# Dynamical vertex approximation —
# a step beyond dynamical mean field theory

**K. Held***

MPI for solid state research, Stuttgart

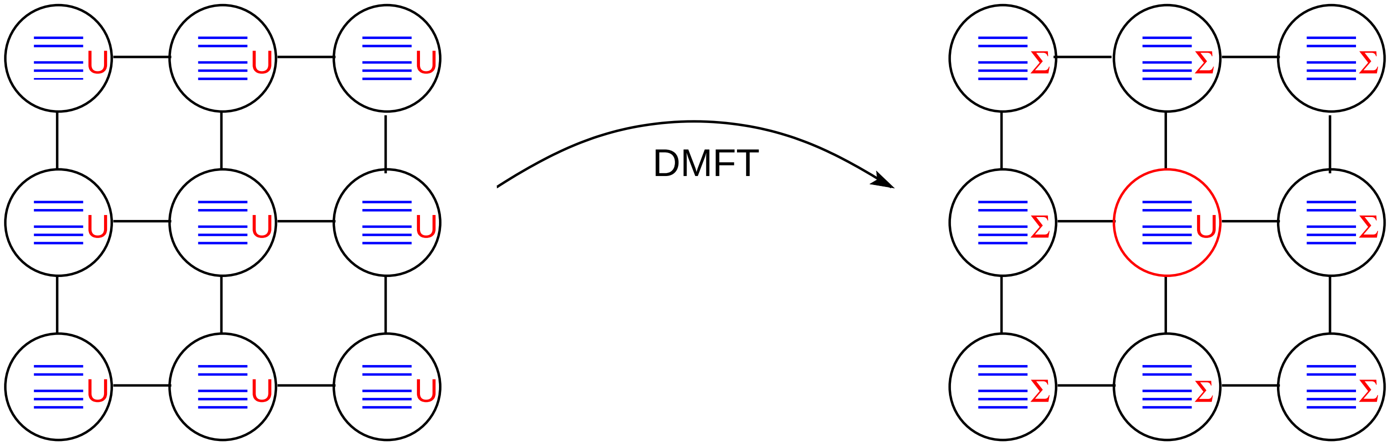
*CORPES07, April 26, 2007*

- **Motivation**
- **Method**
- **Results for 3D, 2D, and 1D Hubbard model**
- **Conclusion and outlook**

* together with A. Toschi, A. Katanin (MPI-FKF), PRB 75, 045118 (2007)

# Motivation

**Dynamical mean field theory**




$\Sigma$ all topologically distinct, but local diagrams

**Success story:** quasiparticle renormalizations, magnetism, kinks ...

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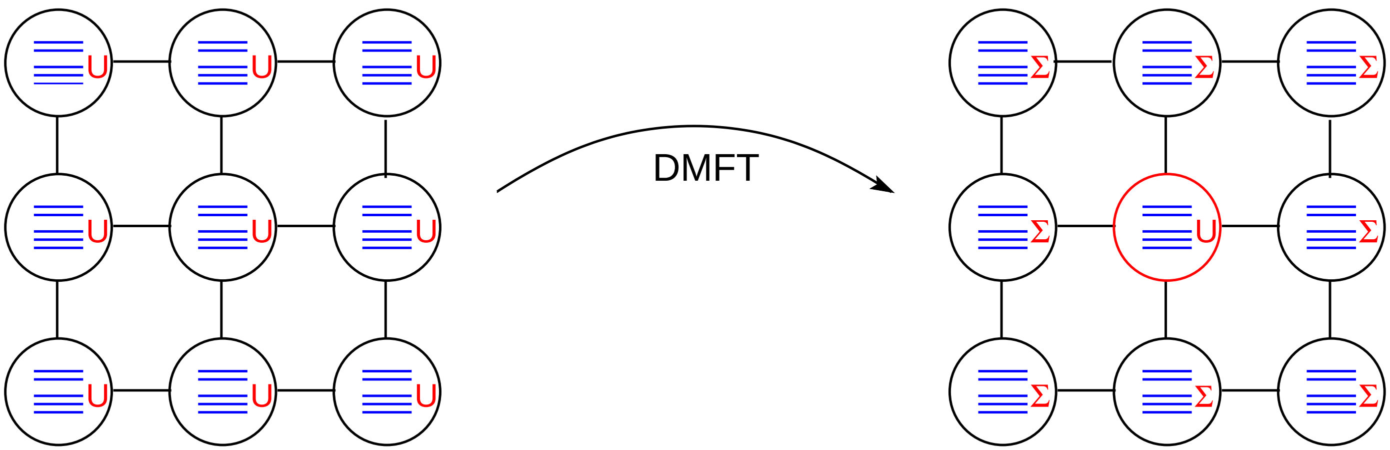


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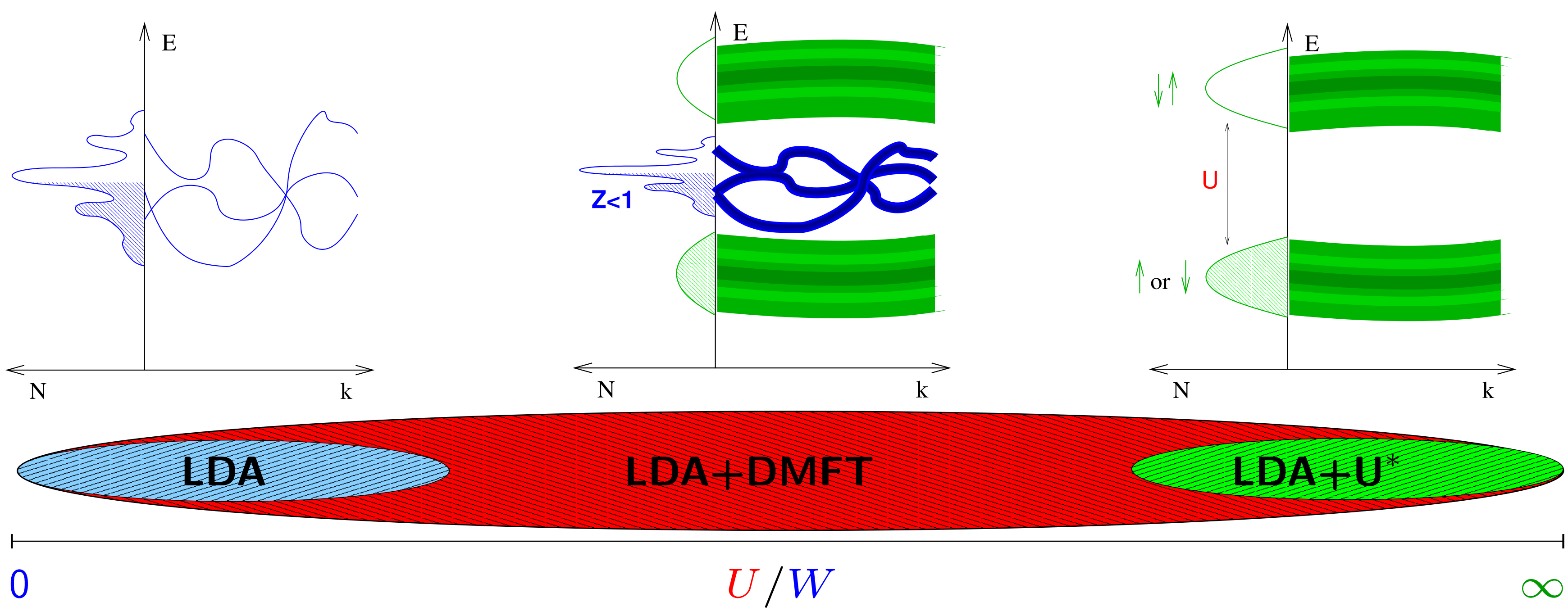

