Center for
Electronic Correlations and Magnetism
University of Augsburg

Theory of correlated fermionic condensed matter

3. Correlation-induced phenomena in electronic systems

a. Kinks in the electronic dispersion

XIV. Training Course in the Physics of Strongly Correlated Systems
Salerno, October 7, 2009

Dieter Vollhardt

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Outline

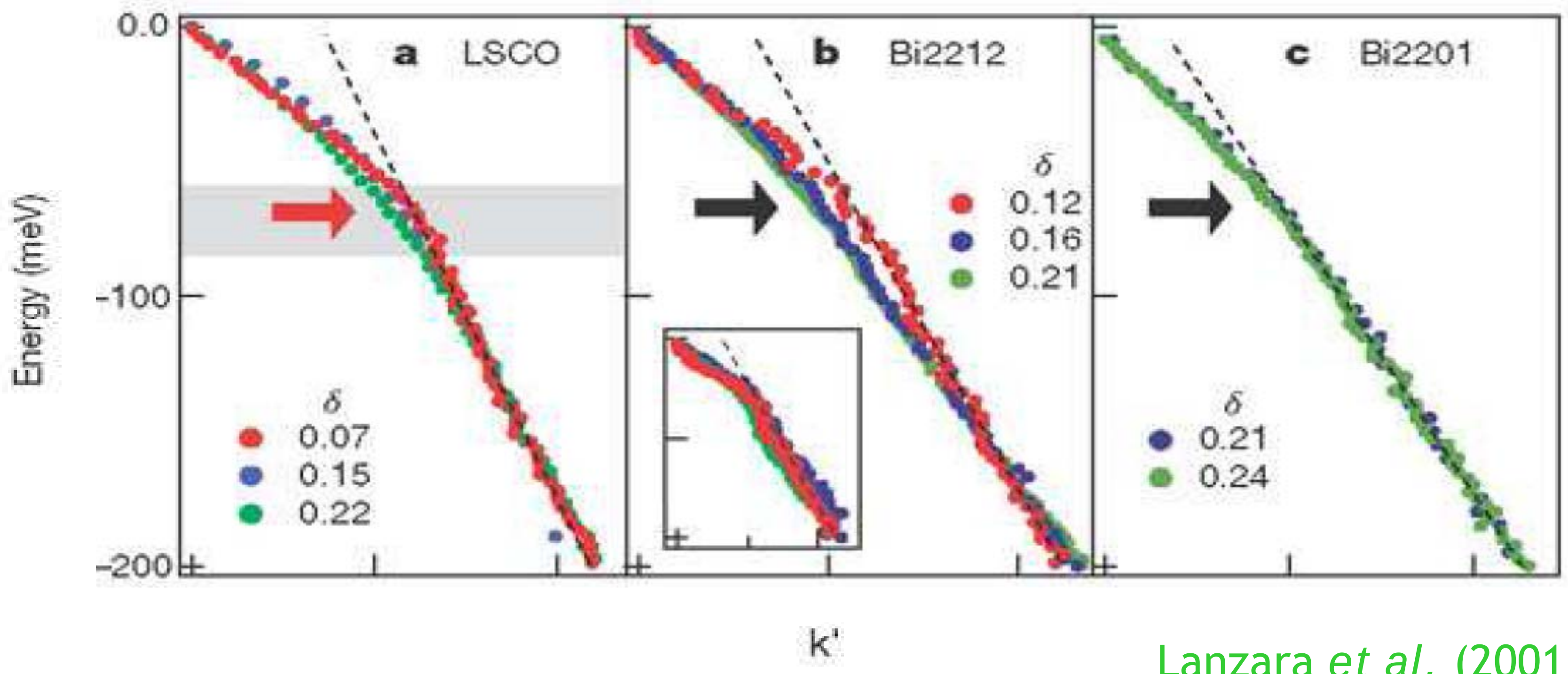
Robust electronic correlation mechanism leading to

- kinks
- waterfalls

in the electronic dispersion

Kinks in high-T_c cuprates

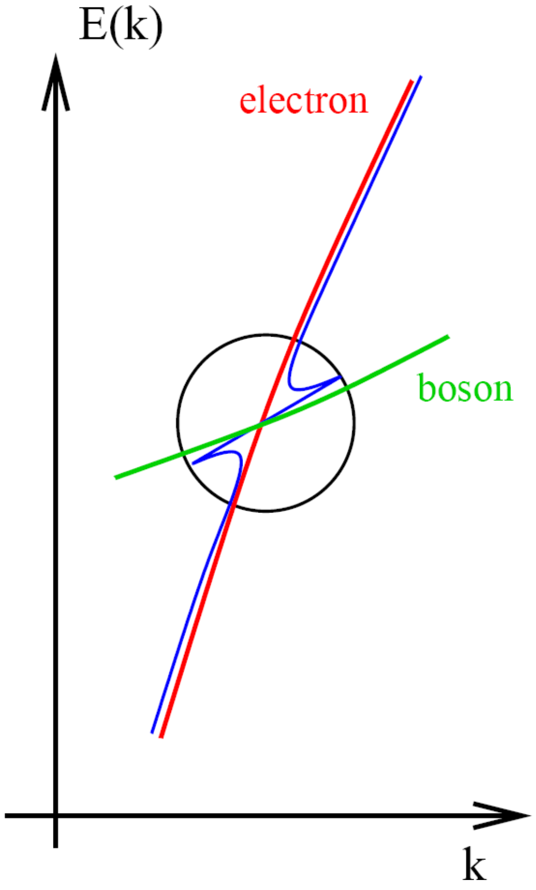
Valla *et al.* (1999)
Bogdanov et al. (2000)



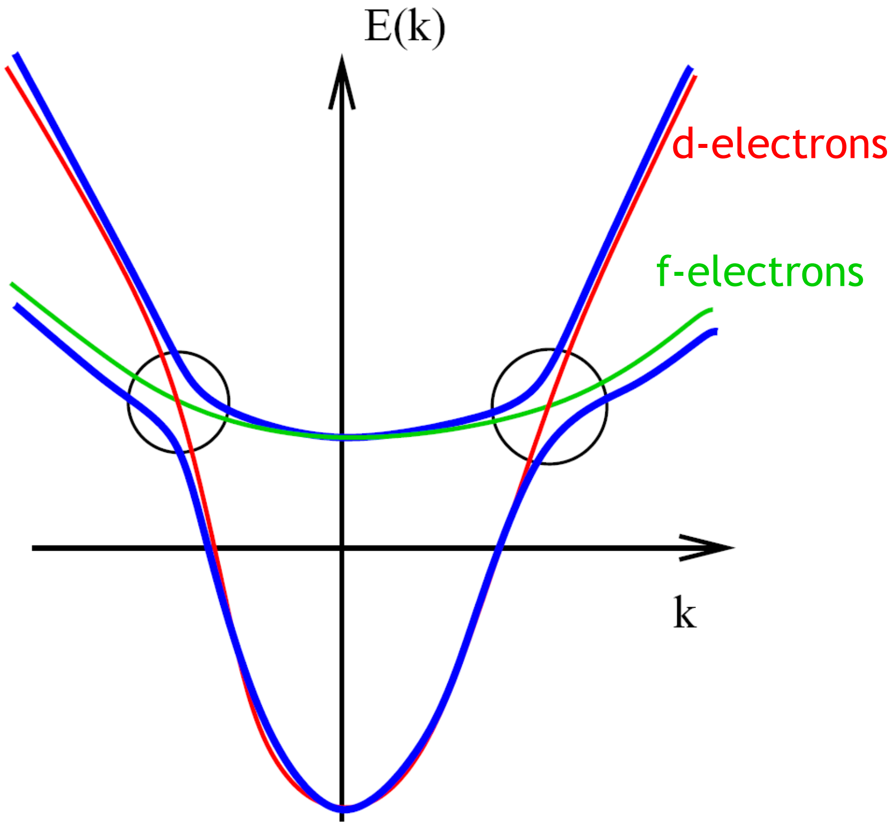
Lanzara *et al.* (2001)

- Kinks at $\omega_* \approx$ 40-70 meV
- Due to coupling of electrons to phonons !?

