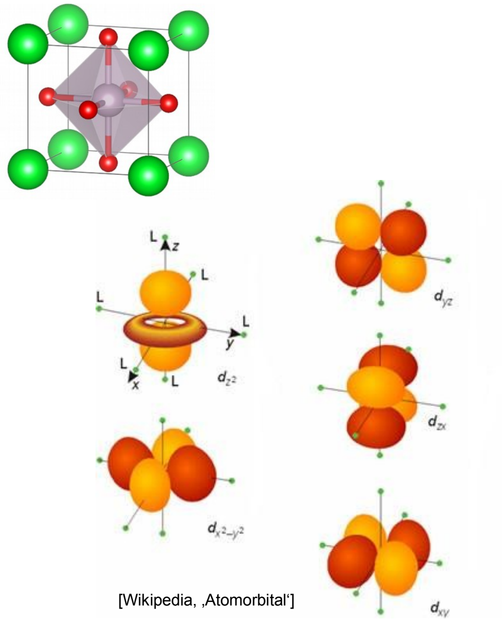
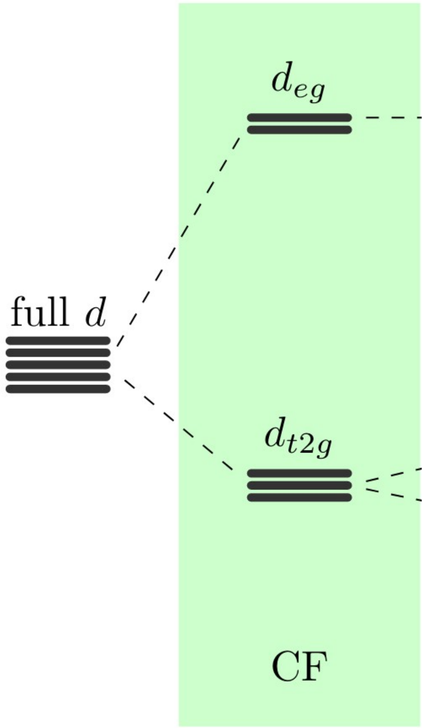
Crystal field vs. spin-orbit coupling



[Wikipedia, ‚Atomorbital']



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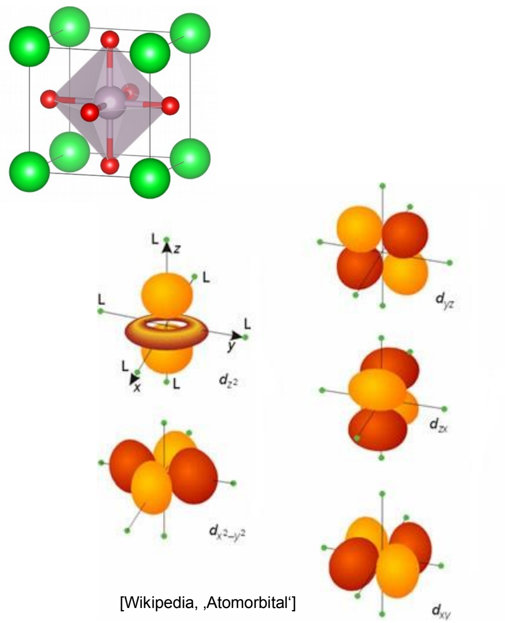

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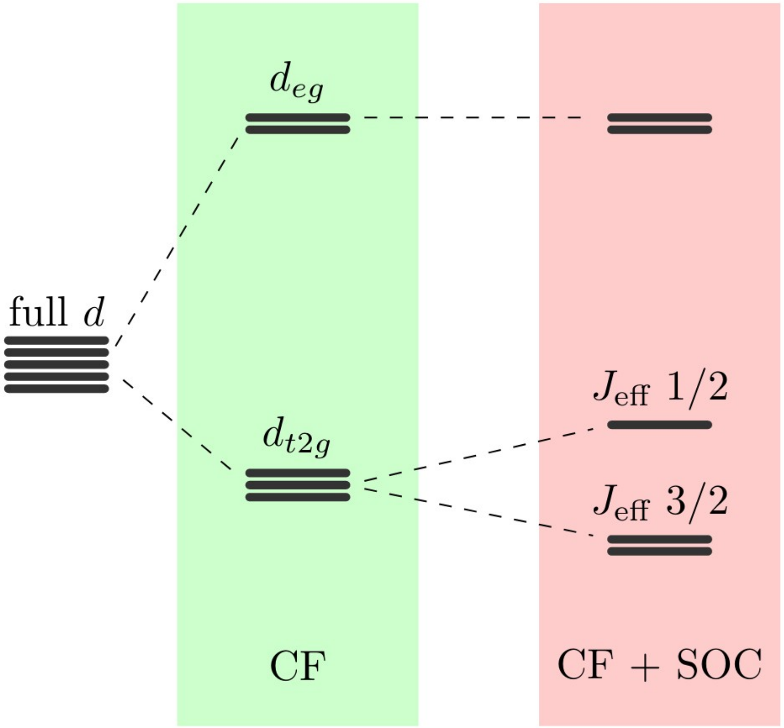

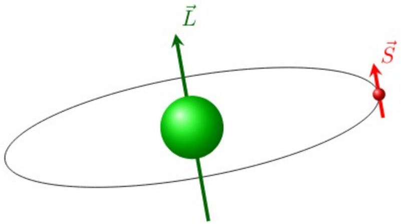

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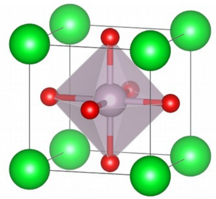

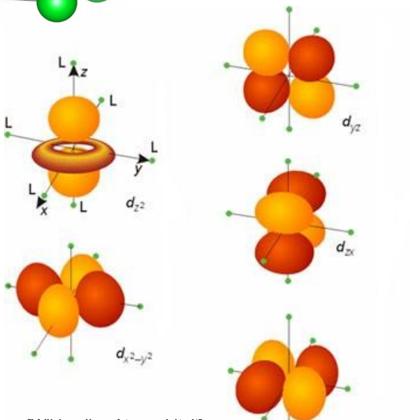

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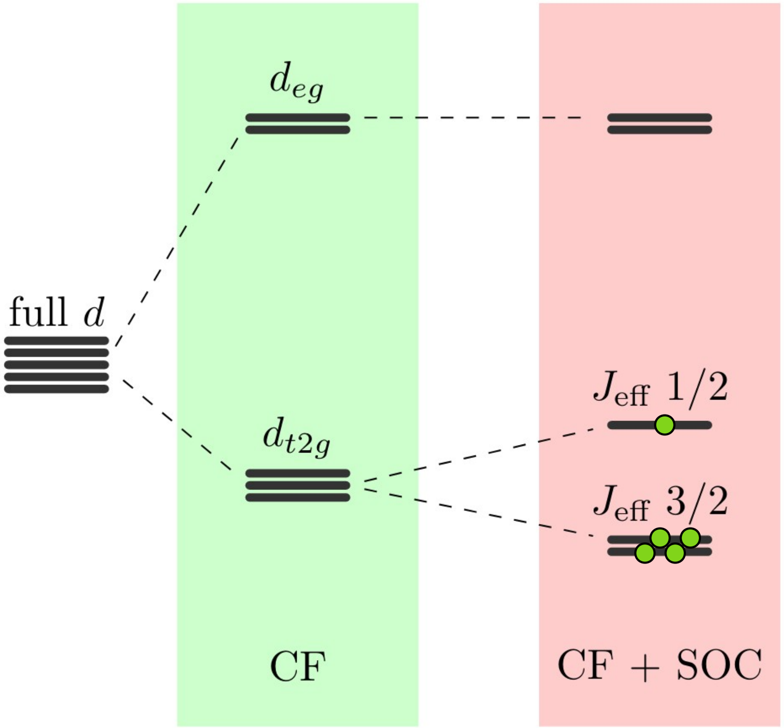
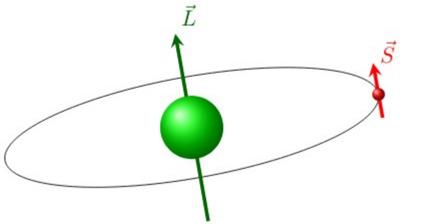


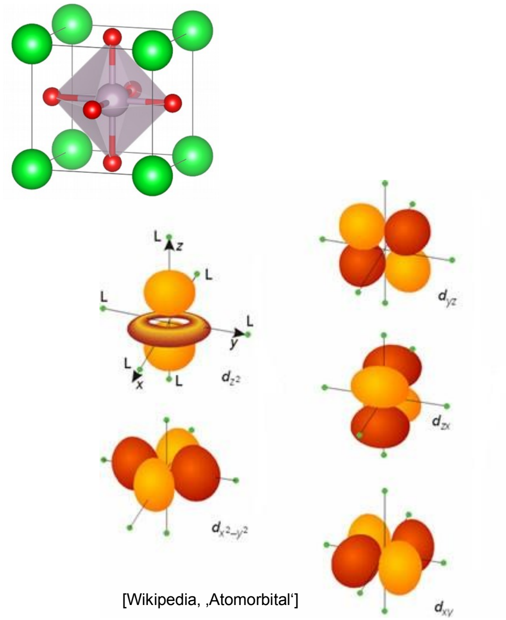


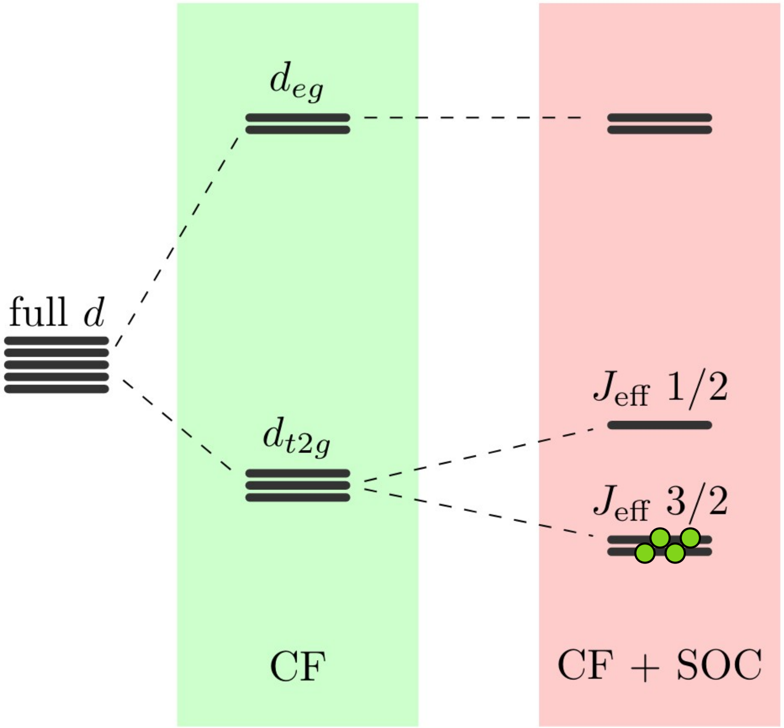
$$H_{\mathrm{SOC}} = \zeta\,(\boldsymbol{L} \cdot \boldsymbol{S})$$

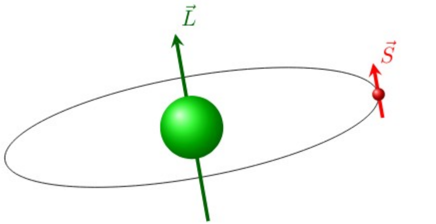
Sr_2IrO_4 ($5d^5$) [1]

[1] B. Kim et al., PRL **101**, 076402 (*2008*)

