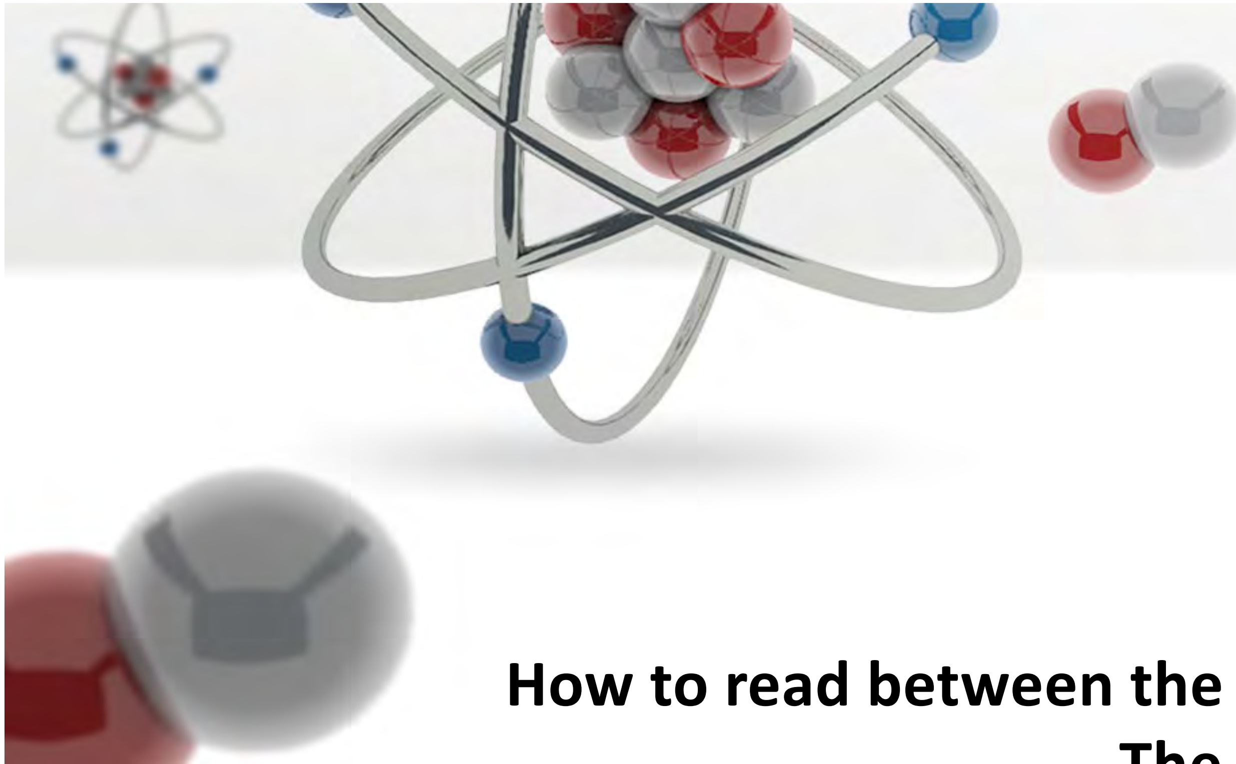

How to read between the lines of electronic spectra: The diagnostics of fluctuations in strongly correlated electron systems

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Seminar Collège de France, 25th May 2021

Max-Planck-Institut für Festkörperforschung

Theory of strongly correlated quantum matter (SCQM)

COLLÈGE DE FRANCE 1530

Fluctuation diagnostics: the collaboration

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How to read between the lines of electronic spectra: the diagnostics of fluctuations in strongly correlated electron systems

Thomas Schäfer[1,2,*] and Alessandro Toschi[3]

PRL 114, 236402 (2015) PHYSICAL REVIEW LETTERS week ending 12 JUNE 2015

Fluctuation Diagnostics of the Electron Self-Energy: Origin of the Pseudogap Physics

O. Gunnarsson,[1] T. Schäfer,[2] J. P. F. LeBlanc,[3,4] E. Gull,[4] J. Merino,[5] G. Sangiovanni,[6] G. Rohringer,[2] and A. Toschi[2]

PHYSICAL REVIEW B 93, 245102 (2016)

Parquet decomposition calculations of the electronic self-energy

O. Gunnarsson,[1] T. Schäfer,[2] J. P. F. LeBlanc,[3] J. Merino,[4] G. Sangiovanni,[5] G. Rohringer,[2,6] and A. Toschi[2]

O. Gunnarsson

A. Toschi

G. Rohringer

TS

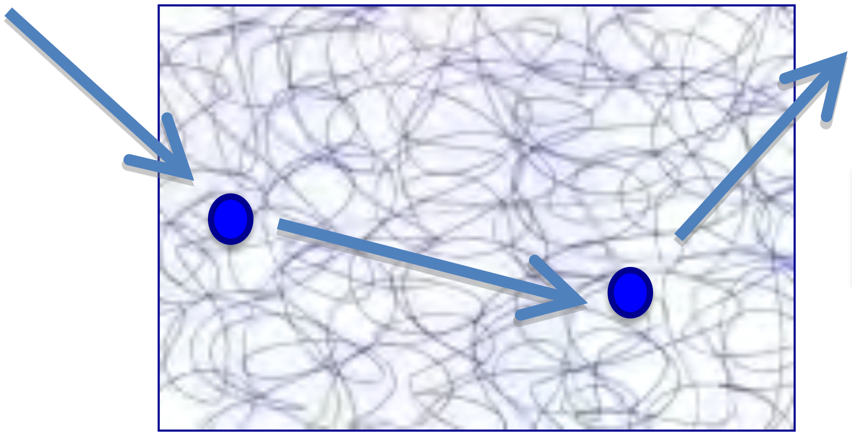
E. Gull

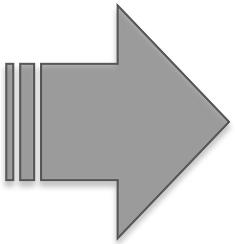
J. LeBlanc

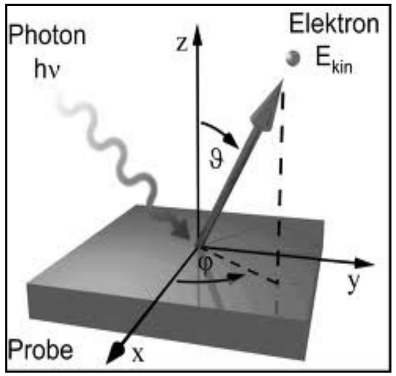
G. Sangiovanni

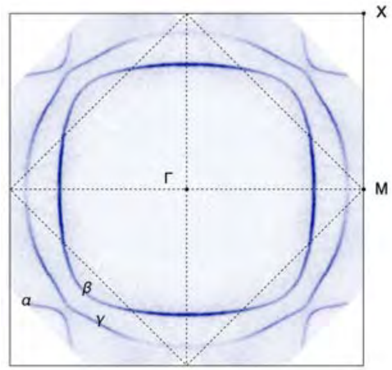
J. Merino

Electronic correlations at the one-particle level: experimental spectra

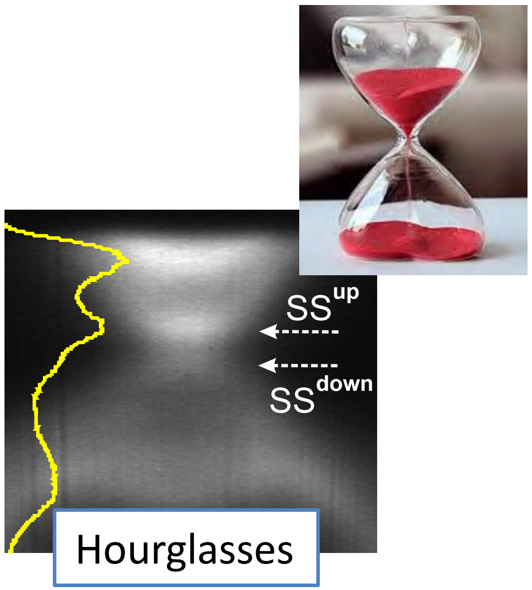


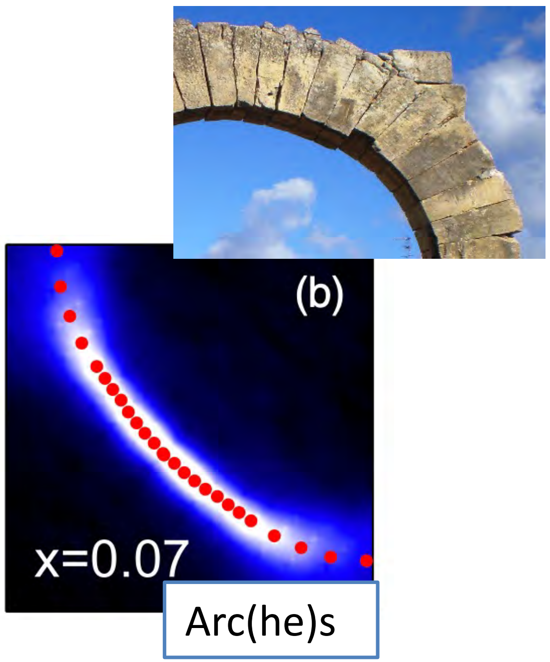


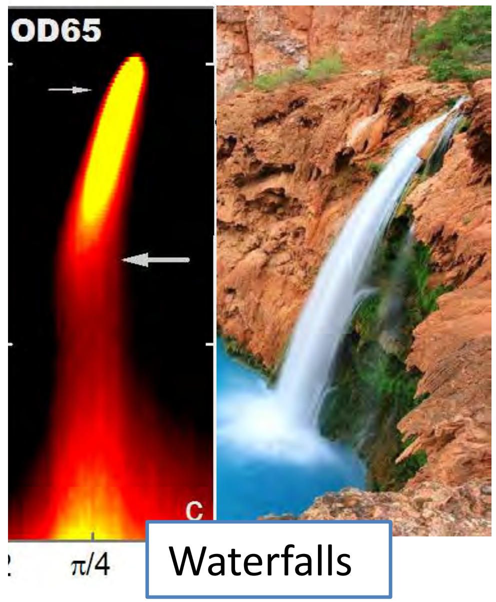




(AR)PES, InvPES, (STM)



