Two-Particle Response (Functions)

Hugo U. R. Strand
hugo.strand@oru.se

Sept 1 (2023)
Centre Port-Royal, Paris

FLATIRON INSTITUTE
Center for Computational Quantum Physics

SIMONS FOUNDATION

Two-Particle Response (Functions)

TPRF

Hugo U. R. Strand
hugo.strand@oru.se

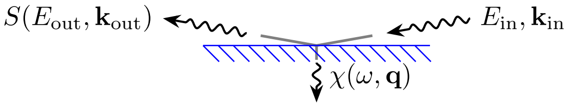
Sept 1 (2023)
Centre Port-Royal, Paris

FLATIRON INSTITUTE
Center for Computational Quantum Physics

SIMONS FOUNDATION

Why two-particles?

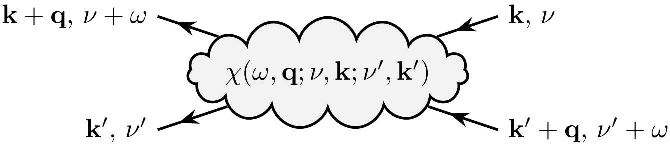
Scattering experiment

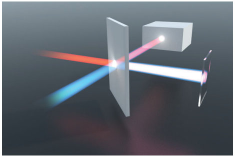


$$\omega = E_{in} - E_{out} \;, \quad \mathbf{q} = \mathbf{k}_{in} - \mathbf{k}_{out}$$

$$S(E_{\mathsf{out}}, \mathbf{k}_{\mathsf{out}}) \propto \chi(\omega, \mathbf{q}) = \sum_{\mathbf{k}\mathbf{k}'} \sum_{\nu\nu'} \chi(\omega, \mathbf{q}; \nu, \mathbf{k}; \nu', \mathbf{k}') \, .$$

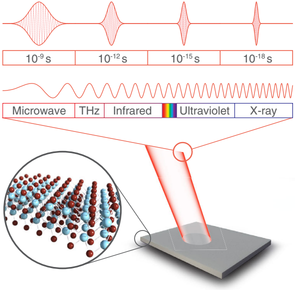
Generalized susceptibility χ

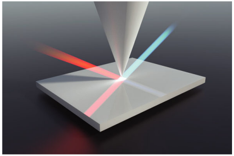




Optical probes

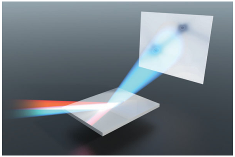
- Probes dielectric properties
- Flexible in implementation (spectral range, detection scheme, environment)
- fs time resolution





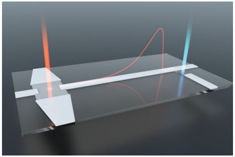
Scanning probes

- Probes optical constants in near-field (SNOM) or tunneling currents (STM)
- fs time resolution
- nm spatial resolution



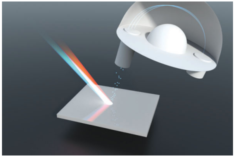
Scattering probes

- Probes structural dynamics and dynamics of electronic degrees of freedom at elemental resonances
- Access to dispersion relations via finite momentum transfer
- fs time resolution



Transport

- Probes transient photoconductivity
- Integrates well into microstructured devices
- Sub-ps time resolution



ARPES

- Probes time- and momentum-resolved carrier dynamics, and the evolution of electronic spectral functions
- Direct probe of electronic temperature
- Tunability of energy vs. time resolution (down to ~15 meV, ~30 fs)

Interacting quantum systems

- Hamiltonian $\hat{H}$ in second quantization

$$\hat{H} = \sum_{ij} t_{ij}\, c_i^\dagger c_j + \sum_{ijkl} U_{ijkl}\, c_i^\dagger c_j^\dagger c_k c_l$$

- Hopping matrix t_{ij}
- Interaction tensor U_{ijkl}

Green's functions

Single particle Green's function

$$G_{a\bar{b}}(\tau_1, \tau_2) = -\langle \mathcal{T} c_a(\tau_1) c_{\bar{b}}^\dagger(\tau_2) \rangle \, ,$$

- create a particle in state b at time τ_2 and
- annihilate a particle in state a at time τ_1.

Two-particle Green's function

$$G^{(2)}_{\bar{a}b\bar{c}d}(\tau_1, \tau_2, \tau_3, \tau_4) = \langle \mathcal{T} c_a^\dagger(\tau_1) c_b(\tau_2) c_c^\dagger(\tau_3) c_d(\tau_4) \rangle$$

higher order processes.

N-particle Green's function

$$G^{(N)}_{a_1 \ldots a_{2N}}(\tau_1, \ldots, \tau_{2N}) = \langle \mathcal{T} c_{a_1}^\dagger(\tau_1) c_{a_2}(\tau_2) \ldots c_{a_{2N-1}}^\dagger(\tau_{2N-1}) c_{a_{2N}}(\tau_{2N}) \rangle$$

External field linear response

Add an external field F to the system coupling to the operator $\hat{B}$

$$\hat{H}_F = \hat{H} + F\hat{B}$$

The linear response of the operator $\hat{A}$

$$\left.\frac{\partial\langle\hat{A}\rangle}{\partial F}\right|_{F=0} = \chi_{AB}$$

is given by the static **susceptibility** $\chi_{AB} = \chi_{AB}(\omega = 0)$.

Where $\chi_{AB}(\omega)$ is the time dependent generalization for $F(t) = Fe^{i\omega t}$.

Generalized susceptibility $\chi_{AB} \to \chi_{ijkl}$

Assume $\hat{A}$ and $\hat{B}$ are quadratic operators

$$\hat{A} = \sum_{ij} A_{ij} \, c_i^\dagger c_j \, , \quad \hat{B} = \sum_{ij} B_{ij} \, c_i^\dagger c_j$$

then χ_{AB} is given by the **generalized susceptibility** χ_{ijkl} as the sum

$$\chi_{AB}(\omega) = \sum_{ijkl} A_{ij} \chi_{ijkl}(\omega) B_{kl}$$

where $\chi_{ijkl}(\omega)$ is a tensor in single particle indices i, j, k, l.

