"Fluctuation diagnostics" of many-electron systems:

How to read between the lines of one-particle spectra

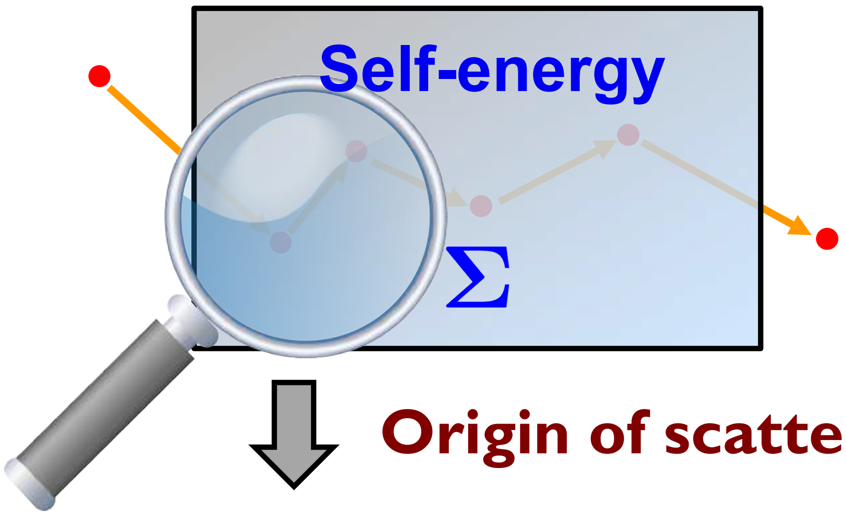
Alessandro Toschi

Workshop - "DMFT and beyond: recent developements",
Paris, 11 June 2019

Collaborators: O. Gunnarsson (Stuttgart), T. Schäfer (Paris/NYC),
G. Rohringer (Moscow), J. Le Blanc (Newfoundland), E. Gull (Ann Arbor/NYC),
J. Merino (Madrid), G. Sangiovanni (Würzburg)

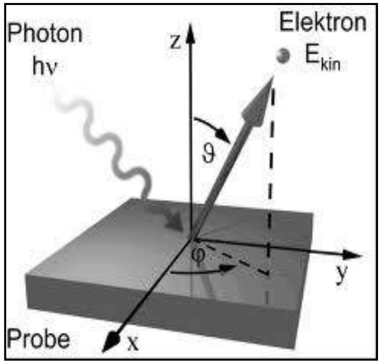
Correlations @ One- and Two-particle level

1P level

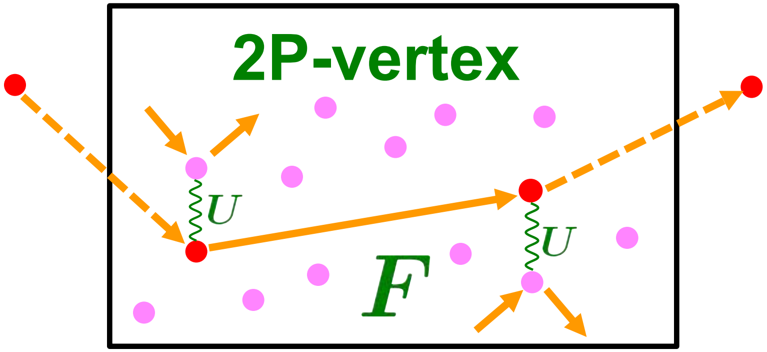


Origin of scattering?

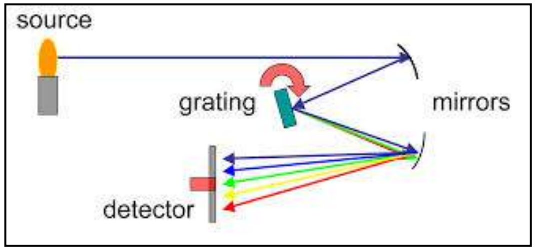
Experiment: (AR)PES, InvPES, STM, …



2P level



Experiment: IR, INS, NMR, …



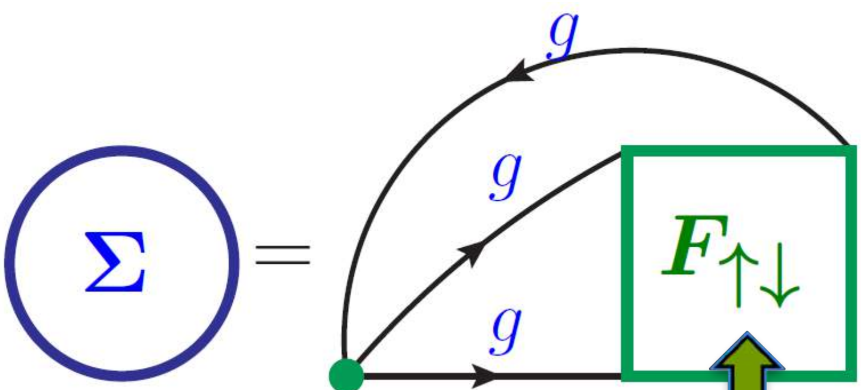
Theory: prerequisites

✦ Computing (on equal footing) **both Σ and F**

[DMFT/DCA, parquet schemes (PA,DΓA,QUADRILEX), DiagMC, DQMC, fRG, …]

How to analyse Σ ?

Our starting point:



1) parquet decomposition

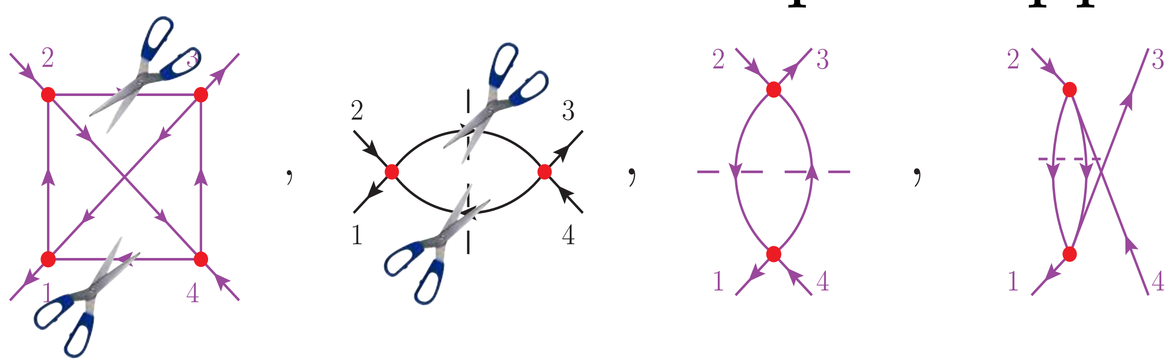
in terms of

2P-irreducible/reducible diagrams

O. Gunnarsson ..., & AT, PRB (2016)

$\Sigma(k)$ =

$$\Lambda_{2PI} + \Phi_{ch} + \Phi_{sp} + \Phi_{pp}$$



How to analyse Σ ?

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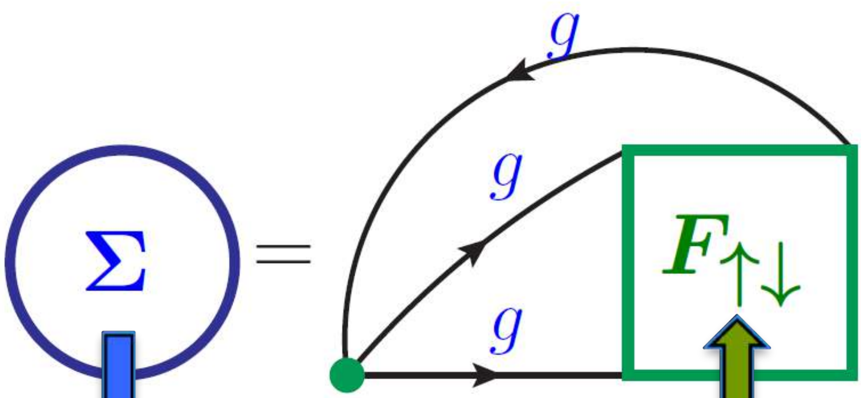


