Center for
Electronic Correlations and Magnetism
University of Augsburg

Kinks in the dispersion of strongly correlated electrons

CORPES'07

MPI-PKS, Dresden, April 27, 2007

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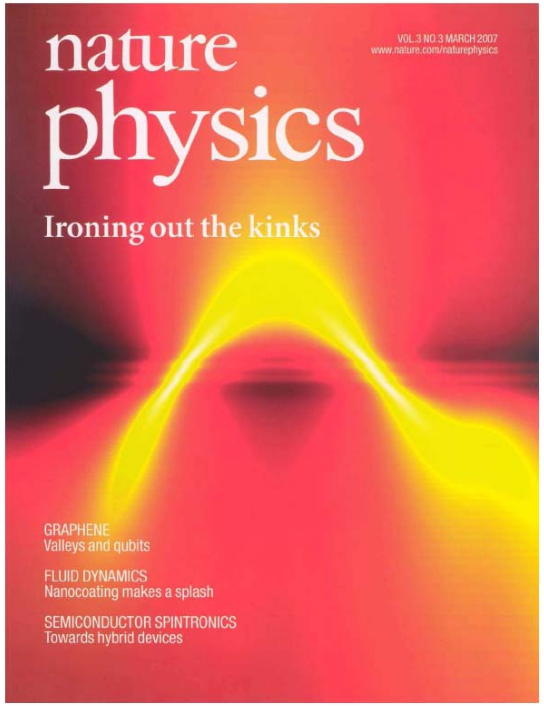
Outline

Robust electronic correlation mechanism leading to

- kinks
- waterfalls

in the electronic dispersion

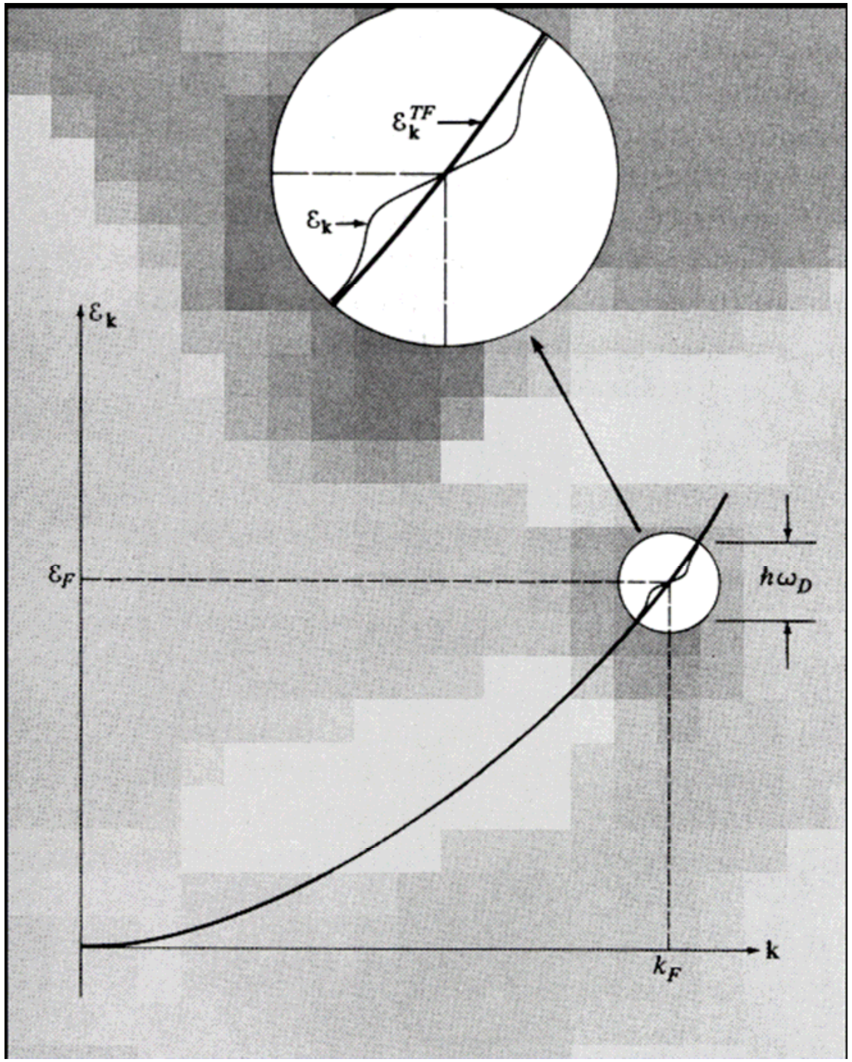
Kinks



Byczuk, Kollar, Held, Yang, Nekrasov, Pruschke, DV

Nature Physics **3,** 168 (March, 2007)

Kinks in conventional superconductivity

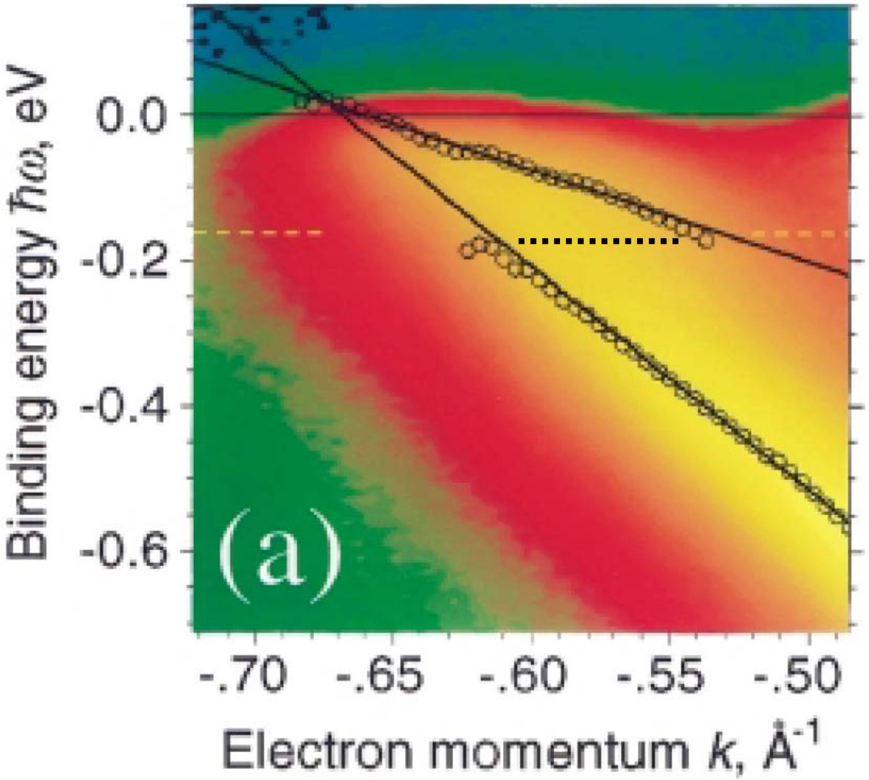


Electron-phonon (boson) correction of electronic dispersion

Ashcroft, Mermin; *Solid State Physics* (1976)

Kinks: Metal surfaces

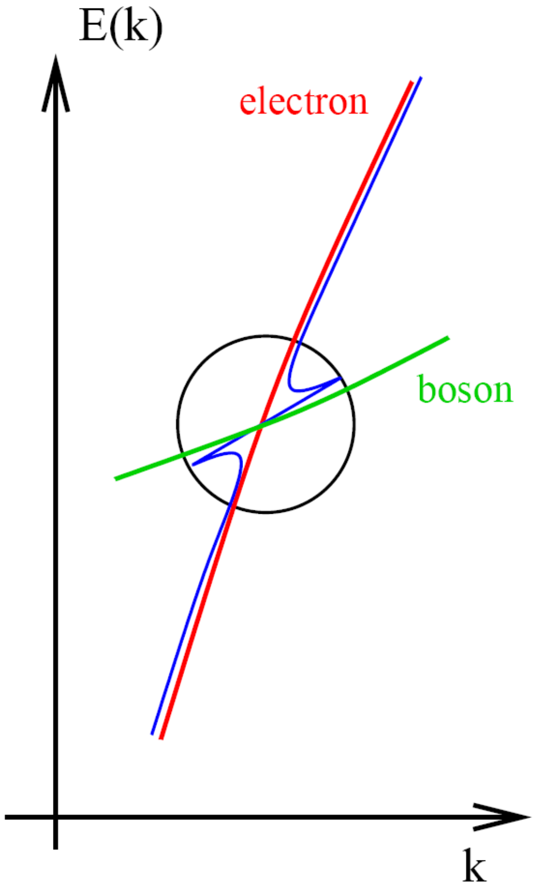
Tungsten

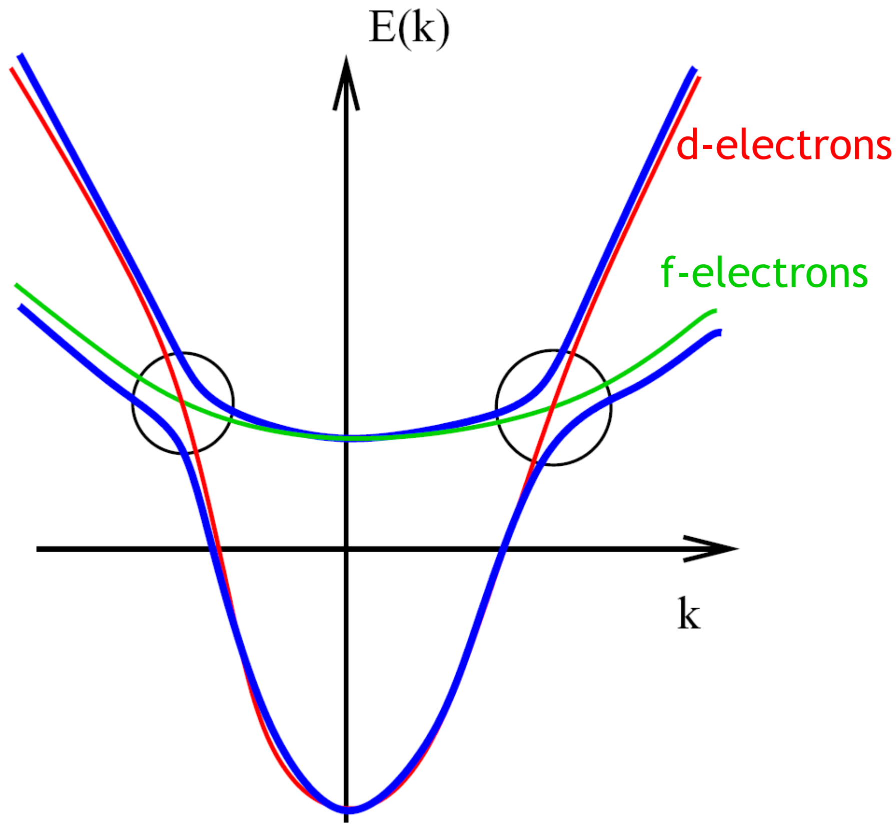


ω_* = 160 meV:
Surface phonon

Rotenberg *et al.* (2000)