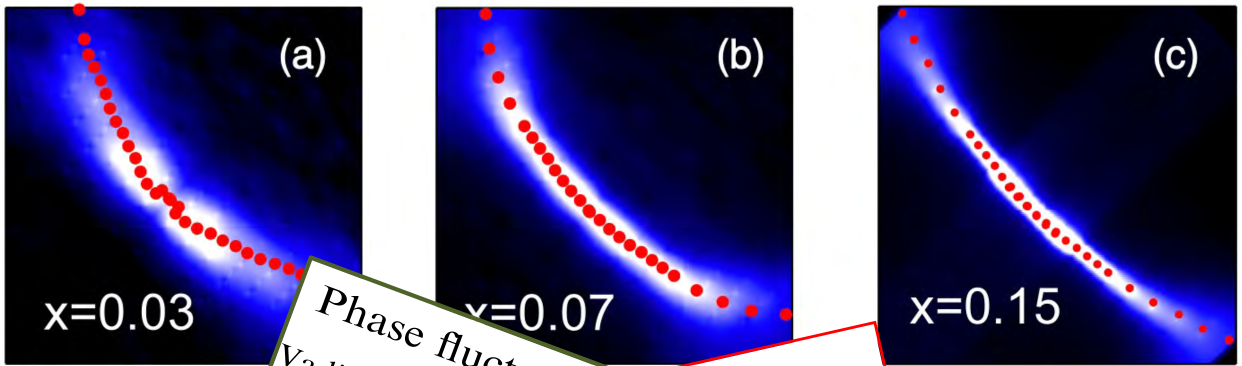


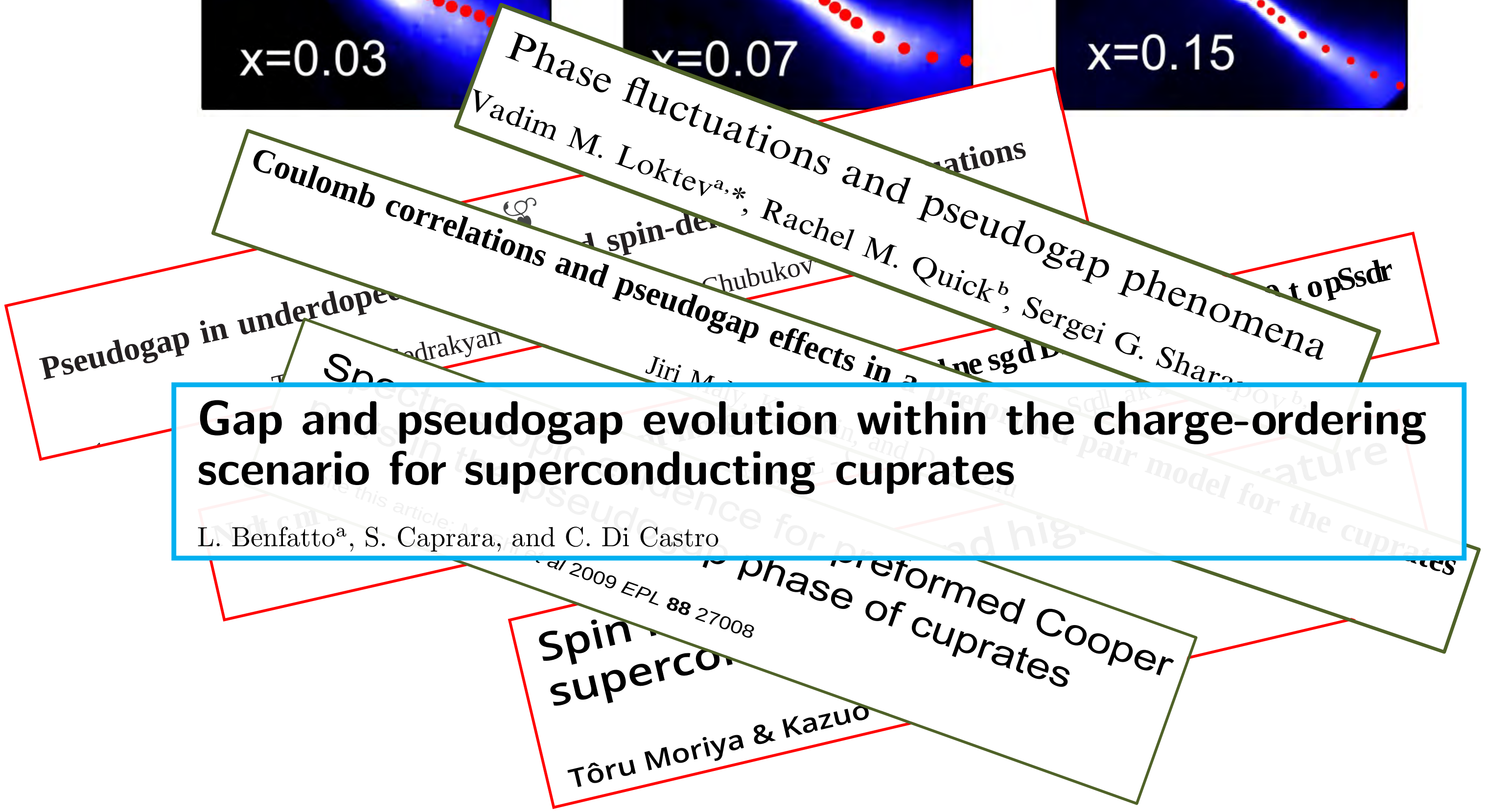


A. Tamai, et al. Phys. Rev. X ***9****, 021048 (2019)*

T. Yoshida, et al., J. Phys. Soc. Jpn. ***81****, 011006 (2012)*

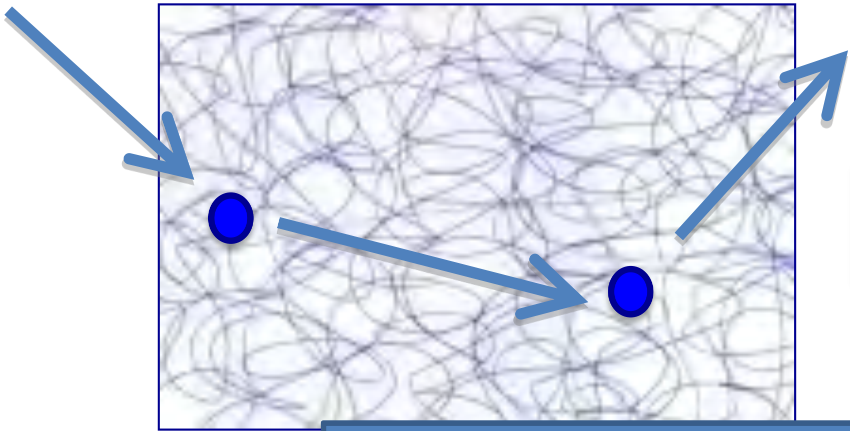
Electronic correlations at the one-particle level: how does the system become excited?

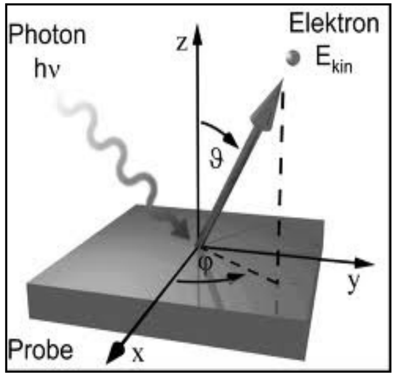


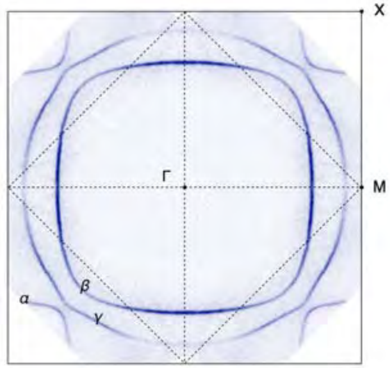


T. Yoshida, et al., J. Phys. Soc. Jpn. **81**, 011006 (2012)

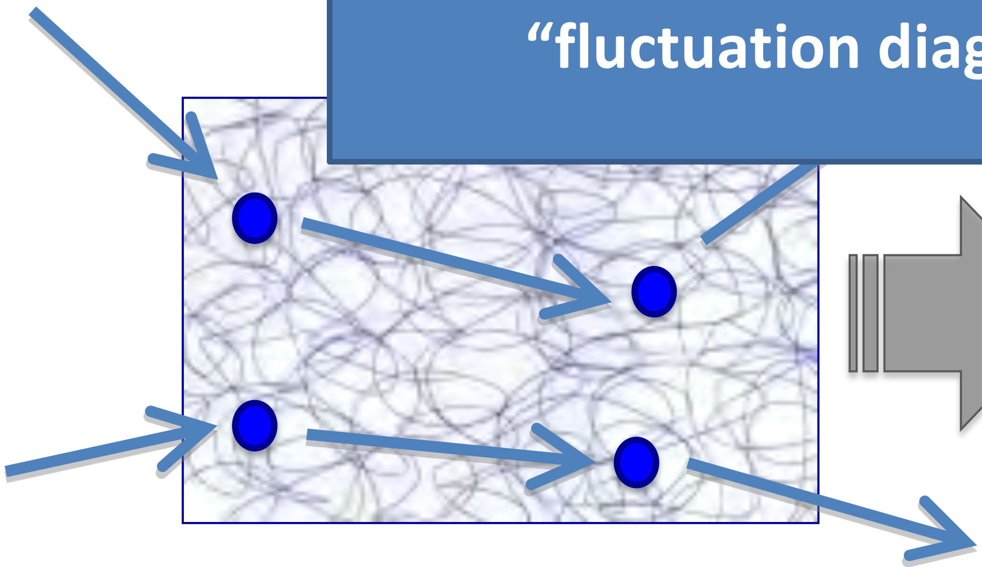
Electronic correlations at the one- and two- particle level: origin of fluctuations

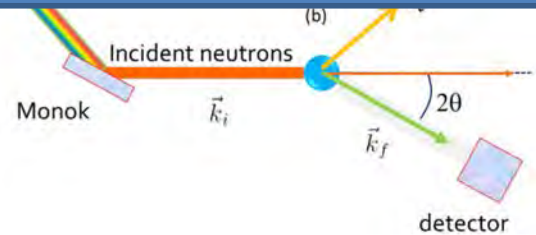




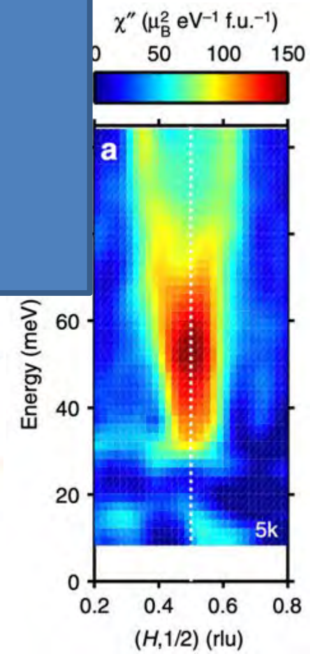


What are possible strategies for a “fluctuation diagnostics” in theory?





IR, INS, NMR

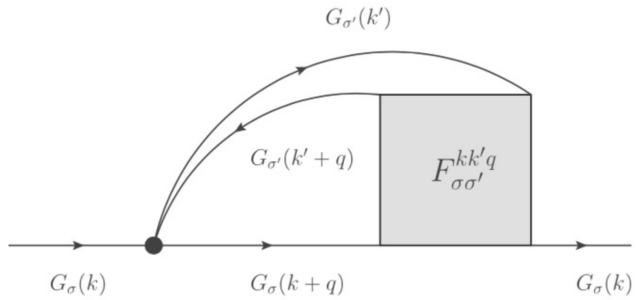


A. Tamai, et al. Phys. Rev. X ***9****, 021048 (2019)*
M.K. Chan, et al., Nat. Comm. ***7****, 10819 (2016)*
S. Petit, EPJ Web of Conferences ***155****, 00007 (2017)*

Outline: diagnostics of fluctuations in correlated systems

Introduction

- Experimental spectra at the one- and two-particle level
- The Hubbard model
- Two-particle level quantities: linear response, vertex and Dyson-Schwinger equation of motion
- **Two general approaches** to tackle complex problems

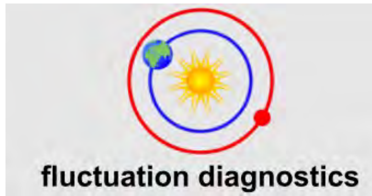


Parquet decomposition

- Parquet equations and description of the method
- Examples
- Breakdown

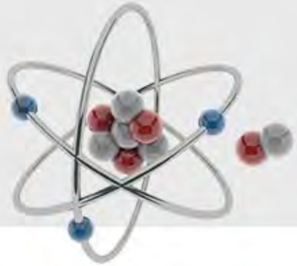
Fluctuation diagnostics

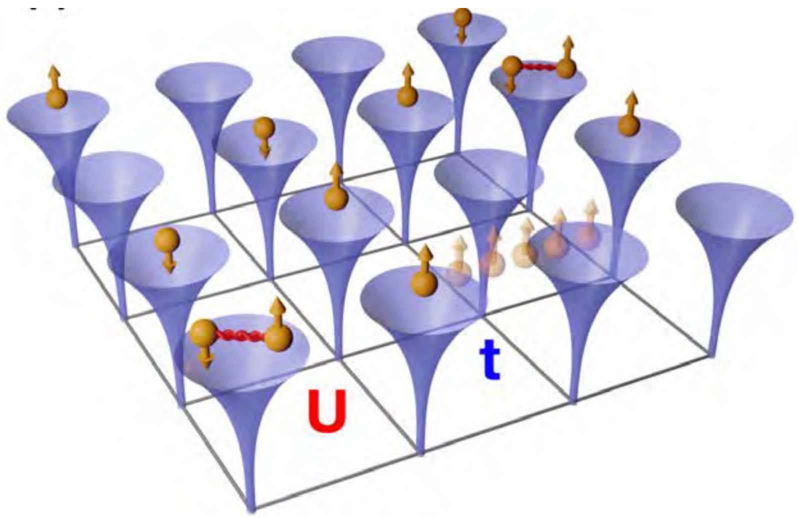
- Partial sums of the Dyson-Schwinger equation of motion
- Examples



Conclusions, outlook and general perspective

Strongly correlated systems: a simple (?) modellization





Hubbard Hamiltonian:

$$H = -t \sum_{\langle ij \rangle \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

-t : hopping

U: **local** Coulomb interaction

In **this talk**: one band, (mostly) 2D, no symmetry broken phases [espc. SU(2)]

Results from:

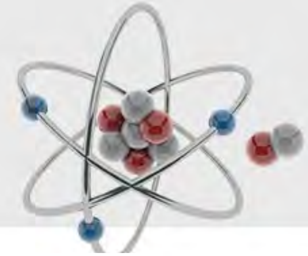
- diagrammatic Monte Carlo (DiagMC) → Seminar of F. Šimkovic
- dynamical mean-field theory (DMFT) → RMP **68**, 13 (1996)
- dynamical cluster approximation (DCA) → RMP **77**, 1027 (2005)
- dynamical vertex approximation (DΓA)
- dual fermion approach (DF)
- triply irreducible local expansion (TRILEX)

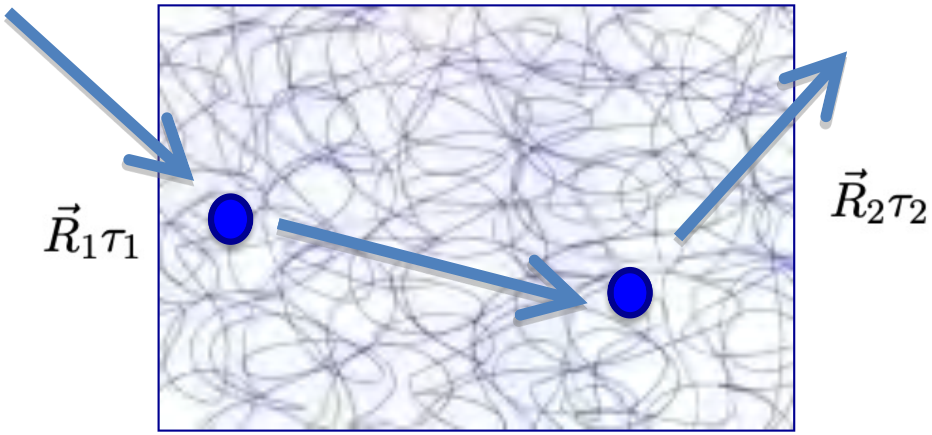
(DΓA, DF, TRILEX) → RMP **90**, 025003 (2018)

*J. Hubbard, Proc. Royal Soc. A, **276**, 238– 257 (1963)*

M. Qin, TS, et al., "The Hubbard model: a computational perspective", arXiv:2104.00064, submitted to Annual Reviews

Quantum field theoretical description of spectra: one-particle Green functions





$$G(\vec{R}_1\tau_1, \vec{R}_2\tau_2) = \left\langle T_\tau \hat{c}^\dagger_{\vec{R}_1}(\tau_1)\hat{c}_{\vec{R}_2}(\tau_2)\right\rangle$$

