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

**K. Held**

MPI-FKF Stuttgart → TU Vienna, as of March 2008

*YKIS, Nov 26, 2007*

**1) Dynamical vertex approximation**

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

**2) Kinks in the dispersion relation of correlated electrons**

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# Thanks to...

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

A. Toschi, A. Katanin – MPI-FKF Stuttgart

PRB 75, 045118 (2007)

## 2) Kinks

Y.-F. Yang – MPI-FKF Stuttgart

K. Byczuk, M. Kollar, D. Vollhardt – Augsburg

I. A. Nekrasov – Ekaterinburg

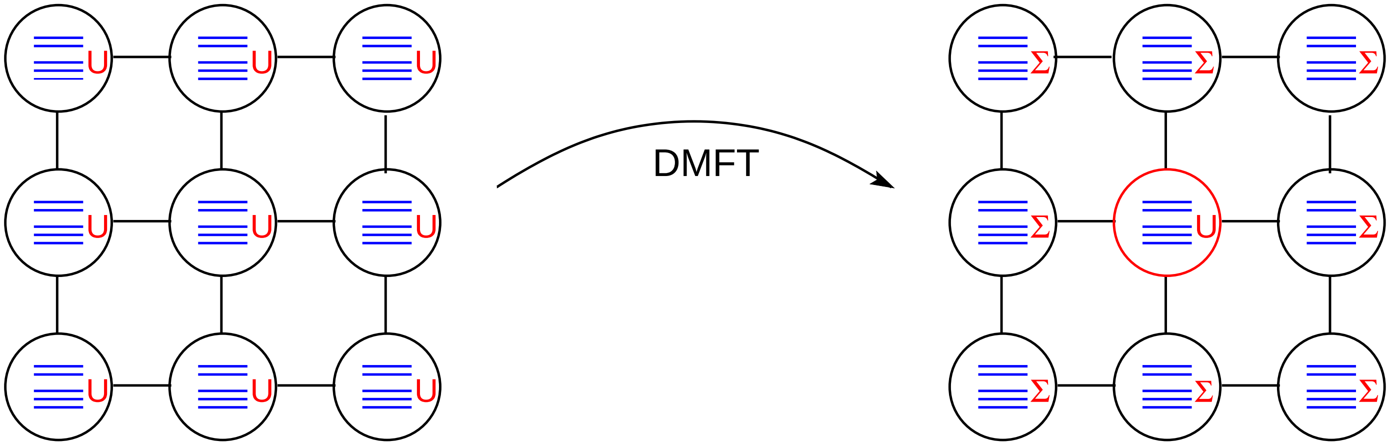
Th. Pruschke – Göttingen

PRB 73, 155112 (2006)

Nature Physics 3 168 (2007)

# Motivation

**Dynamical mean field theory** (Metzner,Vollhardt'89; Georges, Kotliar'92)

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

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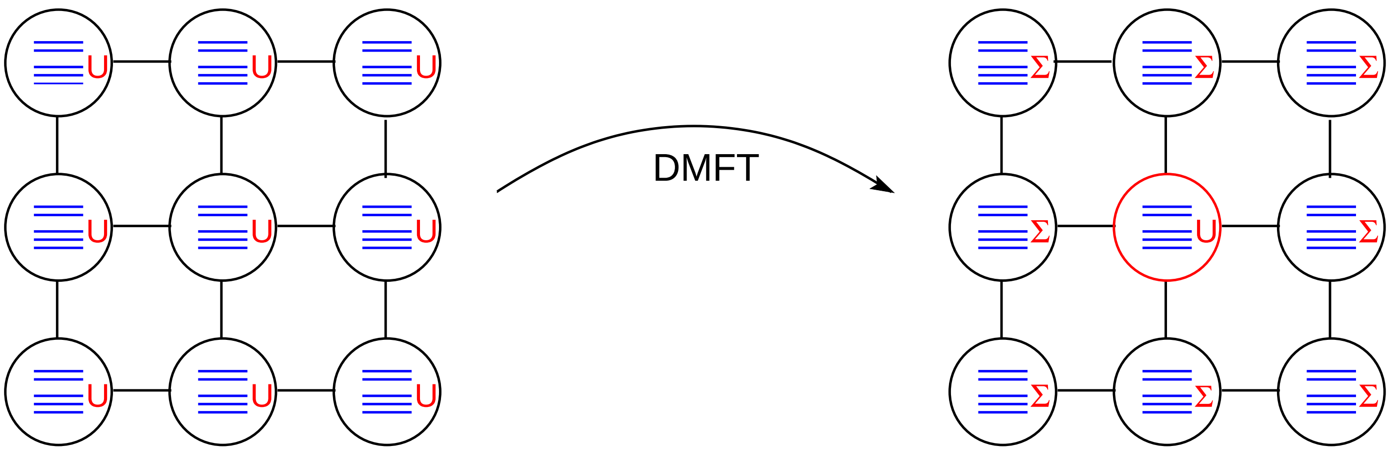


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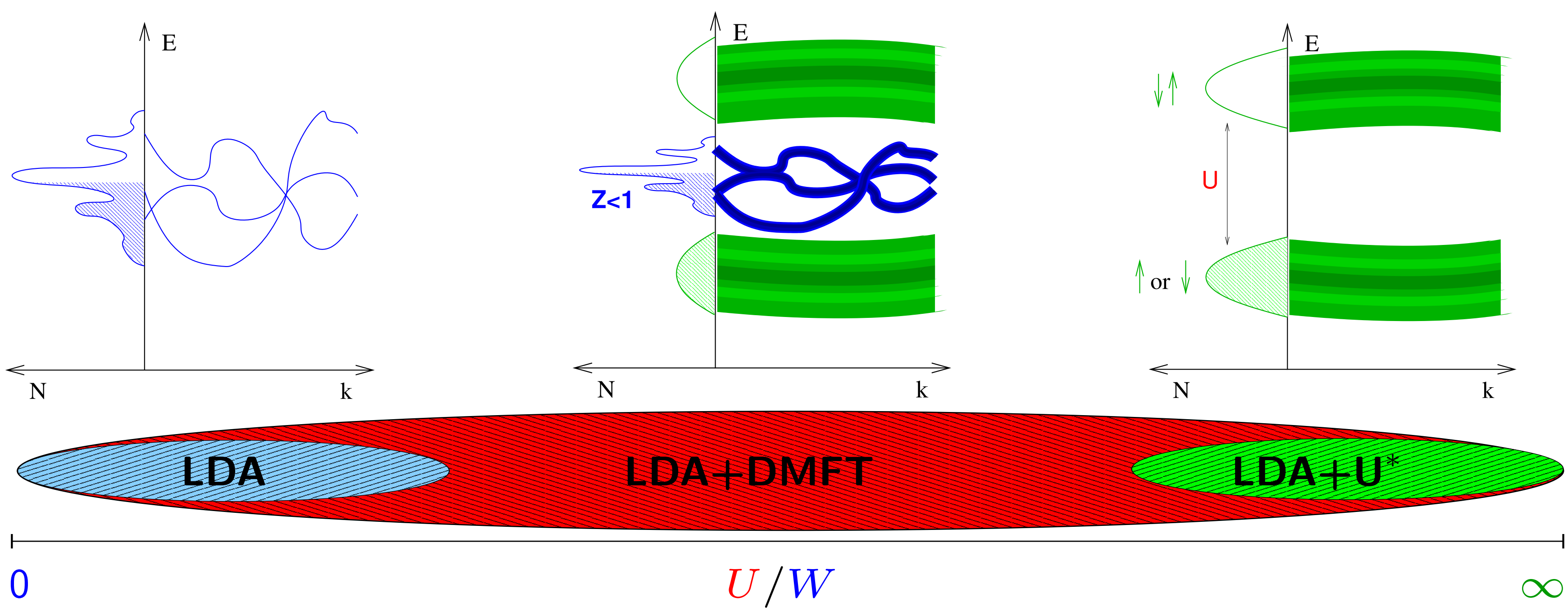

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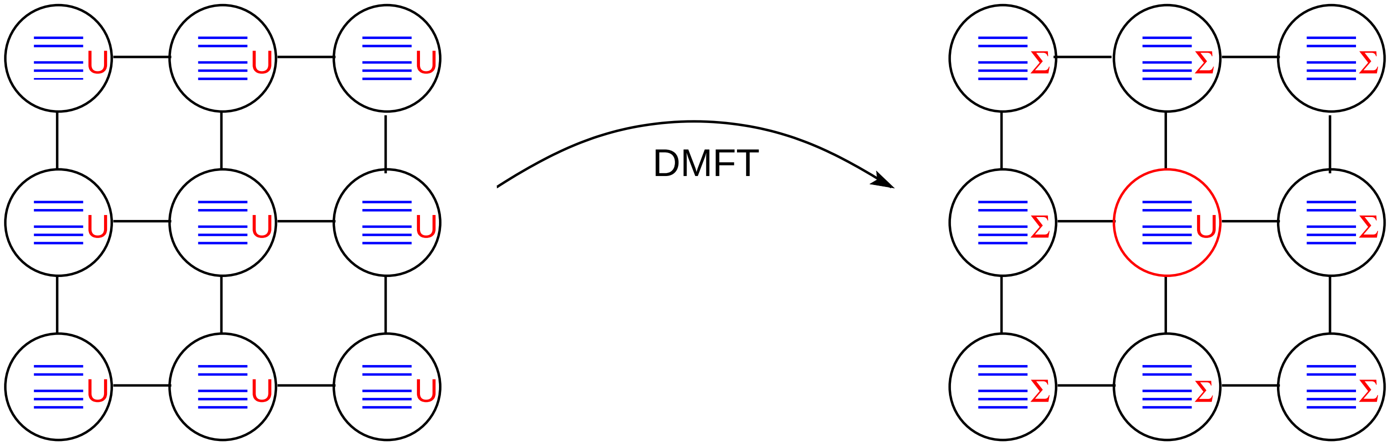



$\Sigma$ all topologically distinct, but local diagrams

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

**Not included:**

non-local correlations

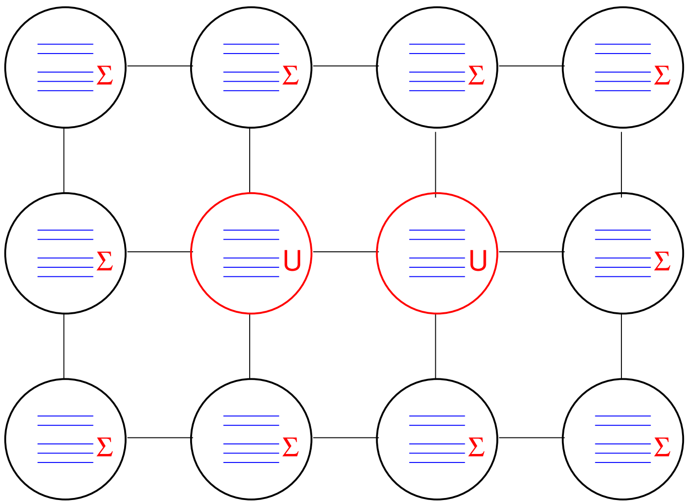
$p$-, $d$-wave superconductivity, spin Peierls

magnons, (quantum) critical behavior ...

$\mathbf{k}$-dependence of $\Sigma$

# beyond DMFT

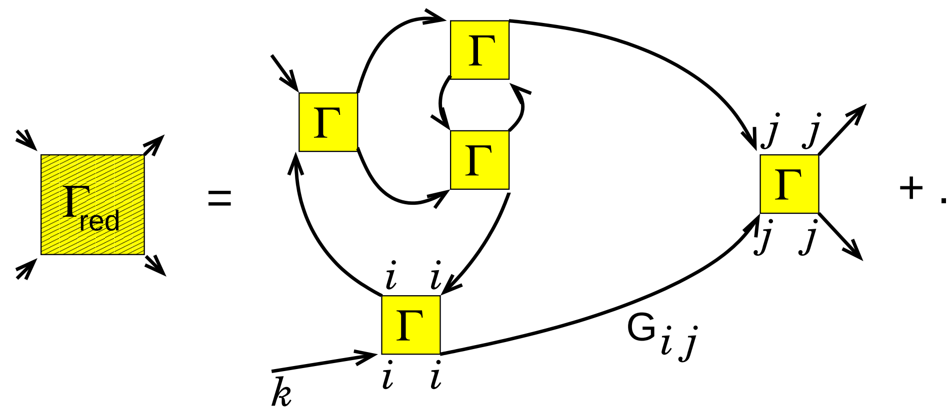
## cluster extensions of DMFT




- 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 ...

