TECHNISCHE UNIVERSITÄT WIEN
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Fluctuation diagnostics of the electron self-energy – origin of the pseudogap physics

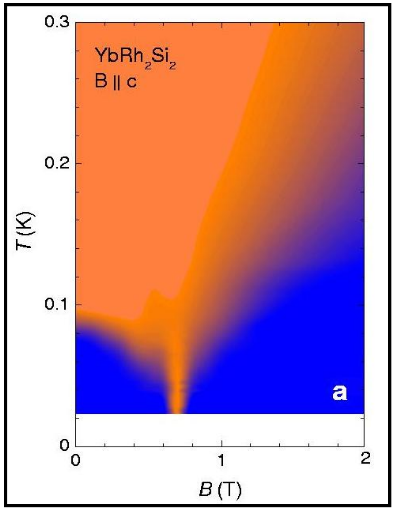
Thomas Schäfer
O. Gunnarsson, J. LeBlanc, E. Gull, J. Merino, G. Sangiovanni, G. Rohringer and A. Toschi

Phys. Rev. Lett. **114**, 236402 (2015)

The New Generation in Strongly Correlated Electron Systems
Trogir, Croatia, 14rd-18th September 2015

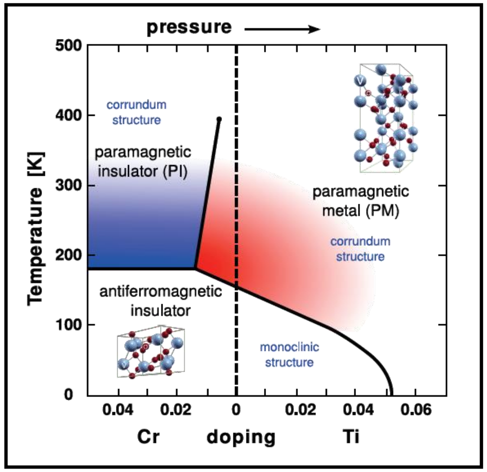
Strong correlations – fascinating physics

1) QUANTUM CRITICALITY



J. Custers et al., Nature (2003)

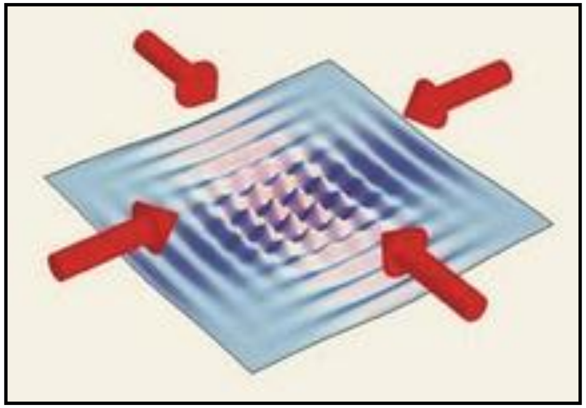
2) MOTT TRANSITION



Mc Whan et al., PRB (1973)

3) HIGH TEMPERATURE SUPERCONDUCTIVITY

4) OPTICAL LATTICES

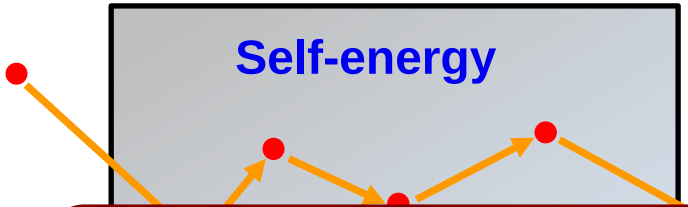


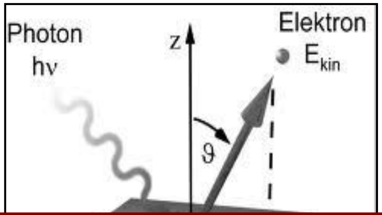
M. Greiner et al., Nature (2008)

Physical origin of spectra

Experiment: (AR)PES, InvPES, STM, ...

1P level



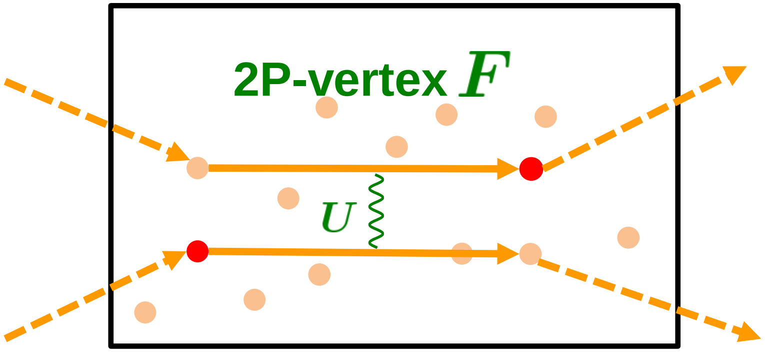


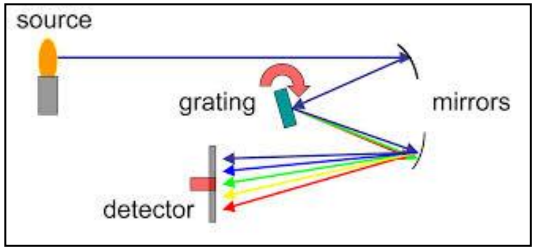
Σ not sufficient for identifying unambigously the underlying physics!

Origin of scattering?

Experiment: IR, INS, NMR, …

2P level





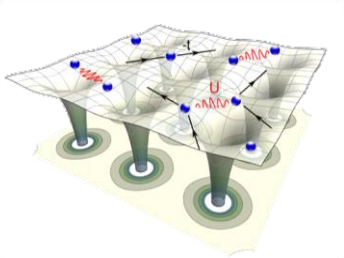
Outline

How to determine origin of spectra theoretically?

- Schwinger-Dyson equation of motion
- Fluctuation diagnostics method

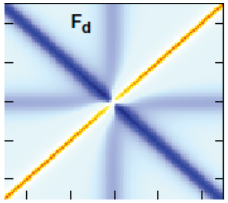
Application: two-dimensional Hubbard model

- Benchmark: **attractive** case
- Pseudogap physics: **repulsive** case



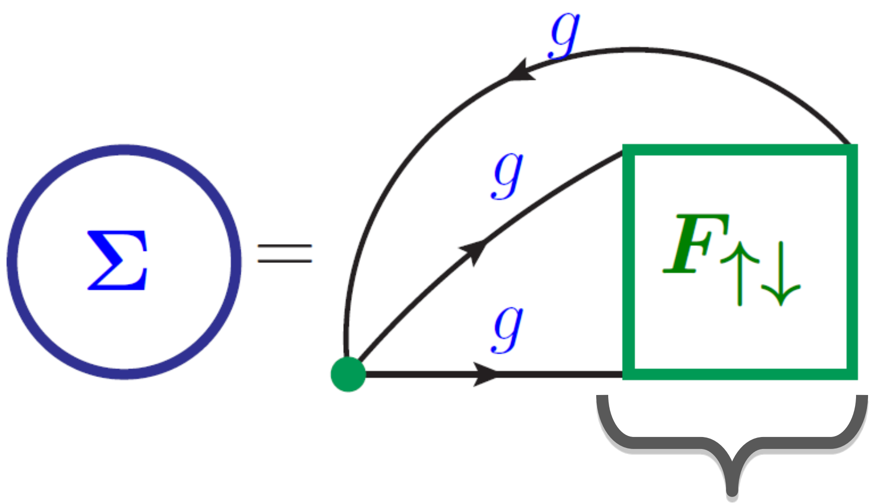
Further insight: weak-coupling analysis

- Analysis of the full vertex
- Consequences for d-wave pairing fluctuations



How to proceed in theory?

