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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- Results for 3D, 2D, and 1D Hubbard model

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Thanks to...

1) Dynamical vertex approximation (DΓA)

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

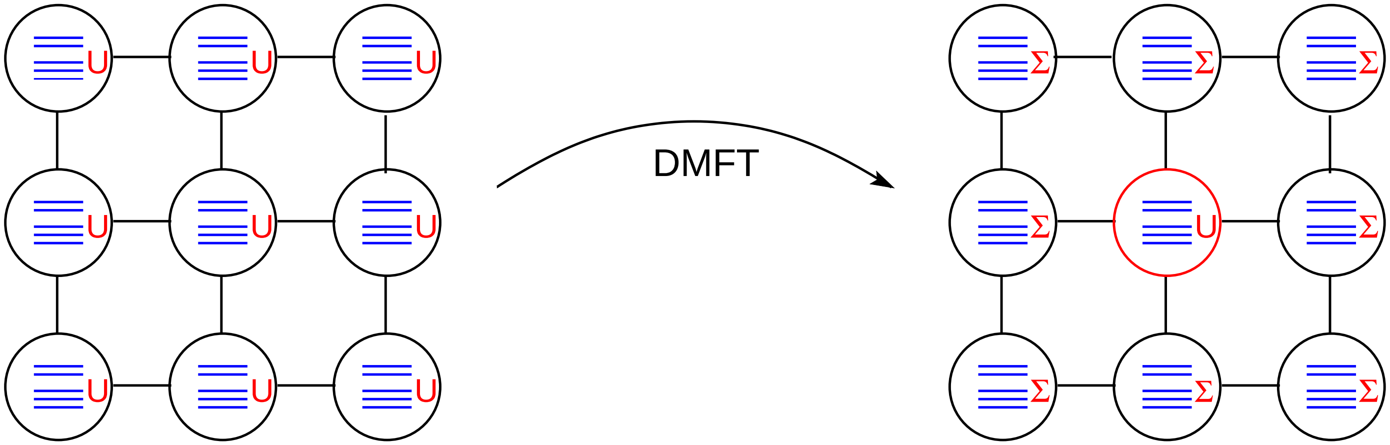
Th. Pruschke – Göttingen

PRB 73, 155112 (2006)

Nature Physics 3 168 (2007)

Motivation

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



Σ all topologically distinct, but local diagrams

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

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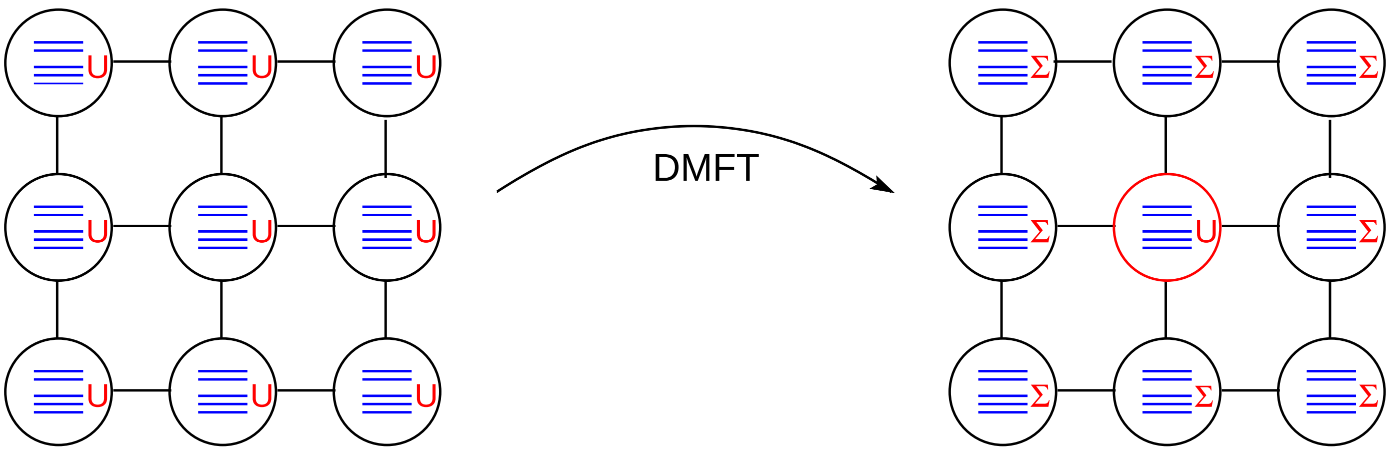

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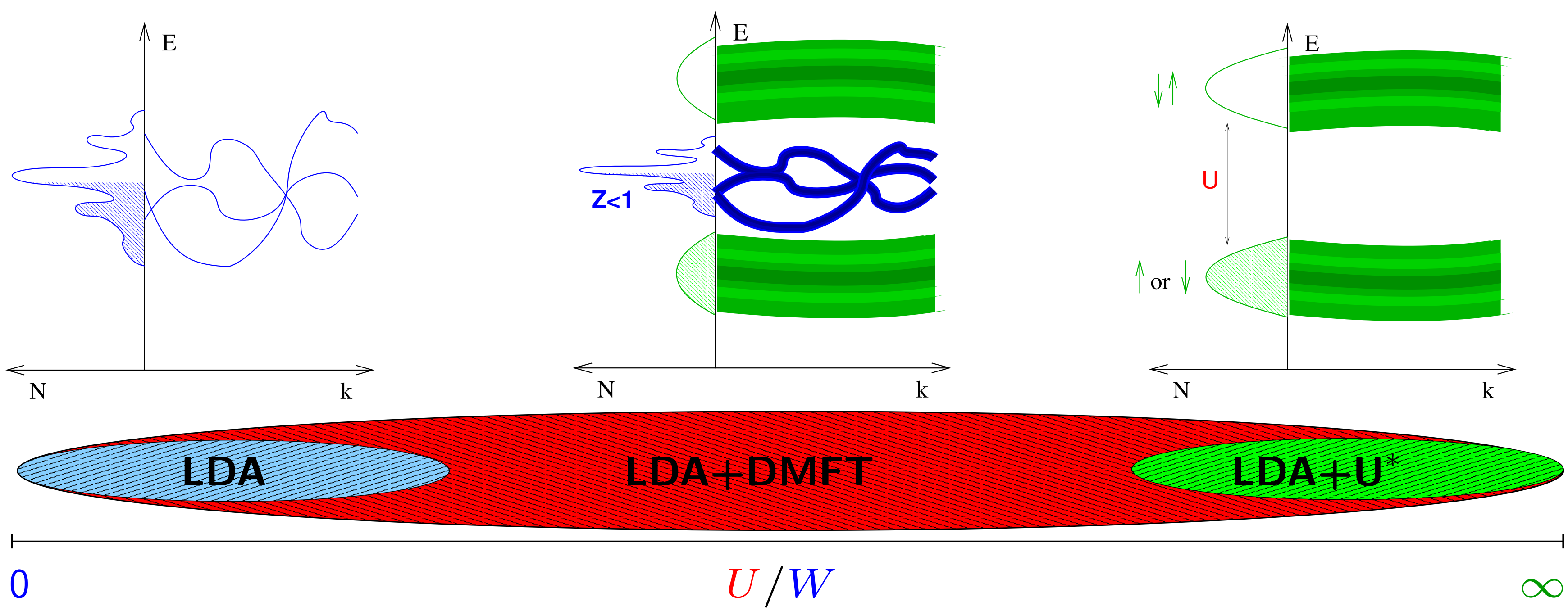

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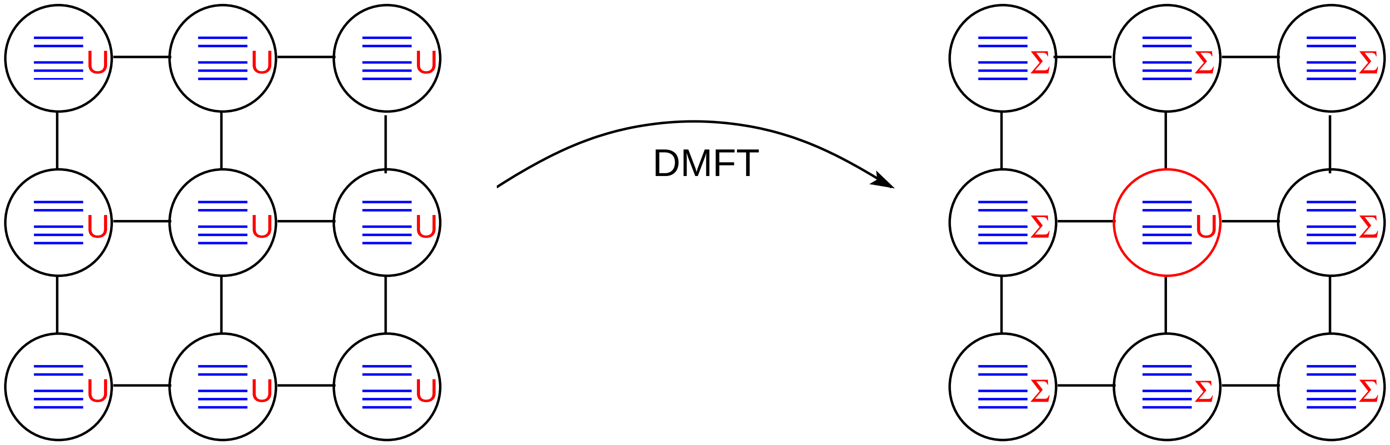


Σ all topologically distinct, but local diagrams

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

Not included:

non-local correlations

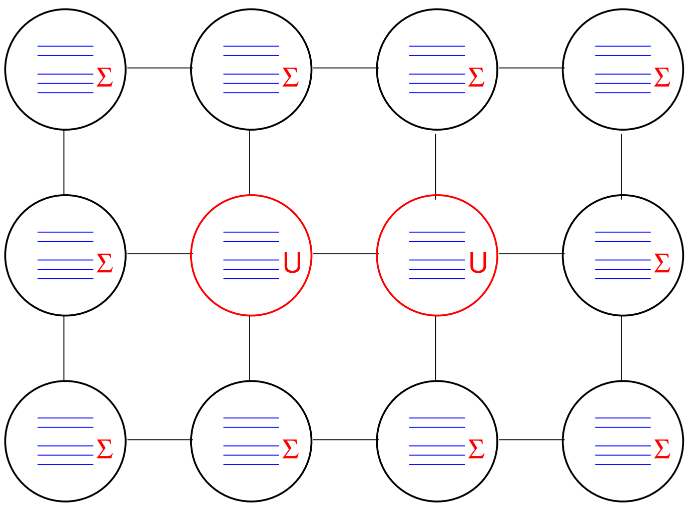
p-, d-wave superconductivity, spin Peierls

magnons, (quantum) critical behavior ...

$\mathbf{k}$-dependence of Σ

beyond DMFT

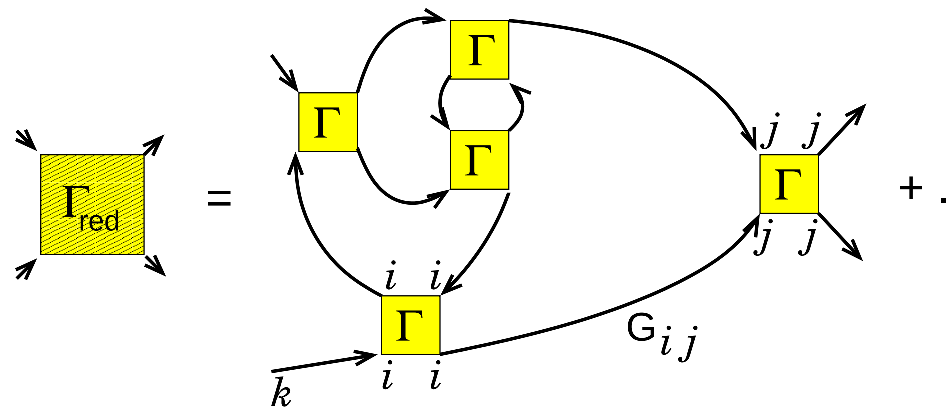
cluster extensions of DMFT



- 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 ...