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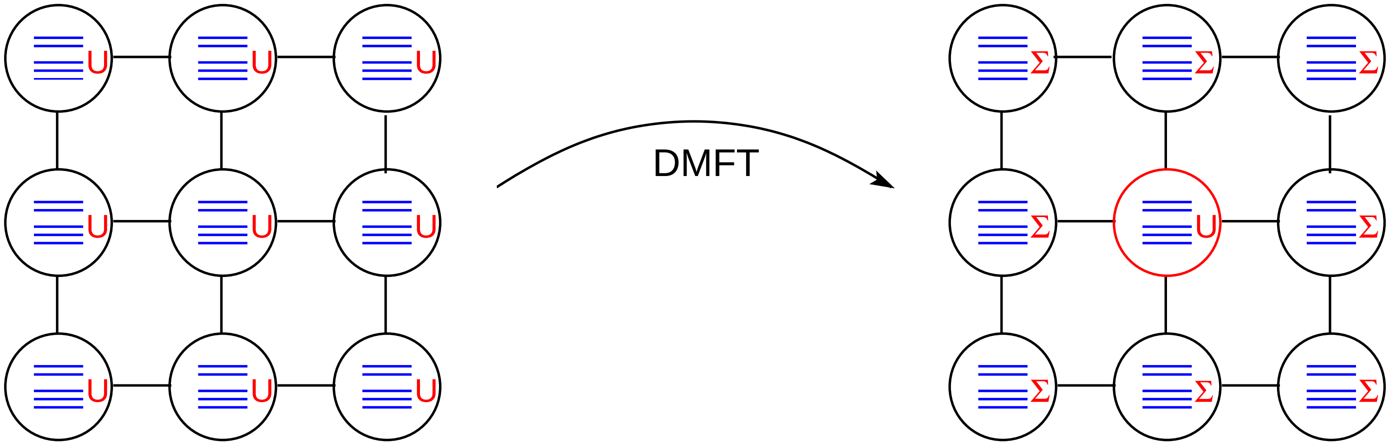



$\Sigma$ all topologically distinct, but local diagrams

**Success story:** quasiparticle renormalizations, magnetism, kinks ...

**Not included:**

non-local correlations

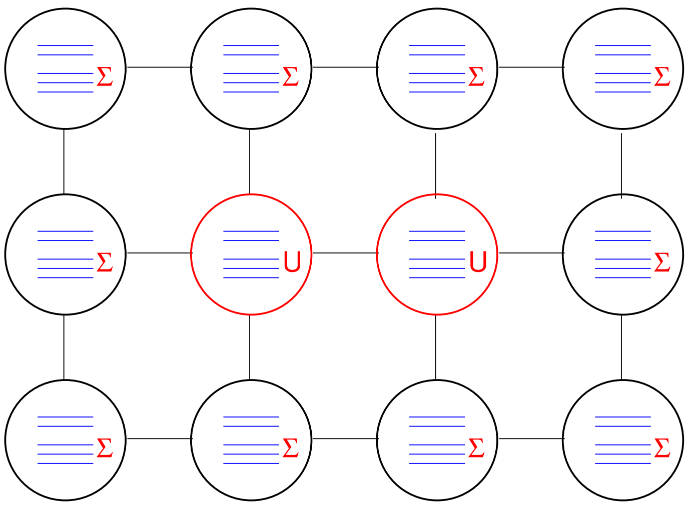
$p$-, $d$-wave superconductivity, spin Peierls

magnons, (quantum) critical behavior ...

ARPES with $\mathbf{k}$-dependent $\Sigma$

# beyond DMFT

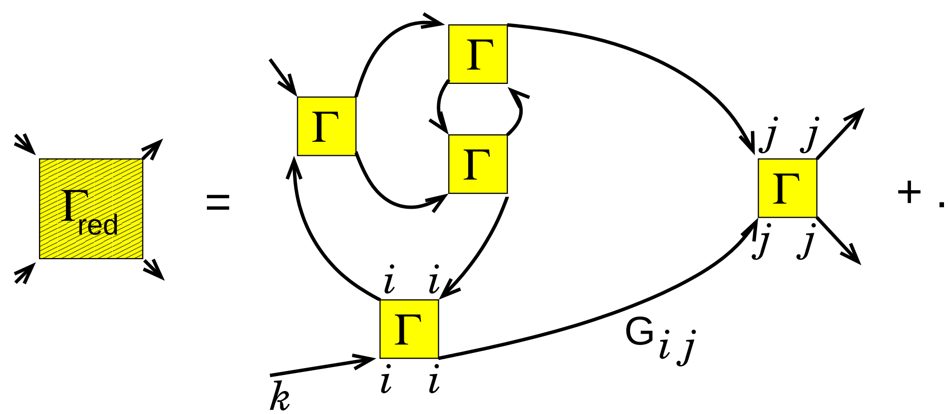
## cluster extensions of DMFT




- 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

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

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

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

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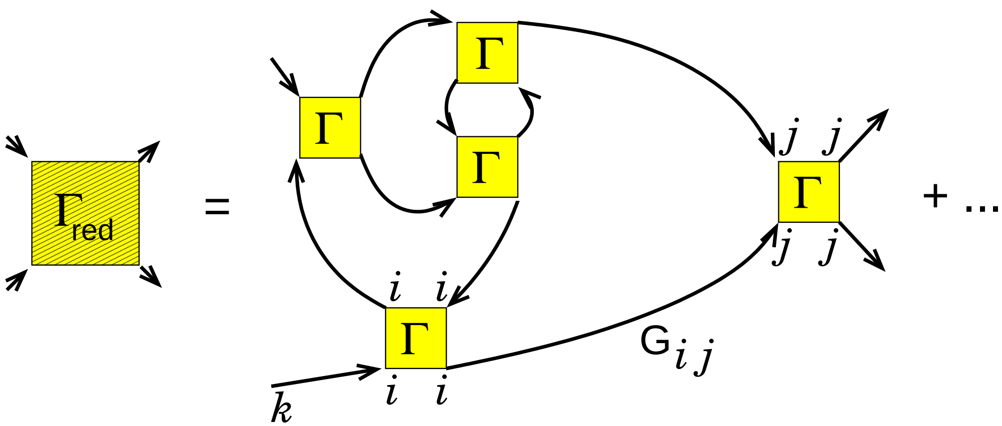