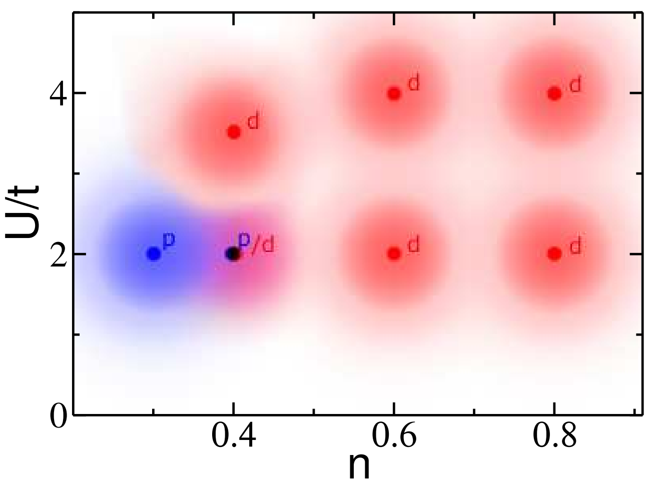
Toschi, Katanin, KH cond-mat/0603100
cf. Kusunose cond-mat/0602451
Slezak *et al.* cond-mat/0603421

# beyond DMFT

dominant superconducting susceptibility

$t$-$t'$ 2D Hubbard model

Arita, KH PRB'06




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

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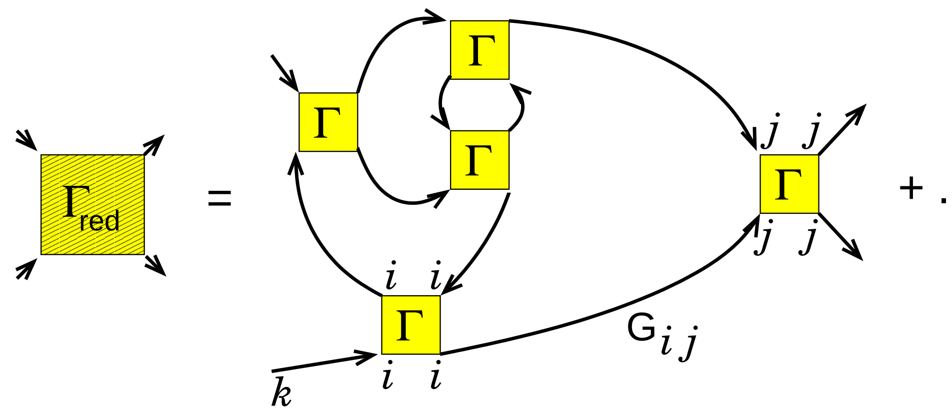


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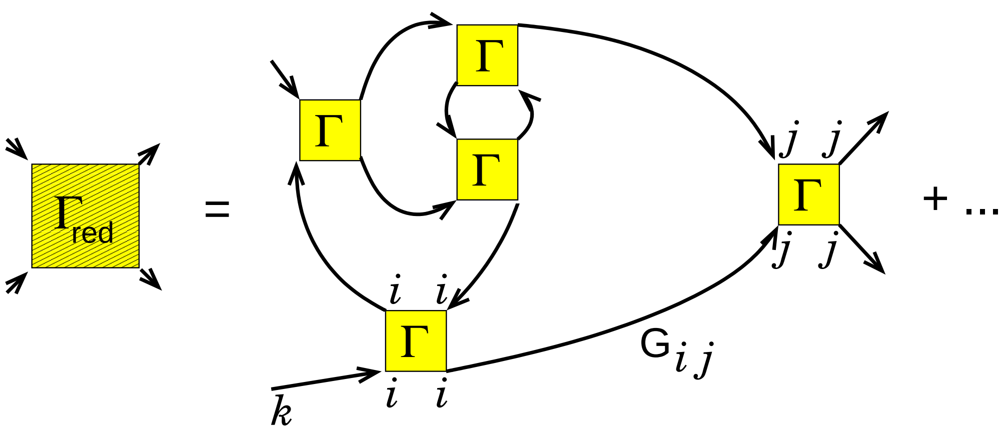


local $\Gamma$, non-local $G$

$\longrightarrow$

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

via parquet equations

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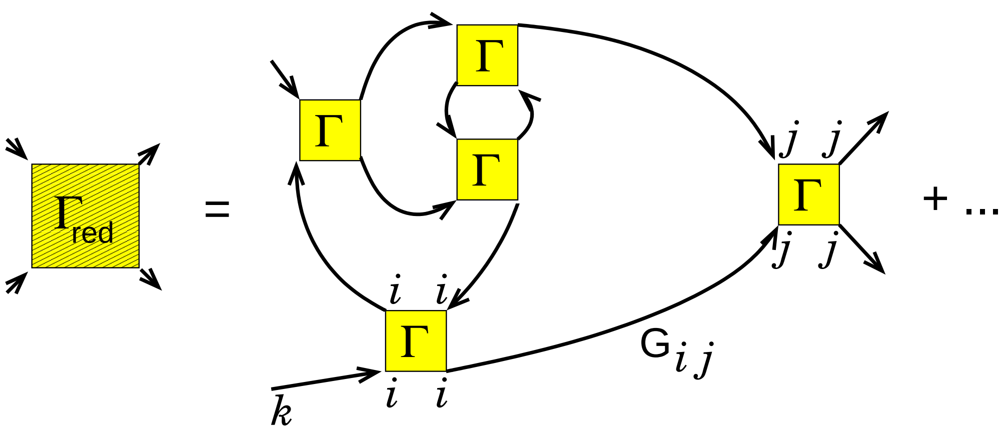


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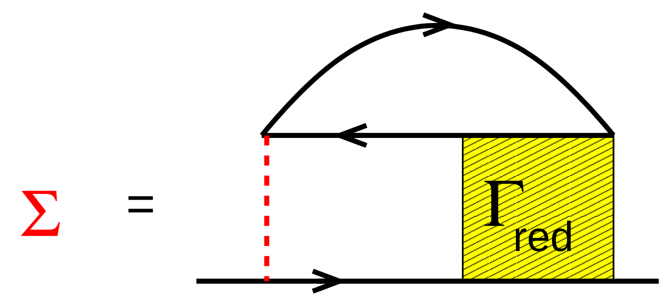


$\Gamma_{\text{red}}$

$\longrightarrow$

non-local $\Sigma$

exact relation (eq. of motion)

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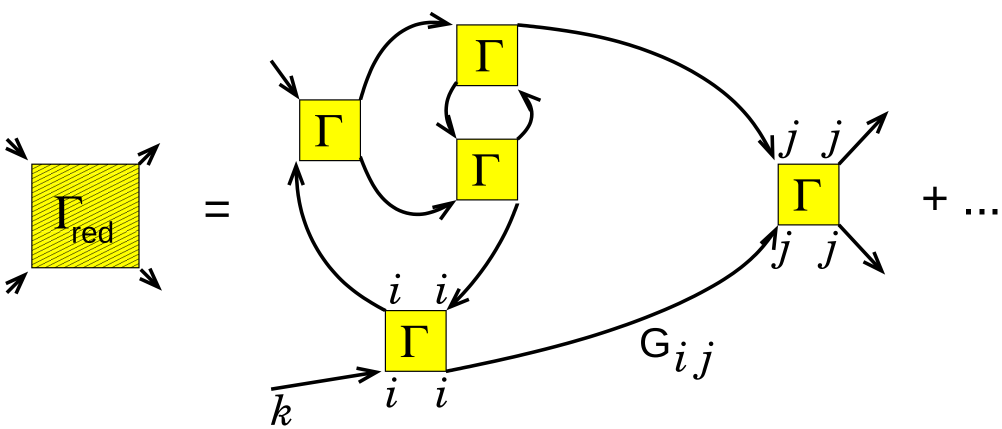


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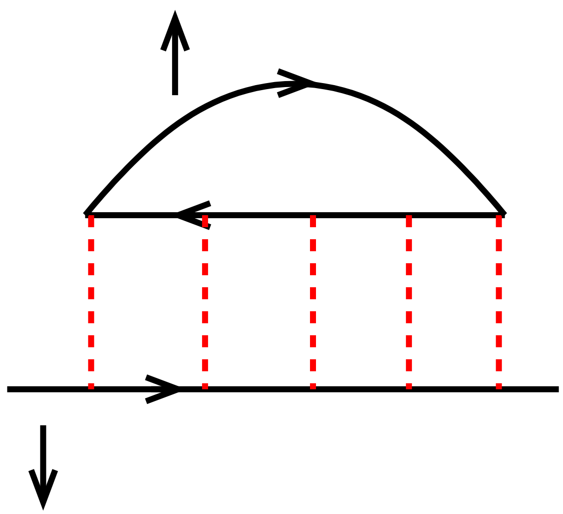

Moriya Edwards-Hertz

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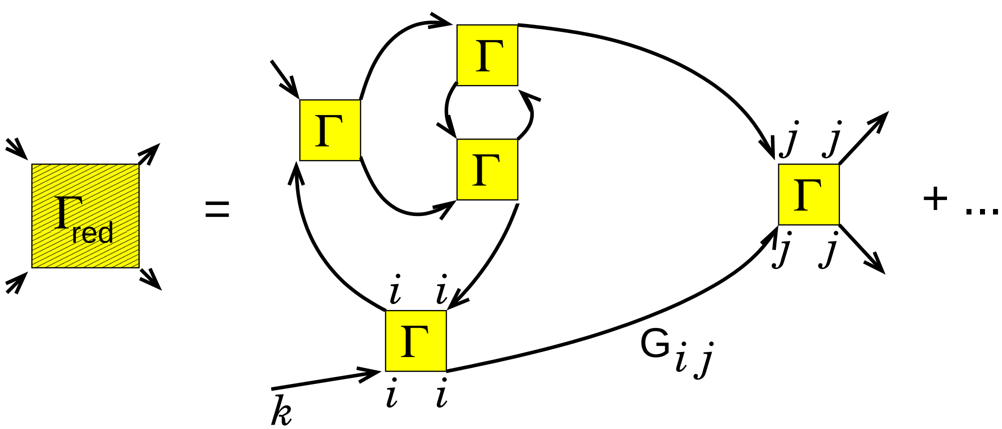


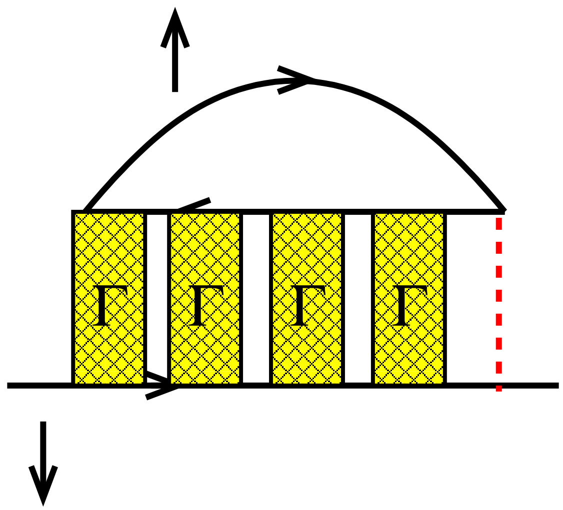


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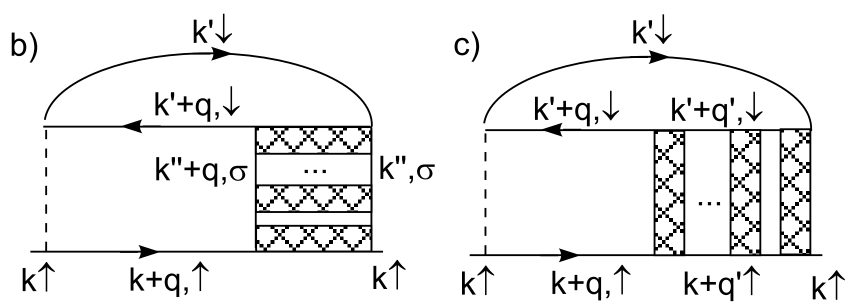
**First step: restriction to ladder diagrams**

