Magnetic response of a Hund's metal within DMFT: Sr_2RuO_4

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Spin Fluctuations in Sr_2RuO_4

Existence from temperature dependence

Theoretical prediction

Experimental verification

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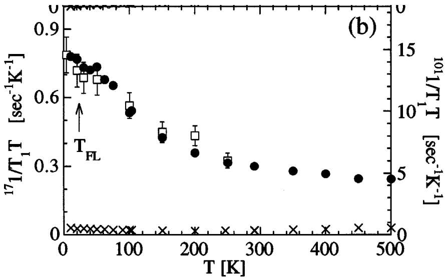
- Nuclear Magnetic Resonance (NMR)

  Imai et al. PRL 81 3006 (1998)



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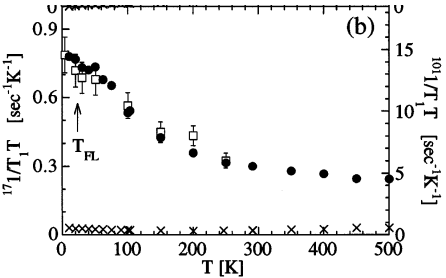

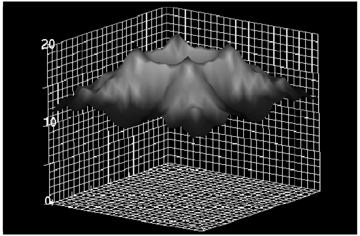

FIG. 1. Calculated bare susceptibility for Sr_2RuO_4.

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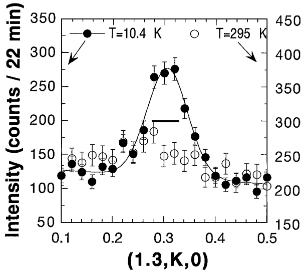
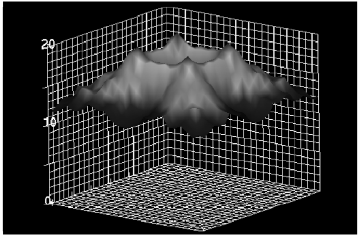
  Sidis et al. PRL 83 3320 (1999)





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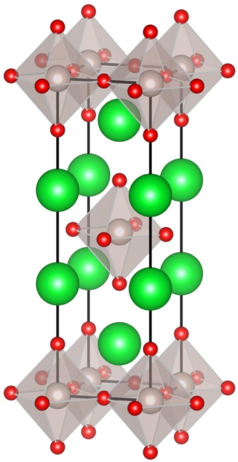
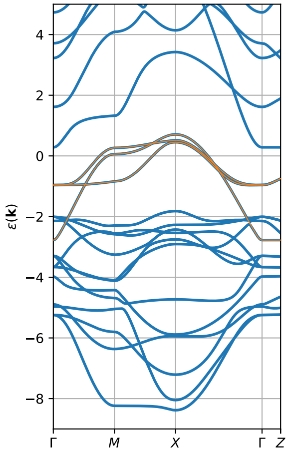
Sr_2RuO_4 atomic & electronic structure

- Planar perovskite (La_2CuO_4 type)
- BC-tetragonal sg-139, I4/mmm

- Three bands with Ru(4d)-t_{2g} symmetry and 4 electrons
- xy (quasi-2D)
- xz, yz (quasi-1D)