local $\Gamma$, non-local $G$

$\longrightarrow$

non-local reducible vertex $\Gamma_{\rm red}$

via parquet equations

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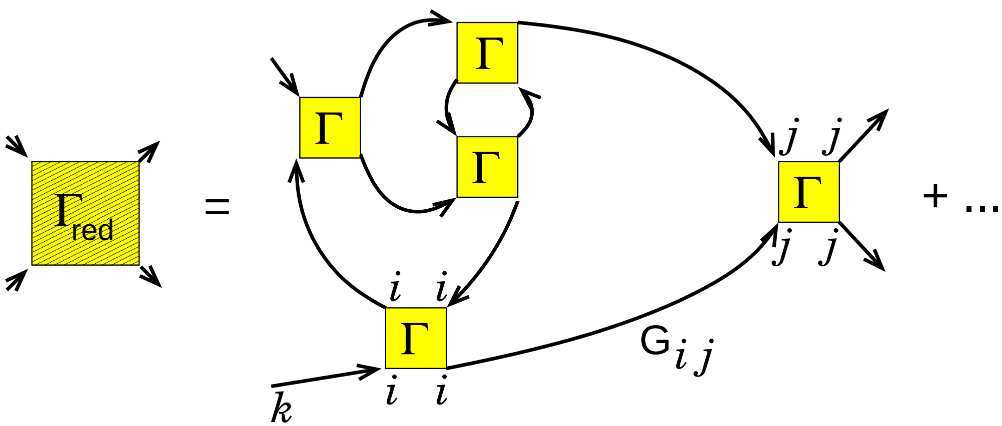


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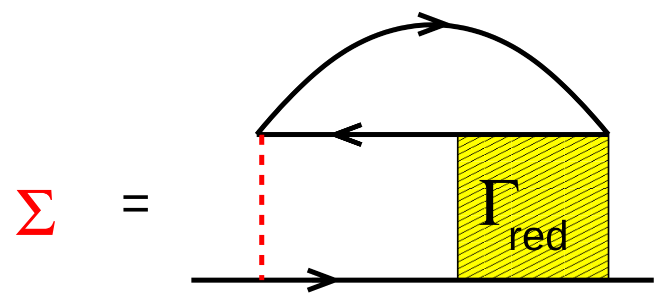


$\Gamma_{red}$

$\longrightarrow$

non-local $\Sigma$

exact relation (eq. of motion)

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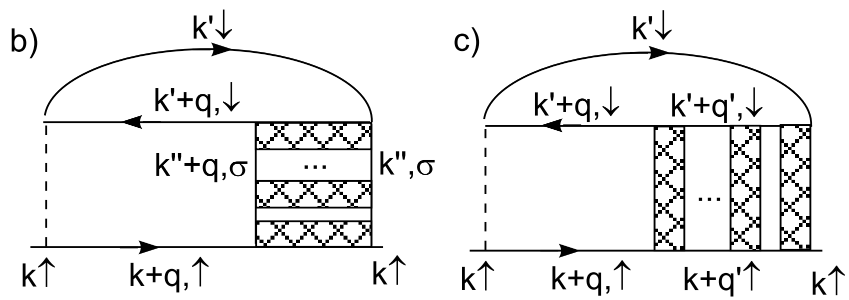
**First step: restriction to ladder diagrams**

$\Sigma \quad =$




lines: non-local $G$

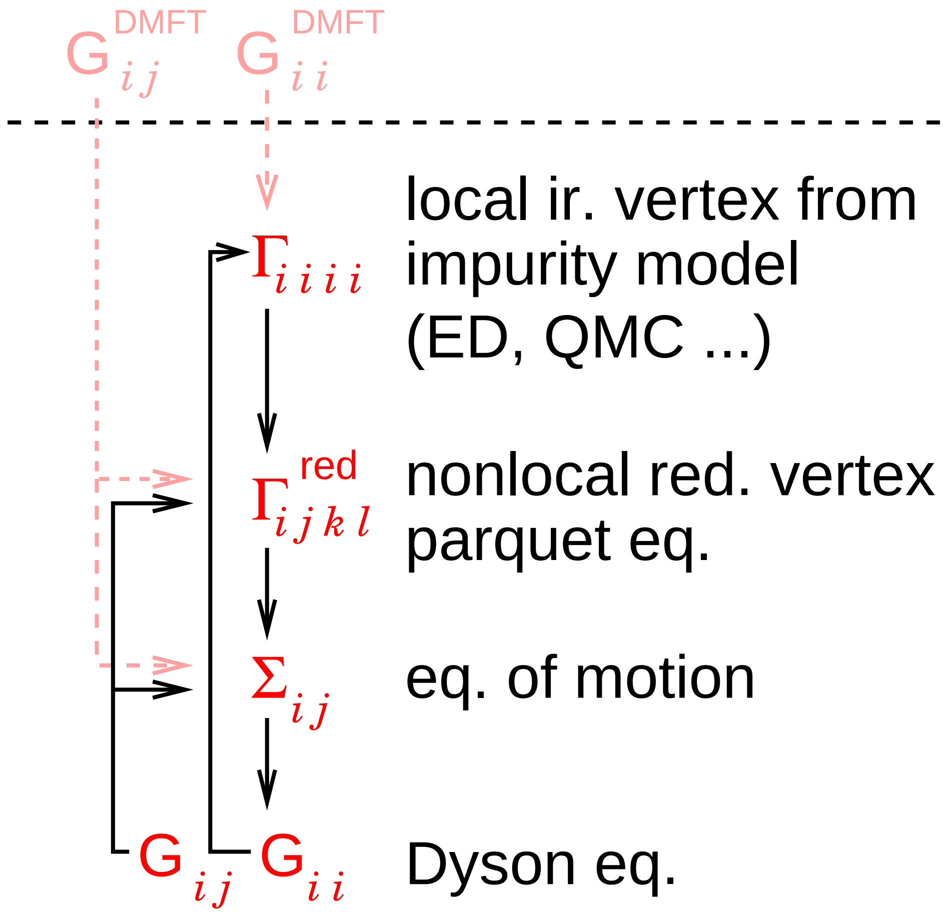
crosshatched: local irreducible vertex in spin/charge channels