$\Sigma$ =




lines: non-local $G$

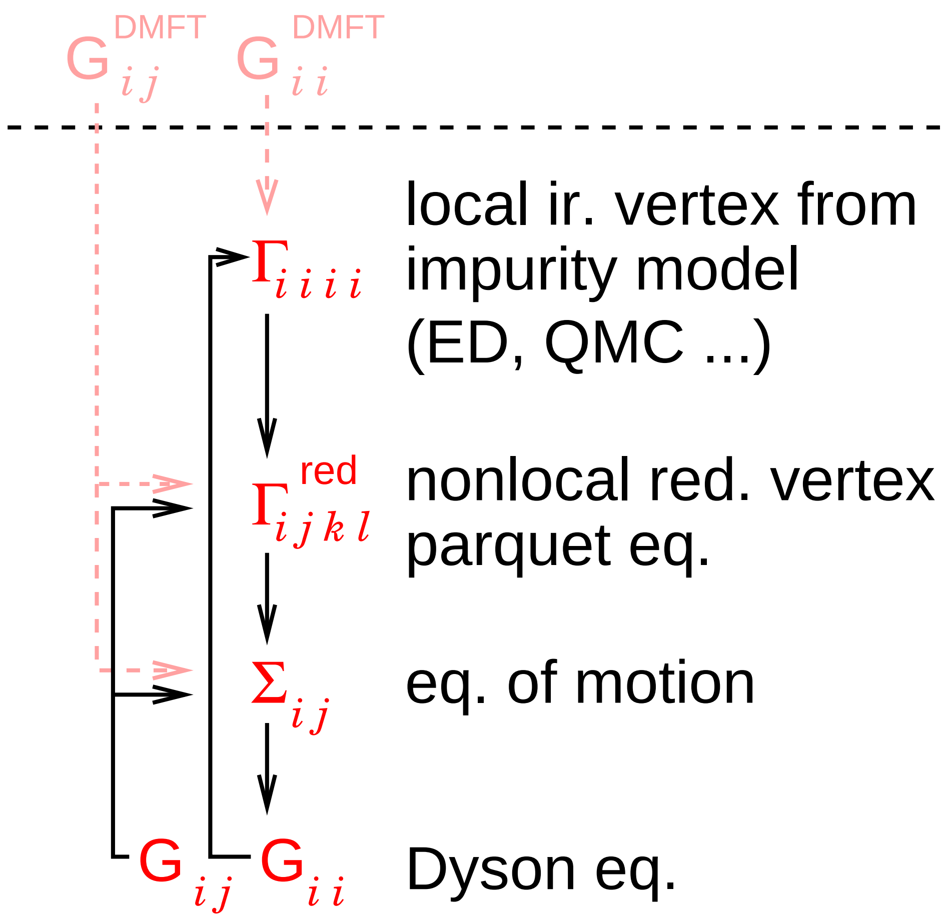
crosshatched: local irreducible vertex in spin/charge channels

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

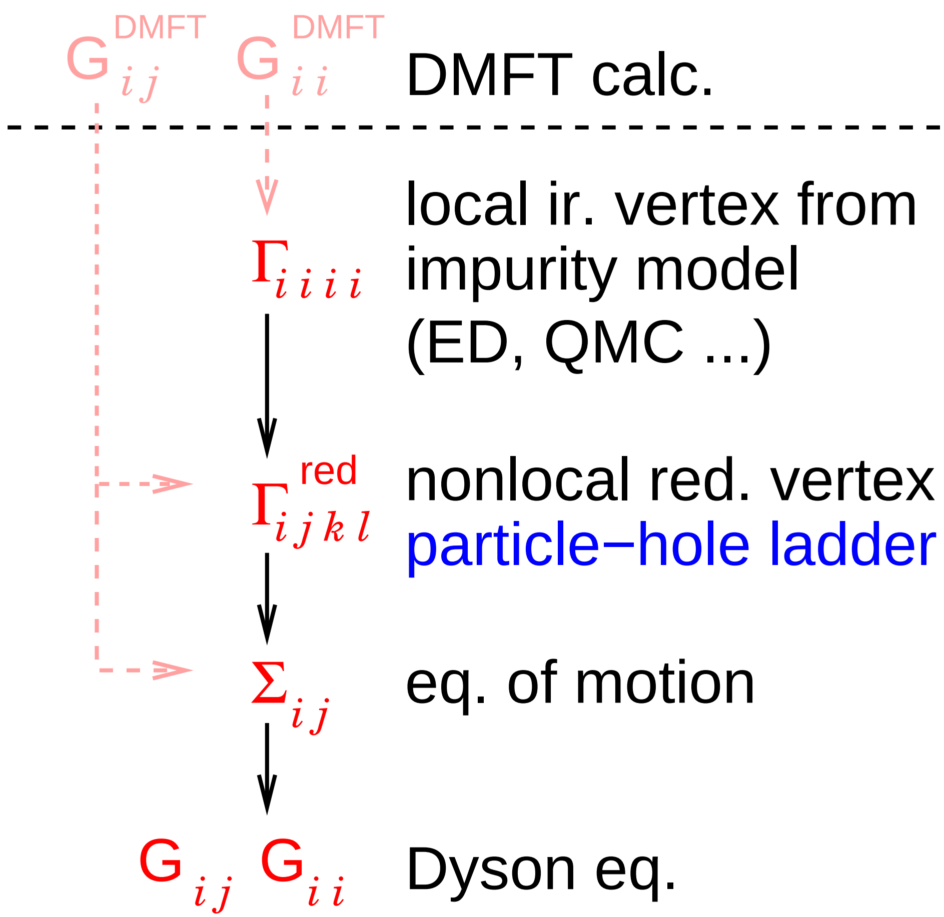
magnons, spin-fluctuations at (A)FM phase transition

$G_{ij}$ from DMFT

# DΓA algorithm



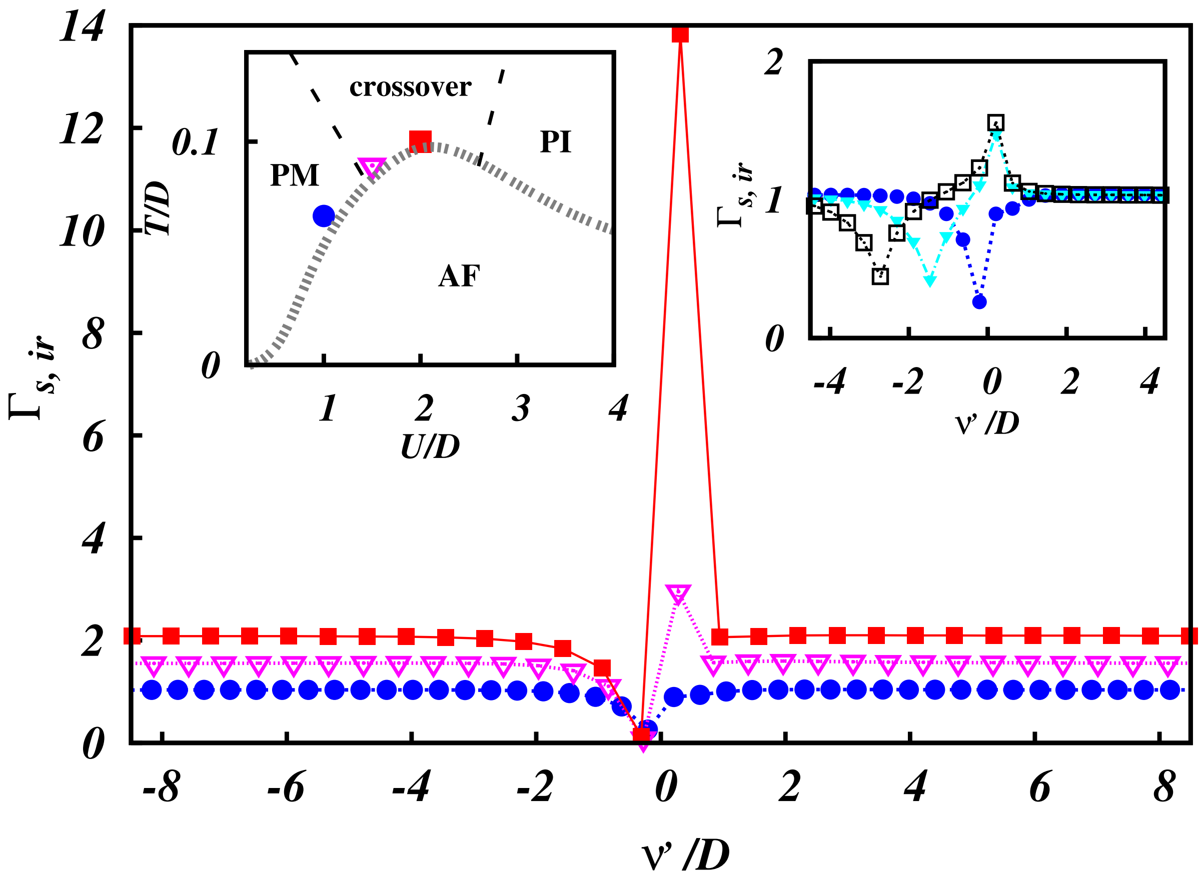
# DΓA algorithm (restriction to ph ladders)



# Results: 3D Hubbard model

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

cubic lattice, exact diagonalization as impurity solver




eff. bandwidth $\equiv$ 2D

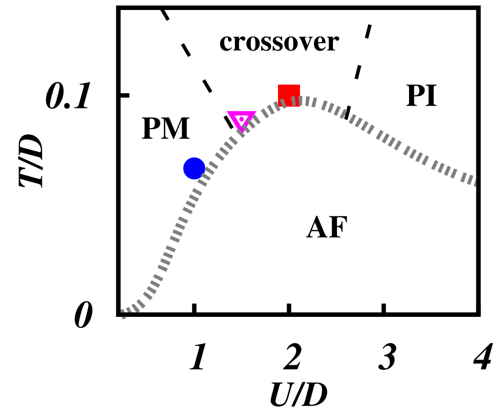
$\omega = 0$

$\nu = \pi T$

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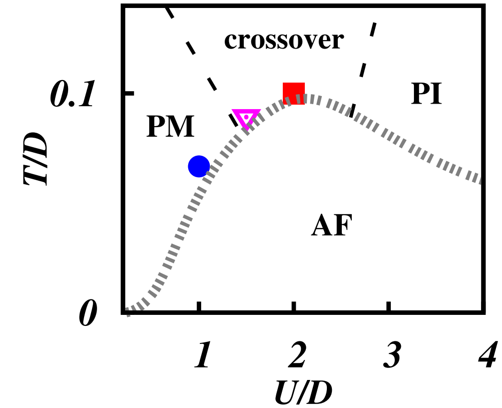


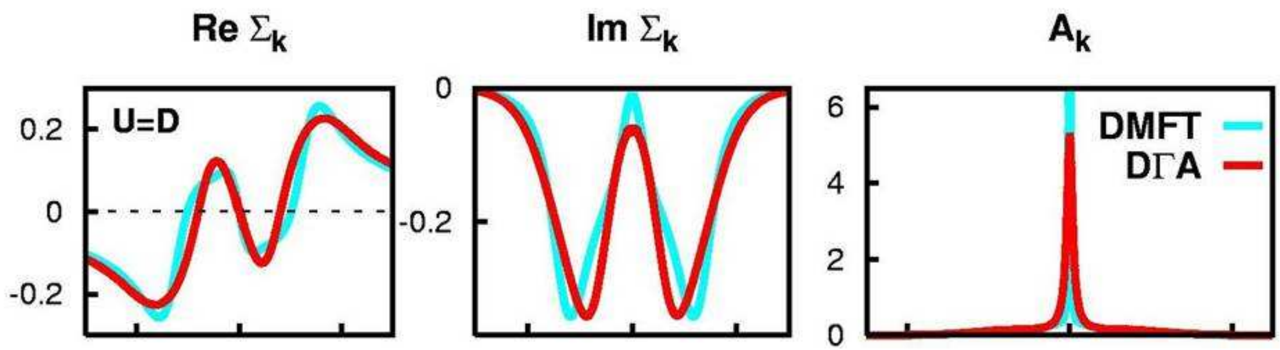


← weak damping of QP peak

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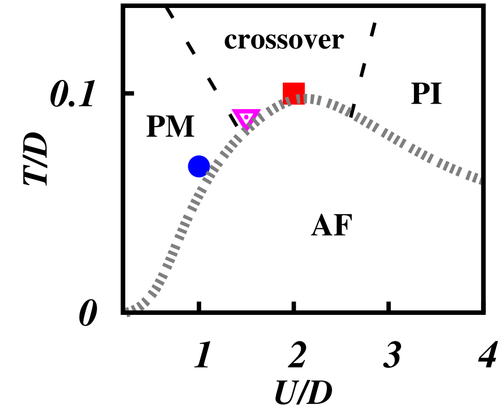


