Two-particle response using parquet equations

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Outline

Introduction

- One-particle *vs* two-particle excitations
- Two-particle response functions
- Vertex corrections – when important?
- Vertex corrections – how to calculate?

Parquet equations

- Why parquet equations?
- Two-particle reducibility and parquet decomposition
- Optical excitations in systems with strong AFM/CDW fluctuations: π-tons

Challenges

- Vertex corrections in real materials?

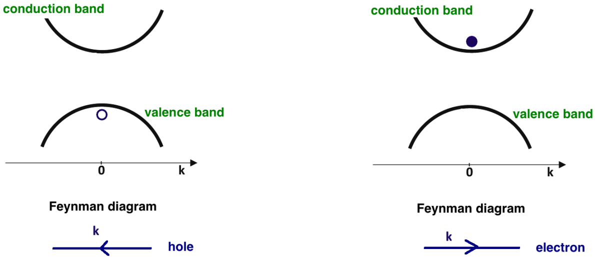
Solutions

- Tiling with triangles (SBE diagrams) and sparse modeling

Summary and outlook

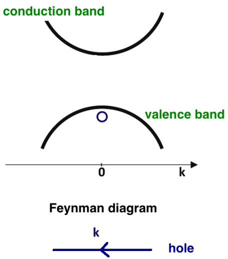
One-particle *vs* two-particle excitations

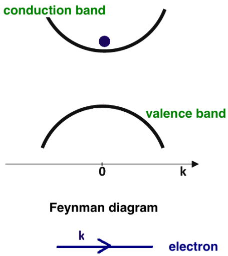
One-particle excitations – (inverse) photoemision



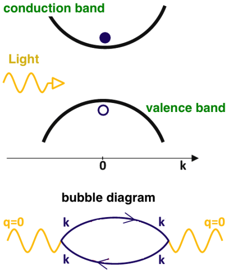
One-particle *vs* two-particle excitations

One-particle excitations – (inverse) photoemission





Two-particle excitations – optical conductivity



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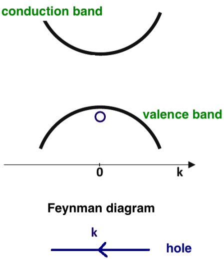

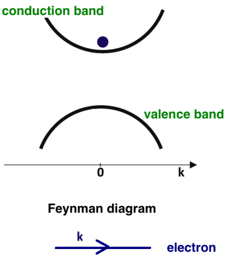

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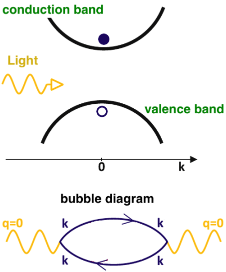
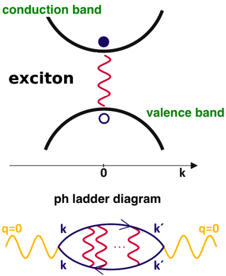
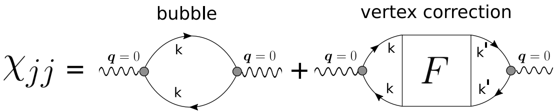


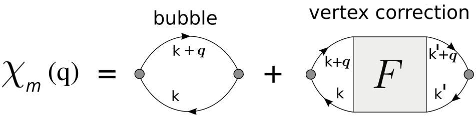


Two-particle response functions

- Optical conductivity $\sigma(\omega) = \frac{\mathrm{Im}\chi_{\boldsymbol{jj}}(\omega)}{\omega}$

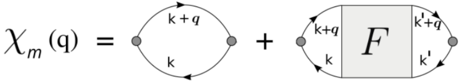


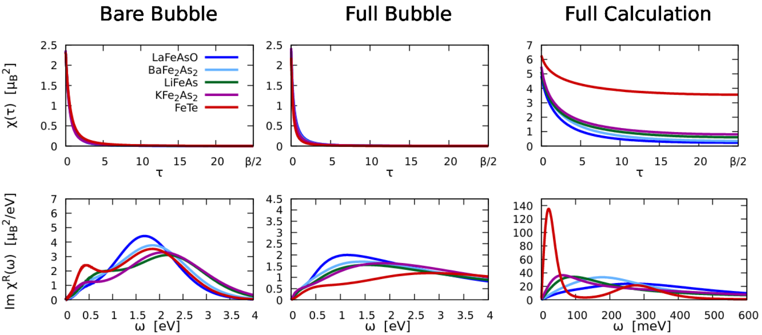
- Magnetic susceptibility $\chi_{\boldsymbol{m}} = \frac{\partial M}{\partial H}$



When they are big

- Spin susceptibility of the 3d-Fe atoms and corresponding absorption spectra at $T \approx 232K$ (method: DFT + DMFT)

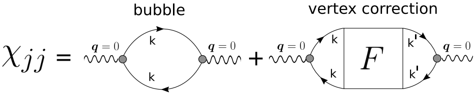


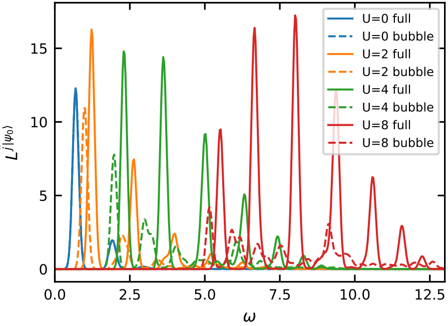


C. Watzenböck et al, Phys. Rev. Lett. 125, 086402 (2020)

When they are big

- Optical conductivity for 8-site chains for different values of the local Coulomb interaction U (method: exact diagonalization)