Known origin of kinks in solid-state physics

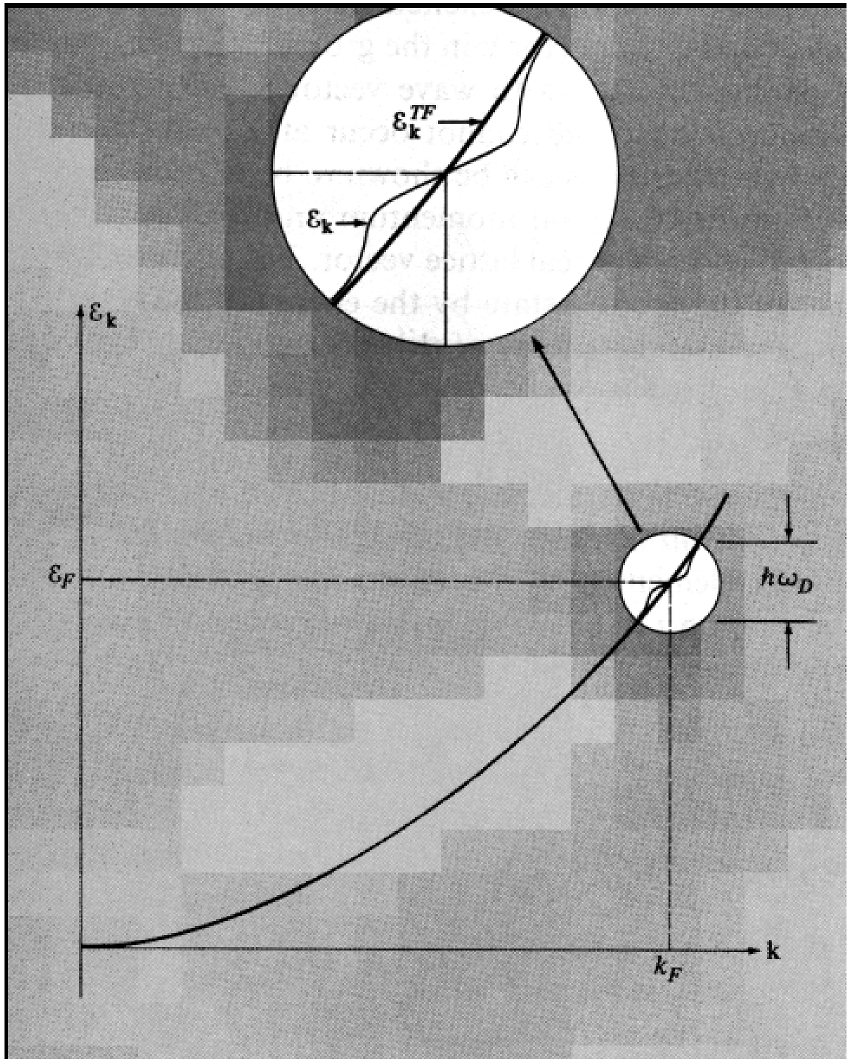


Kinks due to
electron-phonon (boson) coupling



Kinks due to
electron-electron hybridization

Kinks in conventional superconductivity

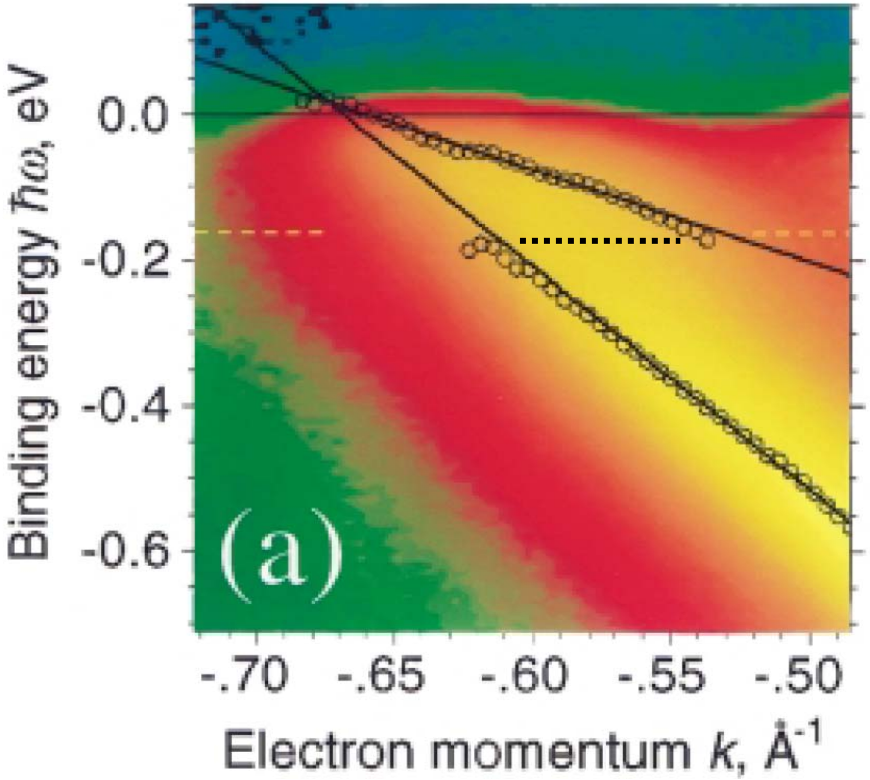


Electron-phonon correction of electronic dispersion

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

Kinks: Metal surfaces

Tungsten



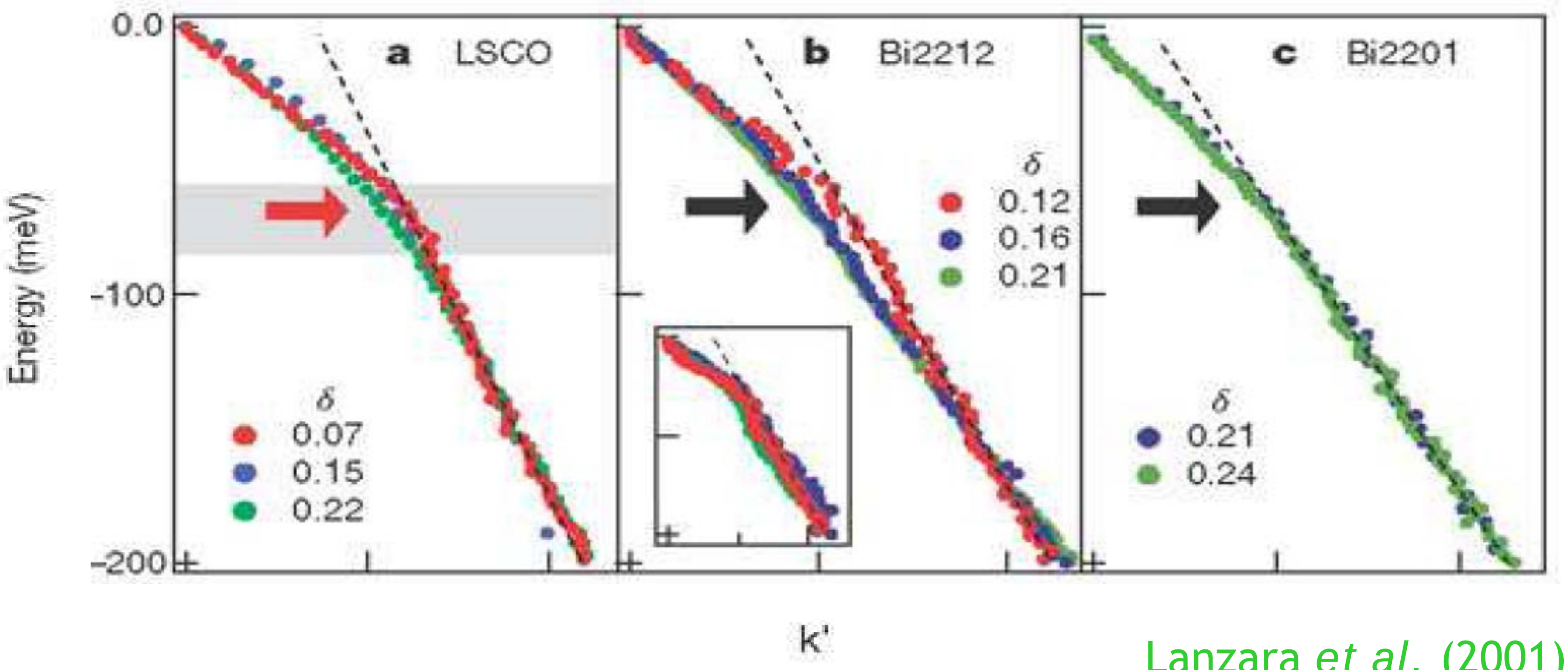
$\omega_* = 160$ meV:
Stiff surface phonon