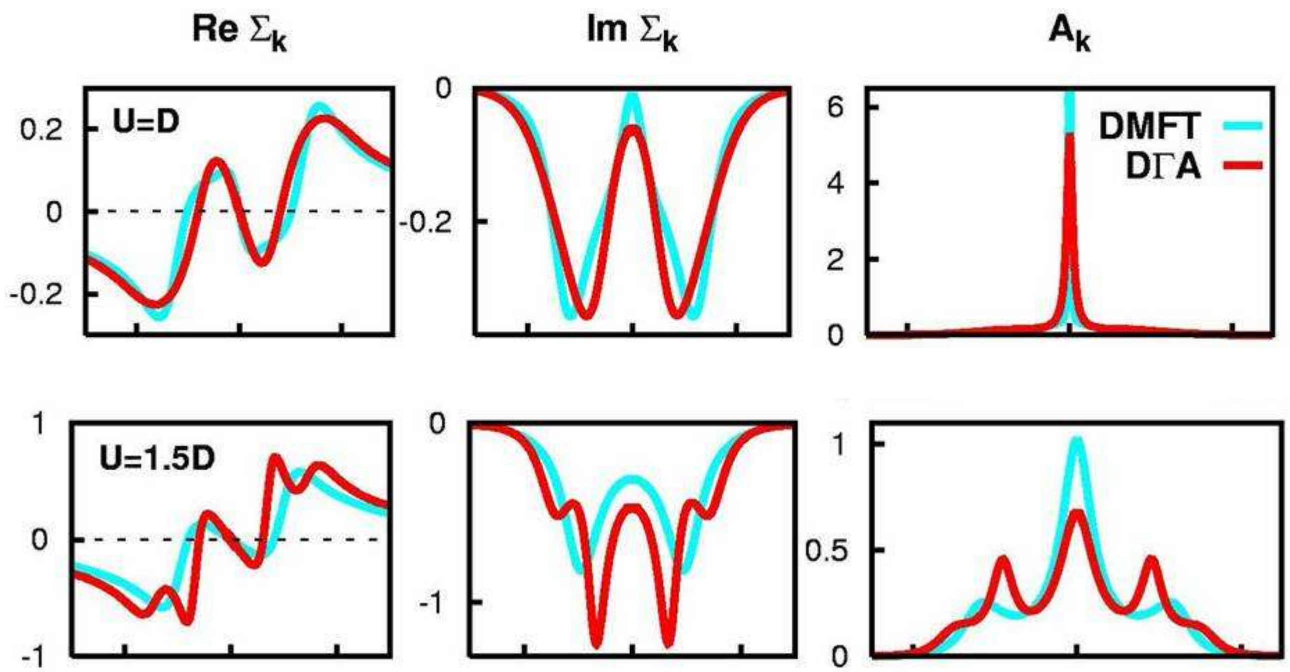


← weak damping of QP peak

← QP-damping strongly enhanced

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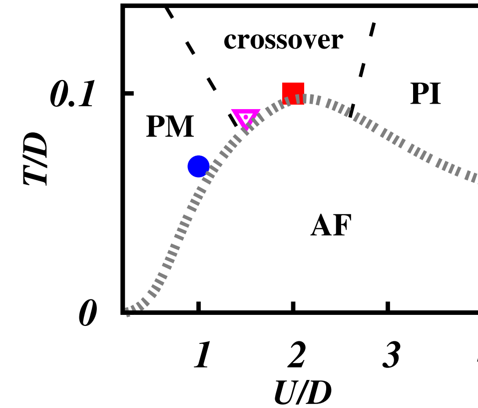
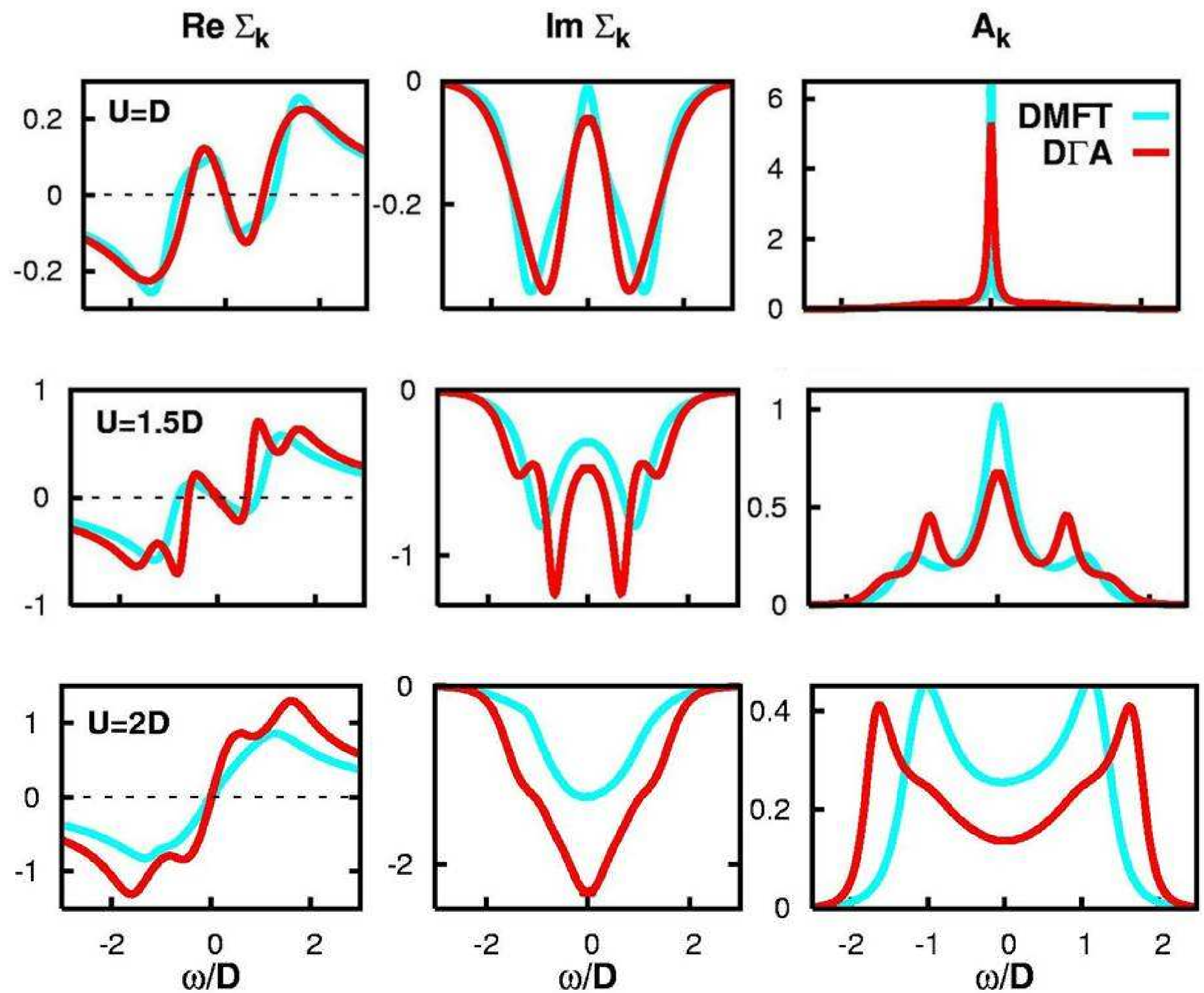


