

# Dynamical mean field theory

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MPI for solid state research, Stuttgart

Bristol, March 30, 2007

- Dynamical mean field theory (DMFT) — an introduction
- LDA+DMFT
- Beyond DMFT

*further reading:*

**DMFT**: Kotliar and Vollhardt, Physics Today **57**, No. 3 (March), 53 (2004).

Georges *et al.*, Rev. Mod. Phys. **68**, 13 (1996).

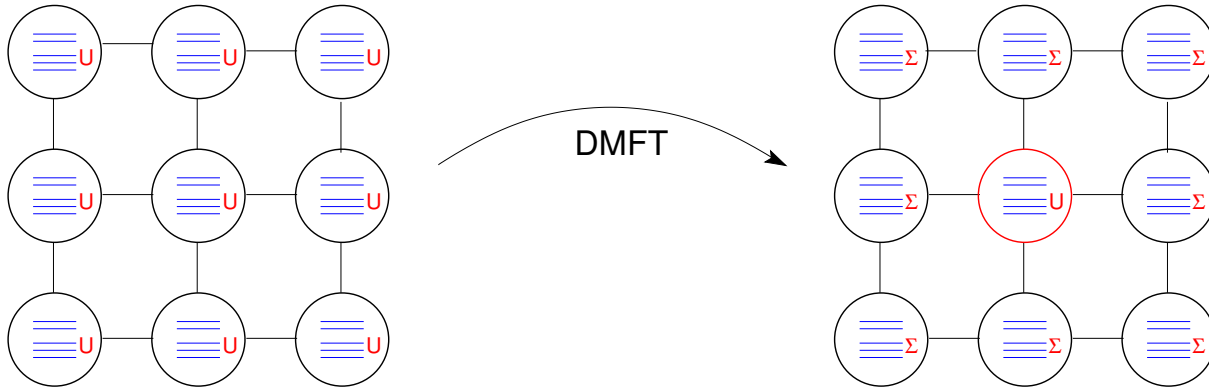
**LDA+DMFT**: Held *et al.*, Psi-k Newslett. **56**, 65 (2003) [phys. stat. sol. (B) **243**, 2599 (2006)].

Kotliar *et al.*, Rev. Mod. Phys. **78**, 865 (2006).

Held, cond-mat/0511293 (to appear in Adv. in Phys.)

# Motivation

## Dynamical mean field theory

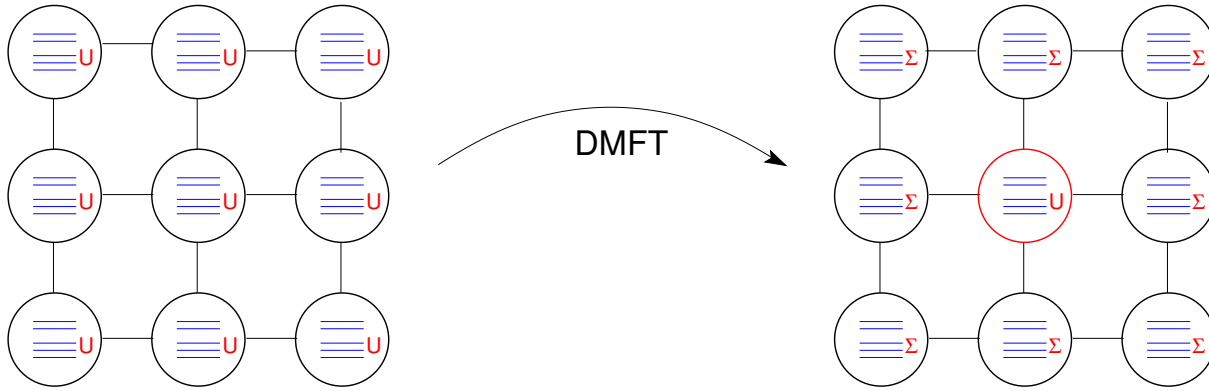


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**Success story:** Mott-Hubbard transition, magnetism, kinks ...

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**Not included:**

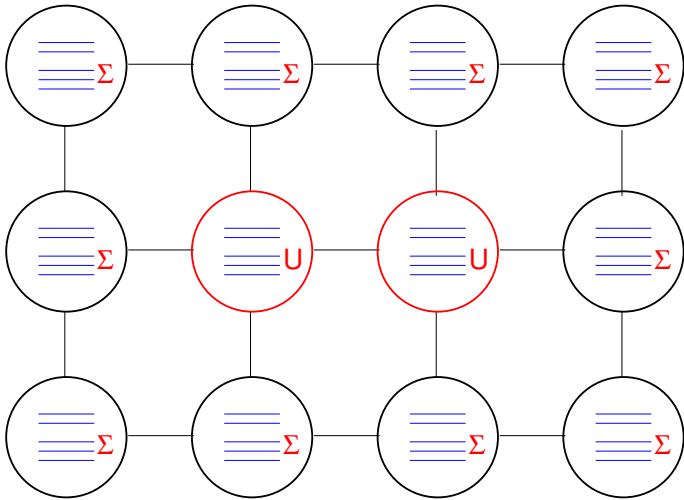
**non-local correlations**

$p$ -,  $d$ -wave superconductivity, spin Peierls

magnons, (quantum) critical behavior ...