Crystal field vs. spin-orbit coupling







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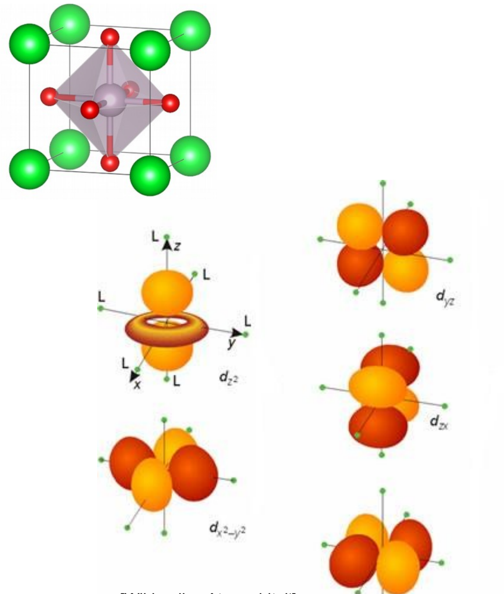

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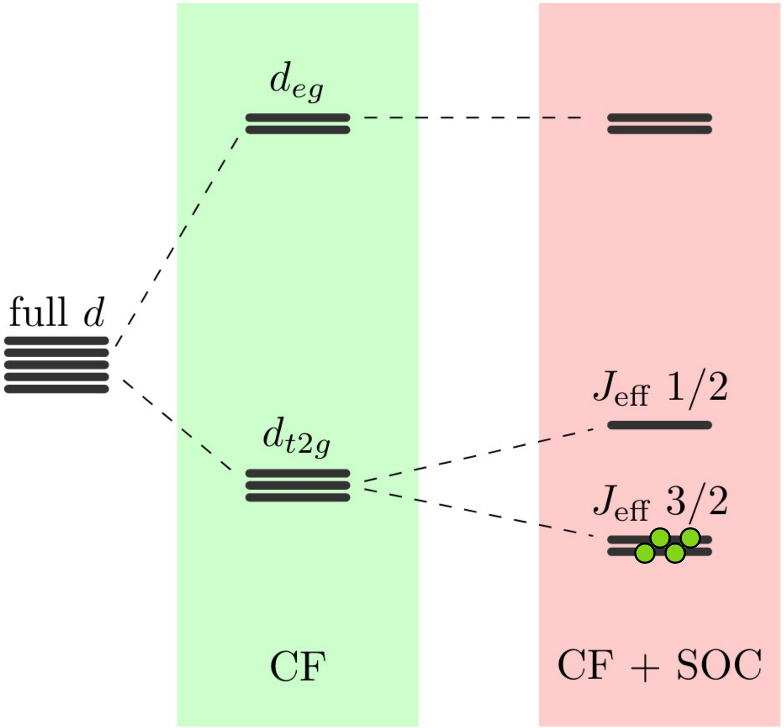

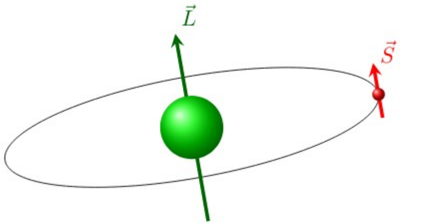

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BUT: In Experiment magnetic!

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Literature results

- Magnetic moment $\mu_{eff} \approx 0.16 - 0.63\ \mu_B$
  - From Curie-Weiss fits [8, 17], muon-spin relaxation [17], RIXS [18]
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Intrinsic:	**Extrinsic:**
- J=0 + excitons - J≠0	J=0 bulk with magnetic impurities

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What we do: Modelling on computer - “*in-silico*”

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Density Functional Theory (DFT)

$$H_{\mathrm{BO}} = \underbrace{-\frac{1}{2}\sum_i \nabla_i^2}_{\text{Kinetic energy}} + \underbrace{\frac{1}{2}\sum_{ij,i\neq j}\frac{1}{|\boldsymbol{r}_i-\boldsymbol{r}_j|}}_{\text{Electron-Electron repulsion}} - \underbrace{\sum_i V_c(\boldsymbol{r}_i)}_{\text{Crystal potential}}$$

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Kinetic energy Electron-Electron repulsion Crystal potential

Hohenberg Kohn Theorem: $\psi(\boldsymbol{r}_1 \ldots, \boldsymbol{r}_N) \leftrightarrow n(\boldsymbol{r})$

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BUT: Iridium, open d shell → Correlations!

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Strong Correlations

Localized electrons (d, f shell) → strong repulsion

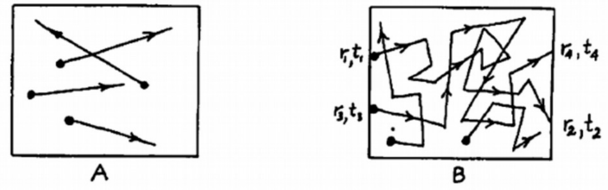

Fig. 0.2 A. *Non-interacting Particles*
B. *Interacting Particles*

[R. Mattuck: A Guide to Feynman Diagrams]

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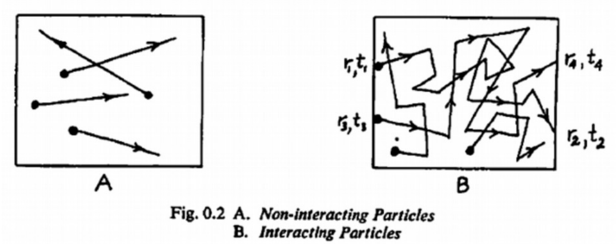

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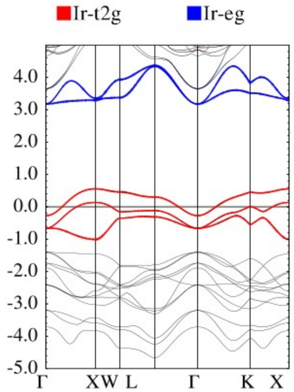
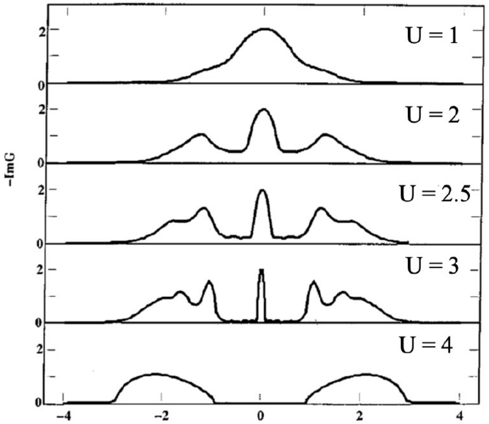


Metal-Insulator transitions,



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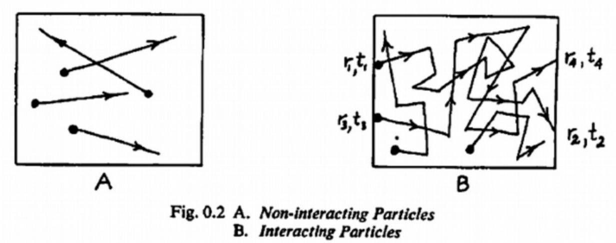

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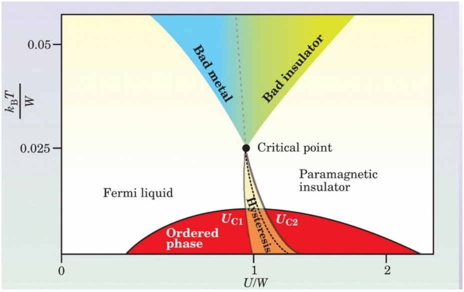
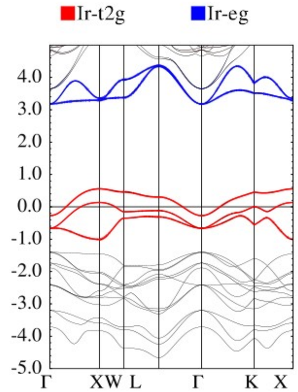
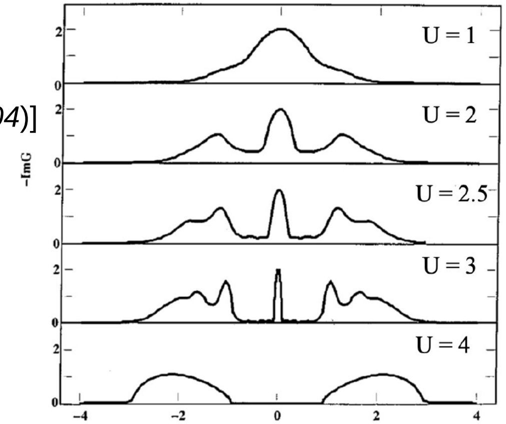


[Kotliar *et al*., Physics Today **57**, 3, 53 (*2004*)]



Metal-Insulator transitions,

complex phase spaces, ...



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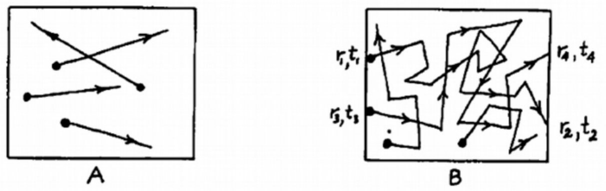

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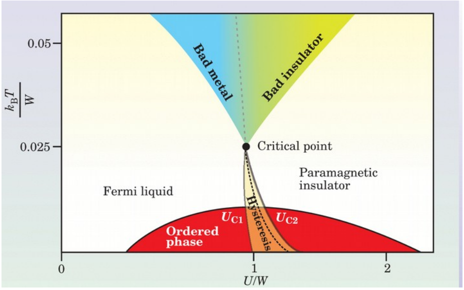

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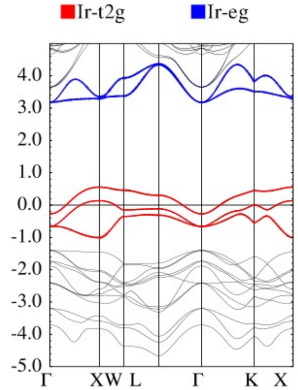

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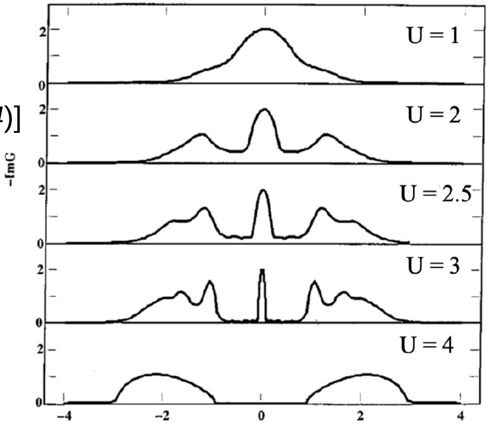

[Zhang *et al.*, PRL **70**, 1666 (*1993*)]

In short:

Single particle picture not justified anymore!