Starting from Dyson-Schwinger equation of motion (EOM)

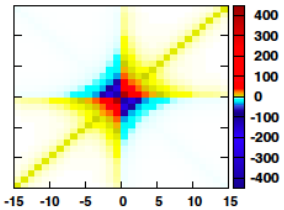


$$F_{\uparrow\downarrow} = \Gamma_{irr} + \phi_{ph} + \phi_{\overline{ph}} + \phi_{pp}$$

par **ition**

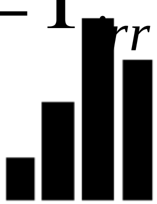
2P cible

$\Gamma_{IRR} \to \infty$



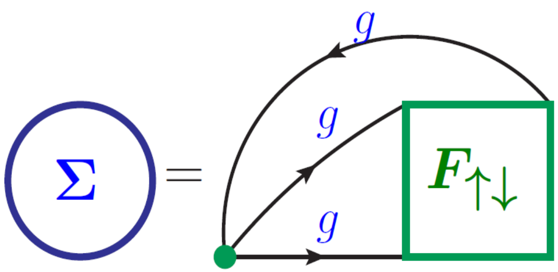
T. Schäfer et al., PRL (2013)

Change of representation



Fluctuation Diagnostics

Rewriting the EOM in different representations...



$$\Sigma(k) = \sum_{k',q} F_{\uparrow\downarrow}(k,k',q)ggg$$

$$q = (\vec{Q},\omega), k = (\vec{K},\nu)$$

Idea: Consider vertex $F_{\uparrow\downarrow}$ in different representations!

$$\boldsymbol{F_{ch}(k,k',q)} = F_{\uparrow\uparrow}(k,k',q) + F_{\uparrow\downarrow}(k,k',q) \quad \text{charge}$$

$$\boldsymbol{F_{sp}(k,k',q)} = F_{\uparrow\uparrow}(k,k',q) - F_{\uparrow\downarrow}(k,k',q) \quad \text{spin}$$

$$\boldsymbol{F_{pp}(k,k',q)} = F_{\uparrow\downarrow}(k,k',q-k-k') \quad \text{particle-particle}$$

Identical results after all **k**- and ω-summations

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

... and partially sum over frequency...

partial summation over all variables except momentum transfer **Q**

$$\tilde{\Sigma}_Q(k) = \sum_{k',\omega} F_r(k,k',q) ggg \quad r = ch, sp, pp \quad \Rightarrow \quad \Sigma(k) = \sum_Q \tilde{\Sigma}_Q(k)$$

Q ⇒ specific **spatial pattern** e^{iQR} ⇒ certain **collective mode** in the **given representation *r*!**

E.g.:

- Q=(π, π), charge representation: *Charge density wave (CDW)*
- Q=(π, π), spin representation: *Antiferromagnetism (AFM)*
- Q=(0,0), spin representation: *Ferromagnetism (FM)*
- Q=(0,0), particle-particle representation: *Superconductivity (SC)*

⇒ **If one of these modes dominates the self-energy:**

$\tilde{\Sigma}_Q(k)$ **strongly peaked at the corresponding Q if one adopts the " correct" representation r!**

" Wrong" representation: weak **Q dependence!**

... or partially sum over momentum.

partial summation over all variables execpt the transfer frequency ω

$$\widetilde{\Sigma}_\omega(k) = \sum_{\boxed{k},Q} F_r(k,k',q)ggg \quad r = ch, sp, pp \quad \Rightarrow \quad \Sigma(k) = \sum_\omega \widetilde{\Sigma}_\omega(k)$$

For a given representation r:

$\widetilde{\Sigma}_\omega(k)$ (almost) ω**-independent** → **short-lived fluctuations**

$\widetilde{\Sigma}_\omega(k)$ (strongly) **peaked at** $\omega = 0$ → **long-lived fluctuations**

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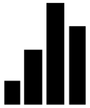

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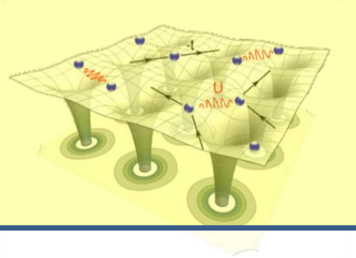
- Benchmark: **attractive** case
- Pseudogap physics: **repulsive** case



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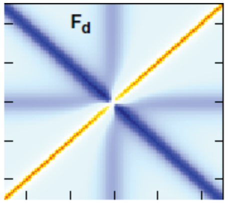
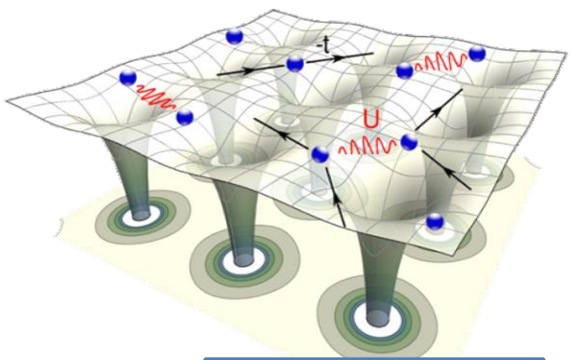


Application to test case: **attractive** Hubbard model

HUBBARD HAMILTONIAN

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



cf. talk by **Agnese Tagliavini**

Benchmark: **attractive** model: **U<0**

physics is well understood in this case!

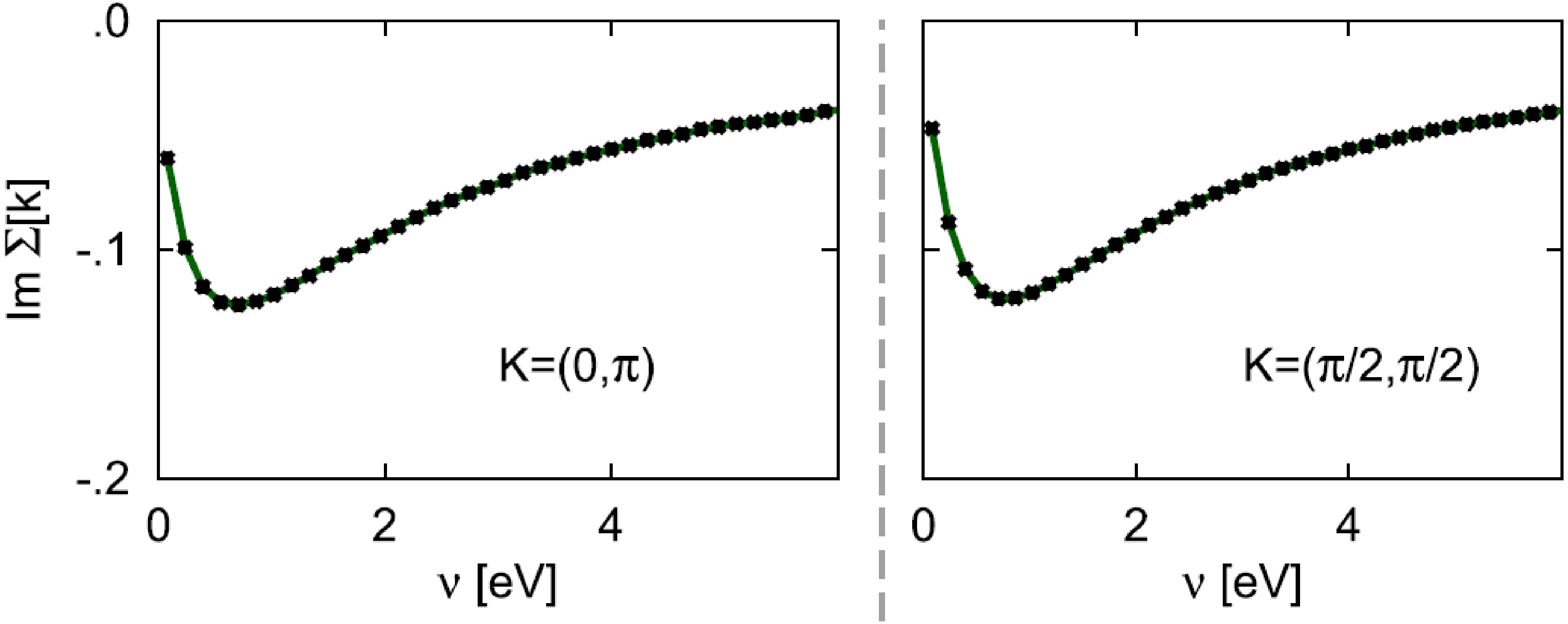
Dominating fluctuations (modes) at half-filling:

Q=(0,0) s-wave pairing (superconductivity) fluctuations

Q=(π, π) (checkerboard) charge-density-wave fluctuations

Application to test case: **attractive** Hubbard model

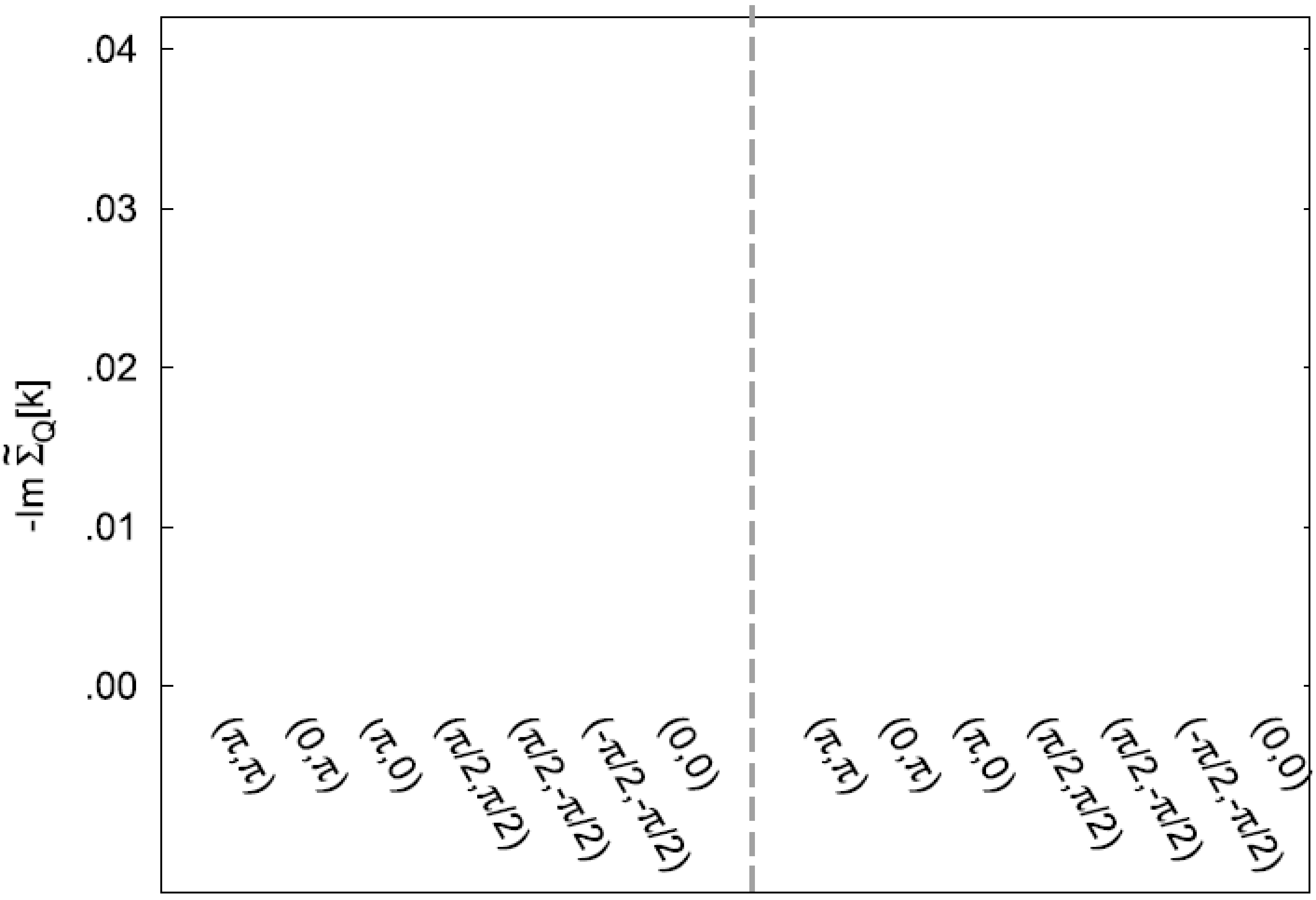
DCA for 2d Hubbard model, N=8, t=-0.25eV, μ=-0.53eV (n=0.87), U=-1eV, T=0.025eV



What does fluctuation diagnostics (FluctDiag) tell us?