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

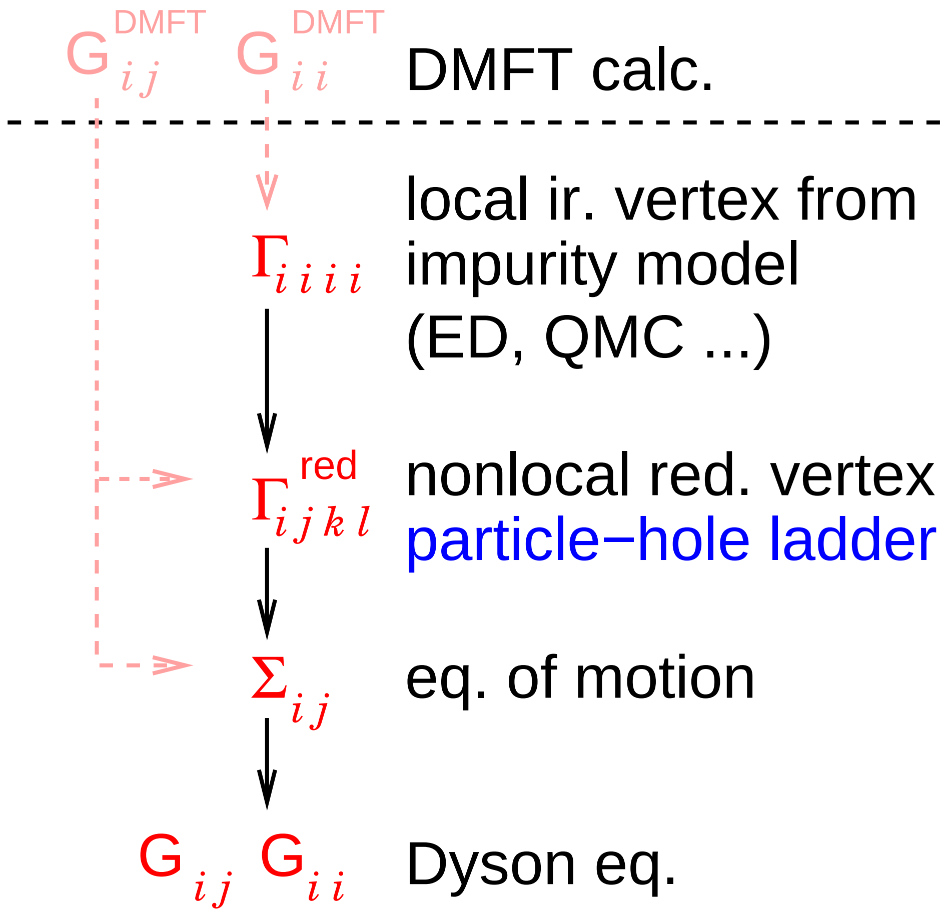
magnons, spin-fluctuations at (A)FM phase transition

$G_{ij}$ from DMFT

# DΓA algorithm



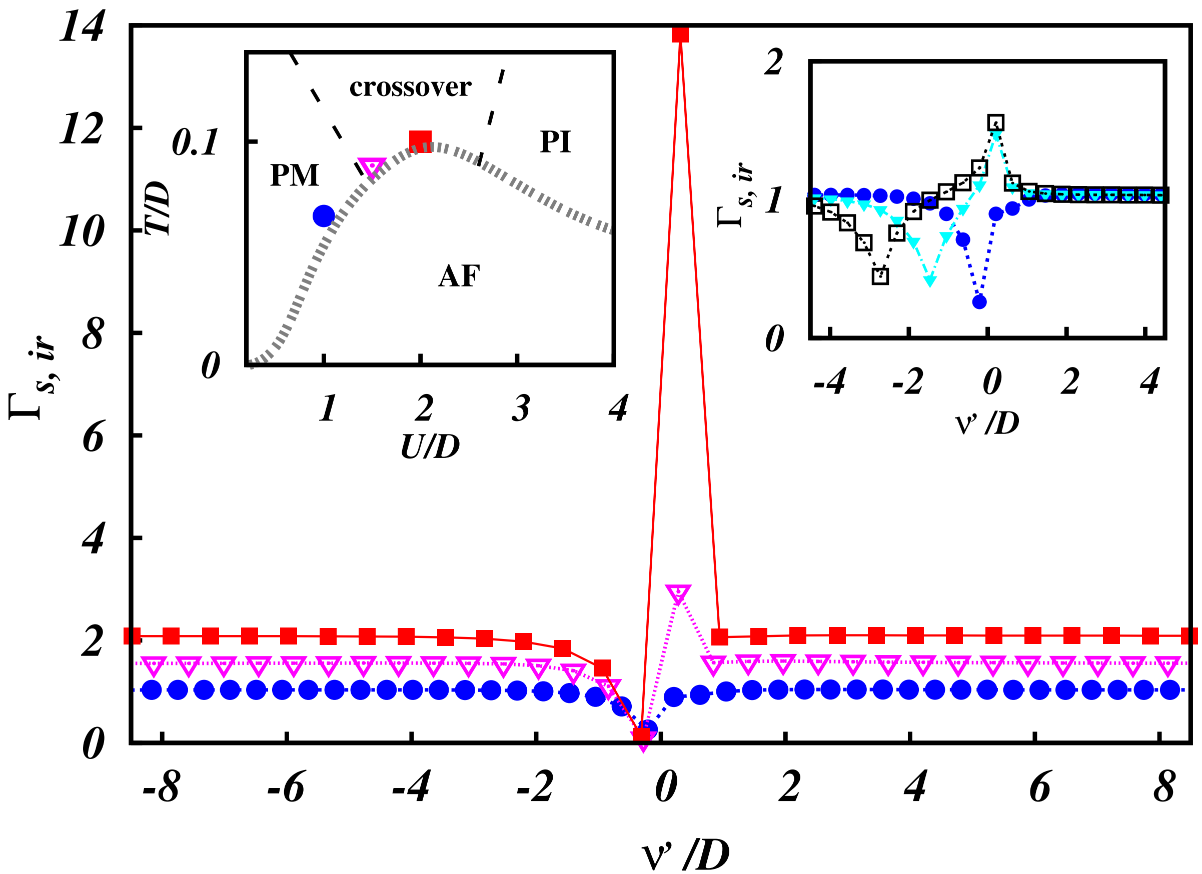
# DΓA algorithm (restriction to ph ladders)