Kink due to electron-phonon coupling



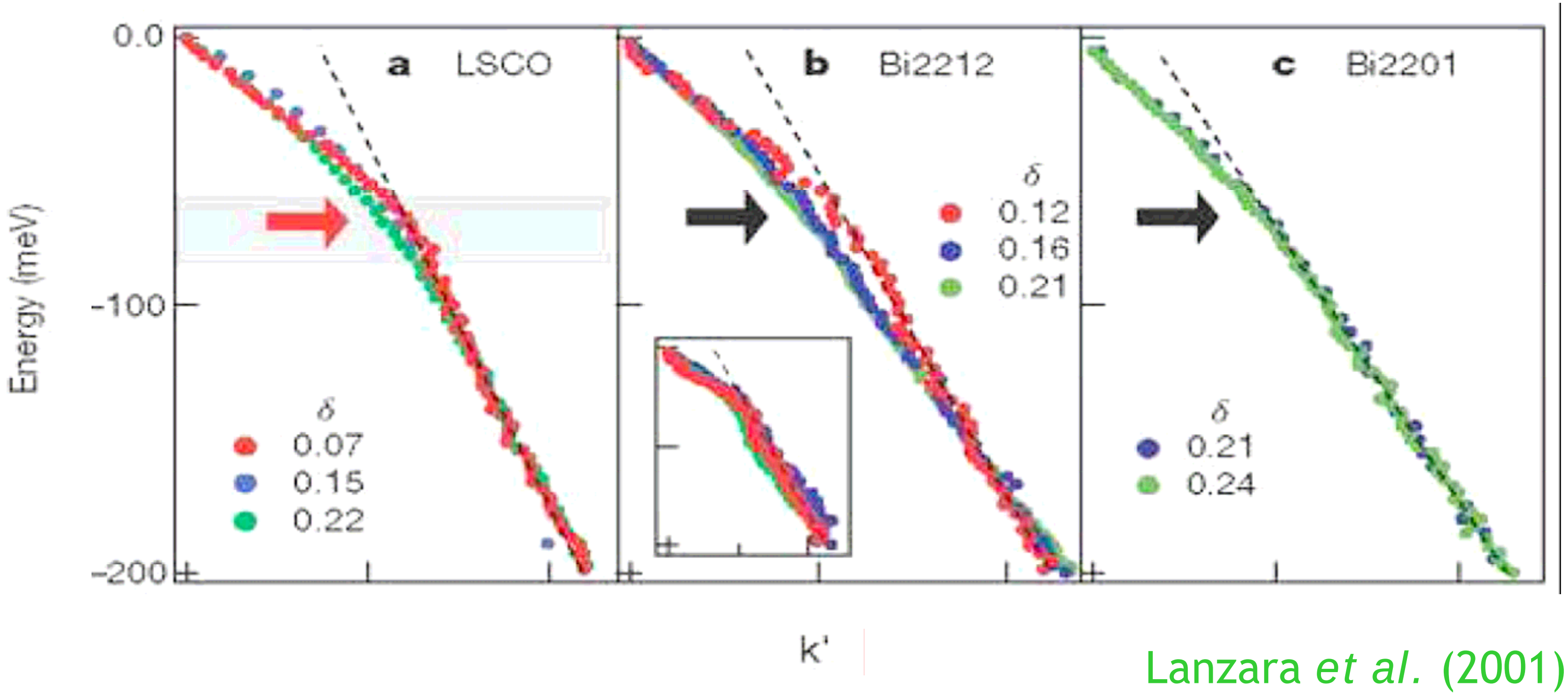


Kinks due to
electron-boson coupling

Kinks due to
electron-electron hybridization

Kinks: High-T_c cuprates

Valla *et al.* (1999)
Bogdanov et al. (2000)



Lanzara *et al.* (2001)

- Kinks at ω_* = 40-70 meV
- Coupling of electrons to phonons or spin fluctuations ?

Kinks due to electronic interaction in high-T_c cuprates (non-phononic)

- Manske, Eremin, Bennemann (2001, 2003, …)

  Coupling of quasiparticles to spin fluctuations

  [FLEX]

- Randeria, Paramekanti, Trivedi (2004)

  Different high/low energy dispersion of nodal quasiparticles (origin?)

  [Gutzwiller projected wave functions]

- Kordyuk *et al.* (2004 –), Borisenko *et al.* (2006)

  Spin-fluctuation mediated electronic interaction

  [KK-consistent extraction of self-energy]

- Kakehashi, Fulde (2005)

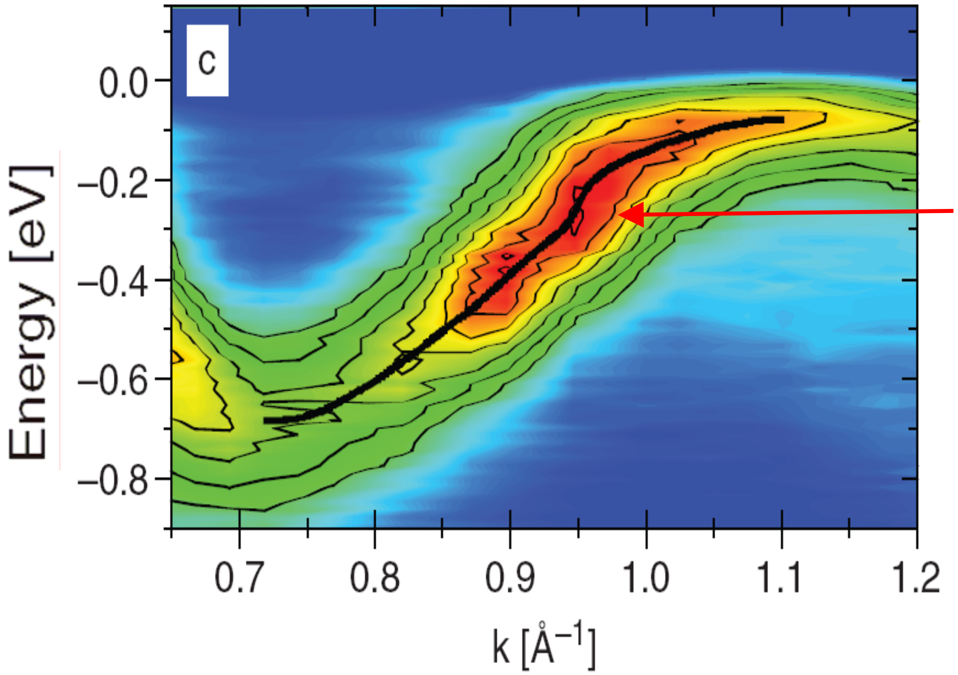
  Coupling of quasiparticles to short-range magnetic fluctuations

  [Self-consistent projection operator method]

k-dependence of self-energy $\Sigma(\mathbf{k},\omega)$ essential

Kinks: Metal surfaces

PES of quasi-1D electronic structures on Platinum(110) surface



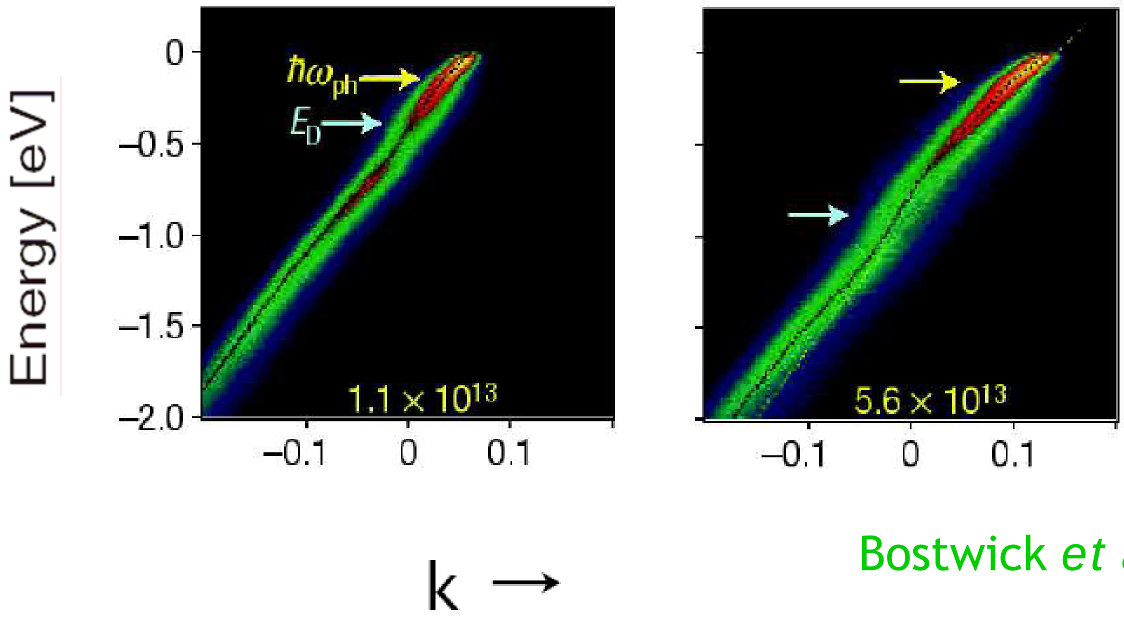
300meV: too high
for phonons or
spin fluctuations

Menzel *et al.* (2005)

Kinks due to coupling of electrons to what?

Kinks: Graphene

Doping by potassium adsorption

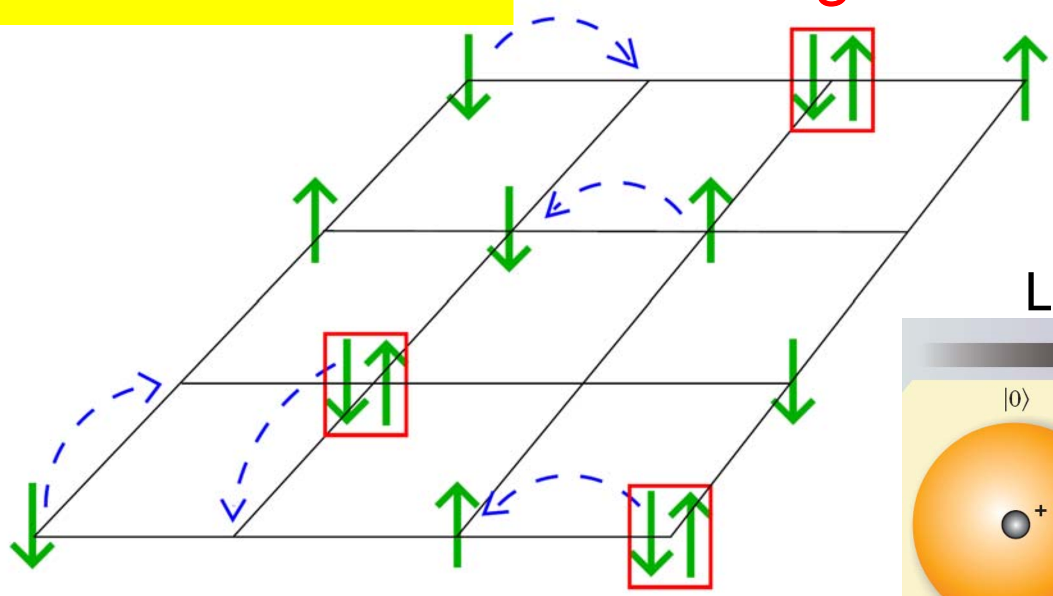


Bostwick *et al.* (2007)

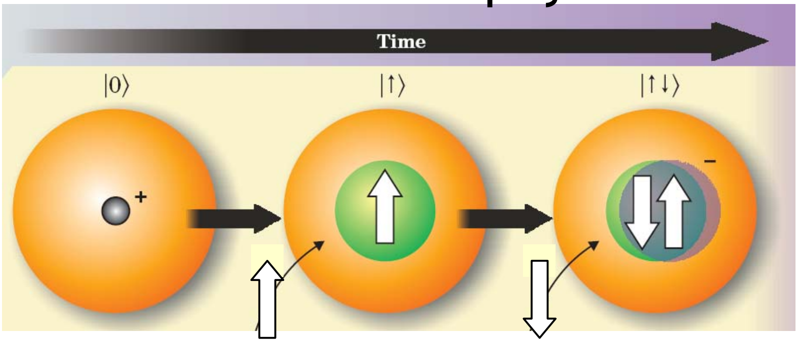
- "Low energy" kinks at 200 meV
- "High energy" kinks at 400-900 meV (near X-ing of Dirac branches, E_D)
- coupling of electrons to plasmons ?