- Strong correlations ARPES & dHvA





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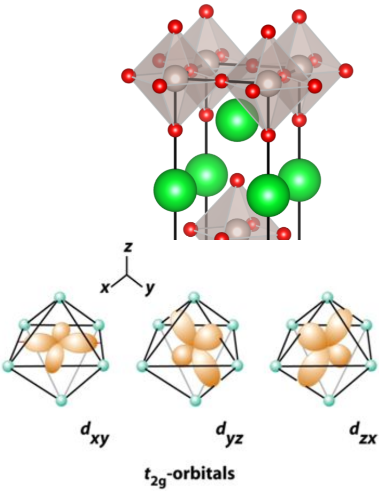
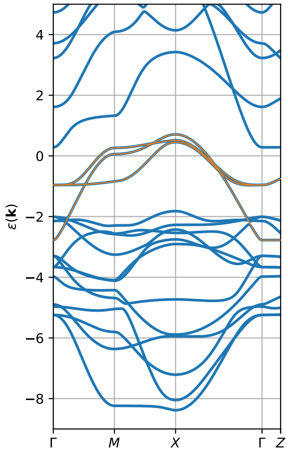
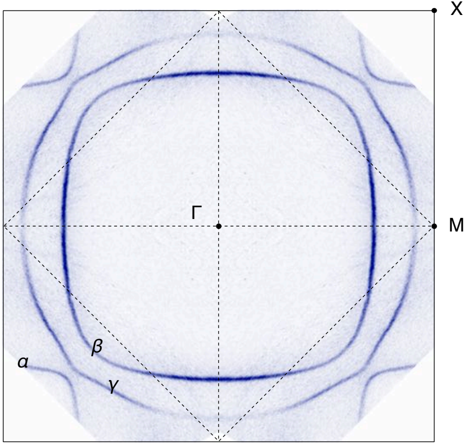




Fermi Surfaces

- α & β sheets, mixtures of xz and yz
- γ sheet, dominantly xy



Tamai, et al., PRX 9 021048 (2019)

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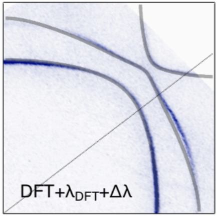
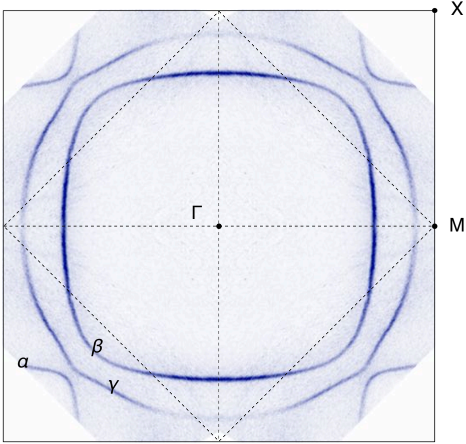


- Correlation effects from DMFT

Mravlje, et al. PRL 106, 096401 (2011)
Zhang, et al. PRL 116, 106402 (2016)
Kim, et al. PRL 120, 126401 (2018)