$$\boxed{\Lambda_{2PI} + \Phi_{ch} + \Phi_{sp} + \Phi_{pp}}$$

$$\boxed{\Sigma_{\Lambda} + \Sigma_{ch} + \Sigma_{sp} + \Sigma_{pp}}$$

1) parquet decomposition

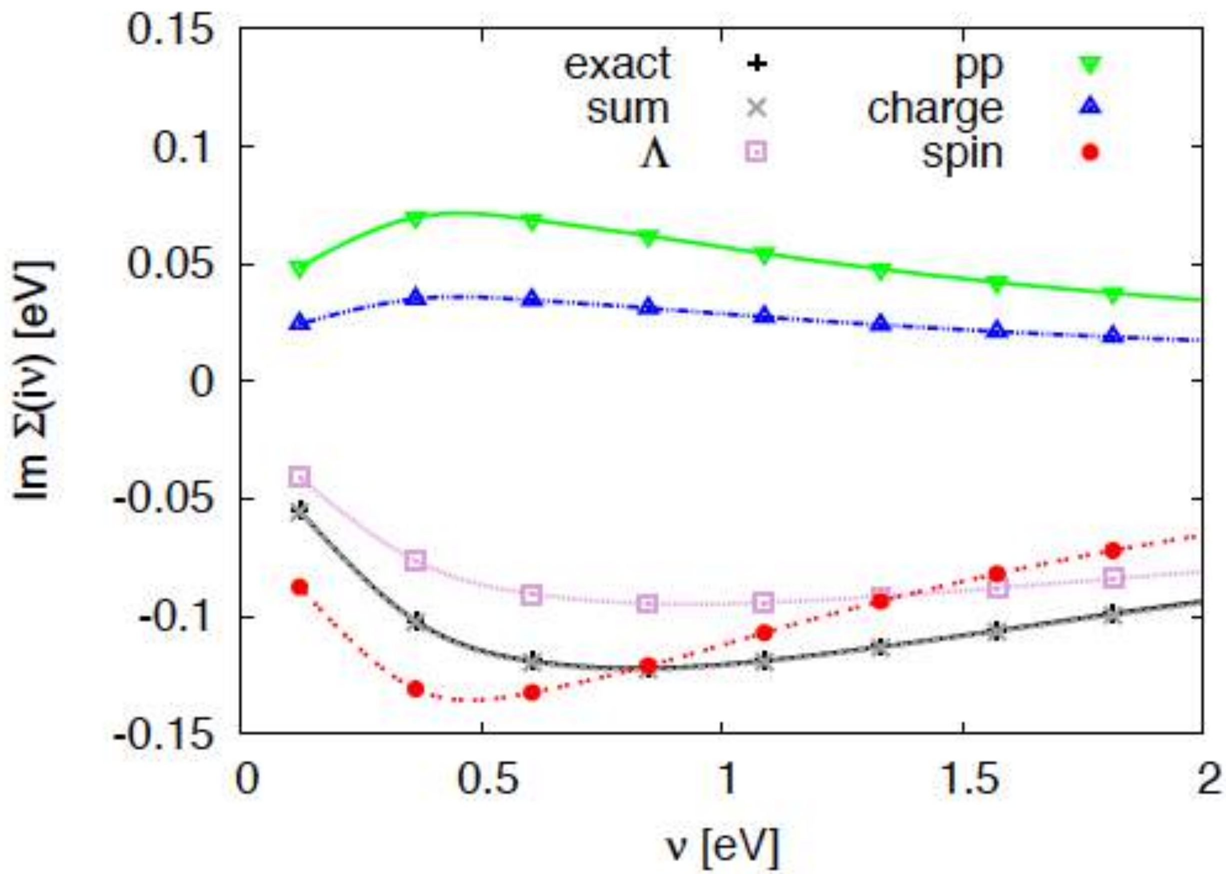
in terms of
2P-irreducible/reducible diagrams

O. Gunnarsson ..., & AT, PRB (2016)

Parquet decomposition: Results

✦ Analysis of a **DMFT** self-energy (similar results also for DCA)

✔ at weak-coupling (U << bandwidth) **reasonable** decomposition



O. Gunnarsson, ... , & AT, PRB (2016)

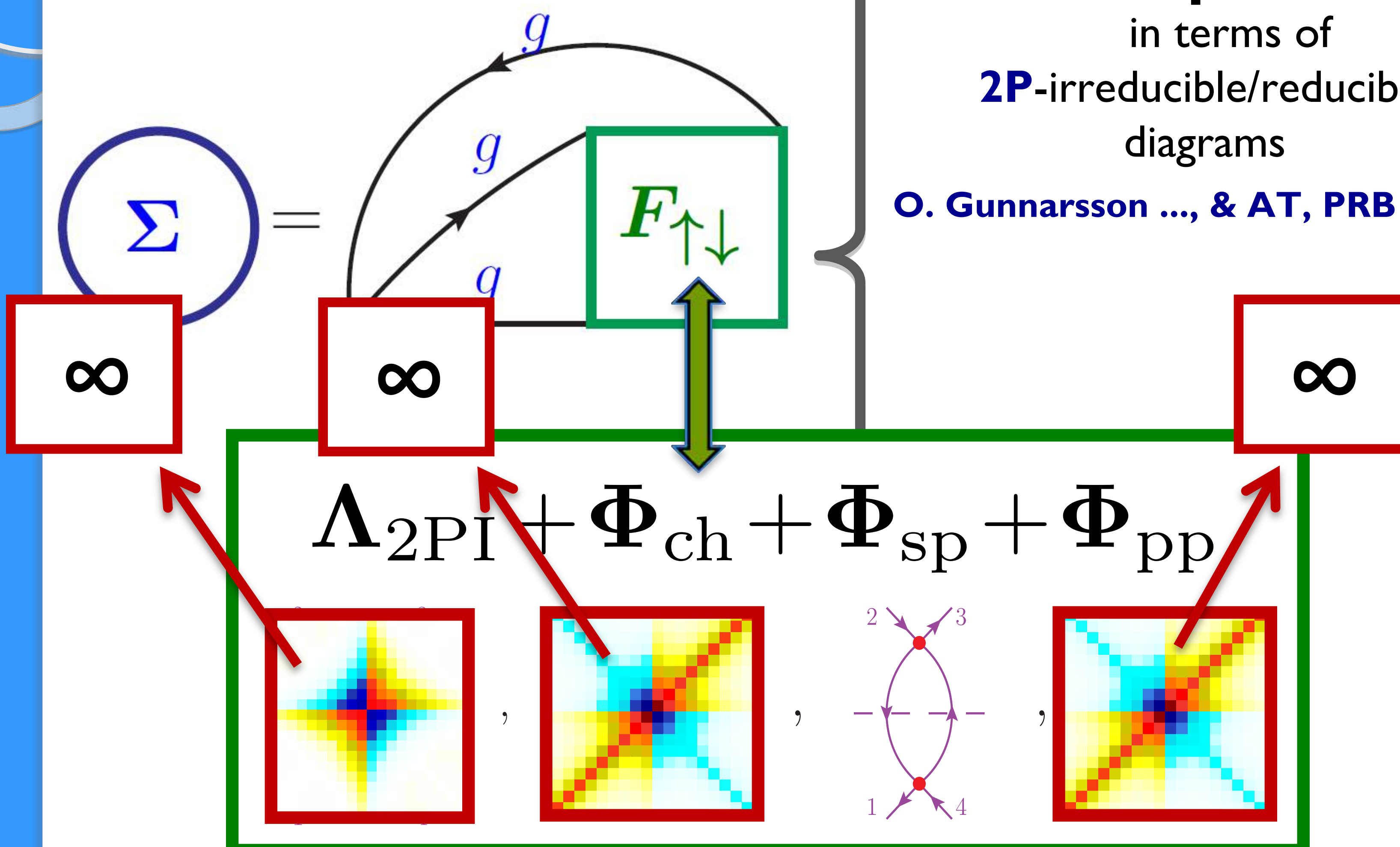
But, it is not that easy …

Our starting point:

1) parquet decomposition

in terms of **2P**-irreducible/reducible diagrams

O. Gunnarsson …, & AT, PRB (2016)

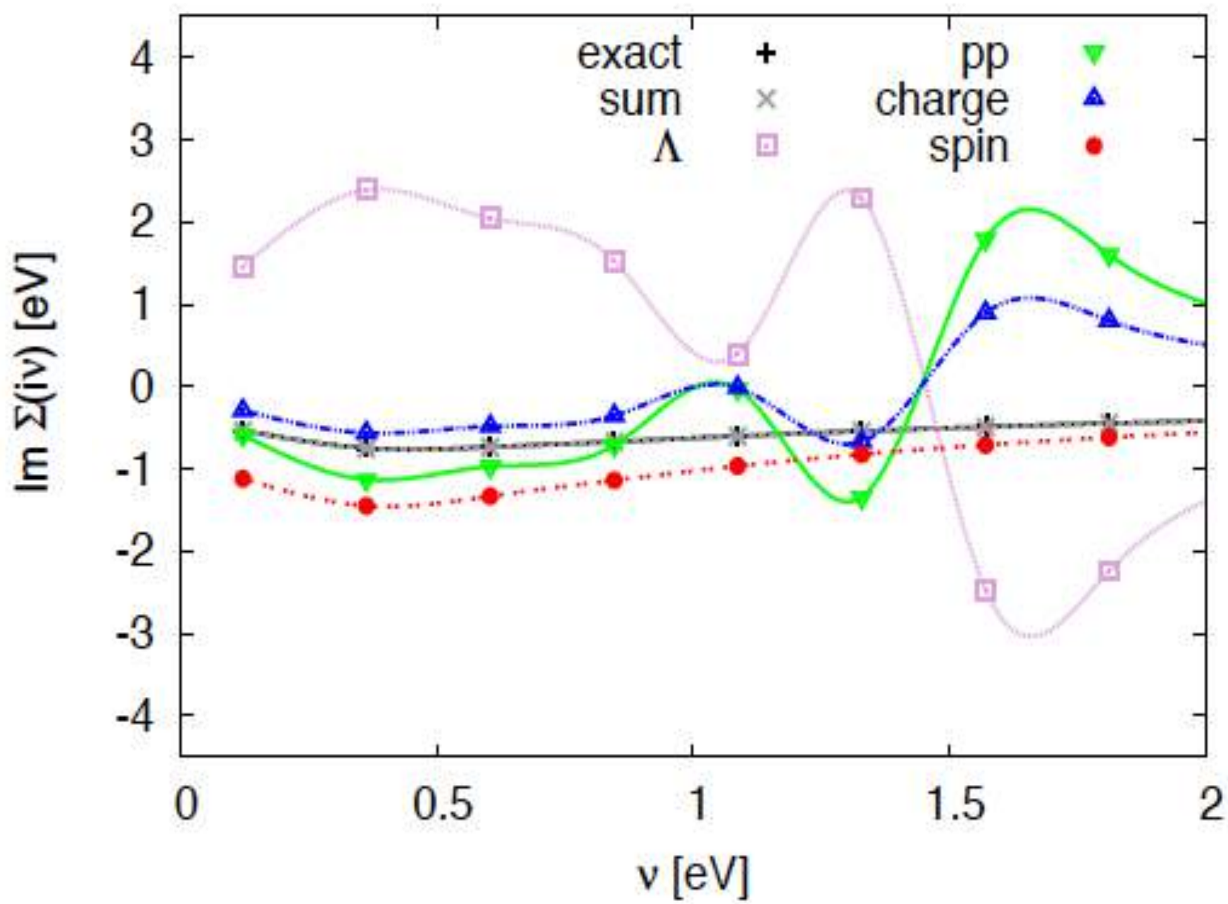


Hubbard: T. Schäfer, …, & AT, PRL, (2013) & O. Gunnarsson …, & AT, PRB (2016)
AIM: P. Chalupa, …, & AT, PRB (2018); Falicov Kimball: V. Janis, *et al.*, PRB (2014