# beyond DMFT

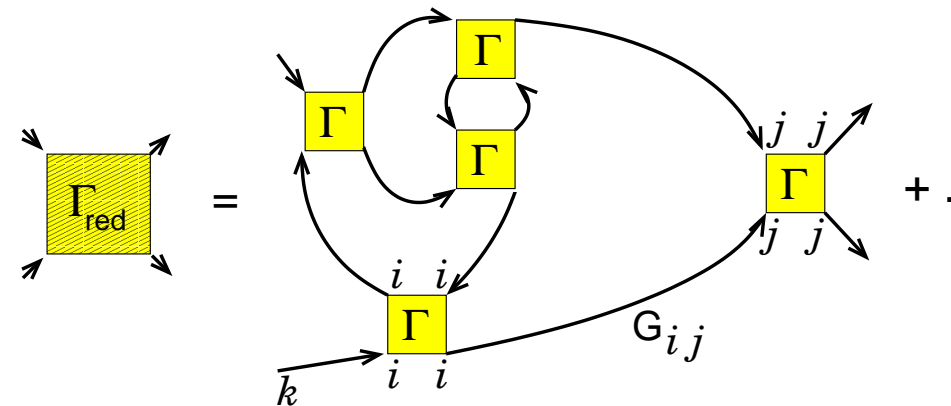
## cluster extensions of DMFT



- non-local **short-range** correlations
- $d/p$ -wave superconductivity

Hettler *et al.*'98, Lichtenstein Katsnelson'00,  
Kotliar *et al.*'01, Potthoff'03

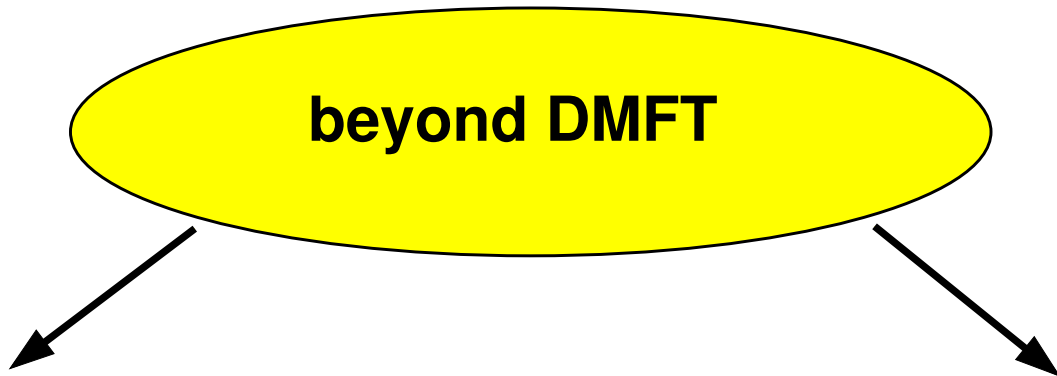
## diagrammatic extensions of DMFT



## dynamical vertex approximation

- non-local **long-range** correlations
- (para-)magnons, phase transitions ...

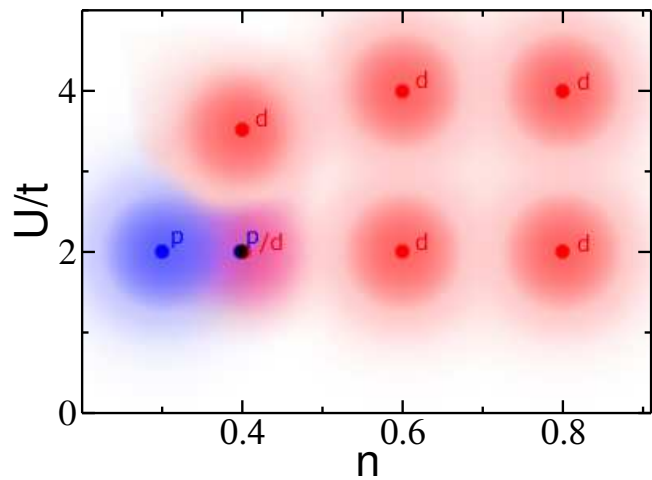
Toschi, Katanin, KH cond-mat/0603100  
cf. Kusunose cond-mat/0602451  
Slezak *et al.* cond-mat/0603421