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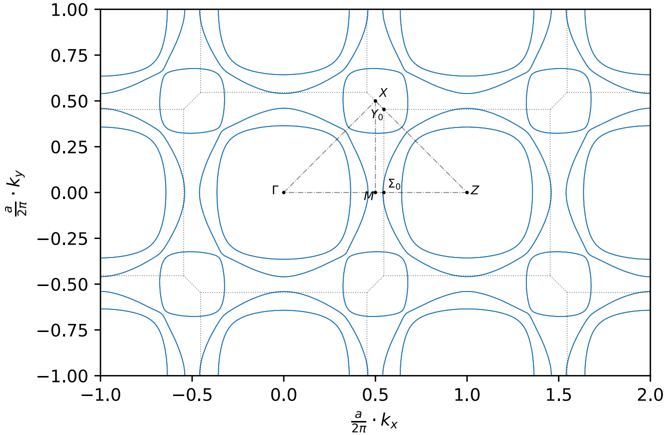
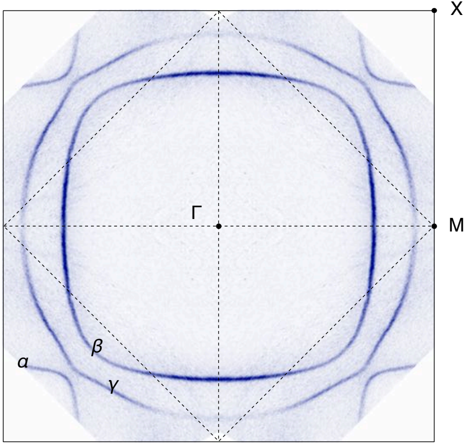
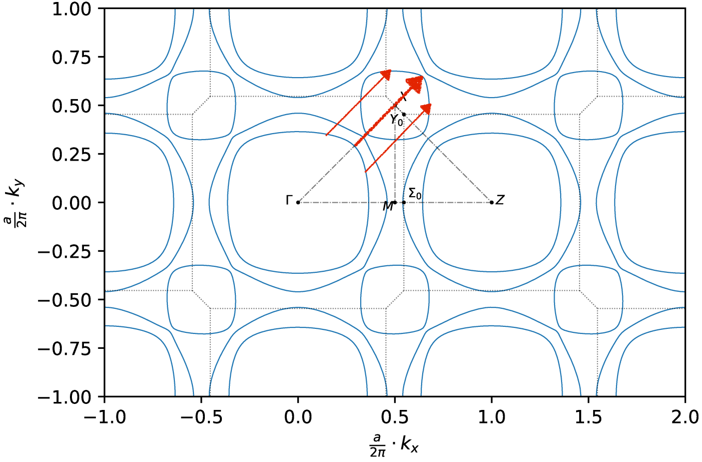


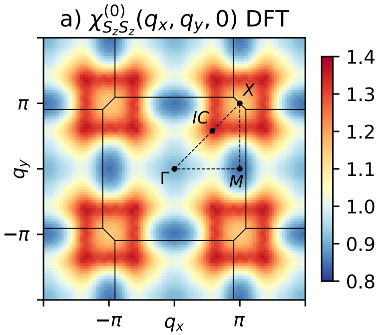


Quizz: Find the “nesting vector”

Tamai, et al., PRX 9 021048 (2019)

Fermi Surface Nesting



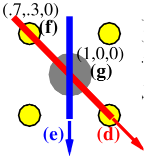


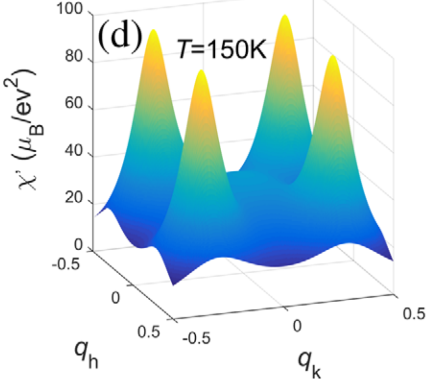
- Nesting vector (red)
- Bare susceptibility

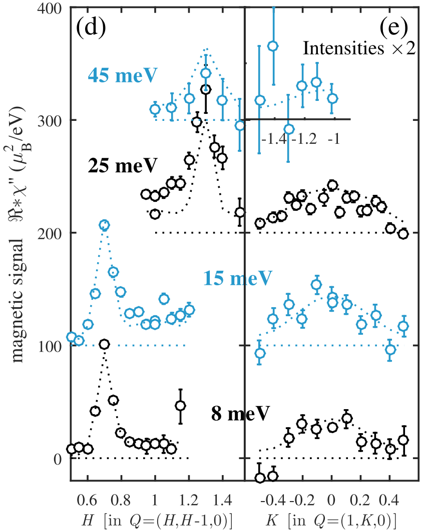
$$\chi^{(0)} = G_0 * G_0$$

Mazin & Singh PRL 82 4324 (1999)

Inelastic Neutron Scattering (INS)







P. Steffens, et al., PRL 122, 047004, (2019)

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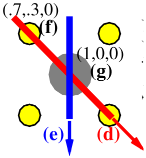