Parquet decomposition: Results

✦ Analysis of a **DMFT** self-energy (similar results also for DCA)

✗ For U ~ bandwidth: “**chaotic,,** decomposition

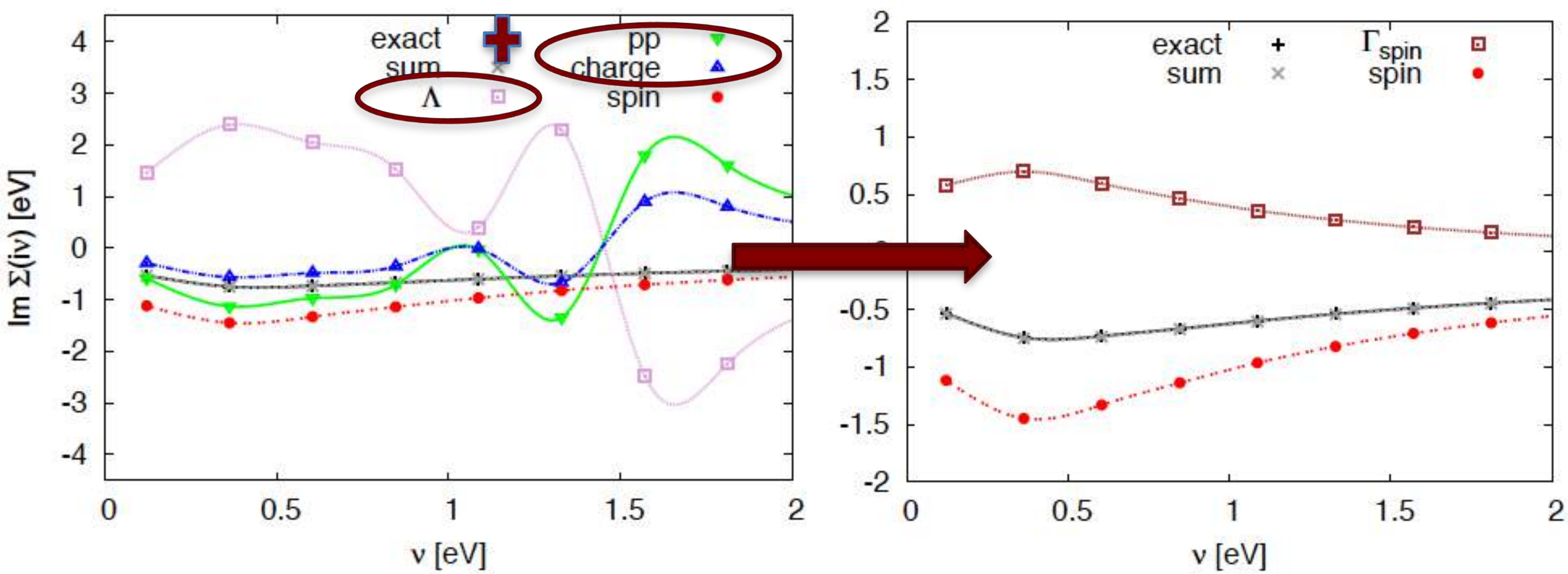


O. Gunnarsson, ... , & AT, PRB (2016)

Parquet decomposition: Results

✦ Analysis of a DMFT self-energy (similar results also for DCA)

✗ For U ~ bandwidth: “**chaotic„** decomposition



✗ **parquet** decomposition

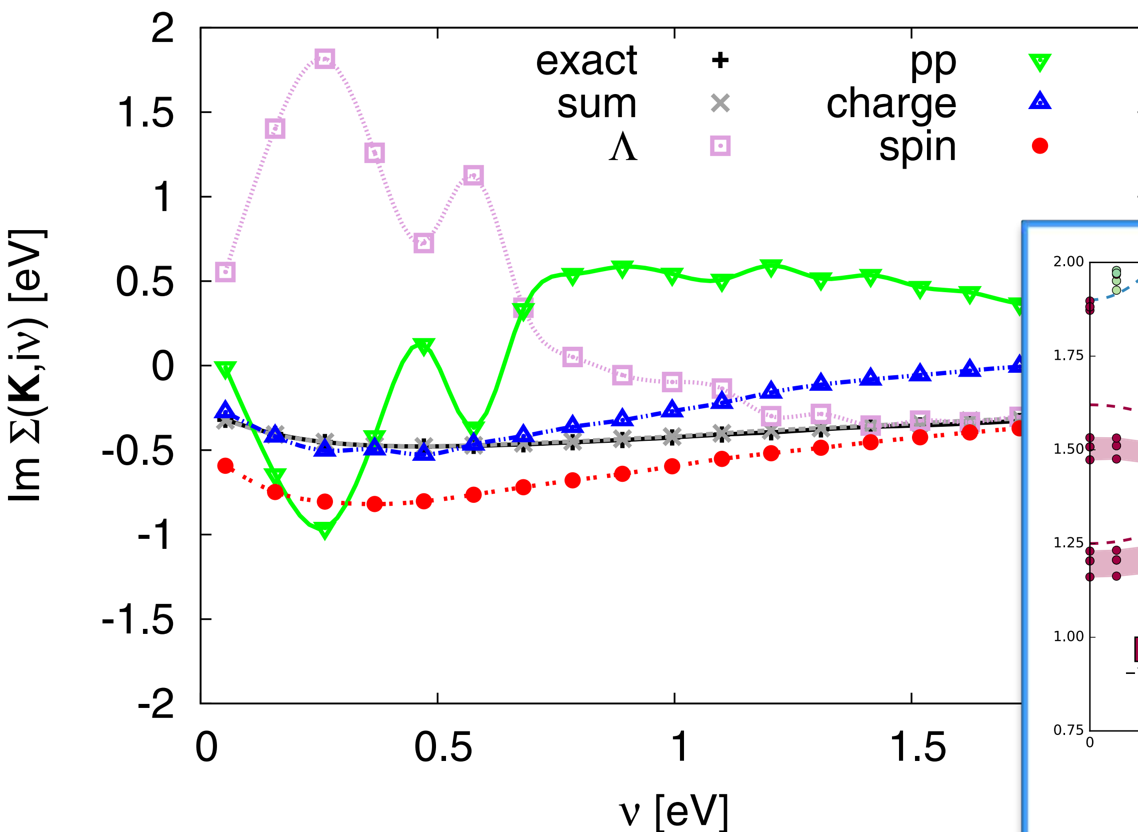
✔ **Bethe-Salpeter** decomposition
(w.r.t. the **dominant** channel)

O. Gunnarsson, … , & AT, PRB (2016)

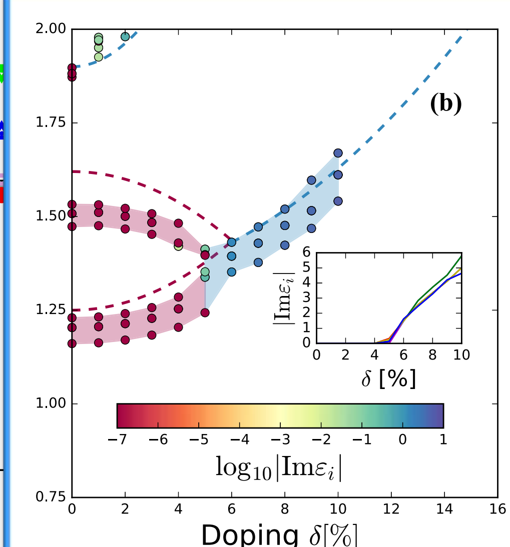
Parquet decomposition: Results

✦ Analysis of a **DCA** self-energy (out-of-half-filling: n =0.94, U = 7t)

✗ a “**chaotic,,** decomposition, **but** only in **pp** and *Λ*



O. Gunnarsson, ... , & AT, PRB (2016)

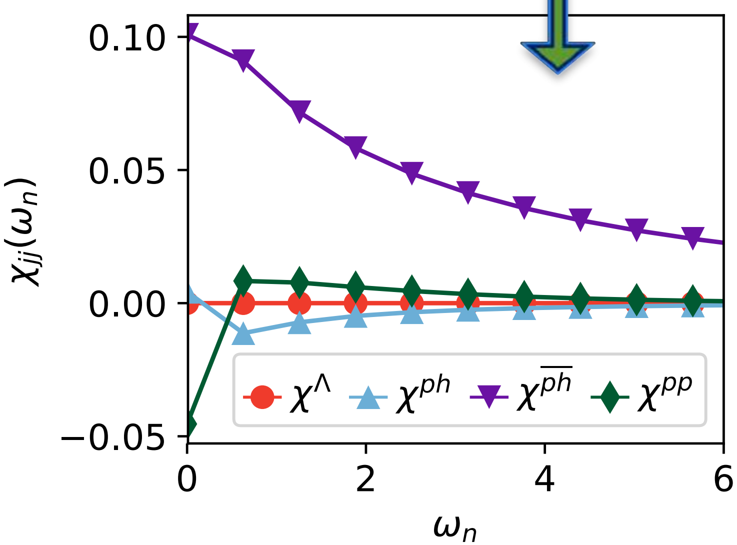


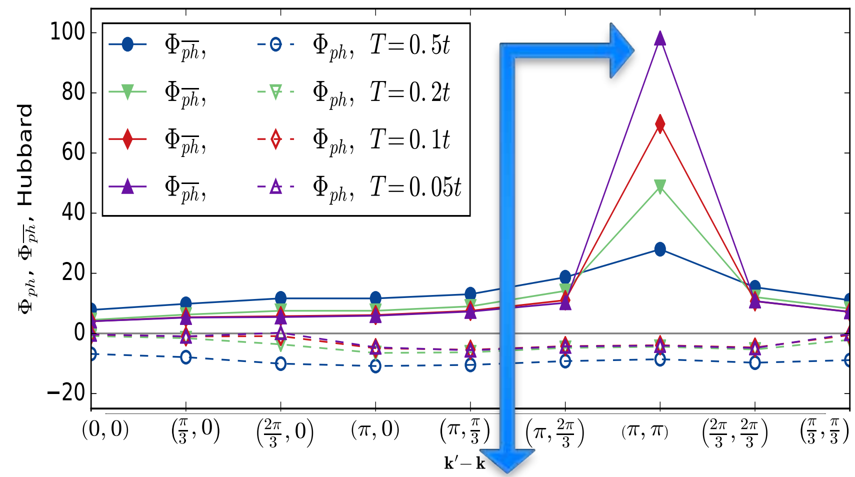
J. Vucicevic, …. & O. Parcollet
PRB (2018)