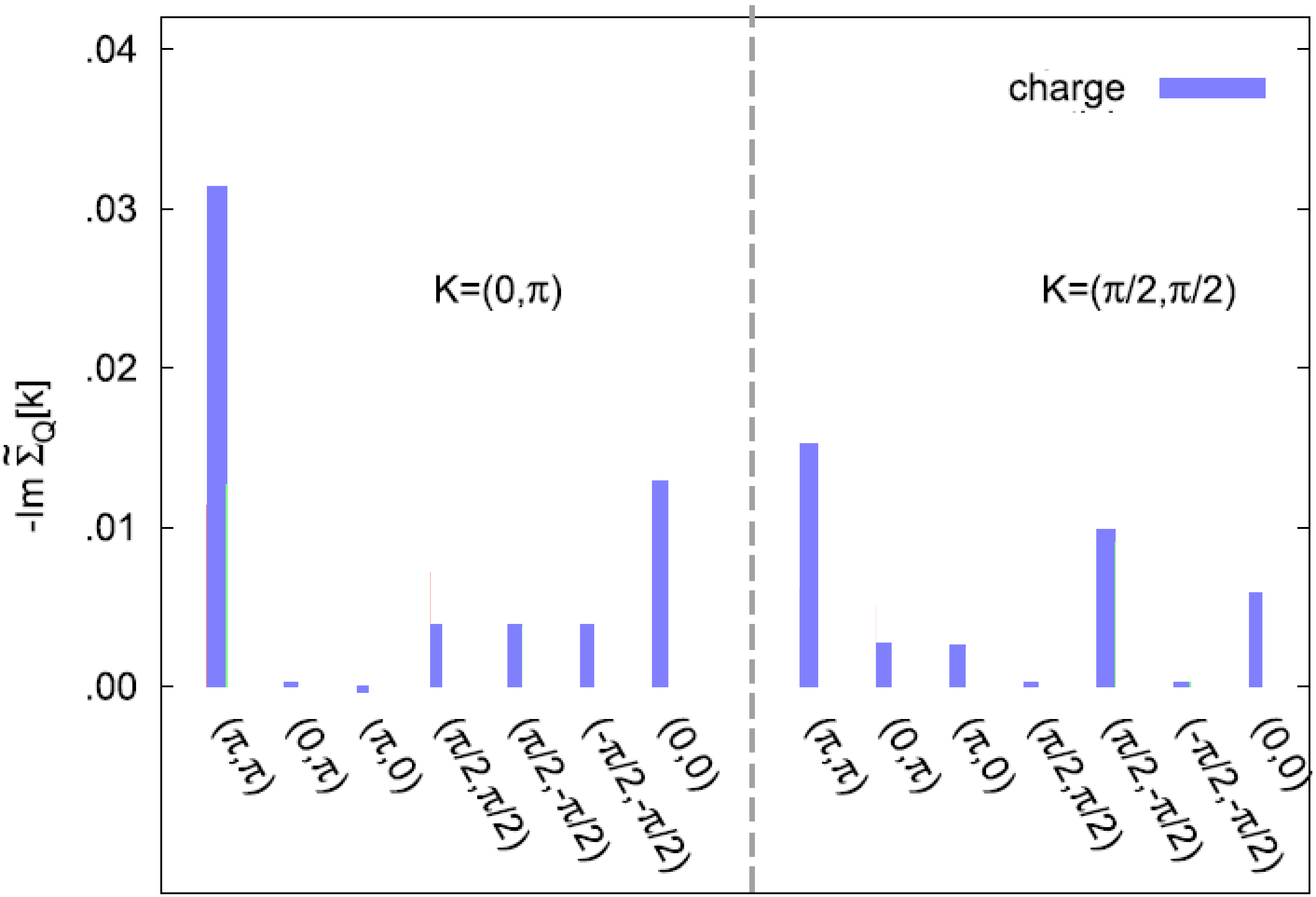
Attractive Hubbard model: FluctDiag

Fluctuation Diagnostics



Attractive Hubbard model: FluctDiag

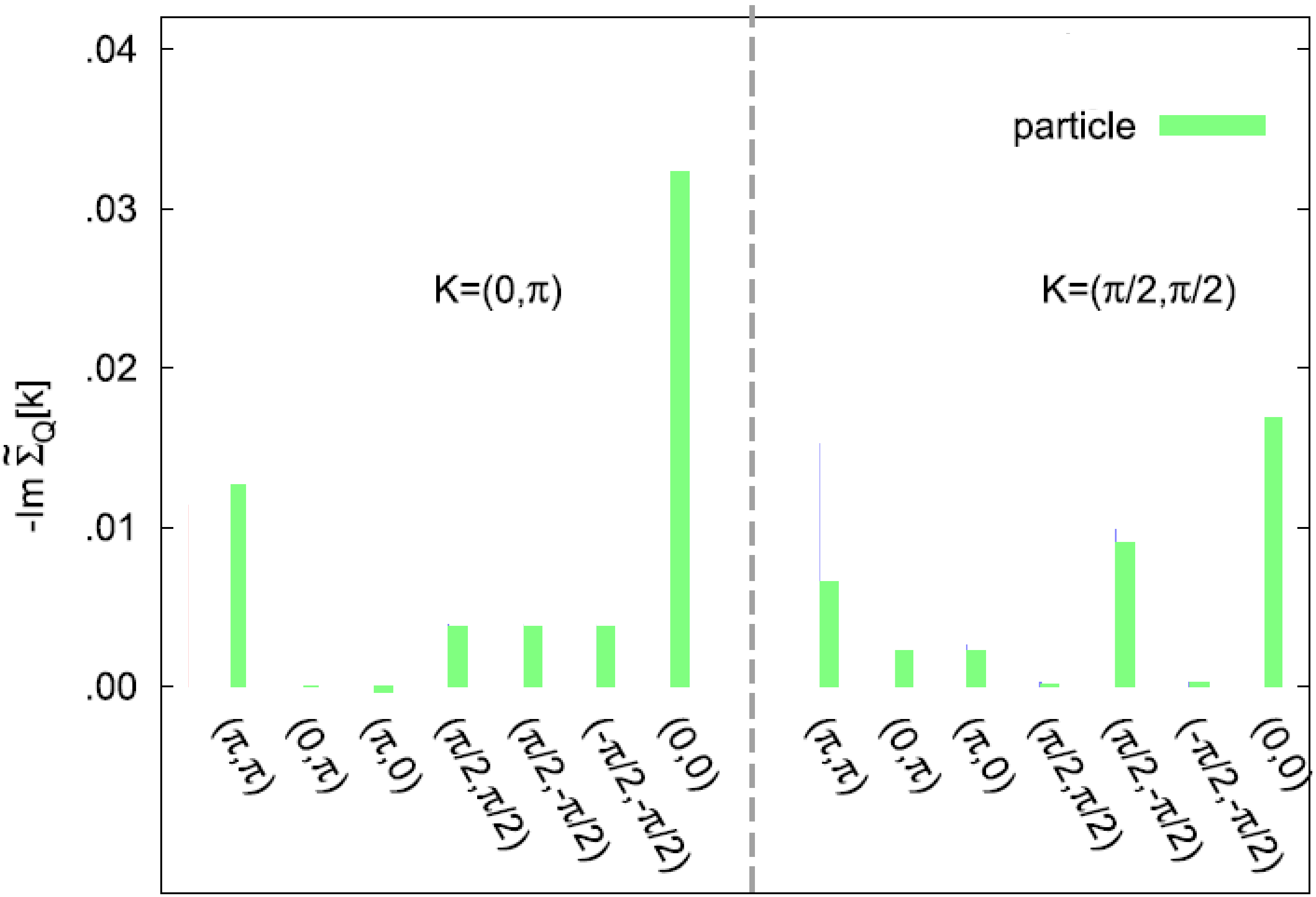
Fluctuation Diagnostics



- **Q=(π, π) charge-density-wave fluctuations**

Attractive Hubbard model: FluctDiag

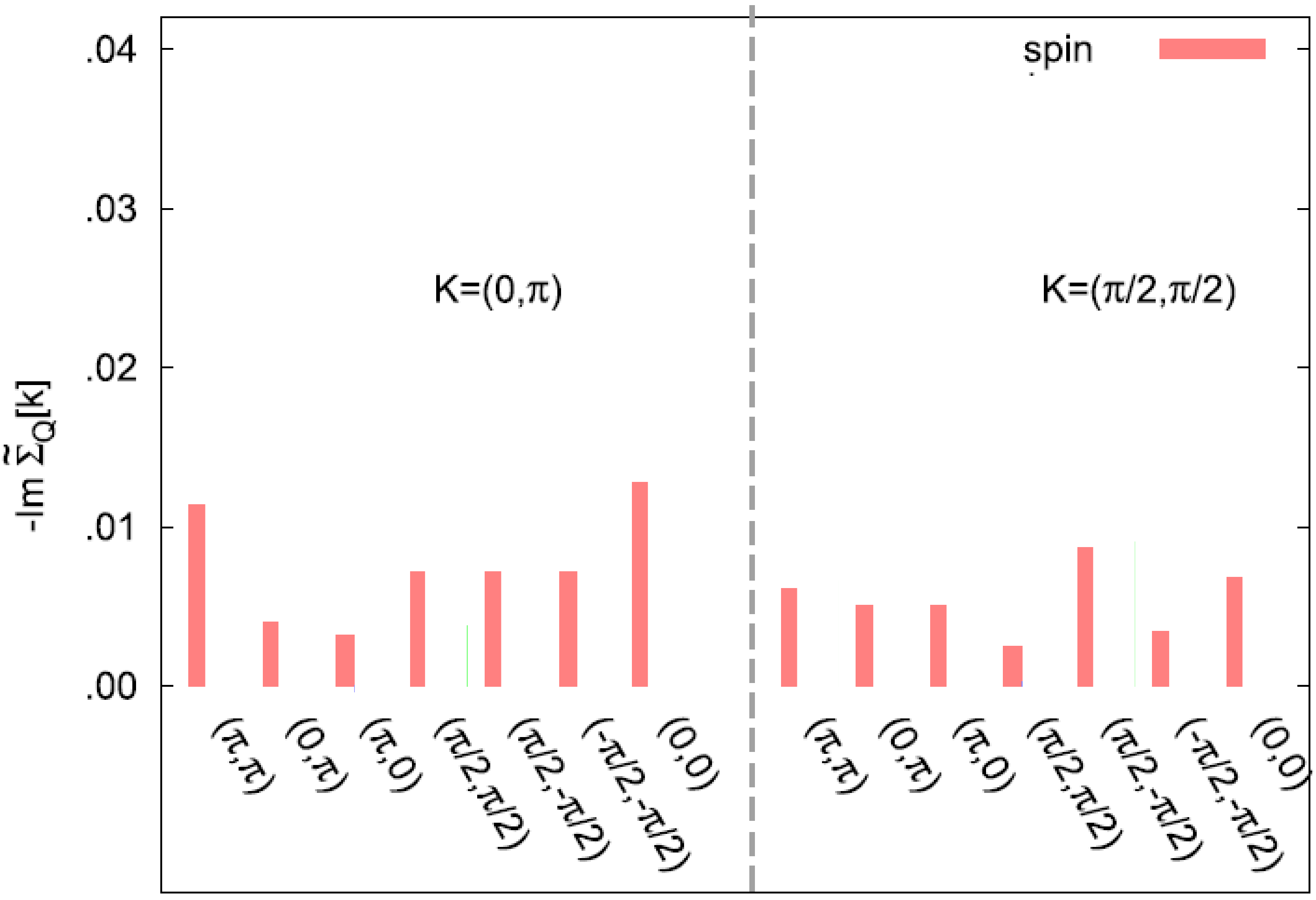
Fluctuation Diagnostics



- **s-wave Q=(0,0) pairing fluctuations**

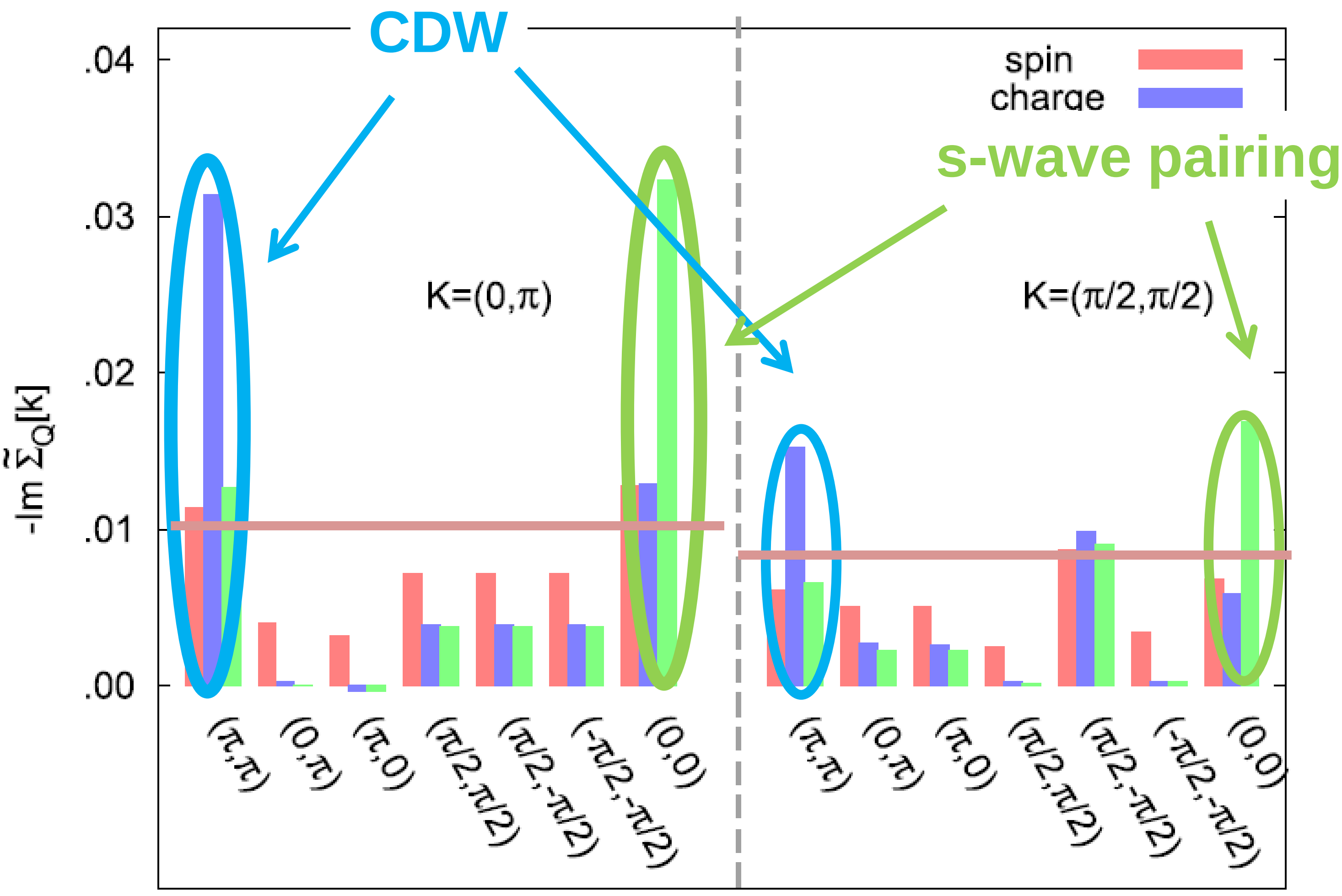
Attractive Hubbard model: FluctDiag

Fluctuation Diagnostics



- **uniform Q distribution in the spin picture**