Rotenberg *et al.* (2000)

Kink due to electron-phonon coupling

Kinks in high-T_c cuprates

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



Lanzara *et al.* (2001)

- Kinks at $\omega_* \approx$ 40-70 meV
- Due to 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)

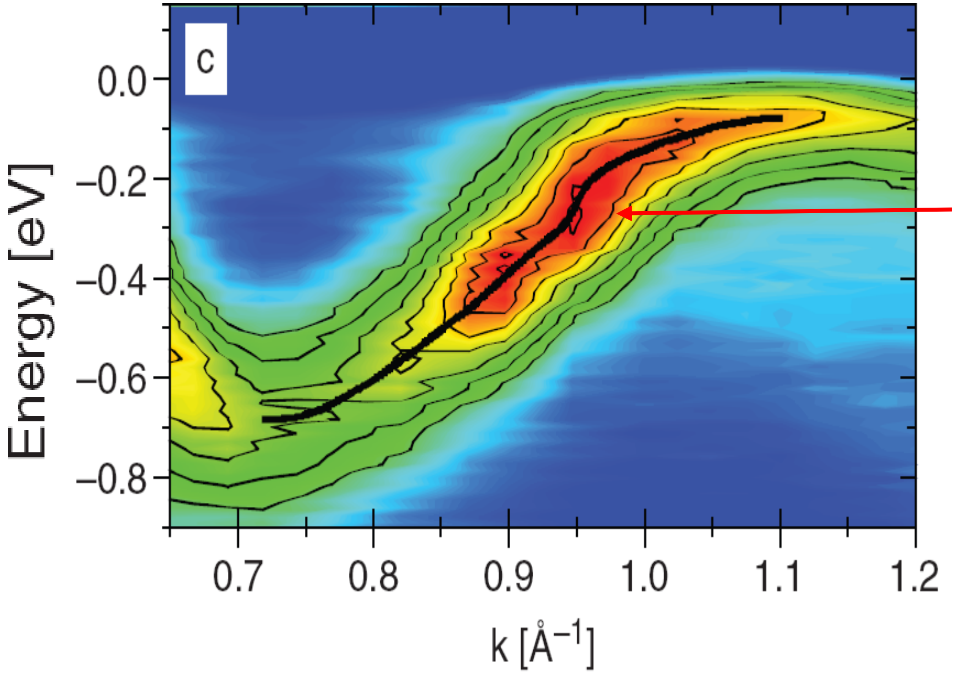
  Coupling of quasiparticles to short-range magnetic fluctuations

  [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



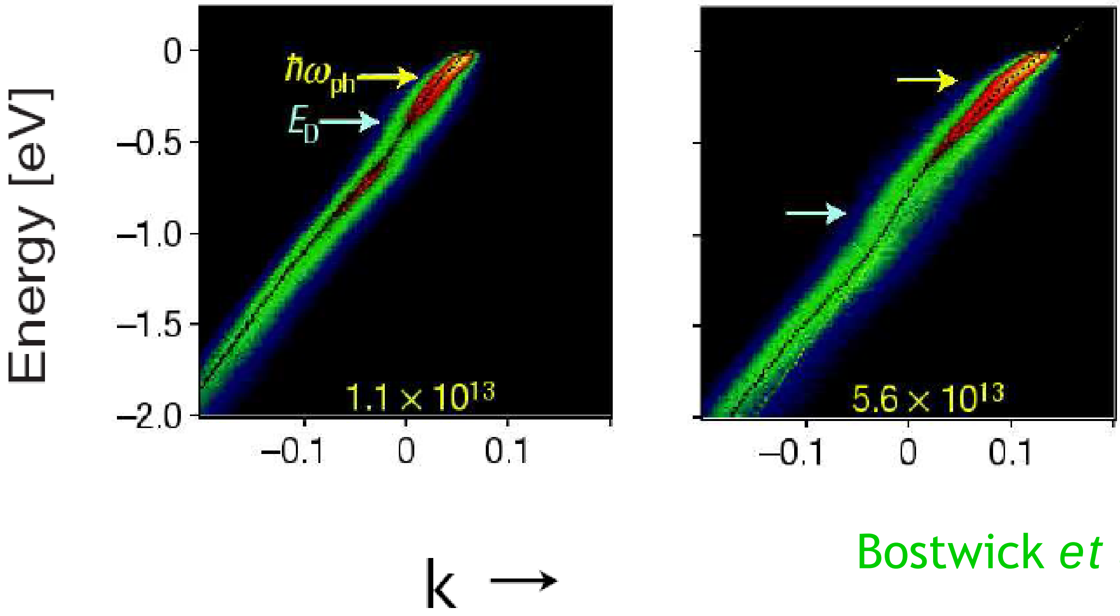
300meV: too high
for phonons or
spin fluctuations

Menzel *et al.* (2005)

Kinks due to coupling of electrons to what?

Kinks: Graphene

Doping by potassium adsorption



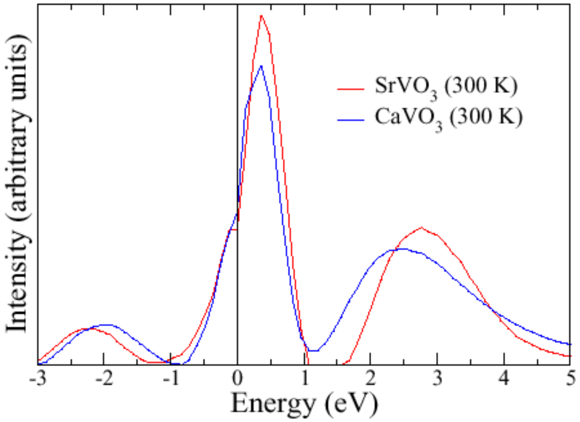
Bostwick *et al.* (2007)

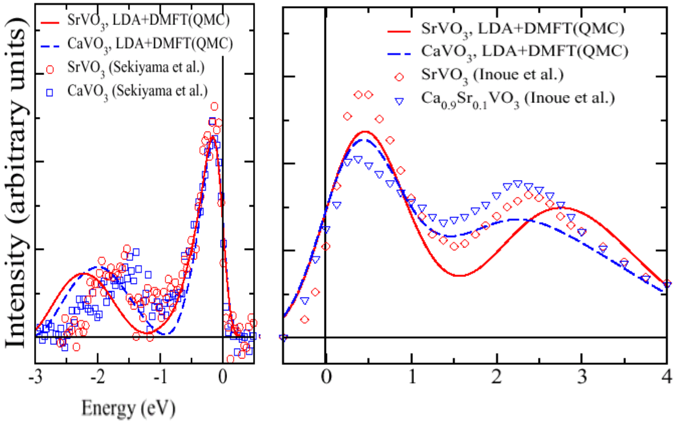
- "Low energy" kinks at 200 meV
- "High energy" kinks at 400-900 meV (near X-ing of Dirac branches, E_D)
- coupling of electrons to plasmons ?