Parquet decomposition of response functions

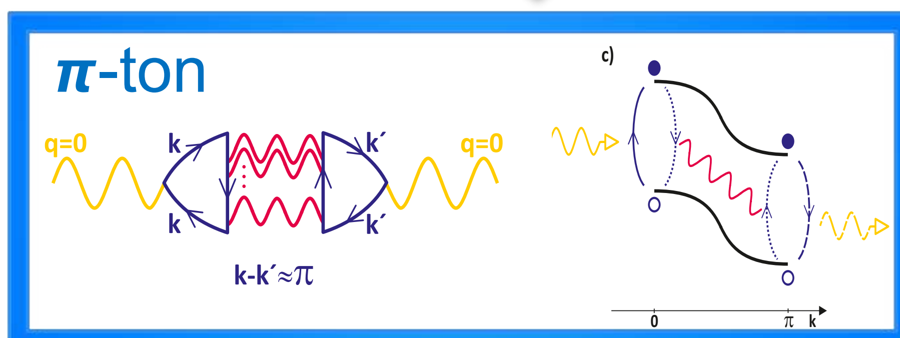
$$\chi_{jj,q} = \frac{2}{\beta N}\sum_k [\gamma^{\mathbf{q}}_{\mathbf{k}}]^2\, G_{q+k}G_k \; + \frac{2}{(\beta N)^2}\sum_{k,k'} \gamma^{\mathbf{q}}_{\mathbf{k}}\gamma^{\mathbf{q}}_{\mathbf{k}'} G_{k'}G_{q+k}F_d^{kk'q}G_{q+k'}G_k$$

$$\mathbf{\Lambda}_{\mathrm{2PI}} + \mathbf{\Phi}_{\mathrm{ph}} + \mathbf{\Phi}_{\overline{\mathrm{ph}}} + \mathbf{\Phi}_{\mathrm{pp}}$$



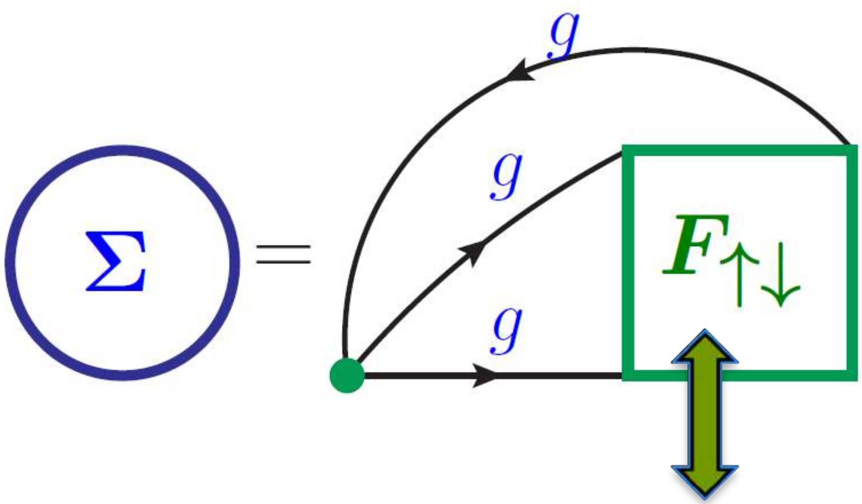


A. Kauch, …. & K. Held
arXiv: 1902..09342 (2019)



How to analyse Σ ?

Our starting point:



change of representation!

O. Gunnarsson, ..., & AT, PRL (2015)

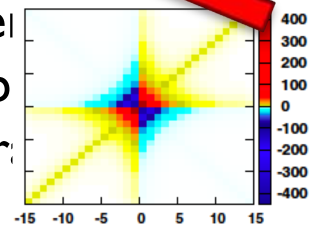
1) ~~parquet decomposition~~

in te

icib

agr

$\Lambda_{2PI}=\infty$



O. Gunnarsson ..., & AT, PRB (2016)

2)

Fluctuation diagnostics

$\Sigma(k,\omega)$

Change of representation of the EOM

$$\Sigma(k) = \frac{Un}{2} - \frac{U}{\beta^2 N} \sum_{k',q} F_{\uparrow\downarrow}(k,k',q)\, g(k')g(k'+q)g(k+q)$$

$$\boxed{\begin{aligned} \boldsymbol{F_{ch}(k,k',q)} &= F_{\uparrow\uparrow}(k,k',q) + F_{\uparrow\downarrow}(k,k',q) \\ \boldsymbol{F_{sp}(k,k',q)} &= F_{\uparrow\uparrow}(k,k',q) - F_{\uparrow\downarrow}(k,k',q) \\ \boldsymbol{F_{pp}(k,k',q)} &= F_{\uparrow\downarrow}(k,k',q-k-k') \end{aligned}}$$

$$\left.\begin{aligned} \Sigma(k) - \Sigma_{\mathrm{H}} &= \frac{U}{\beta^2 N} \sum_{k',q} F_{sp}(k,k';q)\, g(k')g(k'+q)g(k+q) \\ &= -\frac{U}{\beta^2 N} \sum_{k',q} F_{ch}(k,k';q)\, g(k')g(k'+q)g(k+q) \\ &= -\frac{U}{\beta^2 N} \sum_{k',q} F_{pp}(k,k';q)\, g(k')g(q-k')g(q-k) \end{aligned}\right\}$$

identical results

after all

k-summations

&

ω-summations

But: significant info by performing **partial summations**

Fluctuation diagnostics

$$\Sigma(k) - \Sigma_{\mathrm{H}} = \frac{U}{\beta^2 N} \sum_{k',q} F_{sp}(k,k',q)\, g(k')\, g(k'+q)\, g(k+q)$$

$$= -\frac{U}{\beta^2 N} \sum_{k',q} F_{ch}(k,k',q)\, g(k')\, g(k'+q)\, g(k+q)$$

$$= -\frac{U}{\beta^2 N} \sum_{k',q} F_{pp}(k,k',q)\, g(k')\, g(q-k')\, g(q-k)$$

➔ **spin**

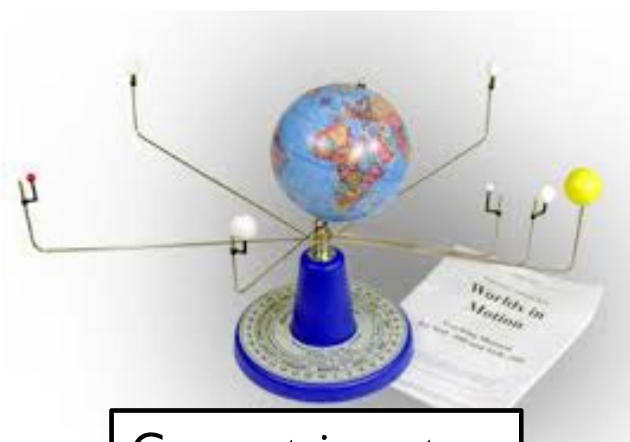
➔ **charge**

➔ **particle**

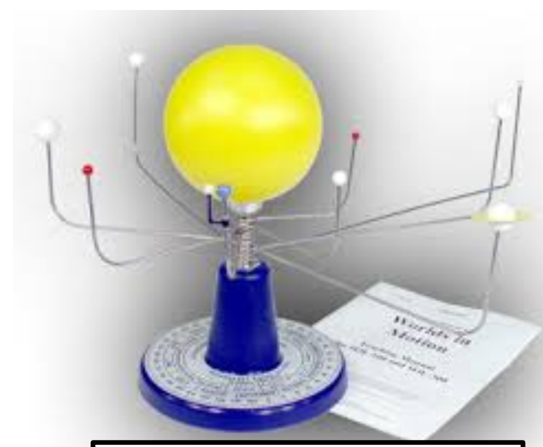
q-resolved histograms

ω-resolved pie-charts

important: **different** representations of the **same** physics:



Geocentric system



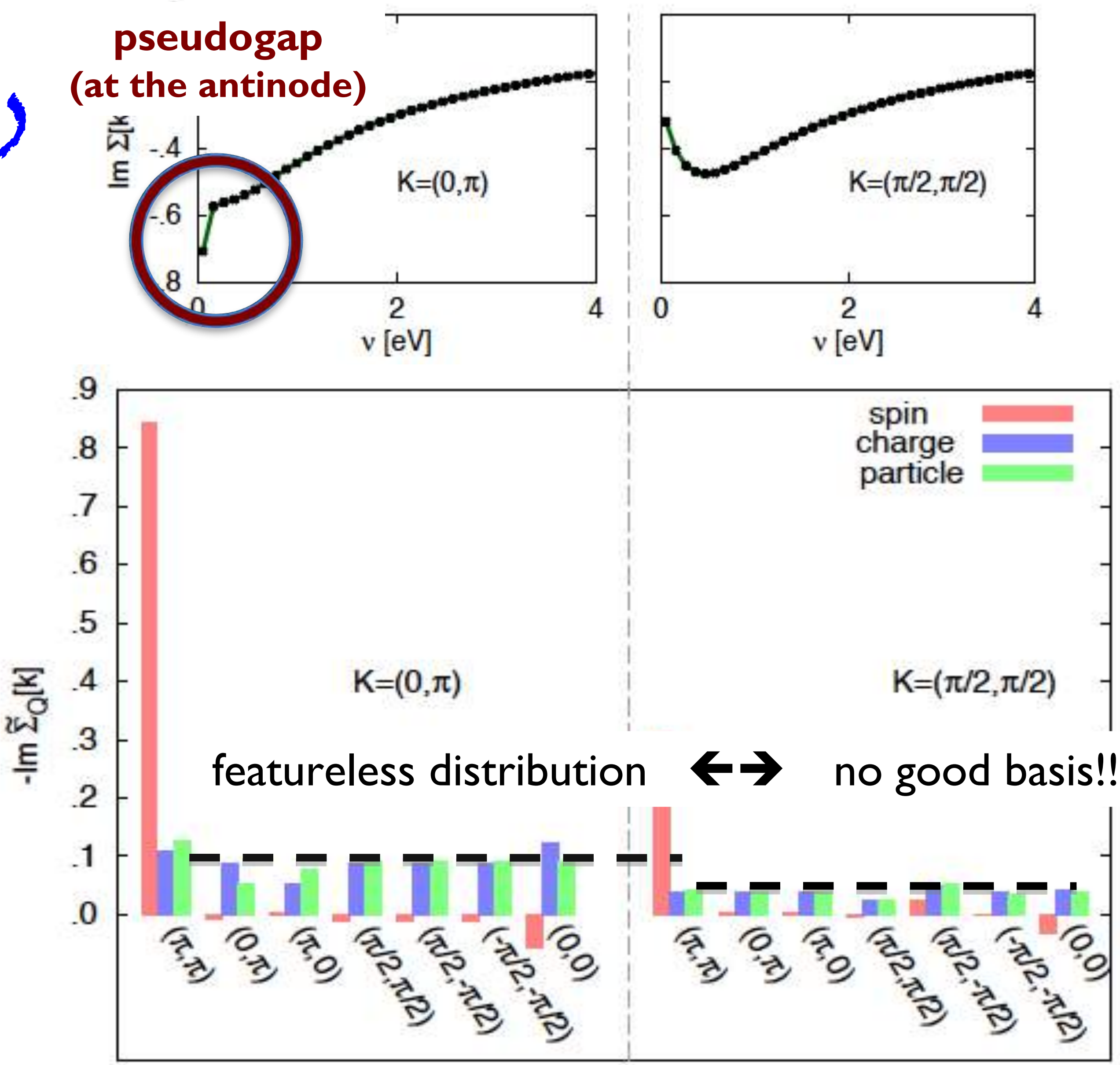
Heliocentric system

Results: pseudogap in the 2D Hubbard model

Fluctuation diagnostics

[DCA calculations, N_c=8 for U= 6t, n=0.94, β=60]

pseudogap
(at the antinode)

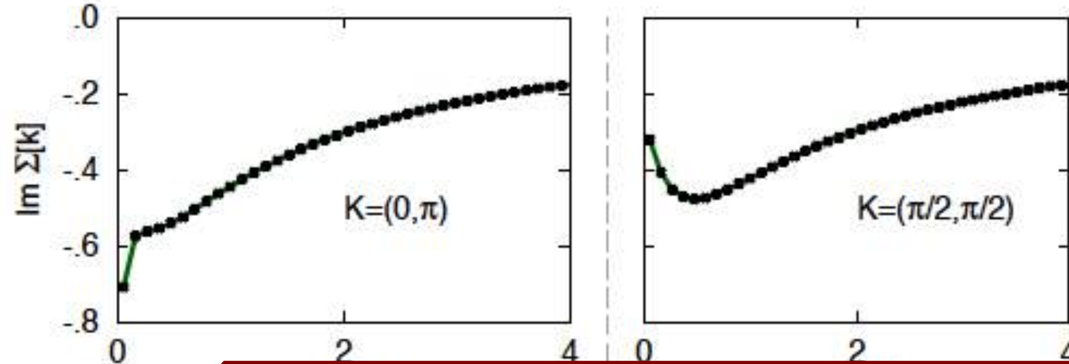


featureless distribution ←→ no good basis!!!

Results: pseudogap in the 2D Hubbard model

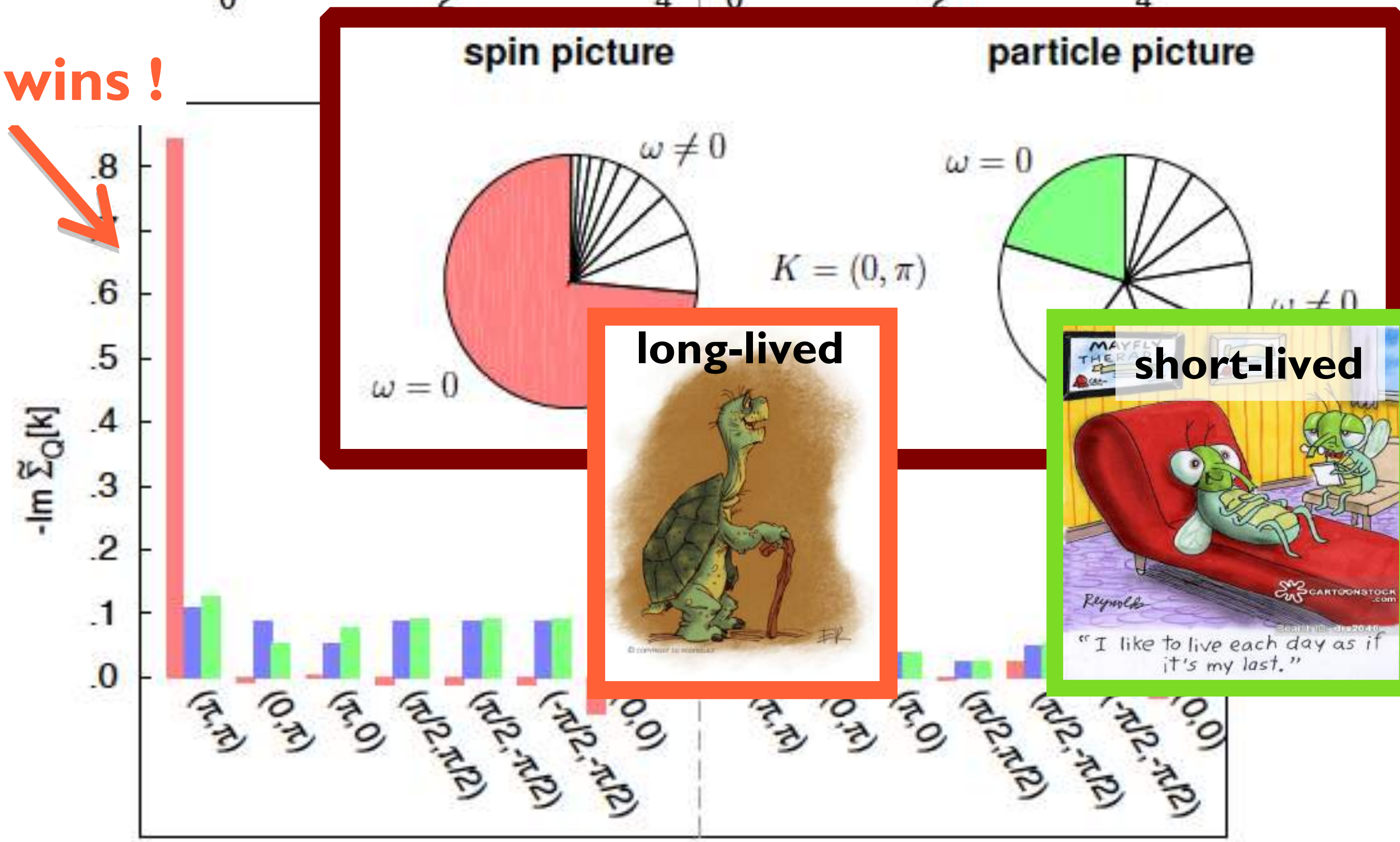
Fluctuation diagnostics

$\Sigma(k,\omega)$



Heliocentric system

Spin wins !



But …. what about d-wave pp-fluctuations?

- *d*-wave pairing correlator

$$\langle \Delta^\dagger \Delta \rangle = \boxed{\sum_{\mathbf{K},\mathbf{K}'} f(\mathbf{K}) f(\mathbf{K}') \langle c^\dagger_{\mathbf{K}\uparrow} c^\dagger_{-\mathbf{K}\downarrow} c_{-\mathbf{K}'\downarrow} c_{\mathbf{K}'\uparrow} \rangle} - \sum_{\mathbf{K}} [f(\mathbf{K})]^2 \langle c^\dagger_{\mathbf{K}\uparrow} c_{\mathbf{K}\uparrow} \rangle \langle c^\dagger_{-\mathbf{K}\downarrow} c_{-\mathbf{K}\downarrow} \rangle$$

with $f(\mathbf{K}) = \cos K_x - \cos K_y$

large if

$$\langle c^\dagger_{\mathbf{K}\uparrow} c^\dagger_{-\mathbf{K}\downarrow} c_{-\mathbf{K}'\downarrow} c_{\mathbf{K}'\uparrow} \rangle \sim f(\mathbf{K}) f(\mathbf{K}')$$

- fluctuation diagnostics

(in *pp*-representation, **Q=0**)

but, then ...

$$\frac{N}{U\beta} \sum_{\nu} [\Sigma(k) - \frac{Un}{2}] g(k) = \sum_{\mathbf{K}',\cancel{\mathbf{Q}}} \langle c^\dagger_{\mathbf{K}\uparrow} c^\dagger_{\cancel{\mathbf{Q}}-\mathbf{K}\downarrow} c_{-\mathbf{K}'\downarrow} c_{\cancel{\mathbf{Q}}+\mathbf{K}'\uparrow} \rangle - \sum_{\mathbf{K}'} \langle c^\dagger_{\mathbf{K}\uparrow} c_{\mathbf{K}\uparrow} \rangle \langle c^\dagger_{\mathbf{K}'\downarrow} c_{\mathbf{K}'\downarrow} \rangle$$

small !

➜ in general: large fluctuations $\not\Leftrightarrow$ equally important effects on Σ !!