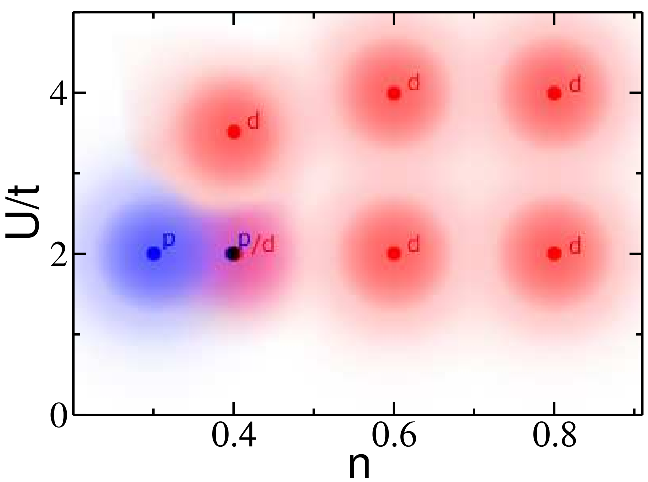
Toschi, Katanin, KH cond-mat/0603100
cf. Kusunose cond-mat/0602451
Slezak *et al.* cond-mat/0603421

beyond DMFT

dominant superconducting susceptibility

t-t' 2D Hubbard model

Arita, KH PRB'06

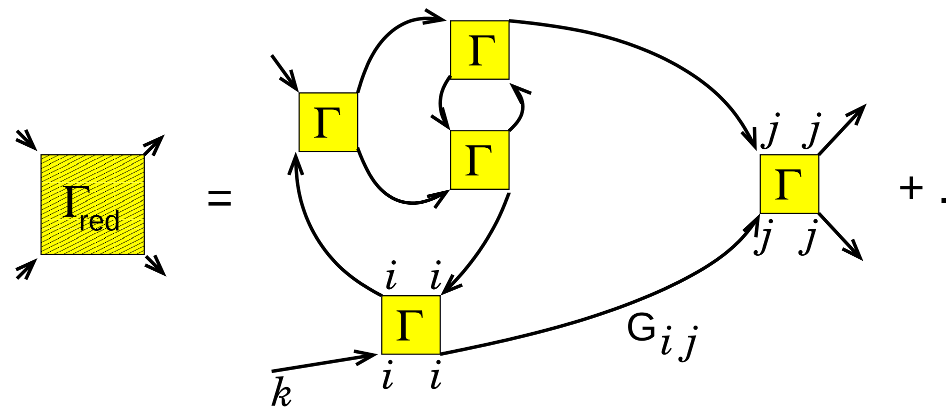


$t' = 0.4t$, $N_c = 4 \times 4 = 16$

- 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



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DMFT: all (topological distinct) local diagram for Σ

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

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$n = \infty \rightarrow$ exact solution

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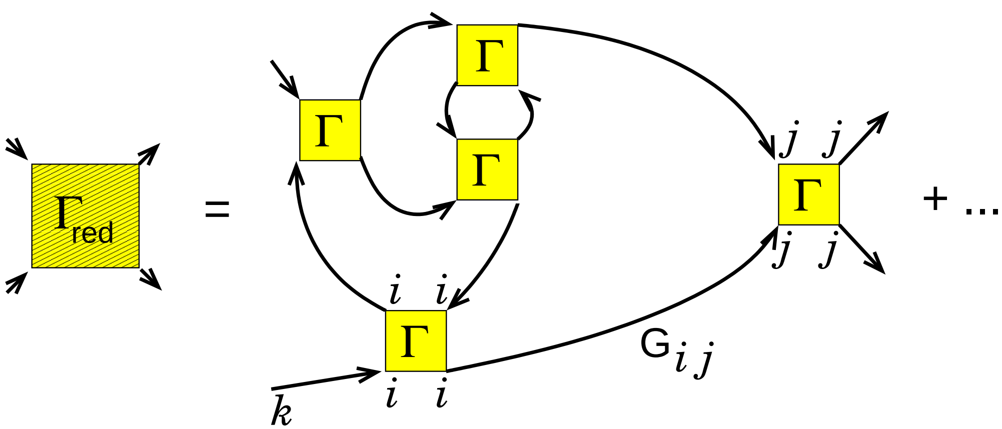

local Γ, non-local G

$\longrightarrow$

non-local reducible vertex Γ_{red}

via parquet equations

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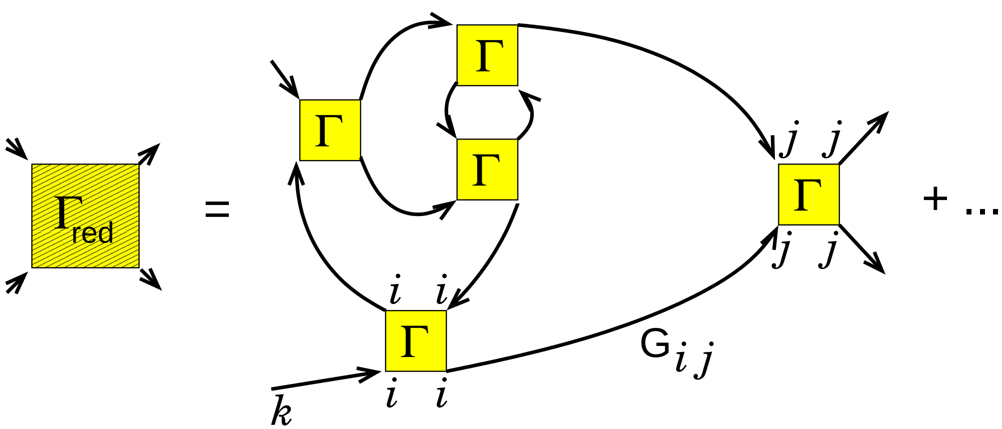

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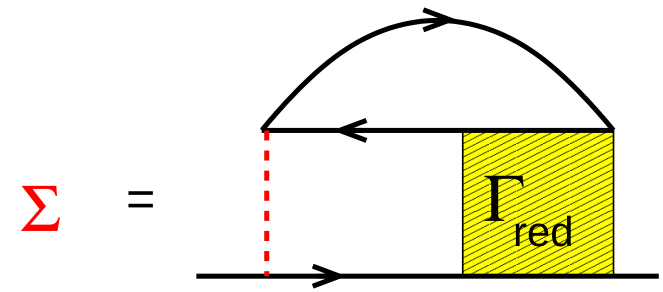

Γ_{red}

$\longrightarrow$

non-local Σ

exact relation (eq. of motion)

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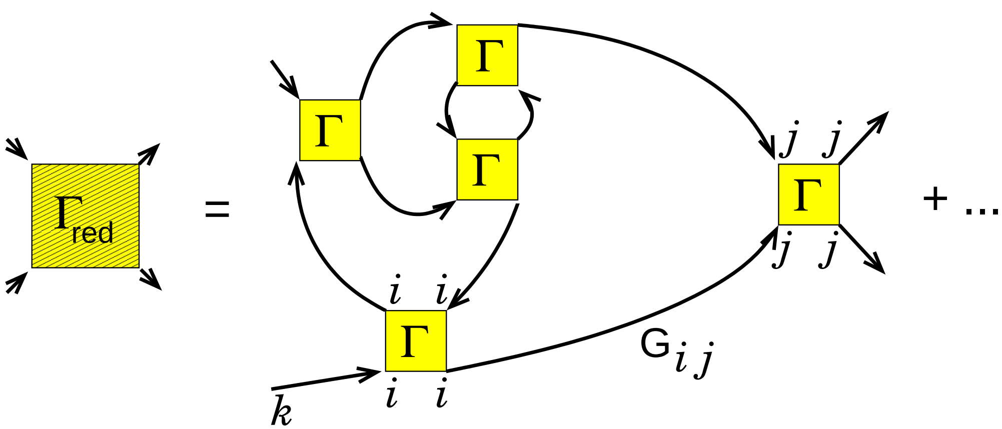

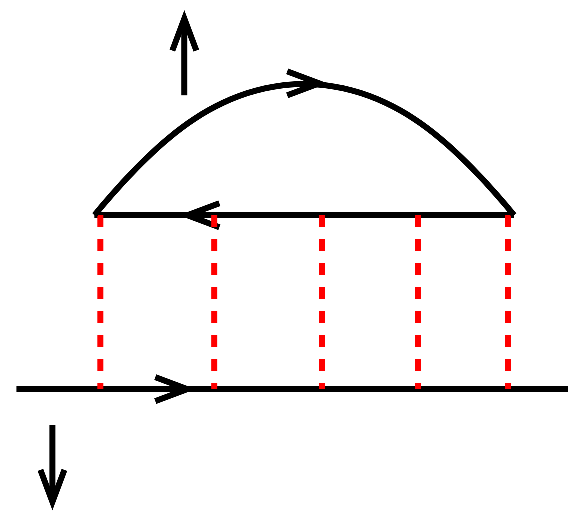

Moriya Edwards-Hertz

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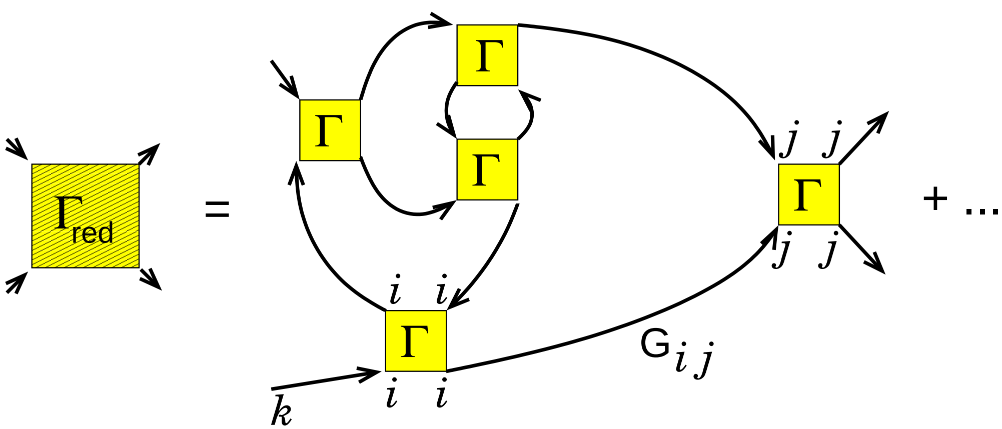

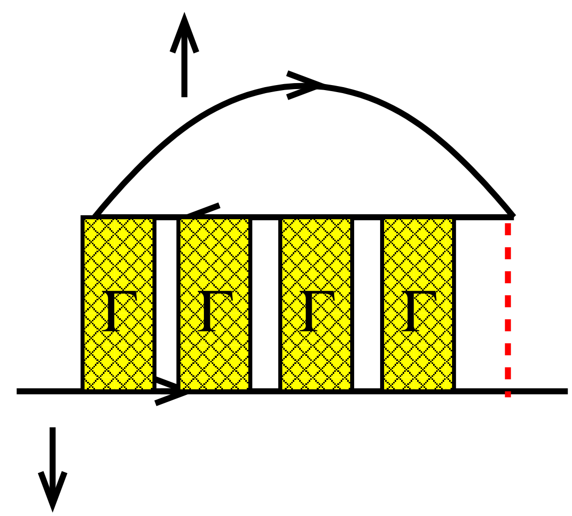

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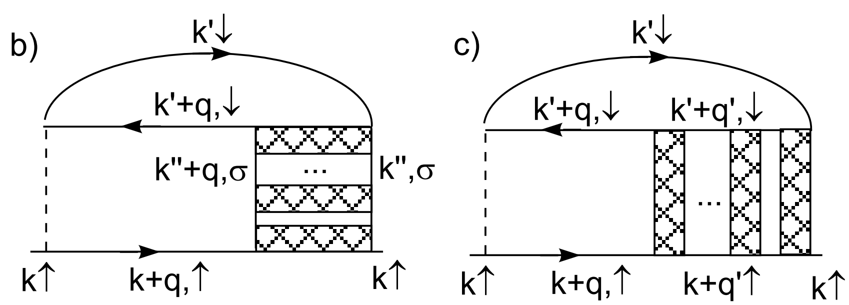
First step: restriction to ladder diagrams