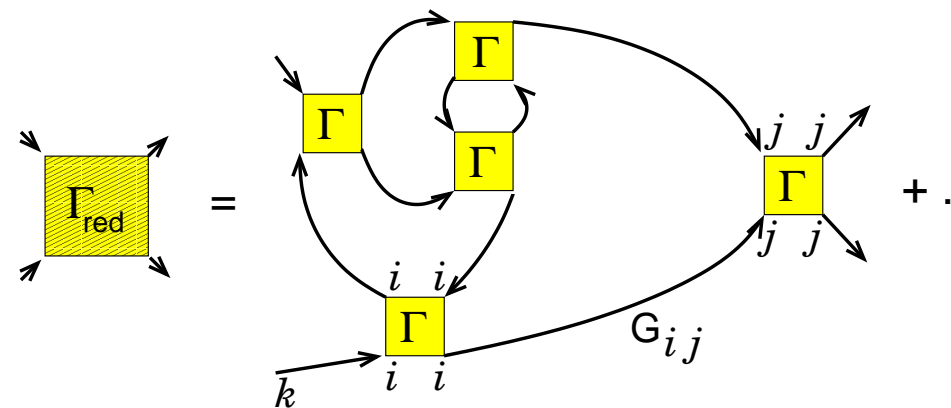
### cluster extensions of DMFT

dominant superconducting susceptibility

in  $t$ - $t'$  2D Hubbard-Modell Arita, Held PRB'06



### diagrammatic extensions of DMFT



### dynamical vertex approximation

- non-local **long-range** correlations
- (para-)magnons, phase transitions ...

$$t' = 0.4t, N_c = 4 \times 4 = 16$$

Toschi, Katanin, KH cond-mat/0603100  
 cf. Kusunose cond-mat/0602451  
 Slezak et al. cond-mat/0603421

# Dynamical vertex approximation (D $\Gamma$ A)

**DMFT:** all (topological distinct) **local** diagram for  $\Sigma$

**Generalization:** all **local** diagrams for  $n$ -particle fully irreducible vertex  $\Gamma$

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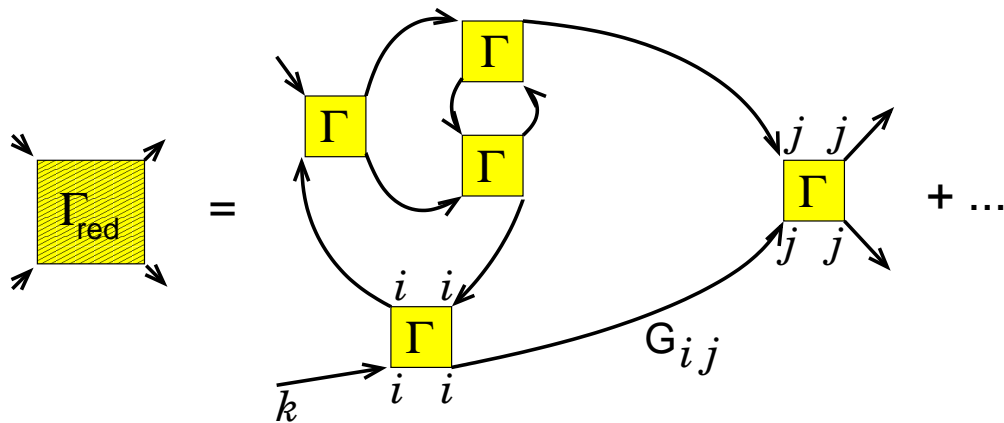
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**local**  $\Gamma$ , **non-local**  $G$

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**non-local** reducible vertex  $\Gamma_{\text{red}}$

via parquet equations

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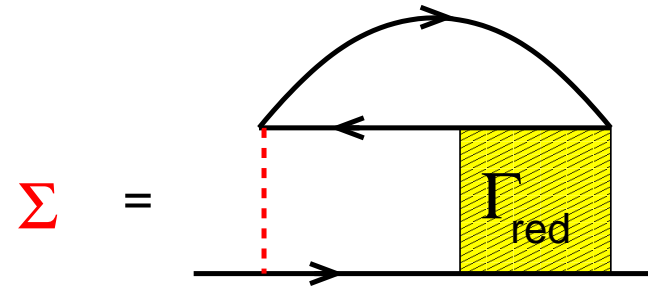
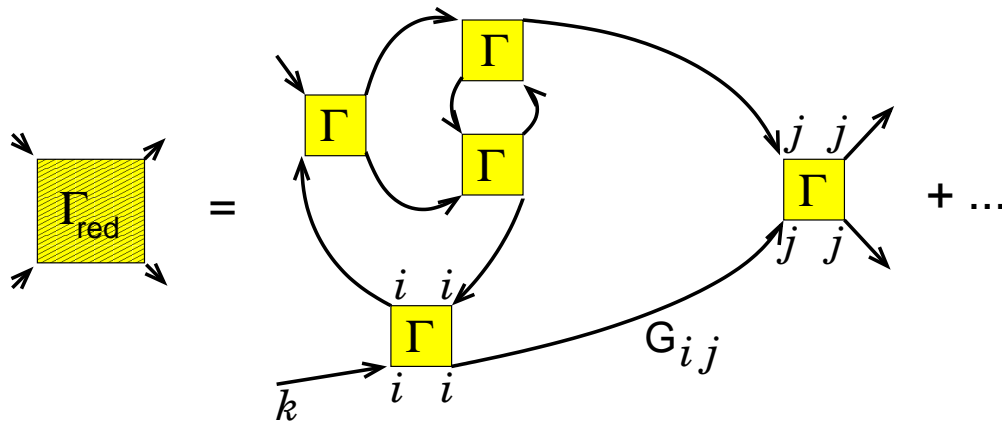
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**non-local**  $\Sigma$

exact relation (eq. of motion)