# Results: 3D Hubbard model

$$H = -{\color{blue}t} \sum_{\langle i,j\rangle\sigma} c^\dagger_{i\sigma} c_{j\sigma} + {\color{blue}U} \sum_i n_{i\uparrow} n_{i\downarrow}$$

cubic lattice, exact diagonalization as impurity solver




eff. bandwidth $\equiv$ 2D

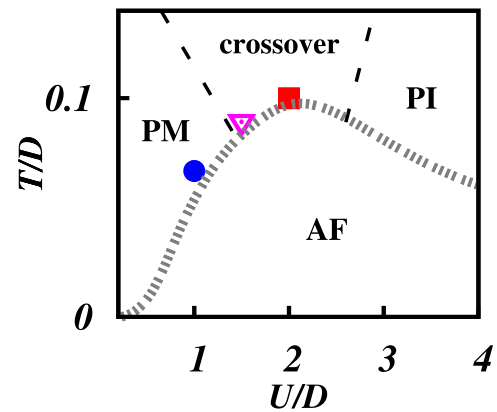
$\omega = 0$

$\nu = \pi T$

$\Gamma_{\mathrm{s,ir}}(\nu, \nu', \omega)$ strongly frequency dependent

# Results: 3D Hubbard model

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



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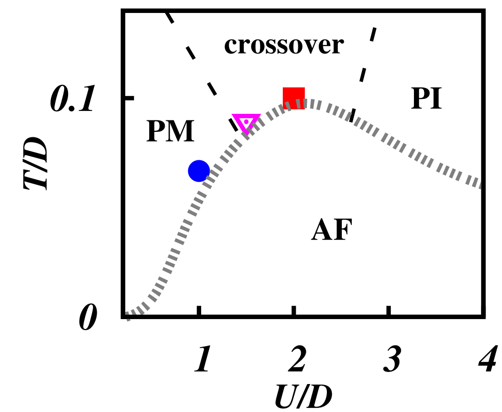


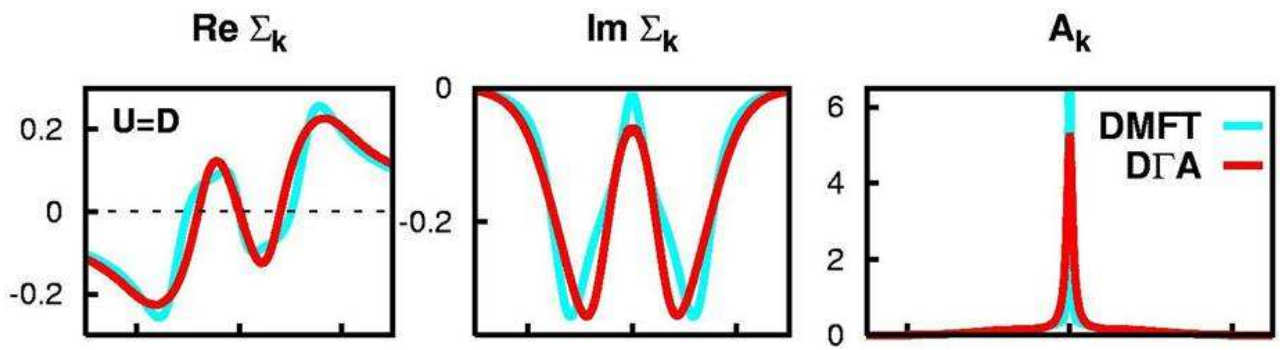


← weak damping of QP peak

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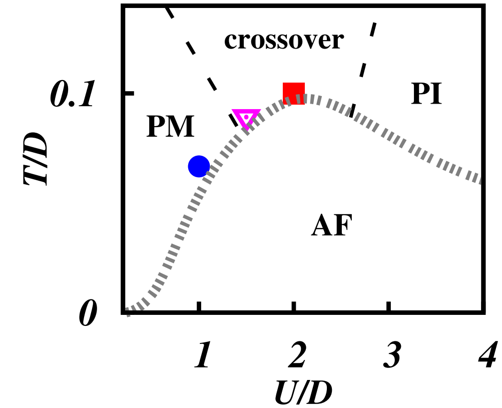