Robust electronic correlation mechanism for kinks

Correlated electrons



Local Hubbard physics:



Hubbard model

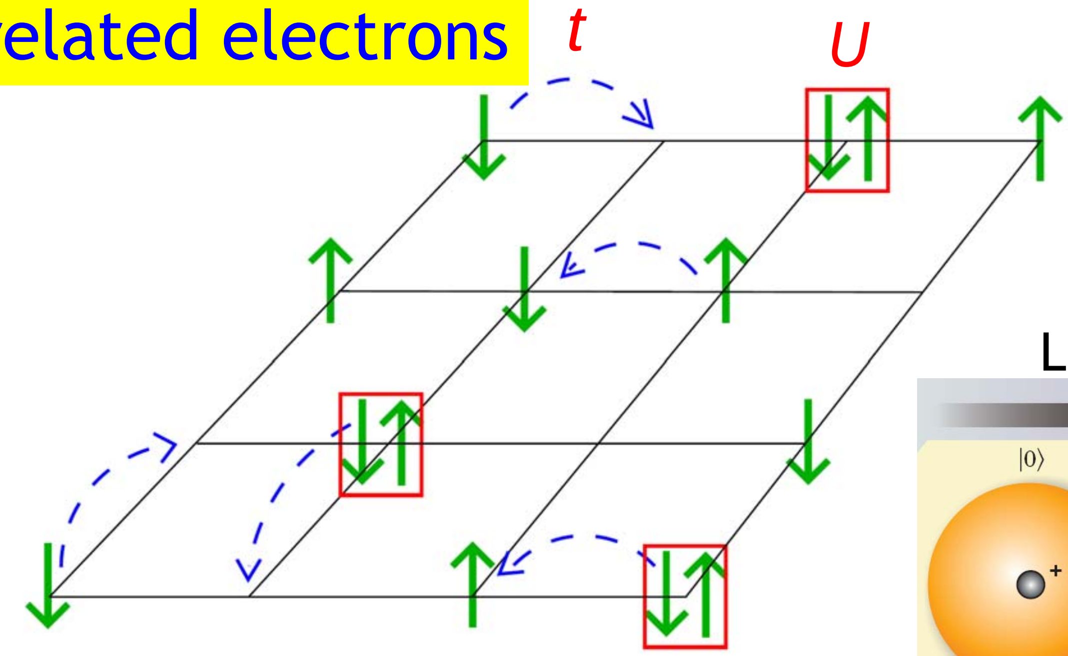
$$H = -t \sum_{\langle \mathbf{i},\mathbf{j} \rangle, \sigma} c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow}$$

$$\langle n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} \rangle \neq \langle n_{\mathbf{i}\uparrow} \rangle \langle n_{\mathbf{i}\downarrow} \rangle$$

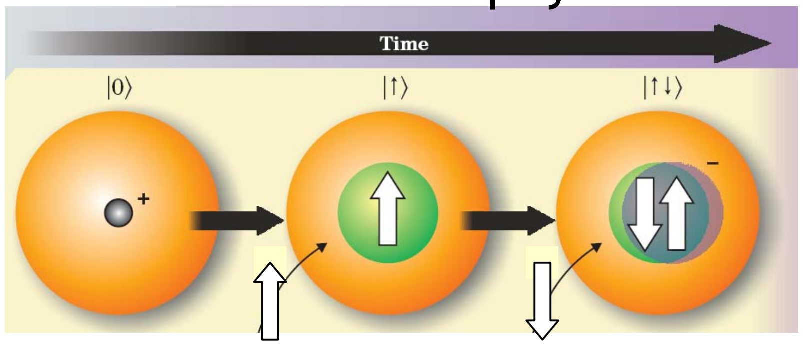
Correlation phenomena:
Metal-insulator transition, ...

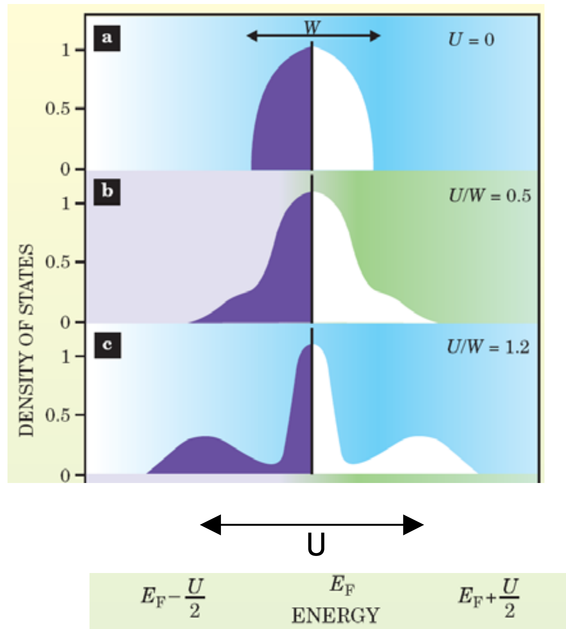
Hartree-Fock (static) mean-field theory generally insufficient

Correlated electrons



Local Hubbard physics:



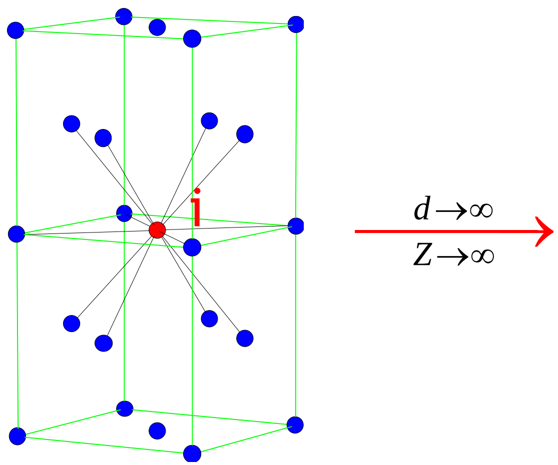


Hubbard model

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

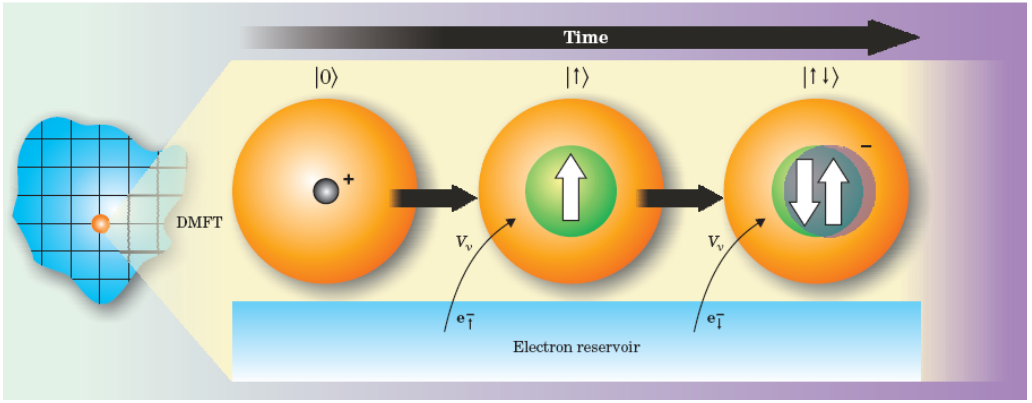
Correlated electrons

d=3; coord. # Z
fcc lattice: Z=12



Dynamical Mean-Field Theory (DMFT)

Proper time resolved treatment
of local electronic interactions



→ LDA+DMFT

Kotliar, DV; **Physics Today (March 2004)**

k- resolved spectra (ARPES) in DMFT

$$\mathbf{G}(\mathrm{k},\omega) = [\omega - \mathbf{\Sigma}(\omega) - \mathbf{H}^{0}_{LDA}(\mathrm{k})]^{-1}$$

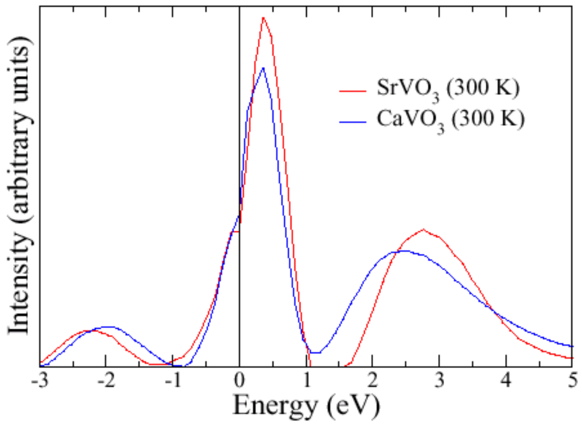
matrices in orbital space

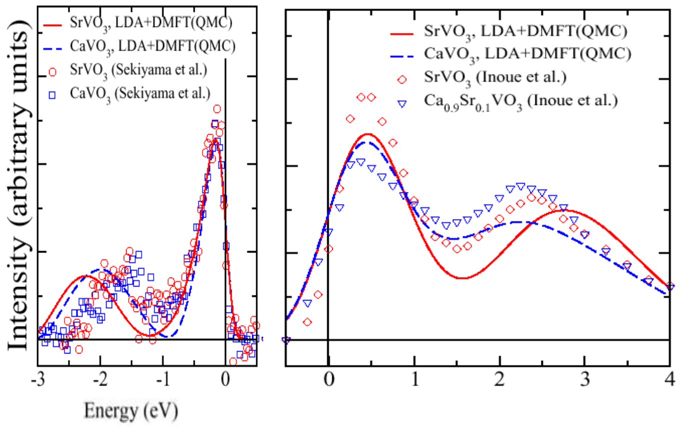
$\rightarrow$ **k**-resolved spectral function