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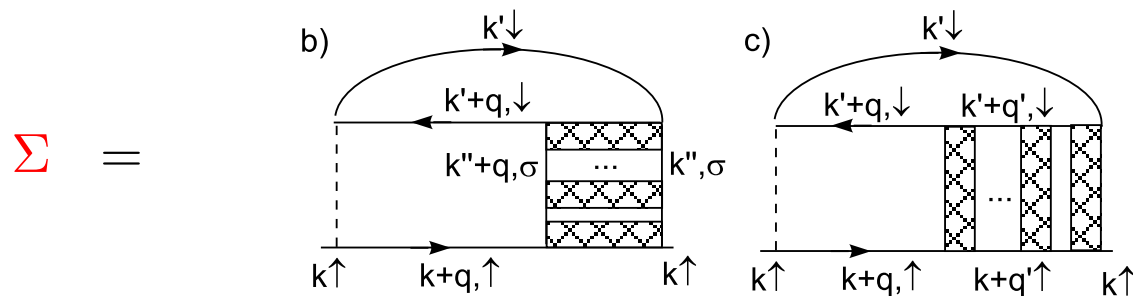
$n = 1 \rightarrow$  DMFT

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**Included: ladder diagrams**



lines: **non-local**  $G$

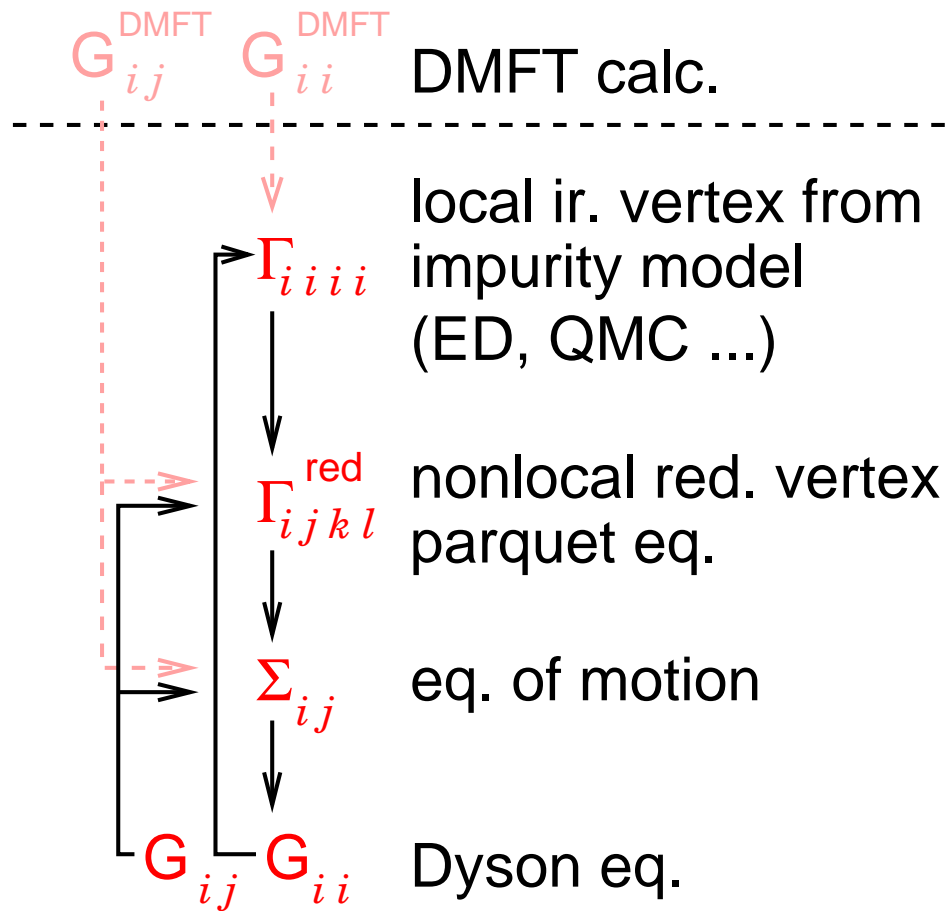
crosshatched: local irreducible vertex in spin/charge channels