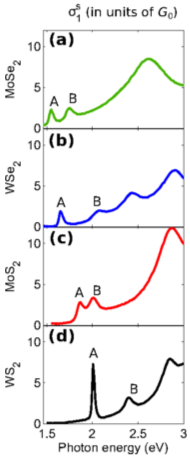


C. Watzenböck, AK, et al, Phys. Rev. B 106, 085135 (2022)

When are vertex corrections important?

When they lead to new, qualitatively distinct, features

Excitons in TM dichalcogenites



Li et al., PRB 90, 205422 (2014)

Theory: *Ridolfi et al., PRB 97, 205409 (2018)*

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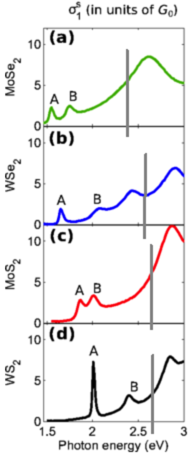

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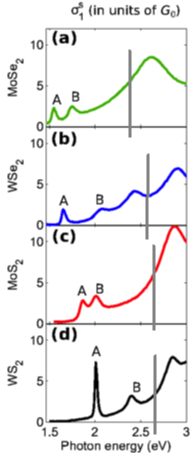

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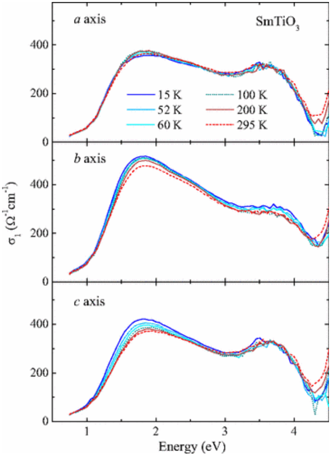
Gap reduction in $SmTiO_3$



One-particle (ARPES) gap $\sim 1.8 - 2.5eV$
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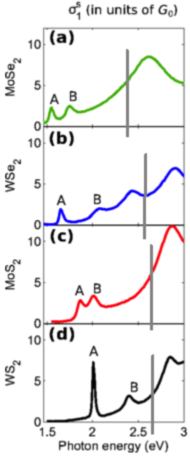

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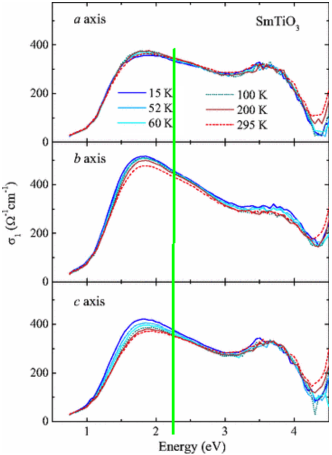

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How can we compute vertex corrections to response functions?

With numerically exact methods

- Exact diagonalization (small clusters)
- DMRG, Matrix Product States (1D or quasi-1D systems)
- Quantum Monte Carlo (small clusters or Anderson impurity model)

With diagrammatic methods

- RPA

$$\chi_m(q) = \chi_0(q) + \chi_0(q) U \chi_0(q) + \chi_0(q) U \chi_0(q) U \chi_0(q) + \ldots = \frac{\chi_0(q)}{1 - U\chi_0(q)}$$

- GW + BSE, FLEX, TPSC, ...

With embedded impurity methods

- Impurity with a dynamical self-consistent bath represents the entire lattice system (DFT + DMFT)
- Impurity problem is solved with exact methods
- Impurity vertices are used in lattice response functions

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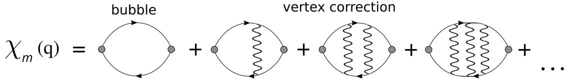

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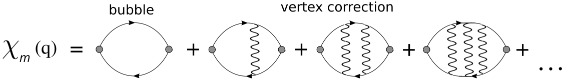

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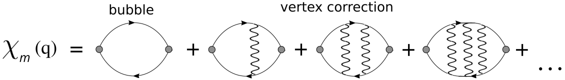

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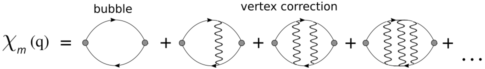

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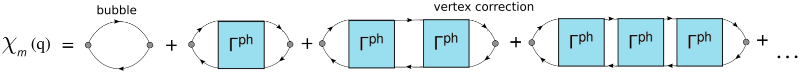
- Impurity vertices are used in lattice response functions: 2P response in DMFT

$$\chi_m(q) = \frac{\chi_0(q)}{1 - \Gamma_{imp}\chi_0(q)}$$

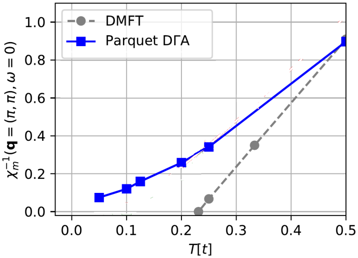


Problems with $\Gamma^{ph} = \Gamma_{imp}$ (no momentum dependence in the vertex)