Fourier transforms
time-/translation invariance

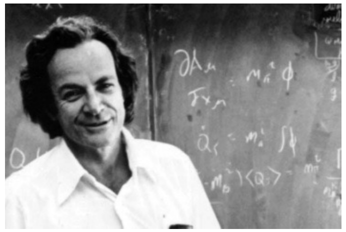
G^k

k=(**k**, iν) four vector
ν = (2n+1)πT, n integer

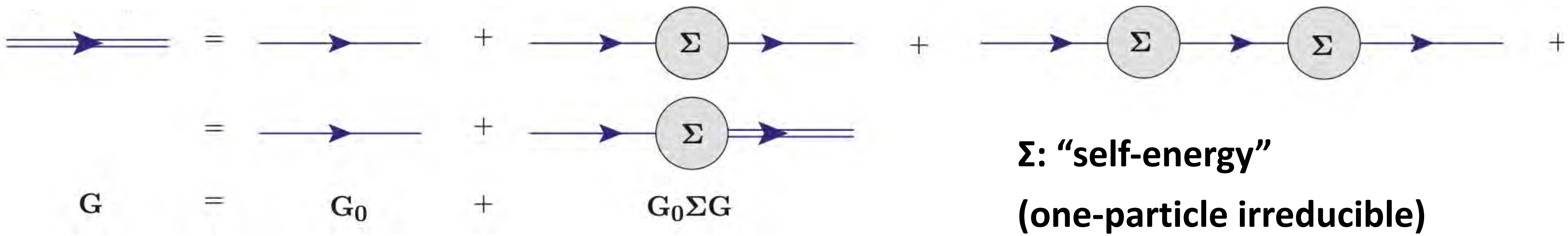
One-particle spectrum: $A(\vec{k},\omega) = -\frac{1}{\pi}\,\mathrm{Im}G_R(\vec{k},\omega)$

G_0 (free) propagation with momentum **k**

U local interaction



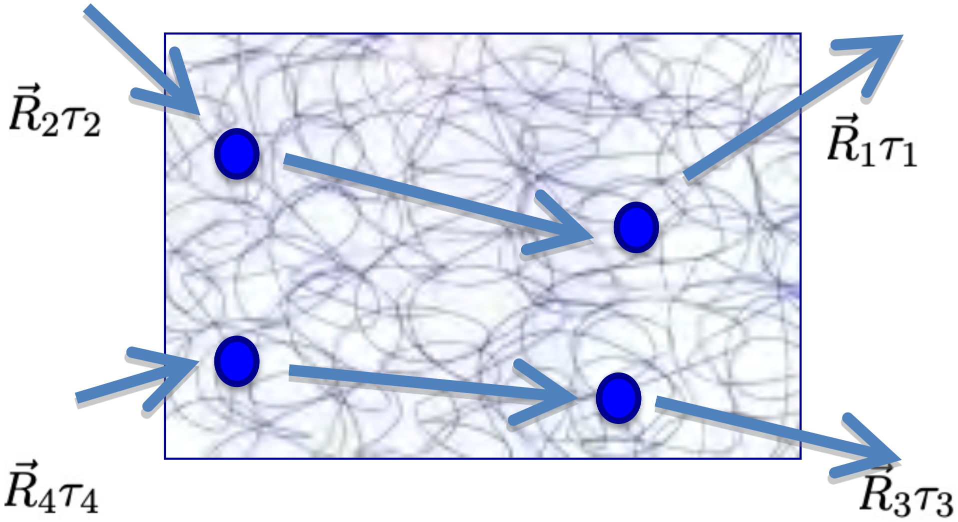
Dyson equation



Σ: “self-energy”

(one-particle irreducible)

Quantum field theoretical description of linear response: two-particle Green functions



$$G_{2,\sigma\sigma'}(\vec{R}_1\tau_1,\vec{R}_2\tau_2,\vec{R}_3\tau_3,\vec{R}_4\tau_4) = \left\langle T_\tau \hat{c}^\dagger_{\vec{R}_1,\sigma}(\tau_1)\hat{c}_{\vec{R}_2,\sigma}(\tau_2) T_\tau \hat{c}^\dagger_{\vec{R}_3,\sigma'}(\tau_3)\hat{c}_{\vec{R}_4,\sigma'}(\tau_4)\right\rangle$$

Fourier transforms (ph convention)
time-/translation invariance

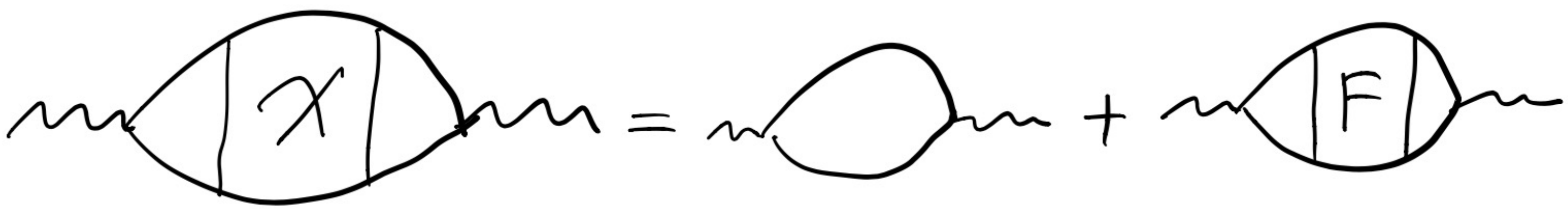
$$G^{kk'q}_{2,\sigma\sigma'}$$

q=(**q**,iω) four vector
ω=2nπT, n integer

$$G^{kk'q}_{2,\sigma\sigma'} = G^{kk'q}_{2,\text{conn},\sigma\sigma'} + G^{kk'q}_{2,\text{disconn},\sigma\sigma'}$$

$$G^{kk'q}_{2,\text{conn},\sigma\sigma'} = -G^k G^{k+q} F^{kk'q}_{\sigma\sigma'} G^{k'} G^{k'+q}$$

Full vertex F



physical susceptibility χ(q,ω)
(e.g. charge, spin, pairing)

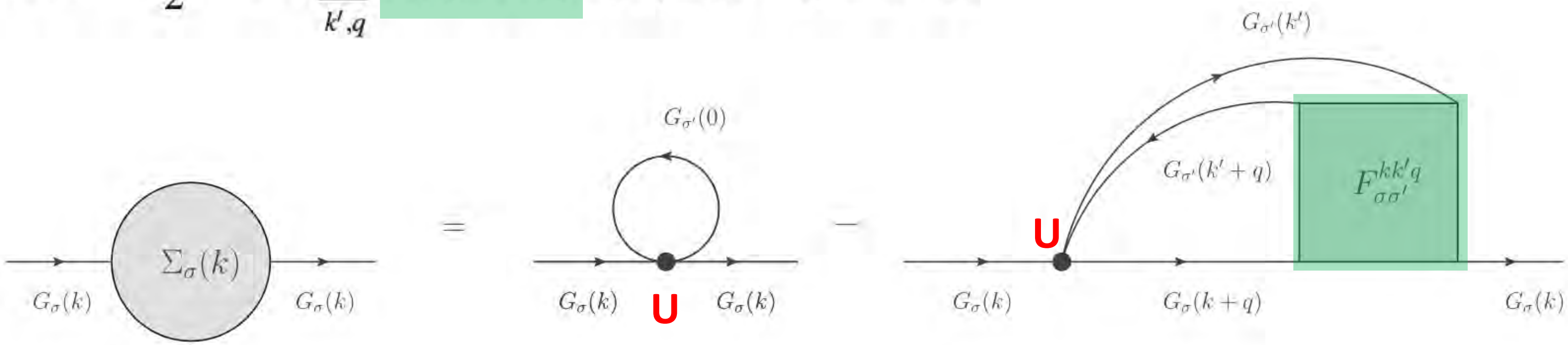
“bubble contribution”

“vertex corrections”

Connecting one- and two-particle level: the Dyson-Schwinger equation of motion (DSE)

$$\Sigma(k) = \frac{Un}{2} - UT^2 \sum_{k',q} F_{\uparrow\downarrow}(k,k',q)\, G(k')\, G(k'+q)\, G(k+q)$$

Full vertex F (from G_2)



How can we tackle the complex problem of analyzing the DSE with F?

Strategies of tackling complex problems: rely on Latin mottos!

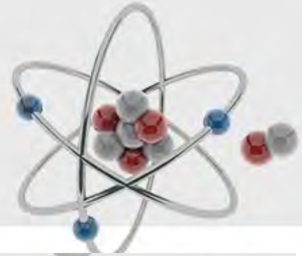
”teach everything”
good start (however, not very constructive)

“divide and rule”

“change what has to be changed”

TS and A. Toschi, J. Phys.: Condens. Matter ***33*** *214001 (2021), Special Issue: Emerging Leaders 2020*

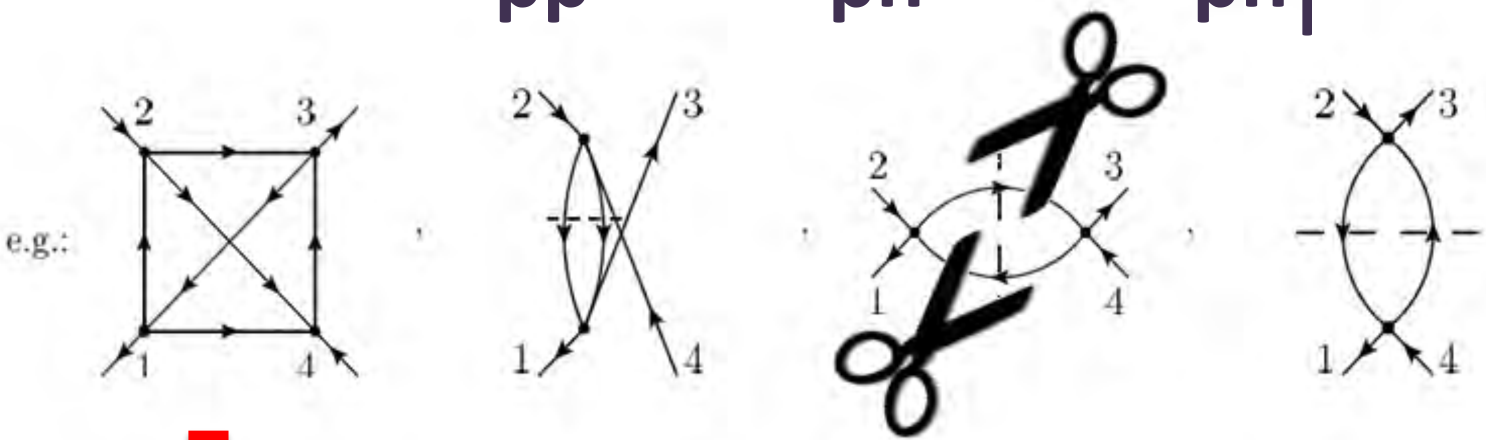
“Divide et impera”: subdividing the full vertex F via the parquet equations



$$\Sigma(k) = \frac{Un}{2} - UT^2 \sum_{k',q} F_{\uparrow\downarrow}(k,k',q)\, G(k')\, G(k'+q)\, G(k+q)$$

$$\mathbf{F} = \Lambda + \Phi_{pp} + \Phi_{ph} + \Phi_{ph_T}$$

All connected 2P diagrams



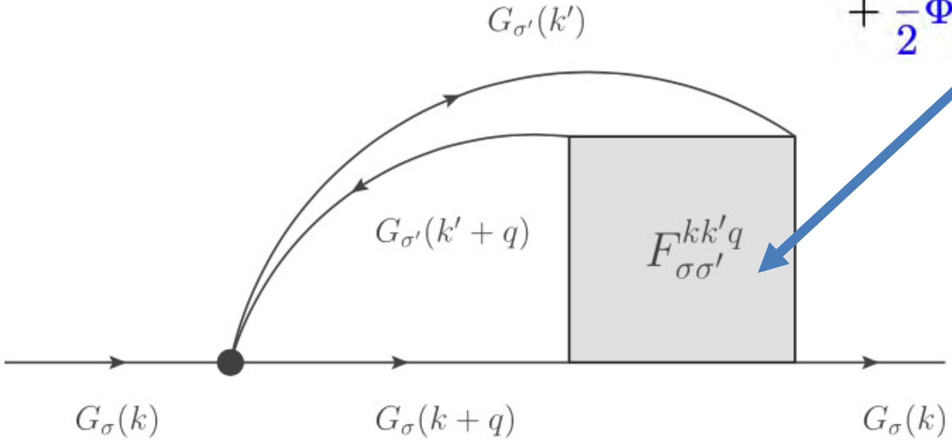
Fully irreducible vertex **Λ**

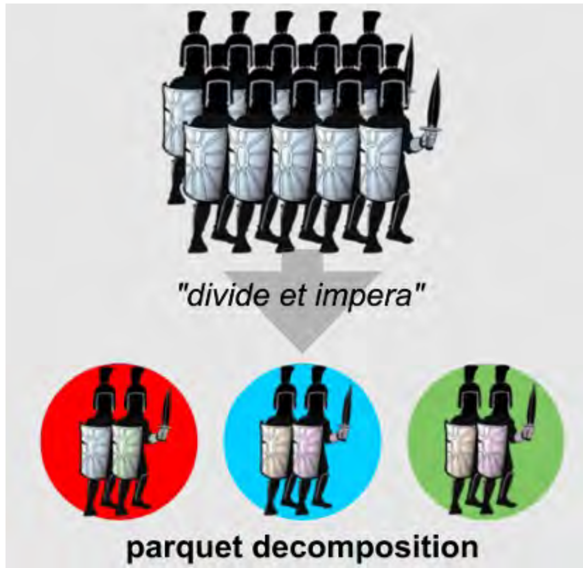
Full vertex **F**
(“scattering amplitude”)

C. de Dominicis and P. C. Martin, J. Math. Phys. ***5****, 14/31 (1964)*

"Divide et impera": the parquet decomposition of the self-energy

$$F_{\uparrow\downarrow}(k,k',q) = \Lambda_{\uparrow\downarrow}(k,k',q) + \Phi_{pp,\uparrow\downarrow}(k,k',k+k'+q) + \frac{1}{2}\Phi_{ch}(k,k',q) - \frac{1}{2}\Phi_{sp}(k,k',q) - \Phi_{sp}(k,k+q,k'-k)$$





$$\Sigma = \Sigma_\Lambda + \Sigma_{\rm pp} + \Sigma_{\rm ch} + \Sigma_{\rm sp}$$