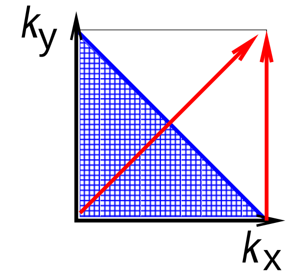




← weak damping of QP peak

← QP-damping strongly enhanced

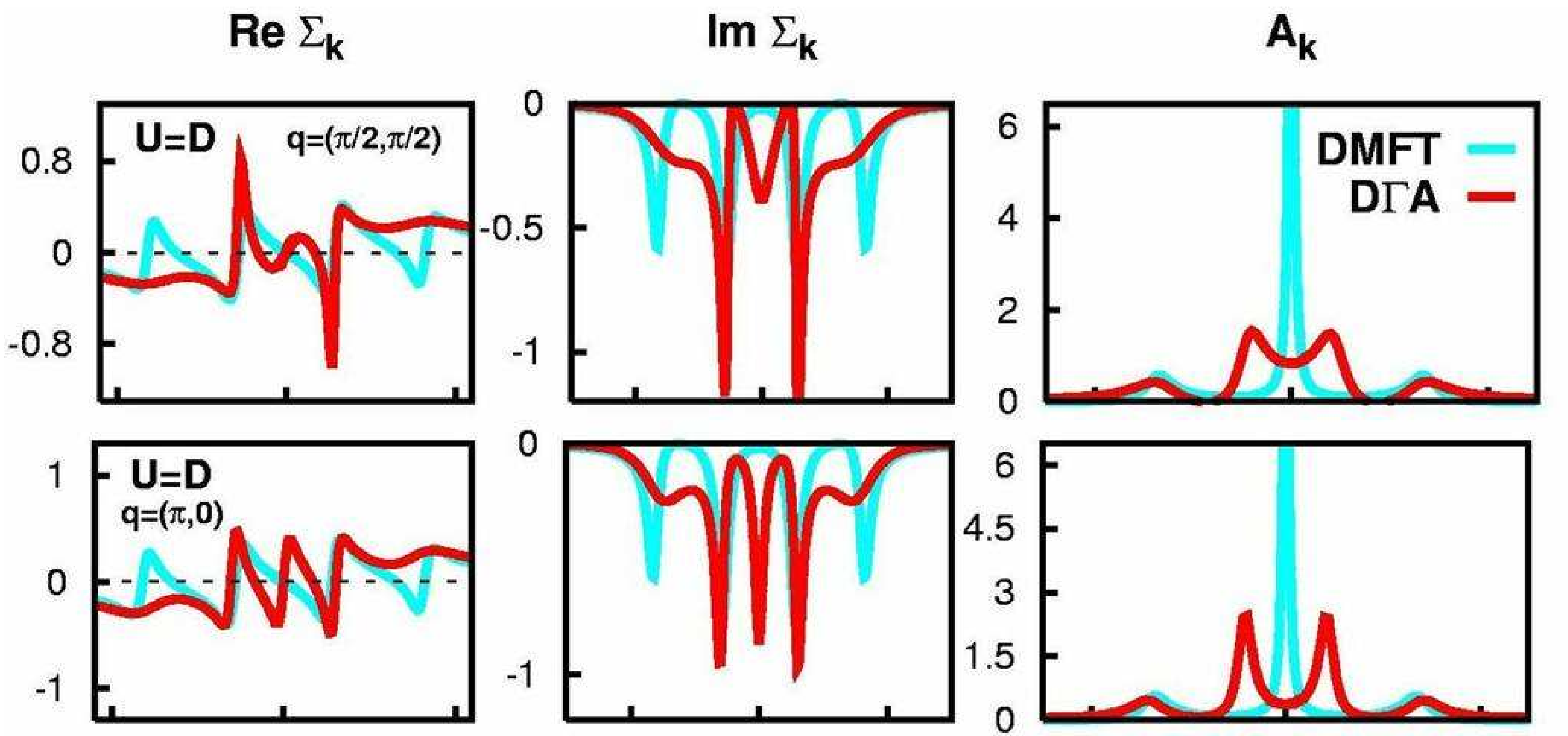
← more insulating

# 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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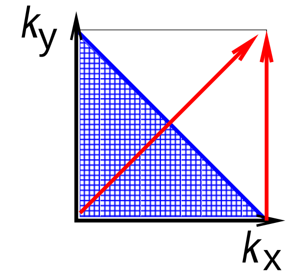
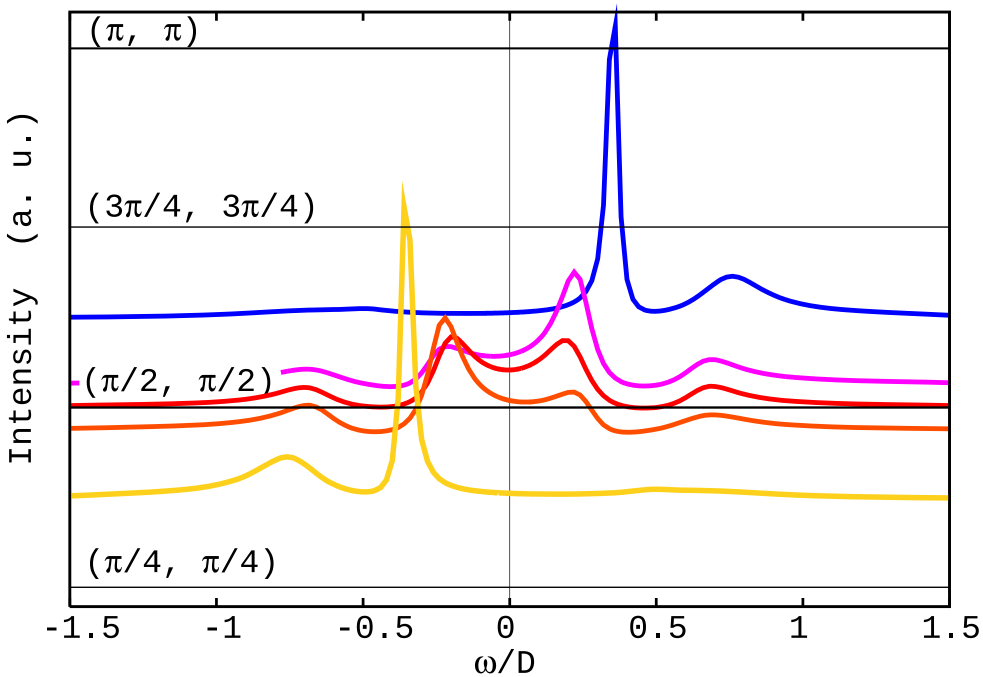
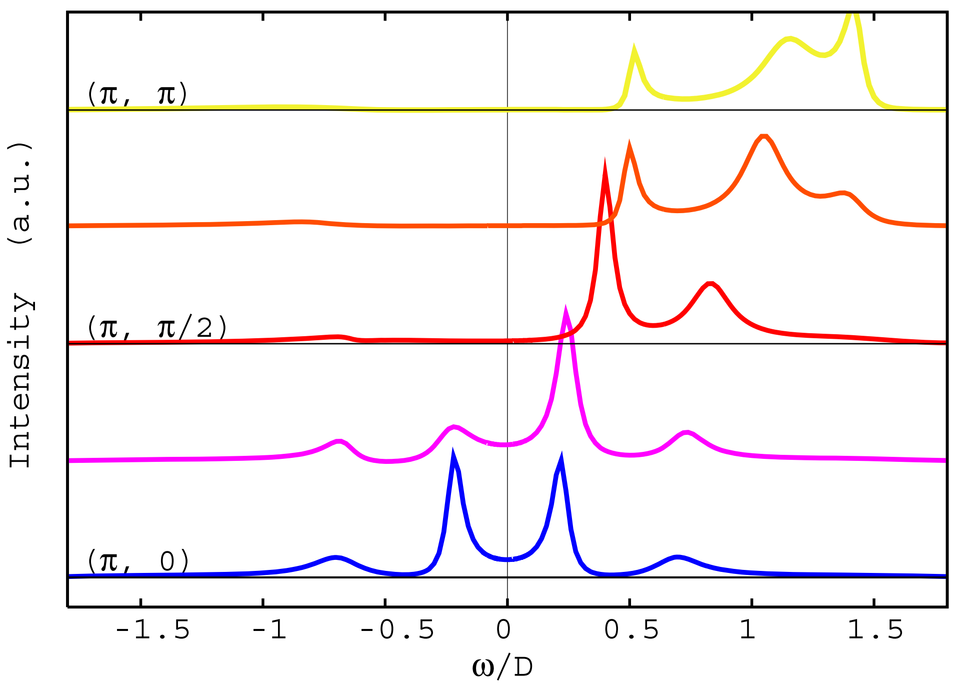


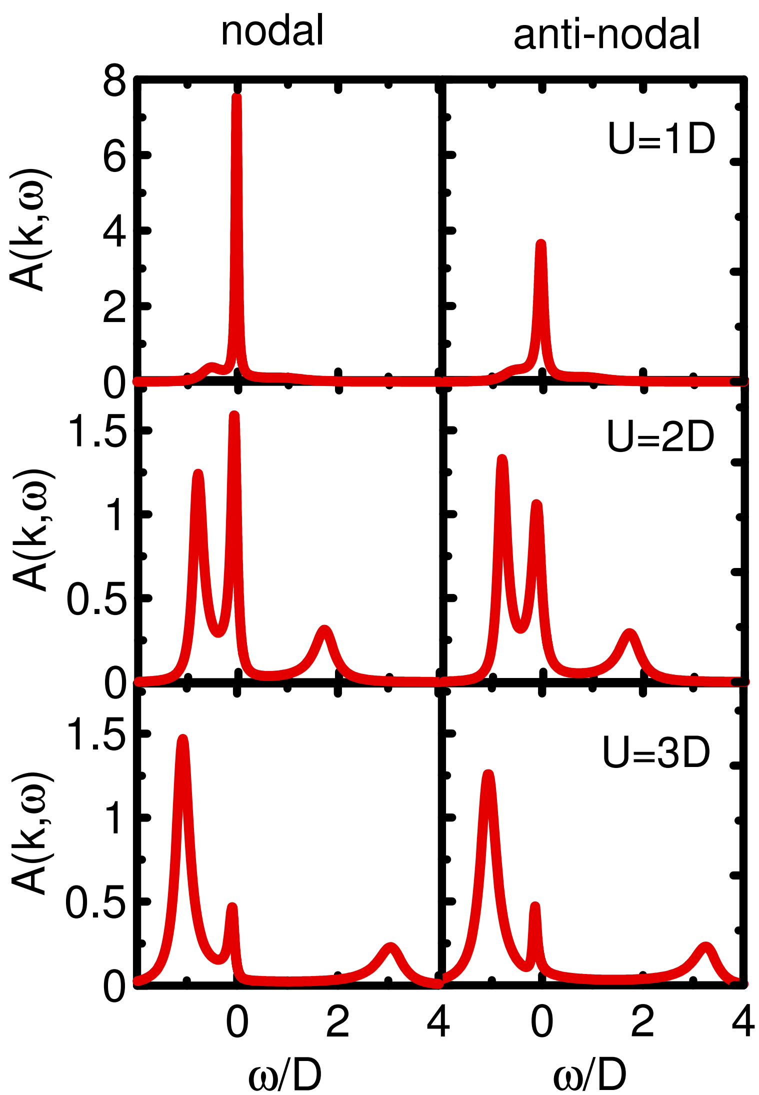

nodal

antinodal



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




$t'/t = 0.3$
$n = 0.8$
$\beta = 100/D$

less anisotropic
at strong coupling

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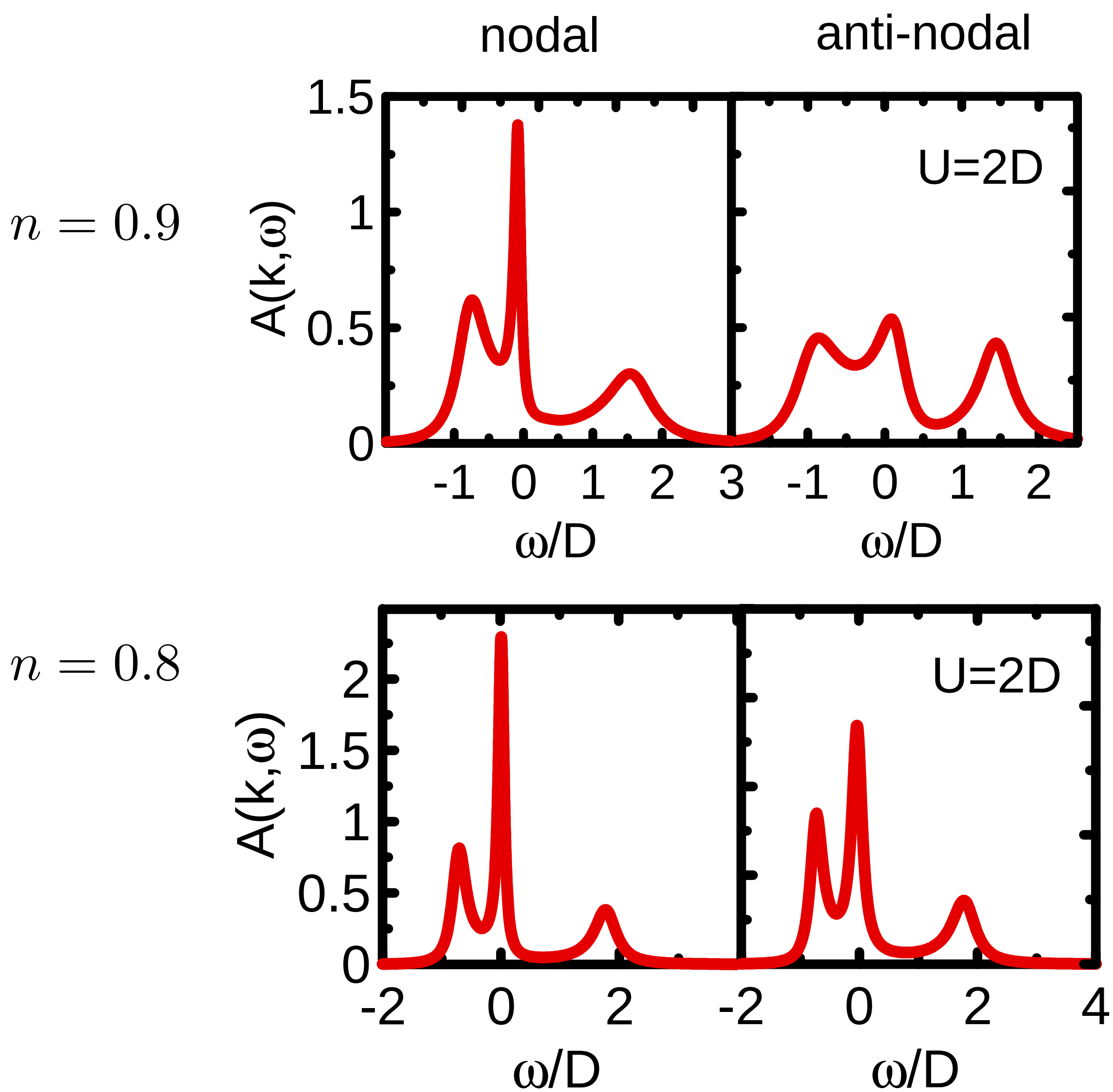