$\Sigma \quad =$



lines: non-local G

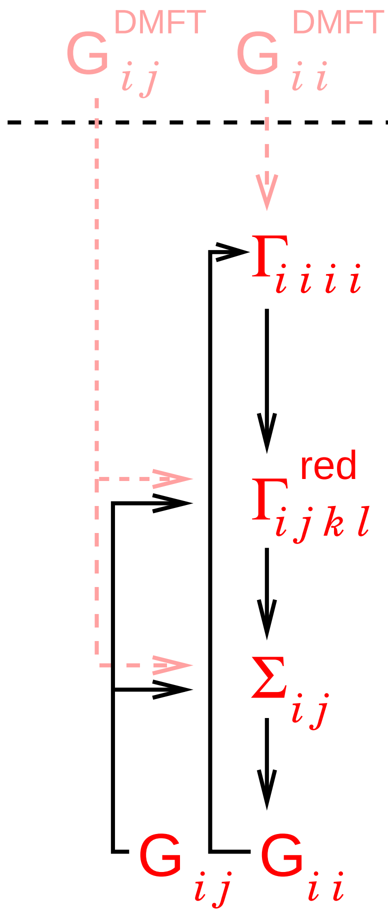
crosshatched: local irreducible vertex in spin/charge channels

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

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

G_{ij} from DMFT

DΓA algorithm



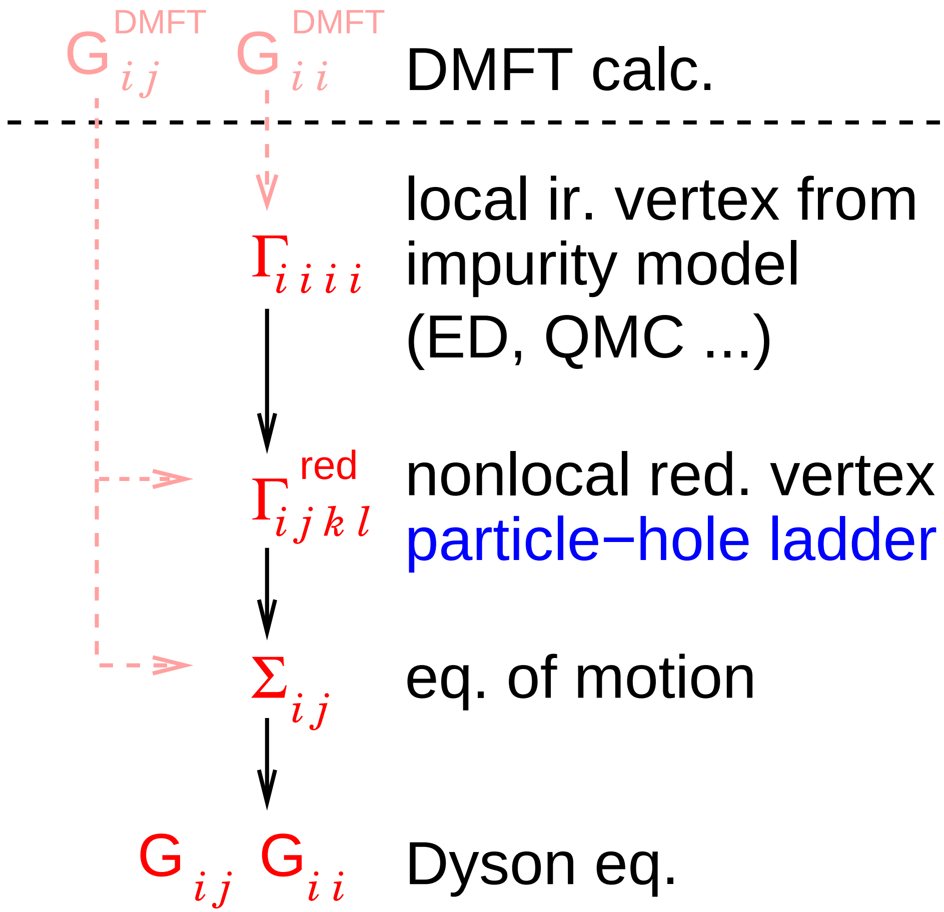
local ir. vertex from impurity model (ED, QMC ...)

nonlocal red. vertex parquet eq.

eq. of motion

Dyson eq.

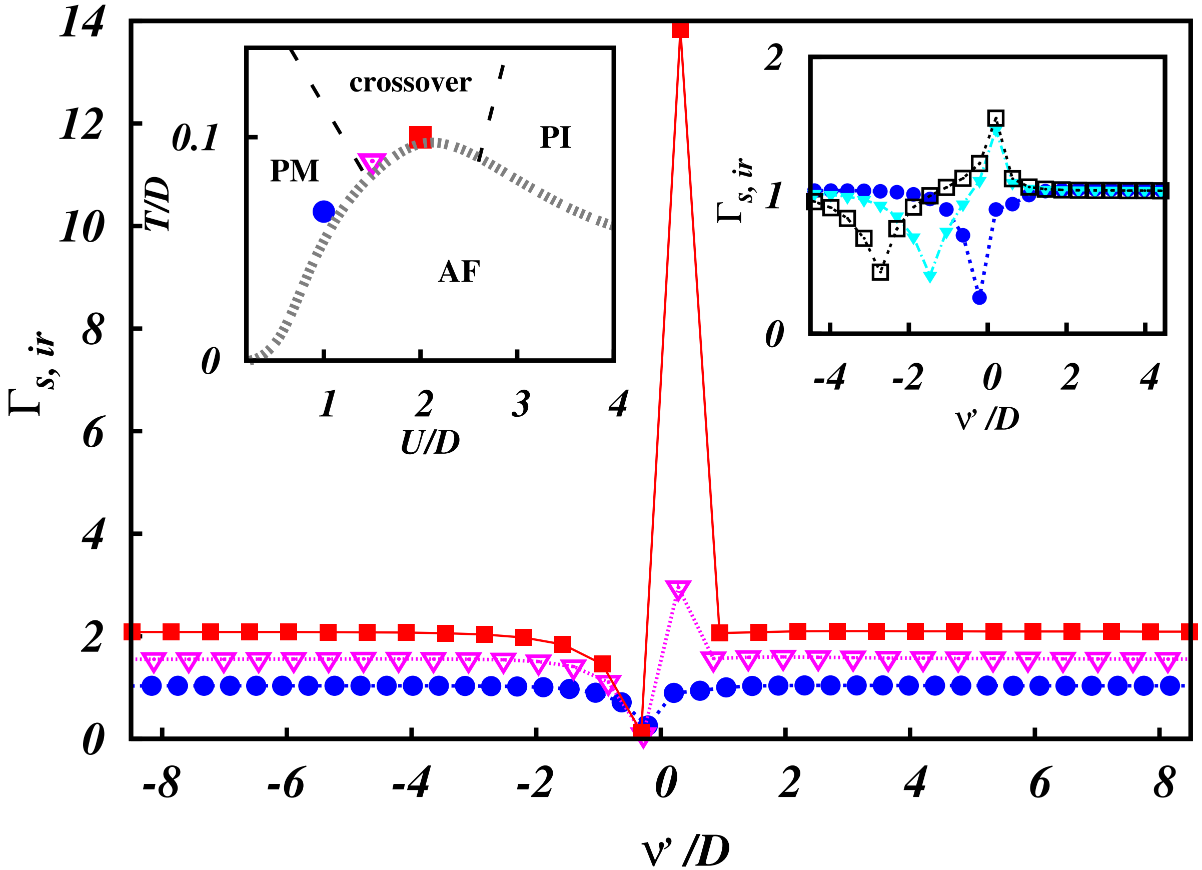
DΓA algorithm (restriction to ph ladders)



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

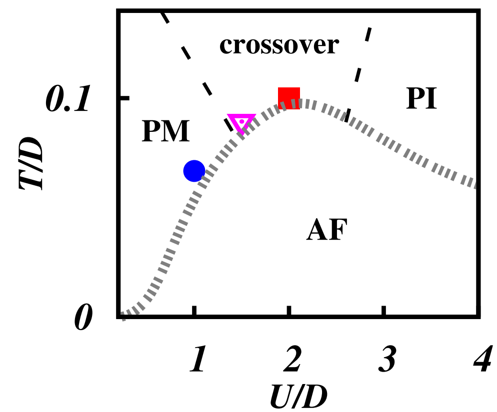


eff. bandwidth ≡ 2D
$\omega = 0$
$\nu = \pi T$

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

Results: 3D Hubbard model

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



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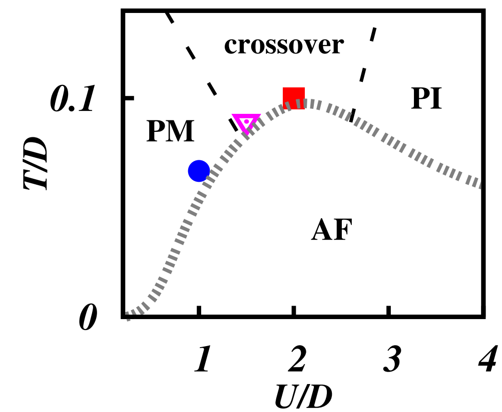

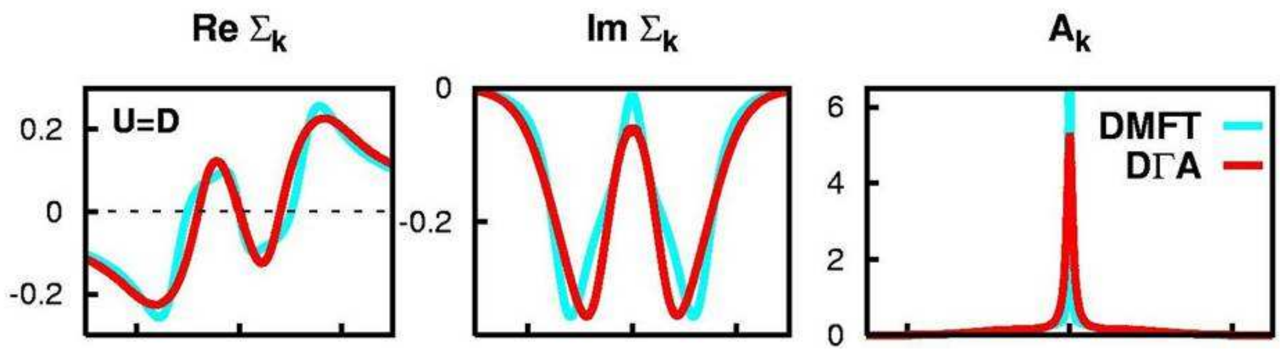

$\longleftarrow$ weak damping of QP peak

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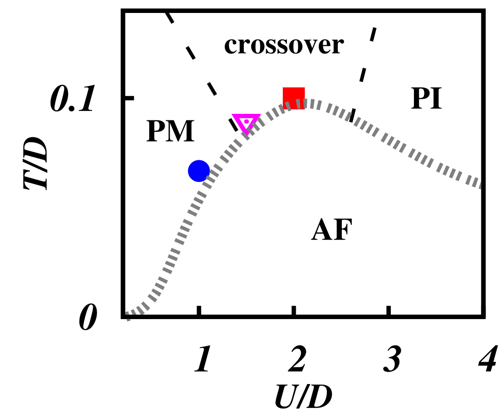