$$\Gamma_{S,C}(\nu, \nu', \omega) = \chi_{0,loc}^{-1} - \chi_{S,C}^{-1}$$

magnons, spin-fluctuations at (A)FM phase transition

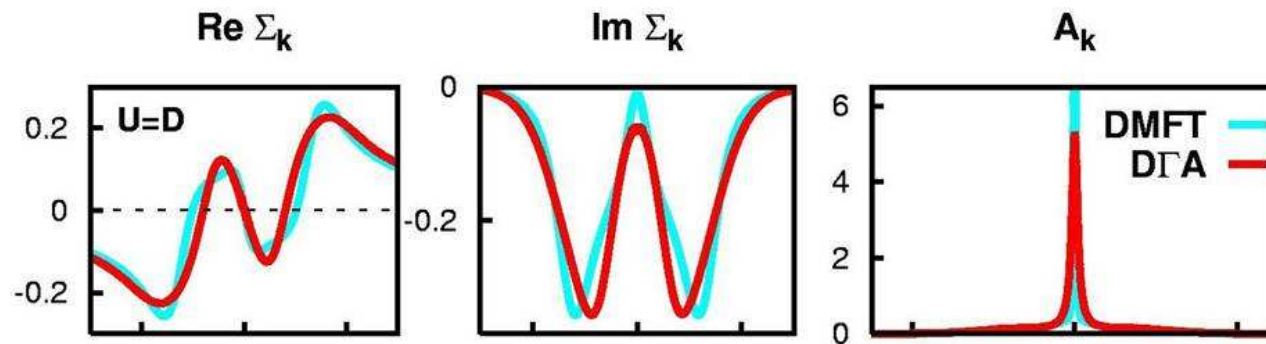
$G_{ij}$  from DMFT

# DΓA algorithm



# Results: 3D Hubbard model

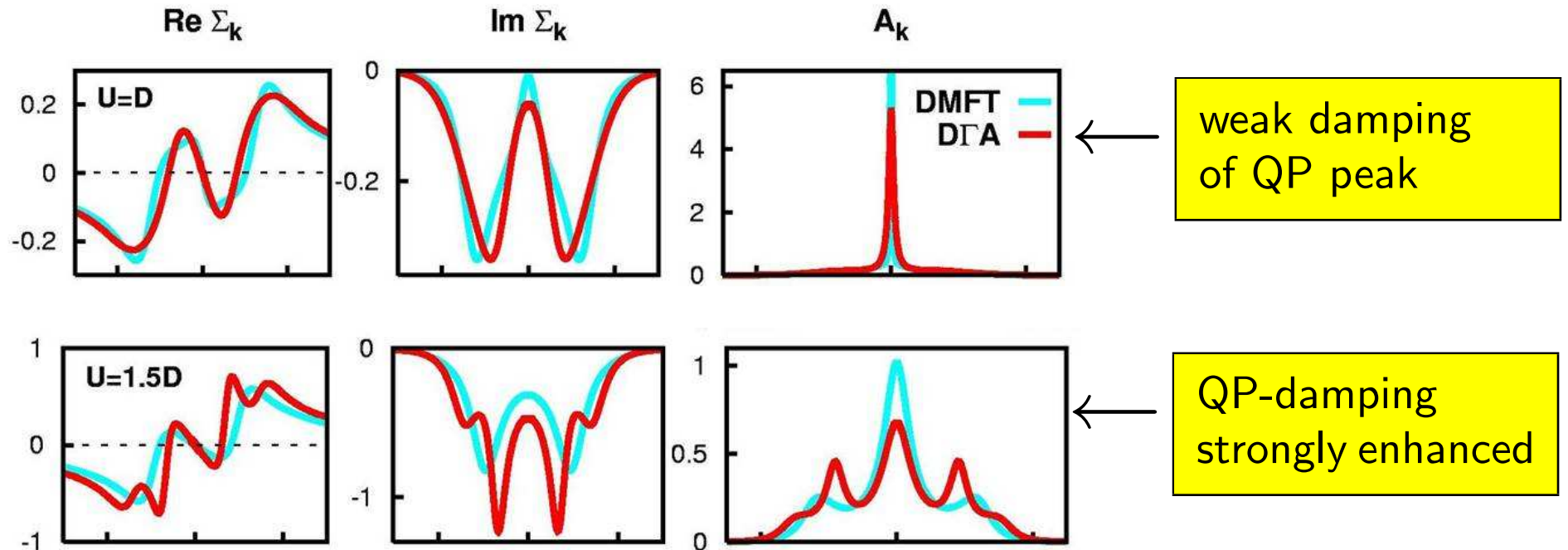
$\Sigma$  and  $A$  for  $\mathbf{k} = (\pi/2, \pi/2, \pi/2)$  (on Fermi surface)