*O. Gunnarsson, TS, et al., Phys. Rev. B **93**, 245102 (2016)*

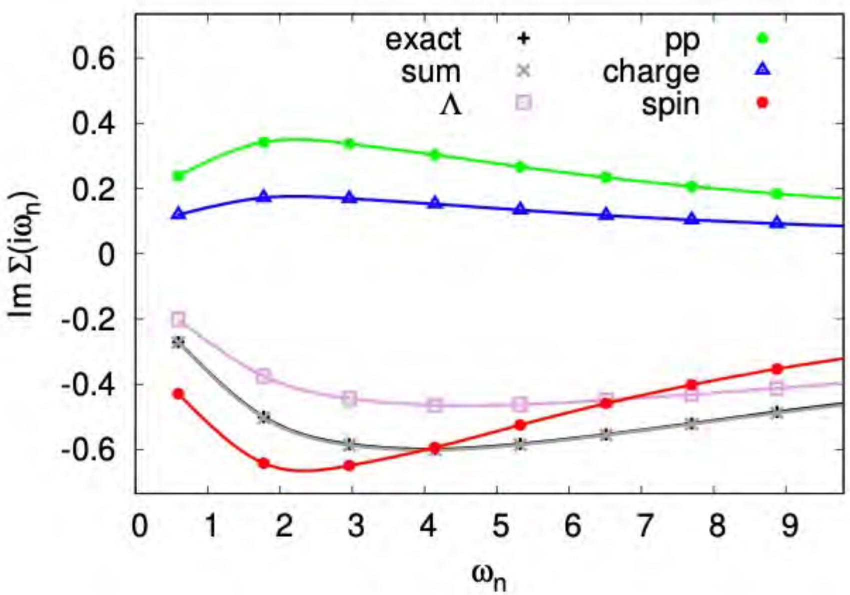
Parquet decomposition: application 1
first DMFT and DCA calculations

Model: Hubbard model

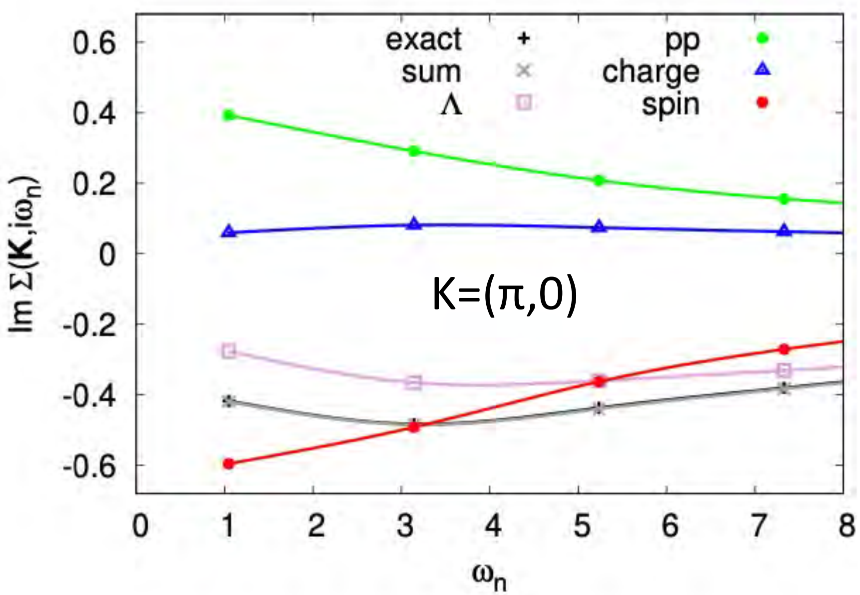
Techniques: DMFT, DCA with N_c=8

$$\Sigma = \Sigma_\Lambda + \Sigma_{pp} + \Sigma_{ch} + \Sigma_{sp}$$

3D cubic, DMFT, n=1, T=0.19t, U=4.9t



2D square, DCA, n=0.85, T=0.33t, U=4t

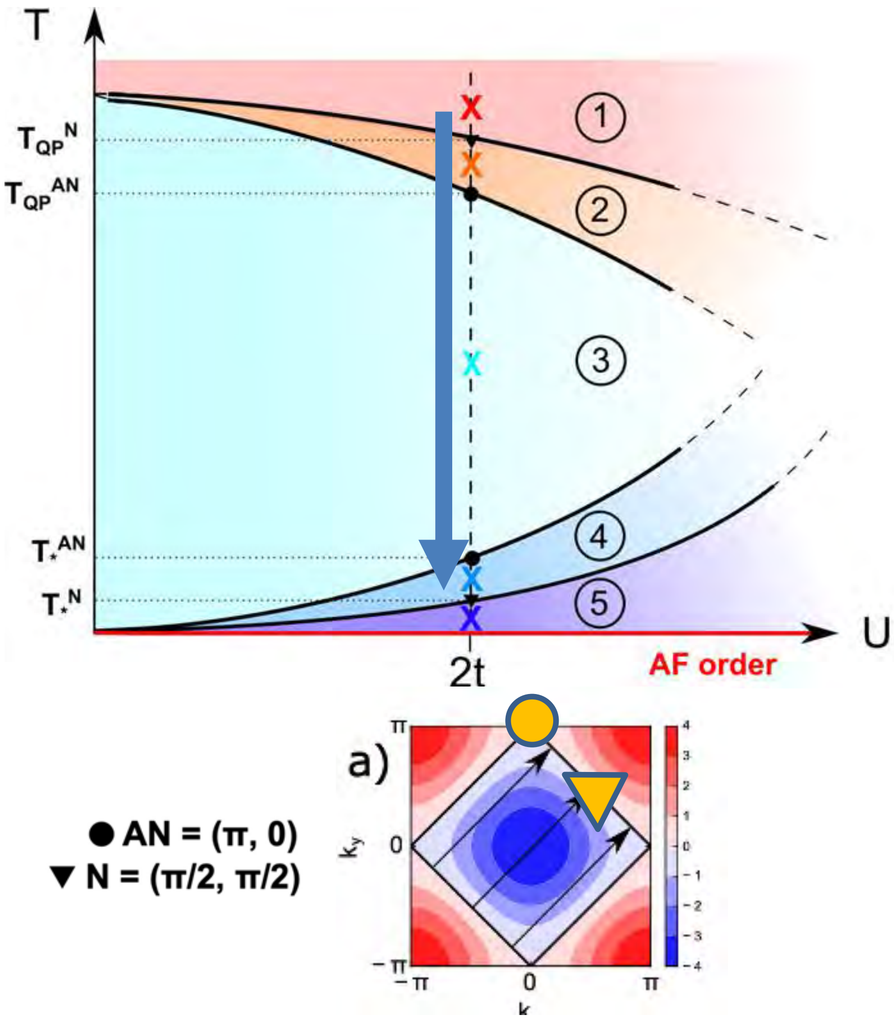


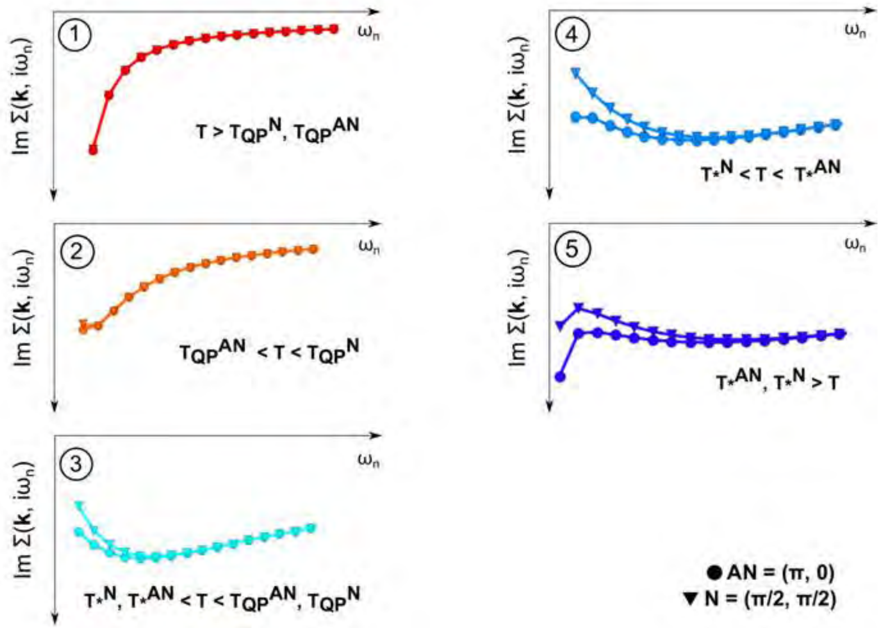
*O. Gunnarsson, TS, et al., Phys. Rev. B **93**, 245102 (2016)*

*TS and A. Toschi, J. Phys.: Condens. Matter **33** 214001 (2021)*

Parquet decomposition: application 2
two magnetic regimes at weak coupling

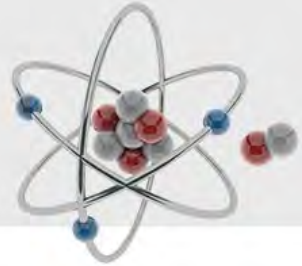
Model: 2D Hubbard, n=1 (half filling), simple square lattice, U=2t



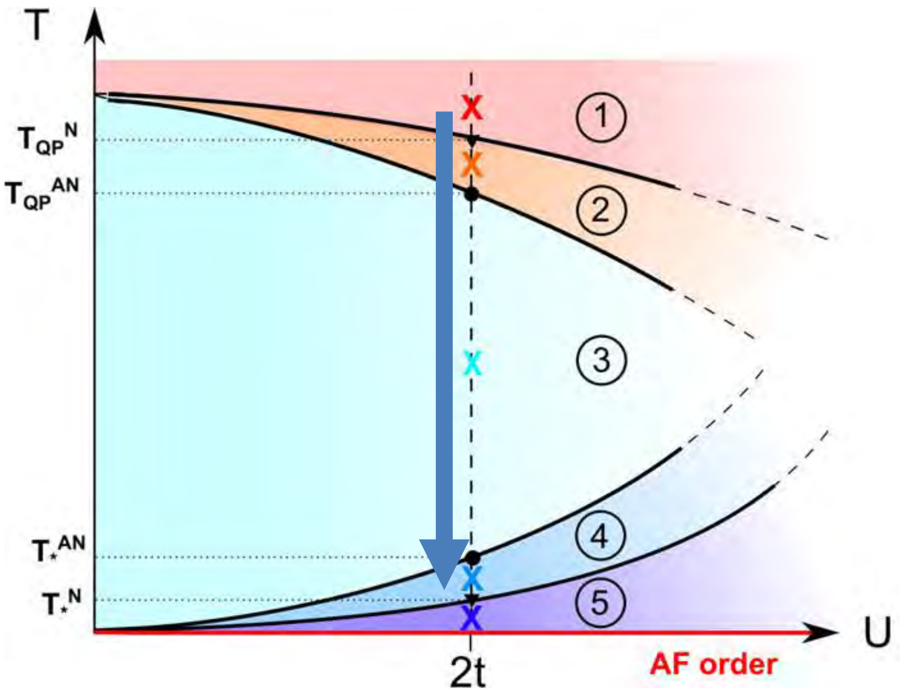


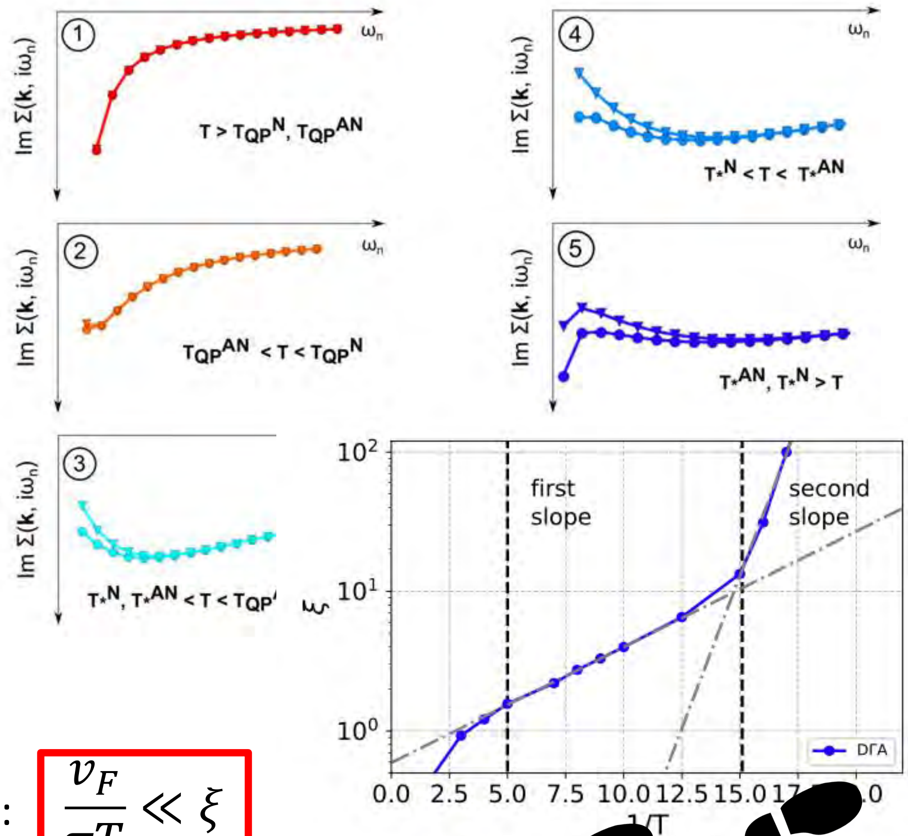
T. Schäfer, et al., Phys. Rev. X ***11****, 01158 (2021)*
TS and A. Toschi, J. Phys.: Condens. Matter ***33*** *214001 (2021)*

Parquet decomposition: application 2
two magnetic regimes at weak coupling



Model: 2D Hubbard, n=1 (half filling), simple square lattice, U=2t

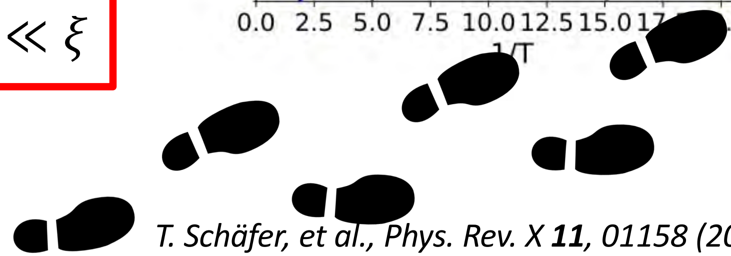




Magnetic correlation length exponentially growing!