less anisotropic
at larger doping

# Results: 1D Hubbard model

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

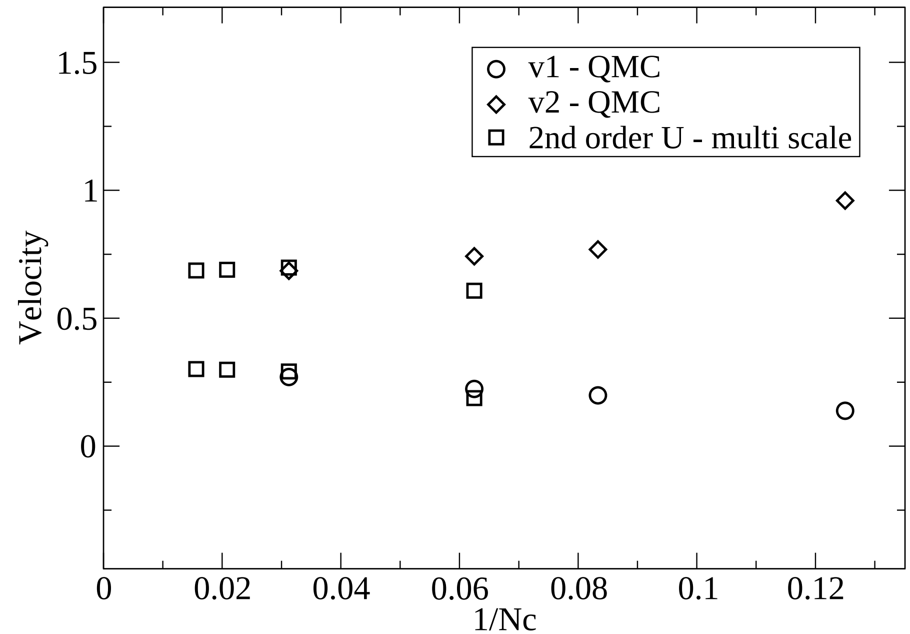
## Spin-charge separation

$U = W = 1$

$k = \pi/2$

$\beta = 31$

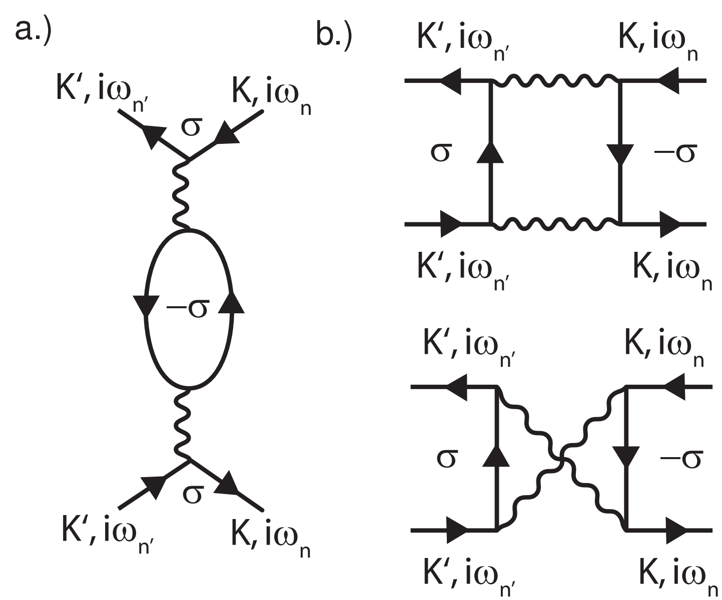
$n = 0.7$




Here, only 2nd order diagrams for vertex

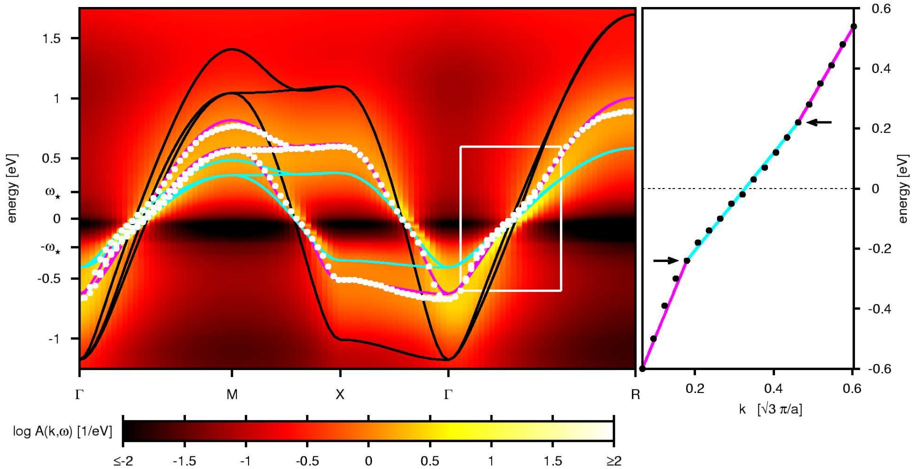
$(q = 0,\ \omega = 0)$

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



# 2) Kinks — direct consequence of strong correlations

Kinks in $SrVO_3$ Nekrasov et al. PRB'06



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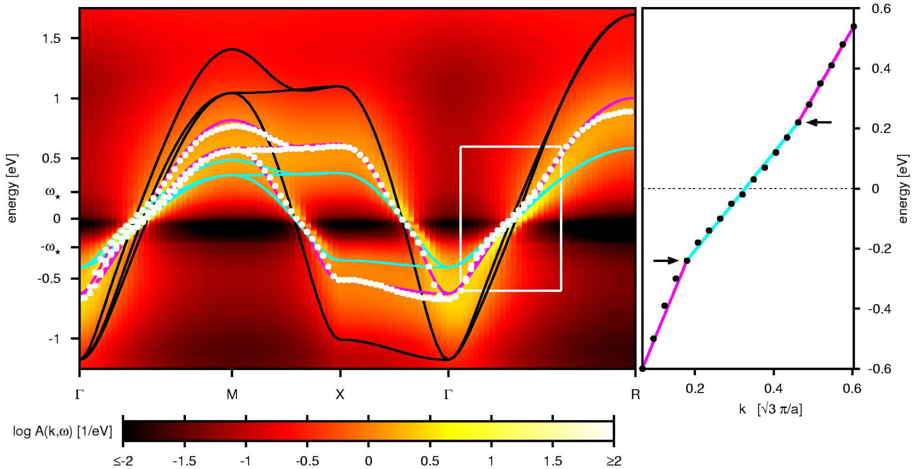
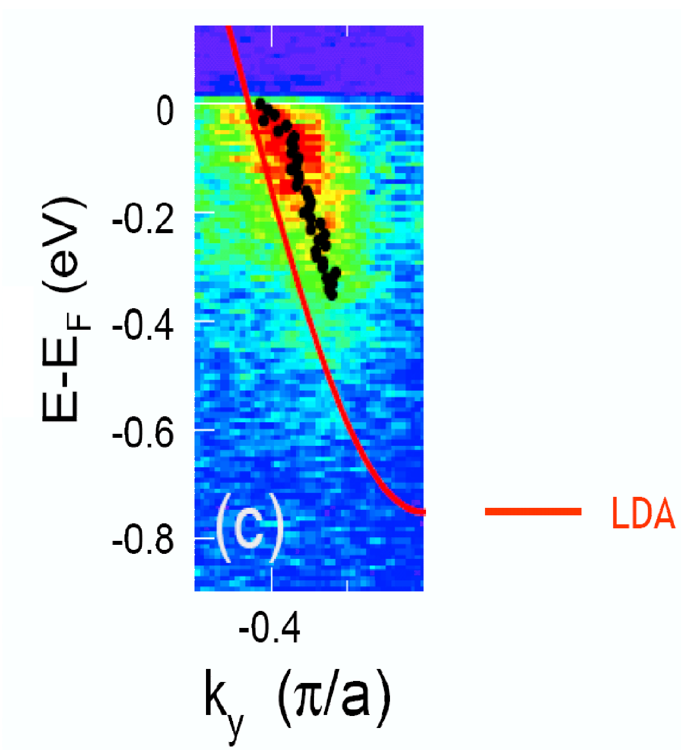



experimentally observed Fujimori et al.'06



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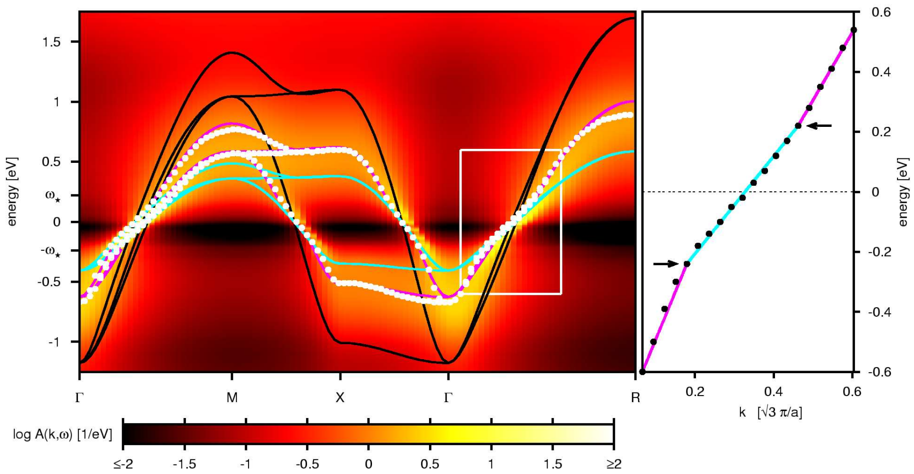
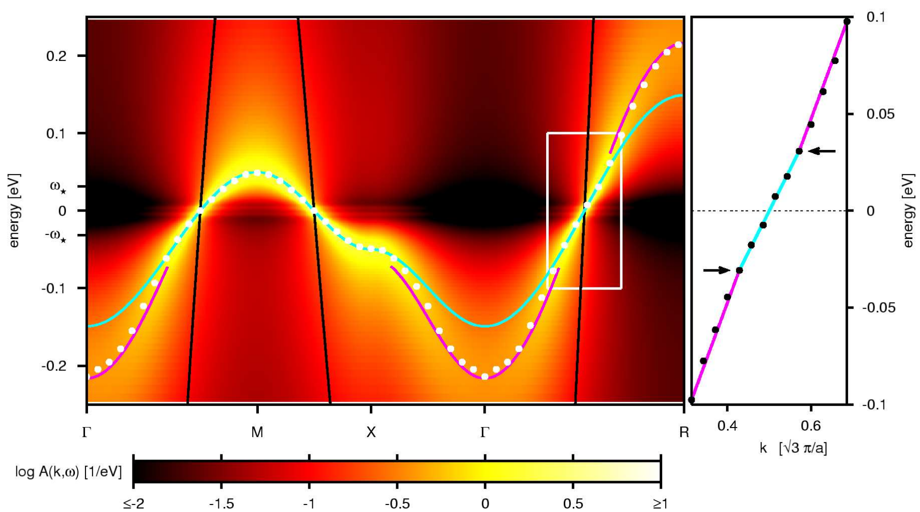



Kinks in the 3D Hubbard model

Byczuk, Kollar, KH, Yang, Nekrasov, Pruschke, Vollhardt Nature Phys.'07



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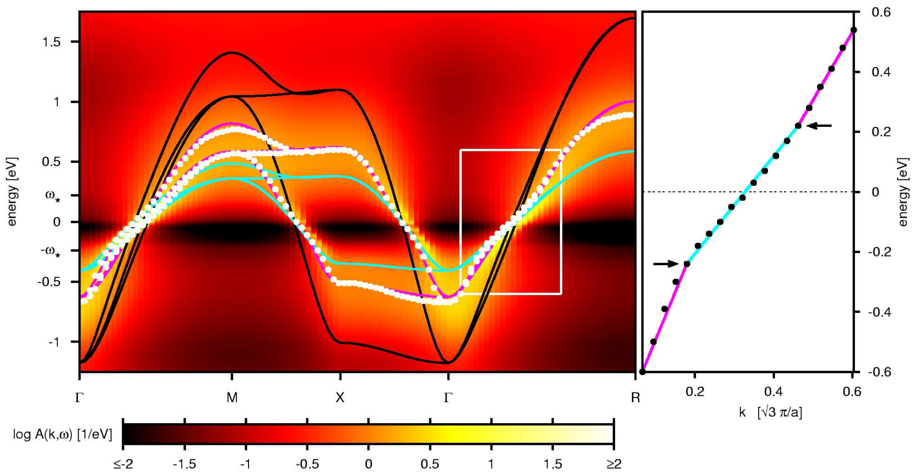


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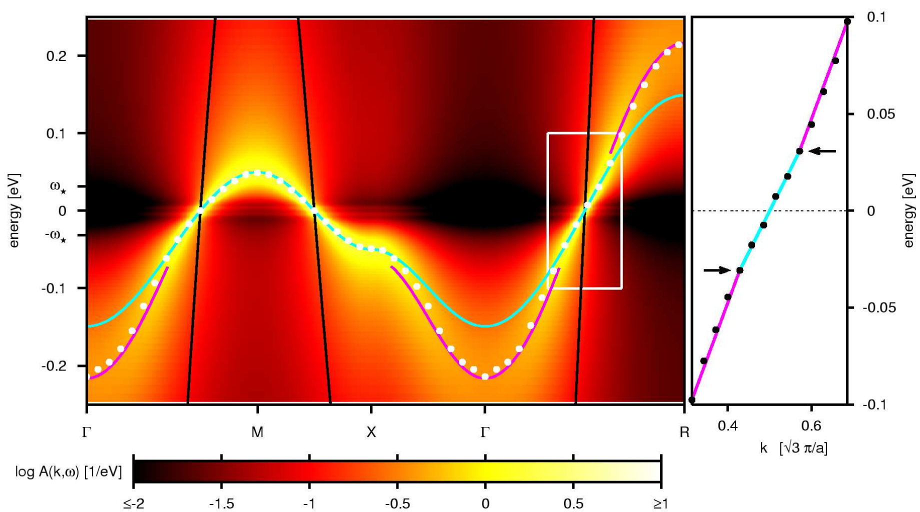
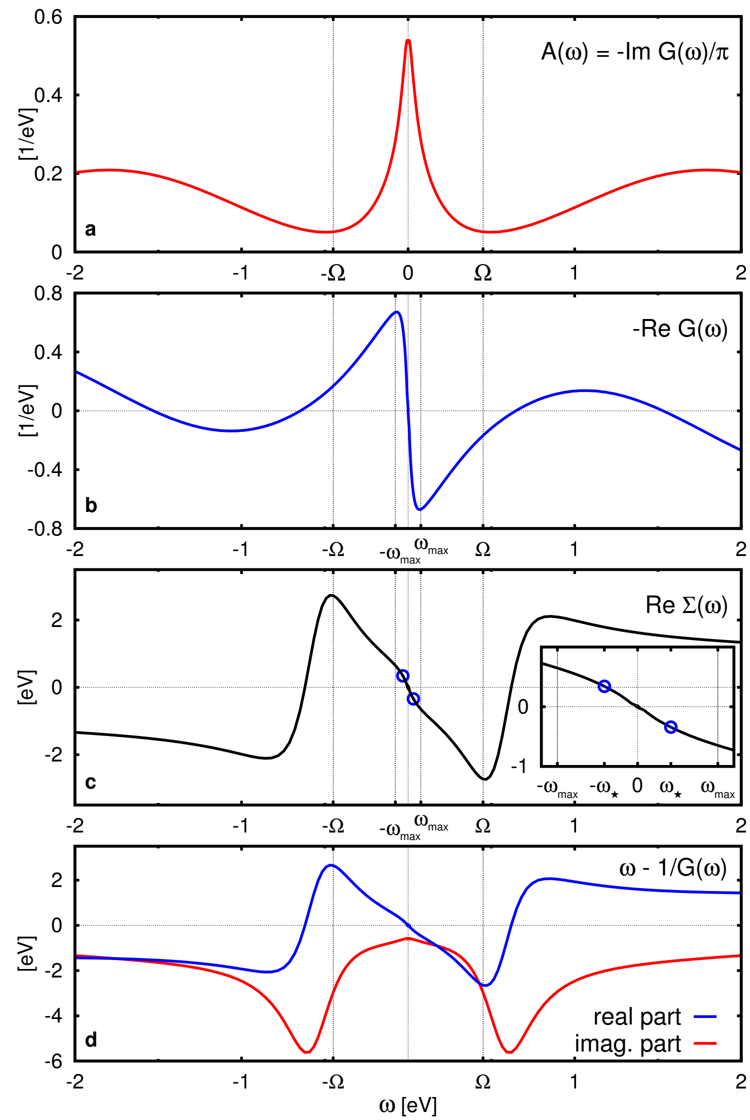