Robust electronic correlation mechanism for kinks

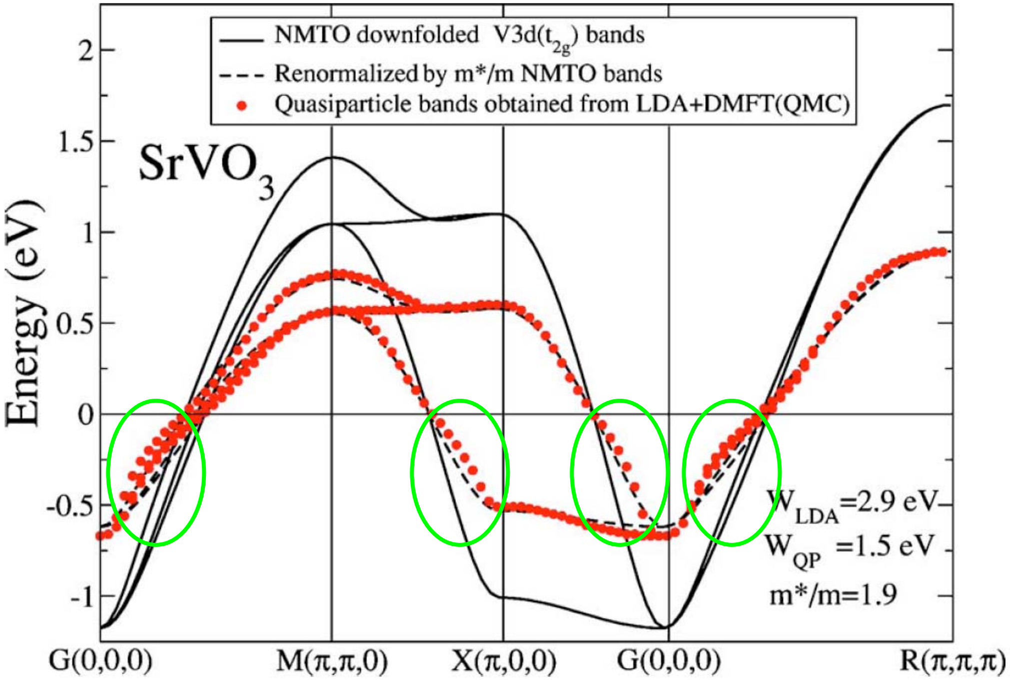
Purely electronic mechanism for kinks: Strong correlations

$SrVO_3$ and $CaVO_3$





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

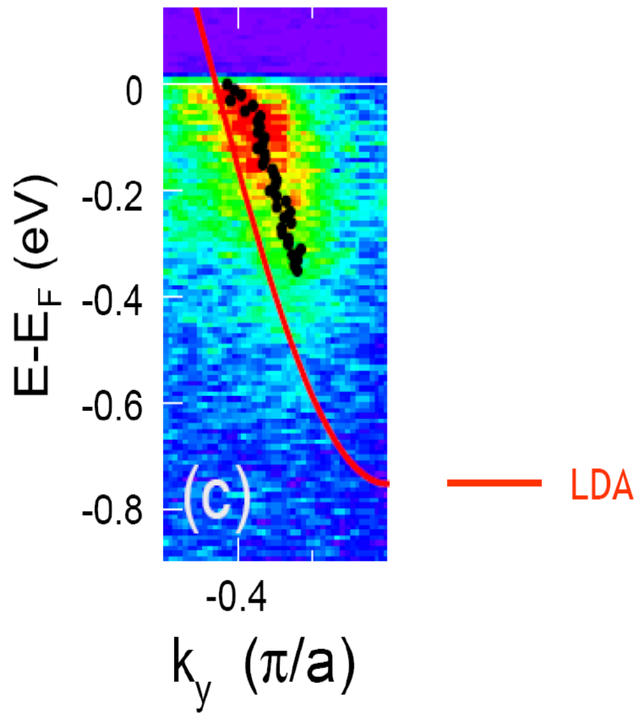


Ekaterinburg – Augsburg – Stuttgart collaboration,
Nekrasov *et al.* (2004, 2006)

Renormalization of LDA-bands by self-energy

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

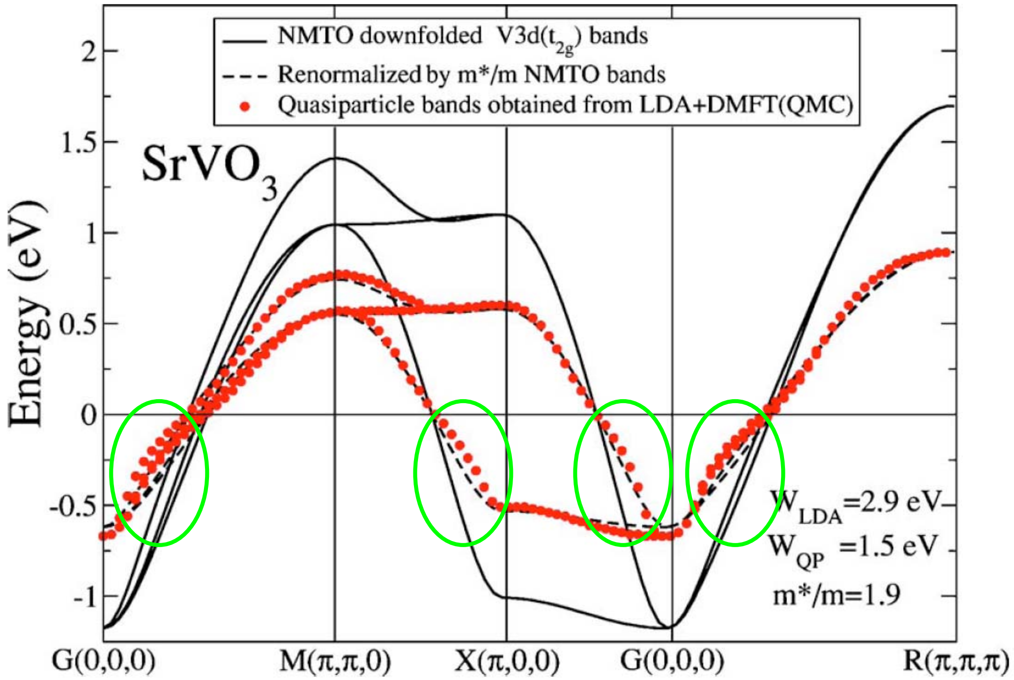
Purely electronic mechanism for kinks: Strong correlations



Yoshida *et al.* (2005)