Generalized susceptibility $\chi_{ijkl} \to \chi_{ijkl}(\tau_1, \tau_2, \tau_3, \tau_4)$

Pass to imaginary time $\omega \to \tau$

$$\chi_{ijkl}(\omega) \to \chi_{ijkl}(\tau)$$

and write χ_{ijkl} as an explicit correlation function

$$\chi_{ijkl}(\tau) = \langle \mathcal{T} (c_i^\dagger c_j)(\tau)(c_k^\dagger c_l) \rangle - \langle c_i^\dagger c_j \rangle \langle c_k^\dagger c_l \rangle$$

Generalized time dependence

$$\chi_{ijkl}(\tau_1, \tau_2, \tau_3, \tau_4) = \langle \mathcal{T} c_i^\dagger(\tau_1) c_j(\tau_2) c_k^\dagger(\tau_3) c_l(\tau_4) \rangle \\ - \langle c_i^\dagger(\tau_1) c_j(\tau_2) \rangle \langle c_k^\dagger(\tau_3) c_l(\tau_4) \rangle$$

Generalized susceptibility $\chi_{ijkl}(\tau_1, \tau_2, \tau_3, \tau_4) \to \chi_{ijkl}(\omega, \nu, \nu')$

$$\chi_{ijkl}(\tau_1, \tau_2, \tau_3, \tau_4) = \langle \mathcal{T} c_i^\dagger(\tau_1) c_j(\tau_2) c_k^\dagger(\tau_3) c_l(\tau_4) \rangle - \langle c_i^\dagger(\tau_1) c_j(\tau_2) \rangle \langle c_k^\dagger(\tau_3) c_l(\tau_4) \rangle$$

Connect to the two-particle Green's function

$$G^{(2)}_{\bar{a}b\bar{c}d}(\tau_1, \tau_2, \tau_3, \tau_4) = \langle \mathcal{T} c_a^\dagger(\tau_1) c_b(\tau_2) c_c^\dagger(\tau_3) c_d(\tau_4) \rangle$$

Rewrite using $G^{(2)}$ and $G_{ij}(\tau) = \langle \mathcal{T} c_i(\tau) c_j^\dagger \rangle$ gives

$$\chi_{ijkl}(\tau_1, \tau_2, \tau_3, \tau_4) = G^{(2)}_{\bar{i}j\bar{k}l}(\tau_1, \tau_2, \tau_3, \tau_4) - G_{ji}(\tau_2 - \tau_1) G_{lk}(\tau_4 - \tau_3)$$

Fourier transform to Matsubara frequency + frequency conservation

$$\chi_{ijkl}(\tau_1, \tau_2, \tau_3, \tau_4) \quad \to \quad \chi_{ijkl}(i\omega, i\nu, i\nu')$$

Non-interacting limit

No interaction $\Rightarrow$ Wick's theorem for the non-interacting $\chi^{(0)}$

$$\chi^{(0)}_{ijkl}(\tau) = \langle \mathcal{T} (c^\dagger_i c_j)(\tau)(c^\dagger_k c_l) \rangle_0 - \langle c^\dagger_i c_j \rangle_0 \langle c^\dagger_k c_l \rangle_0$$
$$= \langle \mathcal{T} c_l(-\tau) c^\dagger_i \rangle_0 \langle \mathcal{T} c_k(\tau) c^\dagger_l \rangle_0 = G^{(0)}_{li}(-\tau) G^{(0)}_{kj}(\tau)$$

The direct product in τ is the cheapest way to compute $\chi^{(0)}(\tau)$.

Implemented for TRIQS lattice Green's functions in TPRF:

- `triqs_tprf.lattice_utils.imtime_bubble_chi0_wk`

Lindhard expression for $\chi^{(0)}$

Insert the non-interacting Green's function

$$G^{(0)}_{ij}(i\nu_n) = [i\nu_n \cdot \mathbf{1} - t]^{-1}_{ij} = \sum_a U^\dagger_{ia} \frac{1}{i\nu_n - \epsilon_a} U_{aj}$$

with $t_{ij} = \sum_a U^\dagger_{ia} \epsilon_a U_{aj}$.

Fourier transform to Matsubara frequency $i\omega_n$

$$\chi^{(0)}_{ijkl}(\tau) = G^{(0)}_{kj}(\tau) G^{(0)}_{li}(-\tau) \;\rightarrow\; \chi^{(0)}_{ijkl}(i\omega_n) = T \sum_{\nu_m} G^{(0)}_{kj}(i\nu_m) G^{(0)}_{li}(i\nu_m + i\omega_n)$$

Insert $G^{(0)}(i\nu_m)$ and sum over m

$$\chi^{(0)}_{ijkl}(i\omega_n) = \sum_{ab} U^\dagger_{ka} U_{aj} U^\dagger_{lb} U_{bi} \, T \sum_{\nu_m} \frac{1}{i\nu_m - \epsilon_a} \frac{1}{i\nu_m + i\omega_n - \epsilon_b}$$

$$= \sum_{ab} U^\dagger_{ka} U_{aj} U^\dagger_{lb} U_{bi} \frac{f(\epsilon_a) - f(\epsilon_b)}{i\omega_n - \epsilon_a + \epsilon_b}$$

Example: Electrons on the square lattice

Nearest neighbour hopping t

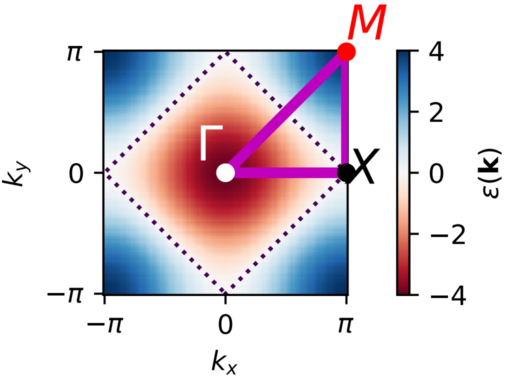
$$\hat{H} = -t \sum_{\langle ij \rangle} c_i^\dagger c_j$$