← weak damping of QP peak

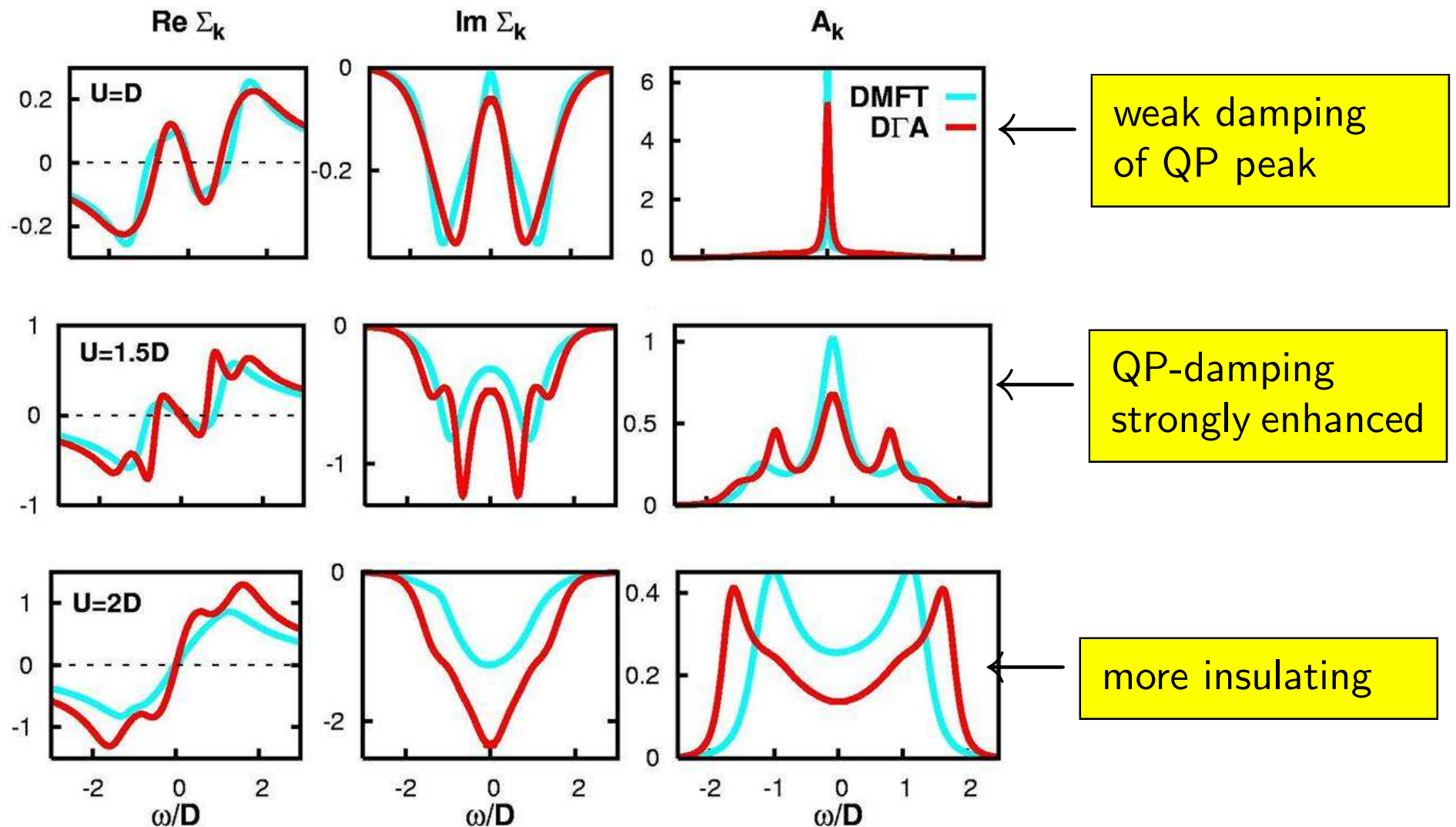
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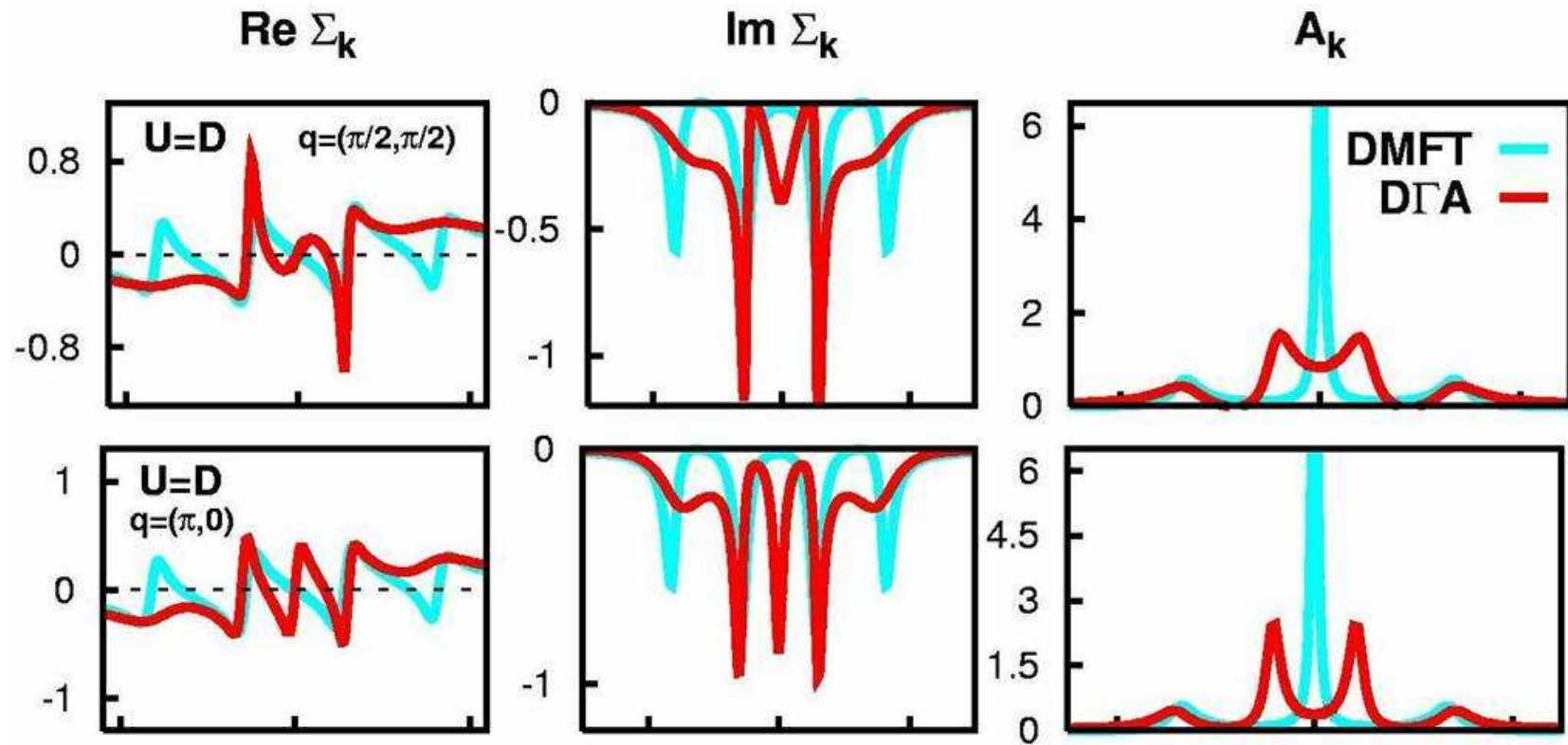