Kinks at $\omega_* \approx$ 100 meV

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

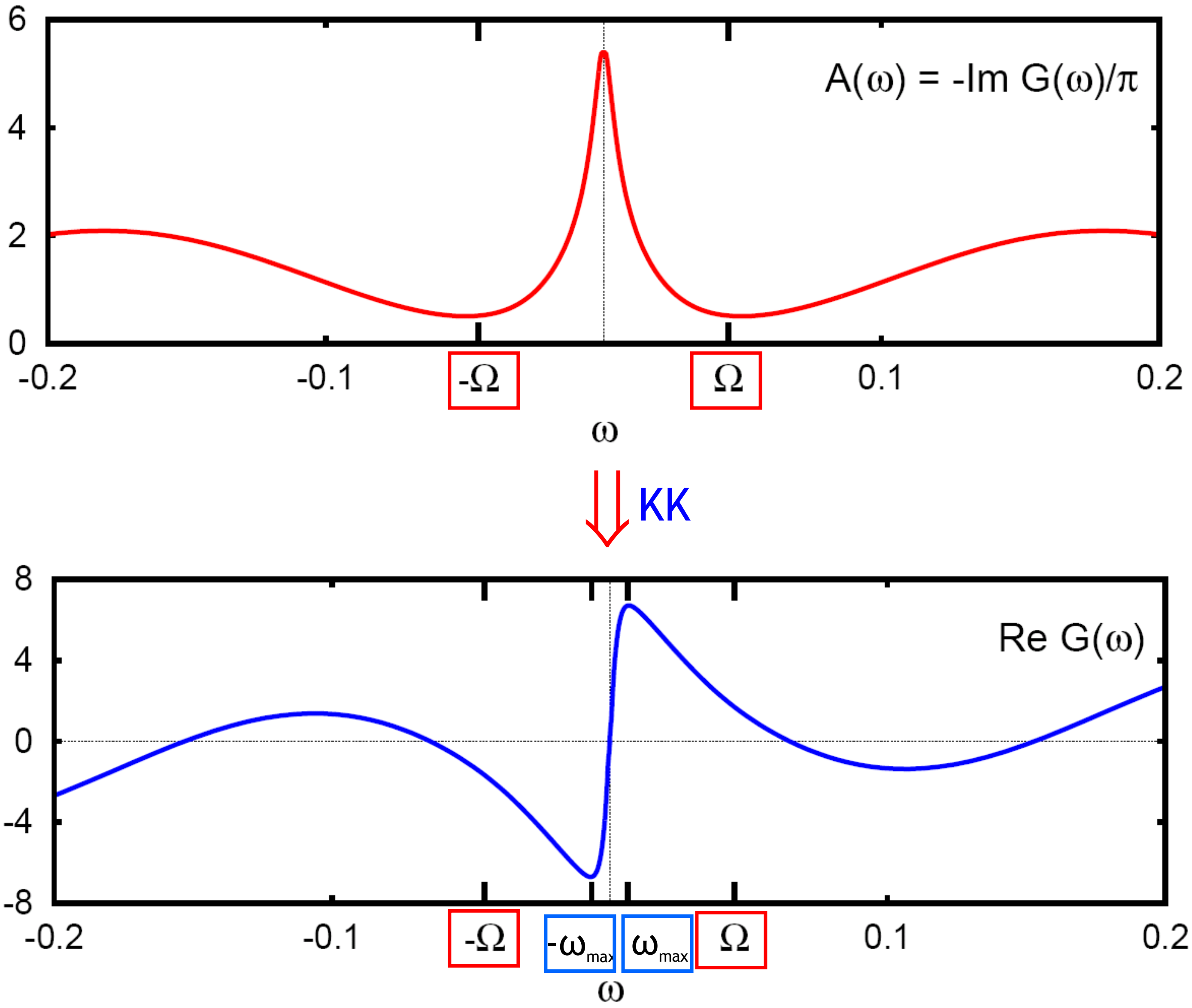


Ekaterinburg – Augsburg – Stuttgart collaboration,
Nekrasov *et al.* (2004, 2006)

Renormalization of LDA-bands by self-energy

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

Strongly correlated paramagnetic metal



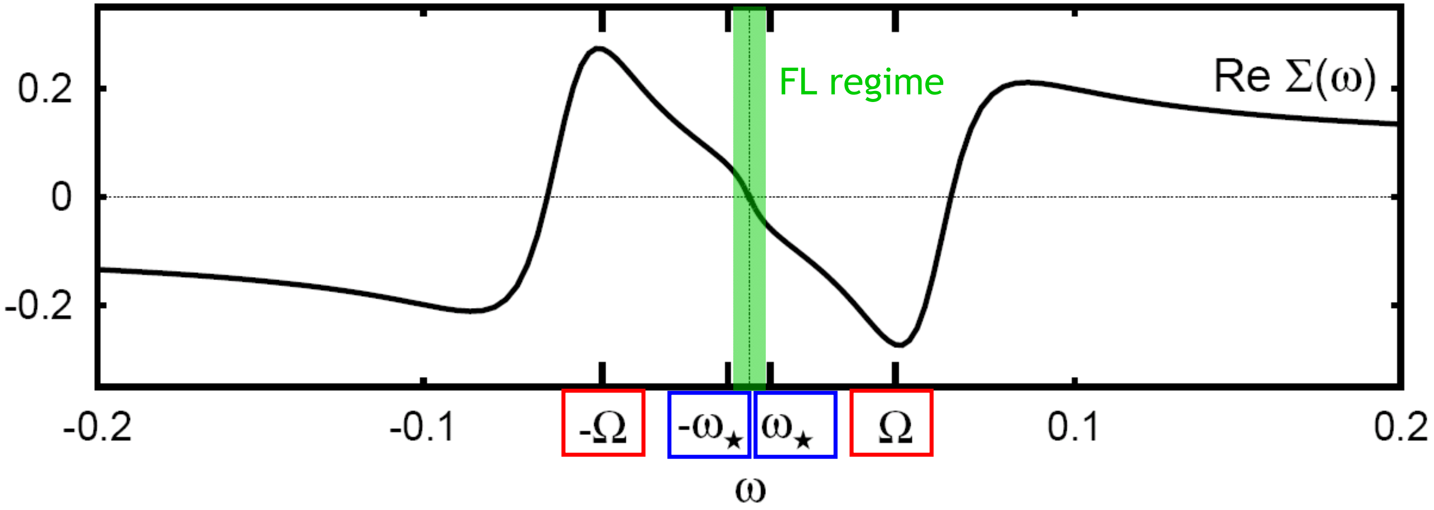
New energy scale ?

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

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

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

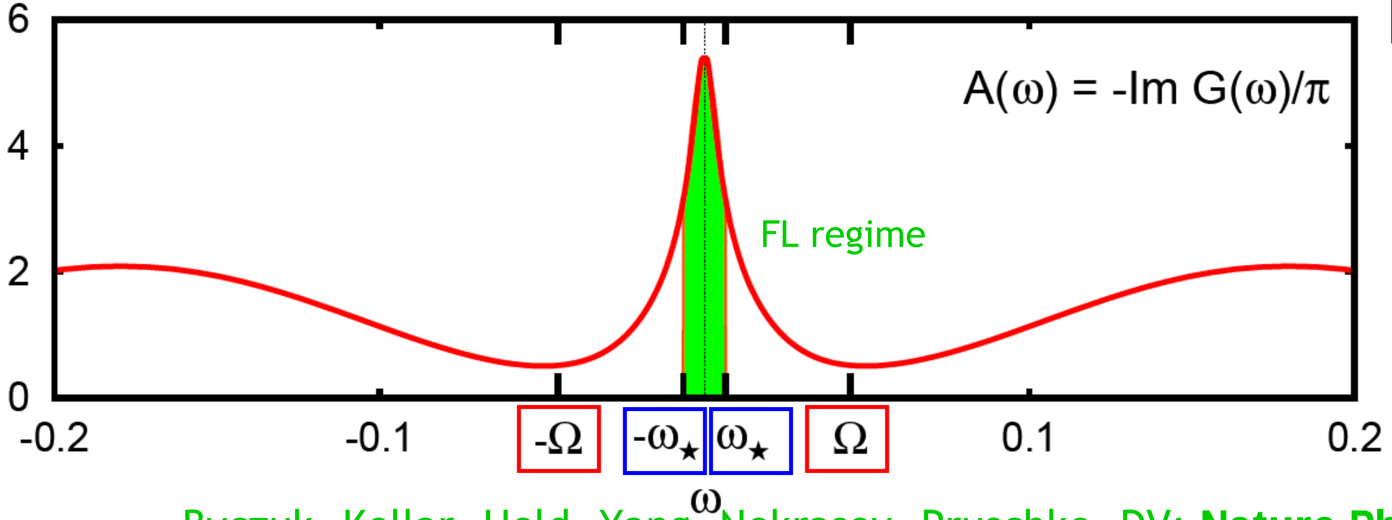
Oudovenko *et al.* (2006)



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

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

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

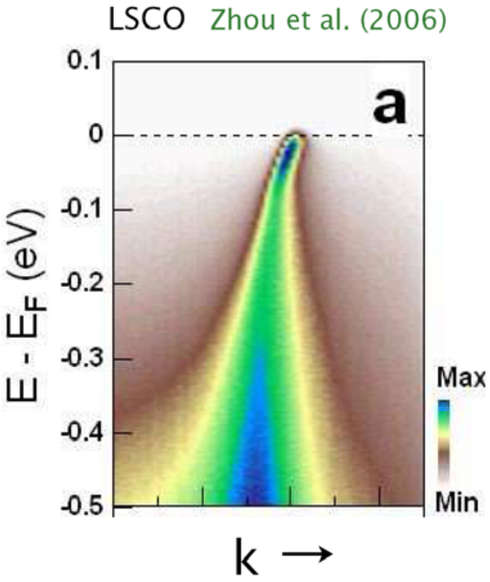


Electronic dispersion *outside* Fermi liquid regime?