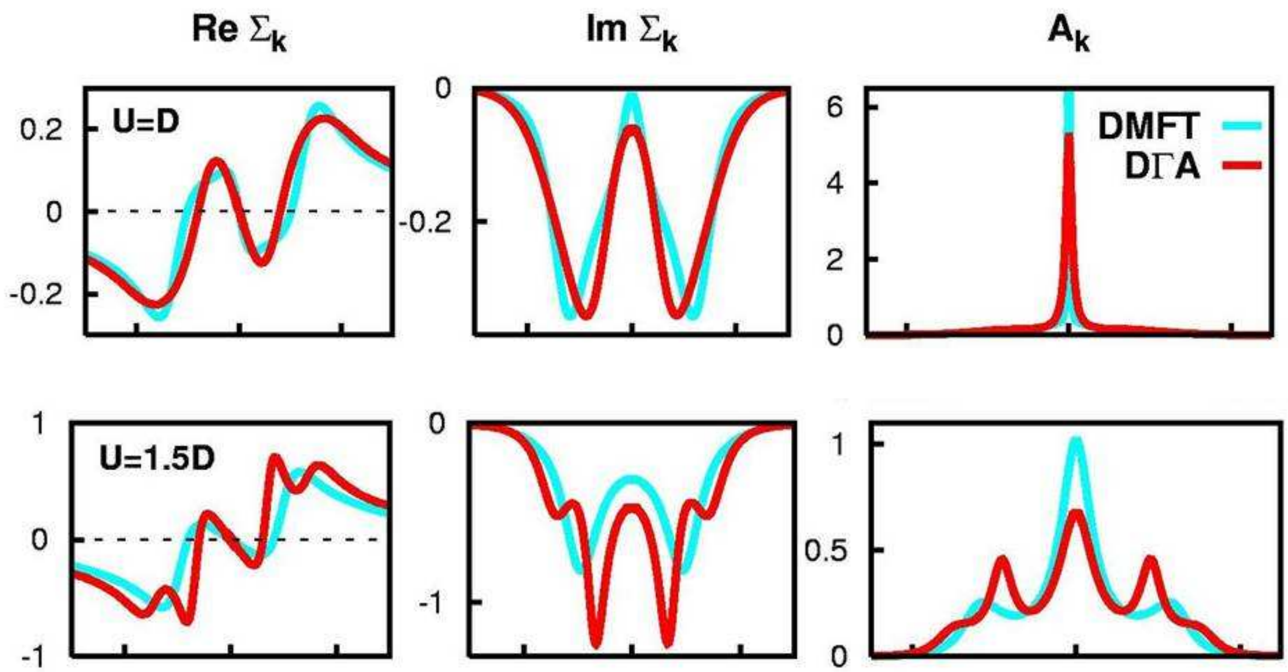


← weak damping of QP peak

← QP-damping strongly enhanced

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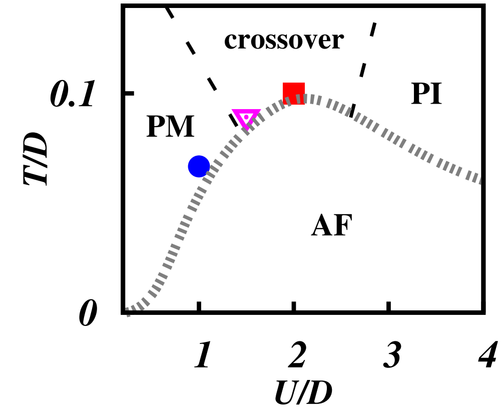
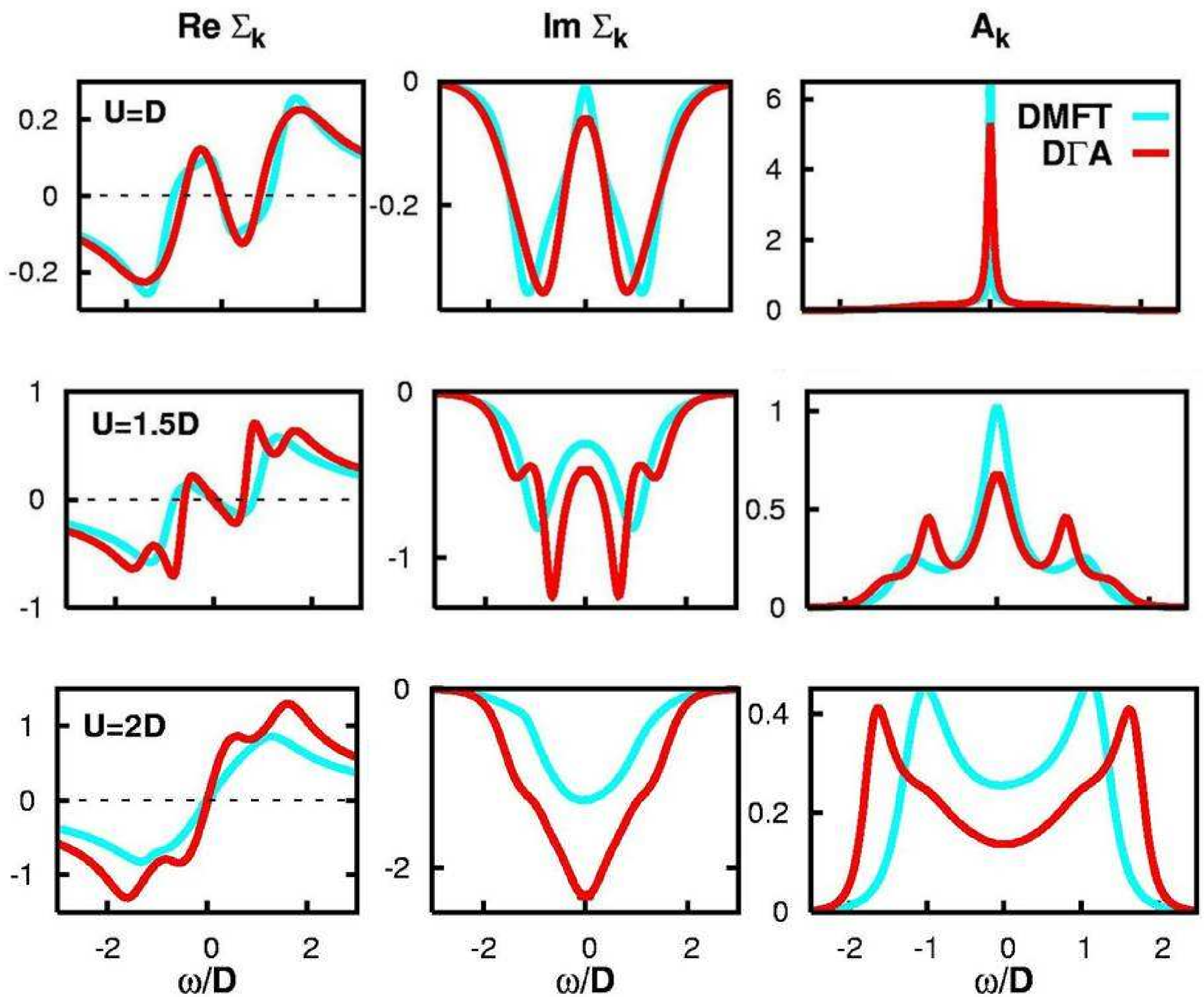