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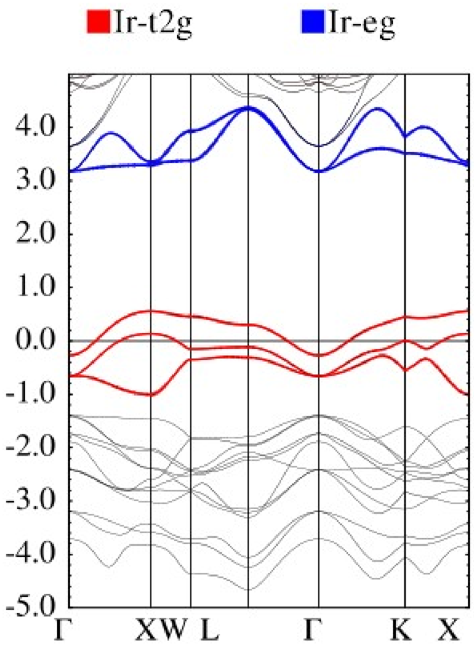
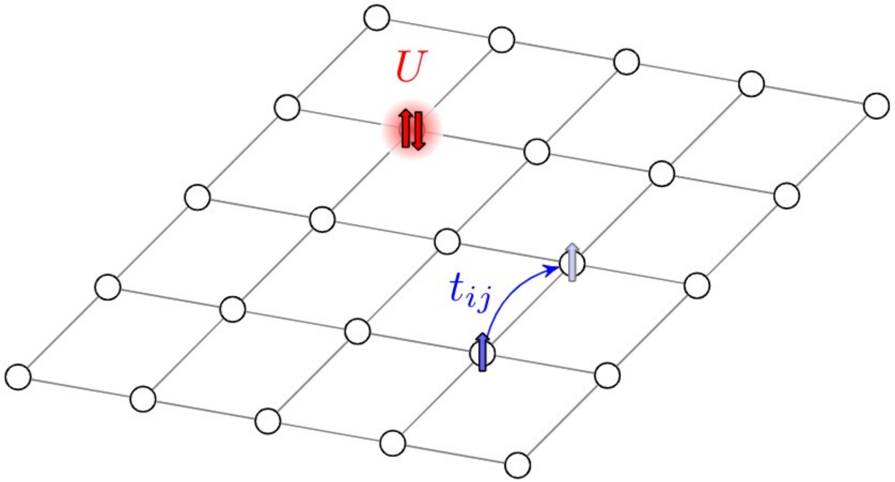
DFT → Local Model

From bands to local levels





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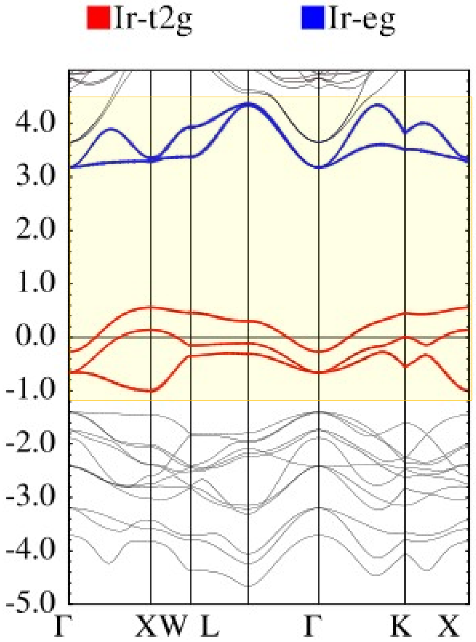

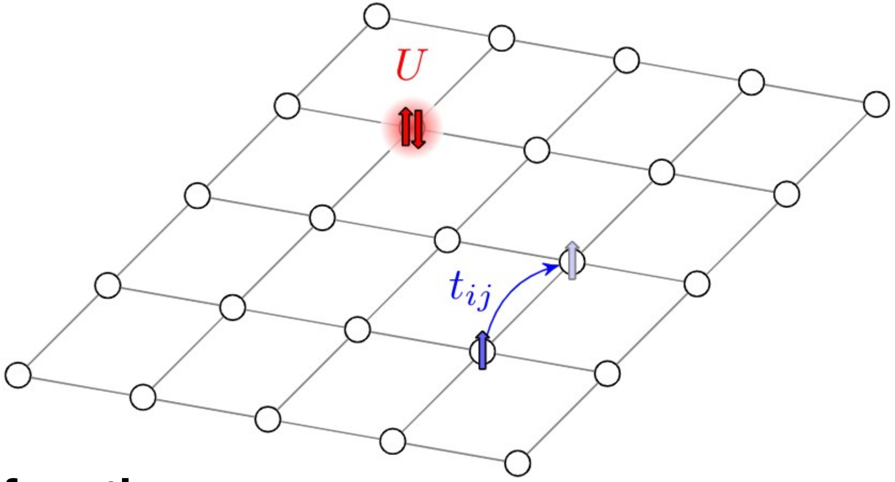

→ (Projective) **Wannier functions**

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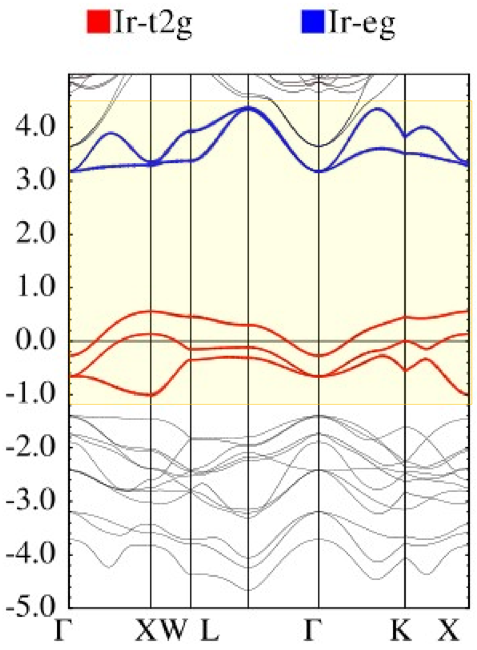
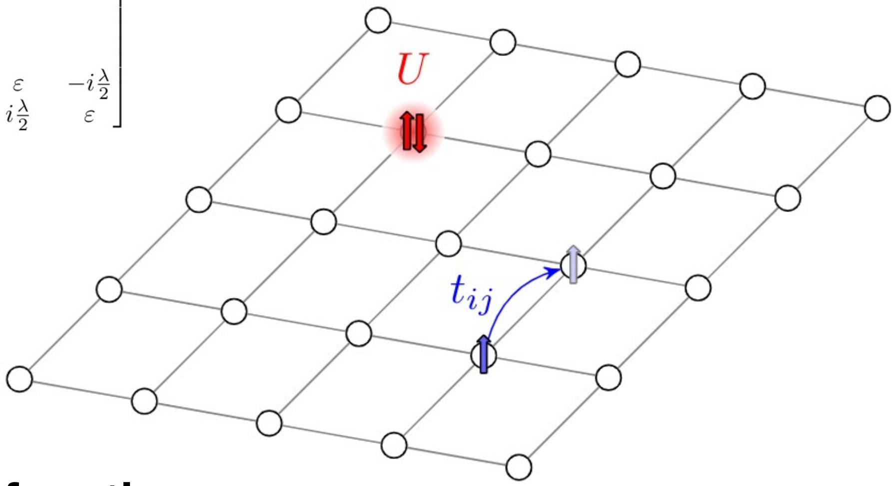


$$H_{\mathrm{loc}} = \begin{array}{c} \begin{array}{cccccc} |d^{\uparrow}_{xy}\rangle & |d^{\uparrow}_{xz}\rangle & |d^{\uparrow}_{yz}\rangle & |d^{\downarrow}_{xy}\rangle & |d^{\downarrow}_{xz}\rangle & |d^{\downarrow}_{yz}\rangle \end{array} \\ \begin{bmatrix} \varepsilon & & & & -i\frac{\lambda}{2} & -\frac{\lambda}{2} \\ & \varepsilon & \frac{\lambda}{2}i & -i\frac{\lambda}{2} & & \\ & -i\frac{\lambda}{2} & \varepsilon & \frac{\lambda}{2} & & \\ & i\frac{\lambda}{2} & \frac{\lambda}{2} & \varepsilon & & \\ i\frac{\lambda}{2} & & & & \varepsilon & -i\frac{\lambda}{2} \\ -\frac{\lambda}{2} & & & & i\frac{\lambda}{2} & \varepsilon \end{bmatrix} \end{array}$$



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Many body theory

Green's function ("Propagator")

$$G^r(t) = -i\Theta(t)\left\langle\left\{c(t),\, c^\dagger(0)\right\}\right\rangle$$

(additional **orbital** / **spin** / **site** indices)

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Link to experiment: **Spectral function**

$$A(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\left\{G(\omega)\right\}$$

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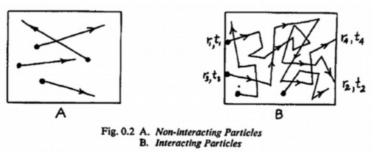

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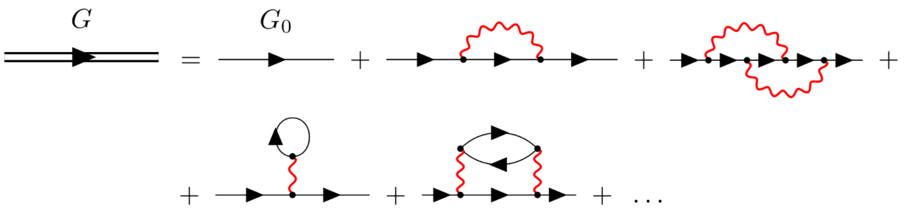
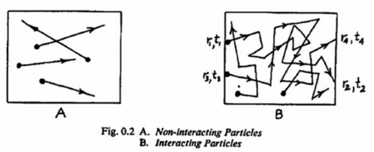


Link to experiment: **Spectral function**

$$A(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\left\{G(\omega)\right\}$$

arXiv:2202.10794

Many body theory



[R. Mattuck: A Guide to Feynman Diagrams]

Green's function ("Propagator")

$$G^r(t) = -i\Theta(t)\left\langle\left\{c(t),\, c^\dagger(0)\right\}\right\rangle$$

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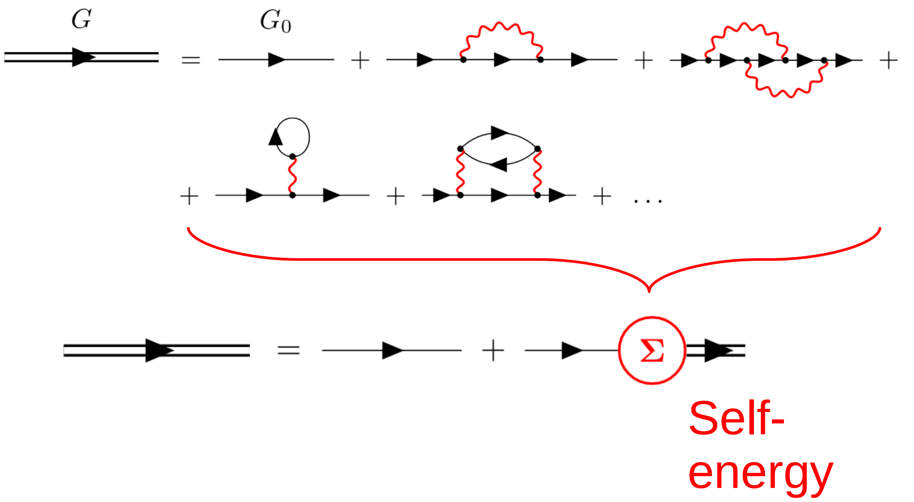

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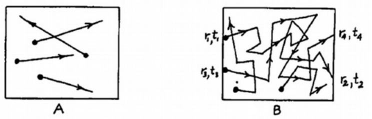

Fig. 0.2 A. Non-interacting Particles
B. Interacting Particles

[R. Mattuck: A Guide to Feynman Diagrams]

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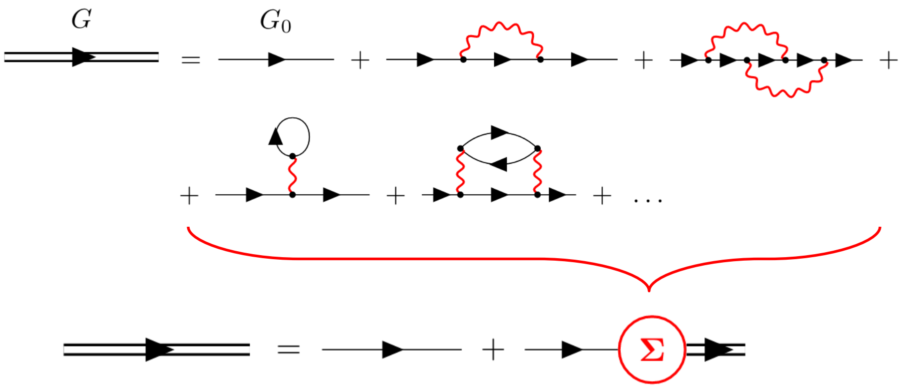