Fourier transform to k-space

$$\hat{H} = \sum_{\mathbf{k}} \epsilon(\mathbf{k}) c_{\mathbf{k}}^\dagger c_{\mathbf{k}}$$

where

$$\epsilon(\mathbf{k}) = -2t \sum_{n \in \{x,y\}} \cos(k_n)$$



High symmetry path $\Gamma - X - M - \Gamma$

Example: Electrons on the square lattice

Nearest neighbour hopping t

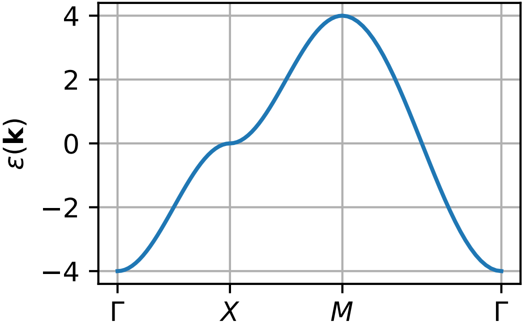
$$\hat{H} = -t \sum_{\langle ij \rangle} c_i^\dagger c_j$$

Fourier transform to k-space

$$\hat{H} = \sum_{\mathbf{k}} \epsilon(\mathbf{k}) c_{\mathbf{k}}^\dagger c_{\mathbf{k}}$$

where

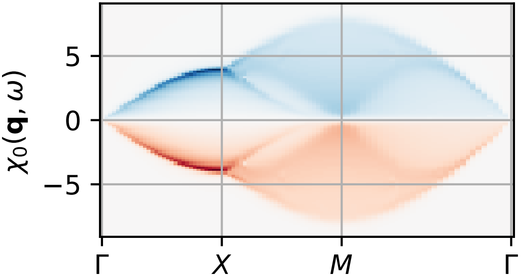
$$\epsilon(\mathbf{k}) = -2t \sum_{n \in \{x,y\}} \cos(k_n)$$



High symmetry path $\Gamma - X - M - \Gamma$

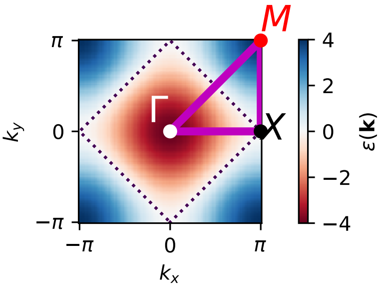
Non-interacting susceptibility $\chi^{(0)}$

$$\chi^{(0)}(\mathbf{r},\tau) = G^{(0)}(\mathbf{r},\tau)G^{(0)}(-\mathbf{r},-\tau) \;\rightarrow\; \chi^{(0)}(\mathbf{q},\omega) = \sum_{\mathbf{k}} \frac{f(\epsilon_{\mathbf{k}}) - f(\epsilon_{\mathbf{q}+\mathbf{k}})}{\omega - \epsilon_{\mathbf{k}} + \epsilon_{\mathbf{k}+\mathbf{q}} + i\delta}$$

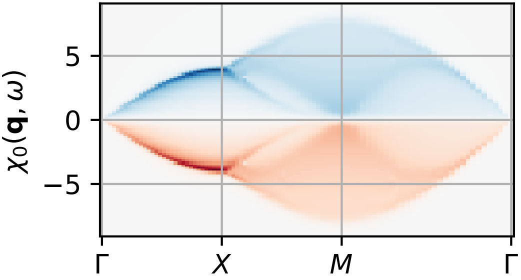


Non-interacting susceptibility $\chi^{(0)}$

$$\chi^{(0)}(\mathbf{r},\tau) = G^{(0)}(\mathbf{r},\tau)G^{(0)}(-\mathbf{r},-\tau) \;\rightarrow\; \chi^{(0)}(\mathbf{q},\omega) = \sum_{\mathbf{k}} \frac{f(\epsilon_{\mathbf{k}}) - f(\epsilon_{\mathbf{q}+\mathbf{k}})}{\omega - \epsilon_{\mathbf{k}} + \epsilon_{\mathbf{k}+\mathbf{q}} + i\delta}$$



Fermi surface nesting



Interacting systems

Bethe-Salpeter equation

$$\chi = \chi_0 + \chi_0 \Gamma \chi \quad \rightarrow \quad (1 - \chi_0 \Gamma)\chi = \chi_0 \quad \rightarrow \quad \chi = (1 - \chi_0 \Gamma)^{-1} \chi_0$$

with the vertex function Γ and $\chi_0 = GG$ (NB! $\chi_0 \neq G^{(0)} G^{(0)}$).

In general $\Gamma = \Gamma_{ijkl}(i\omega, i\nu, i\nu')$ and multiplication is a **matrix product**

$$\chi^{(0)} \Gamma = \sum_{\nu''} \sum_{ab} \chi^{(0)}_{ijab}(i\omega, i\nu, i\nu'') \Gamma_{bakl}(i\omega, i\nu'', i\nu')$$

Compare with the Dyson equation for G

$$G = G^{(0)} + G^{(0)} \Sigma G$$

with self-energy Σ.

Random Phase Approximation (RPA)

First order approximation of the vertex function $\Gamma = \Gamma_{ijkl}(i\omega, i\nu, i\nu')$

Hubbard model with local interaction U (NB! no frequency dependence)

$$\Gamma \propto U$$

Gives χ_{RPA} from the Bethe-Salpeter equation

$$\chi_{RPA} = \chi_0 + \chi_0 U \chi_0 + \chi_0 U \chi_0 U \chi_0 + \chi_0 U \chi_0 U \chi_0 U \chi_0 + \ldots = \chi_0 + \chi_0 U \chi_{RPA}$$

Surprisingly good!?