- Impurity vertices are used in lattice response functions

$$\chi_m(q) = \frac{\chi_0(q)}{1 - \Gamma_{imp}\chi_0(q)}$$

- Violation of Mermin-Wagner theorem for 2D lattice – divergence of AFM susceptibility $\chi_m(q = (\pi, \pi))$ for $T_c > 0$



- Can be cured by using parquet diagrams instead of only ladders – parquet DΓA
  C. Eckhardt et al. Phys. Rev. B 101, 155104 (2020)

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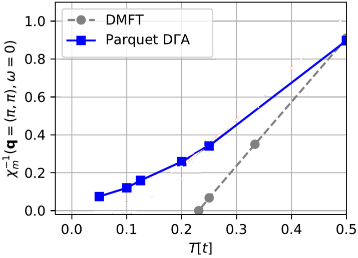

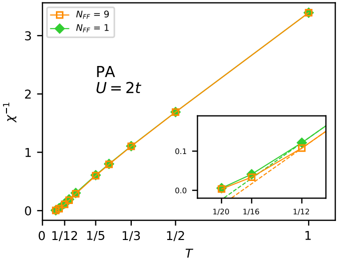

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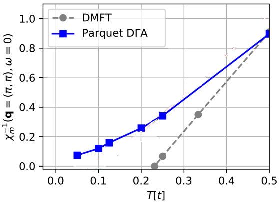
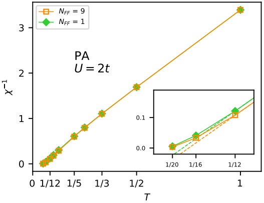


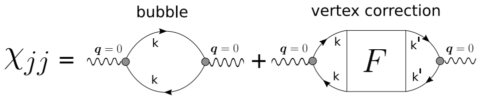


- Can be cured by using parquet diagrams instead of only ladders – parquet DΓA
  C. Eckhardt et al. Phys. Rev. B 101, 155104 (2020)
- By using additionally a sum rule – λ-corrected ladder DΓA
  A. A. Katanin, A. Toschi, and K. Held Phys. Rev. B 80, 075104 (2009)
- By using $\chi_0(q)$ from a ladder DΓA calcualtion (and not DMFT) –
  self-consistent ladder DΓA
  J. Kaufmann et al. Phys. Rev. B 103, 035120 (2021)

Problems with $\Gamma^{ph} = \Gamma_{imp}$ (no momentum dependence in the vertex)

- Impurity vertices are used in lattice response functions

Vertex corrections to optical conductivity



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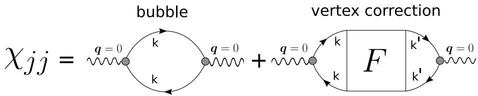

- Vanish for impurity vertex or for a *ph*-ladder constructed from impurity vertex (except for inter-orbital contributions)
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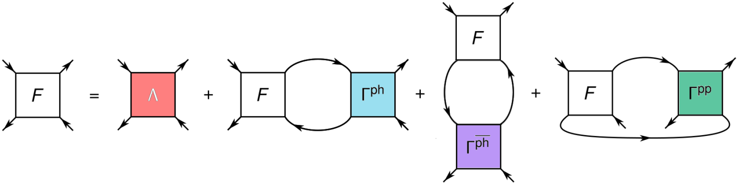
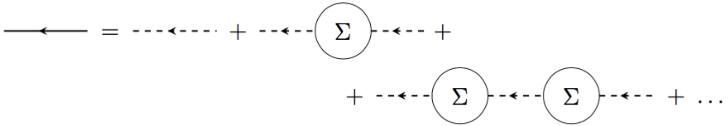
- We use the parquet equation for F with $\Lambda = \Lambda_{imp}$ from DMFT

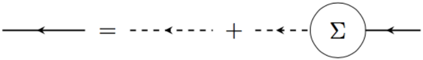


The concept of irreducibility

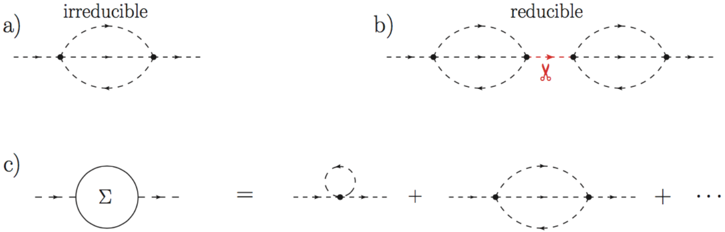
Self-energy Σ is one-particle irreducible



Dyson equation:



One particle irreducibility – cutting one line



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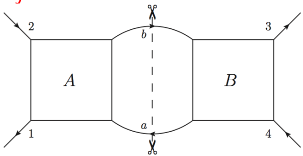
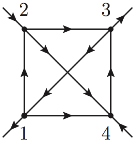
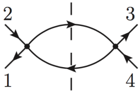