Self-energy

$$\rightarrow G = [G_0^{-1} - \Sigma]^{-1}$$

Dyson's equation

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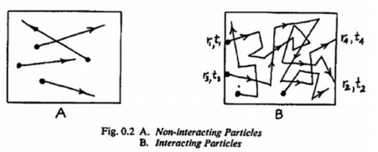

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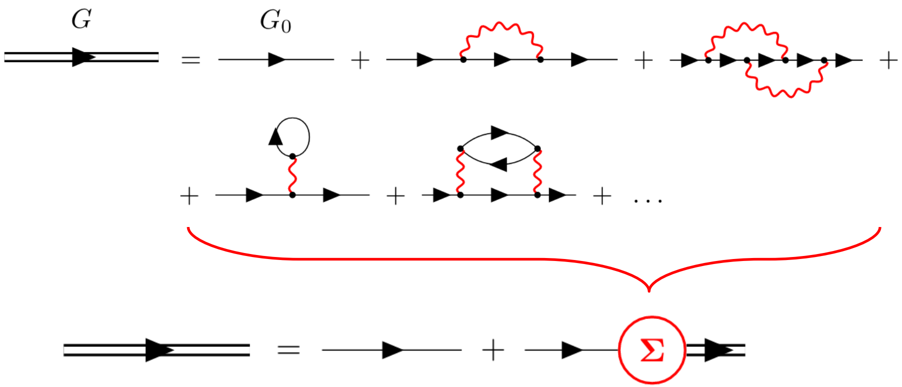

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→ **Dynamical Mean-Field theory**

arXiv:2202.10794

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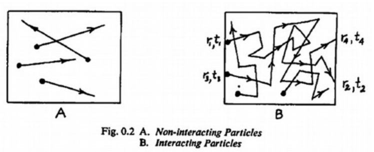

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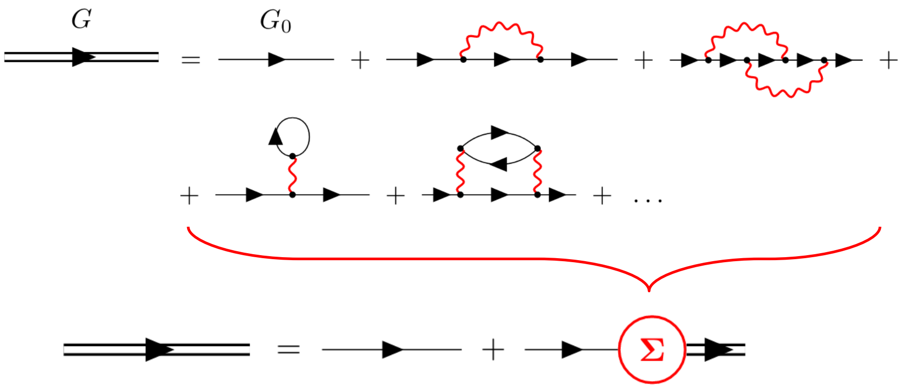

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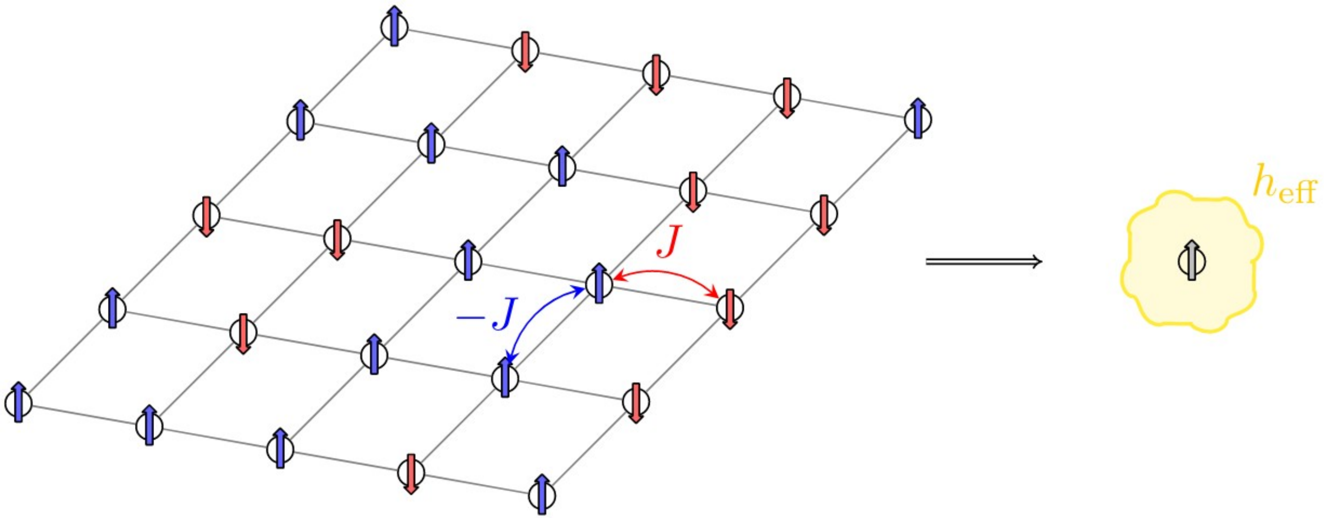
→ **~~Dynamical~~ Mean-Field theory**

arXiv:2202.10794

Classical mean field theory

Ising model (Lattice)

Single spin in effective magnetic field



arXiv:2202.10794

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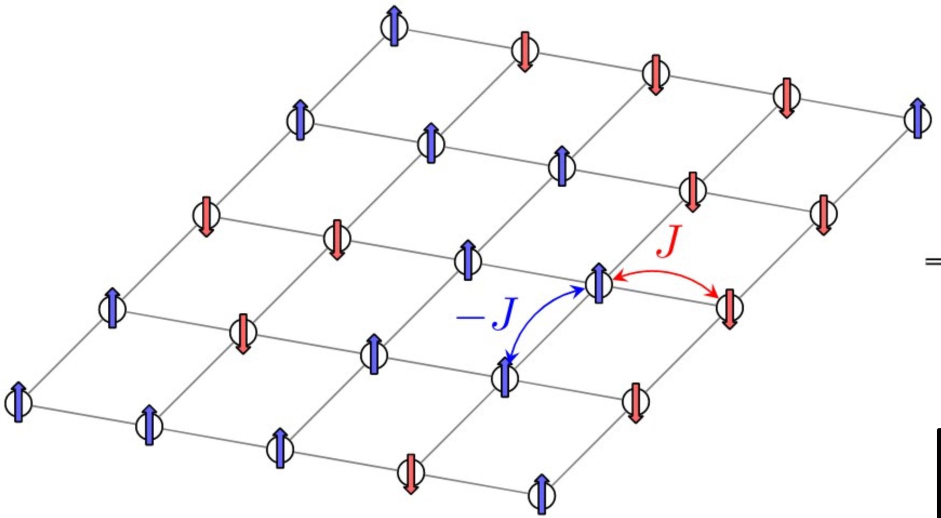

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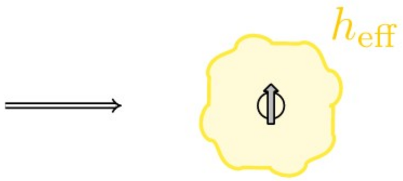
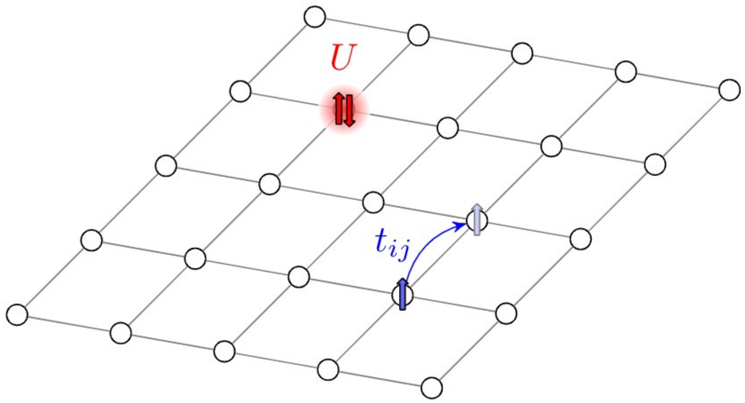


GOAL: Set h_{eff} in a way, that local magnetization is reproduced

arXiv:2202.10794

Dynamical mean field Theory

Hubbard model (Lattice)



arXiv:2202.10794

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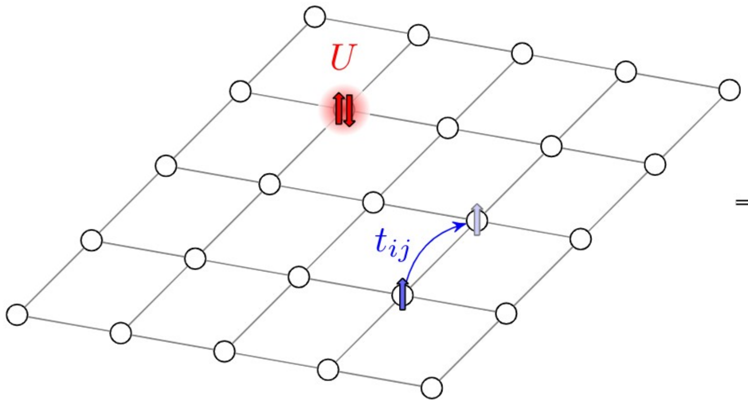
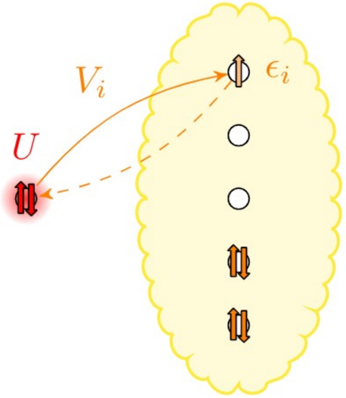


$\Longrightarrow$

Anderson impurity model (AIM)



arXiv:2202.10794

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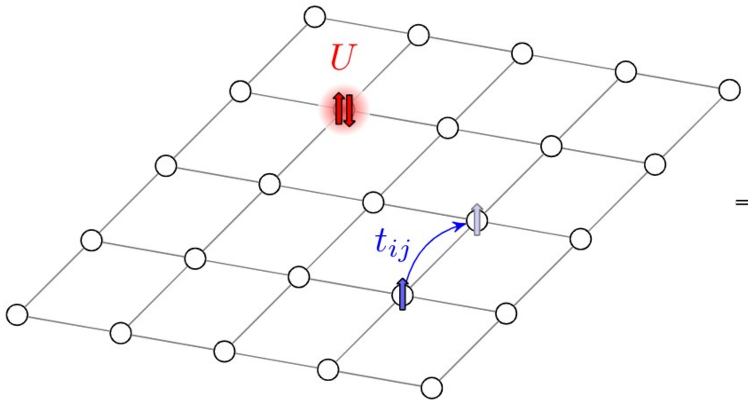

$$G_{\mathrm{loc}}(z) = \sum_{\boldsymbol{k}} \left[z - \epsilon_{\boldsymbol{k}} - \Sigma_{\mathrm{latt}}(\boldsymbol{k}, z) - \mu\right]^{-1}$$