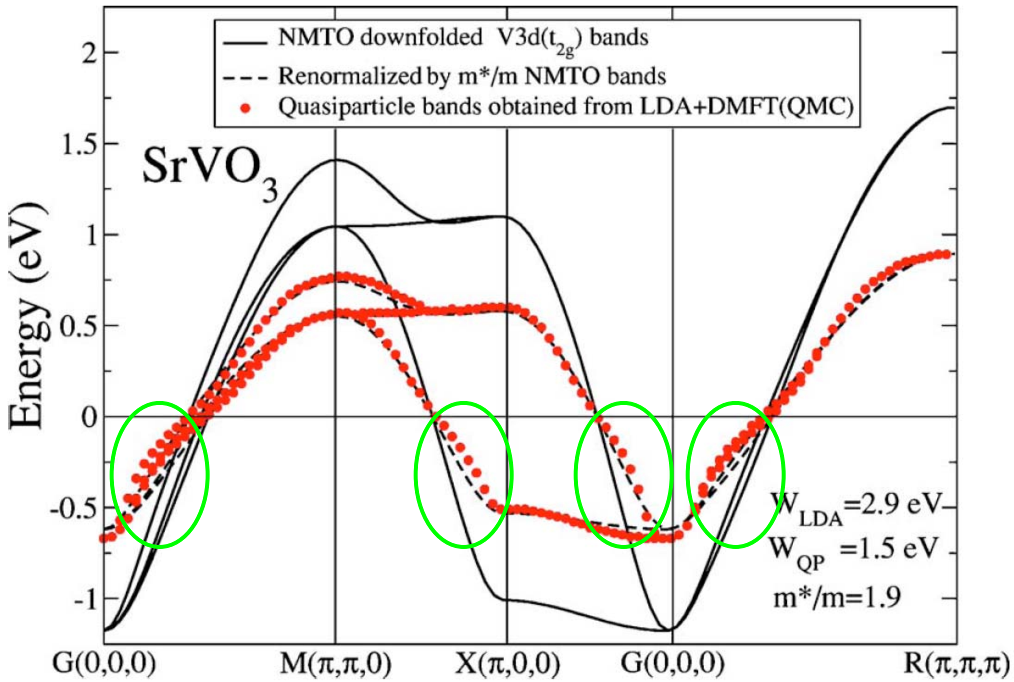
$$A(\mathrm{k},\omega) = -\frac{1}{\pi}\mathrm{Im}\, Tr\,\mathbf{G}(\mathrm{k},\omega)$$

Purely electronic mechanism for kinks: Strong correlations

$SrVO_3$ and $CaVO_3$







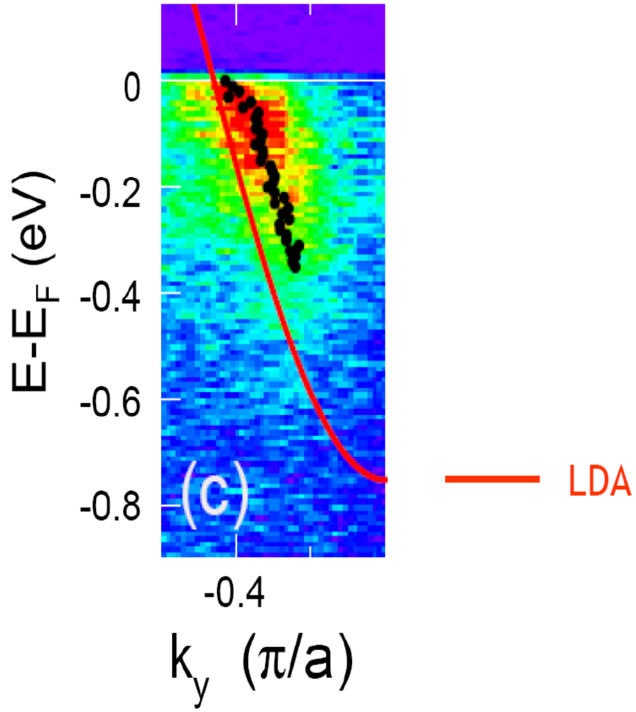
Ekaterinburg – Augsburg – Stuttgart collaboration, Nekrasov *et al.* (2004, 2006)

Renormalization of LDA-bands by self-energy

Kinks at $|\omega_*| \approx 200$ meV

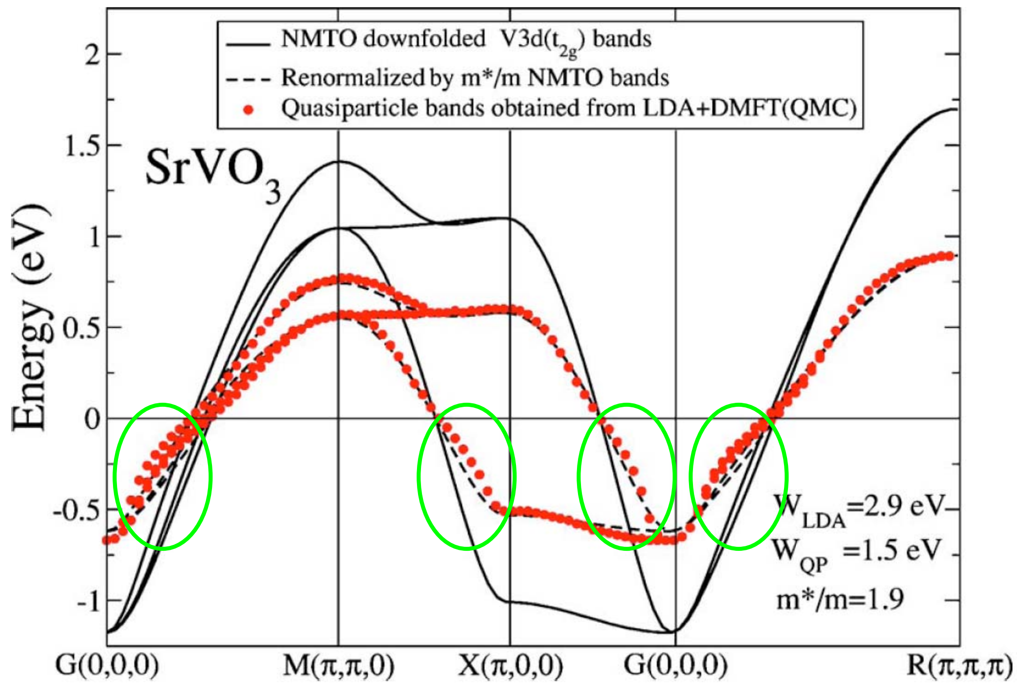
Osaka – Augsburg – Ekaterinburg Collaboration; Sekiyama *et al.* (2004)

Purely electronic mechanism for kinks: Strong correlations



Yoshida *et al.* (2005)

Kinks at $\omega_* \approx 100$ meV



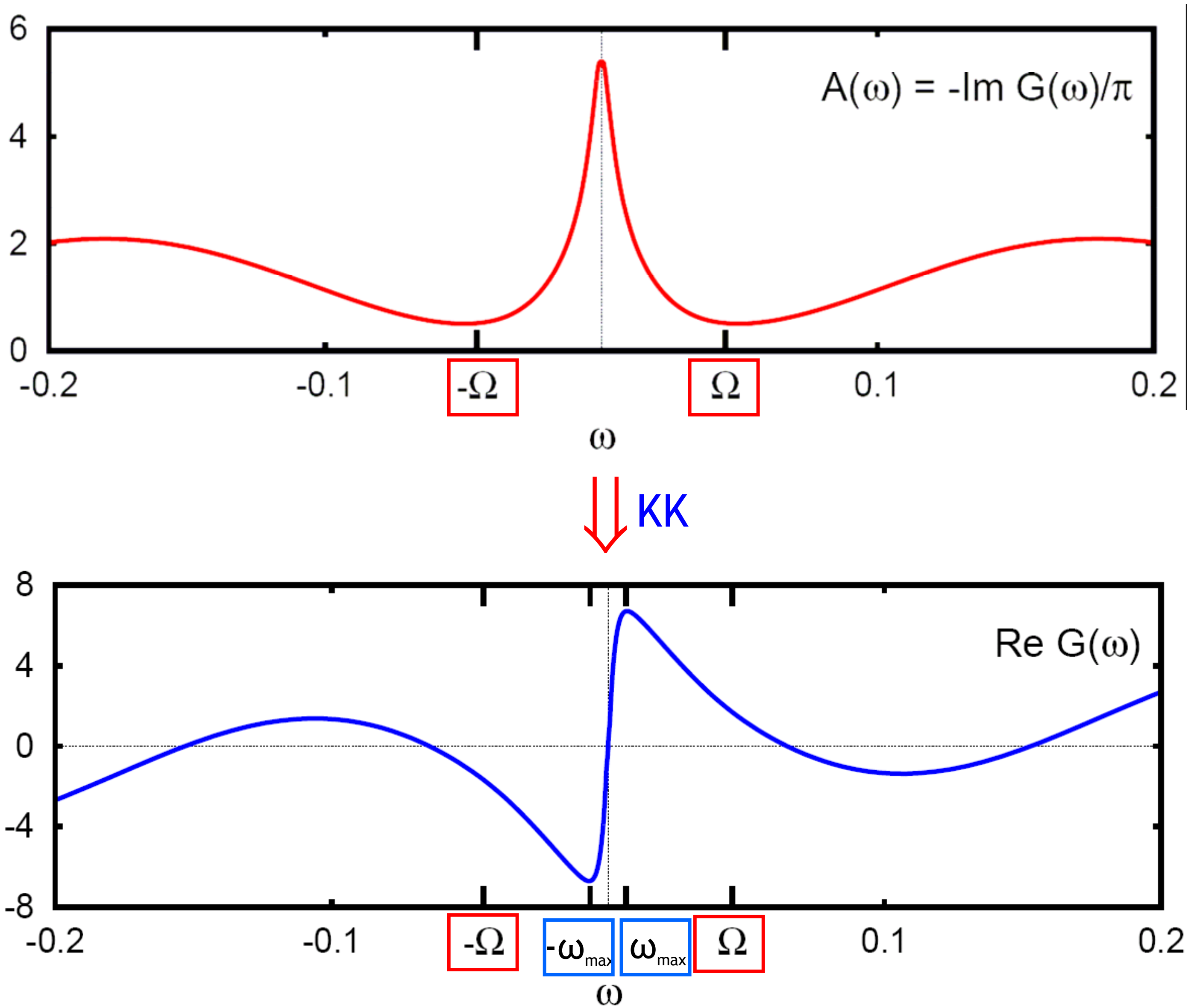
Ekaterinburg – Augsburg – Stuttgart collaboration,
Nekrasov *et al.* (2004, 2006)

Renormalization of LDA-bands by self-energy

Physical origin of kinks in a purely electronic theory with one type of electron ?