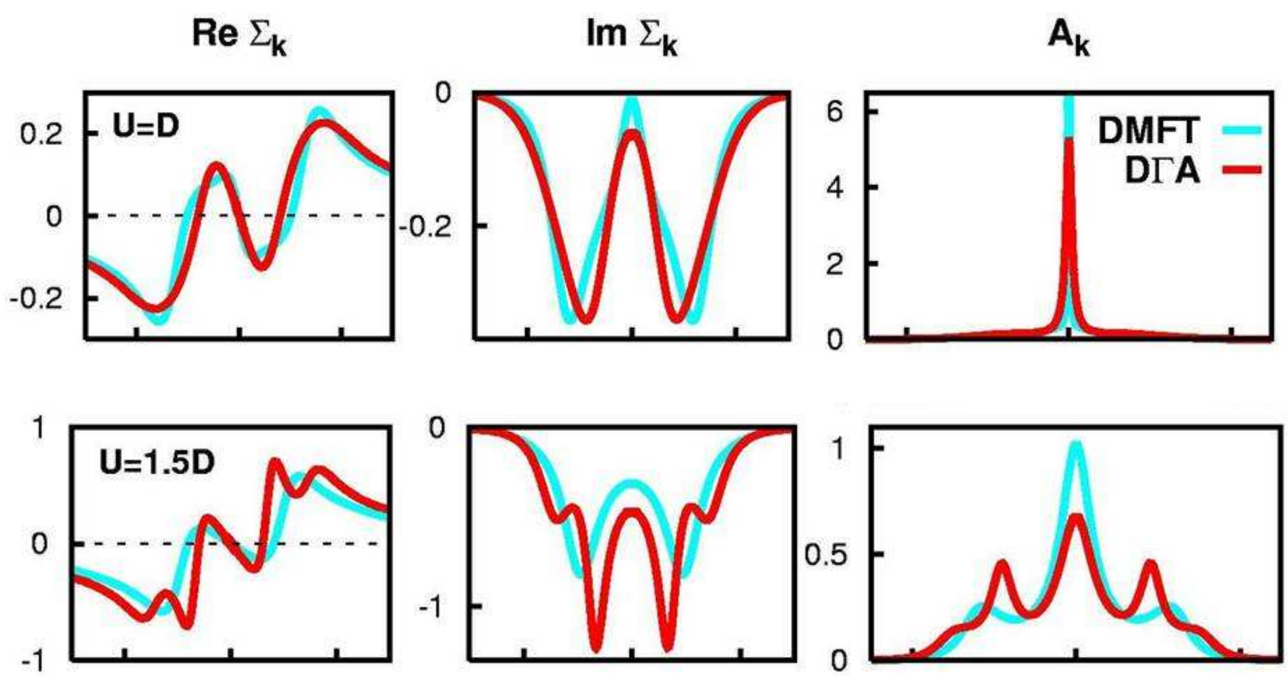

← weak damping of QP peak

← QP-damping strongly enhanced

Results: 3D Hubbard model

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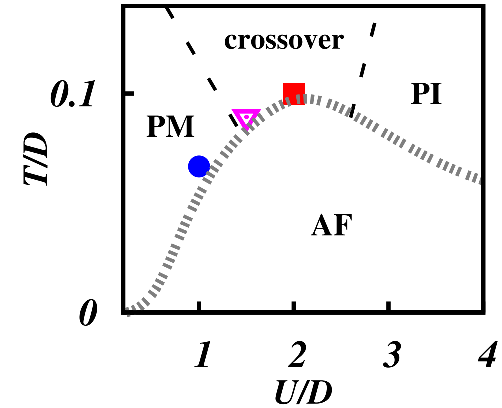
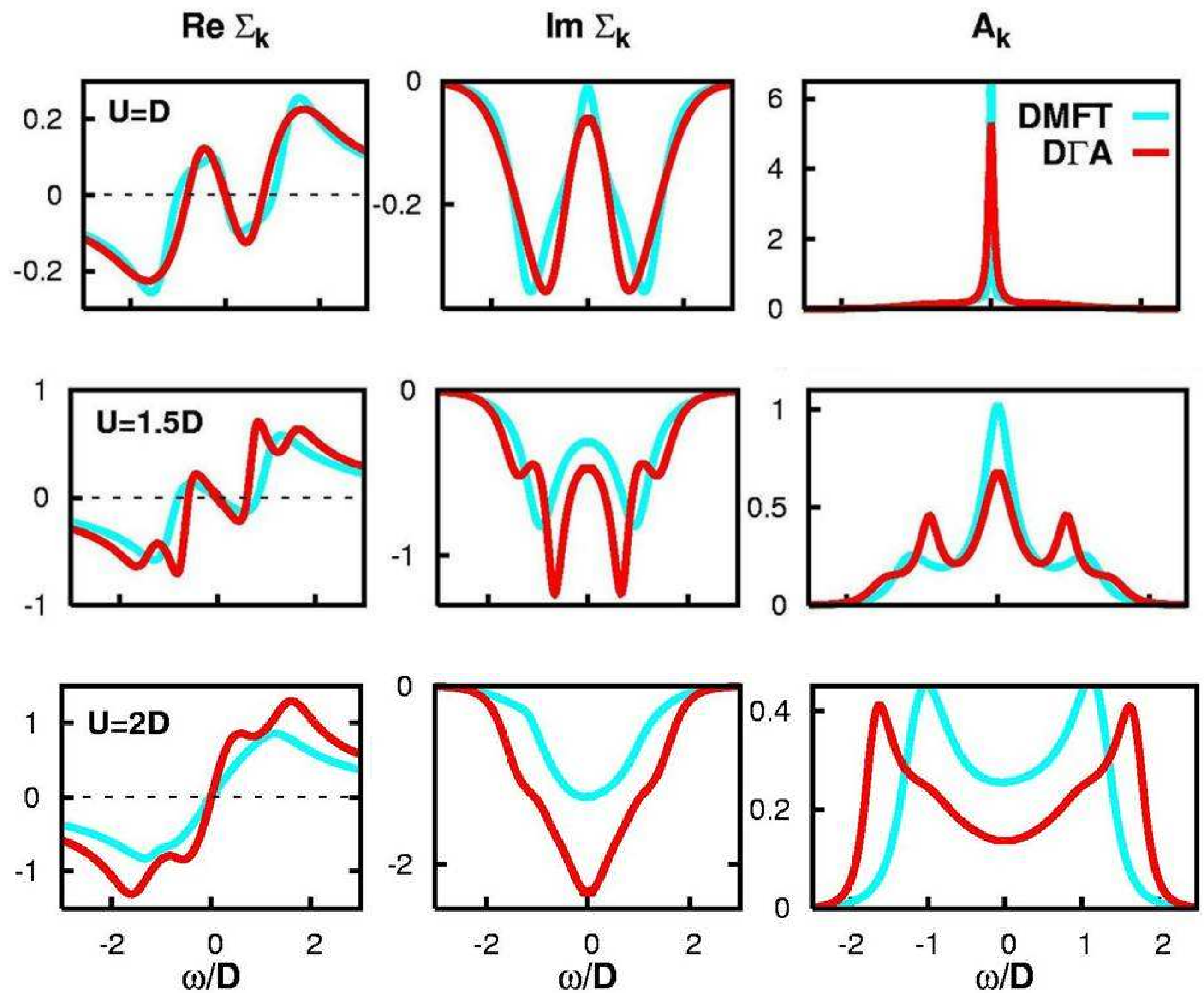


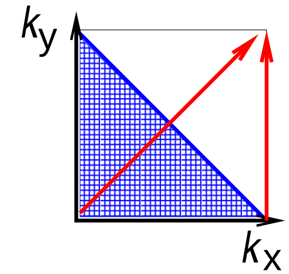


← weak damping of QP peak

← QP-damping strongly enhanced

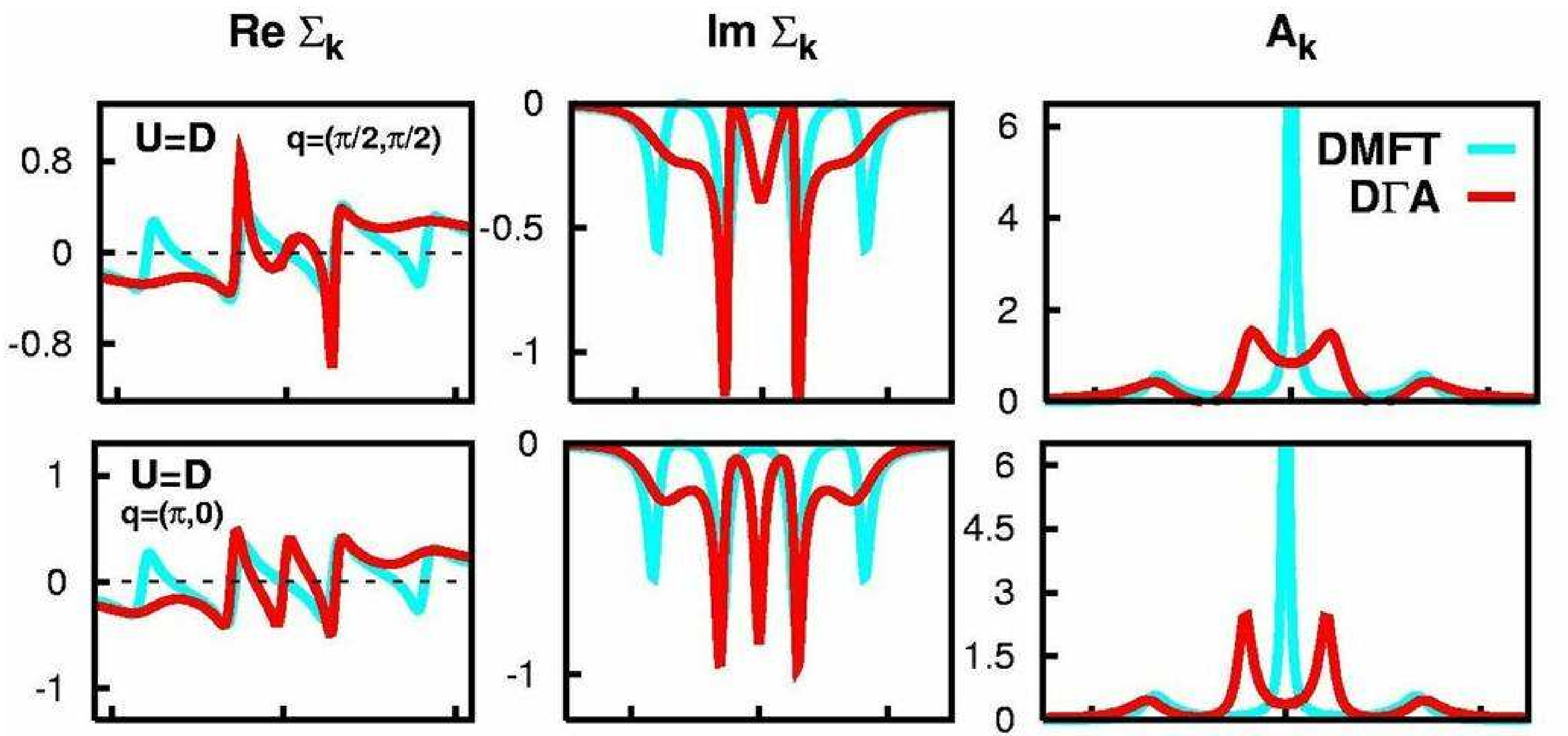
← more insulating

Results: 2D Hubbard model (half-filling)



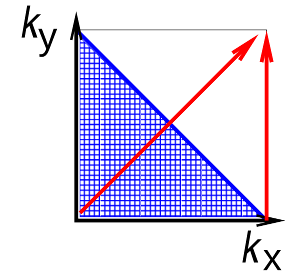
nodal
$\mathbf{k} = (\frac{\pi}{2}, \frac{\pi}{2})$