$\Longrightarrow$

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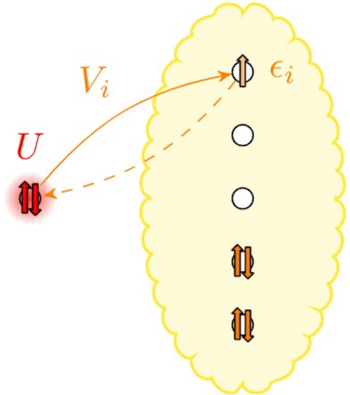

$$G_{\mathrm{imp}}(z) = \left[z - H_{\mathrm{loc}} - \Sigma_{\mathrm{imp}}(z) - \Delta(z)\right]^{-1}$$

($\Delta(z)$ contains V_i, ϵ_i)

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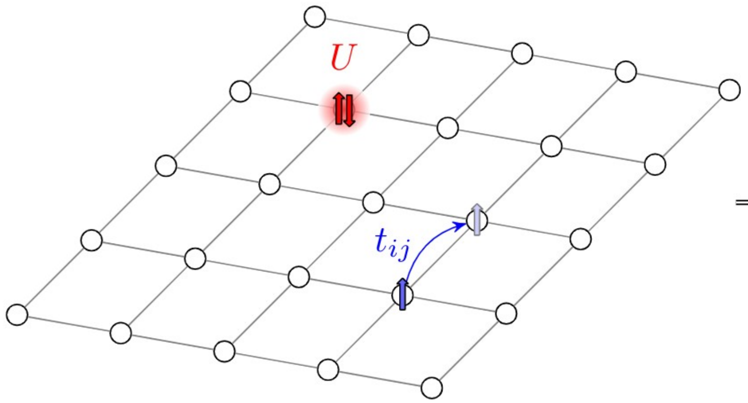

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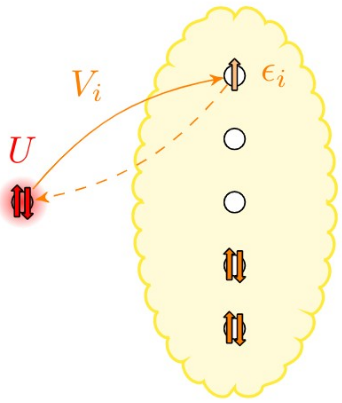

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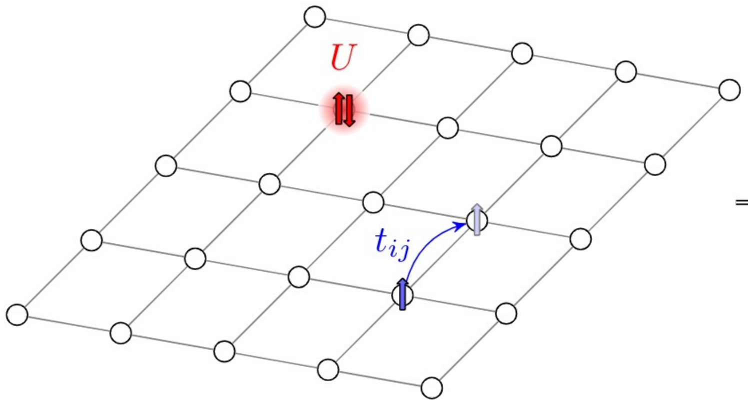

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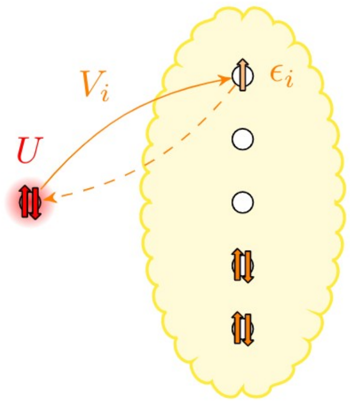

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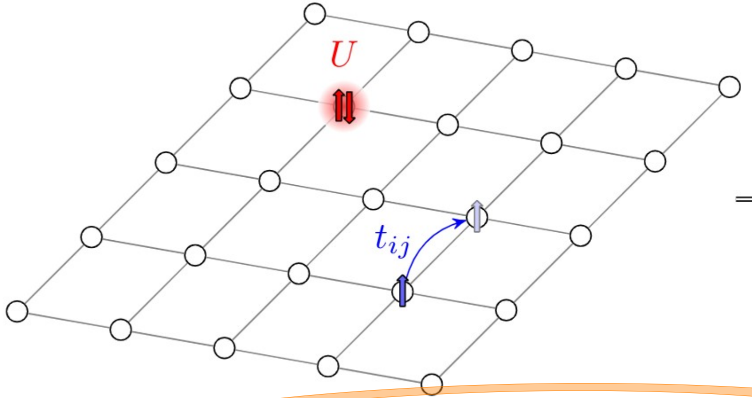

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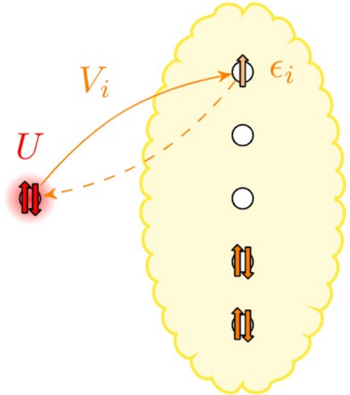

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Solve AIM:

$H_{\text{loc}}, \Delta(z), H_{\text{int}} \Rightarrow G_{\text{imp}}(z), \Sigma_{\text{imp}}(z)$

(linked via Dyson's equation)

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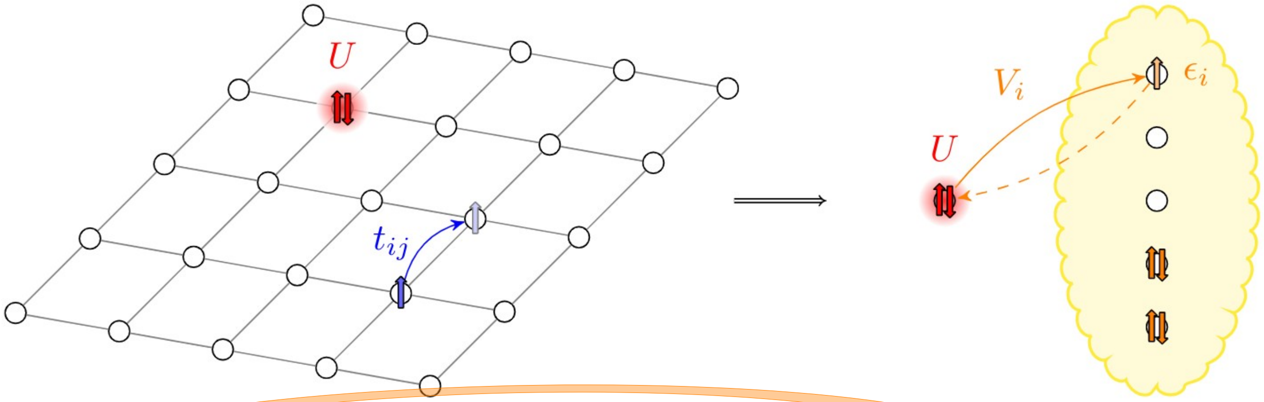
Dynamical mean field Theory

Hubbard model (Lattice) **Anderson impurity model** (AIM)



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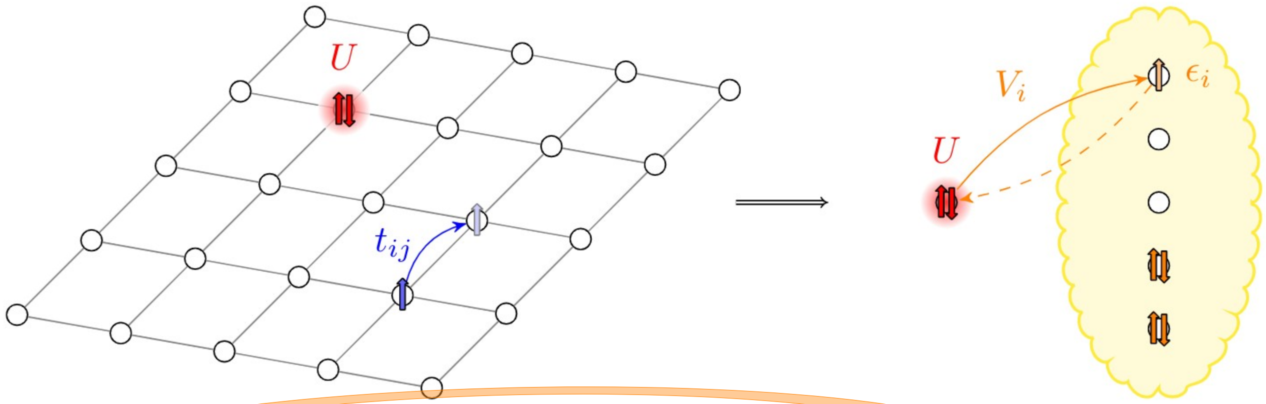

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(linked via Dyson's equation)

BUT: AIM not trivial!

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Impurity Solvers

Different algorithms available

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- **Quantum Monte-Carlo** (QMC)
  - Continous hybridization (inf. bath sites)
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  - Sign problem

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- **Quantum Monte-Carlo** (QMC)
  - Continous hybridization (inf. bath sites)
  - Finite Temperatures
  - Sign problem
  - **BUT:** Bad scaling down to T = O(1K)!

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Hamiltonian based Solvers:

- Discrete bath sites → Many-body Hamiltonian
  - $T = 0$ ground state

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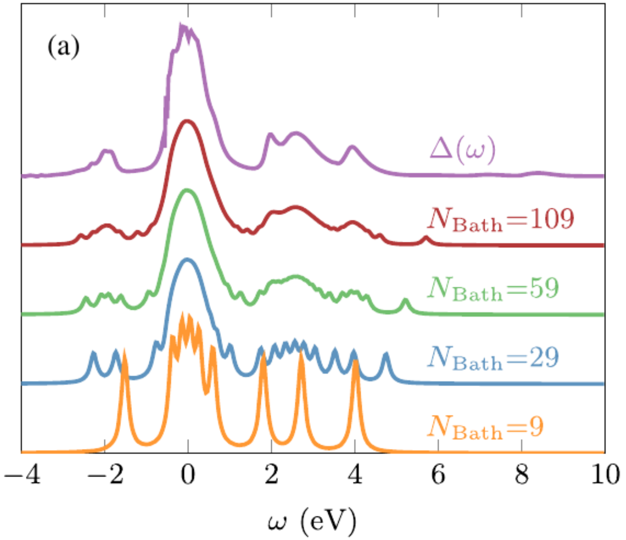
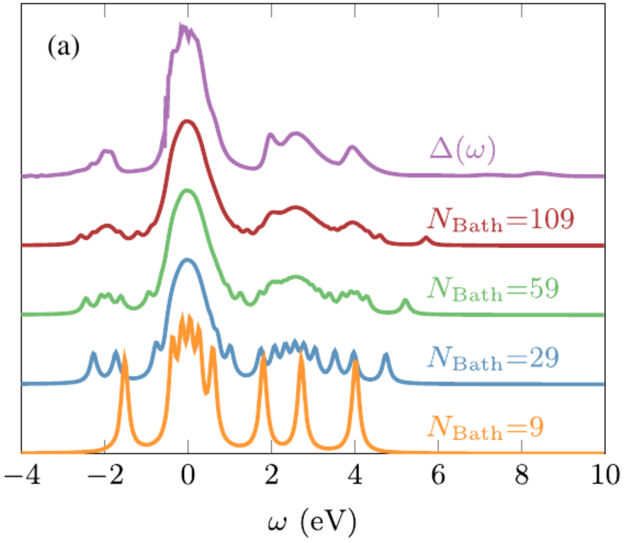