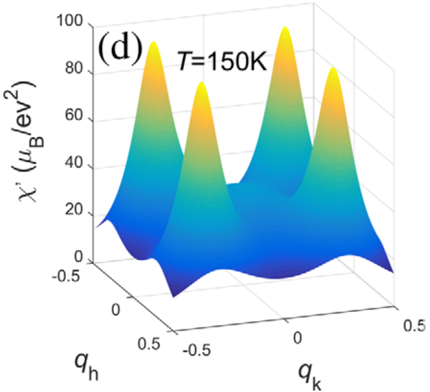

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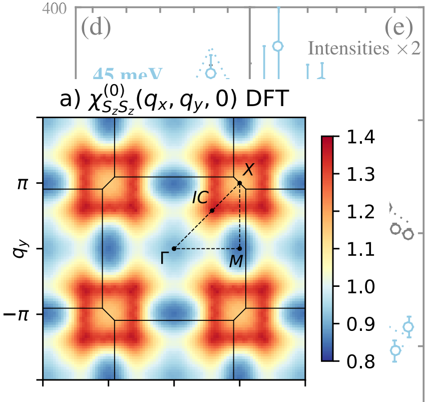

$$\chi(\mathbf{Q}_\Gamma) \gtrsim \chi(\mathbf{Q}_X)$$

$\chi^{(0)}$ is incompatible with INS!

What is the effect strong correlations on the magnetic susceptibility in Sr_2RuO_4?

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Idea:

Compute the DMFT magnetic susceptibility and find out!

Software

- **TRIQS**
  Toolbox for Research on Interacting Quantum Systems
  github.com/TRIQS/triqs
- **TRIQS/cthyb**
  Continous Time Hybridization Expansion Quantum Monte Carlo *(CTHYB)*
  github.com/TRIQS/cthyb
- **TRIQS/tprf**
  Two-Particle Response Function *(TPRF)* toolbox
  github.com/TRIQS/tprf

- **Python, Numpy, Scipy, Matplotlib**

Computing susceptibilities in DMFT

There are two approaches

1. Static suseptibilities $\chi(\mathbf{Q})$ from DMFT calculations in applied field
   - Possible for a single $\mathbf{Q}$ vector at a time
   - Non-zero $\mathbf{Q}$ requires super-cell calculations

1. Dynamical susceptibilities $\chi(\mathbf{Q}, i\omega)$ from the Bethe-Salpeter Equation (BSE)
   - Requires two-particle response functions
   - Requires solving large matrix-equations (BSE)

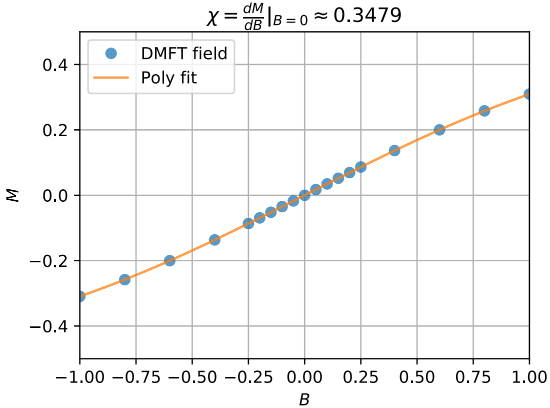
Consider the single-band Hubbard model on the square lattice
with nearest neighbour hopping at half-filling with $t = 1$, $U = 10$, $\beta = 1$.