Mapping the k-space: a Diag-MC study

Fluctuation diagnostics

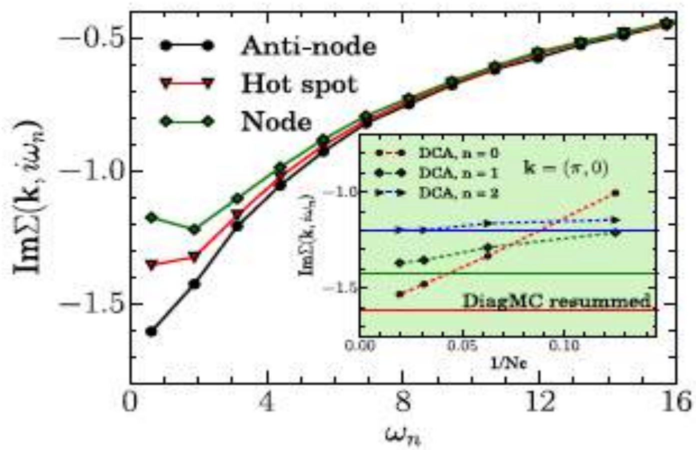
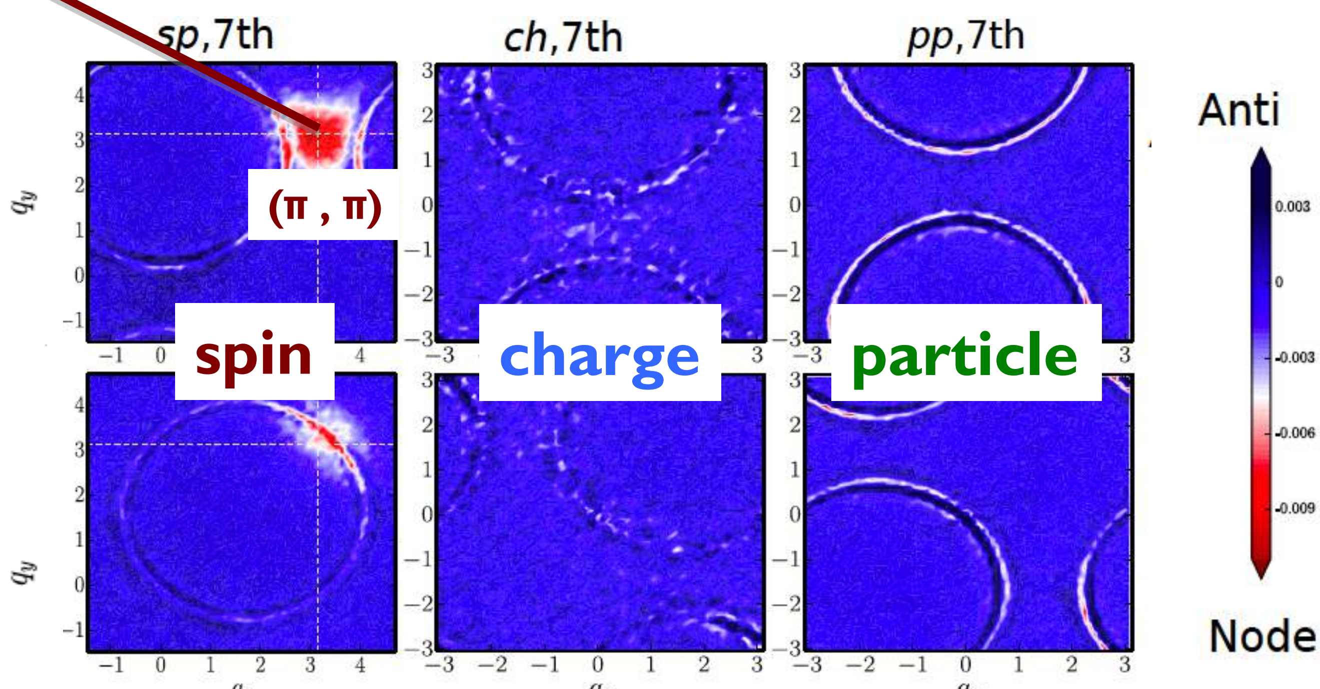


Figure 2. Imaginary part of the self-energy at the node, hot-spot and anti-node at $U = 5.6$, $t' = -0.3$, $n = 0.96$.

AF fluctuations !

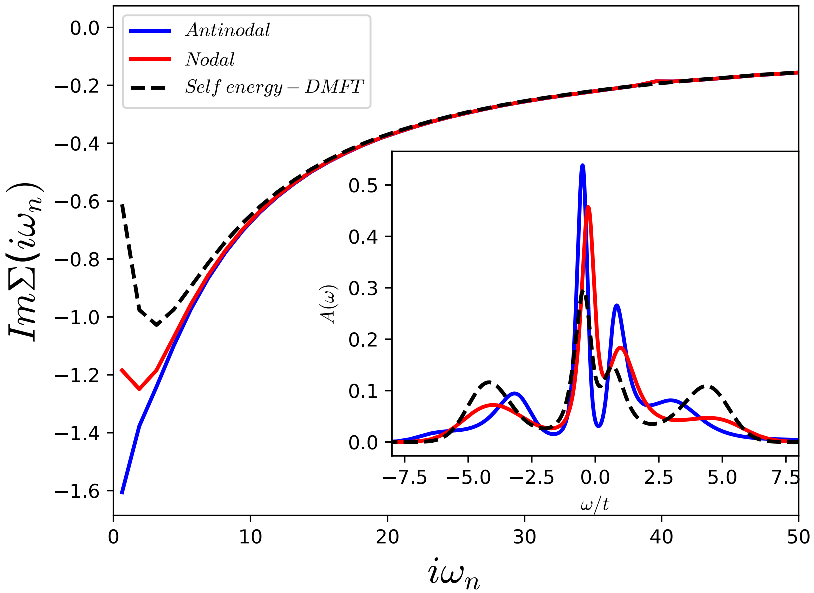


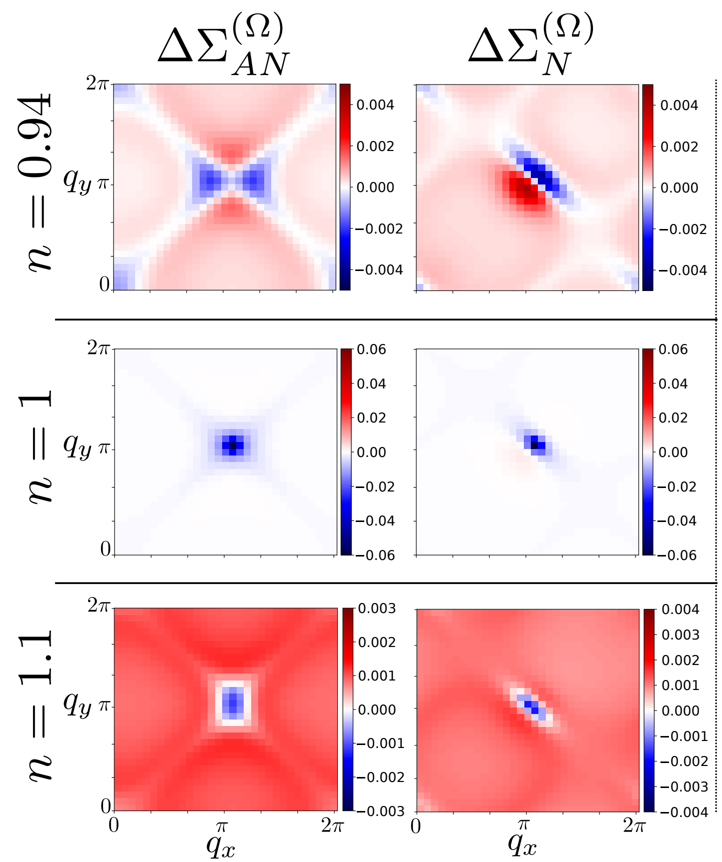
W. Wu, M. Ferrero, A. Georges,& E. Kozik, PRB (2018)

A “brand-new„ Dual-Fermion analysis

✦ Ladder DF analysis of the pseudogap phase
[U= 5.6 t , βt =5, different dopings]

$$\Delta\Sigma_k = Im\Sigma_k(i\omega_0) - Im\Sigma_k(i\omega_1)$$





[B. Arzang, A. Antipov & J. Le Blanc,
arXiv 1905.075462 (2019)]

Fluctuation diagnostics: a very versatile tool !

- *Schwinger-Dyson eq. (with all frequency summation done)*

$$\Sigma(k) + n_0 U = -\frac{U}{N_c g(k)} \sum_{\mathbf{K}'\mathbf{Q}} \int_0^\beta d\tau\, e^{i\nu\tau} \langle c_{\mathbf{K}+\mathbf{Q}\uparrow}(\tau) c^\dagger_{\mathbf{K}'+\mathbf{Q}\downarrow}(\tau) c_{\mathbf{K}'\downarrow}(\tau) c^\dagger_{\mathbf{K}\uparrow} \rangle$$

$$= \frac{1}{g(k)} \sum_{\mathbf{K}'\mathbf{Q}} A_{\uparrow\downarrow}(\mathbf{K},\mathbf{K}',\mathbf{Q};\nu)$$

where

$$A_{\sigma\sigma'}(\mathbf{K},\mathbf{K}',\mathbf{Q};\nu) = \frac{U}{N_c} \int_0^\beta d\tau\, e^{-i\nu\tau} \langle c^\dagger_{\mathbf{K}\sigma}(\tau) c_{\mathbf{K}+\mathbf{Q}\sigma} c^\dagger_{\mathbf{K}'+\mathbf{Q}\sigma'} c_{\mathbf{K}'\sigma'} \rangle$$

sum over fermionic momenta

$$C_{\sigma\sigma'}(\mathbf{K},\mathbf{Q};\nu) = \sum_{\mathbf{K}'} A_{\sigma\sigma'}(\mathbf{K},\mathbf{K}',\mathbf{Q};\nu)$$

standard (BOSONIC)
fluctuation diagnostics

sum over ***bosonic*** *momenta*

$$B_{\sigma\sigma'}(\mathbf{K},\mathbf{K}';\nu) = \sum_{\mathbf{Q}} A_{\sigma\sigma'}(\mathbf{K},\mathbf{K}',\mathbf{Q};\nu)$$

complementary **FERMIONIC**
fluctuation diagnostics

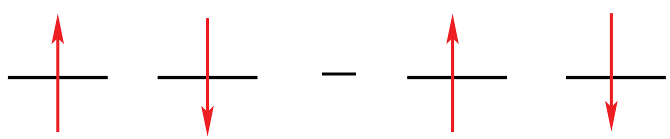
“Fermionic“ fluctuation diagnostics

$$\boxed{B_{\sigma\sigma'}(\mathbf{K},\mathbf{K}';\nu) = \sum_{\mathbf{Q}} A_{\sigma\sigma'}(\mathbf{K},\mathbf{K}',\mathbf{Q};\nu)}$$