[Bauernfeind *et.al*, PRX **7**, 031013 (*2017*)]

Hamiltonian based Solvers:

- Discrete bath sites → Many-body Hamiltonian
  - T = 0 ground state
- **Exact Diagonalization** (ED), e.g. Lanczos
  - Exponential Scaling
  - Only rough bath discretization possible
- Some relief: **Matrix Product States** (MPS)
  - Allows to reduce matrix dimensions
  - DMRG, Time evolution → Use as Solver
  - But: (quasi) 1D structure (1 orbital)



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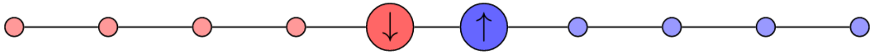
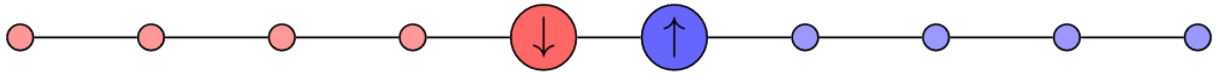


Fork Tensor Product States



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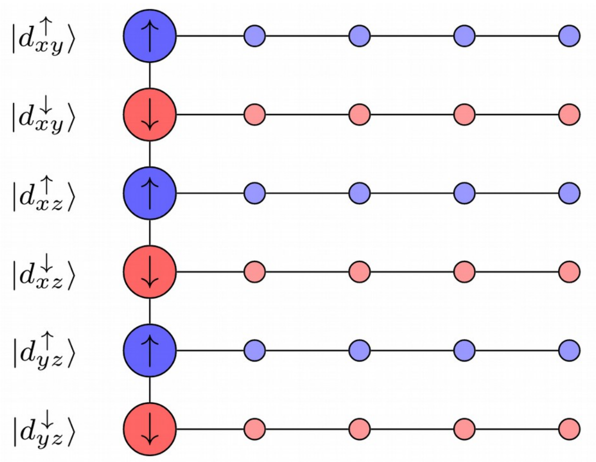

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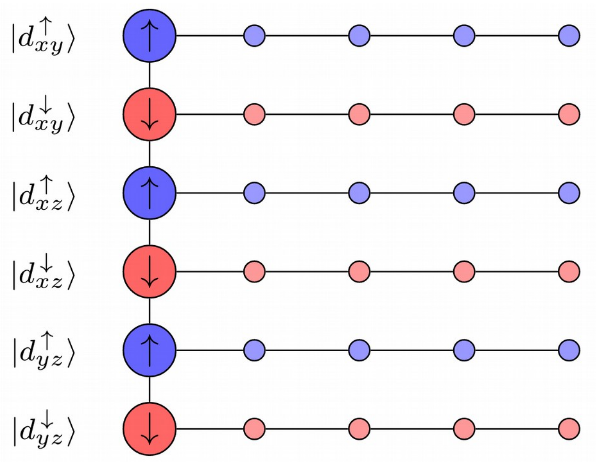
Fork Tensor Product States

- O(100) bath sites per orbital
- DMRG and time evolution possible
- SOC: Off-diagonal hybridization



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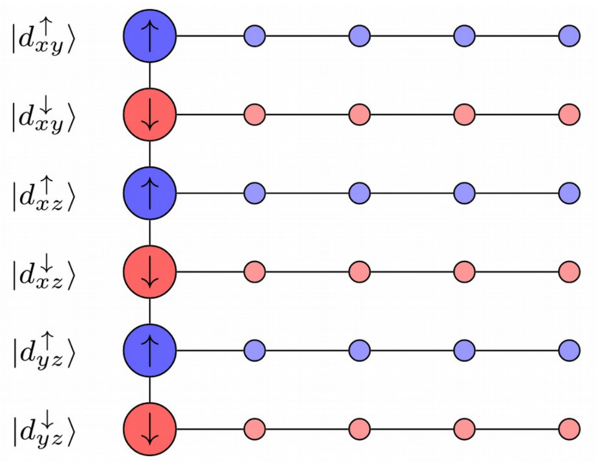

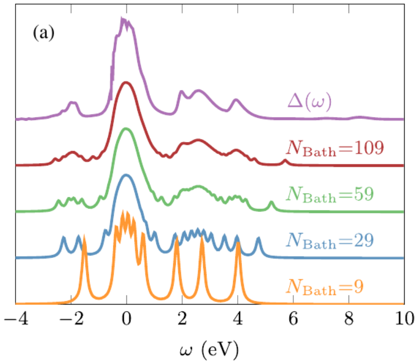

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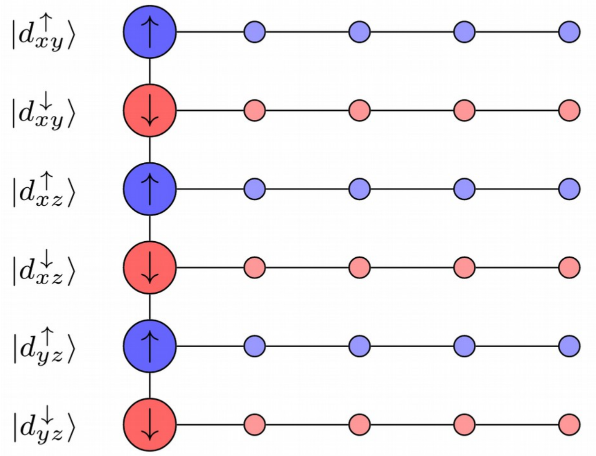

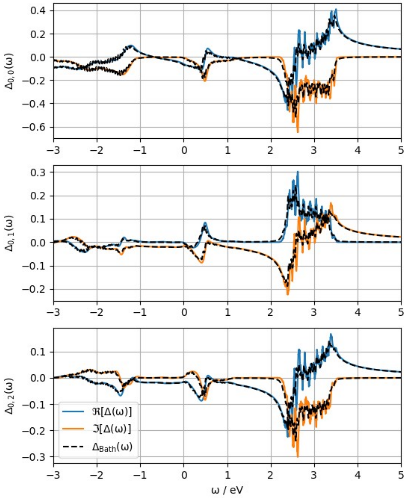

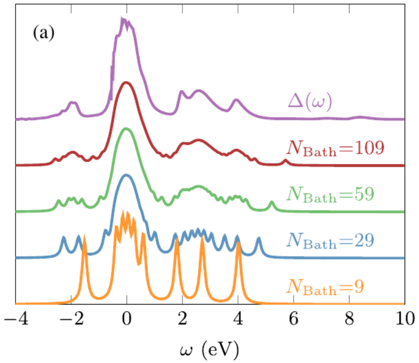

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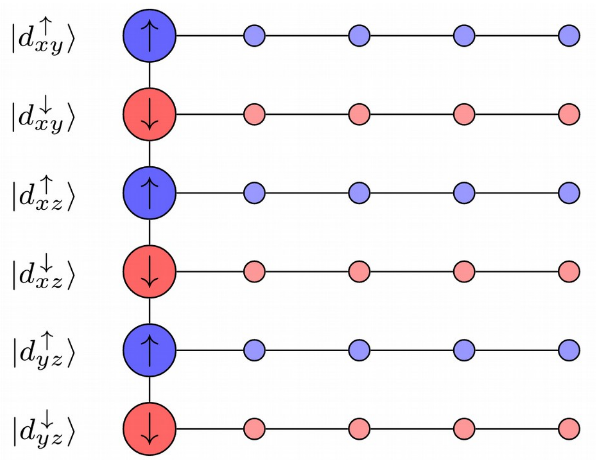
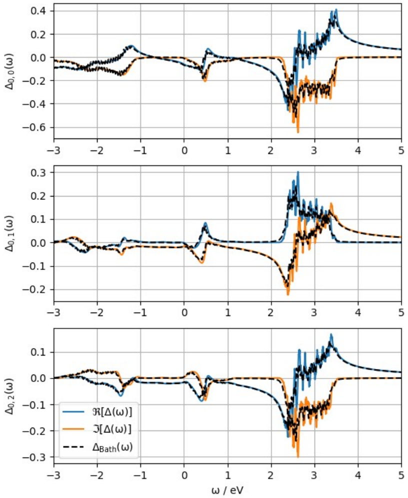
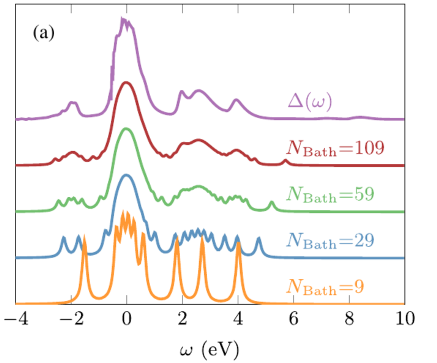


Thanks to Daniel Bauernfeind for implementing the SOC Hamiltonian!





[Bauernfeind *et.al*, PRX **7**, 031013 (*2017*)]

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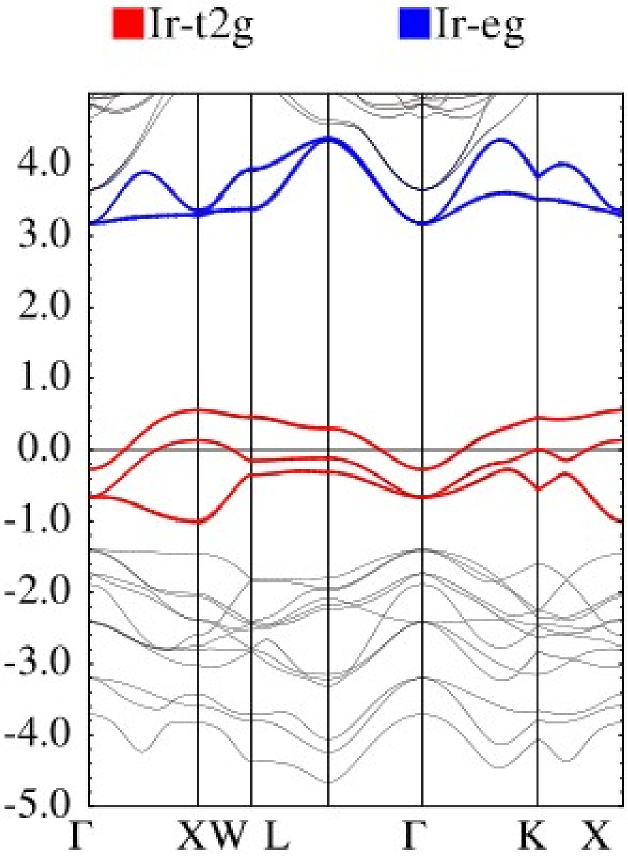
Back to BYIO: DFT results