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

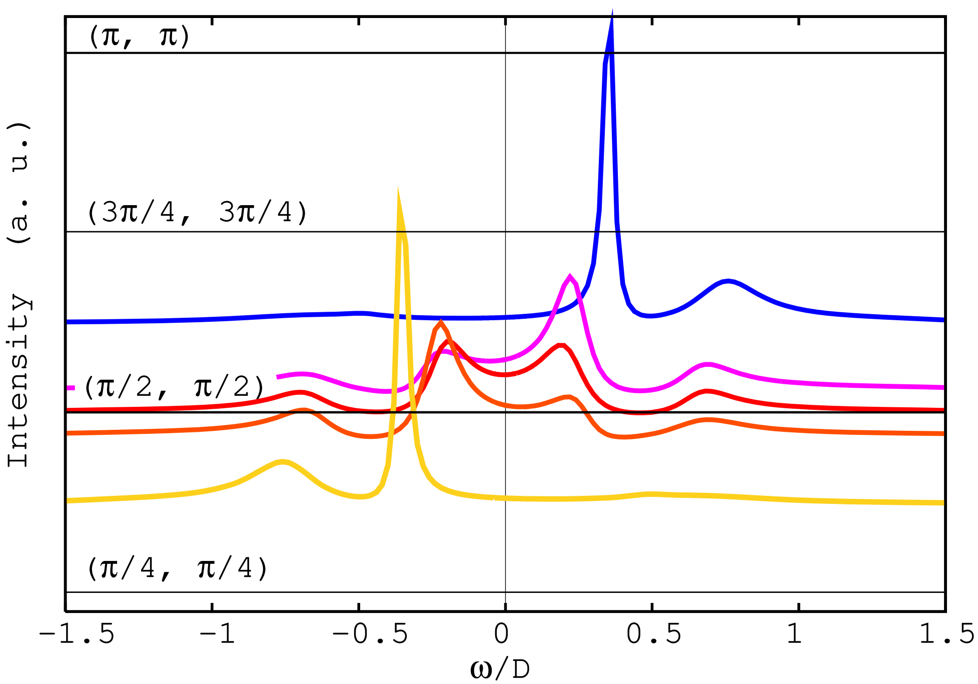


anisotropic pseudogap

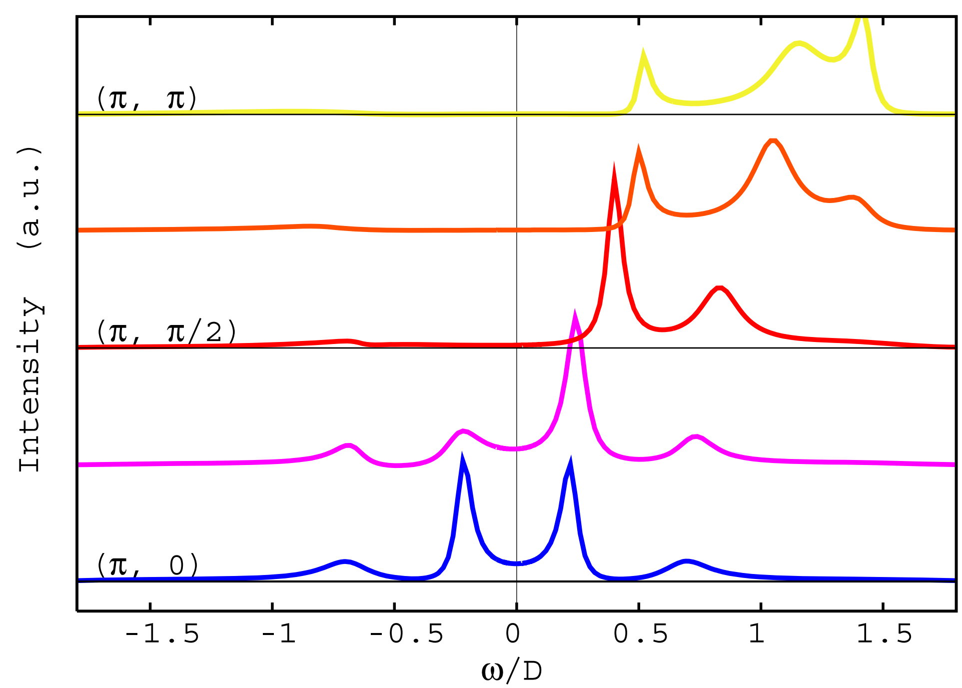
Results: 2D Hubbard model (half-filling)