1. DMFT calculations in applied field

- Many self-consistent DMFT calculations
- Sweeping the applied magnetic field B
- Measure the induced magnetization $M(B)$
- A homogeneous B field gives the $\mathbf{Q} = \mathbf{0}$ response as

$$\chi_{\text{Field}} = \chi(\mathbf{0}) = \left. \frac{dM}{dB} \right|_{B \to 0} \approx 0.3479$$

- For technical details see **TRIQS/tprf** tutorial



2. DMFT susceptibilities from the Bethe-Salpeter Equation

Compute the impurity two-particle ($G^{(2)}$) and single-particle (G) Green's functions

$$G^{(2)}_{abcd}(\omega, \nu, \nu') \equiv \langle \mathcal{T} c^\dagger_a(\nu) c_b(\omega + \nu) c^\dagger_c(\omega + \nu') c_d(\nu') \rangle \, , \quad G_{ab}(\nu) \equiv -\langle \mathcal{T} c_a(\nu) c^\dagger_b \rangle \, ,$$

where $abcd$ are spin-orbital indices and ω, ν and ν' are Matsubara frequencies. Here we will sample both using **TRIQS/cthyb**.

From $G^{(2)}$ and G construct the full χ and bare $\chi^{(0)}$ generalized susceptibilities

$$\chi_{abcd}(\omega, \nu, \nu') = G^{(2)}_{abcd}(\omega, \nu, \nu') - \beta \delta_{0,\omega} G_{ba}(\nu) G_{dc}(\nu') \, ,$$
$$\chi^{(0)}_{abcd}(\omega, \nu, \nu') = -\beta \delta_{\nu,\nu'} G_{da}(\nu) G_{bc}(\omega + \nu) \, .$$

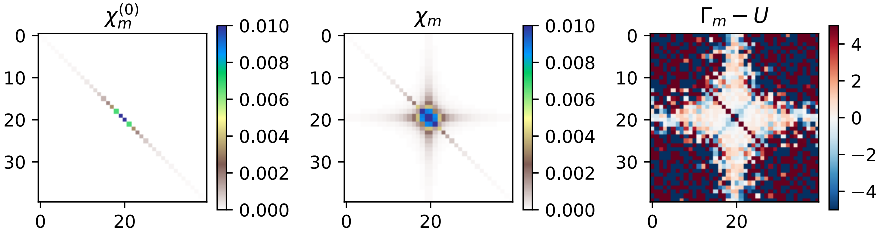
Tools for constructing χ and $\chi^{(0)}$ are available in **TRIQS/tprf**.

2. DMFT susceptibilities from the Bethe-Salpeter Equation

Solve the Bethe-Salpeter Equation (BSE) for the impurity vertex function Γ

$$\chi = \chi^{(0)} + \chi^{(0)}\Gamma\chi \quad \Rightarrow \quad \Gamma_{AB}(i\omega) = [\chi^{(0)}(\omega)]^{-1}_{AB} - [\chi(\omega)]^{-1}_{AB}$$

by matrix inversion with index grouping $\chi_{abcd}(\omega, \nu, \nu') = \chi_{\{\nu ab\}\{\nu' dc\}}(\omega) = \chi_{AB}(\omega)$.



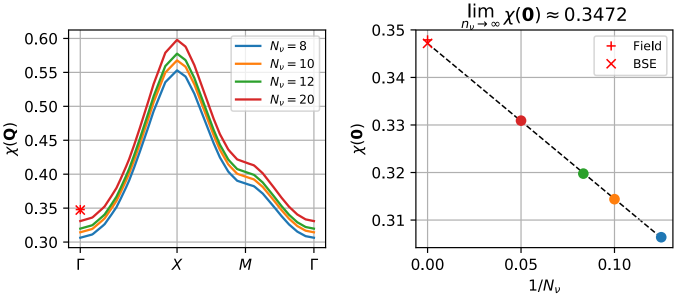
Example: Hubbard model on square lattice using **TRIQS/cthyb** and **TRIQS/tprf**.

2. DMFT susceptibilities from the Bethe-Salpeter Equation

Lattice susceptibility from the BSE in **TRIQS/tprf**

$$\chi(\mathbf{Q}, \omega) = \left[\mathbf{1} - \Gamma(\omega) \chi^{(0)}(\mathbf{Q}, \omega) \right]^{-1} \chi^{(0)}(\mathbf{Q}, \omega) \, ,$$

using the DMFT local vertex $\Gamma(\mathbf{Q}, \omega) \approx \Gamma(\omega)$.