Condition for **pseudogap** at weak coupling (Vilk criterion): $\frac{v_F}{\pi T} \ll \xi$

→ Footprints of spin fluctuations in all observables (on the one- **and** two-particle level)

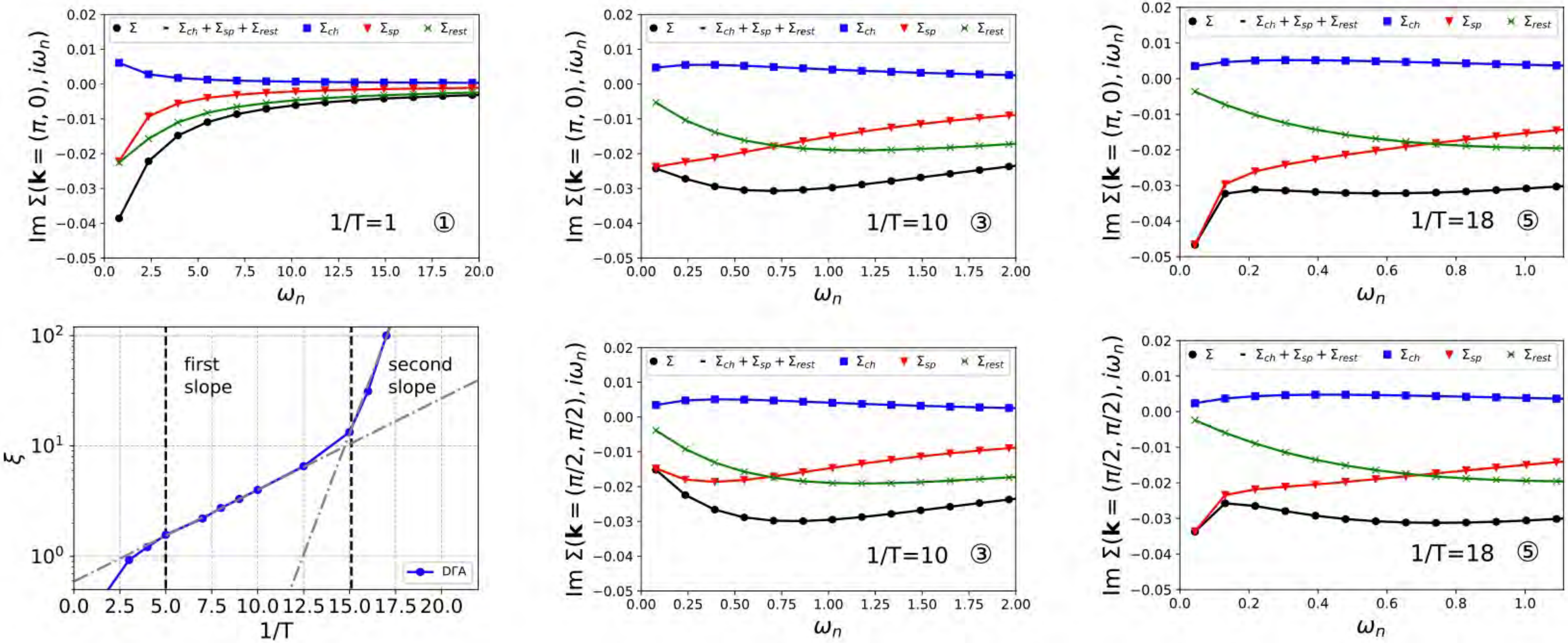


T. Schäfer, et al., Phys. Rev. X ***11****, 01158 (2021)*
TS and A. Toschi, J. Phys.: Condens. Matter ***33*** *214001 (2021)*

Parquet decomposition: application 2
two magnetic regimes at weak coupling

Model: 2D Hubbard, n=1 (half filling), simple square lattice, U=2t
Technique: DΓA (ladder in spin channel)

$$\Sigma = \Sigma_\Lambda + \Sigma_{pp} + \Sigma_{ch} + \Sigma_{sp}$$

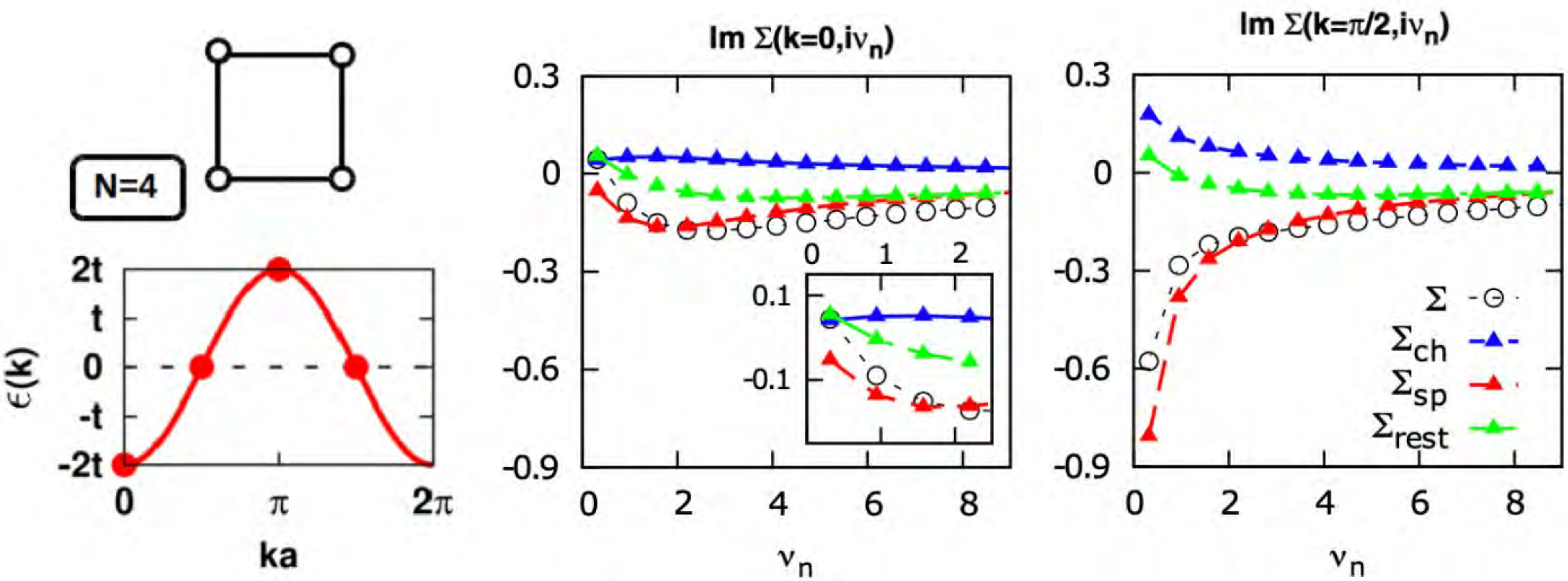


*TS and A. Toschi, J. Phys.: Condens. Matter **33** 214001 (2021)*

Parquet decomposition: application 3
Hubbard nano rings

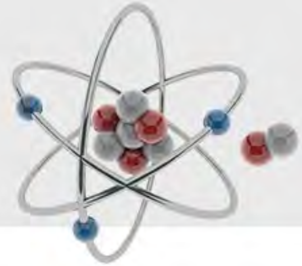
Model: 1D Hubbard nano ring with four sites, n=1 (half filling), U=2t
Technique: DΓA (ladder in spin channel)

$$\Sigma = \Sigma_{\Lambda} + \Sigma_{\mathrm{pp}} + \Sigma_{\mathrm{ch}} + \Sigma_{\mathrm{sp}}$$



A. Valli, TS, et al., Phys. Rev. B ***91****, 115115 (2015)*
TS and A. Toschi, J. Phys.: Condens. Matter ***33*** *214001 (2021)*

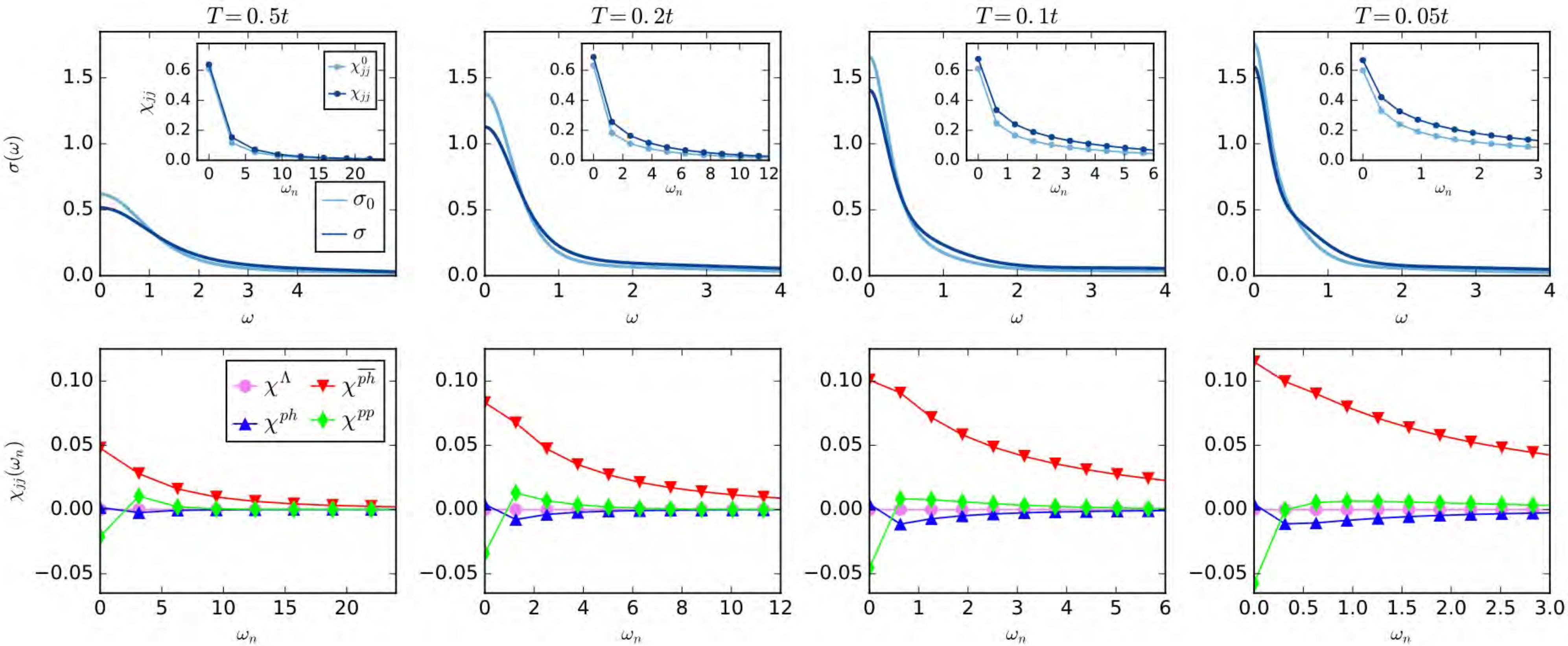
Parquet decomposition: application 4
current-current response functions



Model: 2D Hubbard, n=1, U=4t

Technique: DΓA

$$\chi_r = \chi_0 - \chi_0 \Gamma_r \chi = \chi_0 - \chi_0 F \chi_0 \qquad F = \Lambda + \Phi_{pp} + \Phi_{ph} + \Phi_{\overline{ph}}$$