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

Electronic dispersion E_k

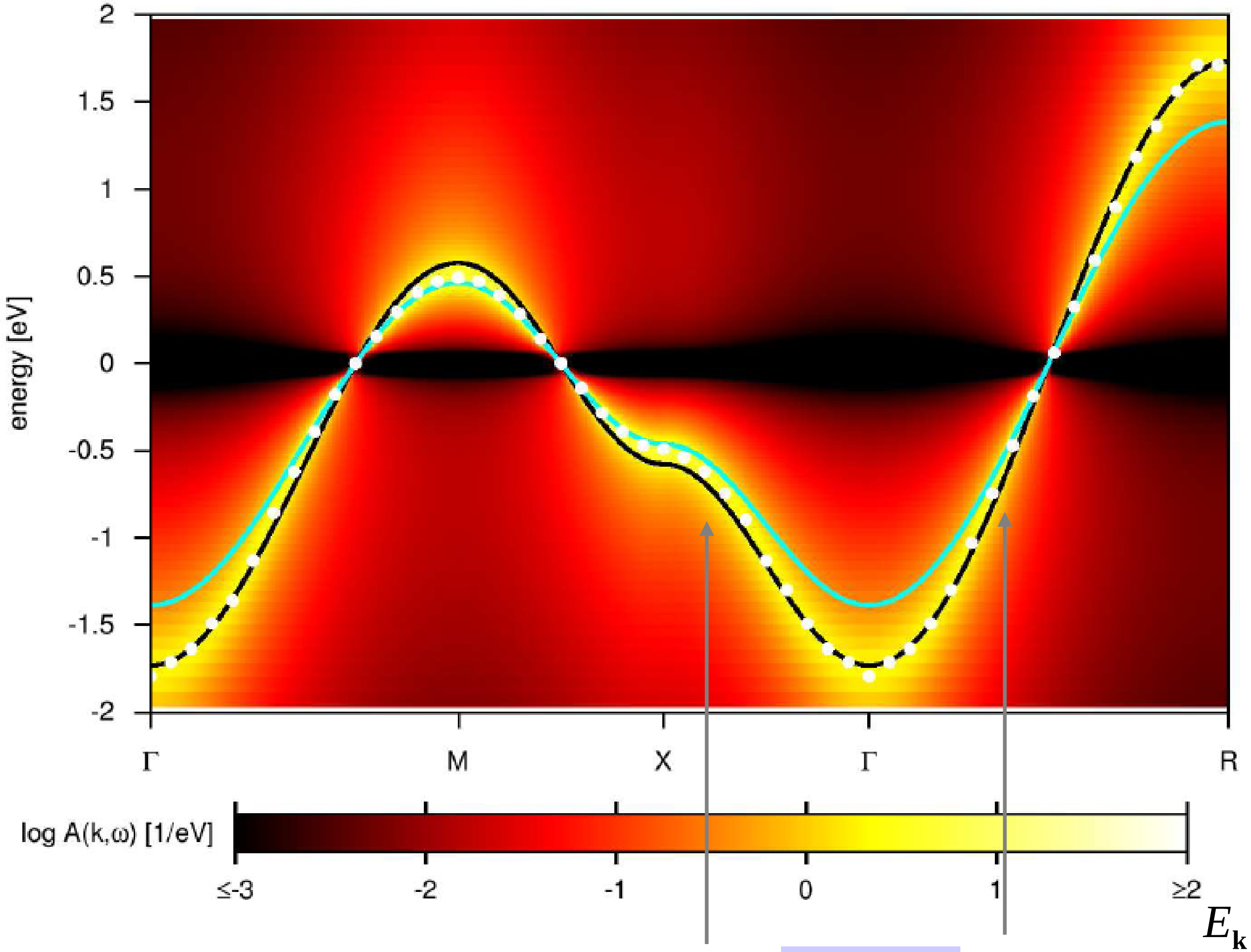
- Dispersion relation: $E_{\mathbf{k}} = \{\omega | A(\mathbf{k},\omega) = \max\}$



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

Electronic dispersion $E_{\mathbf{k}}$: Hubbard model, cubic lattice, DMFT(NRG)

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



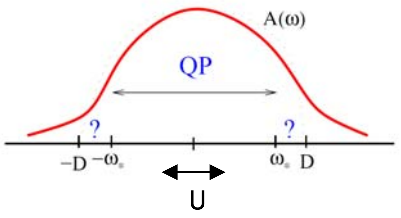
X-over

Fermi liquid dispersion

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

Non-interacting dispersion

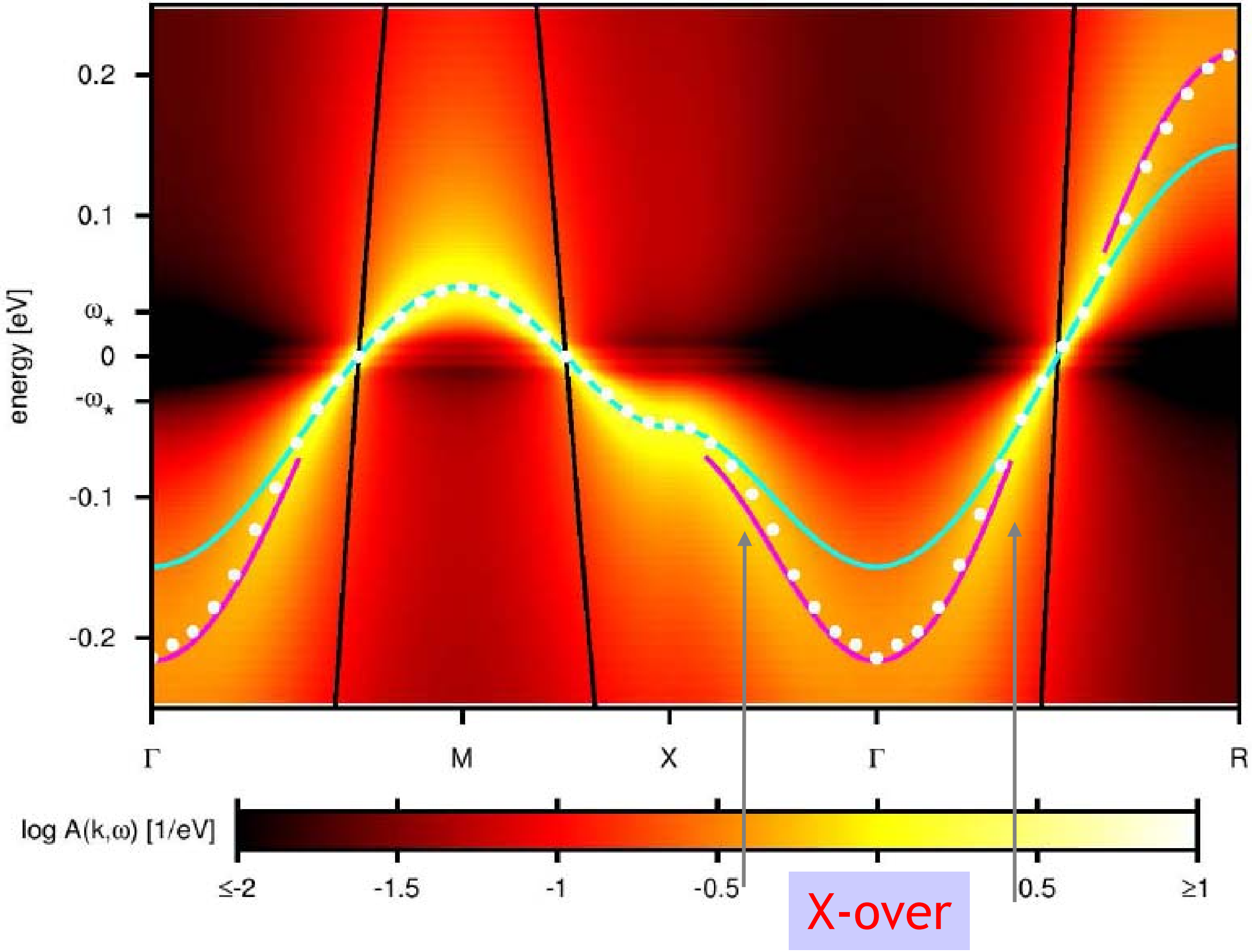
$E_{\mathbf{k}}^0$



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

Electronic dispersion $E_\mathbf{k}$: Hubbard model, cubic lattice, DMFT(NRG)