Low order diagrams

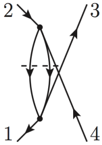
a) fully irreducible



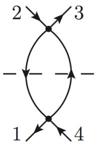
b) particle-hole (*ph*) reducible



c) particle-particle (*pp*) reducible



d) particle-hole vertical ($\overline{ph}$) reducible

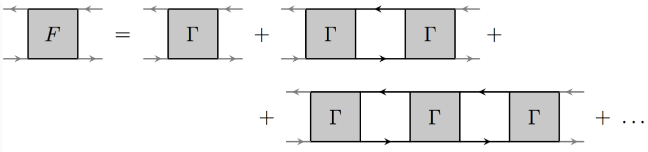


Ladder diagrams and the Bethe-Salpeter equation

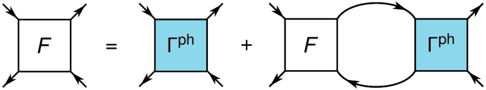
$\color{red}{\Gamma_r}$ – irreducible vertex in a given channel $r = \{ph, \overline{ph}, pp\}$

$$\underbrace{F}_{\text{full vertex}} = \color{red}{\Gamma_r} \color{black}{+} \underbrace{\Phi_r}_{\text{reducible vertex}}$$

Ladder diagrams in a given channel $r = \{ph, \overline{ph}, pp\}$ (here ph is shown)



Bethe-Salpeter equation:



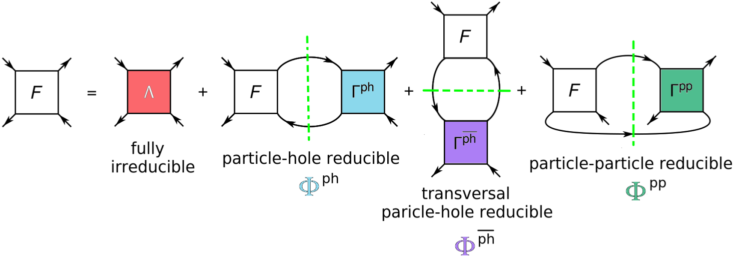
$$F = \color{red}{\Gamma_r} \color{black}{+} \color{red}{\Gamma_r}\color{black}{(GG)_r F}$$

– the reducible vertex is then

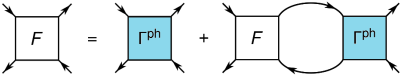
$$\Longrightarrow \Phi_r = \color{red}{\Gamma_r}\color{black}{(GG)_r F}$$

Parquet equations

F is given by contributions from irreducible vertices Λ_{imp}, Γ^{ph}, $\Gamma^{\overline{ph}}$, Γ^{pp} (parquet equation)



Bethe-Salpeter equation (BSE)



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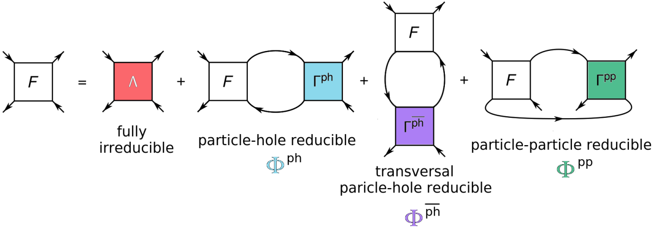

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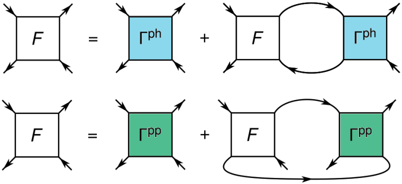

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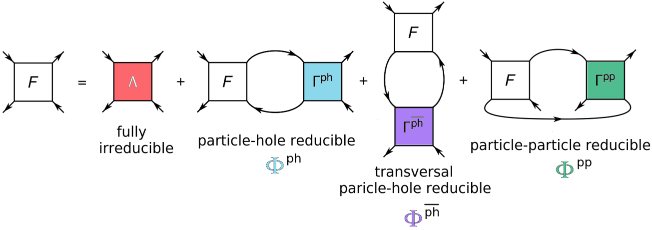
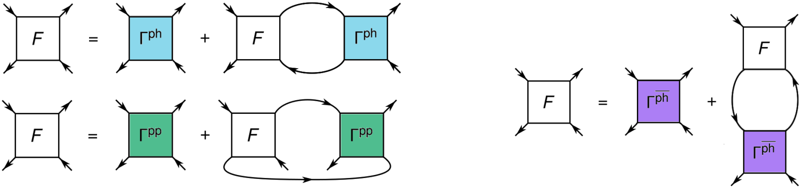
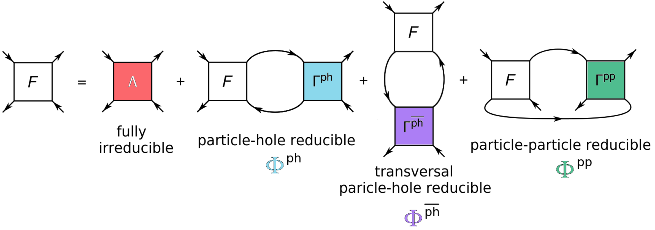


Bethe-Salpeter equations (BSE)



Full set of parquet equations

F is given by contributions from irreducible vertices Λ_{imp}, Γ^{ph}, $\Gamma^{\overline{ph}}$, Γ^{pp} (parquet equation)