Attractive Hubbard model: FluctDiag



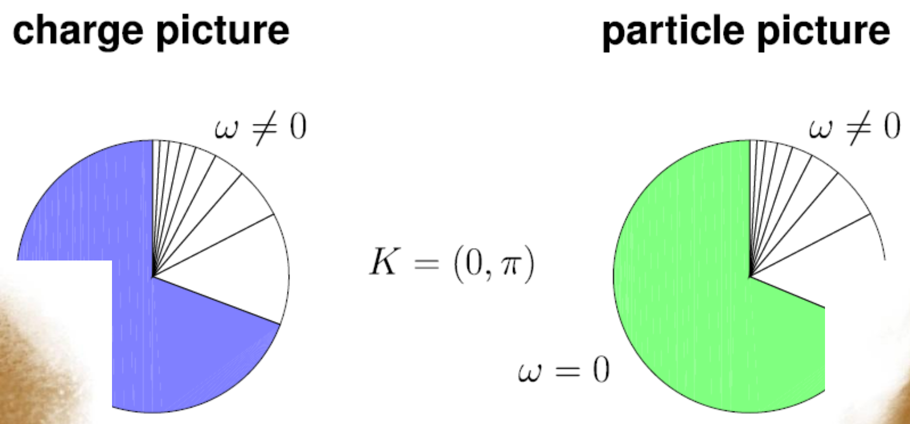
- Q=(π, π) charge-density-wave fluctuations
- s-wave Q=(0,0) pairing fluctuations
- uniform Q distribution in the spin picture

Attractive Hubbard model: FluctDiag

Fluctuation Diagnostics

Are these strong particle-particle and charge fluctuations long-lived?

$\Delta\widetilde{\Sigma}_{\omega}(k)$



r) charge-density-wave fluctu

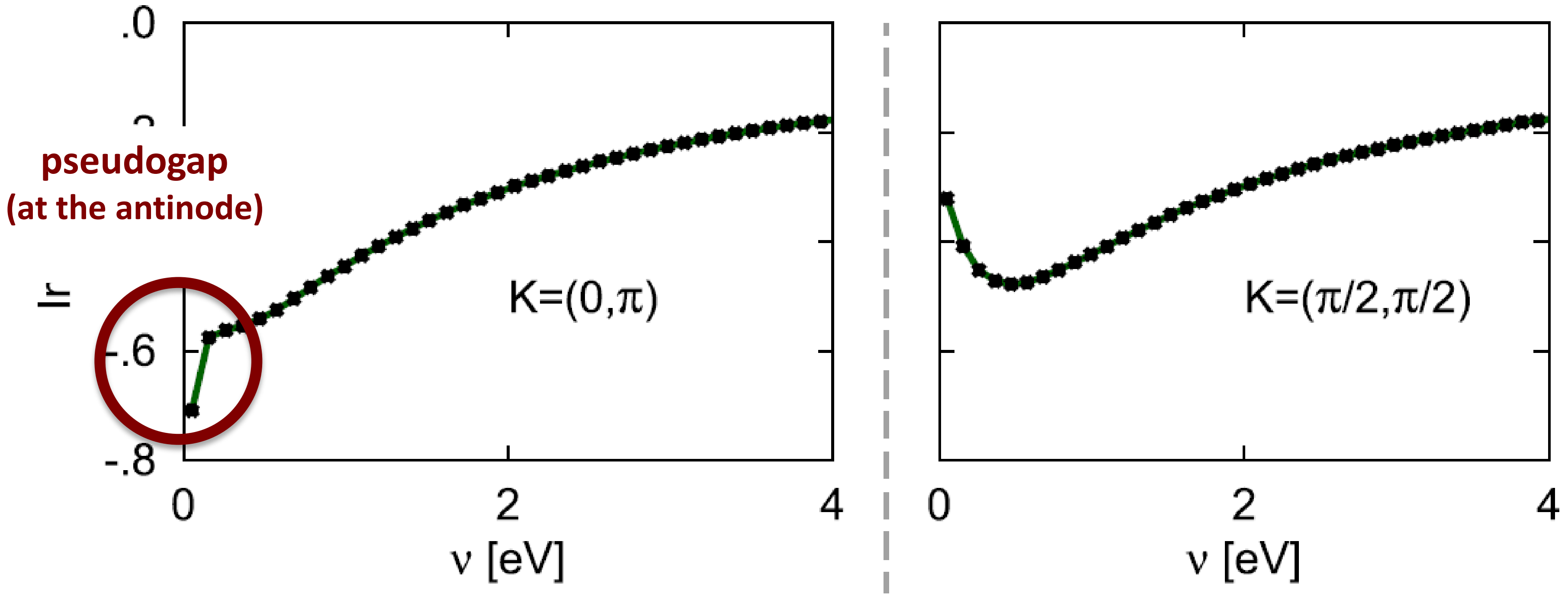
Q=(0,0) pairing fluctuations

n Q distribution in the spin pi

Long-lived charge and pairing fluctuations are present!