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



Non-interacting dispersion

$E^0_\mathbf{k}$

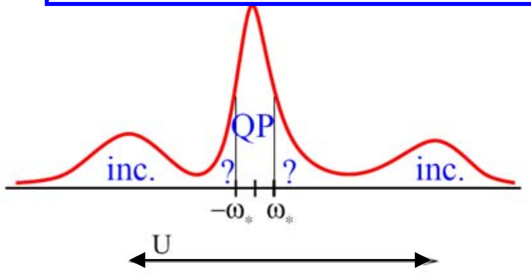
Fermi liquid dispersion

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

Dispersion outside Fermi liquid regime

$E_\mathbf{k} = Z' E^0_\mathbf{k} + c$

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



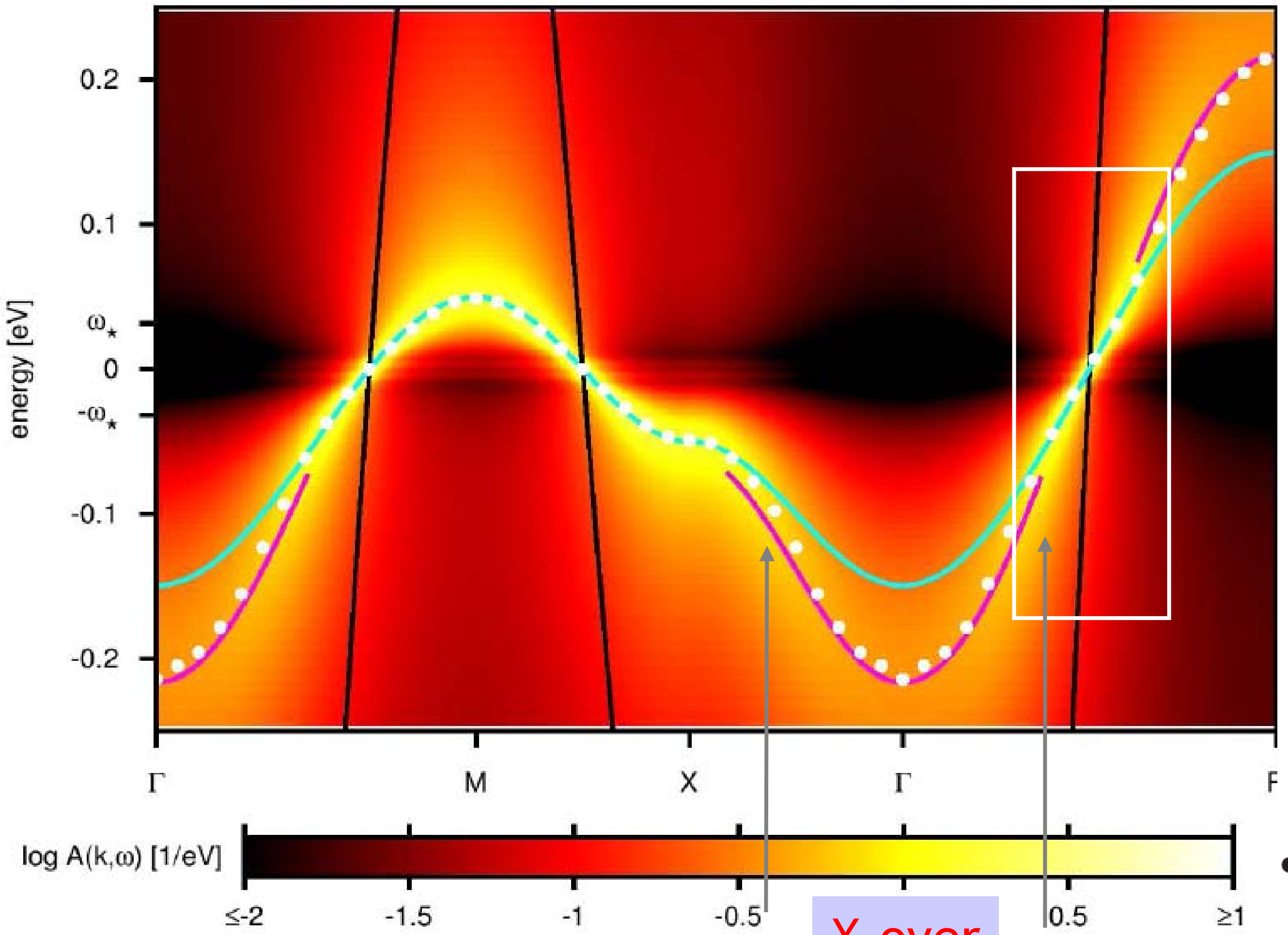
A(ω): three-peak structure

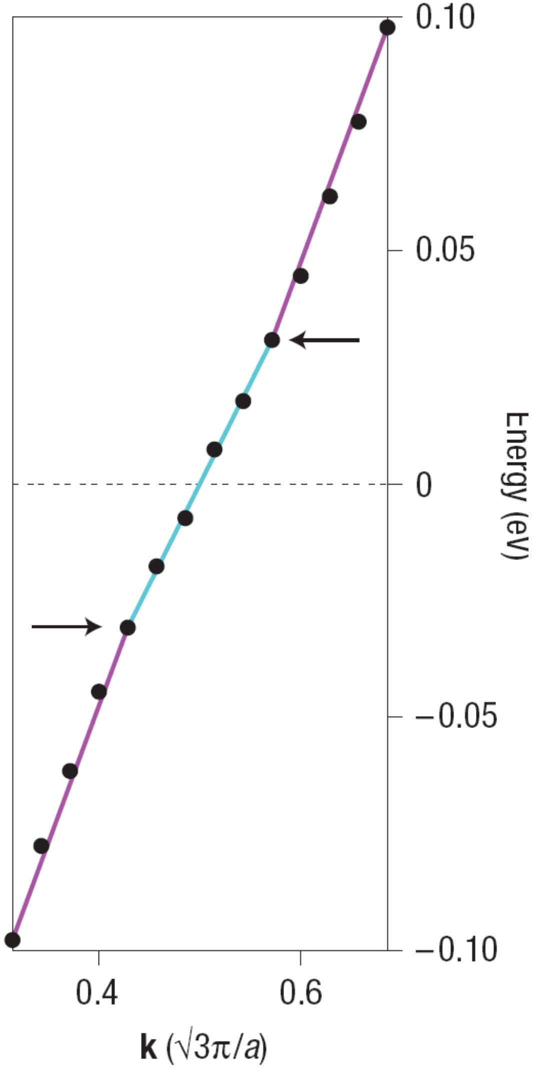
Z' = weight of central peak > Z_{FL}

= 0.135 (moderately correlated)

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

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





X-over

→ 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)