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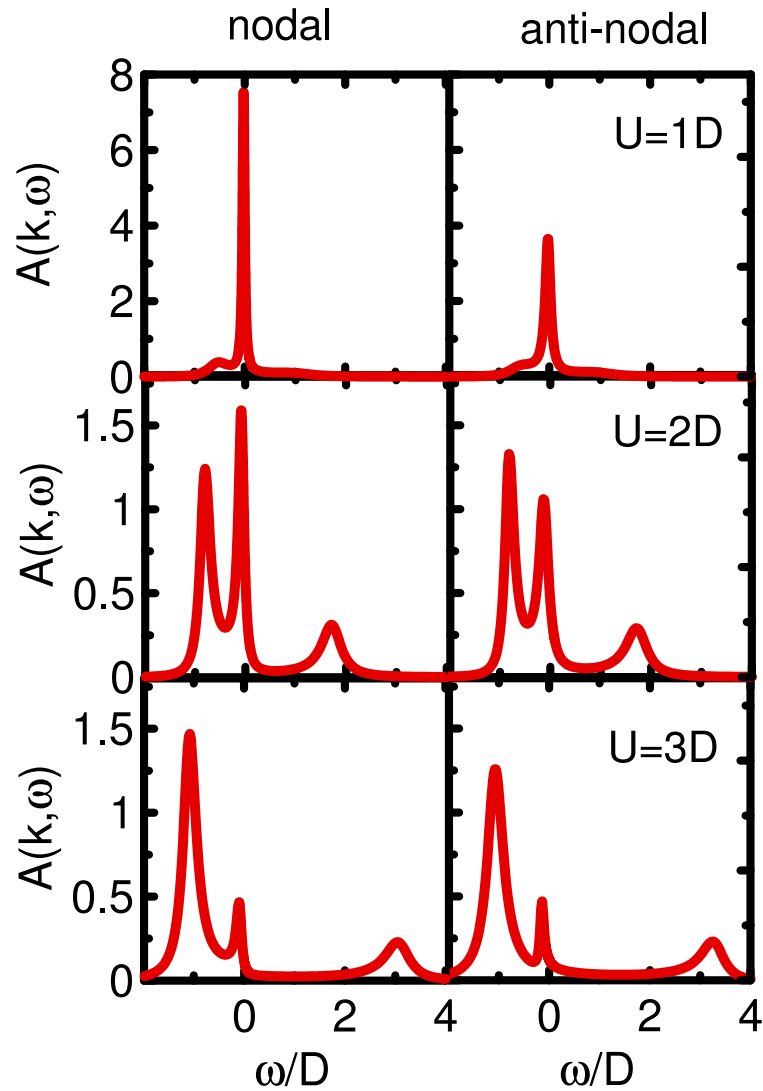