Kinks follow from 3-peak-structure

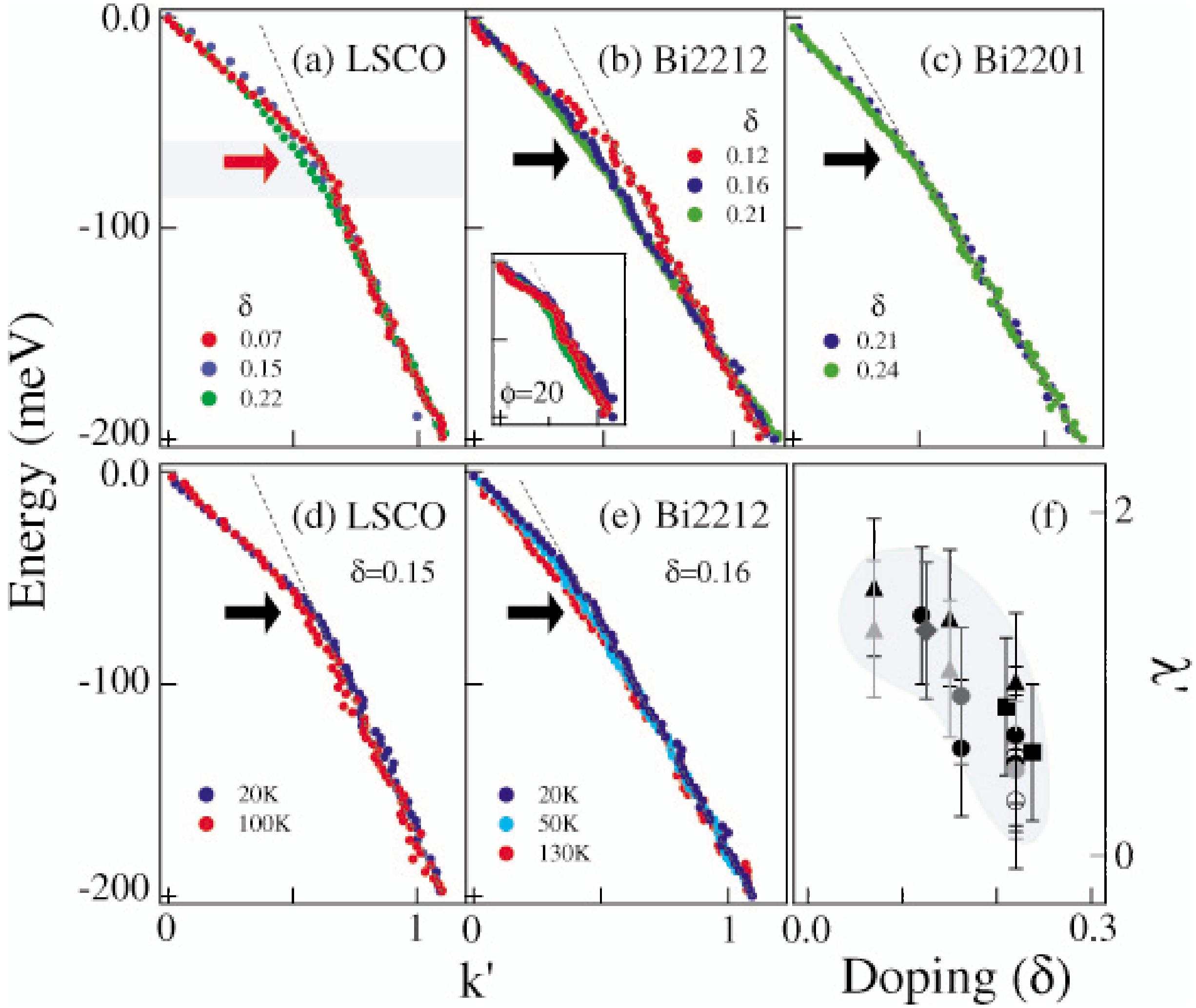



$$\Sigma(\omega) = \omega + \mu - 1/G(\omega) - \Delta(G(\omega))$$

Fermi-liquid regime: $E_{\mathbf{k}} = Z_{\mathrm{FL}}\epsilon_{\mathbf{k}}$ for $|E_{\mathbf{k}}| < \omega_*$

Beyond FL regime: $E_{\mathbf{k}} = Z_{\mathrm{CP}}\epsilon_{\mathbf{k}} \pm c$ for $|E_{\mathbf{k}}| > \omega_*$

# ARPES: low-energy kinks in cuprates

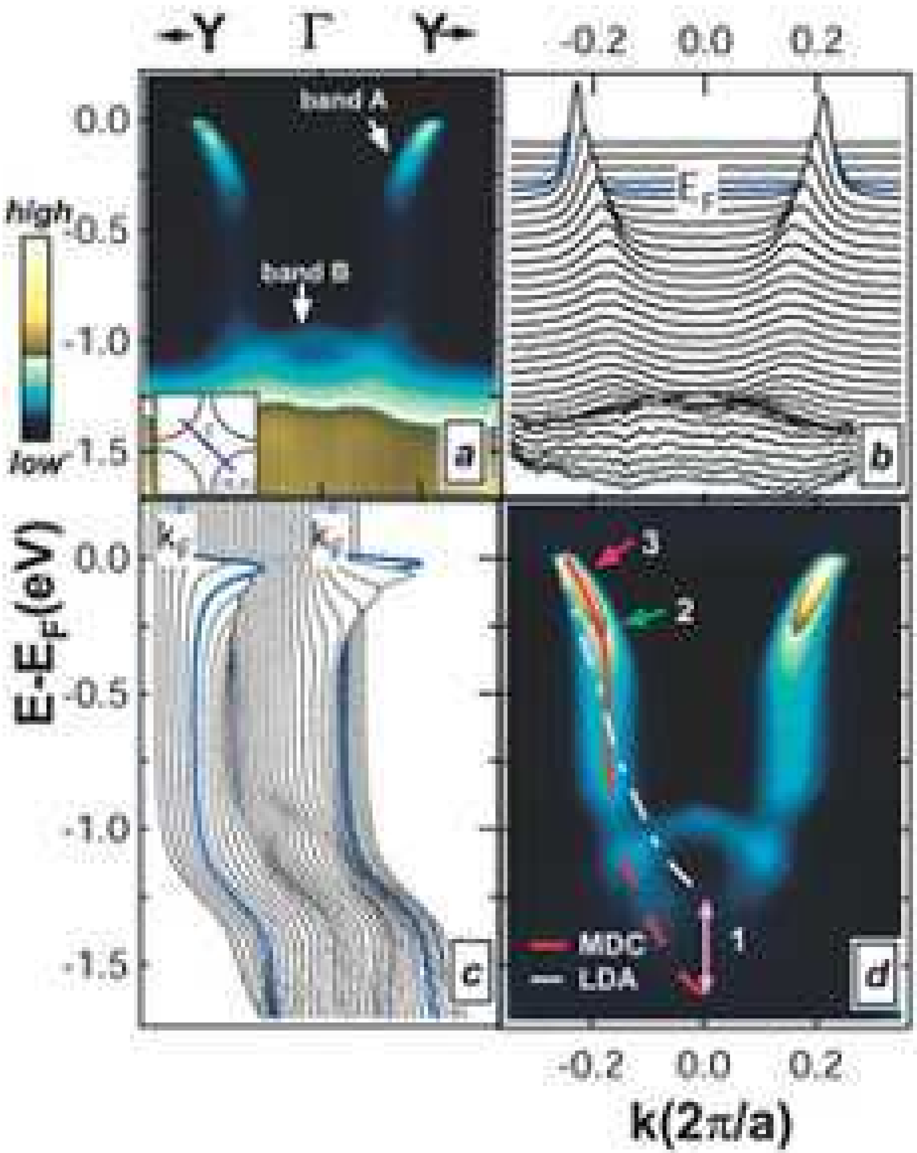



Lanzara *et al.*'01

energy range ∼ 70 meV

# ARPES: high-energy kinks in cuprates

**Bi2201** at $T = 30\text{K}$ ($> T_c$)




Meevasana *et al.* cond-mat/0612541

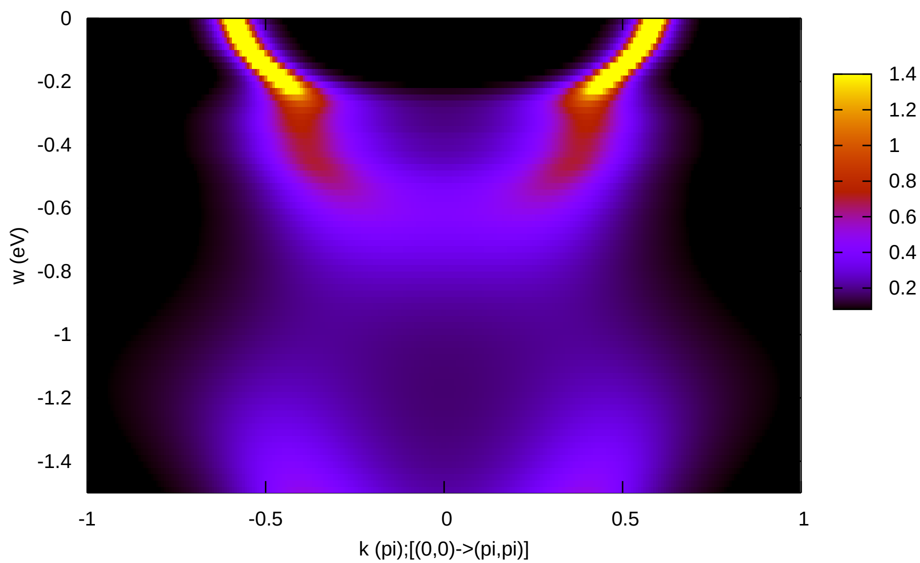
energy range $\sim$ 0.3 eV

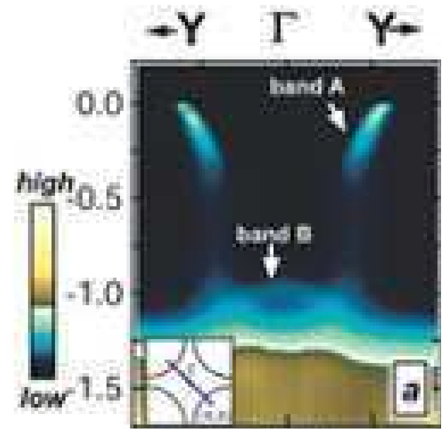
# Connection to high-energy kinks

Yang, Held'07

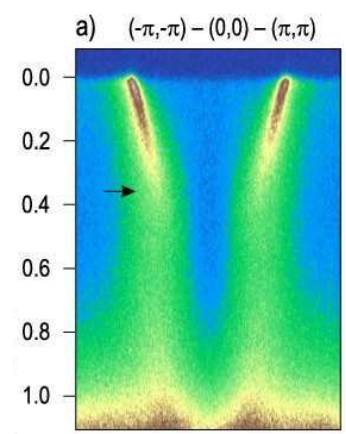
## 2D Hubbard model; DMFT(QMC)