Application to **repulsive** Hubbard model

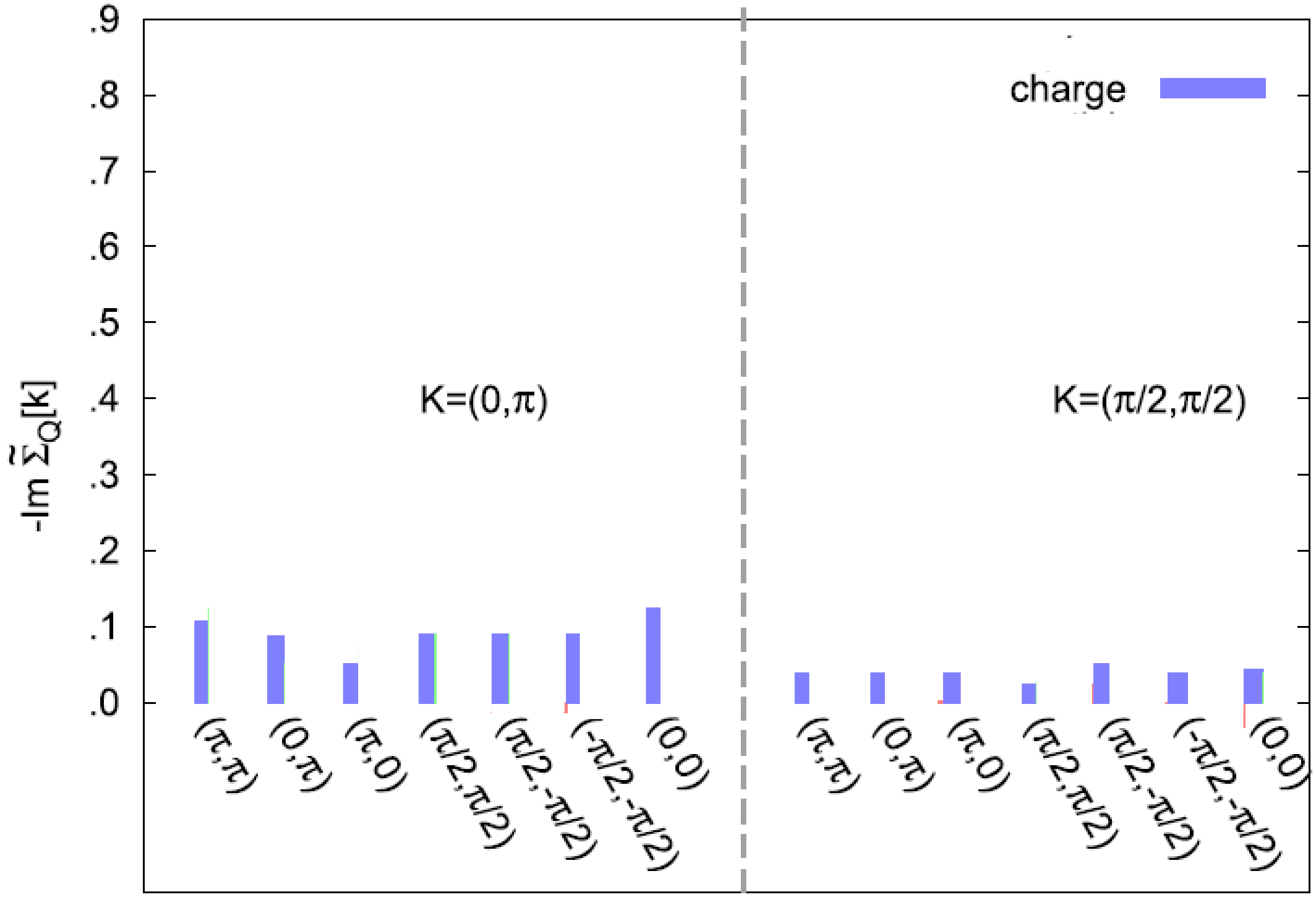
DCA for 2D Hubbard model, N=8, t=-0.25eV, μ=0.8eV (n=1), U=1.6eV, T=0.033eV