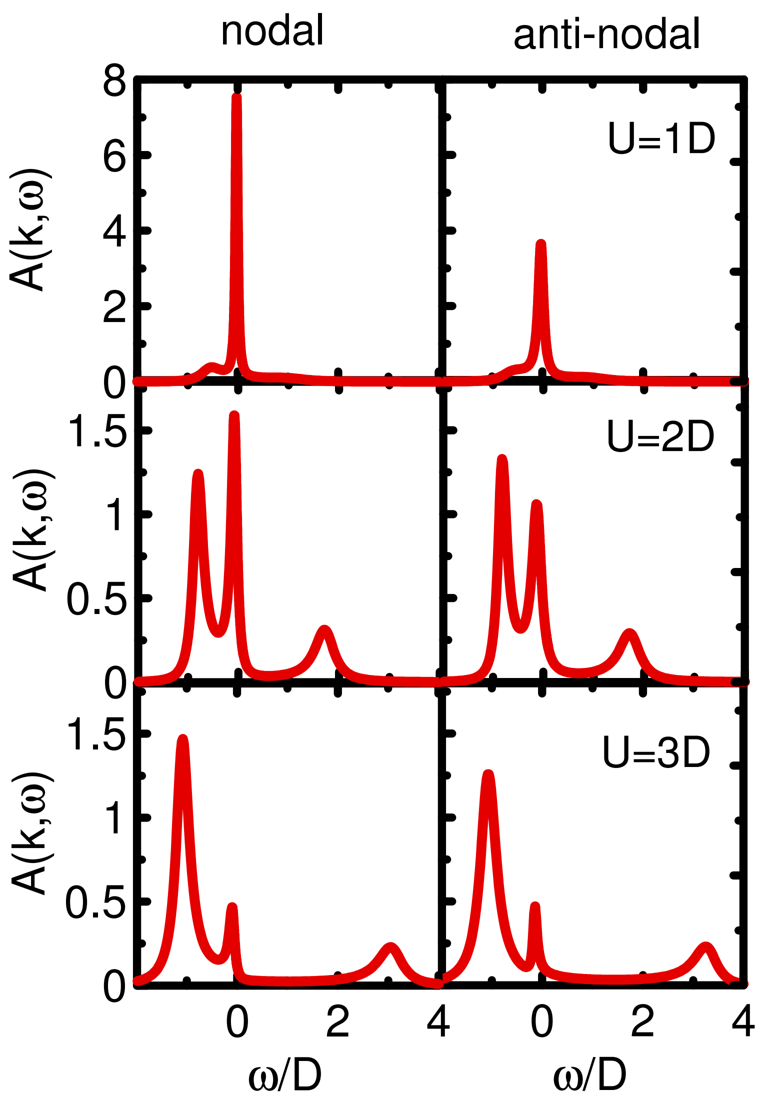
nodal



antinodal



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



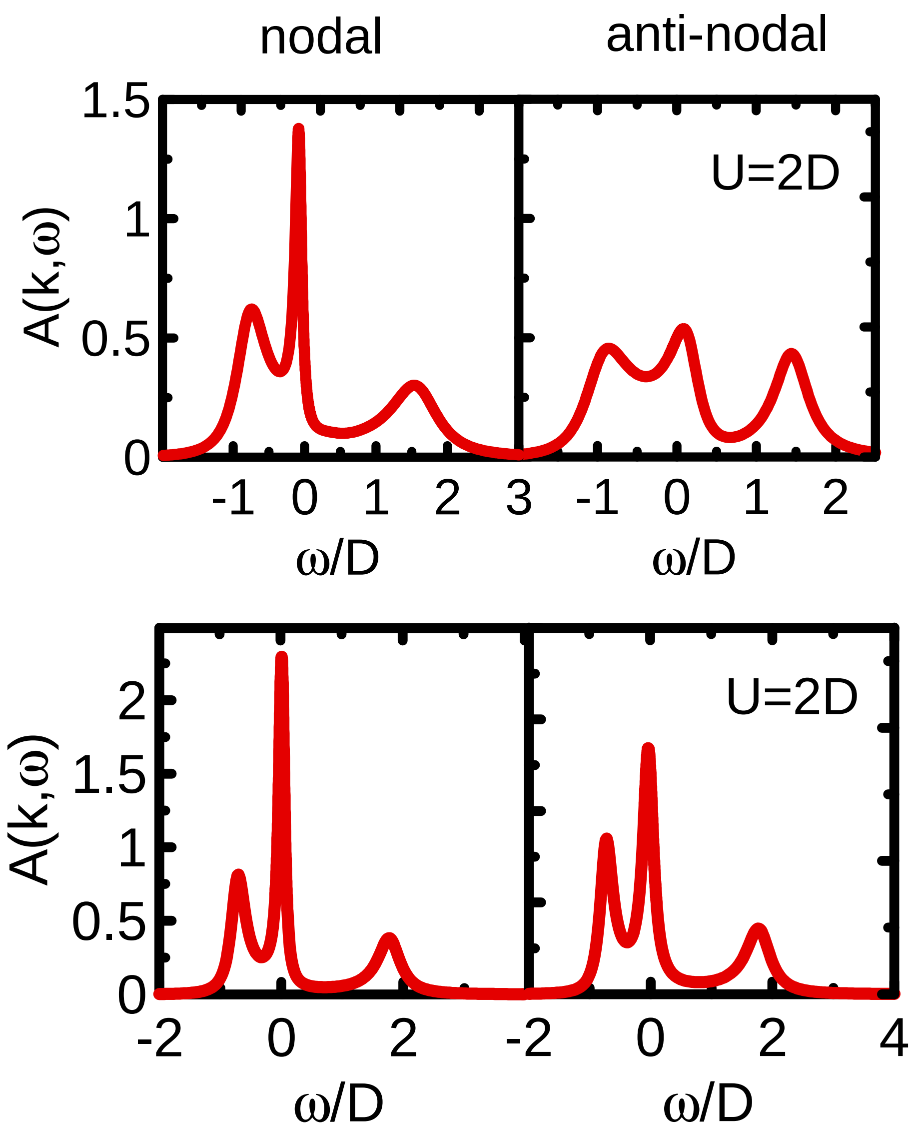
$t'/t = 0.3$
$n = 0.8$
$\beta = 100/D$

less anisotropic
at strong coupling

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

$n = 0.9$

$n = 0.8$



less anisotropic
at larger doping

Results: 1D Hubbard model

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

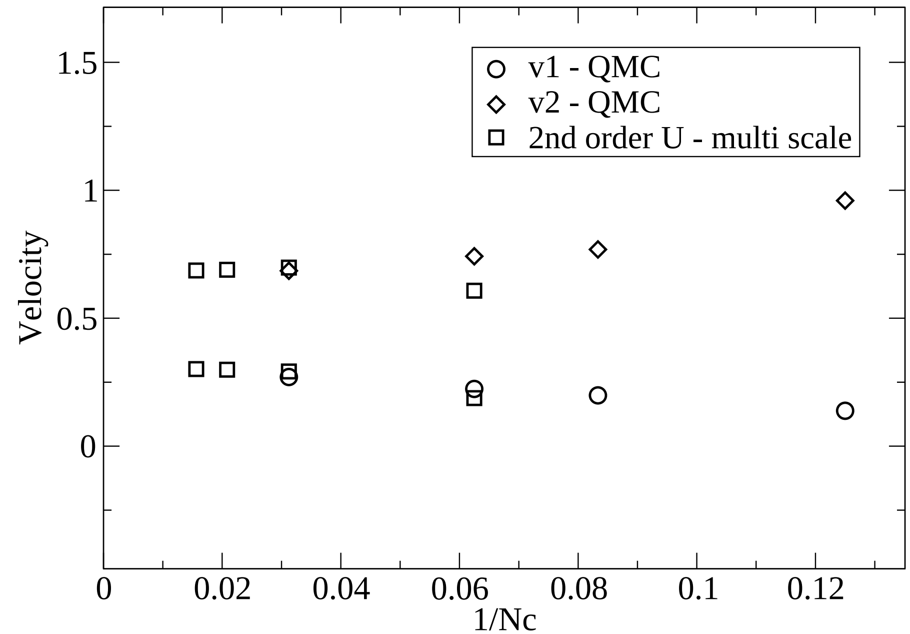
Spin-charge separation

$U = W = 1$

$k = \pi/2$

$\beta = 31$

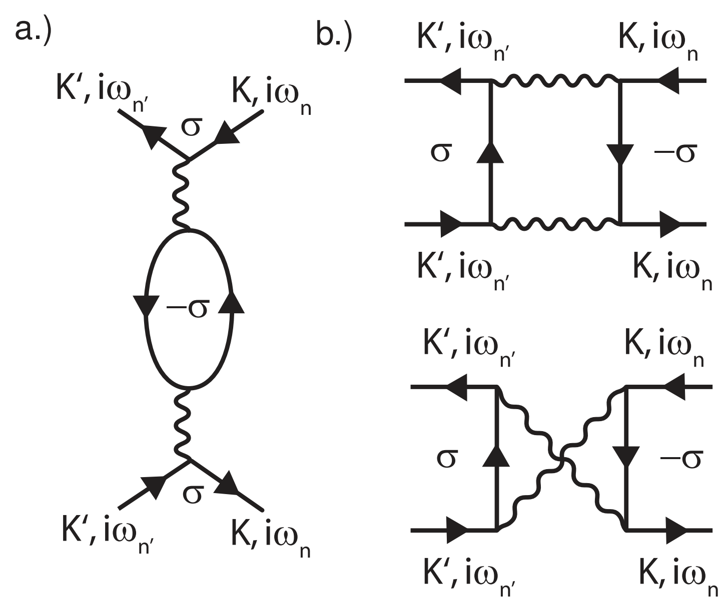
$n = 0.7$



Here, only 2nd order diagrams for vertex

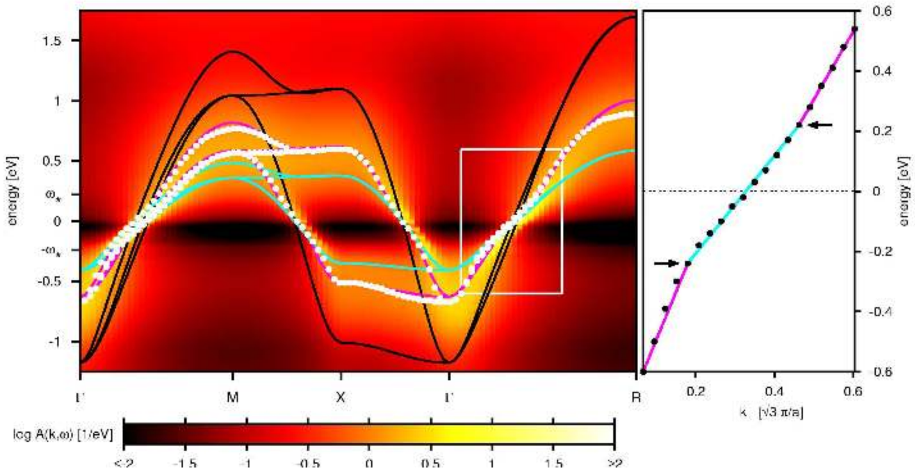
$(q = 0,\ \omega = 0)$

but 8-site DCA for short-range Σ



2) Kinks — direct consequence of strong correlations

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



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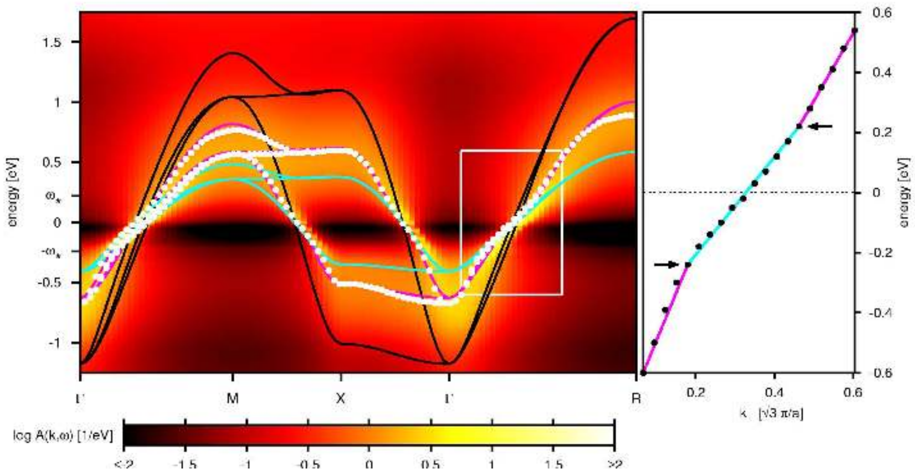
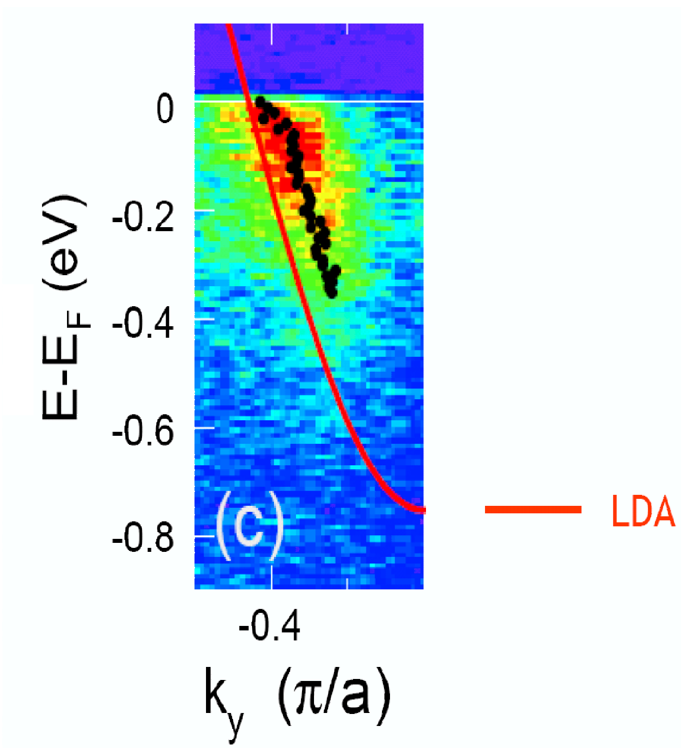


experimentally observed Fujimori et al.'06



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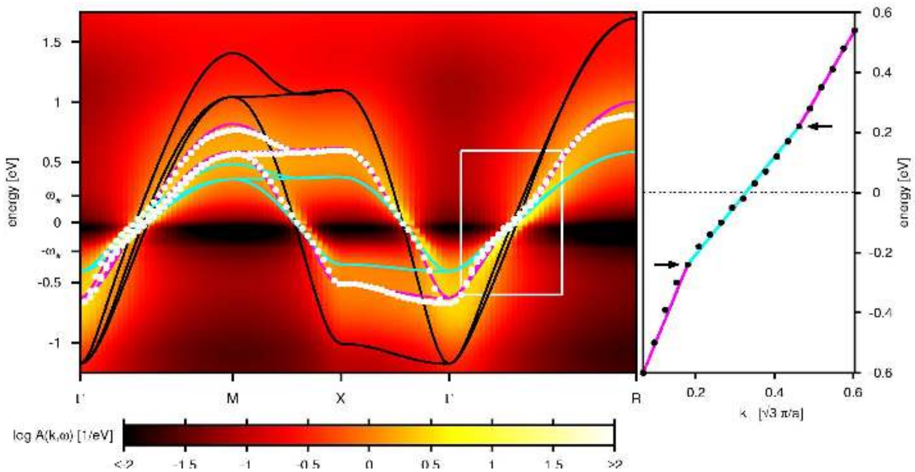
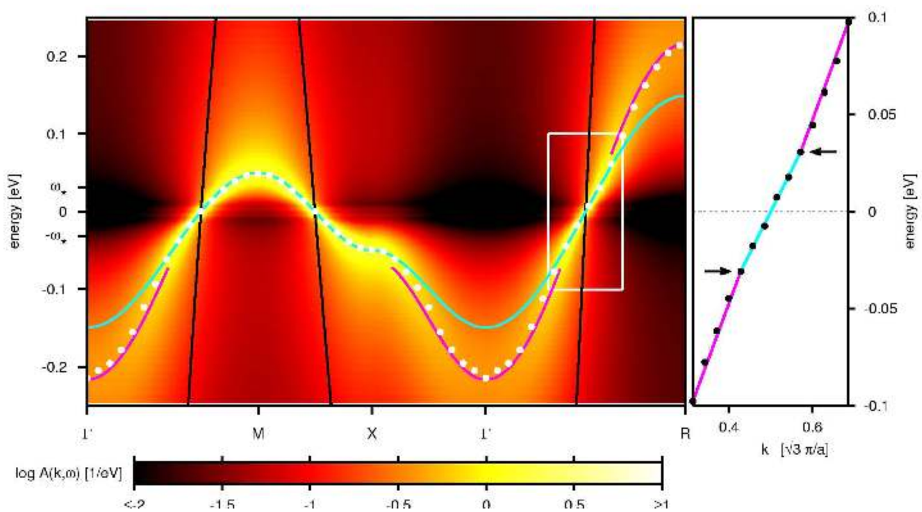


Kinks in the 3D Hubbard model

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



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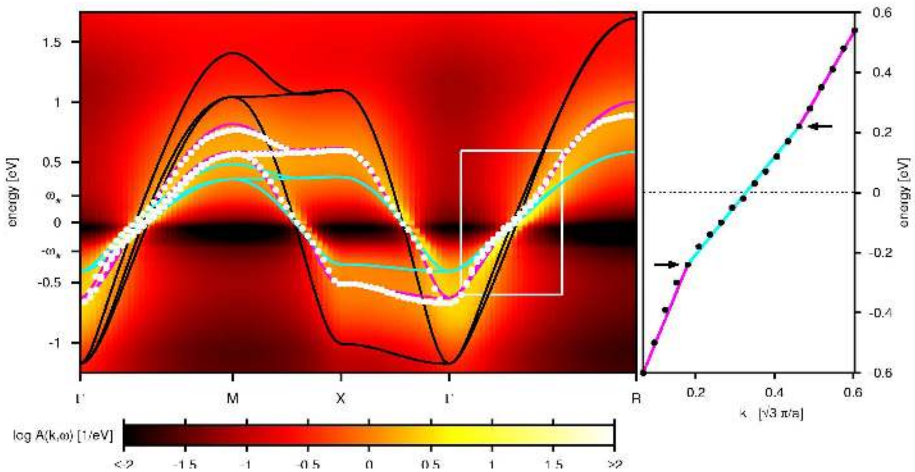