Kinks at $|\omega_*| \approx 200$ meV

Strongly correlated paramagnetic metal



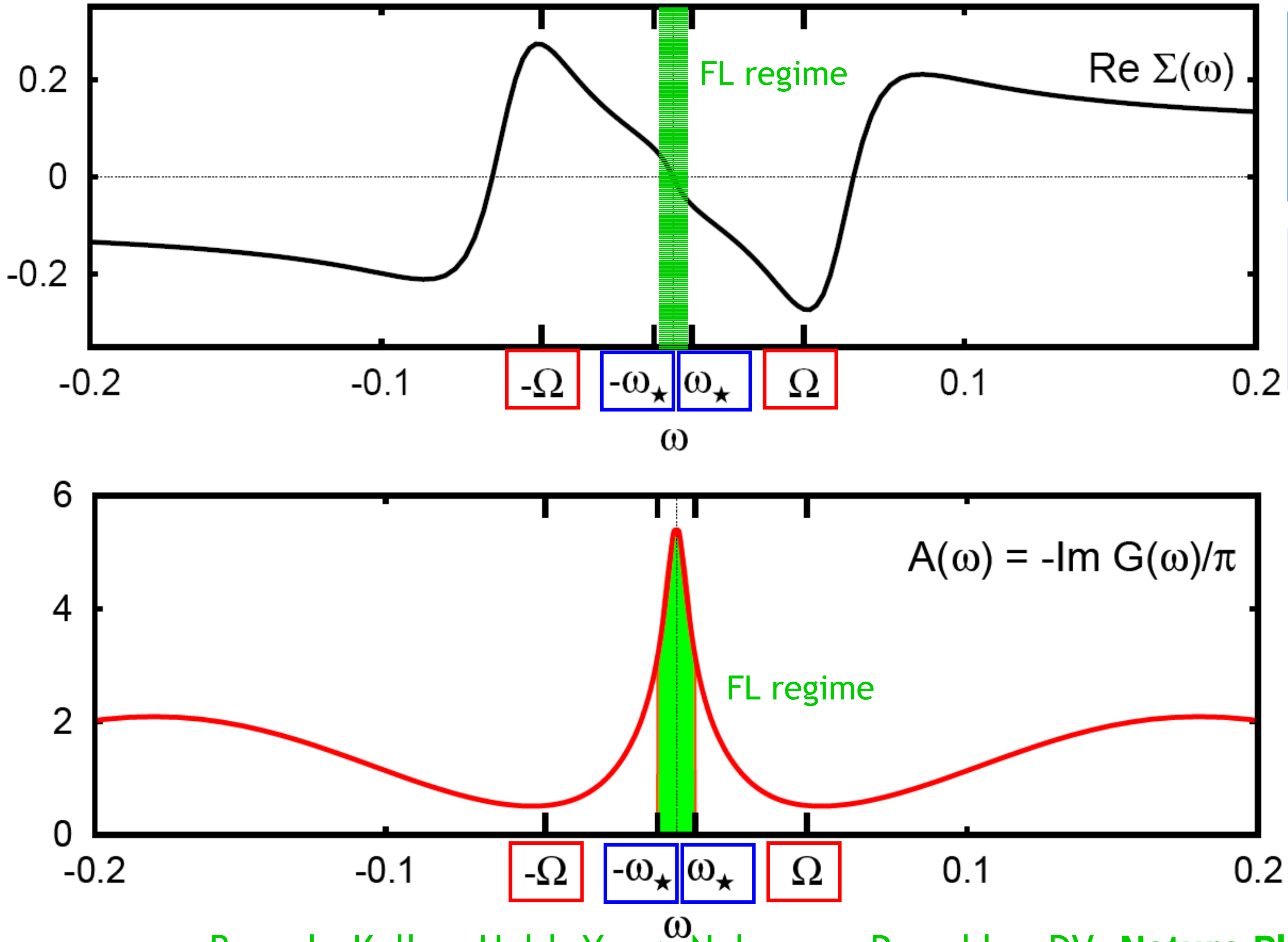
New energy scale ?

Byczuk, Kollar, Held, Yang, Nekrasov, Pruschke, DV; **Nature Phys.** (2007)

$$G(\omega) \xrightarrow{DMFT} \Sigma(\omega) = \underbrace{\left(\omega + \mu - \frac{1}{G(\omega)}\right)}_{\text{linear for } |\omega| \leq \Omega} - \underbrace{\Delta[G(\omega)]}_{\text{linear for } |\omega| \leq \omega_*}$$ hybridization fct.

$\propto G + O(G^2)$

Oudovenko *et al.* (2006)



Fermi liquid regime restricted to $|\omega| \leq \omega_*$

$$\omega_* = (\sqrt{2} - 1)\omega_{max} = (\sqrt{2} - 1) Z_{FL} D_0$$

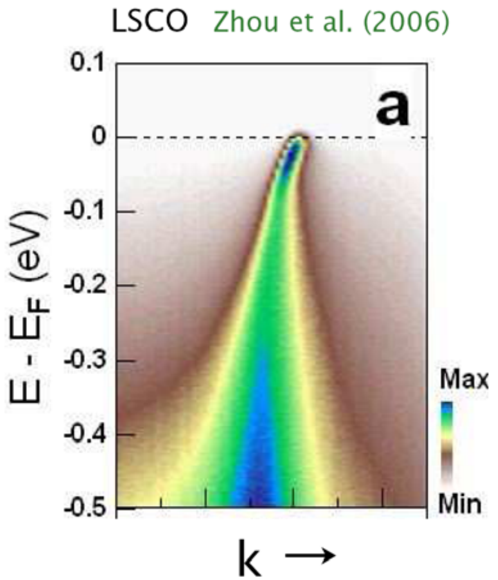
$$\Omega \sim \sqrt{Z_{FL}}$$

Electronic dispersion *outside* Fermi liquid regime?

Byczuk, Kollar, Held, Yang, Nekrasov, Pruschke, DV; **Nature Phys.** (2007)

Electronic dispersion E_k

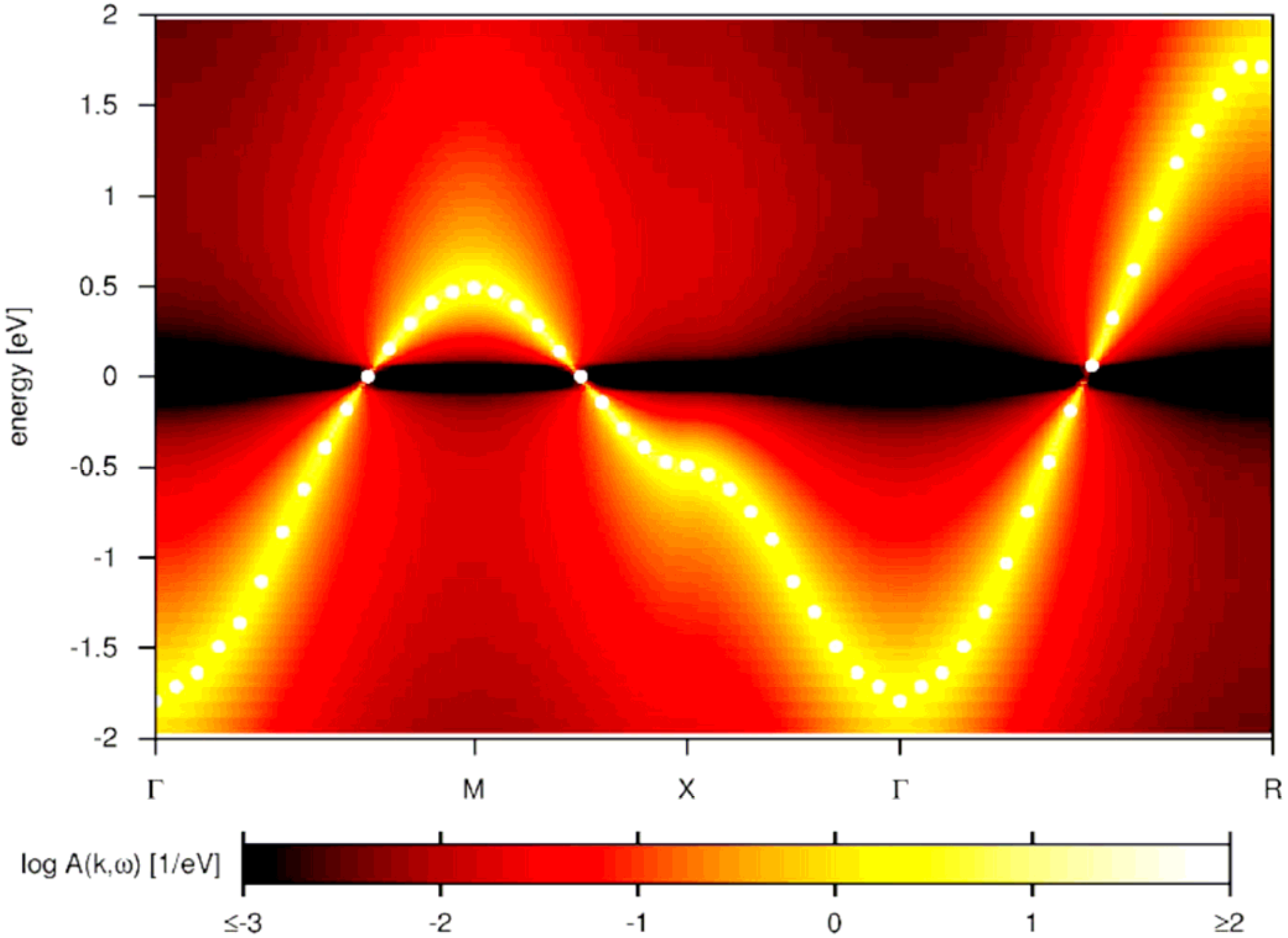
- Dispersion relation: $$E_{\mathbf{k}} = \{\omega | A(\mathbf{k},\omega) = \max\}$$

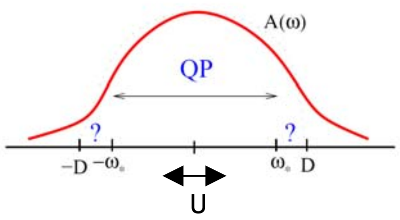


- Integrated spectral function: $A(\omega) = \int d\mathbf{k} A(\mathbf{k},\omega)$

Electronic dispersion E_k: Hubbard model, cubic lattice, DMFT(NRG)