# Results: 2D Hubbard model (half-filling)



anisotropic pseudogap

# Results: 2D Hubbard model (off half-filling)



$$t'/t = 0.3$$

$$n = 0.8$$

$$\beta = 100/D$$

less anisotropic  
at strong coupling

# Results: 1D Hubbard model

Slezak, Jarrell, Maier, Deisz cond-mat/0603421

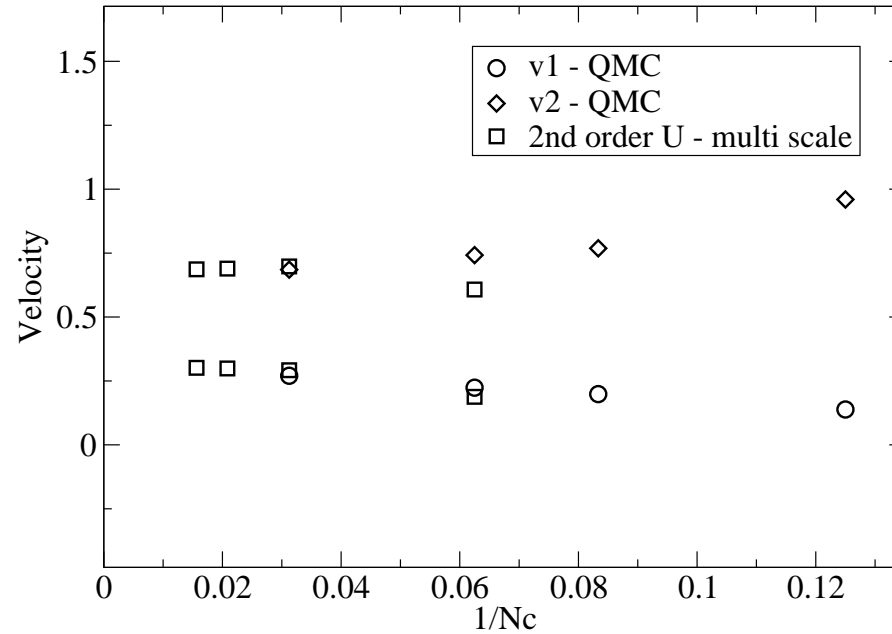
## Spin-charge separation

$$U = W = 1$$

$$k = \pi/2$$

$$\beta = 31$$

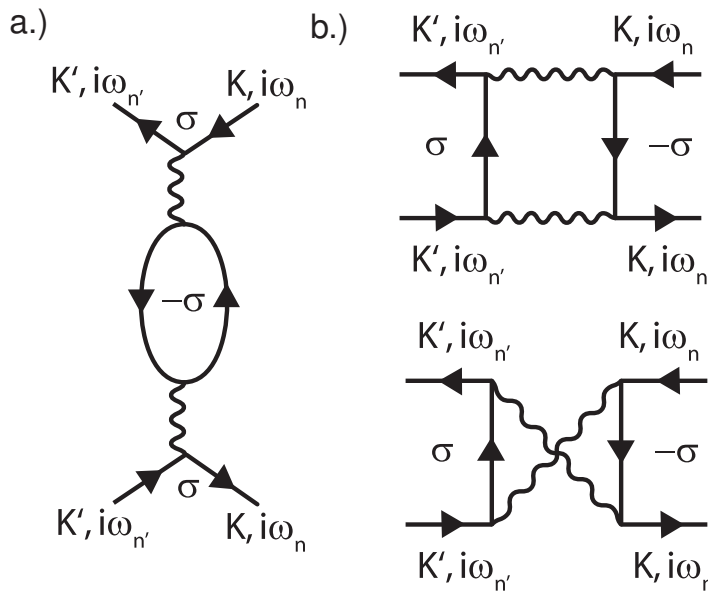
$$n = 0.7$$



Here, only 2nd order diagrams for vertex

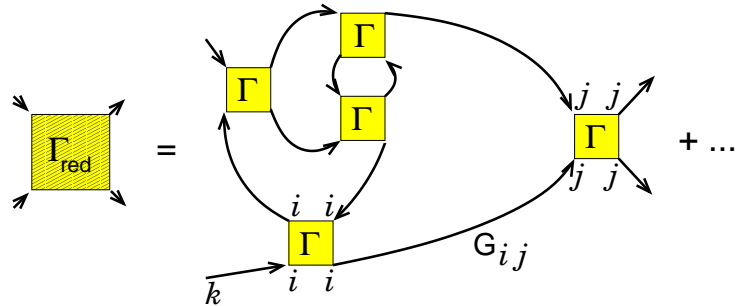
$$(q = 0, \omega = 0)$$

but 8-site DCA for short-range  $\Sigma$



# Conclusion

- $D\Gamma A$  assumption: **local** 2-particle irreducible  $\Gamma$



- $D\Gamma A$  can access **short-** and **long-range** correlations

- Results: **pseudogap** in 2D

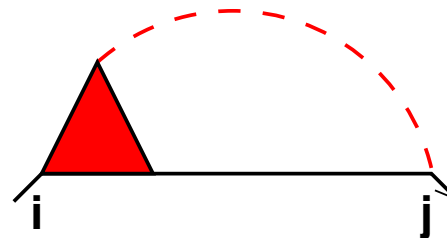
**Mott-Hubbard transition** modified by **AF fluctuations**

# Outlook

- Physics: **magnons**, interplay between **AFM** and **superconductivity**, **QCP**

- Realistic **multi-orbital** calculations possible

- *Ab initio* calculations with  $D\Gamma A$



includes DMFT, GW, and vertex corrections beyond