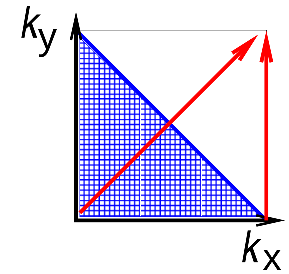




← weak damping of QP peak

← QP-damping strongly enhanced

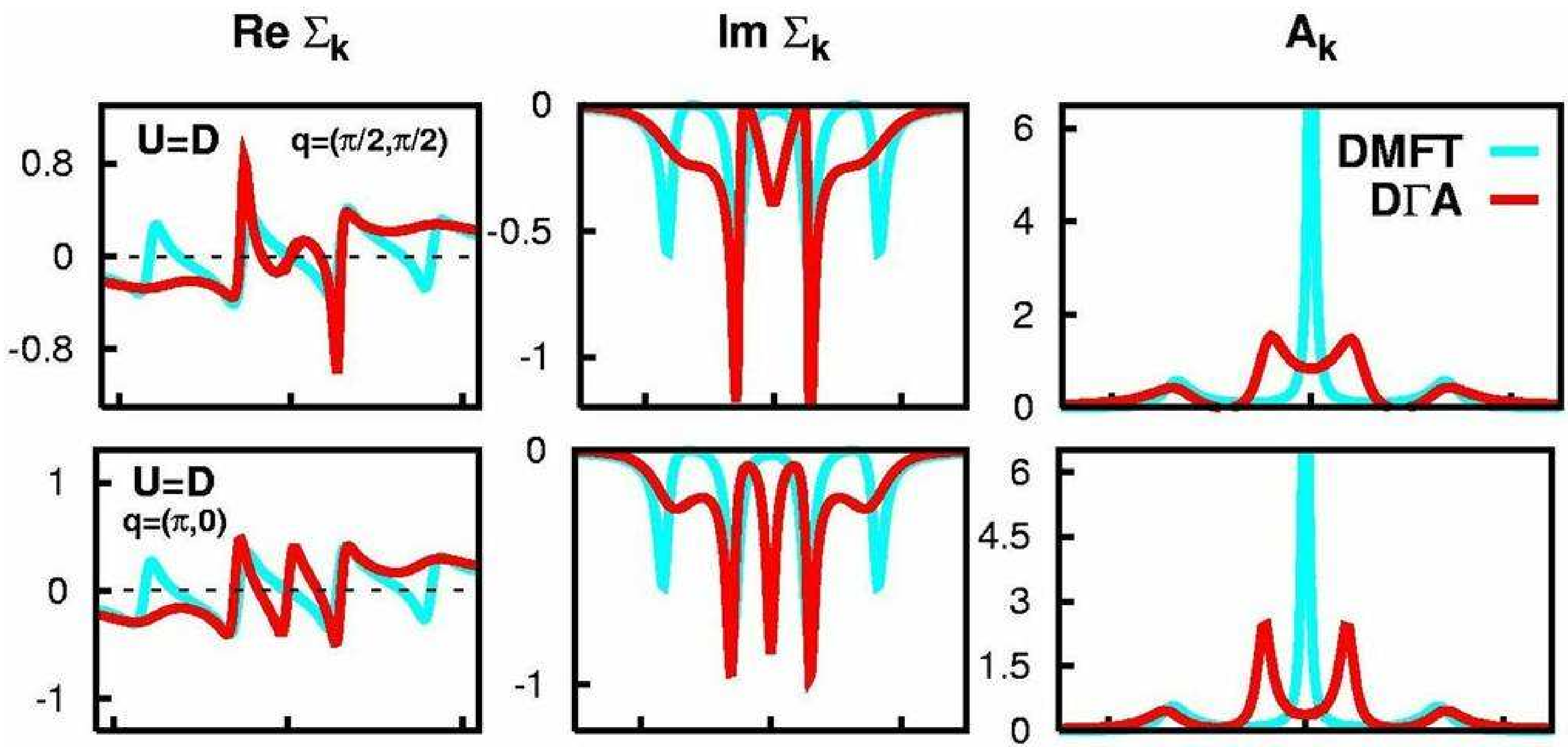
← more insulating

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




nodal
$\mathbf{k} = (\frac{\pi}{2}, \frac{\pi}{2})$

anti-nodal
$\mathbf{k} = (\pi, 0)$




anisotropic pseudogap

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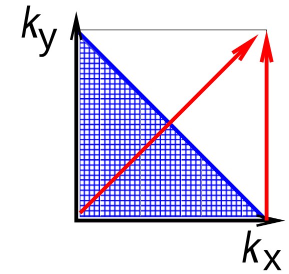
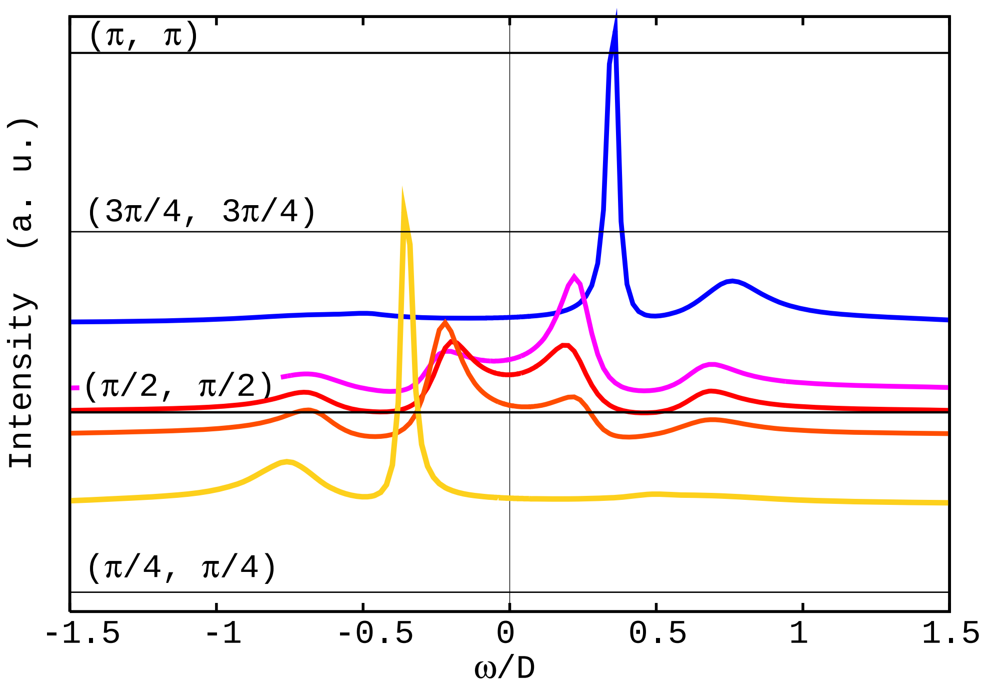
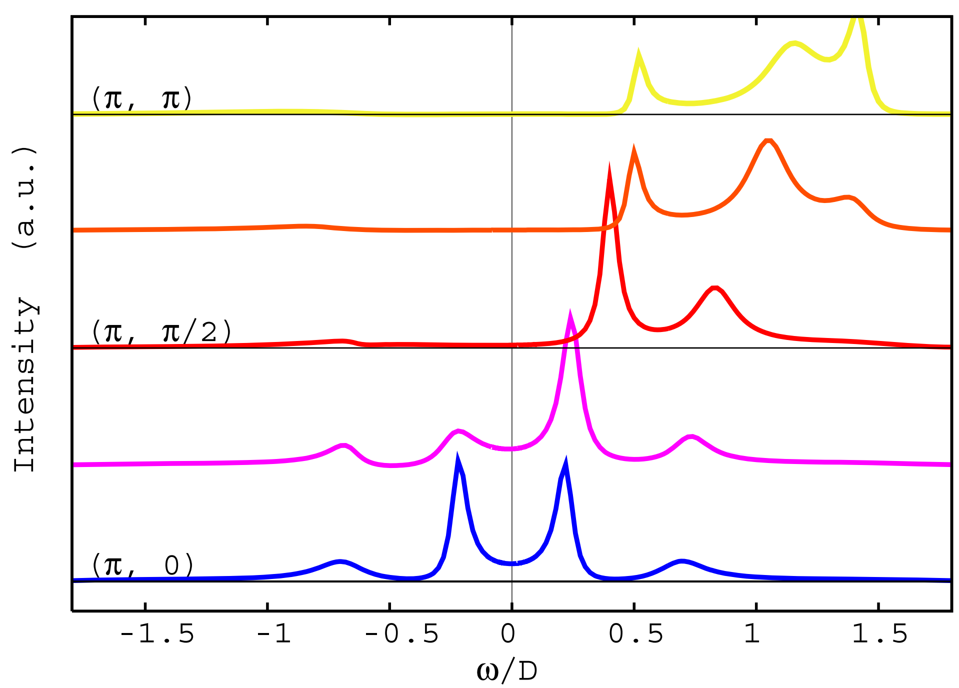