1) Weak correlations: $U=0.29W$, $Z_{FL}=0.8$





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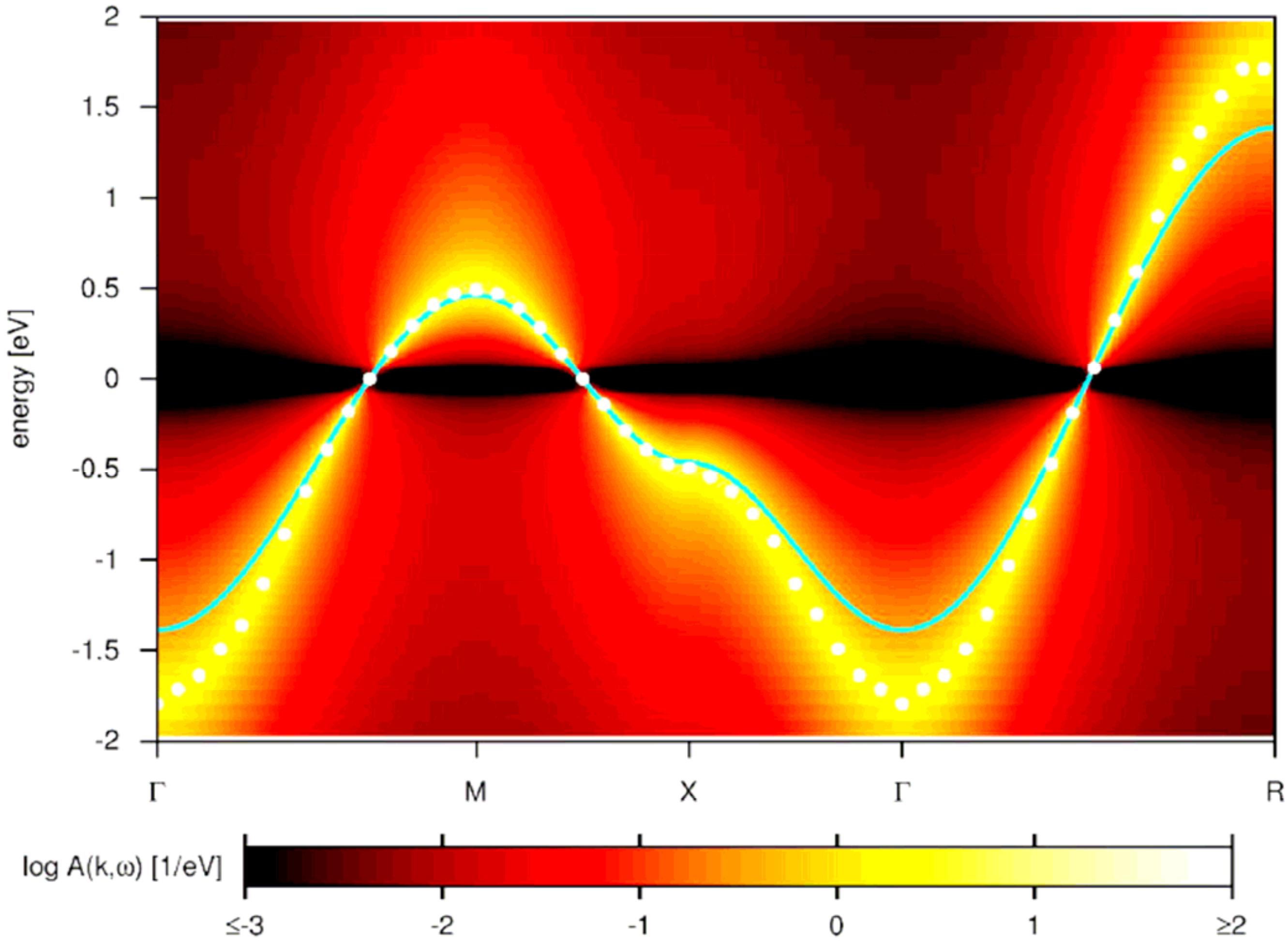
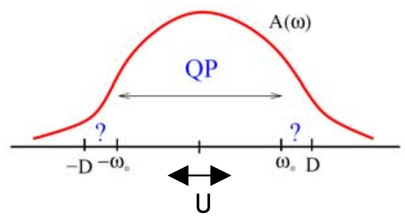


Fermi liquid dispersion

$$E_{\mathbf{k}} = Z_{FL} E_{\mathbf{k}}^0$$



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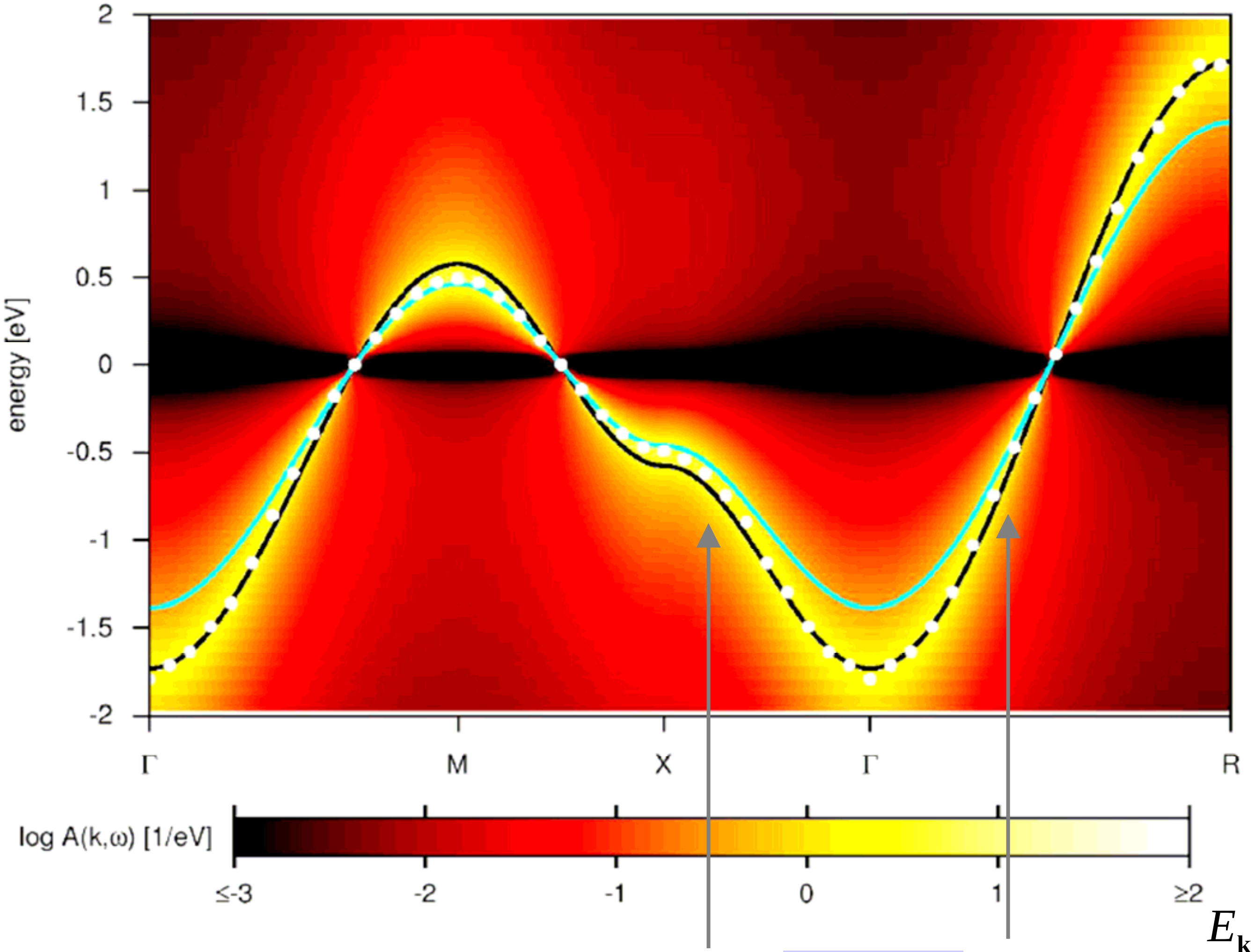


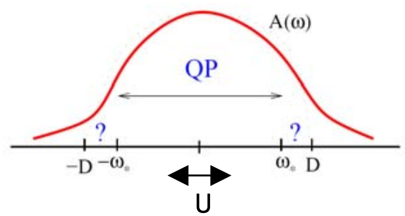
X-over

Fermi liquid dispersion

$$E_{\mathbf{k}} = Z_{FL} E_{\mathbf{k}}^{0}$$

Non-interacting dispersion

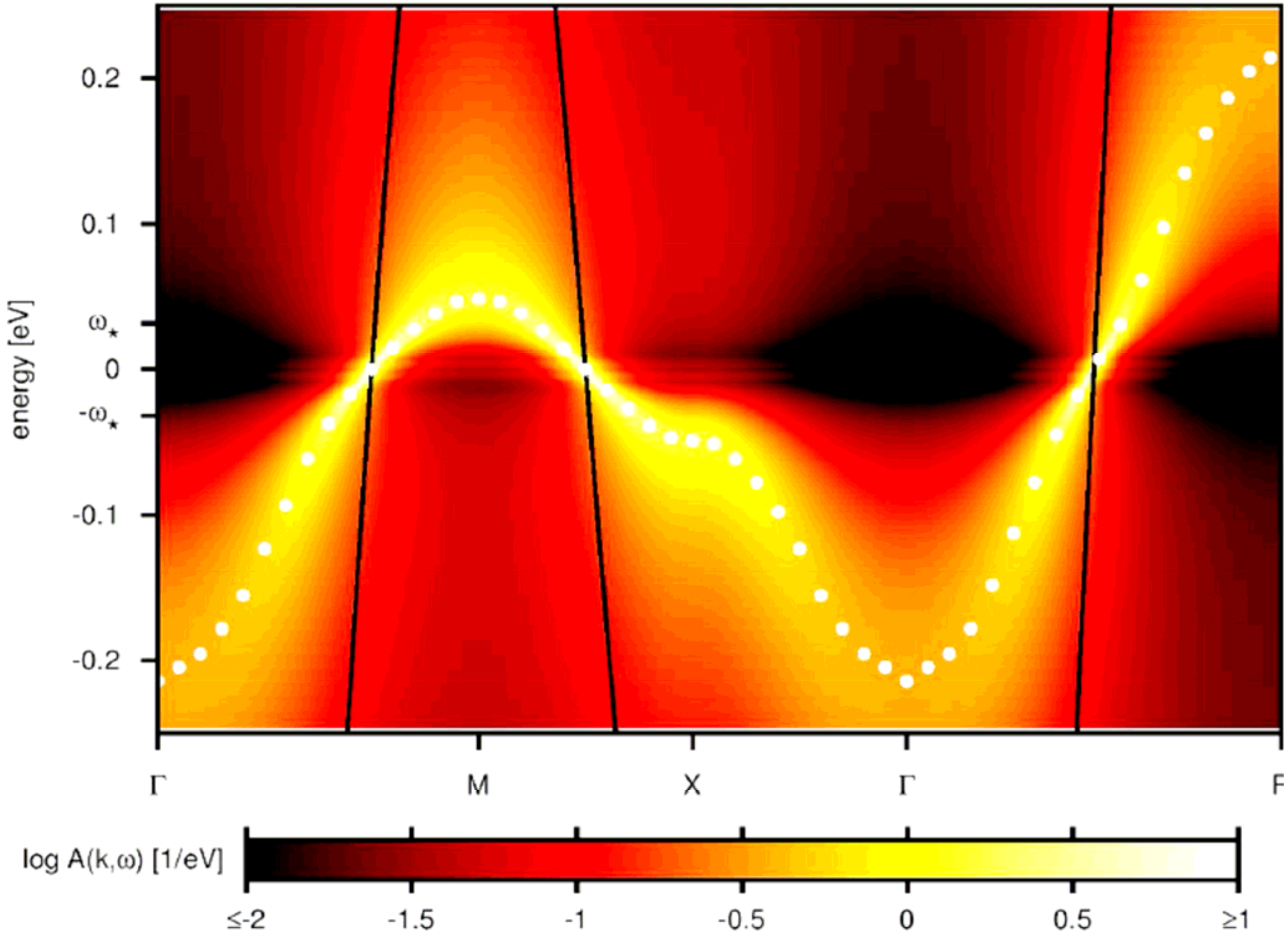
$$E_{\mathbf{k}}^{0}$$



$$E_{\mathbf{k}} = \begin{cases} Z_{FL} E_{\mathbf{k}}^{0}; & \left|E_{\mathbf{k}}\right| \le \omega_{*} \\ E_{\mathbf{k}}^{0}\ ; & \left|E_{\mathbf{k}}\right| \ge \omega_{*} \gg \mathrm{U} \end{cases}$$

Electronic dispersion E_k: Hubbard model, cubic lattice, DMFT(NRG)