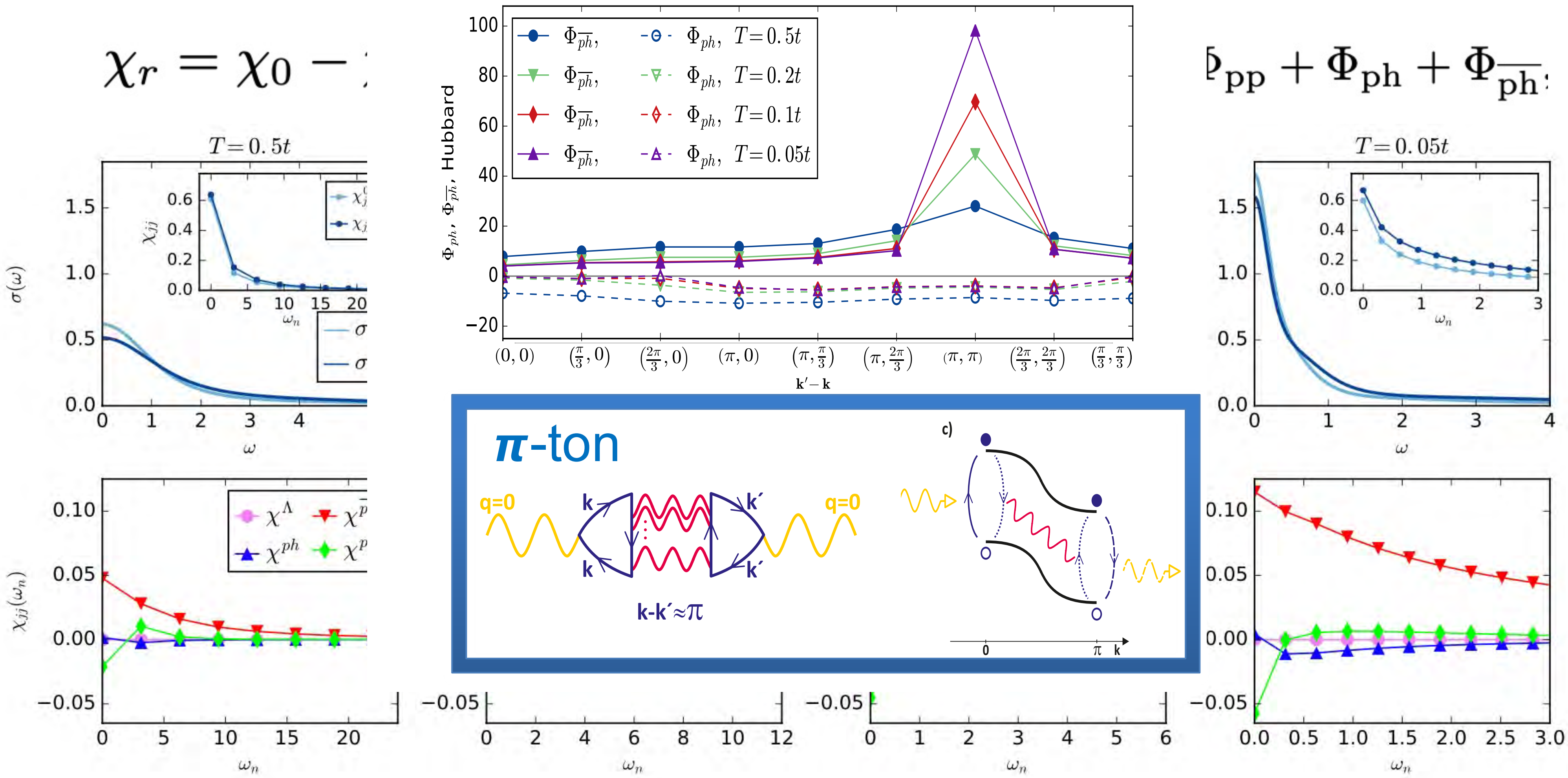
A. Kauch, et al., Phys. Rev. Lett. ***124***,*047401 (2020)*

TS and A. Toschi, J. Phys.: Condens. Matter ***33*** *214001 (2021)*

Parquet decomposition: application 4
current-current response functions

Model: 2D Hubbard, n=1, U=4t

Technique: DΓA



A. Kauch, et al., Phys. Rev. Lett. ***124****,047401 (2020)*

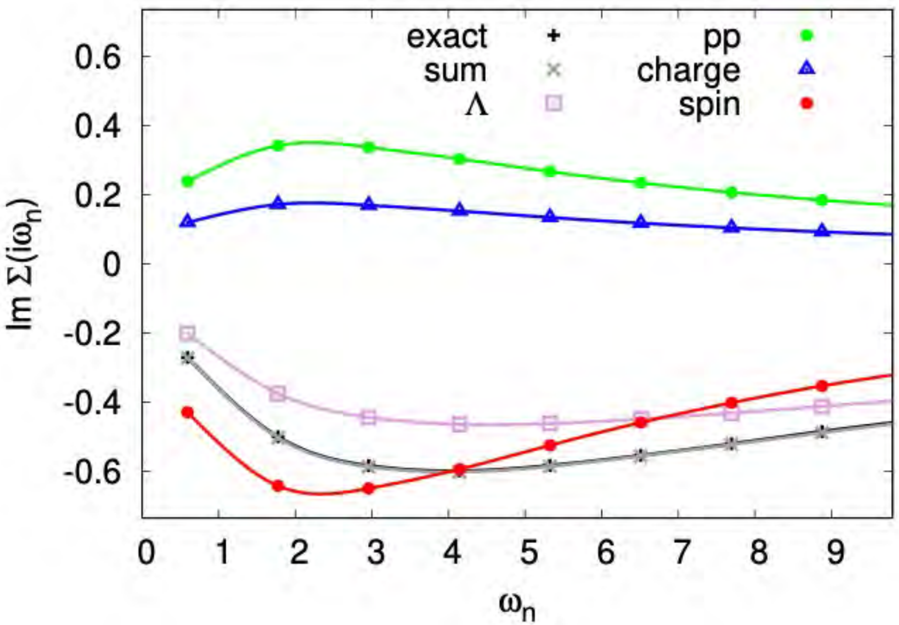
TS and A. Toschi, J. Phys.: Condens. Matter ***33*** *214001 (2021)*

Parquet decomposition: from weak to strong coupling

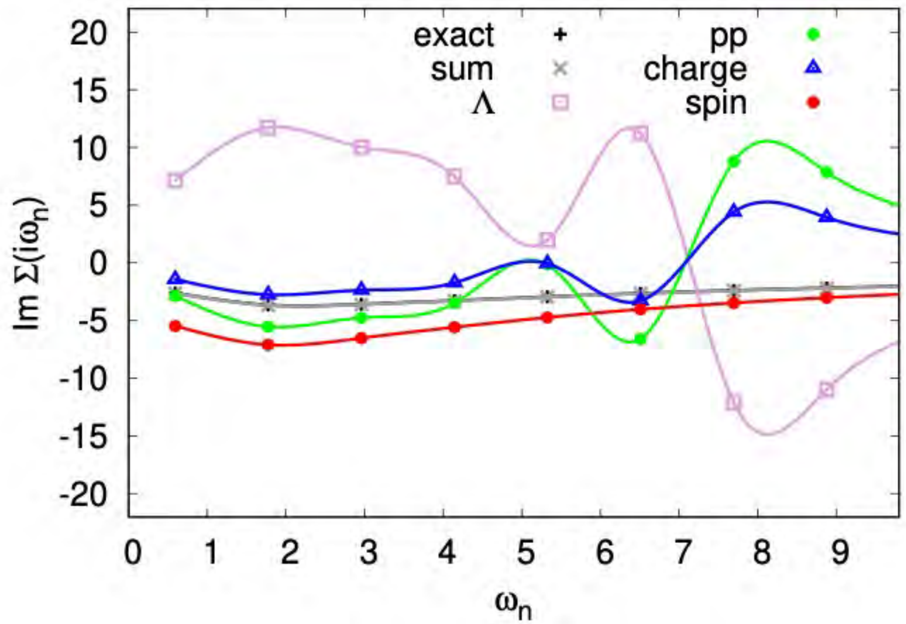
Model: 3D Hubbard, n=1 (half filling), simple cubic lattice, T=0.19t
Technique: DMFT

$$\Sigma = \Sigma_\Lambda + \Sigma_{\rm pp} + \Sigma_{\rm ch} + \Sigma_{\rm sp}$$

U=4.9t

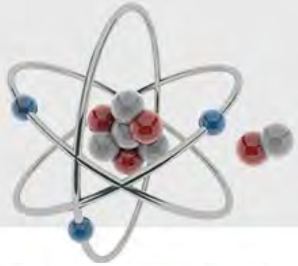


U=9.8t

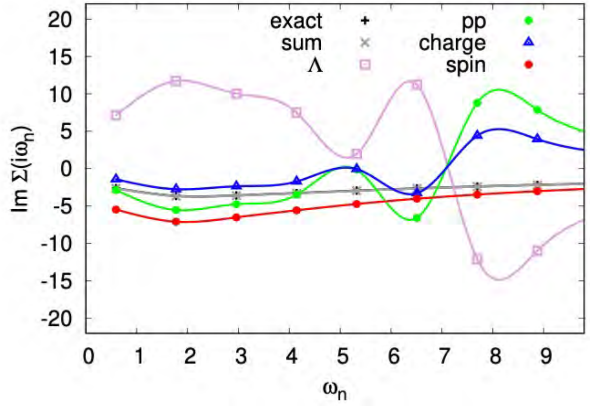


*O. Gunnarsson, TS, et al., Phys. Rev. B **93**, 245102 (2016)*
*TS and A. Toschi, J. Phys.: Condens. Matter **33** 214001 (2021)*

Parquet decomposition: from weak to strong coupling



Model: 3D Hubbard, n=1 (half filling), simple cubic lattice, T=0.19t
Technique: DMFT



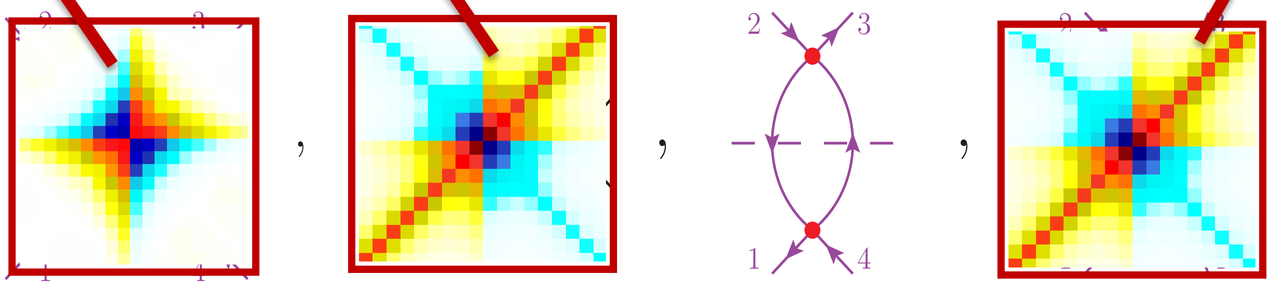
Reason: divergences of vertex parts of the parquet decomposition

∞ ∞ ∞

F

Well behaved

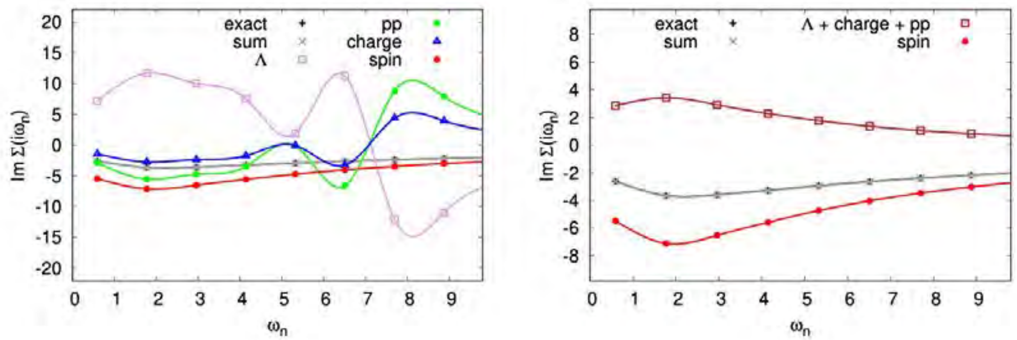
$$\Lambda_{2PI} + \Phi_{ch} + \Phi_{sp} + \Phi_{pp}$$



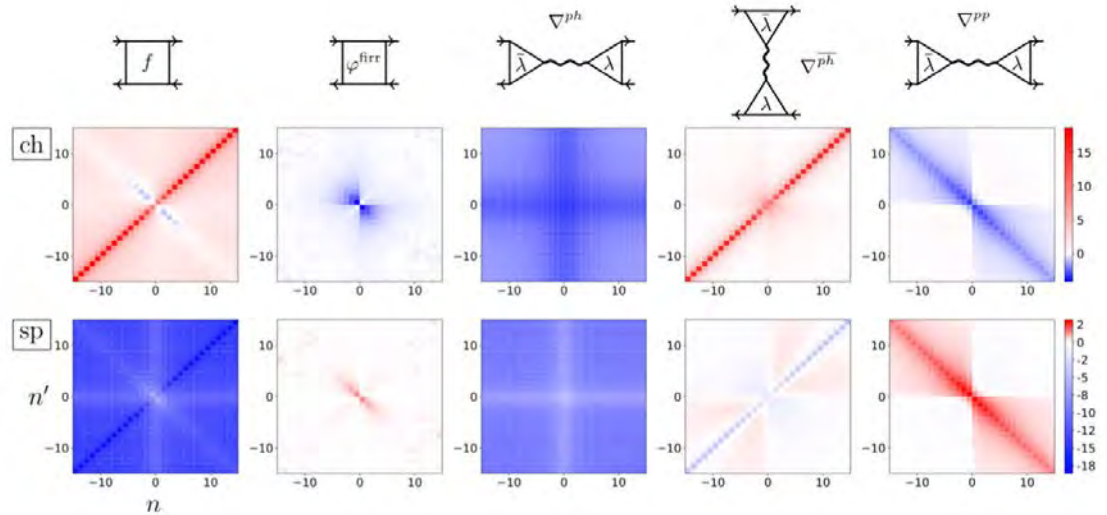
O. Gunnarsson, TS, et al., Phys. Rev. B ***93****, 245102 (2016)*
TS, et al. Phys. Rev. Lett. ***110****, 246405 (2013), TS, et al., Phys. Rev. B* ***94****, 235108 (2016), O. Gunnarsson et al., Phys. Rev. Lett.* ***119****, 056402 (2017), …*

How to circumvent the divergences?

Bethe-Salpeter summations (well behaved dominant channel)



Different decomposition (not parquet, but, e.g. single boson exchange)



*F. Krien, et al., Phys. Rev. B **100**, 155149 (2019)*

*O. Gunnarsson, TS, et al., Phys. Rev. B **93**, 245102 (2016)*
*TS, et al. Phys. Rev. Lett. **110**, 246405 (2013), TS, et al., Phys. Rev. B **94**, 235108 (2016), O. Gunnarsson et al., Phys. Rev. Lett. **119**, 056402 (2017), …*
*J. Vučičević et al., Phys. Rev. B **97**, 125141 (2018),*

Strategies of tackling complex problems: rely on Latin mottos!