Captures excitations like

- **Plasmons**, collective charge fluctuations
- **Magnons**, anti-ferromagnetic and ferromagnetic instabilities

Square lattice

Hubbard interaction

$$U = 2$$

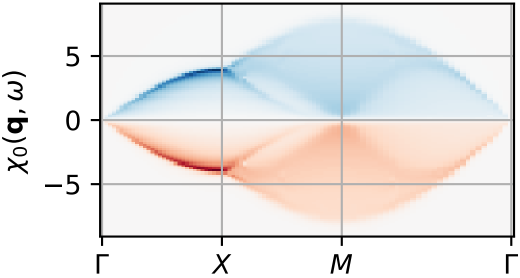
Half-filling $\langle n \rangle = 1$

Bare susceptibility

$$\chi_0 = GG$$

RPA susceptibility

$$\chi_{RPA} = \frac{\chi_0}{1 - U\chi_0}$$



Square lattice

Hubbard interaction

$$U = 2$$

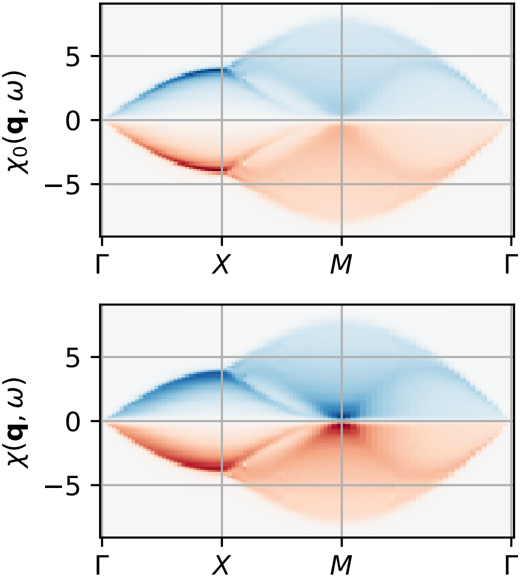
Half-filling $\langle n \rangle = 1$

Bare susceptibility

$$\chi_0 = GG$$

RPA susceptibility

$$\chi_{RPA} = \frac{\chi_0}{1 - U\chi_0}$$



Single band Hubbard and spin rotational invariance

- $\chi_{ijkl}(\mathbf{q},\omega)$ with $i,j,k,l \in \{\uparrow,\downarrow\}$
- Spin rotational invariance $\Leftrightarrow SU(2)$ symmetry
- Completely determined by two **components**

$$\chi_{ch} = \chi_{NN} = \sum_{ijkl} N_{ij}\chi_{ijkl}N_{kl}\,, \quad N_{ij} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\chi_{sp} = \chi_{S_zS_z} = \sum_{ijkl} S^{(z)}_{ij}\chi_{ijkl}S^{(z)}_{kl}\,, \quad S^{(z)}_{ij} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Let $\chi_{iijj} = \chi_{ij}$ then

$$\chi_{ch} = \chi_{\uparrow\uparrow} + \chi_{\uparrow\downarrow} + \chi_{\downarrow\uparrow} + \chi_{\downarrow\downarrow}$$

$$\chi_{sp} = \chi_{\uparrow\uparrow} - \chi_{\uparrow\downarrow} - \chi_{\downarrow\uparrow} + \chi_{\downarrow\downarrow}$$

RPA bubble diagrams for $\chi_{\uparrow\uparrow}$ and $\chi_{\uparrow\downarrow}$

$$\chi^{(0)}_{\sigma\sigma} = \chi^{(0)}_{\sigma} = G_\sigma G_\sigma\,, \quad \chi^{(0)}_{\uparrow} = \chi^{(0)}_{\downarrow}\,, \quad \chi^{(0)} = \chi^{(0)}_{\uparrow} + \chi^{(0)}_{\downarrow}$$

$$\chi_{\uparrow\uparrow} \approx \chi^{(0)}_{\uparrow} + \chi^{(0)}_{\uparrow}(-U)\chi^{(0)}_{\downarrow}(-U)\chi^{(0)}_{\uparrow} + \\ + \chi^{(0)}_{\uparrow}(-U)\chi^{(0)}_{\downarrow}(-U)\chi^{(0)}_{\uparrow}(-U)\chi^{(0)}(-U)\chi^{(0)}_{\uparrow} + \ldots$$

$$\chi_{\uparrow\uparrow} \approx \frac{\chi^{(0)}}{2} + (-U)^2\left(\frac{\chi^{(0)}}{2}\right)^3 + (-U)^4\left(\frac{\chi^{(0)}}{2}\right)^5 + \ldots$$

$$\chi_{\uparrow\downarrow} \approx \chi^{(0)}_{\uparrow}(-U)\chi^{(0)}_{\downarrow} + \chi^{(0)}_{\uparrow}(-U)\chi^{(0)}_{\downarrow}(-U)\chi^{(0)}_{\uparrow}(-U)\chi^{(0)} + \\ + \chi^{(0)}_{\uparrow}(-U)\chi^{(0)}_{\downarrow}(-U)\chi^{(0)}_{\uparrow}(-U)\chi^{(0)}(-U)\chi^{(0)}_{\uparrow}(-U)\chi^{(0)} + \ldots$$

$$\chi_{\uparrow\downarrow} \approx (-U)\left(\frac{\chi^{(0)}}{2}\right)^2 + (-U)^3\left(\frac{\chi^{(0)}}{2}\right)^4 + (-U)^5\left(\frac{\chi^{(0)}}{2}\right)^6 + \ldots$$

RPA bubble diagrams for χ_{ch} and χ_{sp}

$$\chi_{ch} = \chi_{\uparrow\uparrow} + \chi_{\uparrow\downarrow} + \chi_{\downarrow\uparrow} + \chi_{\downarrow\downarrow} = 2\left(\chi_{\uparrow\uparrow} + \chi_{\uparrow\downarrow}\right) \approx \frac{\chi^{(0)}}{1 + \frac{U}{2}\chi^{(0)}}$$

$$\chi_{sp} = \chi_{\uparrow\uparrow} - \chi_{\uparrow\downarrow} - \chi_{\downarrow\uparrow} + \chi_{\downarrow\downarrow} = 2\left(\chi_{\uparrow\uparrow} - \chi_{\uparrow\downarrow}\right) \approx \frac{\chi^{(0)}}{1 - \frac{U}{2}\chi^{(0)}}$$

The bubble diagrams break the conservation laws

$$\frac{T}{N_q}\sum_{\mathbf{q},\omega_n} \chi_{ch}(\mathbf{q}, i\omega_n) = \langle(\hat{n}_\uparrow + \hat{n}_\downarrow)^2\rangle - \langle\hat{n}_\uparrow + \hat{n}_\downarrow\rangle^2$$

$$\frac{T}{N_q}\sum_{\mathbf{q},\omega_n} \chi_{sp}(\mathbf{q}, i\omega_n) = \langle(\hat{n}_\uparrow - \hat{n}_\downarrow)^2\rangle - \langle\hat{n}_\uparrow - \hat{n}_\downarrow\rangle^2$$

Two-particle self-consistent approach (TPSC)

The two-particle self-consistent (TPSC) approach uses

$$\chi_{ch} = \frac{\chi^{(0)}}{1 + \frac{U_{ch}}{2}\chi^{(0)}}, \quad \chi_{sp} = \frac{\chi^{(0)}}{1 - \frac{U_{sp}}{2}\chi^{(0)}}$$

with U_{ch} and U_{sp} determined using the conservation laws.