- Linear convergence with N_ν
- Extrapolate to $1/N_\nu \to 0$
- Compare with applied field @ $\mathbf{Q} = \mathbf{0}$

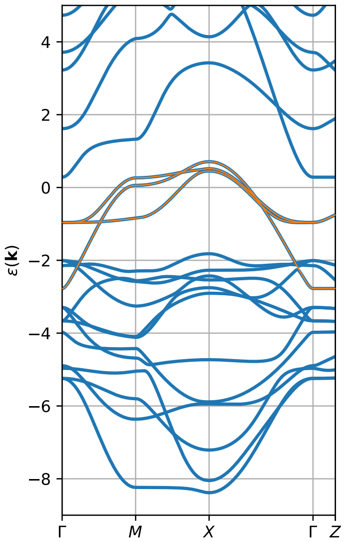
$$\chi_{\text{BSE}}(\mathbf{0}) \approx 0.3472$$
$$\chi_{\text{Field}}(\mathbf{0}) \approx 0.3479$$

- Quantitative agreement
- Thermodynamic consistency

Hafermann et al. PRB 90 235105 (2014)

Application to magnetic susceptibility of Sr_2RuO_4

- DFT + Wannierization
- Three band effective t_{2g} model
- Kanamori interaction U=2.3eV, J=0.4eV
- Dynamical Mean-Field Theory (DMFT)
- Applied field in super-cells 1×1, $\sqrt{2} \times \sqrt{2}$, $\sqrt{2} \times \sqrt{5}$
- Dynamical vertex corrections $\Gamma_{abcd}(i\omega, i\nu, i\nu')$
- Lattice susceptibility $\chi_{abcd}(\mathbf{Q})$ from BSE
- arXiv:1904.07324



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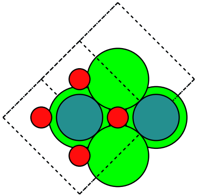

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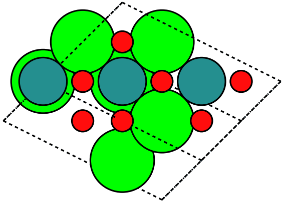

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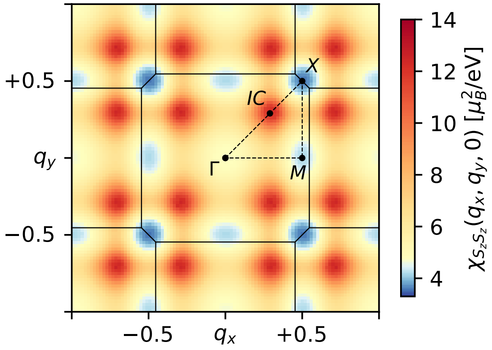
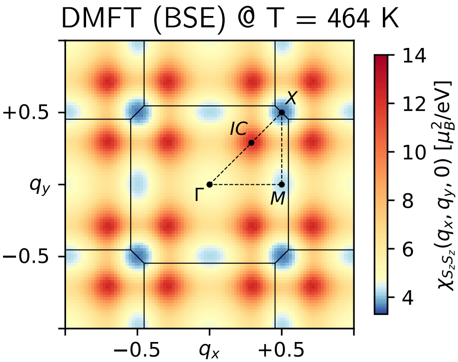
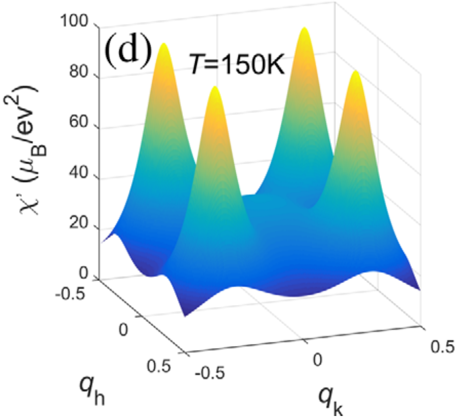