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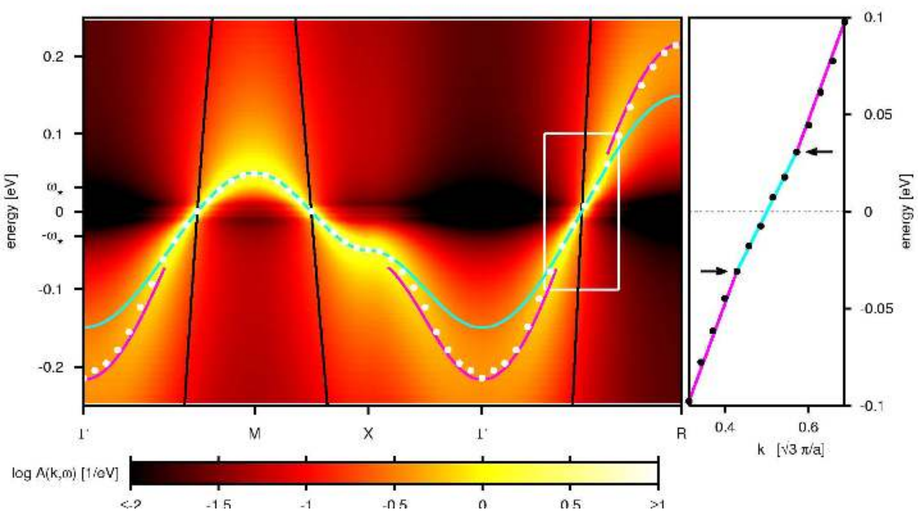
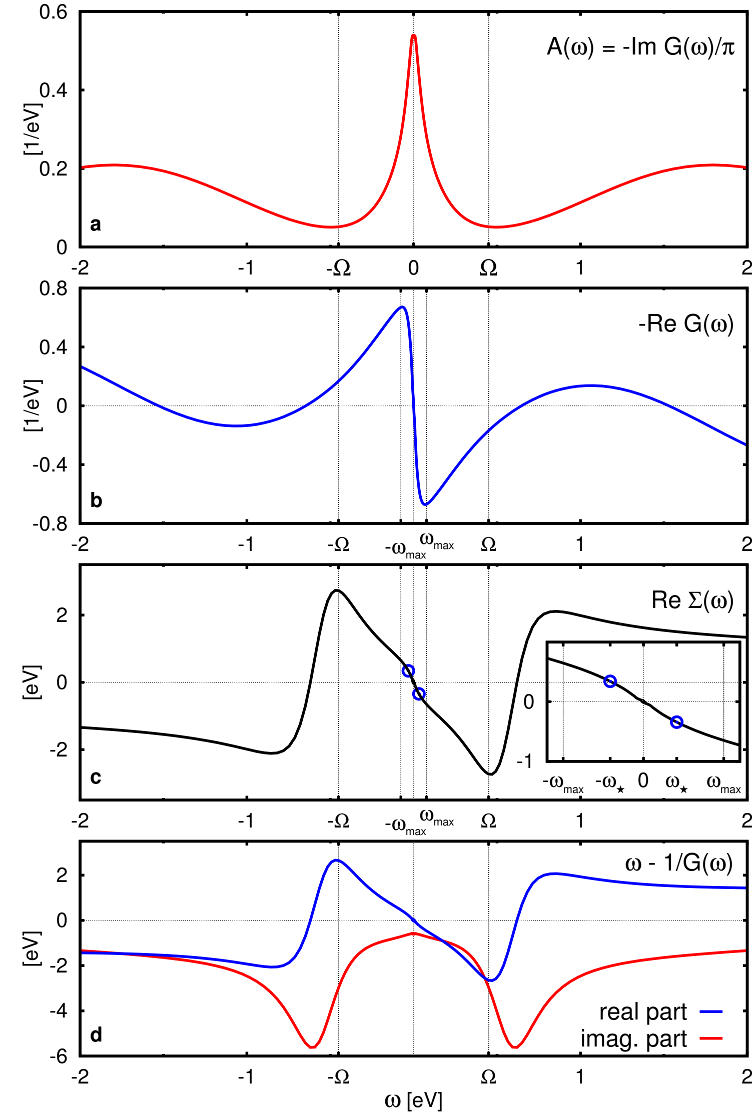


Kinks follow from 3-peak-structure

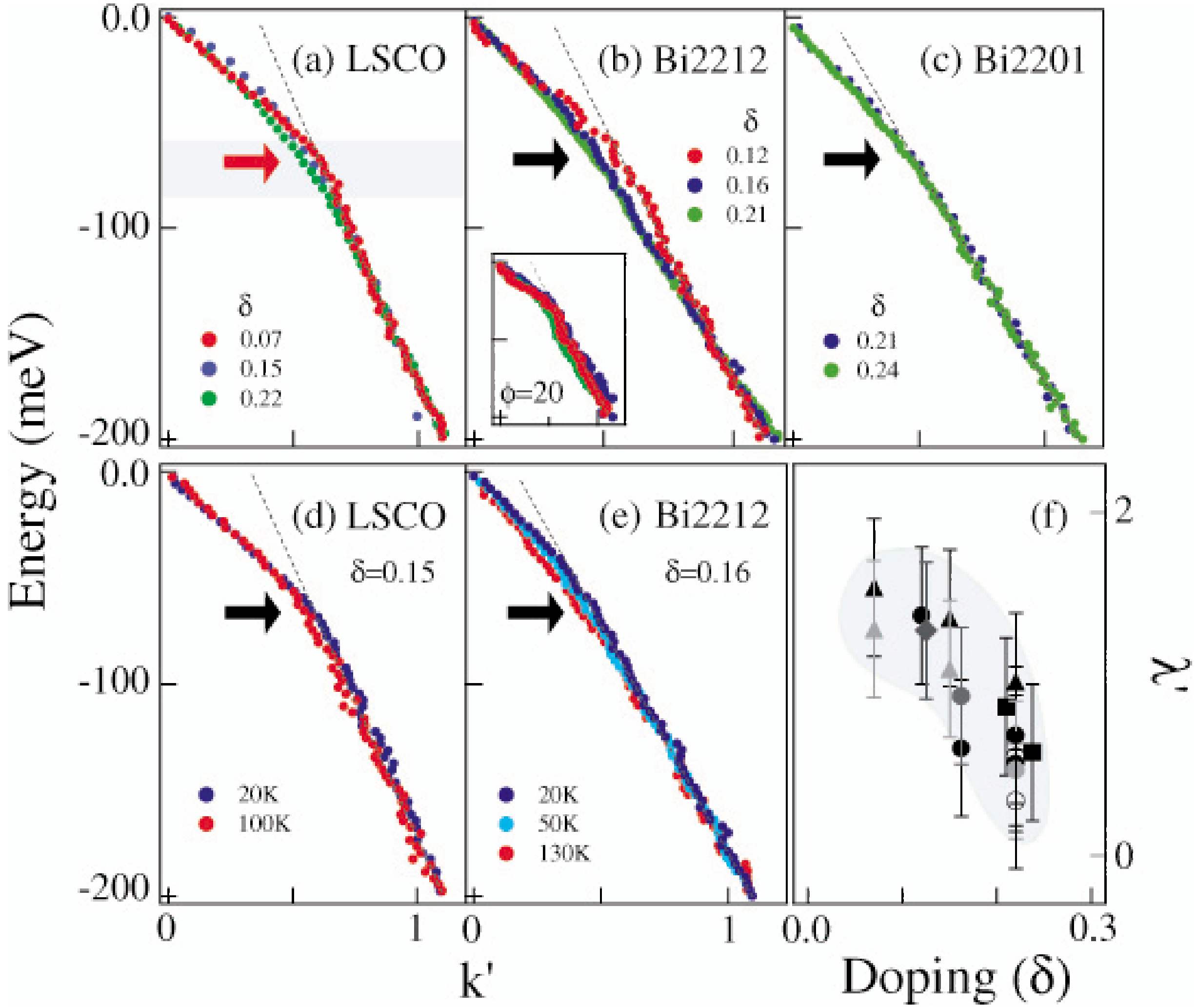


$$\Sigma(\omega) = \omega + \mu - 1/G(\omega) - \Delta(G(\omega))$$

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

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

ARPES: low-energy kinks in cuprates

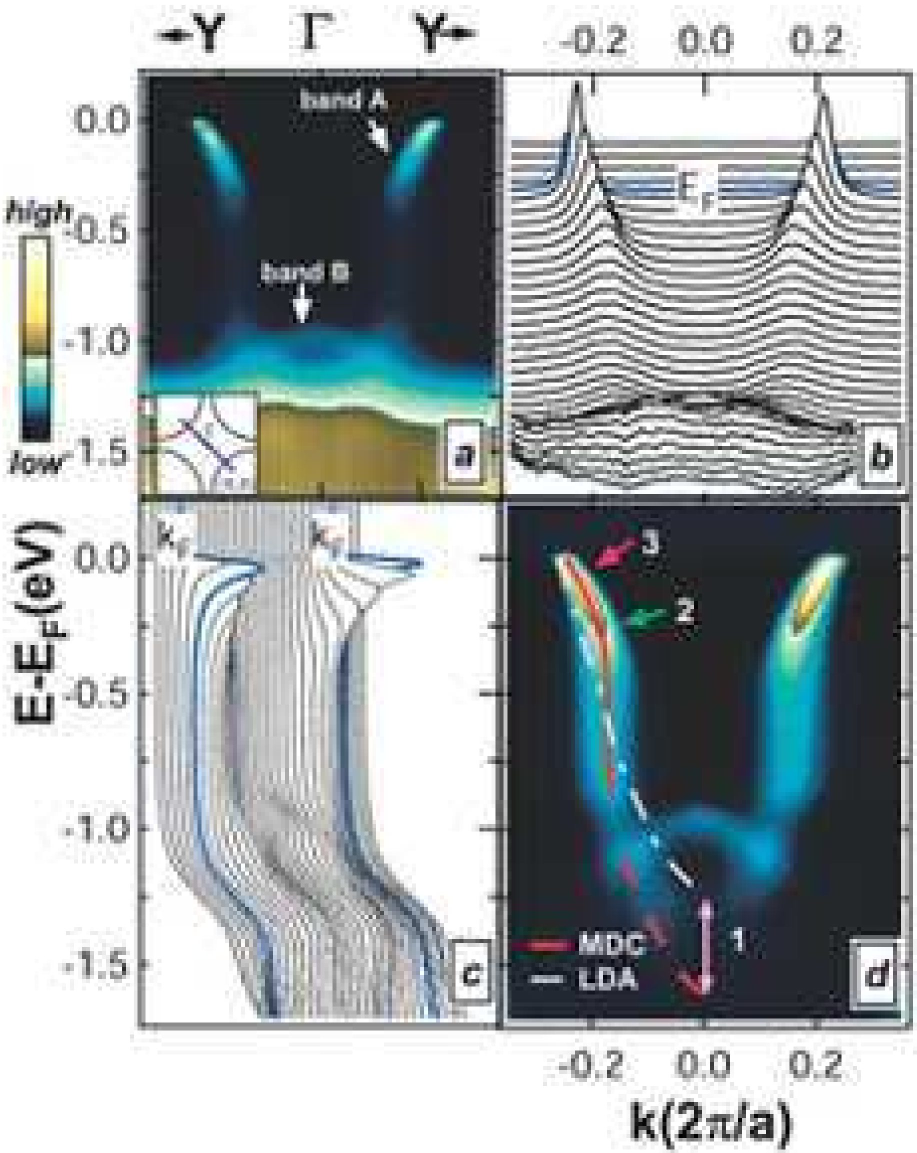


Lanzara *et al.*'01

energy range ∼ 70 meV

ARPES: high-energy kinks in cuprates

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



Meevasana *et al.* cond-mat/0612541

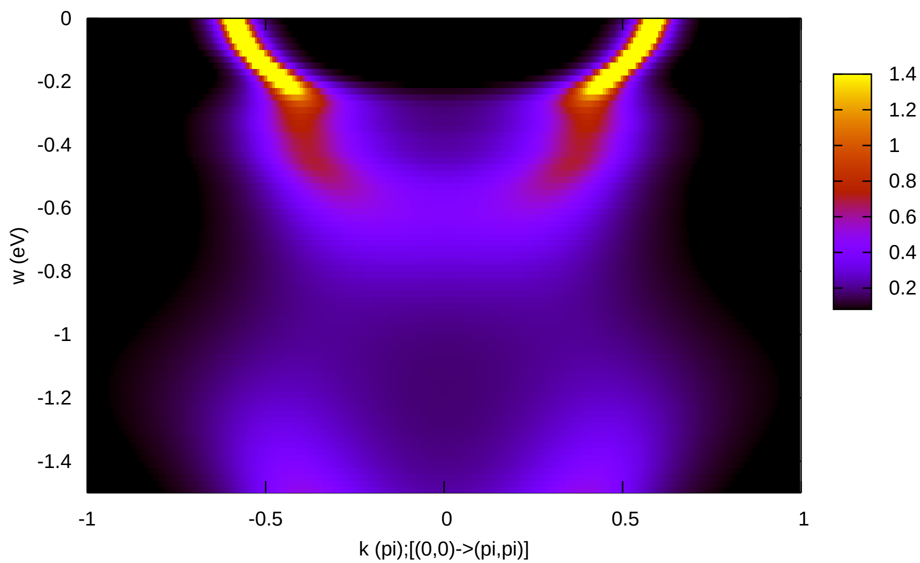
energy range ∼ 0.3 eV

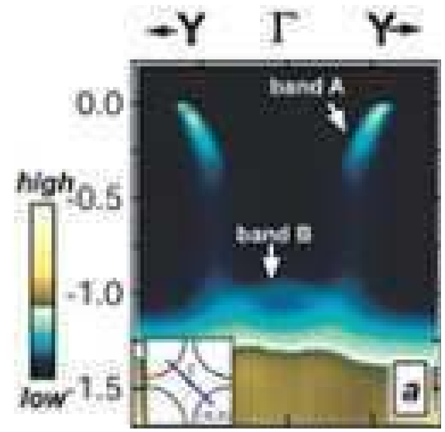
Connection to high-energy kinks

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)