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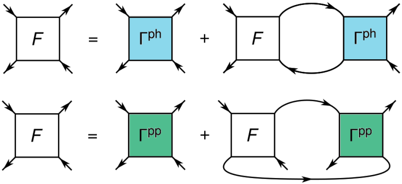
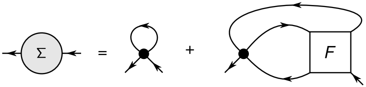


Schwinger-Dyson equation (SDE)



+ Dyson equation

C. DeDominicis, P.C. Martin, J.Math.Phys. 5, 31 (1964), N. Bickers, Int.J.Mod.Phys.B 05, 253 (1991)

Full set of parquet equations:

- Parquet equation

$$F = \Lambda + \Phi_{ph} + \Phi_{\overline{ph}} + \Phi_{pp}$$

- Bethe-Salpeter equation

$$\Phi_r = \Gamma_r (GG)_r F$$

- Schwinger-Dyson equation

$$\Sigma = \Sigma_{HF} + U\ GGG\ F$$

and Dyson equation $G = [G_0^{-1} - \Sigma]^{-1}$

Input:

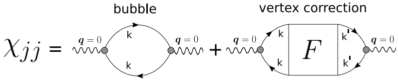
- Fully irreducible vertex $\mathbf{\Lambda}$, (e.g. from DMFT)
- Non-interacting Green's function G_0 (from a model Hamiltonian or DFT)

C. De Dominicis, P. C. Martin, J. Math. Phys. 5, 31 (1964)
N. Bickers, Int. J. Mod. Phys. B 05, 253–270 (1991)
K.-M. Tam et al. Phys. Rev. B 87, 013311 (2013)

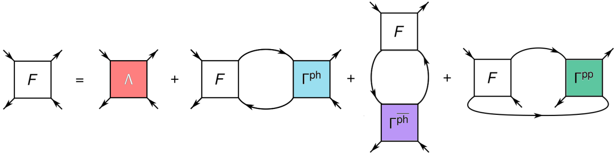
G. Li, AK, P. Pudleiner, K. Held, Comp. Phys. Comm. 241, 146–154 (2019)
C. Eckhardt, C. Honerkamp, K. Held, and AK, PRB 101, 155104 (2020)
F. Krien, AK, and K. Held, PRR 3, 013149 (2021)
F. Krien, AK, EPJB 95, 69 (2022)

Contributions to optical conductivity

- Optical conductivity: $\sigma(\omega) = \frac{\mathrm{Im}\chi_{\boldsymbol{jj}}(\omega)}{\omega}$

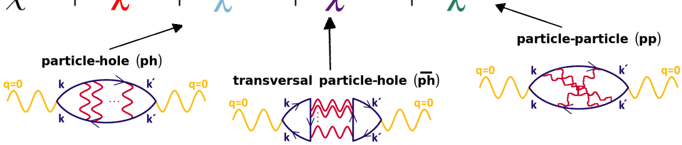


- Parquet equation



- Parquet decomposition of χ_{jj}

$$\chi_{jj} = \chi^0 + \chi^{\Lambda} + \chi^{ph} + \chi^{\overline{ph}} + \chi^{pp}$$



Contributions to optical conductivity

- Parquet decomposition of χ_{jj}

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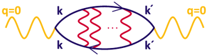
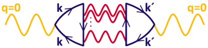
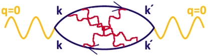
particle-hole (ph)

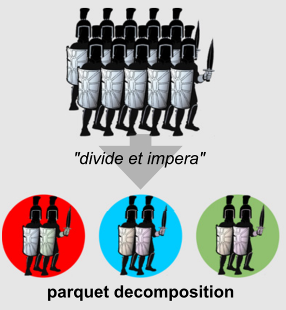


transversal particle-hole ($\overline{ph}$)



particle-particle (pp)

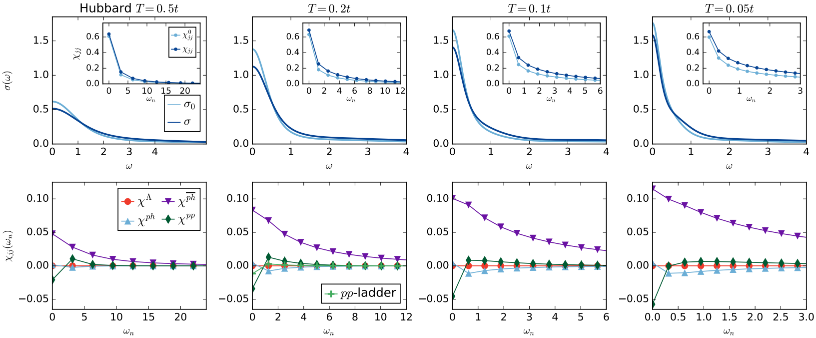




"Divide et impera", T. Schäfer, A.Toschi, J.Phys.: Cond..Mat. 33, 214001 (2021)

Vertex corrections to optical conductivity

- Hubbard model, square lattice, half-filling, $\sigma(\omega)$ for different T from parquet DΓA



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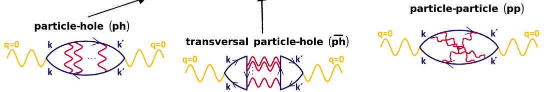