➡ **What can fluctuation diagnostics tell us?**

Repulsive Hubbard model: FluctDiag

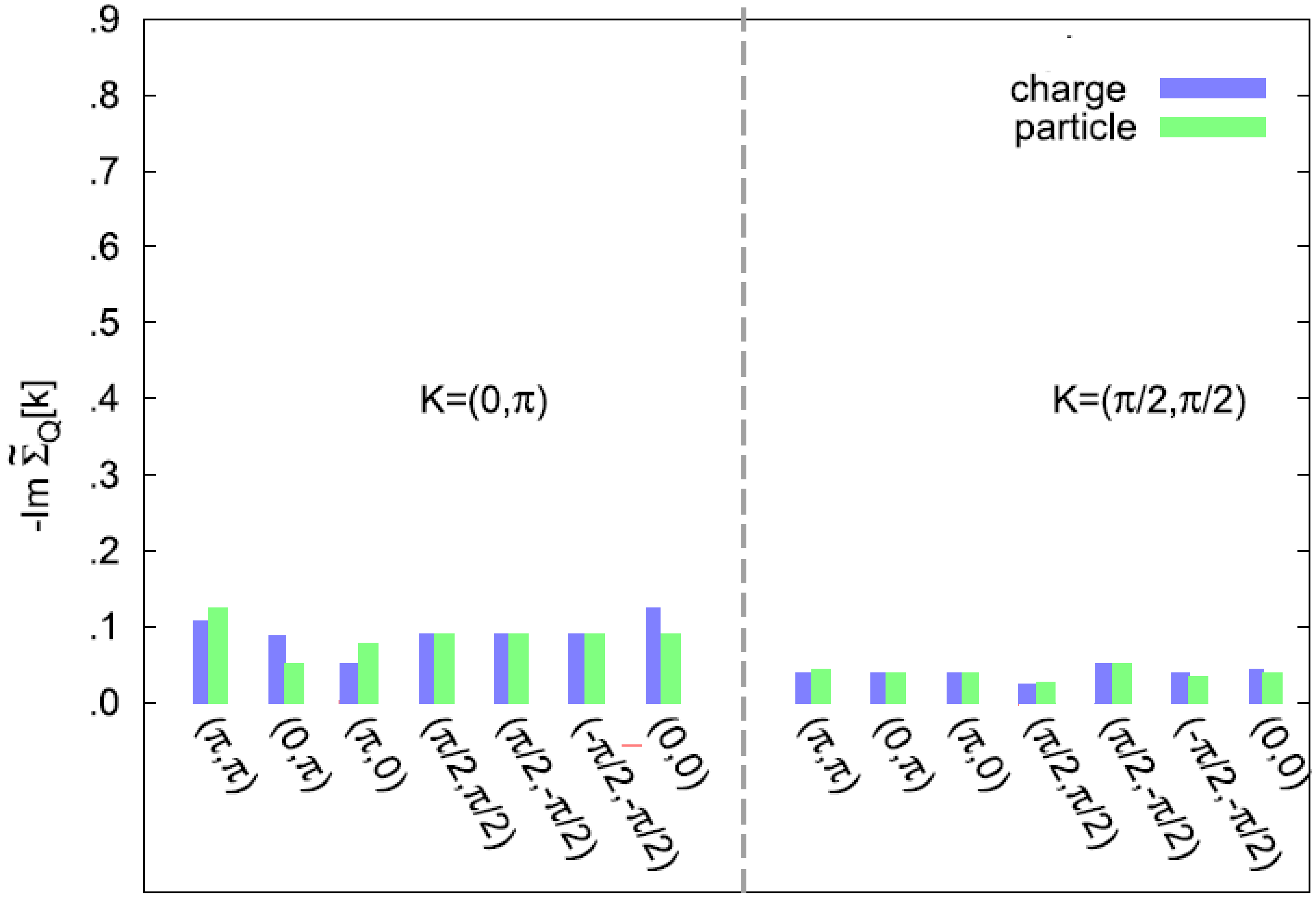
Fluctuation Diagnostics



- **Uniform Q distribution in the charge**

Repulsive Hubbard model: FluctDiag

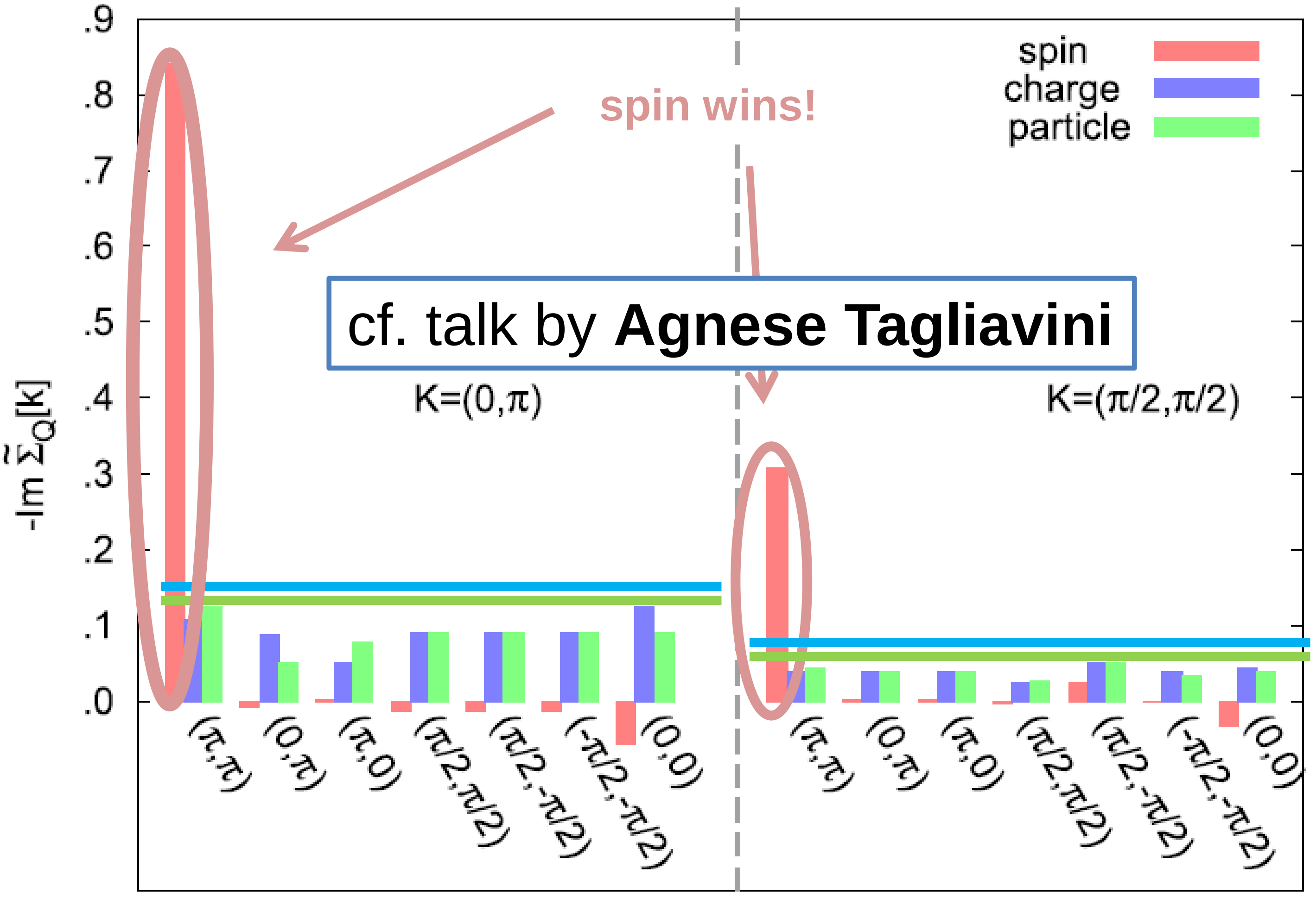
Fluctuation Diagnostics



- **Uniform Q distribution in the charge and particle-particle picture**

Repulsive Hubbard model: FluctDiag

Fluctuation Diagnostics



- Q=(π, π) antiferromagnetic spin fluctuations
- Momentum differentiation
- **Uniform Q distribution in the charge and particle-particle picture**

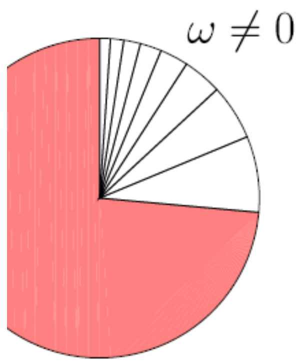
Repulsive Hubbard model: FluctDiag

Fluctuation Diagnostics

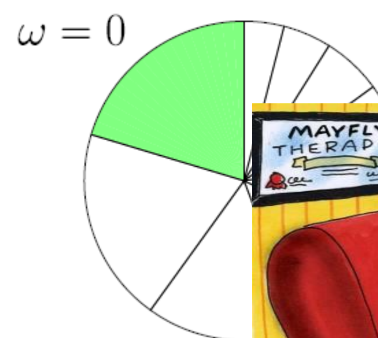
Are these strong spin fluctuations long-lived?

$\Delta\widetilde{\Sigma}_{\omega}(k)$

spin picture | **particle picture**



$K = (0, \pi)$



π) antiferromagnetic spin fluctuatic

Long-lived spin fluctuations are responsible for the pseudogap and momentum differentiation in the self-energy! (for the DCA of the single band Hubbard model)

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Fluctuation Diagnostics

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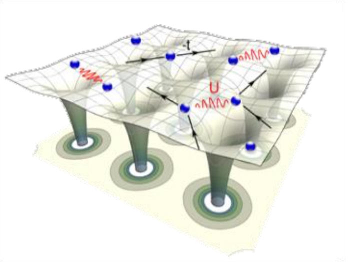
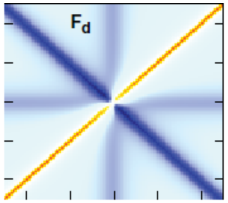


Further insight: weak-coupling analysis

- Analysis of the full vertex
- Consequences for d-wave pairing fluctuations



“Spirit” of the FluctDiag

Fluctuation Diagnostics

A well-defined spin mode appears from the “ wrong“ charge/particle-particle perspective as short-lived/short-ranged charge/particle-particle fluctuations!

Compare: Geocentric vs. Heliocentric model!

Geocentric system

Heliocentric system

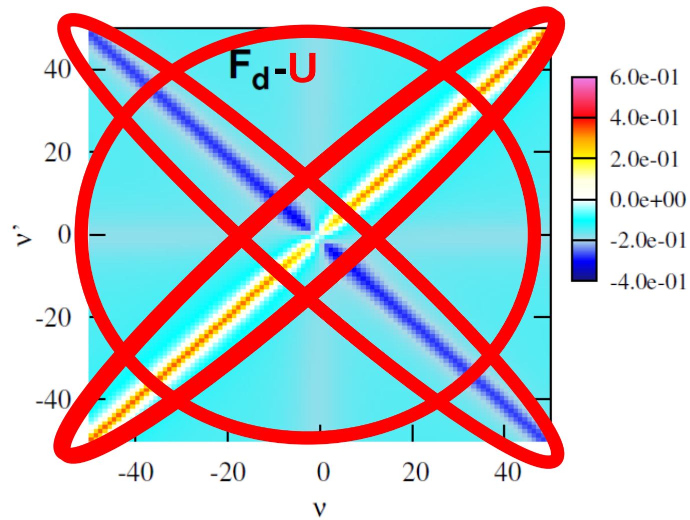
Both are possible, but only one gives a **simple description** of the physics!

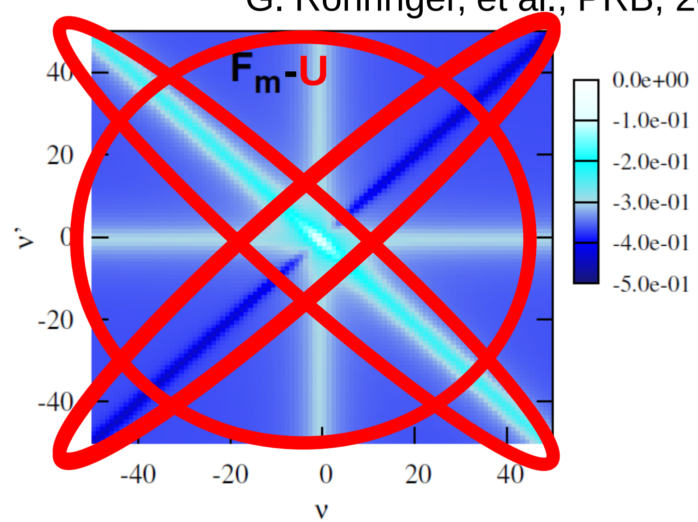
Further insight: weak coupling analysis

Fluctuation Diagnostics

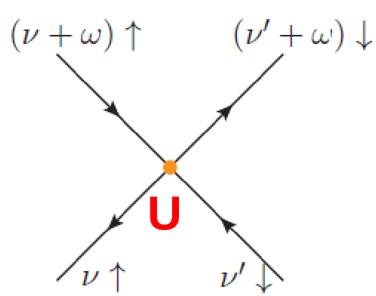
Approximation of the vertex by its main structures (here for the local vertex):

G. Rohringer, et al., PRB, 2012.

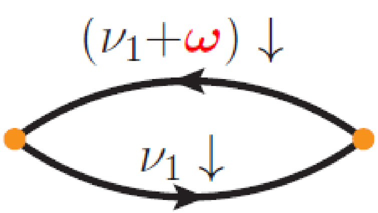




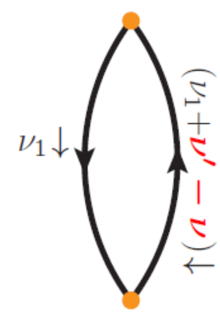
Perturbative analysis of the main structures:



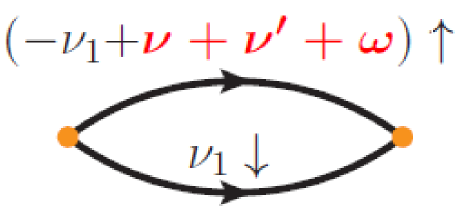
subtracted



constant background



main diagonal



secondary diagonal

Main structures of the 1PI vertex correspond to physical response functions (susceptibilities)!