Gives an approximation valid for weak coupling that obeys

- the Pauli principle and
- the Mermin-Wagner theorem
  (on the absence of magnetism in 2D at finite temperature)

Treated in detail by the TRIQS/tutorials

- `https://github.com/TRIQS/tutorials/`

Square lattice in magnetic field

Local Hubbard interaction U

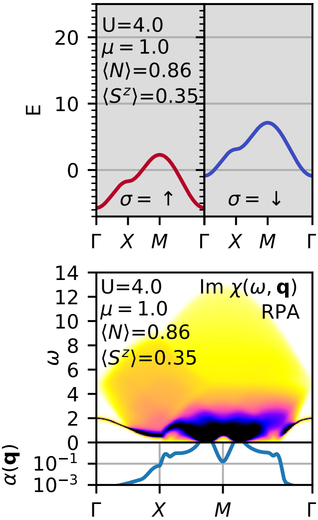
Magnetic field $B = 2$

First order

- Hartree + RPA

Non-perturbative

- DMFT + BSE



E van Loon, HURS, arXiv:2303.03468

Square lattice in magnetic field

Local Hubbard interaction U

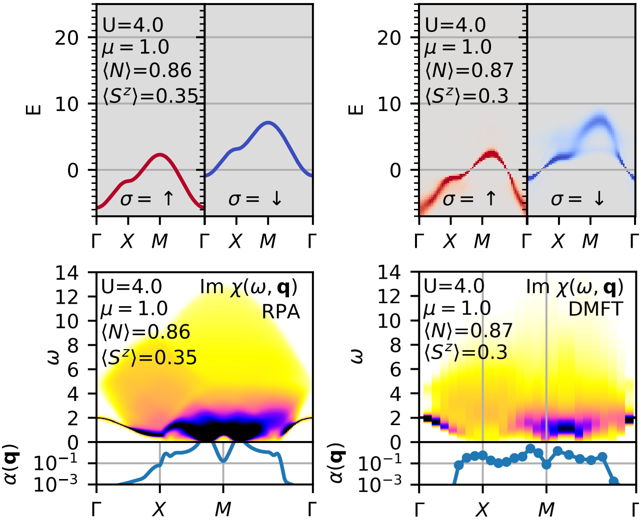
Magnetic field $B = 2$

First order

- Hartree + RPA

Non-perturbative

- DMFT + BSE



Bethe-Salpeter equation in DMFT

Bethe-Salpeter equation

$$\chi = \chi^{(0)} + \chi^{(0)} * \Gamma * \chi$$

Approximate

$$\Gamma(\mathbf{q}, \omega; \mathbf{k}, \nu, \mathbf{k}', \nu') \approx \Gamma_{imp}(\omega, \nu, \nu')$$

From the inverse of the DMFT impurity problem Bethe-Salpeter equation

$$[\Gamma_{imp}(\omega)]_{\nu\nu'} = [\chi_{imp}(\omega)]^{-1}_{\nu\nu'} - [\chi^{(0)}_{imp}(\omega)]^{-1}_{\nu\nu'}$$

Insert in the lattice Bethe-Salpeter equation

$$\chi(\mathbf{q}, \omega) = \chi_0 + \chi_0 * \Gamma_{imp} * \chi$$

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)

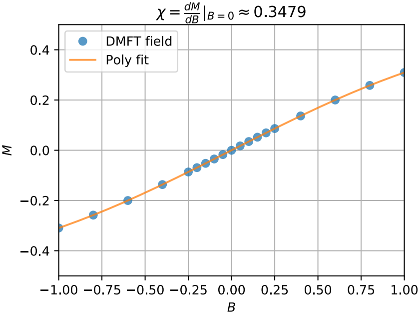
Consider the single-band Hubbard model on the square lattice with nearest neighbour hopping at half-filling with $t = 1$, $U = 10$, $\beta = 1$.

1. DMFT calculations in applied field

- Many self-consistent DMFT calculations
- Sweeping applied magnetic field B
- Measure 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

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

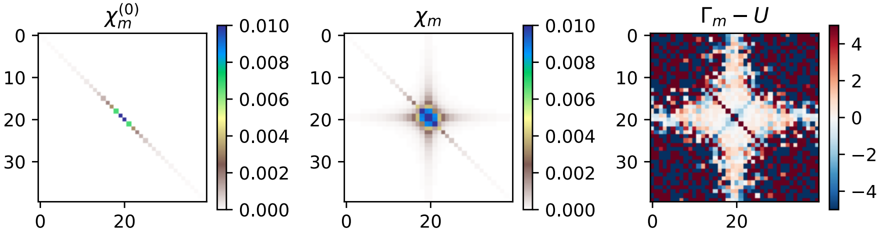
Tools for constructing χ and $\chi^{(0)}$ are available in **TRIQS/tprf**.

2. DMFT susceptibilities from the Bethe-Salpeter Equation

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

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

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



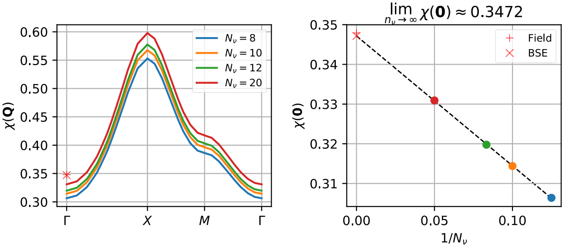
Example: Hubbard model on square lattice using **TRIQS/cthyb** and **TRIQS/tprf**.