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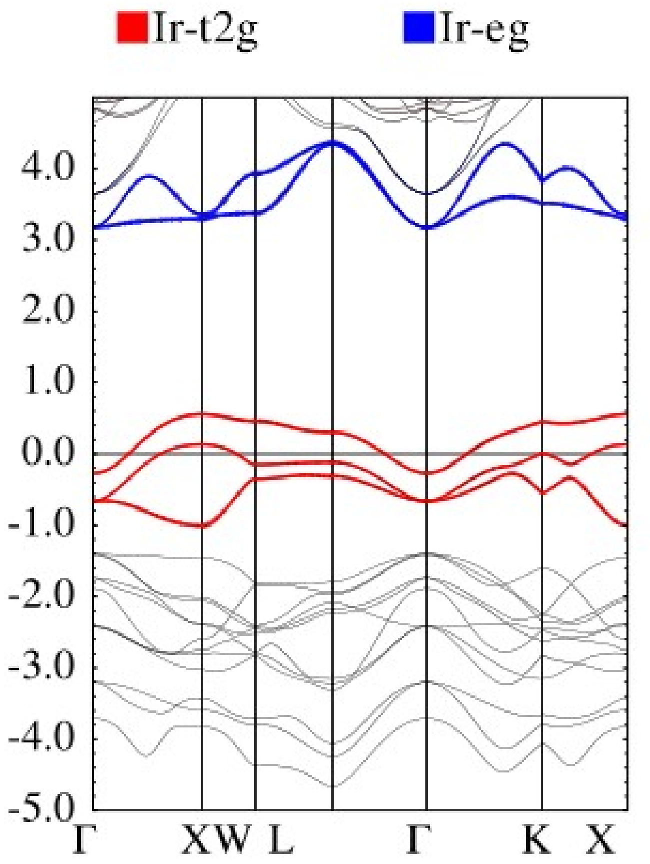
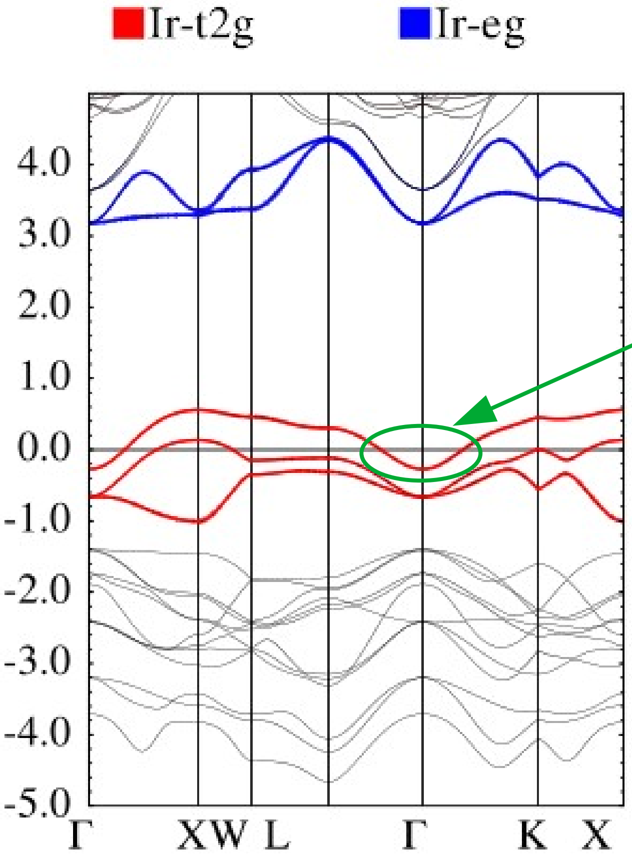
Back to BYIO: DFT results



$\lambda \approx 0.3$ eV

arXiv:2202.10794

Back to BYIO: DFT results

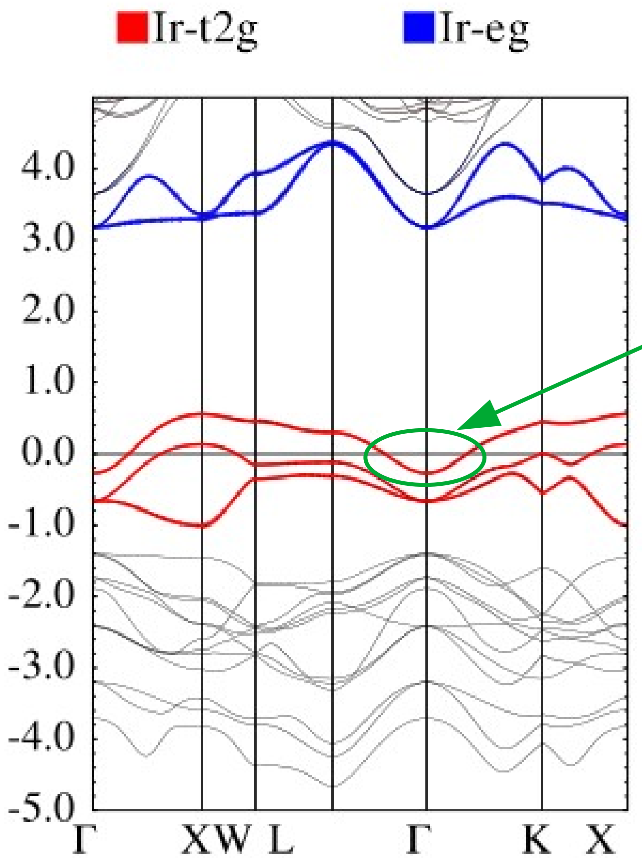


$$n^{\mathrm{DFT}}_{J^{\mathrm{eff}}_{1/2}} = 0.17$$

λ ≈ 0.3 eV

arXiv:2202.10794

Back to BYIO: DFT results



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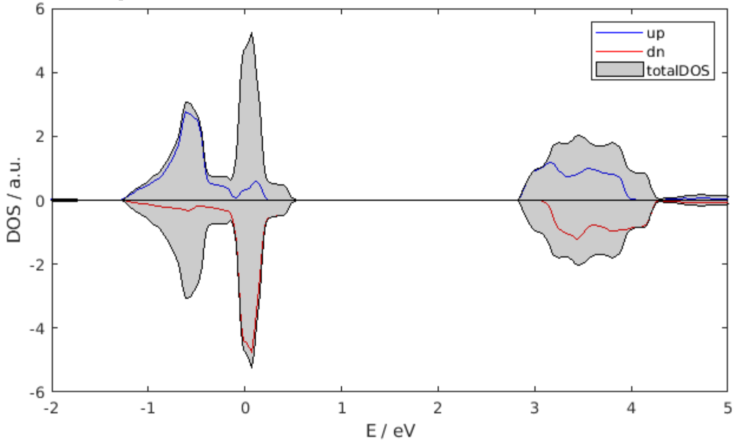
$\lambda \approx 0.3$ eV

Supercell calculation:



→ Ordered moment of 1.07 μ_B

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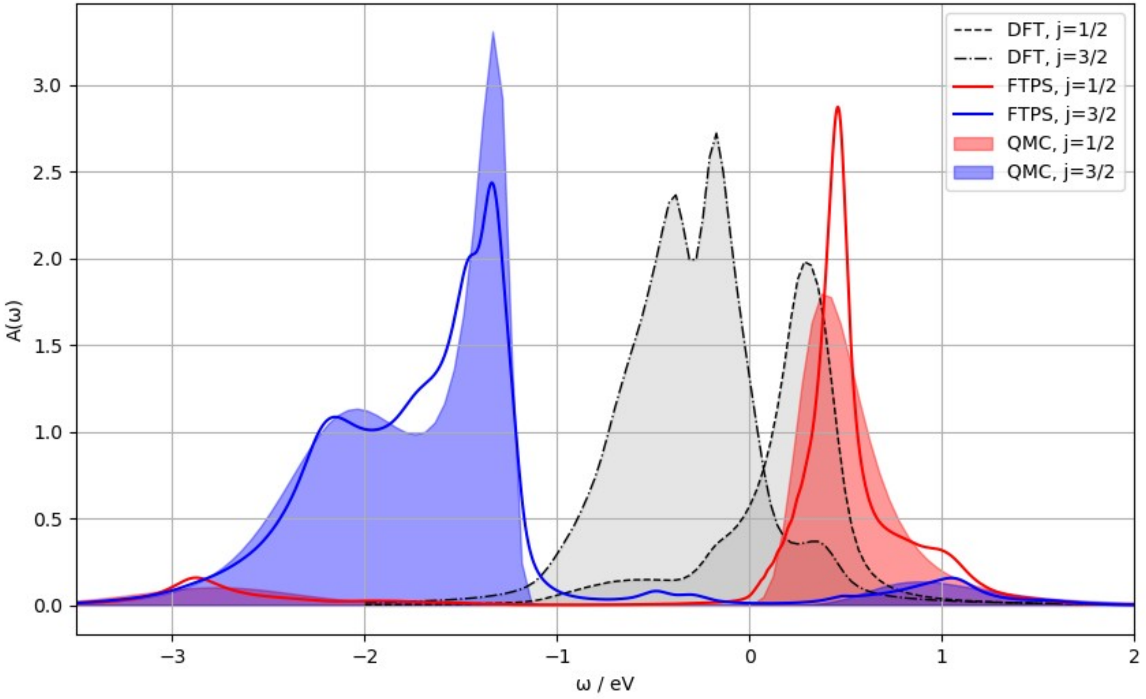
DMFT results



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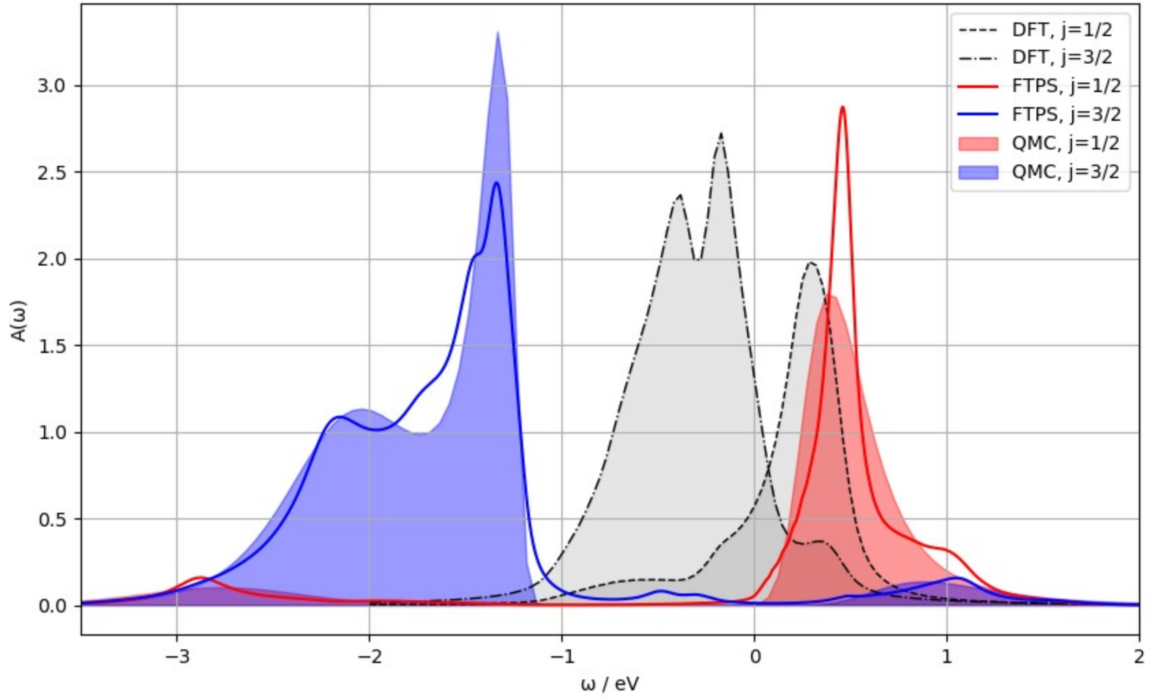