Further insight: weak coupling analysis

Fluctuation Diagnostics

$$F_{sp}(k,k',q) \approx -U - U^2 \left[\chi_{sp}(q) + \frac{1}{2}\chi_{sp}(k'-k) - \frac{1}{2}\chi_{ch}(k'-k) + \chi_{pp}(k+k'+q) \right]$$

C. Karrasch, et al., J. Phys.: Condensed Matter, 2008. and C. Husemann and M Salmhofer, PRB, 2009.

$\chi_r(\mathbf{Q},\omega) \Longrightarrow$ **linear response to external forcing field associated with channel *r***

$r = ch \rightarrow$ **chemical potential** $r = sp \rightarrow$ **(staggered) magnetic field** $r = pp \rightarrow$ **pairing field**

At second order phase transition: $\chi_r(\mathbf{Q}=\mathbf{Q}_0, \omega=0) \Rightarrow \infty$

$\mathbf{Q}_0 \Rightarrow$ defines spatial pattern of the corresponding ordered phase!

(Q=(π,π) for AFM and CDW, Q=(0,0) for FM and SC)

Further insight: weak coupling analysis

Fluctuation Diagnostics

Assume $\chi_{sp}(\vec{q},\omega=0)$ to be the dominant contribution in the EOM

$$F_{sp}(k,k',q) \approx -U - U^2\left[\chi_{sp}(q) + \frac{1}{2}\chi_{sp}(k'-k) - \frac{1}{2}\chi_{ch}(k'-k) + \chi_{pp}(k+k'+q)\right]$$

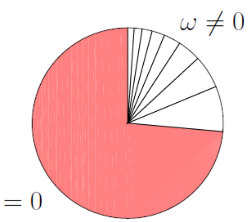
$$F_{ch}(k,k',q) \approx U + U^2\left[-\chi_{ch}(q) + \frac{3}{2}\chi_{sp}(k'-k) + \frac{1}{2}\chi_{ch}(k'-k) - \chi_{pp}(k+k'+q)\right]$$

Two exemplary perspectives after partial summation

$$\sum_{k',(Q/\omega)}$$

In "proper" (spin) channel:

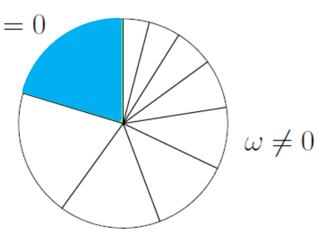
peaked Q and ω distribution



$$\widetilde{\Sigma}_{\omega}(k) \sim \widetilde{\Sigma}_{Q}(k) \sim \chi_{AF}/N_c$$

In "wrong" (e.g. charge) channel:

democratic Q and ω distribution



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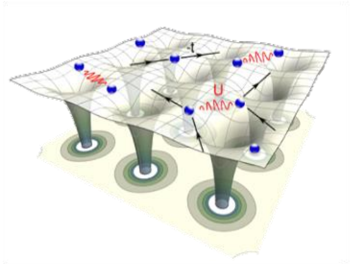

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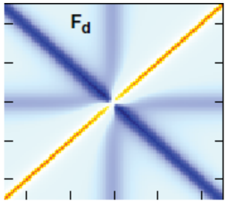
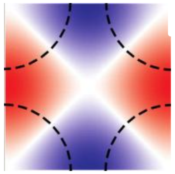


Role of d-wave pairing fluctuations

Fluctuation Diagnostics

d-wave pairing operator: $\Delta^\dagger = \sum_{\mathbf{K}} f(\mathbf{K}) c^\dagger_{\mathbf{K}\uparrow} c^\dagger_{-\mathbf{K}\downarrow}$, $f(\mathbf{K}) =$  [1)]

d-wave pairing fluctuations: $\langle \Delta^\dagger \Delta \rangle \sim \sum_{\mathbf{K},\mathbf{K}'} f(\mathbf{K}) f(\mathbf{K}') \langle c^\dagger_{\mathbf{K}\uparrow} c^\dagger_{-\mathbf{K}\downarrow} c_{-\mathbf{K}'\downarrow} c_{\mathbf{K}'\uparrow} \rangle$

Vicinity of d-wave instability: enhanced d-wave pairing fluctuations

Also large contribution to self-energy?

large $\langle \Delta^\dagger \Delta \rangle$ ⇒ $\mathrm{sgn}\left\langle c^\dagger_{K\uparrow} c^\dagger_{-K\downarrow} c_{K'\downarrow} c_{K'\uparrow} \right\rangle = \mathrm{sgn}\, f(K) f(K')$

EOM rewritten: $\frac{U}{\beta} \sum_\nu \Sigma(k) g(k) = \sum_{\mathbf{K}',\mathbf{Q}} \langle c^\dagger_{\mathbf{K}\uparrow} c^\dagger_{\mathbf{Q}-\mathbf{K}\downarrow} c_{-\mathbf{K}'\downarrow} c_{\mathbf{Q}+\mathbf{K}'\uparrow} \rangle$

$f(K')$ **not** present!

d-wave pairing fluctuations couple inefficiently to the self-energy due to d-wave form factor!
(for purely local U>0)

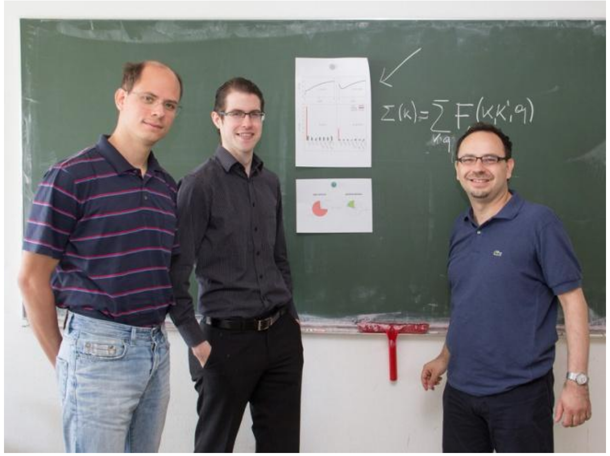
1) Nat. Sc. Rep. 2, 381 (2012)

FluctDiag team

O. Gunnarsson

J. Merino

G. Sangiovanni



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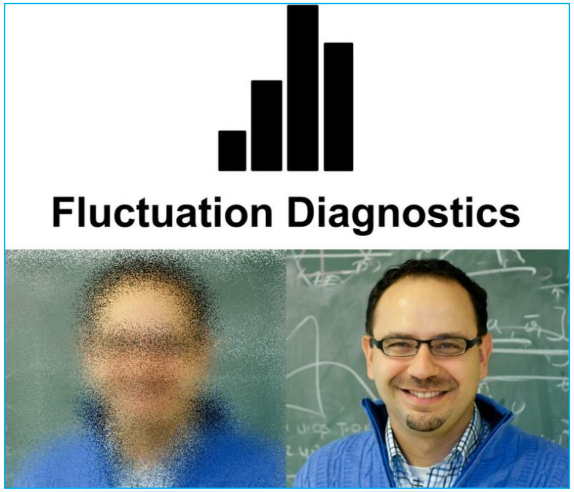
Fluctuation diagnostics of the electron self-energy – origin of the pseudogap physics, PRL 114, 236402 (2015)

Conclusions and outlook

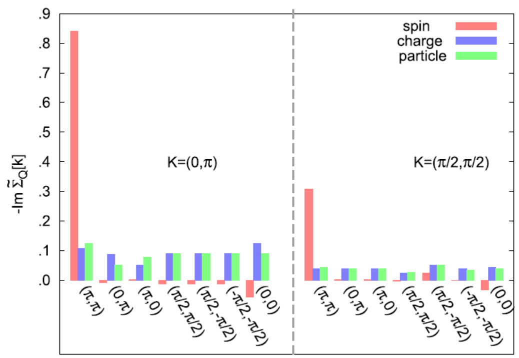


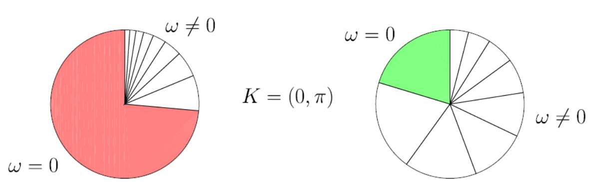
Method of determining physical processes defining spectra

- Rewriting equation of motion: Fluctuation diagnostics

Application to 2D U>0 Hubbard model (in DCA)

- **Pseudogap** due to strong **spin fluctuations**
- **Inefficient coupling of d-wave pairing**





Outlook: non-local interactions (extended Hubbard), multi-orbital physics

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