2. DMFT susceptibilities from the Bethe-Salpeter Equation

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

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

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 @ $\mathbf{Q} = \mathbf{0}$

  $\chi_{\mathrm{BSE}}(\mathbf{0}) \approx 0.3472$

  $\chi_{\mathrm{Field}}(\mathbf{0}) \approx 0.3479$

- Quantitative agreement
- Thermodynamic consistency

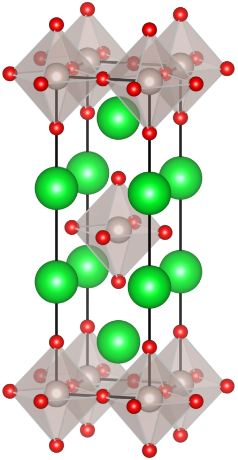
Hafermann et al. PRB 90 235105 (2014)

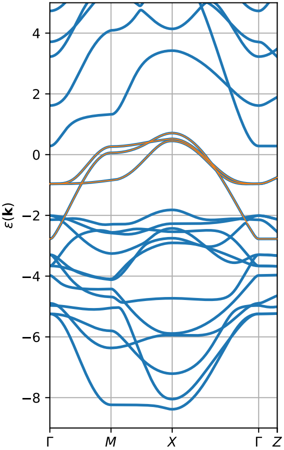
Real materials application example

DFT+DMFT+BSE

Sr_2RuO_4 atomic & electronic structure

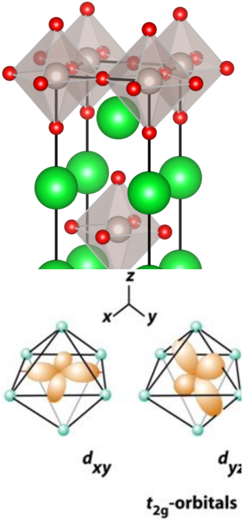
- Planar perovskite (La_2CuO_4 type)
- BC-tetragonal sg-139, I4/mmm
- Three bands with Ru(4d)-t_{2g} symmetry and 4 electrons
- xy (quasi-2D)
- xz, yz (quasi-1D)
- Strong correlations ARPES & dHvA

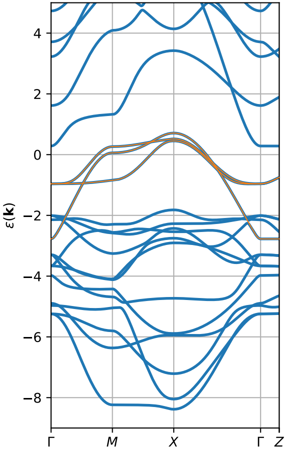




Sr_2RuO_4 atomic & electronic structure

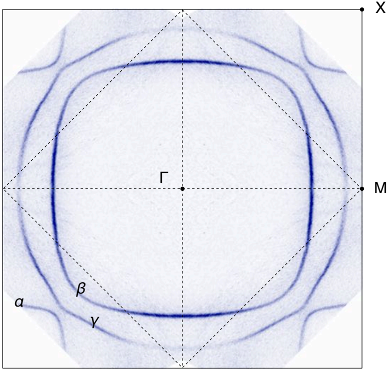
- Planar perovskite (La_2CuO_4 type)
- BC-tetragonal sg-139, I4/mmm
- Three bands with Ru(4d)-t_{2g} symmetry and 4 electrons
- xy (quasi-2D)
- xz, yz (quasi-1D)
- Strong correlations ARPES & dHvA





Fermi Surfaces

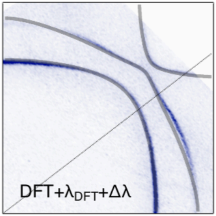
- α & β sheets, mixtures of xz and yz
- γ sheet, dominantly xy



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

Fermi Surfaces

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

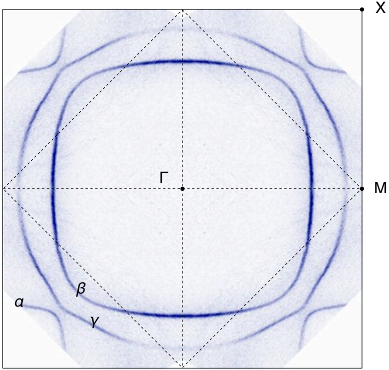


- Correlation effects from DMFT

  Mravlje, et al. PRL 106, 096401 (2011)

  Zhang, et al. PRL 116, 106402 (2016)

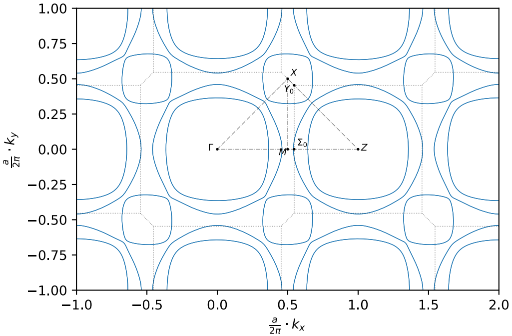
  Kim, et al. PRL 120, 126401 (2018)

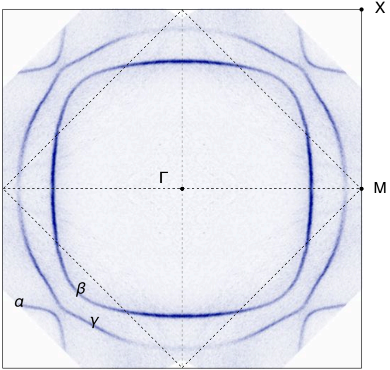


Tamai, et al., PRX 9 021048 (2019)

Fermi Surfaces

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

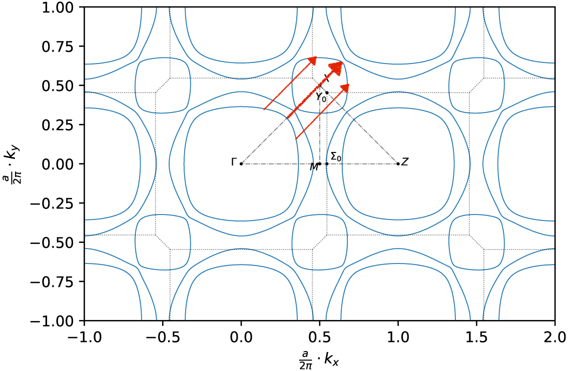


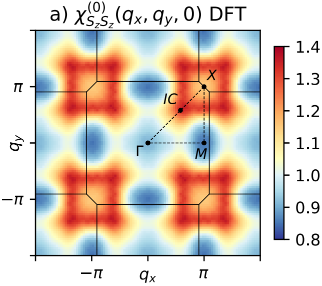


Tamai, et al., PRX 9 021048 (2019)