1) Strong correlations : $U=0.96W$, $Z_{FL}=0.086$

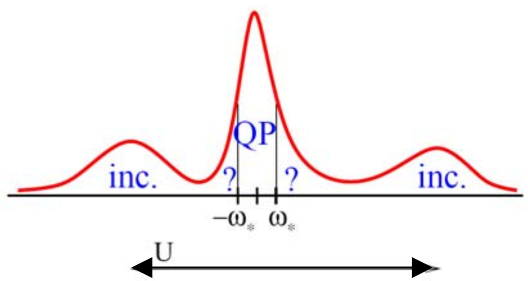


Non-interacting dispersion $E^0_{\mathbf{k}}$

$A(\omega)$: three-peak structure

Z' = weight of central peak > Z_{FL}

= 0.135 (moderately correlated)



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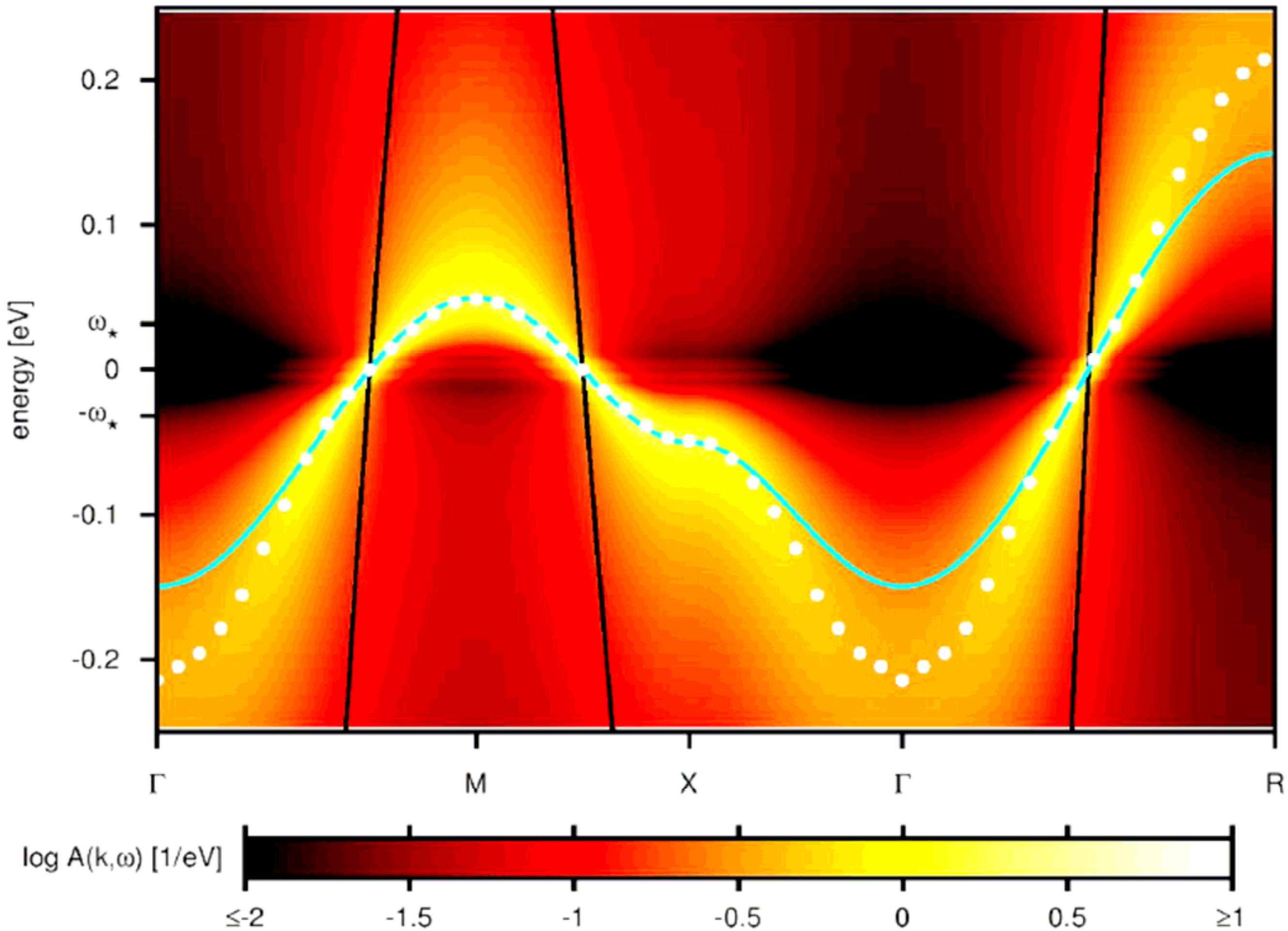
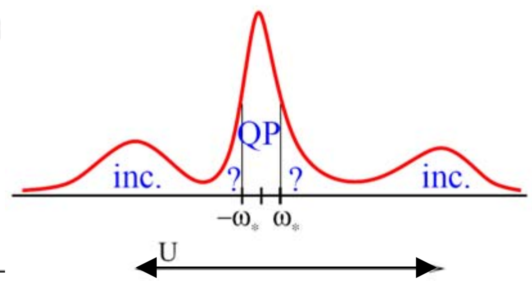


Non-interacting dispersion $E_{\mathbf{k}}^{0}$

Fermi liquid dispersion $E_{\mathbf{k}} = Z_{FL} E_{\mathbf{k}}^{0}$

A(ω): three-peak structure
Z' = weight of central peak > Z_{FL}
= 0.135 (moderately correlated)



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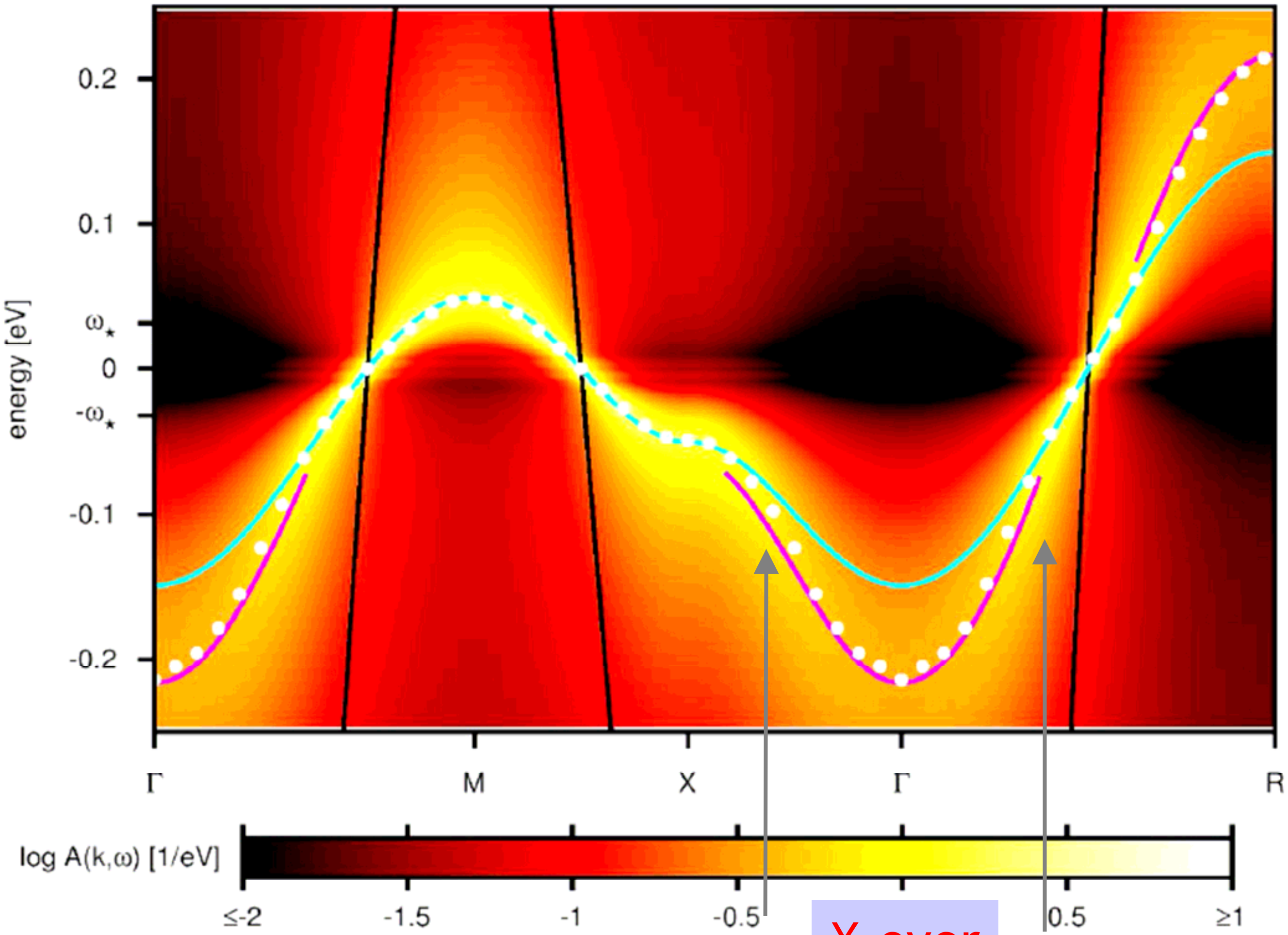


X-over

Non-interacting dispersion
$E^0_{\mathbf{k}}$

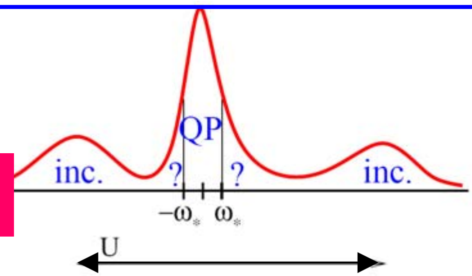
Fermi liquid dispersion
$E_{\mathbf{k}} = Z_{FL} E^0_{\mathbf{k}}$

Dispersion outside
Fermi liquid regime
$E_{\mathbf{k}} = Z' E^0_{\mathbf{k}} + c$

$$E_{\mathbf{k}} = \begin{cases} Z_{FL} E^0_{\mathbf{k}} \; ; \; |E_{\mathbf{k}}| \le \omega_* \\ Z' E^0_{\mathbf{k}} + c \; ; \; |E_{\mathbf{k}}| \ge \omega_* \ll U \end{cases}$$

A(ω): three-peak structure
Z' = weight of central peak > Z_{FL}
= 0.135 (moderately correlated)