Spin susceptiblitiy $\chi_{S_z S_z}(\mathbf{Q})$



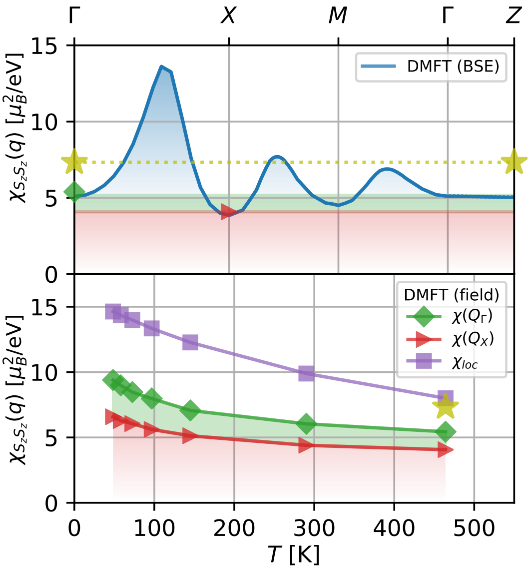


- Qualitative agreement Γ vs X!

P. Steffens, et al.,
PRL 122, 047004, (2019)

Spin susceptiblitiy $\chi_{S_z S_z}(\mathbf{Q})$

- Incommensurate (IC) & ridge response
- **Quasi Local/Ferromagnetic** Background response (red) >50% of $\mathbf{Q}$-average (stars)
- $\chi(\mathbf{Q}_\Gamma) > \chi(\mathbf{Q}_X)$ (green)
- Lower temperature (T↓)
  - Background ↑
  - Local response ↑
  - $\chi(\mathbf{Q}_\Gamma)/\chi(\mathbf{Q}_X) \sim 4/3$

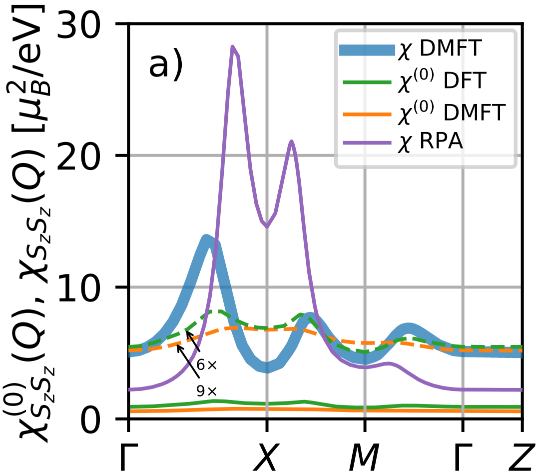


Comparison to simpler approximations

- DMFT lattice susceptibility: χ DMFT
- Bare DFT bubble: $\chi^{(0)}$ DFT (Density Functional Theory)
- Bare DMFT bubble: $\chi^{(0)}$ DMFT
- Random Phase Approximation: χ RPA

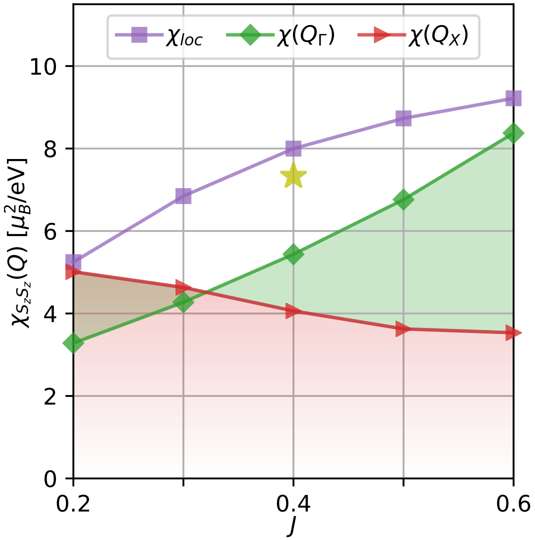
- Only χ DMFT reproduces experment $\chi(\mathbf{Q}_\Gamma) > \chi(\mathbf{Q}_X)$

- **DMFT dynamical vertex** $\Gamma(\omega, \nu, \nu')$ effects are essential!