Quizz: Find the "nesting vector"

Fermi Surface Nesting



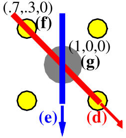


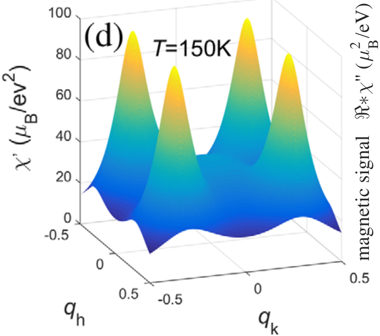
- Nesting vector (red)
- Bare susceptibility
$\chi^{(0)} = G_0 * G_0$

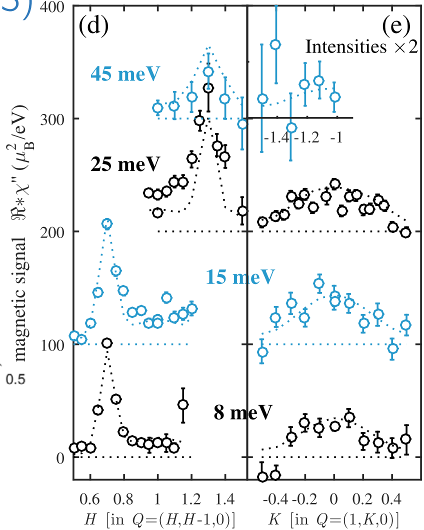
Mazin & Singh

PRL 82 4324 (1999)

Inelastic Neutron Scattering (INS)

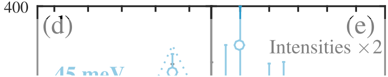


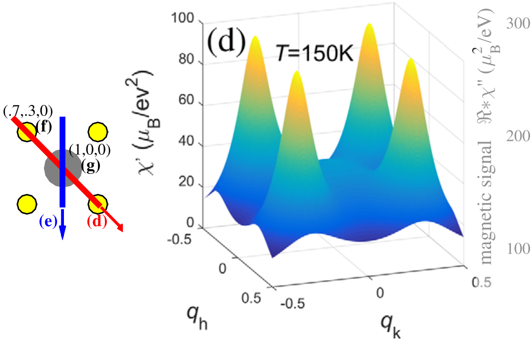


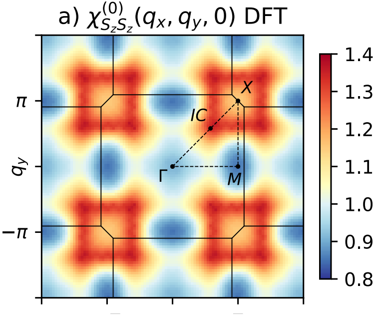


P. Steffens, et al., PRL 122, 047004, (2019)

Inelastic Neutron Scattering (INS)







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

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

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

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

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

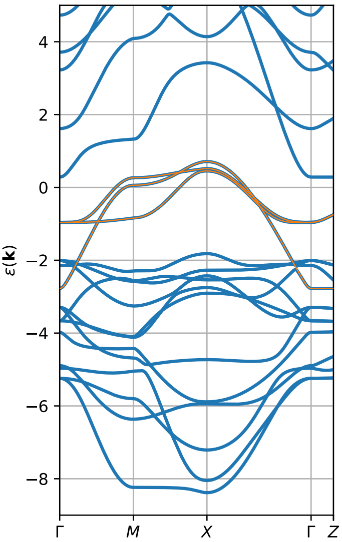
Idea:

Compute the DMFT magnetic susceptibility and find out!

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

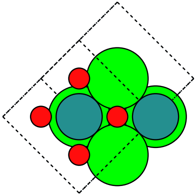
- Applied field in super-cells
  1×1, $\sqrt{2} \times \sqrt{2}$, $\sqrt{2} \times \sqrt{5}$
- Dynamical vertex corrections
  $\Gamma_{abcd}(i\omega, i\nu, i\nu')$
- Lattice susceptibility
  $\chi_{abcd}(\mathbf{Q})$ from BSE



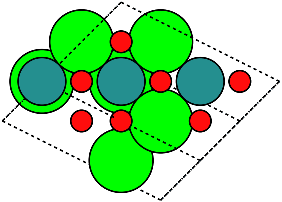
HURS, Zingl, Wentzell, Parcollet, Georges PRB 100, 125120 (2019)

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



- 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

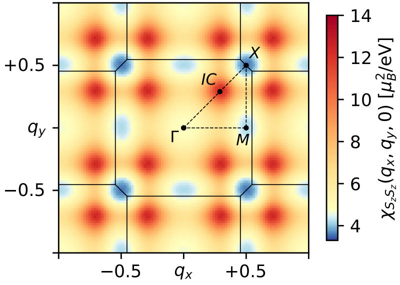


HURS, Zingl, Wentzell, Parcollet, Georges PRB 100, 125120 (2019)

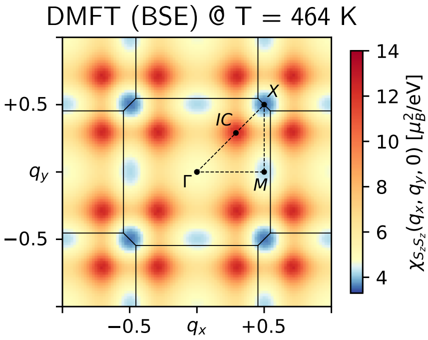
Application to magnetic susceptibility of Sr_2RuO_4

- DFT + Wannierization
- Three band effective t_{2g} model
- Kanamori interaction
  U=2.3eV, J=0.4eV
- Dynamical Mean-Field Theory