Not DMFT specific



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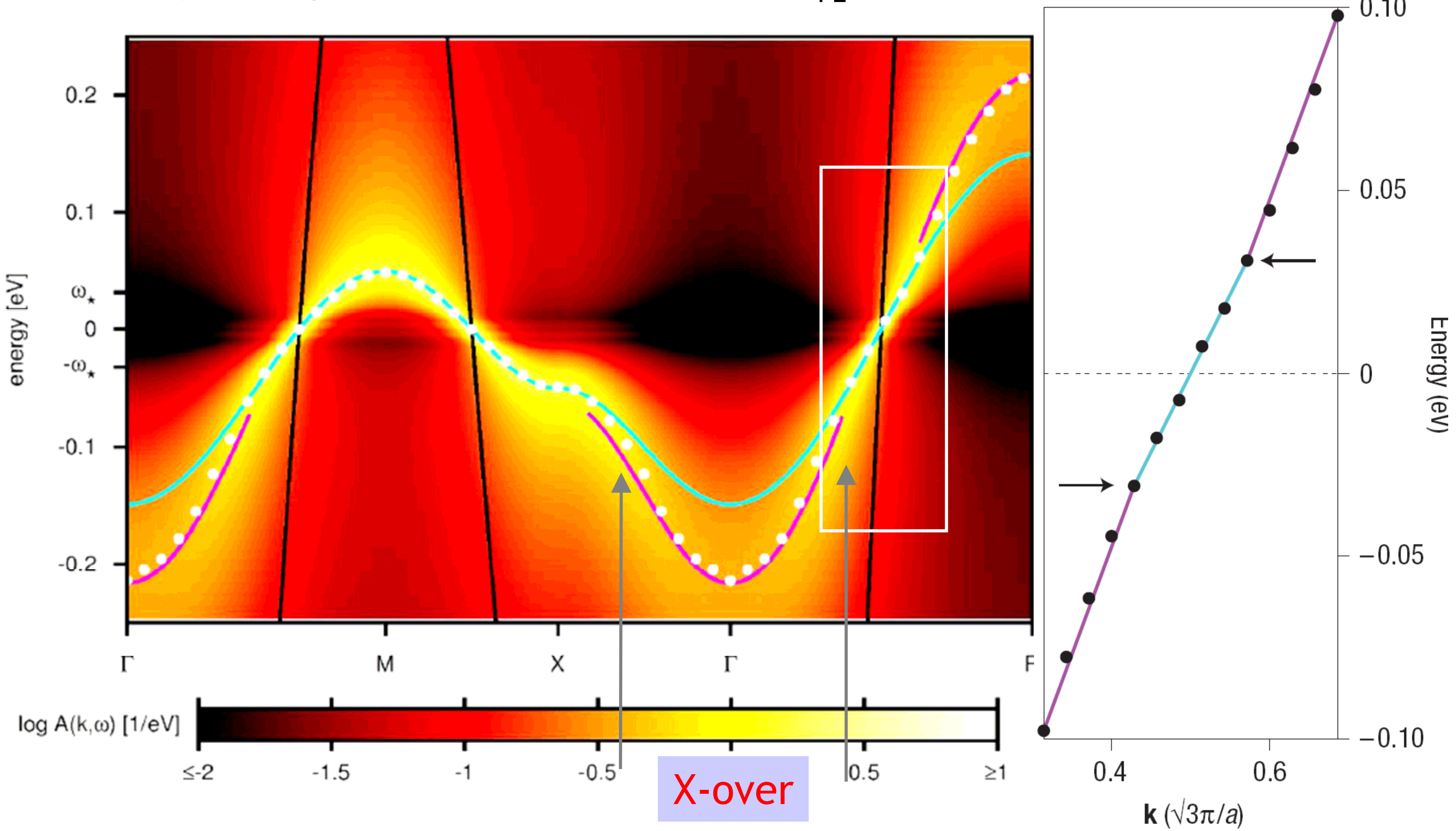


→ Kinks

Characteristics of the kinks

E.g.: p-h symmetric case

- Kink energy:

$$\omega_* = (\sqrt{2} - 1) Z_{FL} \left[\frac{\mathrm{Im}(1/G_0)}{\mathrm{Re}(G_0'/G_0^2)} \right]_{\omega = E_F^0}$$

inside central peak

- Intermediate energy regime:

$$Z' = Z_{FL} \left[\frac{1}{\mathrm{Re}(G_0'/G_0^2)} \right]_{\omega = E_F^0}$$

= weight of central peak in A(ω)

→ change in slope (Z'/Z_{FL}) independent of interaction

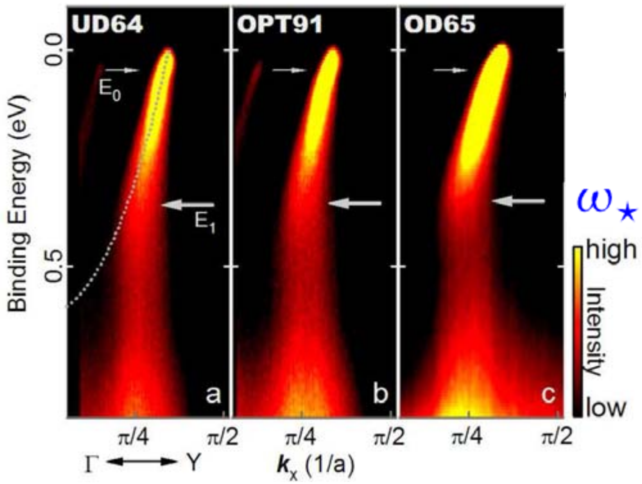
- Curvature at kink: $\mathrm{Im}\,\Sigma''(\omega_*) \propto (Z_{FL})^2$

→ sharpness of kink $\propto (Z_{FL})^{-2}$

→ kinks sharpen with increasing interaction

Waterfalls

"Waterfalls" in the electronic dispersion



Bi2212

$\omega_\star \approx$ 300-400 meV

Graf *et al.* (2006)
Graf, Gweon, Lanzara (2006)

Wang, Tan, Wan (2006) X-over from QP to LHB [t-J model, slave bosons]

Macridin, Jarrell, Maier, Scalapino (2007)

Coupling of quasiparticles to spin fluctuations [DCA]

Zhu, Aji, Shekhter, Varma (2007)

Quantum-critical fluctuations of loop-current phase; cut-off ω_c

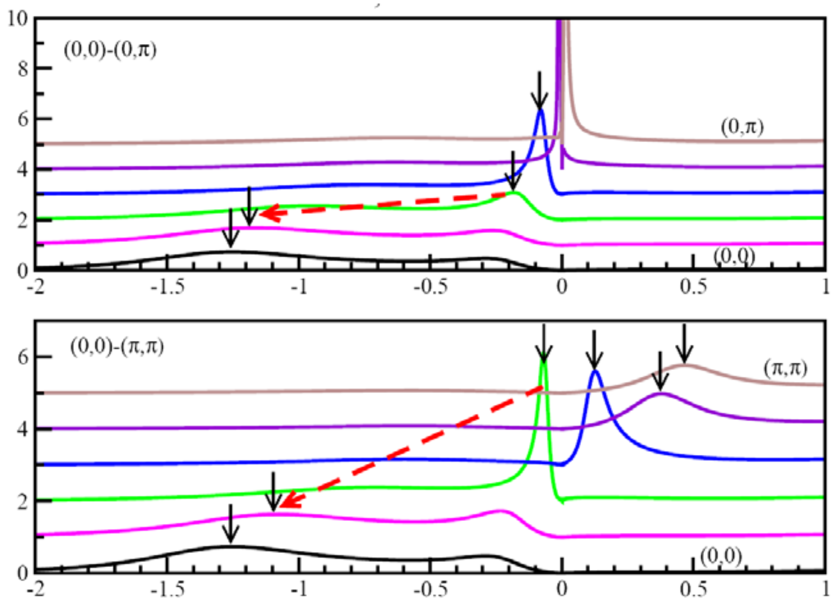
Kordyuk *et al.* (2007), Inosov *et al.* (2007)

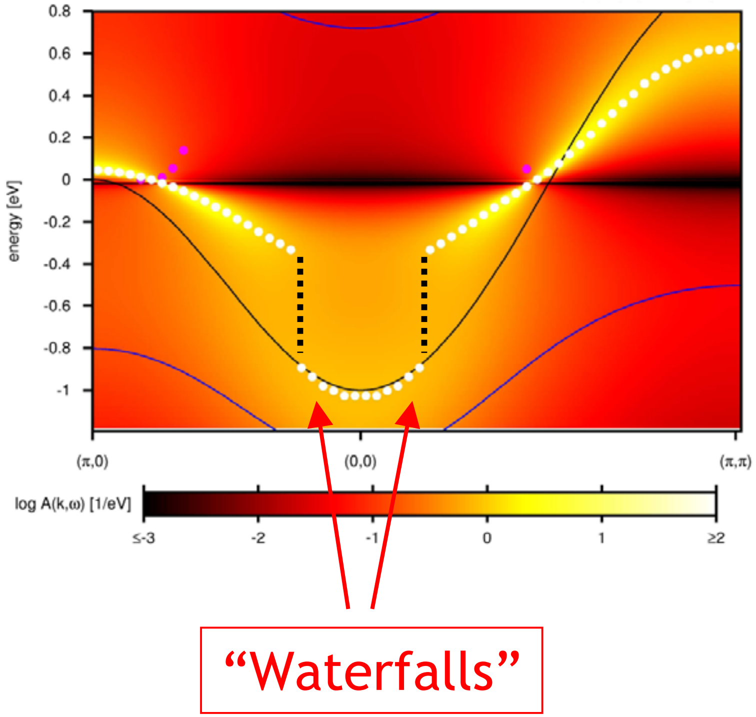
Matrix element effects important

Electronic dispersion E_k: Hubbard model, square lattice, DMFT(NRG)

U=8t, n=0.79

Byczuk, Kollar (2007, unpublished)

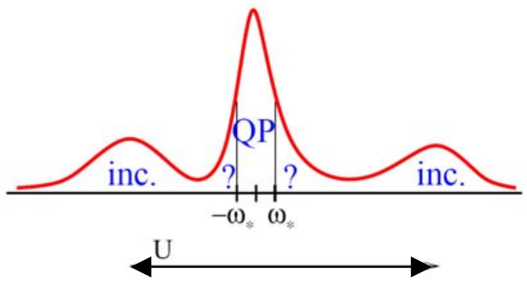




Dispersion jumps from central peak to lower Hubbard band

see also Held, Yang (2007, unpublished)

Conclusions



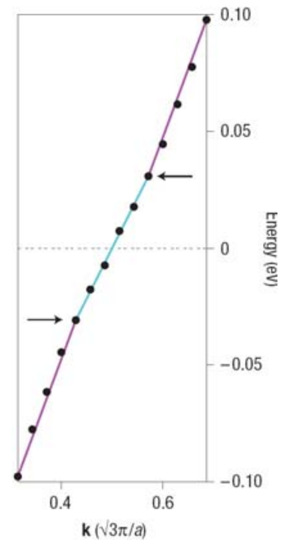
$$E_{\mathbf{k}} = \begin{cases} Z_{FL} E_{\mathbf{k}}^0 \; ; & |E_{\mathbf{k}}| \le \omega_* \\ Z' E_{\mathbf{k}}^0 + c \; ; & |E_{\mathbf{k}}| \ge \omega_* \ll U \end{cases}$$

1. Kinks in the electronic dispersion

- Purely electronic mechanism
- Generic for strong correlations
- 3-peak spectral function A(ω) sufficient
- New energy scale

  $\omega_* = Z_{FL}$ x (bare energy scale)

  inside central peak
- FL regime terminates at ω_*
- Intermediate energy scale with $Z' > Z_{FL}$
- Robust mechanism based on local physics
- Valid beyond DMFT
- Does not rule out other kinks



2. Waterfalls in the electronic dispersion

- Dispersion jumps from central peak to LHB