At large U, low-T $(\nu = \pi/\beta \ll |U|/2)$ *:*

$$B_{\uparrow\downarrow}(\mathbf{K},\mathbf{K}';\nu) = -\frac{2}{N_c}\langle n_{\mathbf{K}'\downarrow}\rangle - \frac{4}{N_c^2}\sum_{\mathbf{R}_1\neq\mathbf{R}_2} e^{i(\mathbf{K}-\mathbf{K}')\cdot(\mathbf{R}_1-\mathbf{R}_2)} \quad \langle E_0(N_{\mathrm{el}})|c^{\dagger}_{\mathbf{R}_2\downarrow}c_{\mathbf{R}_2\uparrow}c^{\dagger}_{\mathbf{R}_1\uparrow}c_{\mathbf{R}_1\downarrow}|E_0(N_{\mathrm{el}})\rangle$$

By considering strong ***singlet-correlation*** *on the bonds (precursors of an RVB state):*

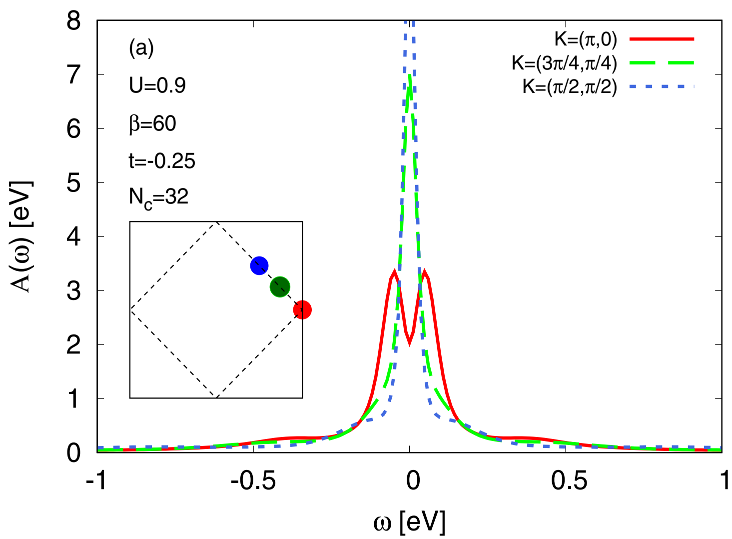


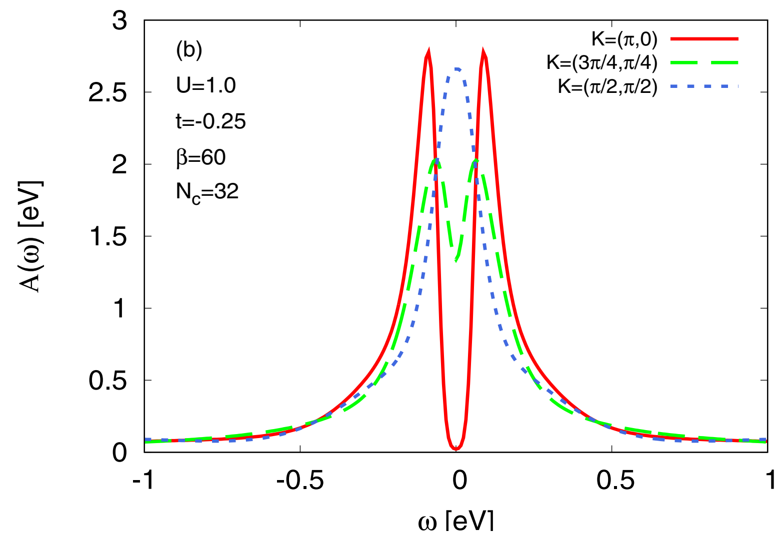
$$= \frac{1}{\sqrt{2}}\left(c^{\dagger}_{\mathbf{R}_1\uparrow}c^{\dagger}_{\mathbf{R}_2\downarrow} - c^{\dagger}_{\mathbf{R}_1\downarrow}c^{\dagger}_{\mathbf{R}_2\uparrow}\right)|\mathrm{vac}\rangle$$

$$B_{\uparrow\downarrow}(\mathbf{K},\mathbf{K}';\nu) \begin{cases} \mathbf{K}' = \mathbf{K} + (\pi,\pi) & \rightarrow \text{ large } \textbf{negative} \text{ values} \\ \mathbf{K}' = \mathbf{K} & \rightarrow \text{ smaller (slightly positive) values} \end{cases}$$

O. Gunnarsson, ... , & AT, PRB (2018)

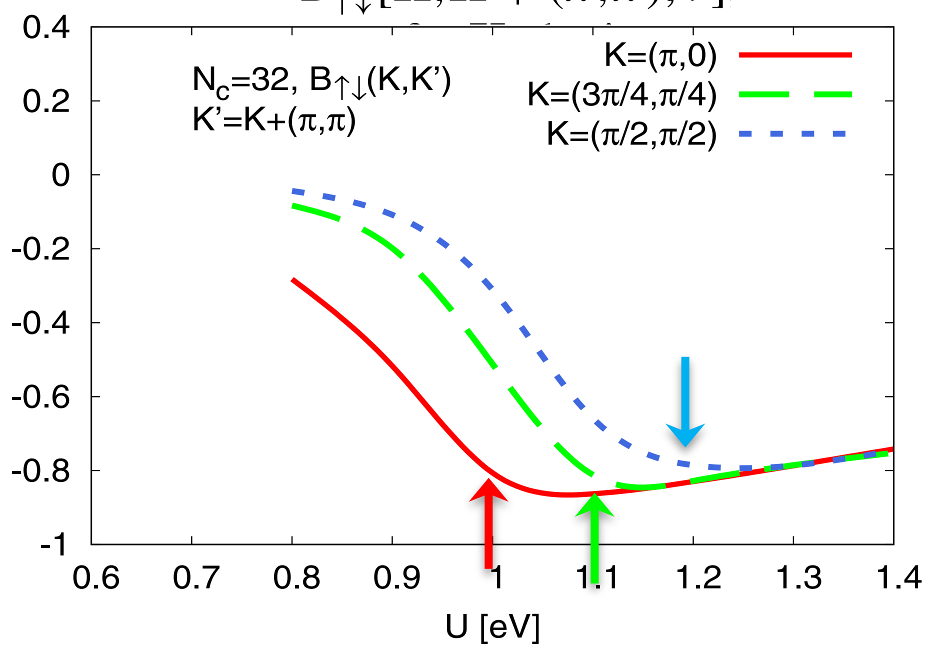
“Fermionic“ fluctuation diagnostics: DCA results





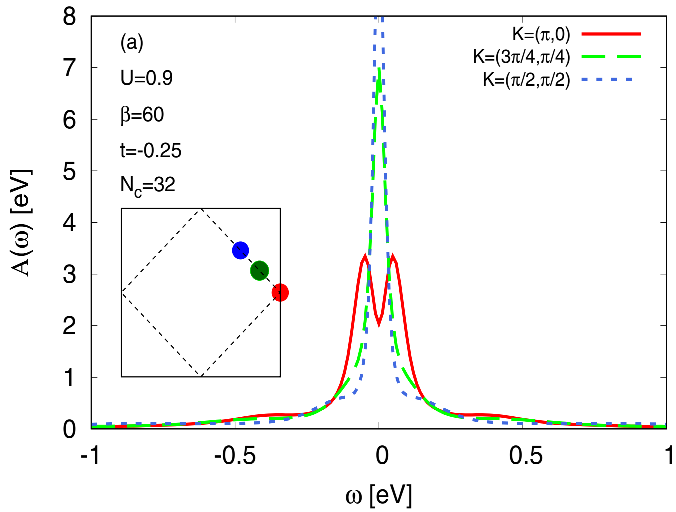
[in unit of: 4t =1 eV]

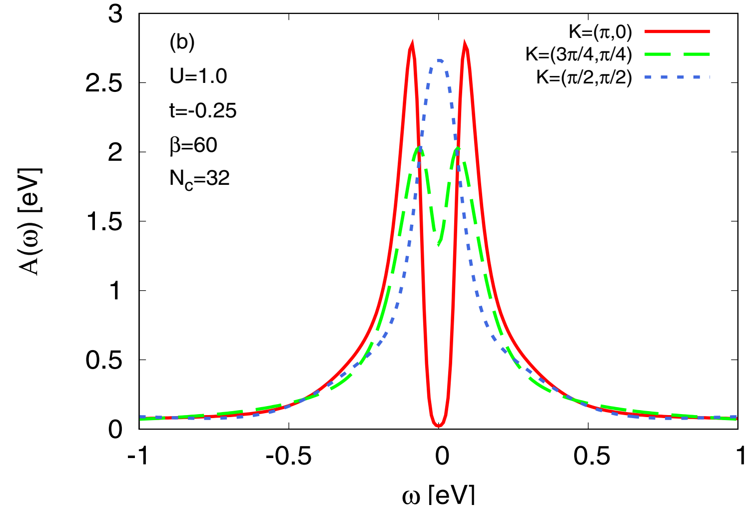
$B_{\uparrow\downarrow}[\mathbf{K},\mathbf{K}+(\pi,\pi);\nu]$