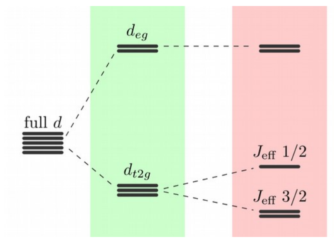

	$\langle J^2 \rangle$	$n_{J^{\text{eff}}_{1/2}}$
AL	0.00	0.00
QMC	0.19	0.11
FTPS	0.20	0.12

$$n^{\text{DFT}}_{J^{\text{eff}}_{1/2}} = 0.17$$

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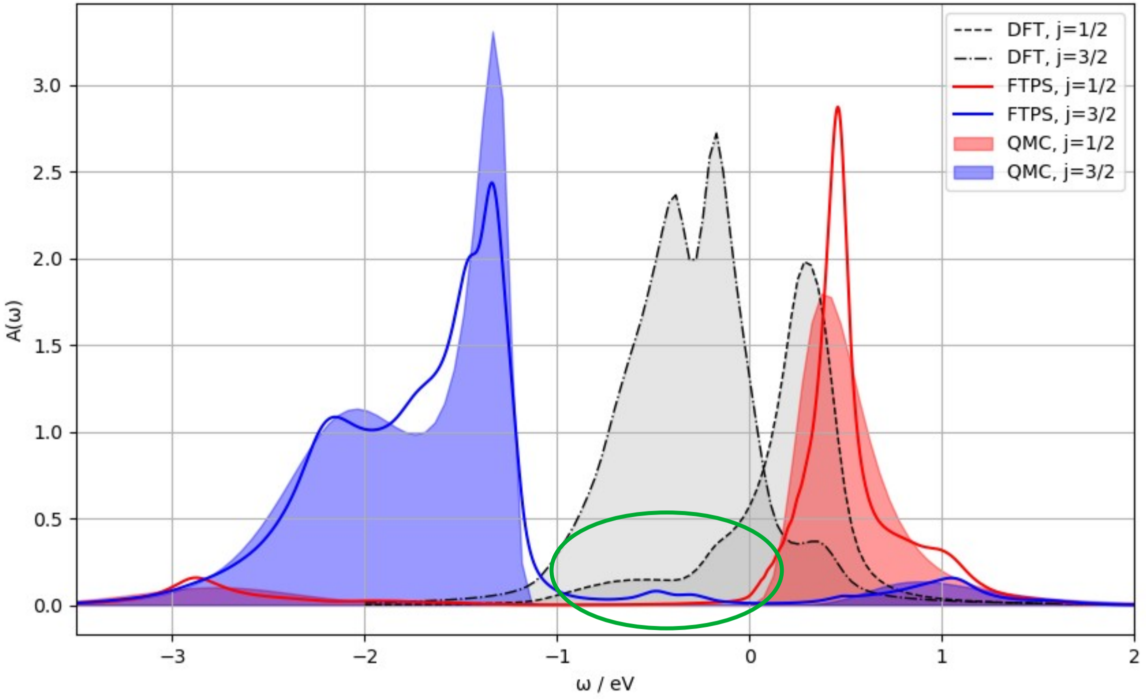
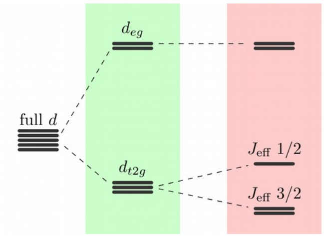
DMFT results



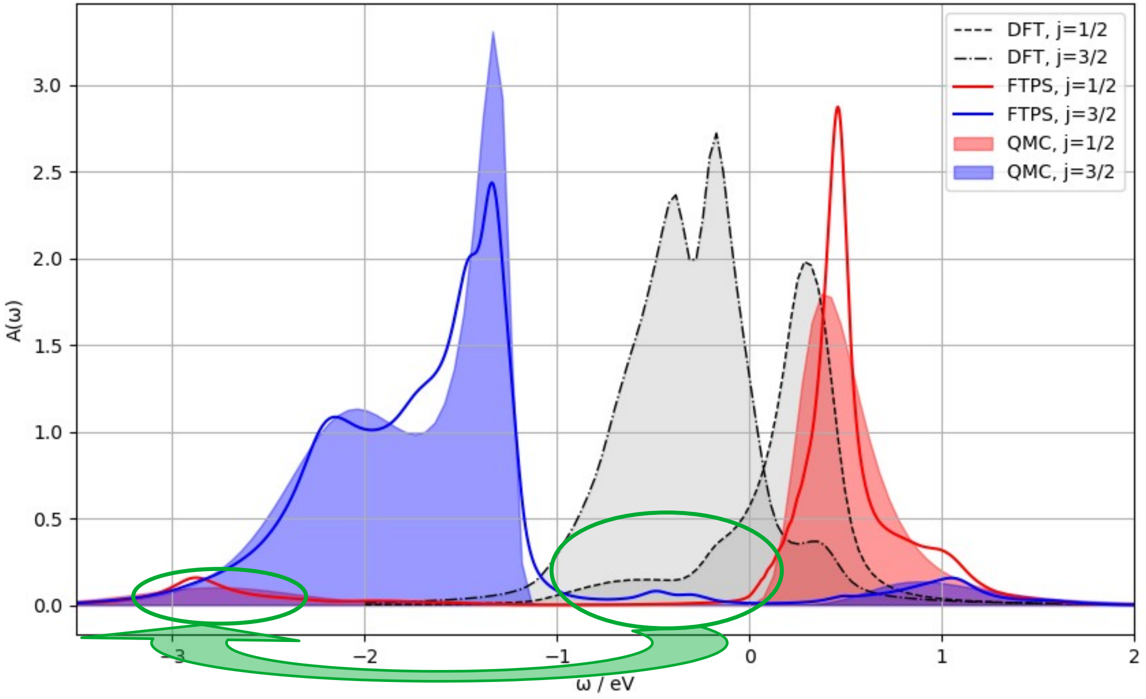


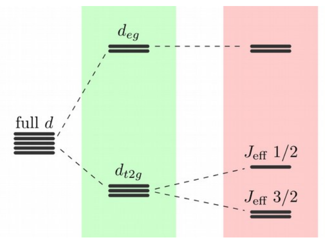
	$\langle J^2 \rangle$	$n_{J^{\text{eff}}_{1/2}}$
AL	0.00	0.00
QMC	0.19	0.11
FTPS	0.20	0.12

$$n^{\text{DFT}}_{J^{\text{eff}}_{1/2}} = 0.17$$

arXiv:2202.10794

DMFT results





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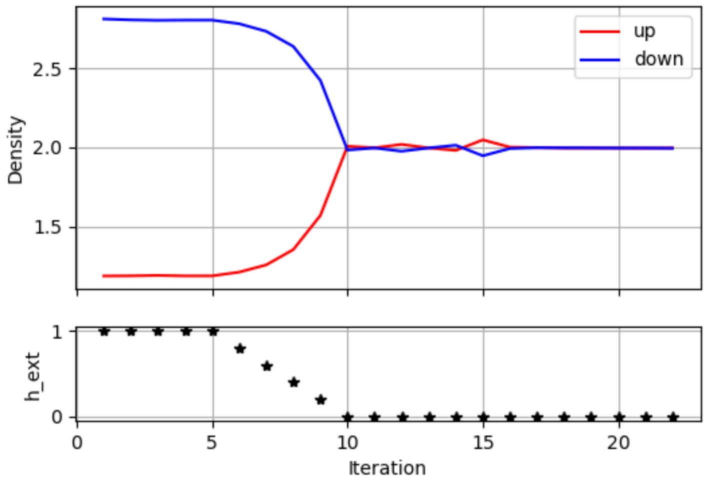
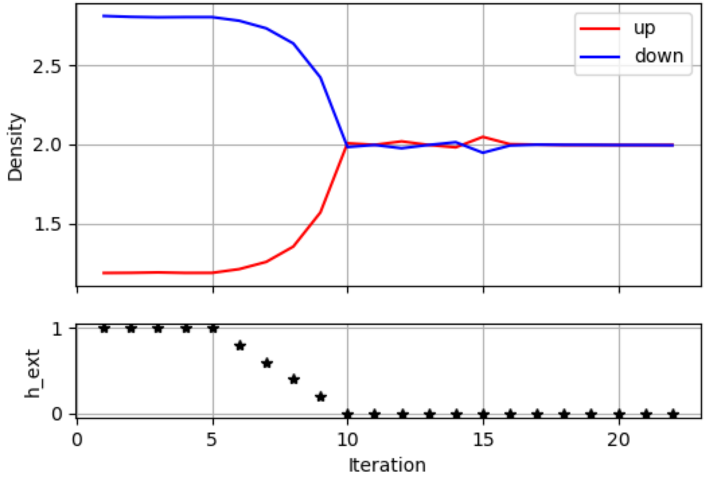


arXiv:2202.10794

DMFT results

At T = 0 :

- Type I AFM: no ordering
- FM unit cell: no ordering
  - No alternating solution
  - **ANY** ordering unlikely



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DMFT results

- Small moment present
  - Independent of temperature
  - Band-structure effect
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  - Mean field should give finite transition temperature for any finite coupling

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Why?

arXiv:2202.10794

Solver itself works

- Benchmark: **Sr_2MgOsO_6**
  - Os $5d^2$
  - AFM ordering at 110K [42]

[42] Yuan et al., Inorganic chem. **54**, 3422 (*2015*)

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- Benchmark: **Sr_2MgOsO_6**
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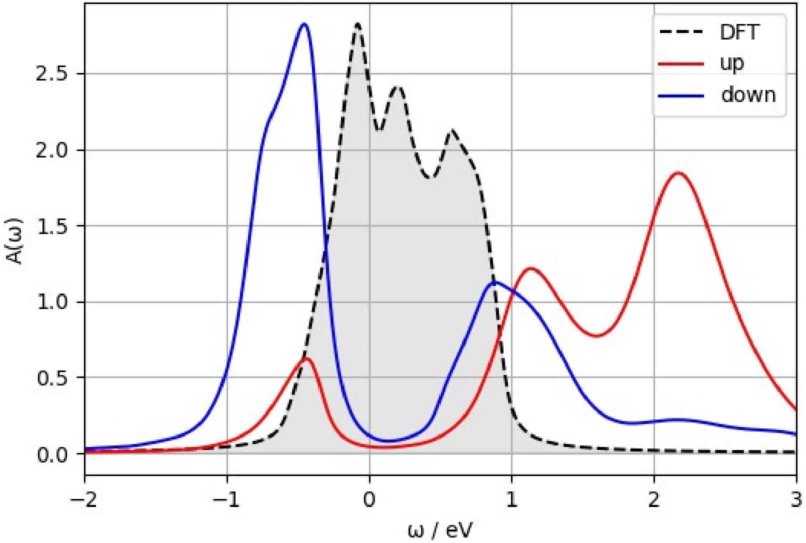

[42] Yuan et al., Inorganic chem. **54**, 3422 (*2015*)

Explanaitons for no ordering

- Non-local singlets (RVB) [17]

[17] A. Nag et al., PRB **98**, 014431 (*2018*)

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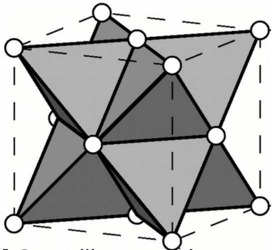

[Gvozdikova et al., arxiv.org/abs/cond-mat/0502255]

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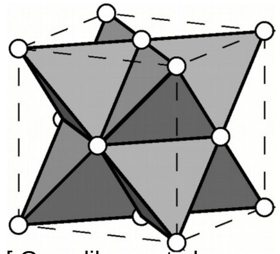
- Frustration
  - Geometric frustration (fcc sublattice)
  - Configurational frustration



[Gvozdikova et al., arxiv.org/abs/cond-mat/0502255]

Magnetic Config	SYIO ΔE (meV/fu)	BYIO ΔE (meV/fu)
NM	27.14	23.34
FM	20.78	11.15
Type I	0.0	0.0
Type III	3.45	2.72

[Bhowal *et al.*, PRB **92**, 121113 (*2015*)]

Recap

- Small moment present
  - Independent of temperature
  - Band-structure effect
- No long-range ordering
  - Mean field should give finite transition temperature for any finite coupling

(Configurational) frustrations & dynamic correlations prevent one stable ordered magnetic ground state!

Acknowledgements


Daniel Bauernfeind


Johannes Graspeuntner


Markus Richter


Markus Aichhorn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arXiv:2202.10794