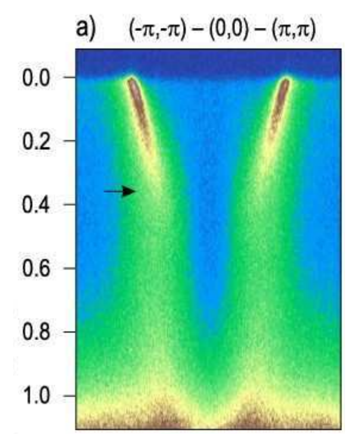




Meevasana *et al.*'06

cf. Macridin *et al.*'07

cf. Byczuk, Kollar, Vollhardt'07



Inosov *et al.*'07

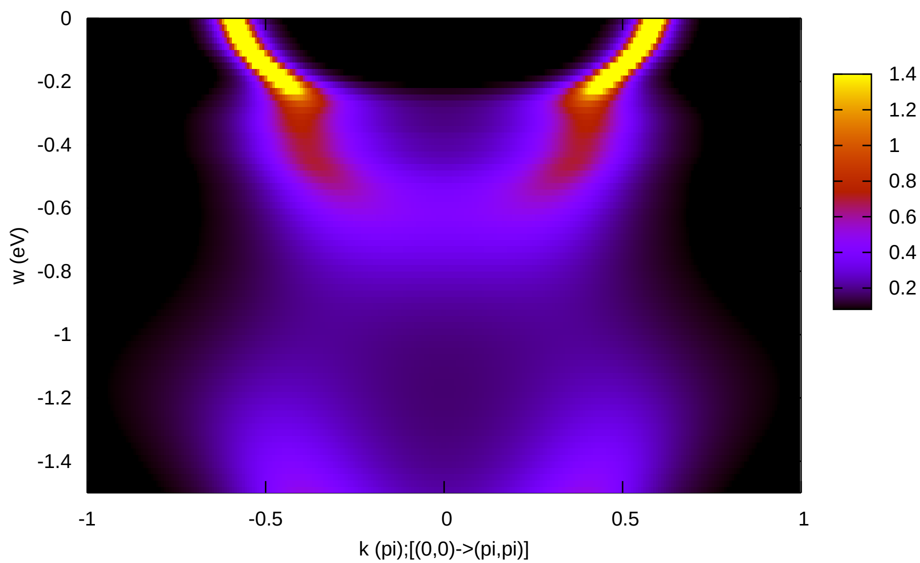
Kink position correct
but two features kink+waterfall

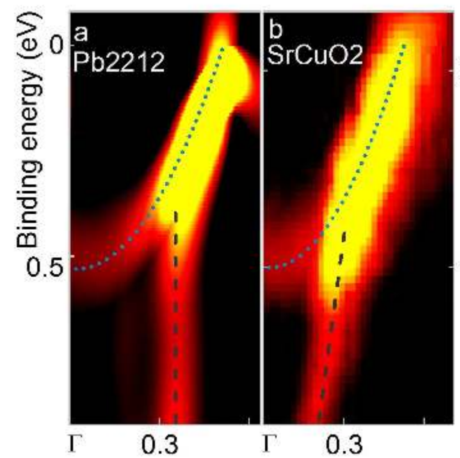
Connection to high-energy kinks

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)





Graf *et al.*'06

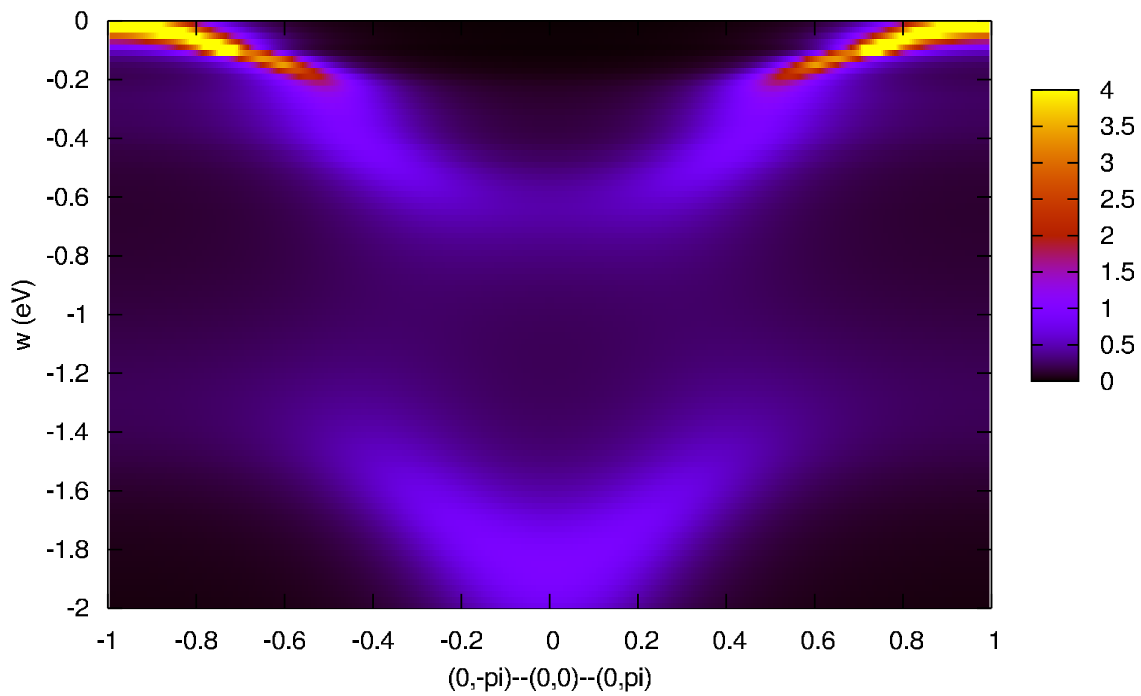
cf. Macridin *et al.*'07

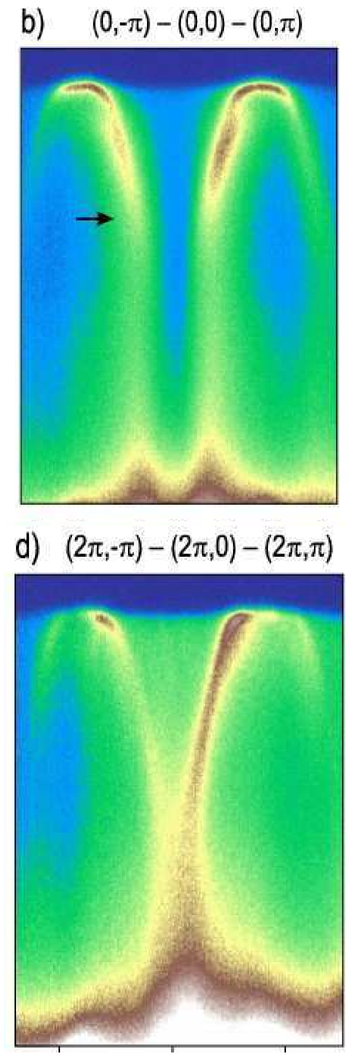
cf. Byczuk, Kollar, Vollhardt'07

Kink position correct
but two features kink+waterfall

High-energy kinks in anti-nodal direction

Yang, Held'07



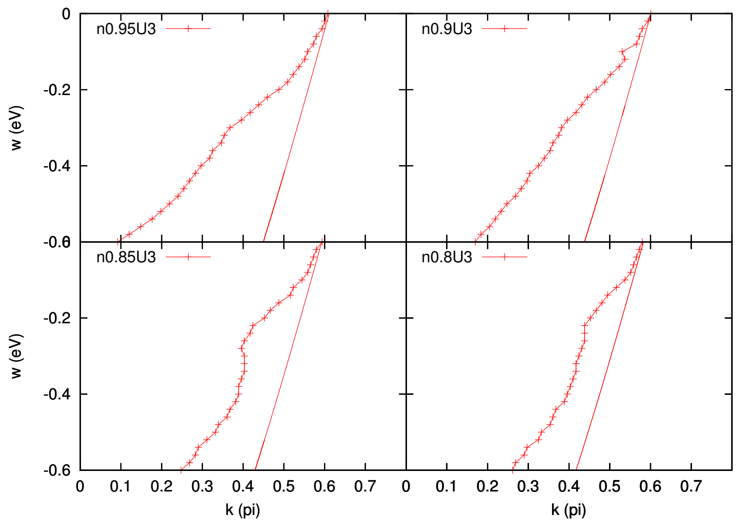


Inosov *et al.*'07

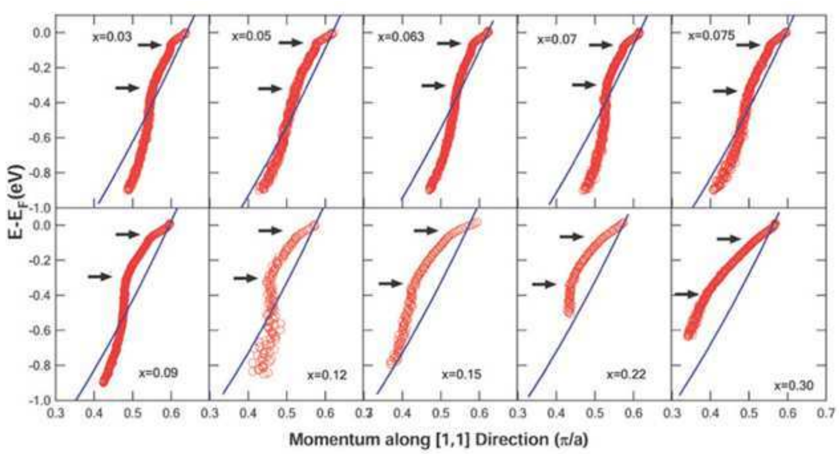
Kinks more pronounced at higher doping

Yang, Held'07

Theory:



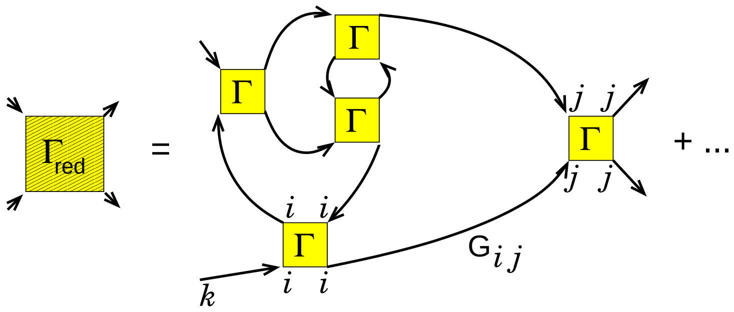
Experiment:



Meevasana *et al.*'06

Conclusion — DΓA

- DΓA assumption: local 2-particle irreducible Γ



- DΓA can access short- and long-range correlations

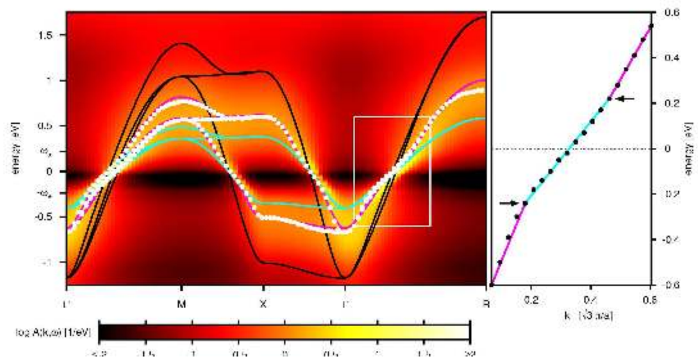
- Pseudogap in 2D; Mott transition in 3D

Outlook

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

- Realistic multi-orbital calculations possible

Conclusion – kinks



- Kinks direct consequence of strong correlations

  $\longrightarrow$ 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