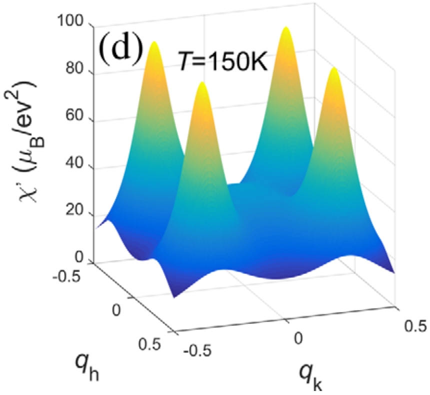
- Applied field in super-cells
  1×1, $\sqrt{2} \times \sqrt{2}$, $\sqrt{2} \times \sqrt{5}$
- Dynamical vertex corrections
  $\Gamma_{abcd}(i\omega, i\nu, i\nu')$
- Lattice susceptibility
  $\chi_{abcd}(\mathbf{Q})$ from BSE



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



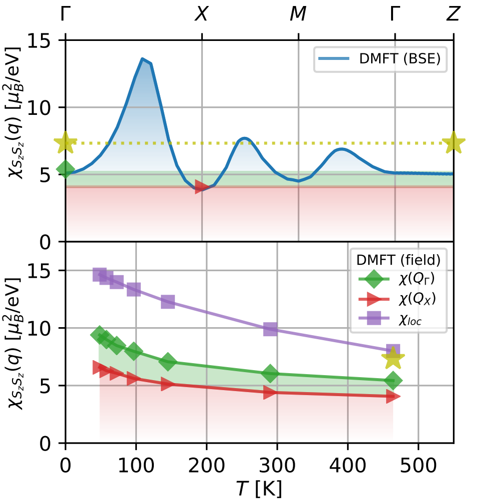
- Qualitative agreement Γ vs X!



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

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

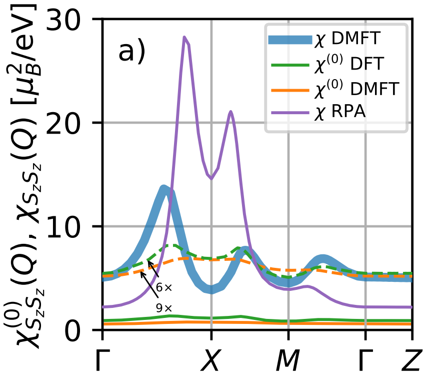
- Incommensurate (IC) & ridge response
- **Quasi Local/Ferromagnetic** Background response (red) >50% of $\mathbf{Q}$-average (stars)
- $\chi(\mathbf{Q}_\Gamma) > \chi(\mathbf{Q}_X)$ (green)
- Lower temperature (T↓)
  - Background ↑
  - Local response ↑
  - $\chi(\mathbf{Q}_\Gamma)/\chi(\mathbf{Q}_X)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



HURS, Zingl, Wentzell, Parcollet, Georges PRB 100, 125120 (2019)

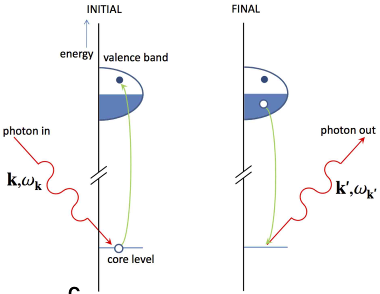
Comparison to simpler approximations

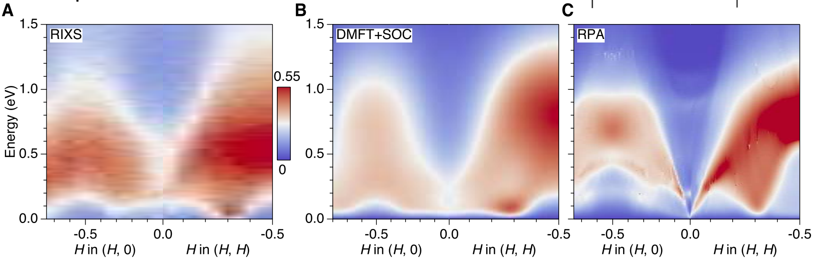
- DMFT lattice susceptibility: χ DMFT
- Bare DFT bubble: $\chi^{(0)}$ DFT (Density Functional Theory)
- Bare DMFT bubble: $\chi^{(0)}$ DMFT
- Random Phase Approximation: χ RPA
- Only χ DMFT reproduces expermient $\chi(\mathbf{Q}_\Gamma) > \chi(\mathbf{Q}_X)$
- **DMFT dynamical vertex** $\Gamma(\omega, \nu, \nu')$ effects are essential!



Sr_2RuO_4 Resonant Inelastic X-ray Scattering (RIXS)

- Direct RIXS
- Photon in photon out
- Core level $\leftrightarrow$ valence band
- Excitation and relaxation
- Instantaneous approximation
- Hund's metal spin & orbital separation





Sr_2RuO_4 Dual BSE formulation

Compute χ using χ_{imp} plus correction

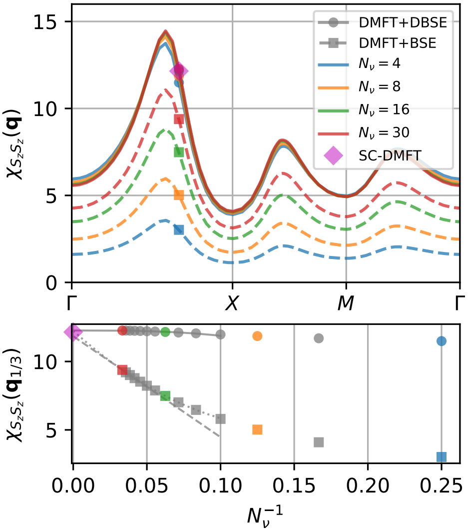
$$\chi = \chi_{imp} + L \frac{\tilde{\chi}_0}{1 - \tilde{\chi}_0 F} L$$

with χ_{imp}, F and L from independent measurements.

Improved convergence

- BSE $\mathcal{O}(1/N_\nu)$
- DBSE $\mathcal{O}(1/N_\nu^3)$

Tutorial and tools available @ `https://triqs.github.io/tprf/unstable/`



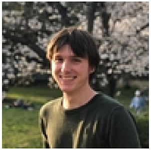
E van Loon, HURS, arXiv:2306.05157

Two-Particle Response Function (TPRF) Collaborators

Nils Wentzell

Alexander Hampel

Stefan Käser



Yann in 't Veld

Olivier Parcollet

Erik van Loon

Philipp Hansmann

Malte Rösner

The End