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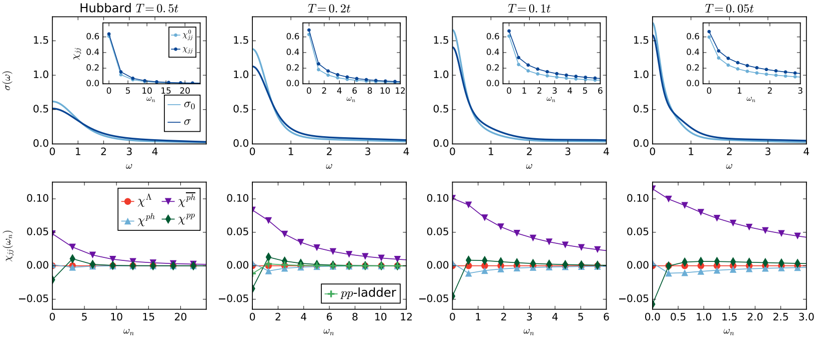


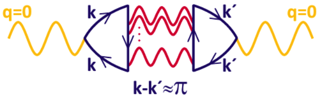
- What can we learn from parquet equations? Vertex corrections are dominated by conttibutions from transversal particle-hole diagrams at momentum (π, π)

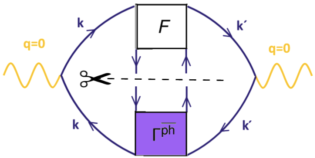
AK et al., PRL 124, 047401 (2020)

Optical excitations in systems with strong AFM/CDW fluctuations

Interpretation:

- Light at q $= 0$ couples to magnetic or density fluctuations at q $= (\pi, \pi)$





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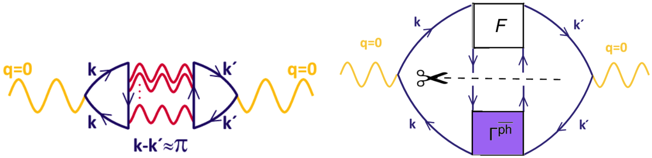
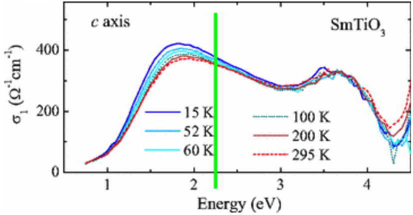


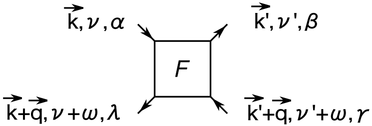
SmTiO$_3$???



Gössling et al., PRB 78, 075122 (2008)

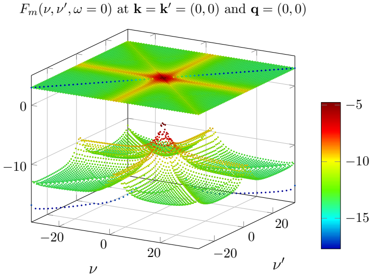
Two-particle response for materials

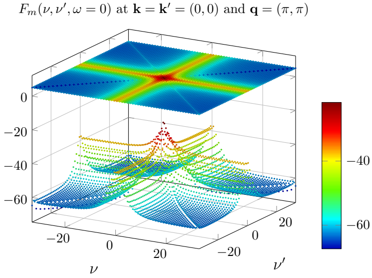
- Challenge : Memory! – scattering vertices of two particles depend on 4 spin-orbital indices, 3 momenta and 3 energies (frequencies)



- For one orbital, 80 frequencies and 56×56 momentum slices a single vertex needs 240 Petabytes!

Full vertex F_m in the 2D Hubbard model on square lattice





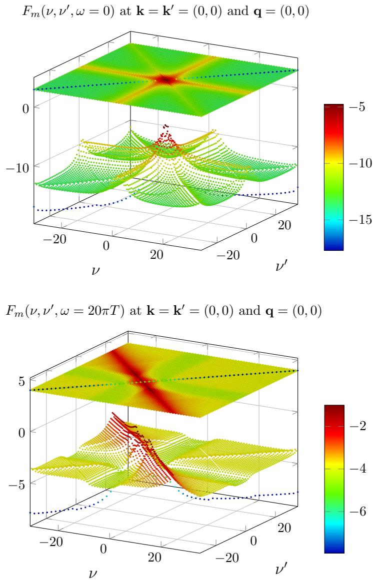
- Each vertex is a function of 3 frequencies and 3 momenta
- There are also 4 spin indices. We use here so-called spin diagonal notation, i.e.

$$F_m = F_{\uparrow\uparrow\uparrow\uparrow} - F_{\uparrow\uparrow\downarrow\downarrow}$$