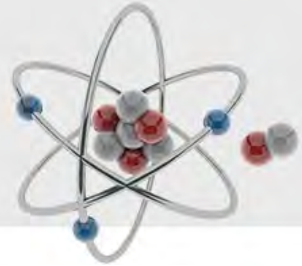
”teach everything”
good start (however, not very constructive)

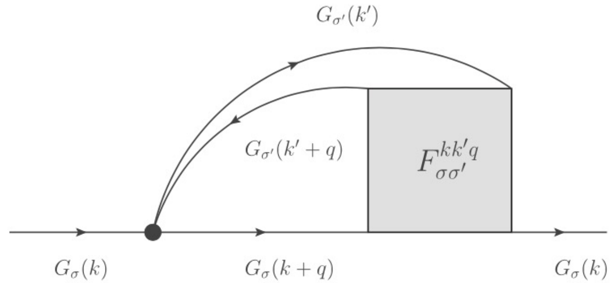
“divide and rule”

“change what has to be changed”

TS and A. Toschi, J. Phys.: Condens. Matter ***33*** *214001 (2021), Special Issue: Emerging Leaders 2020*

“Mutatis mutandis”: changing the representation of the DSE…

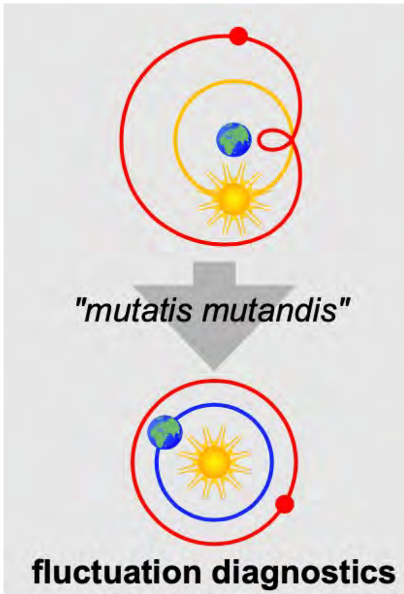




$$
\begin{aligned}
\Sigma(k) - \frac{Un}{2} &= \\
&= UT^2 \sum_{k',q} F_{\uparrow\downarrow}(k,k';q)\, G(k')G(k'+q)G(k+q), \\
&= -UT^2 \sum_{k',q} F_{\rm sp}(k,k';q)\, G(k')G(k'+q)G(k+q) \\
&= \quad UT^2 \sum_{k',q} F_{\rm ch}(k,k';q)\, G(k')G(k'+q)G(k+q) \\
&= -UT^2 \sum_{k',q} F_{\rm pp}(k,k';q)\, G(k')G(q-k')G(q-k)
\end{aligned}
$$

Equivalent due to SU(2)-symmetry and crossing relations

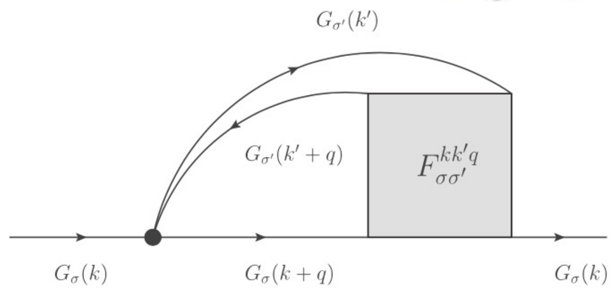
Same result, if all sums are performed – what about partial sums?



O. Gunnarsson, TS, et al., Phys. Rev. Lett. ***114****, 236402 (2015)*

"Mutatis mutandis": … and performing partial sums…

$$\Sigma(k) - \frac{Un}{2} = $$
$$= UT^2 \sum_{k',q} F_{\uparrow\downarrow}(k,k';q)\, G(k')G(k'+q)G(k+q)$$



… omitting the sum over the transfer momentum **Q**

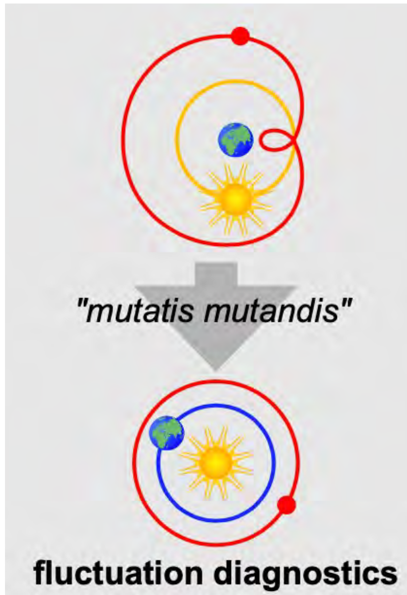
$$\tilde{\Sigma}(k)_{\mathbf{Q}} - \frac{Un}{2} = $$ → histograms

$$= -UT^2 \sum_{k',i\Omega_n} F_{\rm sp}(k,k';q)\, G(k')G(k'+q)G(k+q)$$

… omitting the sum over the bosonic frequency $i\Omega_n$

$$\tilde{\Sigma}(k)_{i\Omega_n} - \frac{Un}{2} = $$ → pie charts

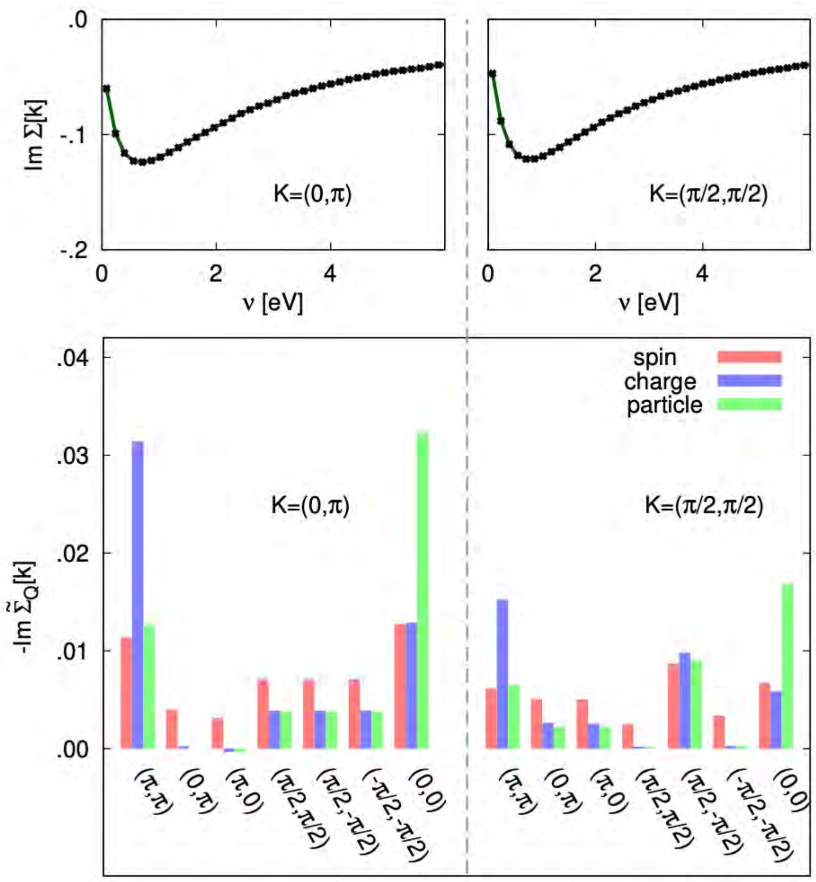
$$= -UT^2 \sum_{k',\mathbf{Q}} F_{\rm sp}(k,k';q)\, G(k')G(k'+q)G(k+q)$$

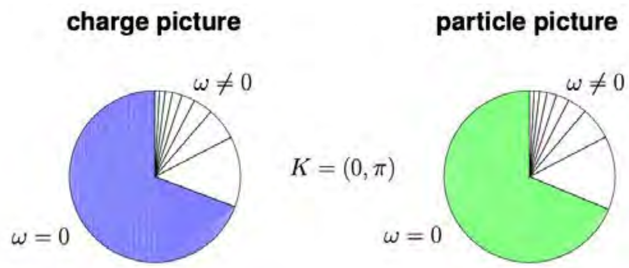


O. Gunnarsson, TS, et al., Phys. Rev. Lett. ***114****, 236402 (2015)*

Fluctuation diagnostics: application 1
The attractive Hubbard model

Model: 2D Hubbard, n=0.87, square lattice, T=0.1t, U=-4t
Technique: DCA, N_c=8





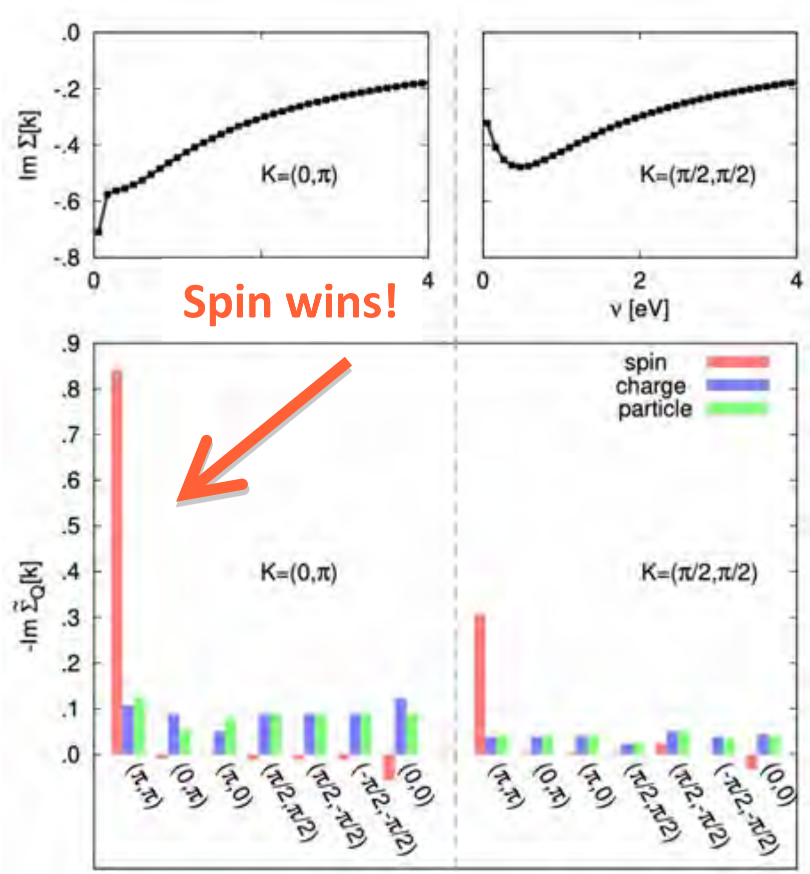
Charge and pp fluctuations well-defined and long-lived!

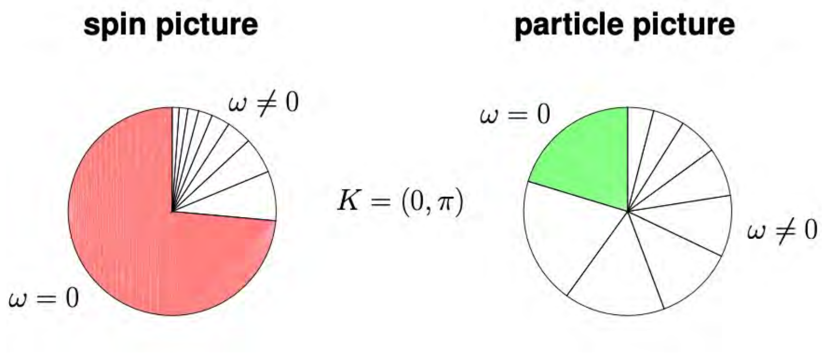
O. Gunnarsson, TS, et al., Phys. Rev. Lett. ***114****, 236402 (2015)*

Fluctuation diagnostics: application 2
The repulsive Hubbard model: origin of the pseudogap

Model: 2D Hubbard, n=0.94, square lattice, t'=-0.15t, T=0.067t, U=7t

Technique: DCA, N_c=8





long-lived

short-lived

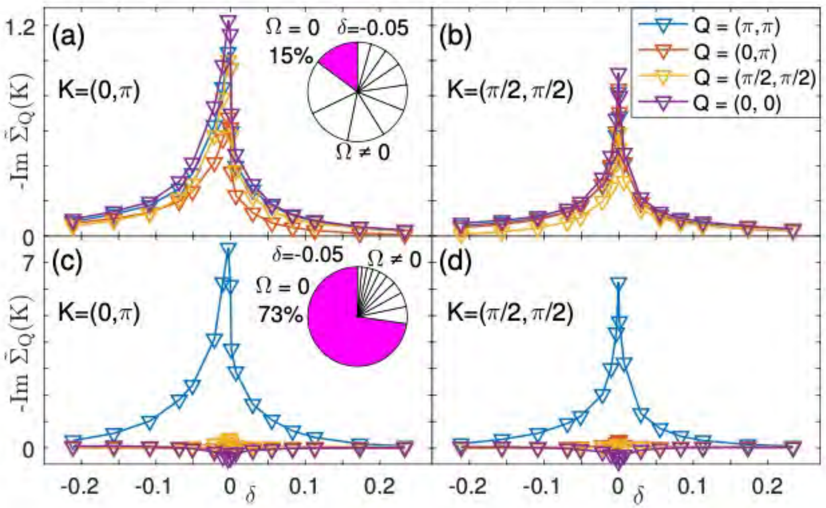
O. Gunnarsson, TS, et al., Phys. Rev. Lett. ***114****, 236402 (2015)*

Fluctuation diagnostics: application 2
The repulsive Hubbard model: origin of the pseudogap