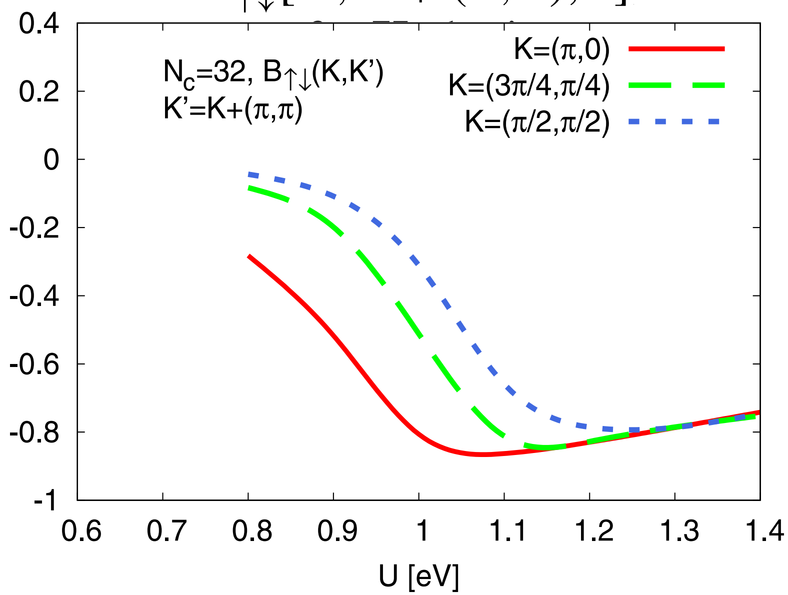
[O. Gunnarsson, ..., & AT, PRB (2018)]

“Fermionic" fluctuation diagnostics: results

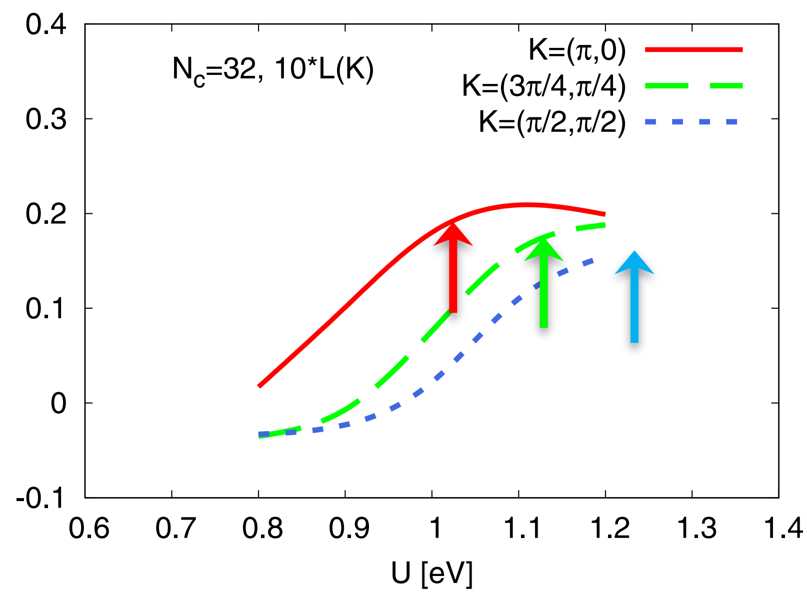




$$B_{\uparrow\downarrow}[\mathbf{K},\mathbf{K}+(\pi,\pi);\nu]$$



$$L(\mathbf{K}) = \langle n_{\mathbf{K}\uparrow} n_{\mathbf{K}\downarrow} \rangle - \langle n_{\mathbf{K}\uparrow} \rangle \langle n_{\mathbf{K}\downarrow} \rangle$$



New insights for … ladder-based calculations !

- *Here: for single-site **TRILEX*** [T. Ayral and O. Parcollet, PRB (2015)]

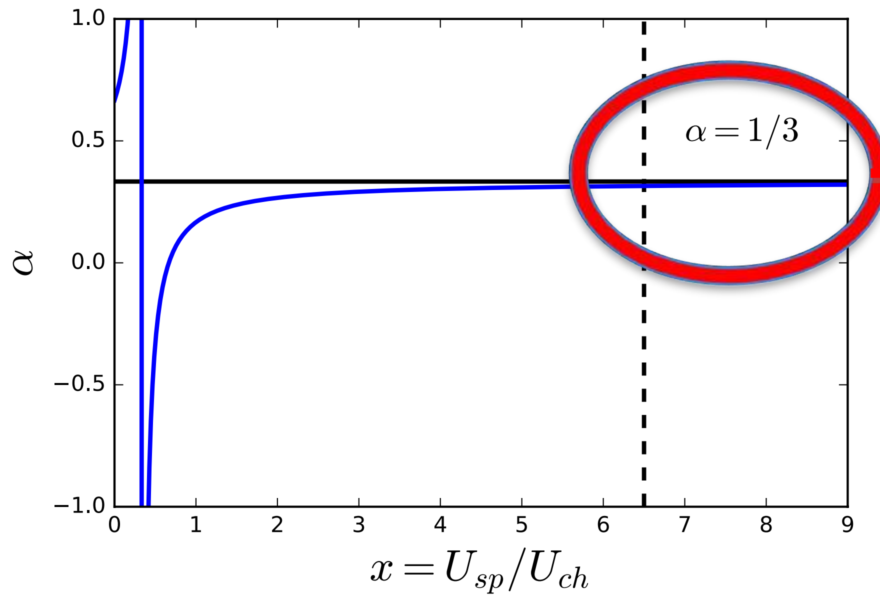
Heisenberg decoupling of the (purely local) Coulomb interaction U: $\begin{cases} U_{ch} = (3\alpha - 1)U \\ U_{sp} = (\alpha - 2/3)U \end{cases}$

$\Rightarrow \alpha = \frac{x-2/3}{3x-1}$ with $x = U_{sp}/U_{ch}$

ratio of partial self-energies of leading fluctuations:

x = -Im $\tilde{\Sigma}_{sp,\mathbf{Q}=(\pi,\pi)}(\mathbf{K} = (\pi, 0), i\omega_0)$/-Im $\tilde{\Sigma}_{ch,\mathbf{Q}=(0,0)}(\mathbf{K} = (\pi, 0), i\omega_0) \approx 6.5$

$$\Rightarrow \alpha(x = 6.5) = 0.32 \approx 1/3$$

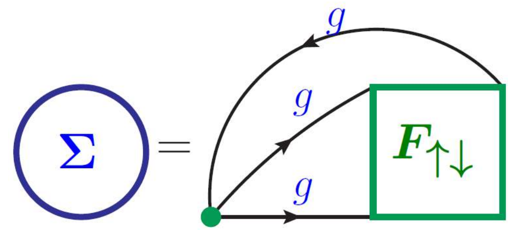


Significant **improvement** of the physical description !

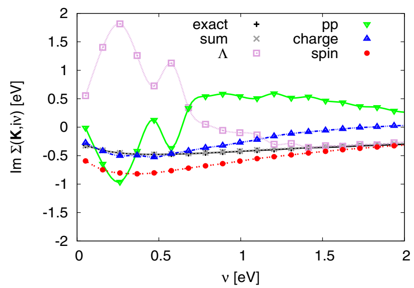
[T. Schäfer, ..., & O. Parcollet, unpublished (2019)]

Summary, Conclusion & …

✦ How to read *between the lines* of one-particle spectra?



parquet decomposition

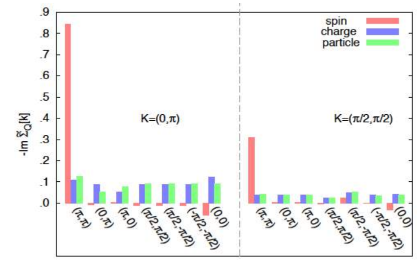


✗ numerically heavier (inversions)

✗ unstable for increasing U

✔ generalizable to response functions

Fluctuation diagnostics



✔ numerically lighter

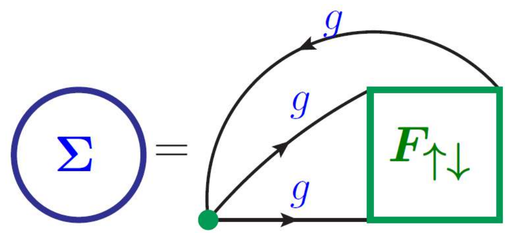
✔ flexible/everywhere applicable

? how "generalizable" ?

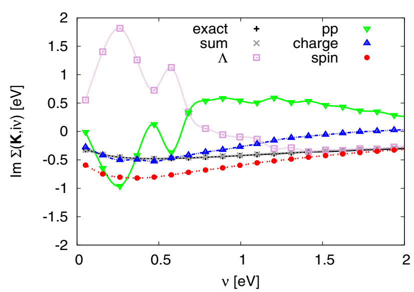
Coming soon: review paper on most recent developements/perspectives by T. Schäfer & AT on *Journal of Physics: Condensed Matter*

Summary, Conclusion & …

✦ How to read *between the lines* of one-particle spectra?



parquet decomposition

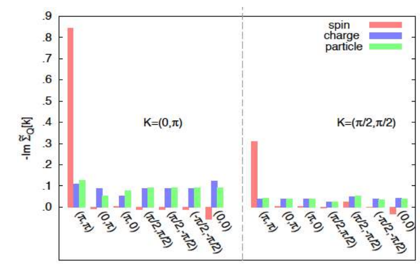


✗ numerically heavier (inversions)

✗ unstable for increasing U

✔ generalizable to response functions

Fluctuation diagnostics



✔ numerically lighter

✔ flexible/everywhere applicable

? how "generalizable" ?

Outlook:

- *Non-local interactions*
- *Symmetry-broken phases*
- *Multi-orbital systems (Hund's metals)*