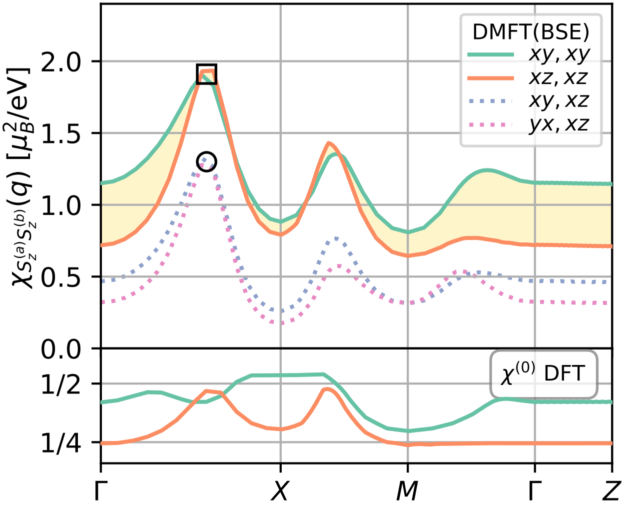
Role of Hund's coupling

- Hund's J interaction: Tune around $J = 0.4$ eV
- $\chi(\mathbf{Q}_\Gamma)$ and $\chi_{loc} \Uparrow$
- $\chi(\mathbf{Q}_X) \downarrow$
- $J \lesssim 0.32$ qualitative change
- Hund's physics controls $\chi(\mathbf{Q}_\Gamma) > \chi(\mathbf{Q}_X)$



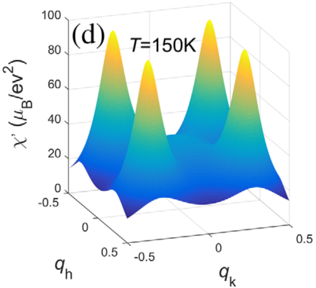
Orbital contributions

- $\chi_{S_z^{(\alpha)} S_z^{(\beta)}}(\mathbf{Q})$
  $\alpha, \beta \in \{xy, xz, yz\}$
- All orbitals @ $\mathbf{Q}_{IC}$ (square)
  (c.f. DFT w. only xz, yz)
  Boehnke, et al., EPL 122 57001
- 50% inter-orbital response
- Γ enhancement from xy

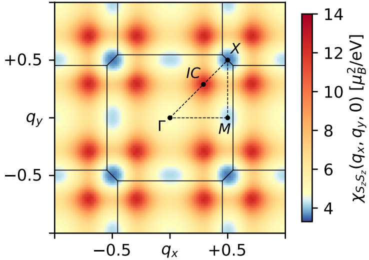


Summary

- Dynamical Mean Field Theory
- Magnetic resp. $\chi_{S_z S_z}(\mathbf{Q})$
- Hund's metal Sr_2RuO_4
- Suppression of AFM @ X
- Hund's coupling drive:
  - Quasi Ferromagnetic fluct.
  - $\chi(\mathbf{Q}_\Gamma) > \chi(\mathbf{Q}_X)$
- Strong orbital mixing
- xy gives Γ enhancement
- For details see arXiv:1904.07324



INS: P. Steffens, et al., PRL 122, 047004, (2019)



DMFT (BSE) @ T = 464 K
HURS et al. arXiv:1904.07324