$n = 0.85$, $U = 3$, $t = 0.435$, $t' = -0.1$, $t'' = 0.038$, $T = 1/40$ (eV)




Meevasana *et al.*'06




Inosov *et al.*'07

cf. Macridin *et al.*'07

cf. Byczuk, Kollar, Vollhardt'07

Kink position correct
but two features kink+waterfall

# Connection to high-energy kinks

Yang, Held'07

## 2D Hubbard model; DMFT(QMC)

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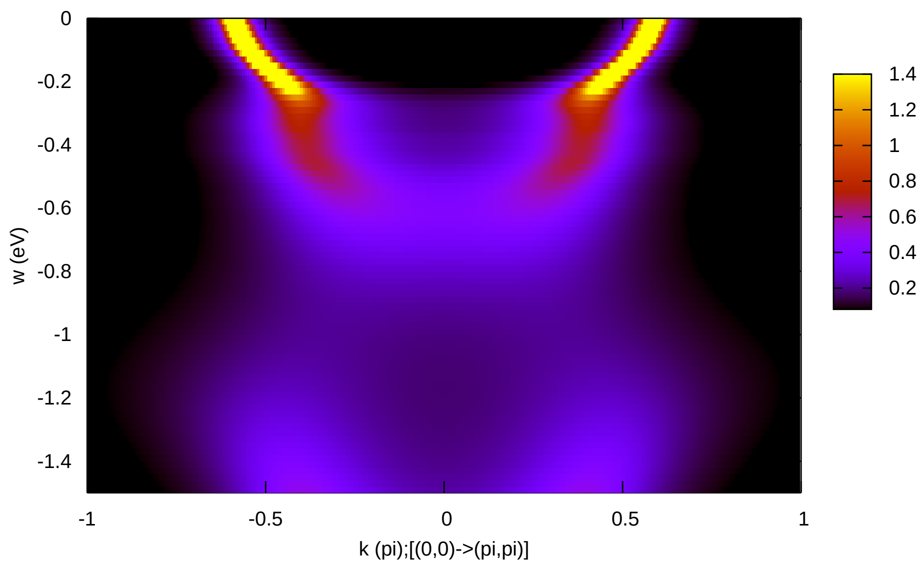
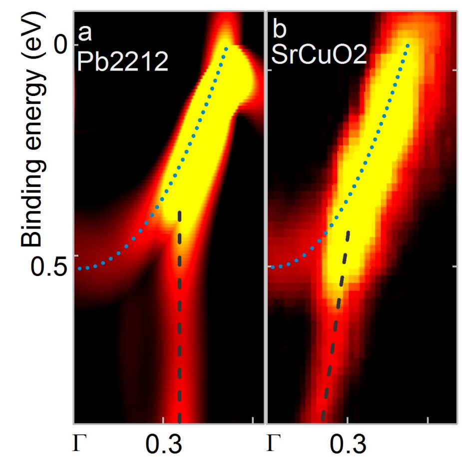



Graf *et al.*'06

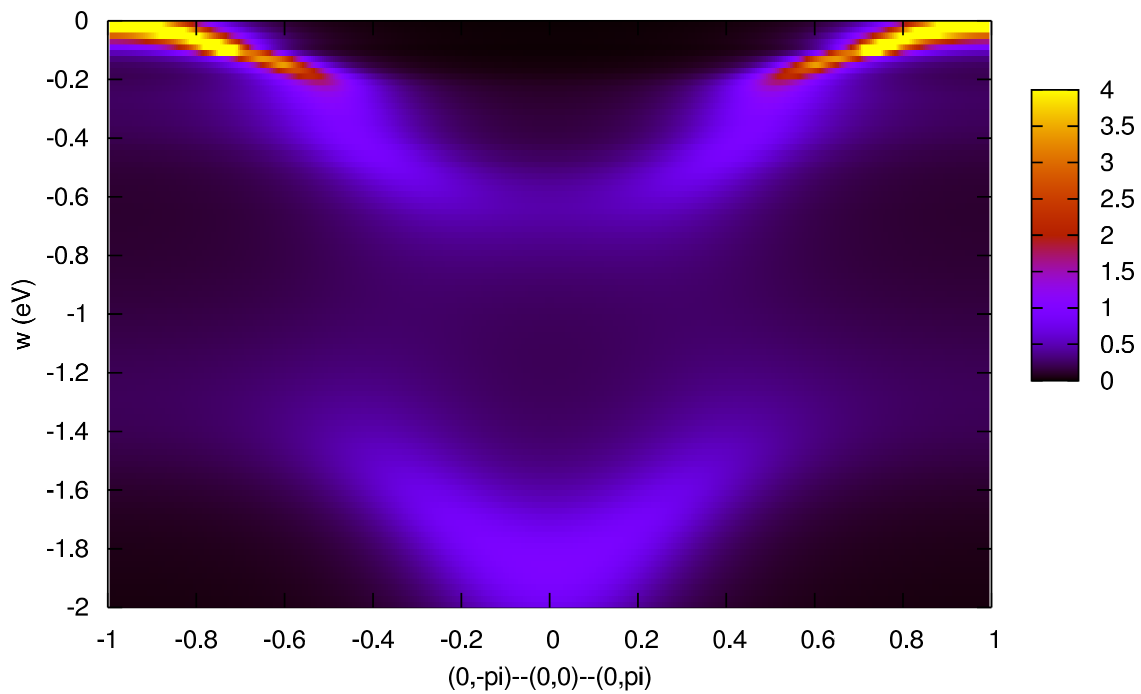
cf. Macridin *et al.*'07

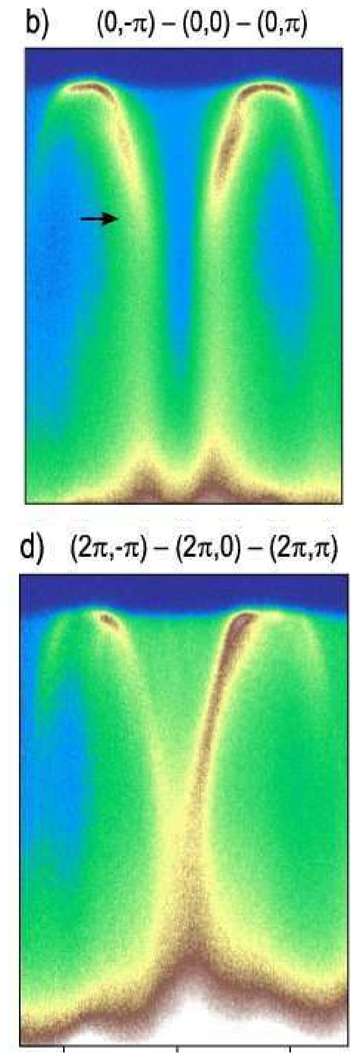
cf. Byczuk, Kollar, Vollhardt'07

Kink position correct
but two features kink+waterfall

# High-energy kinks in anti-nodal direction

Yang, Held'07



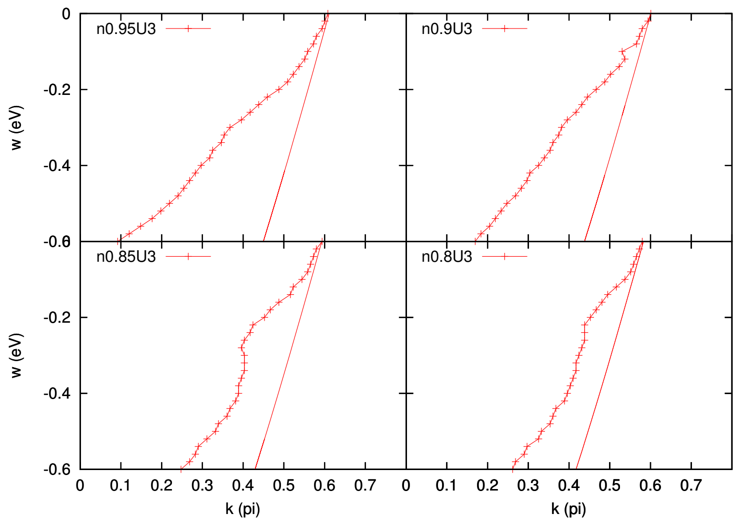




Inosov *et al.*'07

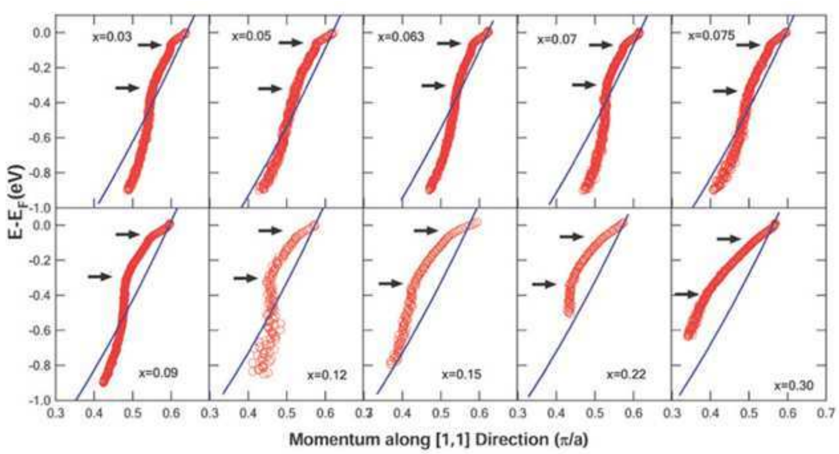
# Kinks more pronounced at higher doping

Yang, Held'07

## Theory:



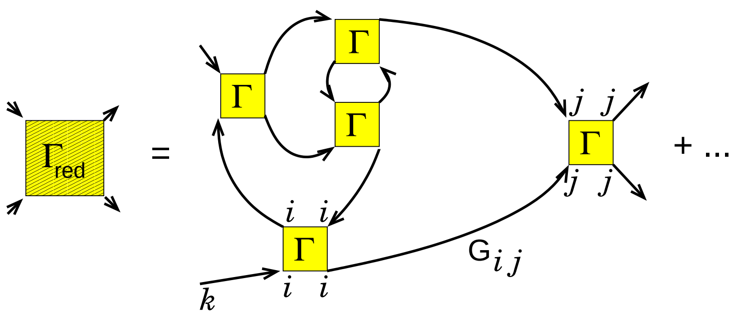

## Experiment:




Meevasana *et al.*'06

# Conclusion — DΓA

- DΓA assumption: local 2-particle irreducible $\Gamma$




- DΓA can access short- and long-range correlations

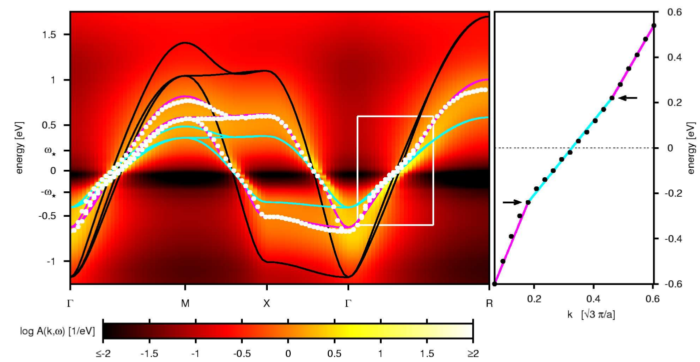
- Pseudogap in 2D; Mott transition in 3D

# Outlook

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

- Realistic multi-orbital calculations possible

# Conclusion – kinks




- Kinks direct consequence of strong correlations

  $\rightarrow$ kinks are everywhere (three peak structure)

- Fermi-liquid regime: $E_{\mathbf{k}} = Z_{\mathrm{FL}} \epsilon_{\mathbf{k}}$ for $|E_{\mathbf{k}}| < \omega_*$

  Beyond Fermi-liquid regime: $E_{\mathbf{k}} = Z_{\mathrm{CP}} \epsilon_{\mathbf{k}} \pm c$ for $|E_{\mathbf{k}}| > \omega_*$

- Connection to high-energy kinks/waterfalls in cuprates