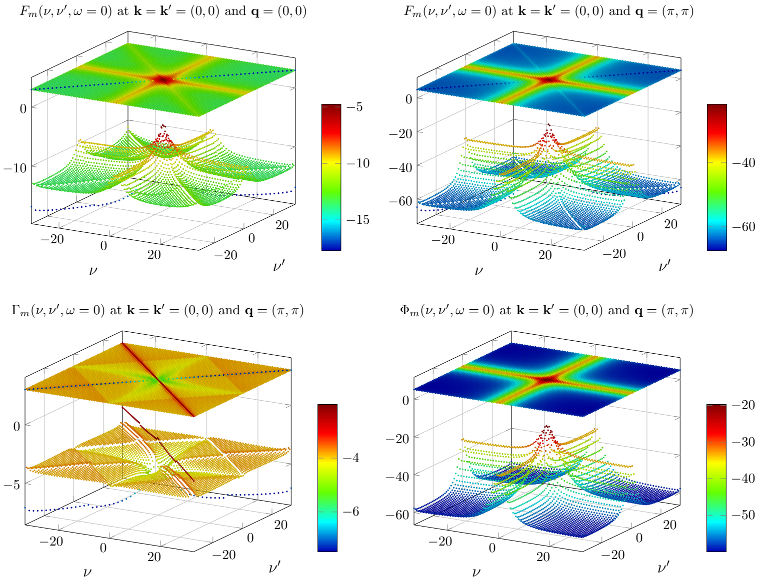
- The parameters are $U = 4t$, $T = 0.1t$, $n = 1$
- Approximation for the fully irreducible vertex is $\Lambda = U$, i.e. parquet approx.
- The results were obtained with *victory* code for 6×6 momenta

G. Li, AK, P. Pudleiner, K. Held, Comp. Phys. Comm. 241, 146–154 (2019)

Full vertex F_m in the 2D Hubbard model on square lattice



Vertices in the 2D Hubbard model on square lattice



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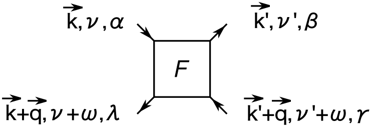


- For one orbital, 80 frequencies and 56 × 56 momentum slices a single vertex needs 240 Petabytes!

SOLUTIONS:

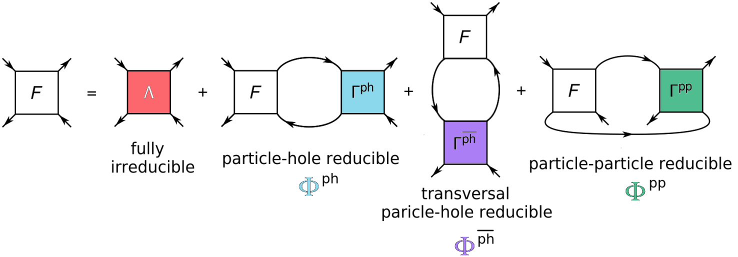
- Momentum dependence reduced to only a few functions: form factors
  C. Eckhardt, C. Honerkamp, K. Held, and AK, PRB 101, 155104 (2020),
  T. Schäfer et al, PRX 11, 011058 (2021)

- Smart reformulation with smaller frequency range (single-boson exchange)
  F. Krien, AK, and K. Held, PRR 3, 013149 (2021),
  F. Krien, AK, EPJB 95, 69 (2022)

- Dimensionality reduction by using IR and QTTs (work in progress)
  M. Wallerberger et al, PRR 3, 033168 (2021),
  H. Shinaoka et al, PRX 13, 021015 (2023)

Parquet equations

Parquet equation



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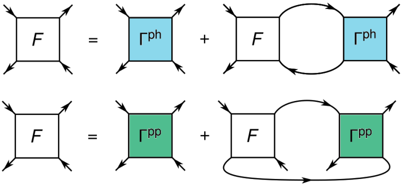
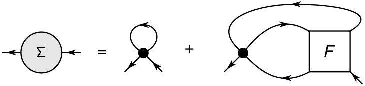


Schwinger-Dyson equation (SDE)



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Parquet equations

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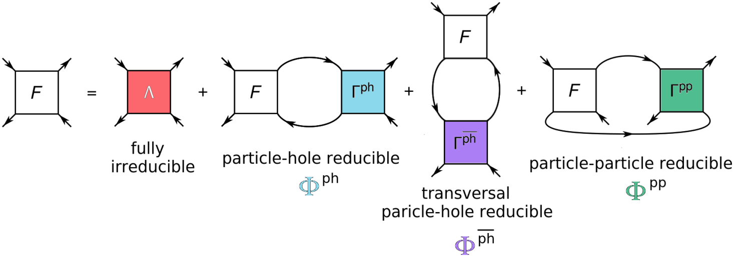
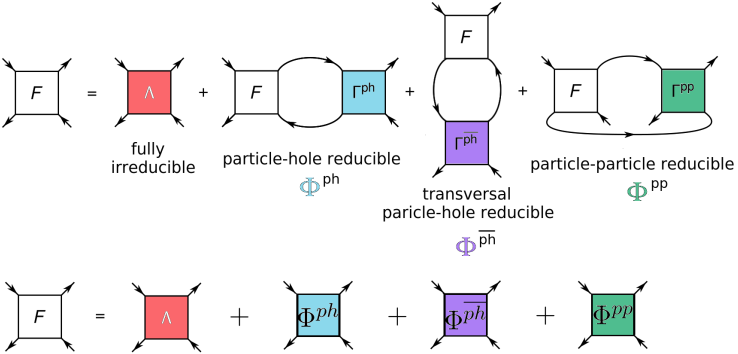
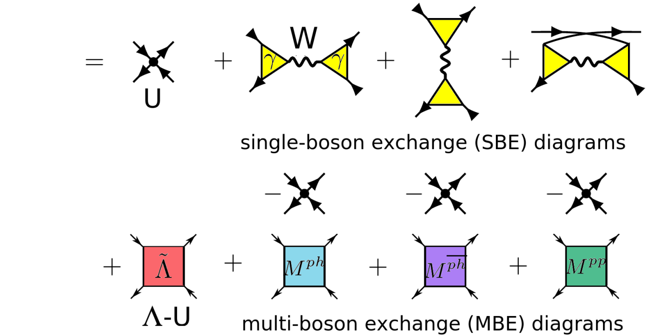