Model: 2D Hubbard, square lattice, t'=-0.15t, T=0.1t, U=7t

Technique: DCA with N_C=8

Charge picture

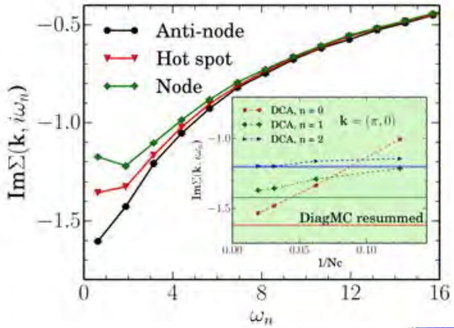


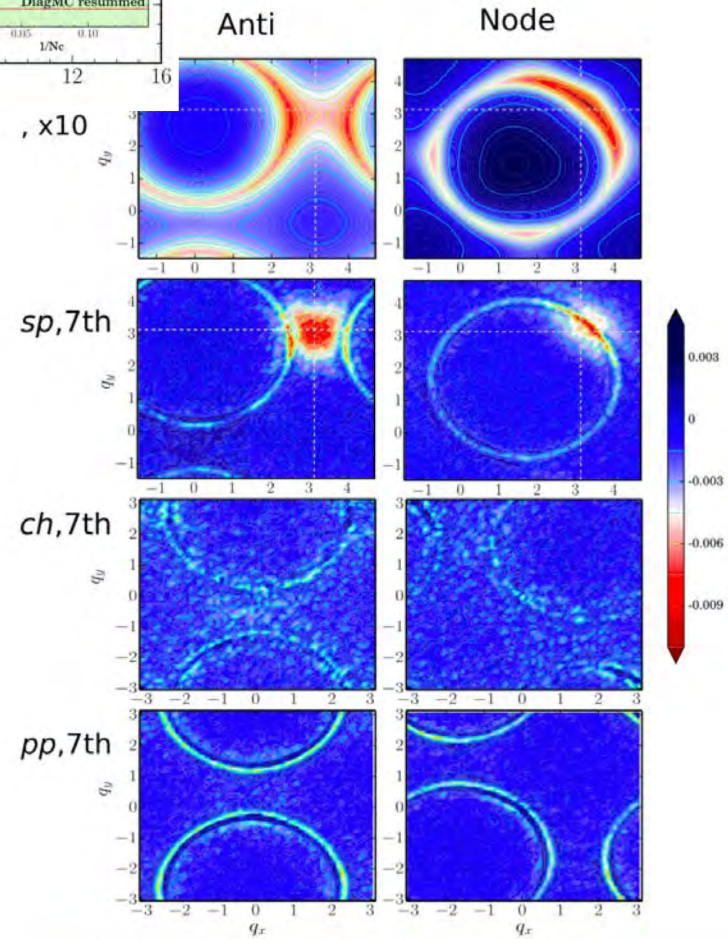
Spin picture

n=0.94

t'=-0.3t, T=0.2t, U=5.6t

DiagMC





X. Dong, et al., Phys. Rev. B ***100****, 235107 (2019)*

W. Wu, et al., Phys. Rev. B ***96****, 041105(R) (2017)*

Fluctuation diagnostics: application 2
Origin of the pseudogap: 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 !

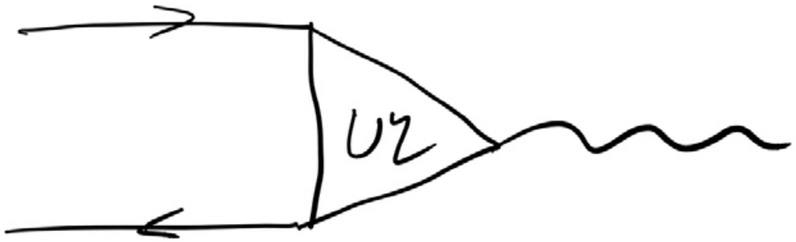
O. Gunnarsson, TS, et al., Phys. Rev. Lett. ***114****, 236402 (2015)*

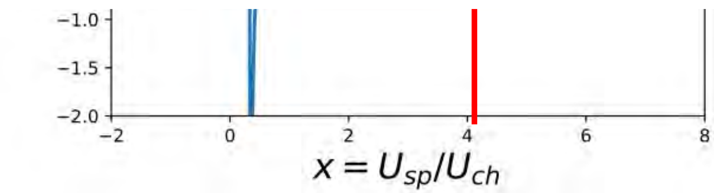
Fluctuation diagnostics: application 3
Estimation of Fierz parameter

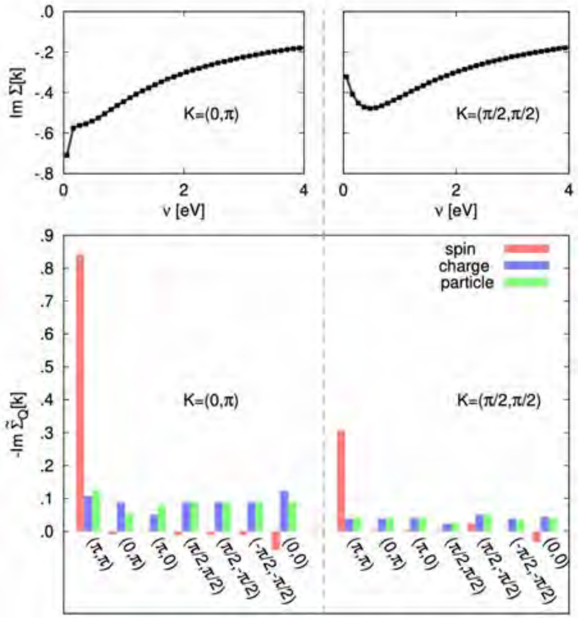
TRILEX: mixed fermionic-bosonic language

$$U n_\uparrow n_\downarrow = \frac{1}{2} U_{\text{ch}} nn + \frac{1}{2} U_{\text{sp}} \vec{s}\vec{s}, \qquad U = U_{\text{ch}} - 3U_{\text{sp}}$$

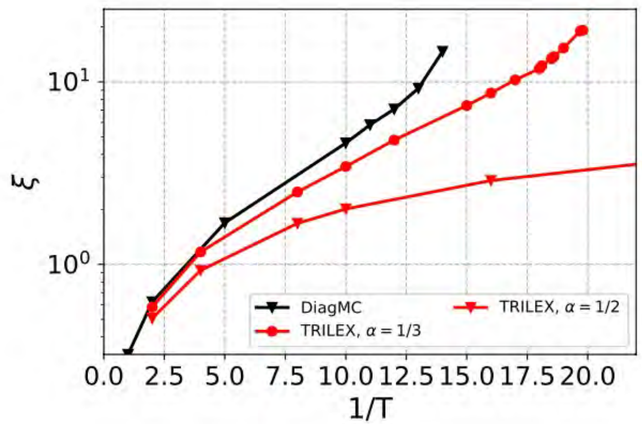
$$U_{\text{ch}} = (3\alpha - 1)U$$
$$U_{\text{sp}} = (\alpha - 2/3)U \qquad x \equiv U_{\text{sp}}/U_{\text{ch}}$$





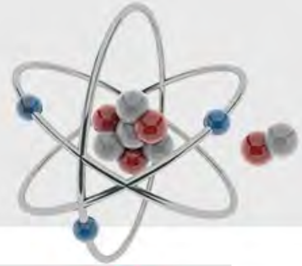


$$\frac{\text{Im}\,\tilde{\Sigma}_{\text{sp}}(\mathbf{k} = (\pi, 0), i\omega_0)}{\text{Im}\,\tilde{\Sigma}_{\text{ch}}(\mathbf{k} = (\pi, 0), i\omega_0)} \approx 4$$

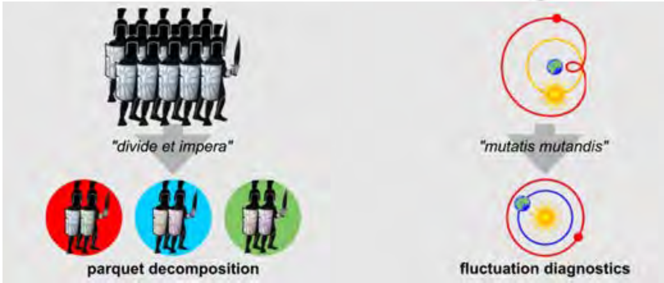


*T. Ayral and O. Parcollet, Phys. Rev. B **92**, 115109 (2015), Phys. Rev. B **93**, 235124 (2016)*
*TS and A. Toschi, J. Phys.: Condens. Matter **33** 214001 (2021)*

Conclusions and perspective

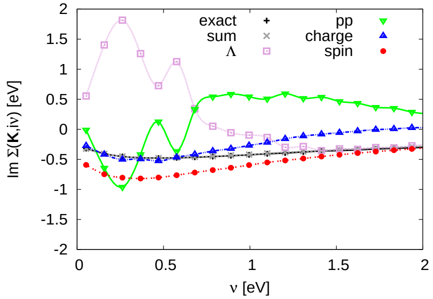


- General strategies for insight in the origins of correlated spectra via the Dyson-Schwinger equation of motion

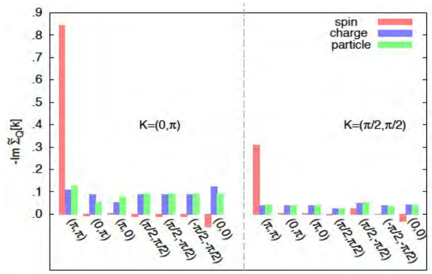


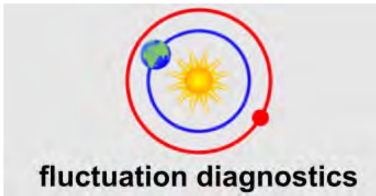
- Prerequisite: access to (unbiased) one- and two-particle Green function

- Parquet decomposition
  - Numerically heavier (parquet inversions)
  - Unstable for increasing U
  - Generalizable to response functions

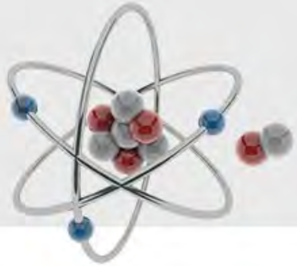


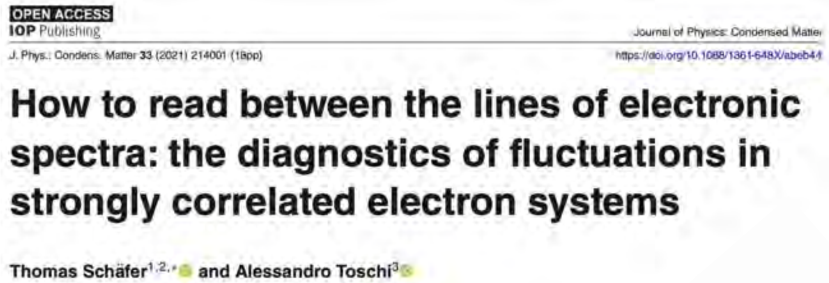
- Fluctuation diagnostics
  - Relatively lightweighed
  - Flexible / applicable everywhere





Conclusions and perspective

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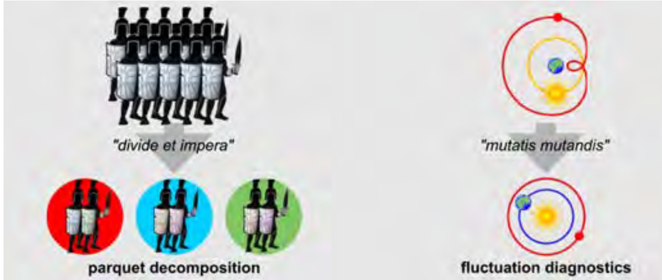
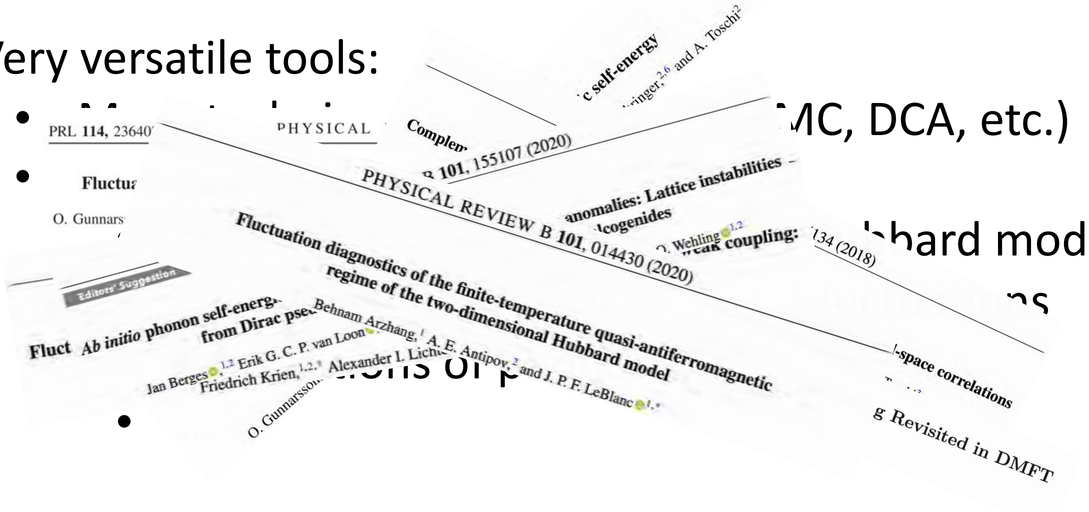
J. Phys.: Condens. Matter 33 (2021) 214001 (18pp)
https://doi.org/10.1088/1361-648X/abeb44

How to read between the lines of electronic spectra: the diagnostics of fluctuations in strongly correlated electron systems

Thomas Schäfer[1,2,*] and Alessandro Toschi[3]



- Very versatile tools:
  - ...MC, DCA, etc.)
  - ...bbard model
  - ...ns
  - ...ions of p...
    -



- Outlook
  - Multiorbital systems
  - Symmetry-broken phases
  - Cluster diagnostics, symmetry diagnostics

TS and A. Toschi, J. Phys.: Condens. Matter ***33*** *214001 (2021)*
Special Issue: Emerging Leaders 2020

C. D. Friedrich, "Wanderer über dem Nebelmeer" (1818)