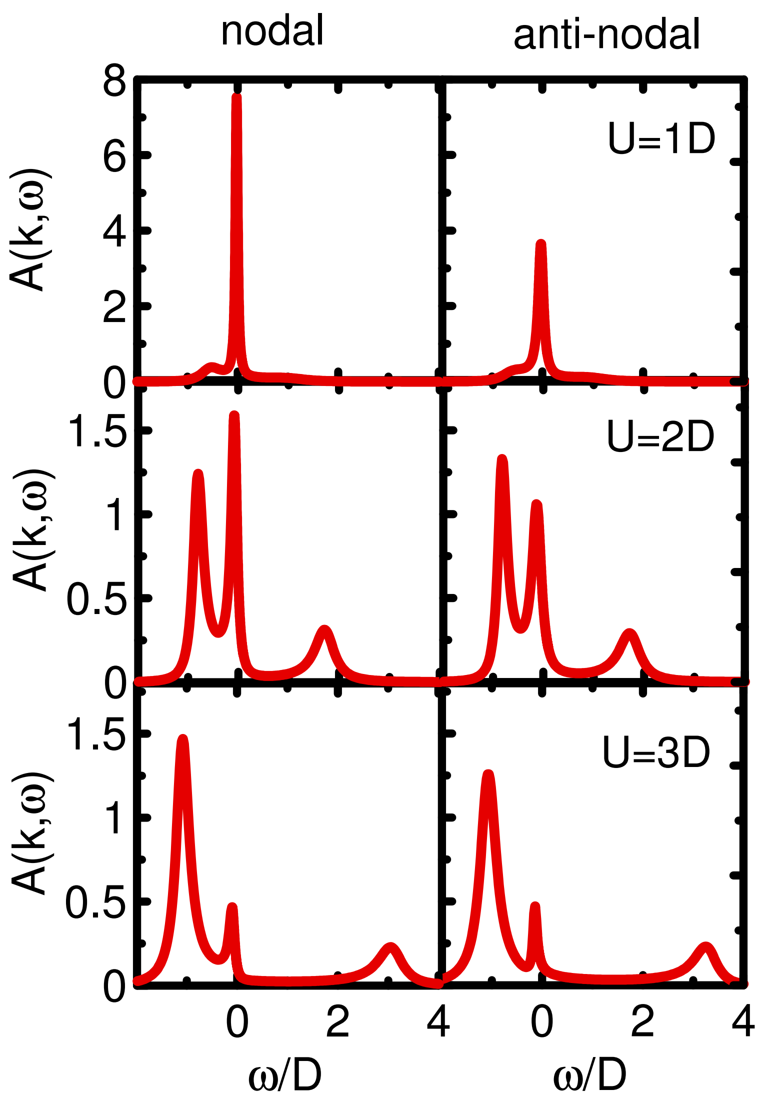

nodal

antinodal



# 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

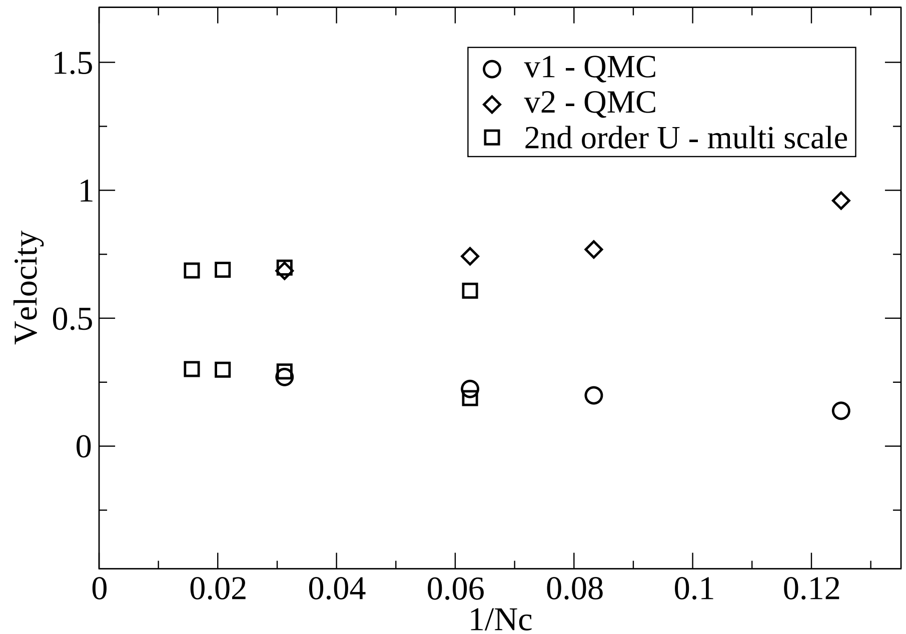
## Spin-charge separation

$U = W = 1$

$k = \pi/2$

$\beta = 31$

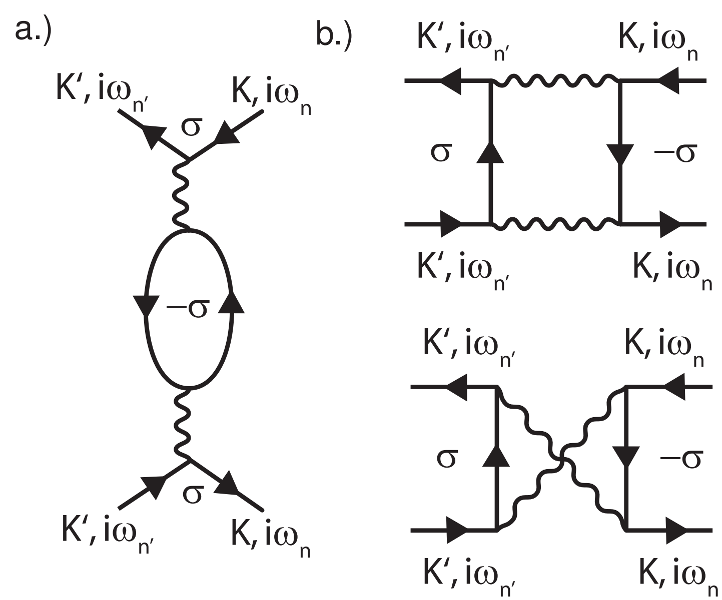
$n = 0.7$




Here, only 2nd order diagrams for vertex

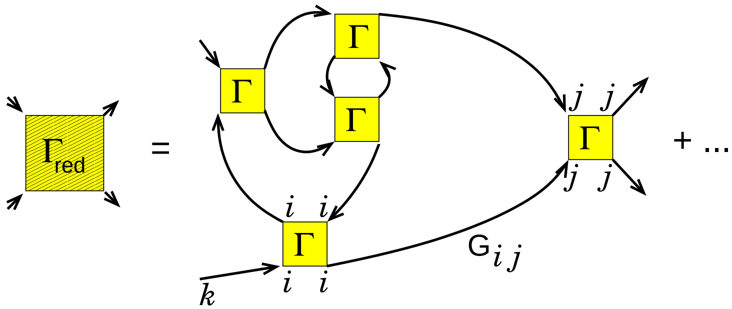
$(q = 0,\ \omega = 0)$

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



## Conclusion

- DΓA assumption: local 2-particle irreducible Γ




- DΓA can access short- and long-range correlations

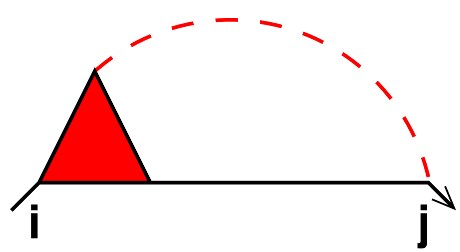
- Results: pseudogap in 2D
  Mott-Hubbard transition modified by AF fluctuations

## Outlook

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

- Realistic multi-orbital calculations possible

- *Ab initio* calculations with DΓA




includes DMFT, GW, and vertex corrections beyond