Parquet equation



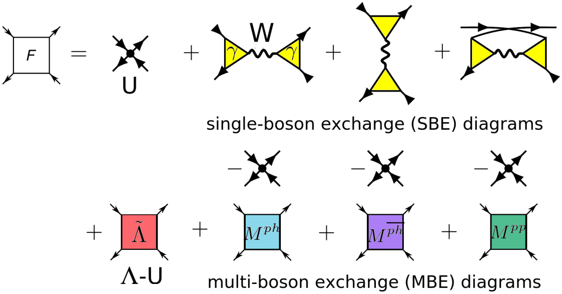
Tiling with triangles

Parquet equation



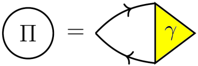
F. Krien, AK , K. Held, Phys. Rev. Res. 3, 013149 (2021),
F. Krien, AK, EPJ B 95, 69 (2022)

Parquet equation

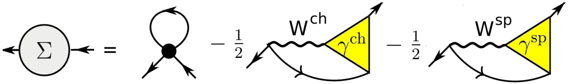


- Effective interaction W is given by polarisation $\Pi = GG\gamma$

$$W = \frac{U}{1 - U\Pi} \qquad \text{and}$$



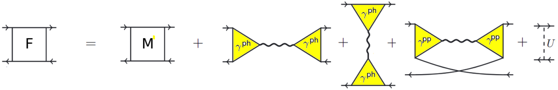
- Schwinger-Dyson equation modifies to: $\Sigma = \Sigma_{HF} + GW\gamma$



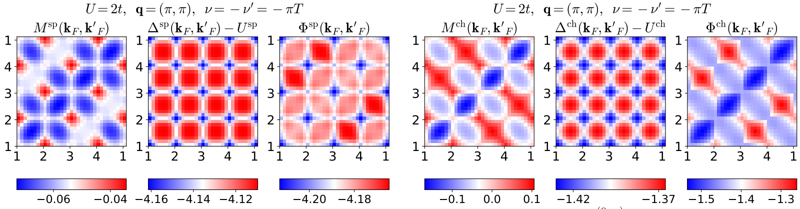
Tiling with triangles – unifies parquet equations with $GW\gamma$

Advantages of triangles reformulation

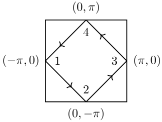
- Clear connection to $GW\gamma$ method
- Physical interpretation in terms of boson-exchange diagrams: SBE vs MBE



- MBE diagrams (M's) require much smaller frequency boxes, which allows for better momentum resolution (currently 16×16, *F. Krien, AK, EPJ B 95, 69 (2022)*)

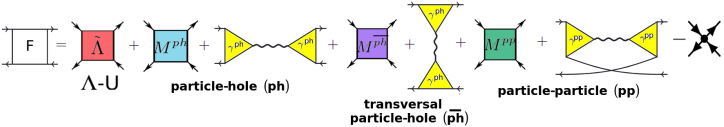


Δ is here the SBE contribution
and the momenta are along the Fermi surface:



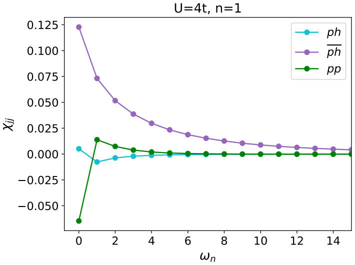
Boson-exchange decomposition of optical conductivity

- M's are the multi-boson contributions (MBE), $\gamma W \gamma$'s are the single-boson contributions (SBE) in each channel (ph, $\overline{ph}$, pp)

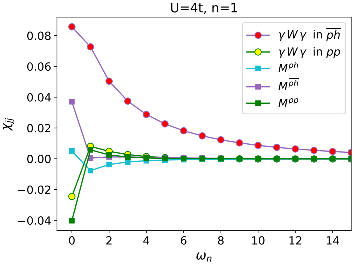


$$\chi_{jj} = \chi^0 + \chi^{\Lambda} + \chi^{ph} + \chi^{\overline{ph}} + \chi^{pp}$$

Parquet decomposition



Boson-exchange decomposition



Summary and outlook

Vertex corrections

- Two-particle response often requires taking into account vertex corrections
- DFT + DMFT or ladder DΓA are very successful in computing two-particle response for materials
- For optical conductivity parquet equations are important

We found with parquet equations

- Important vertex corrections: π-tons
- π-ton contributions to optical conductivity should be universally present in materials with strong π-fluctuations (AFM, CDW)
- Still open question: Can simpler methods describe π-ton vertex corrections?

Outlook: New advances in the parquet method

- Dimensionality reduction by using sparse modeling and/or tensor decomposition