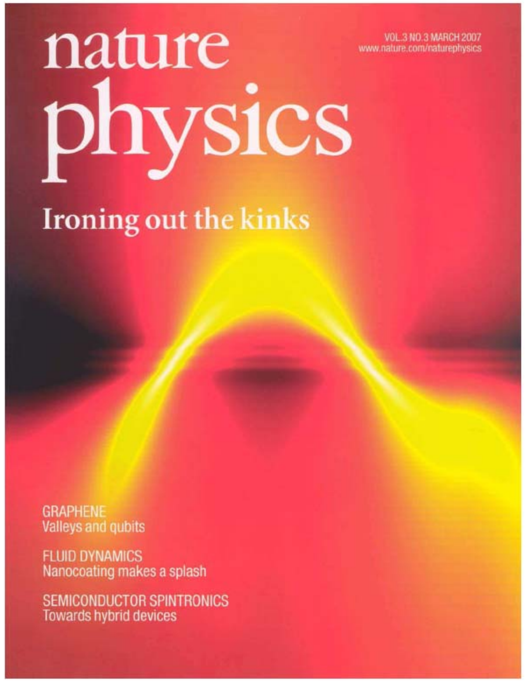
→ change in slope (Z'/Z_{FL}) independent of interaction

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

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

→ kinks sharpen with increasing interaction

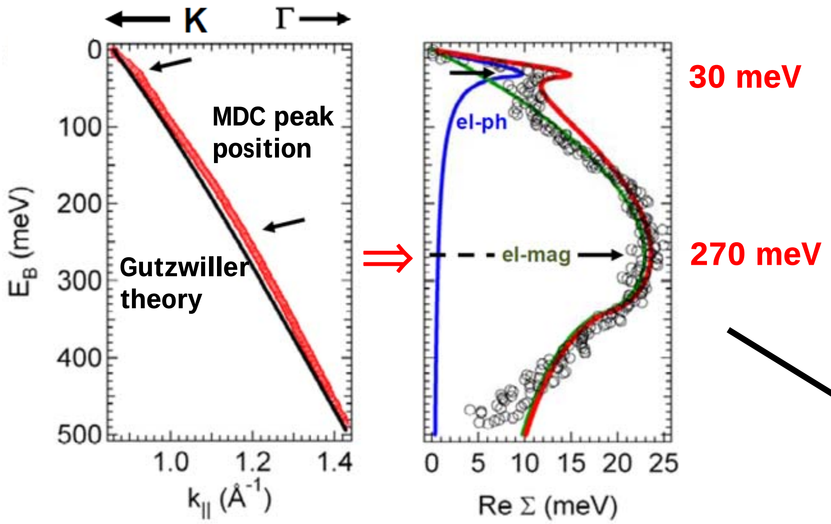
Kinks

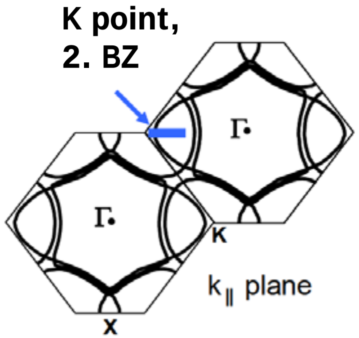


Byczuk, Kollar, Held, Yang, Nekrasov, Pruschke, DV
Nature Physics **3,** 168 (March, 2007)

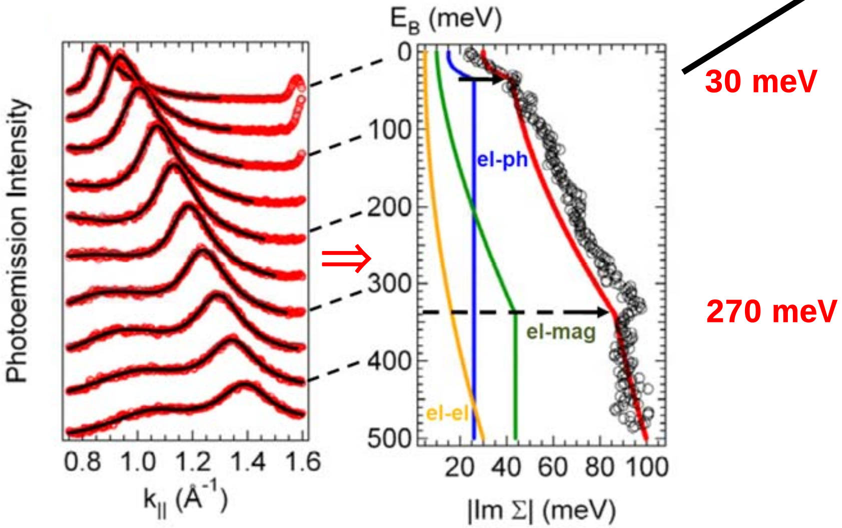
Kinks in high-resolution ARPES of Ni(110)

Hofmann, Cui, Schäfer, Meyer, Höpfner, Blumenstein, Paul, Patthey, Rotenberg, Bünemann, Gebhard, Ohm, Weber, Claessen (2009)





Consistent with KK-relation
→ “electron–magnon” coupling

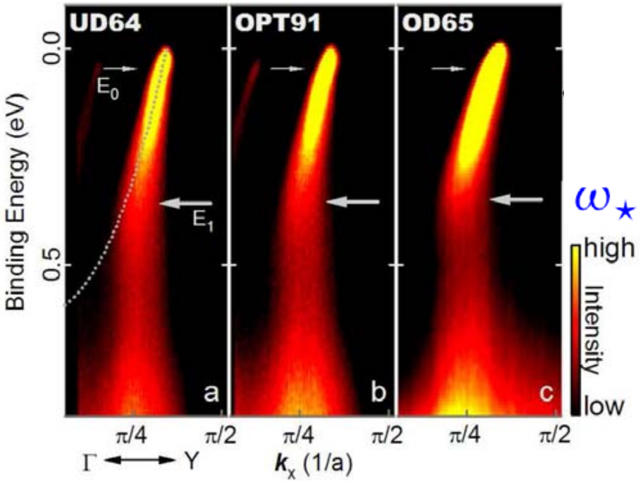


Energy scale for magnons
in Ni (large k) ~ 270-370 meV

Byczuk *et al.* (2007):
Kink energy caused by
local spin fluctuations ω* ~ 300 meV

Waterfalls

“Waterfalls” in the electronic dispersion



Bi2212

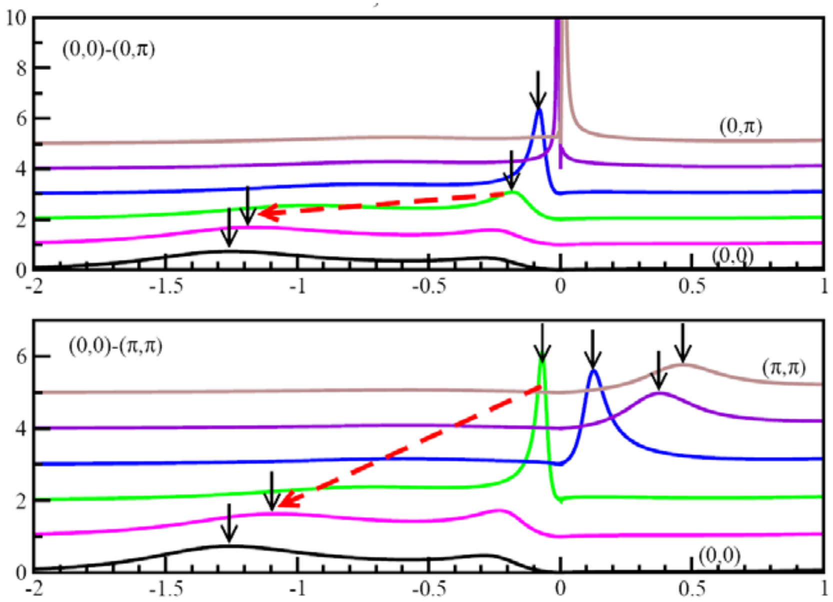
$\omega_\star \approx$ 300-400 meV

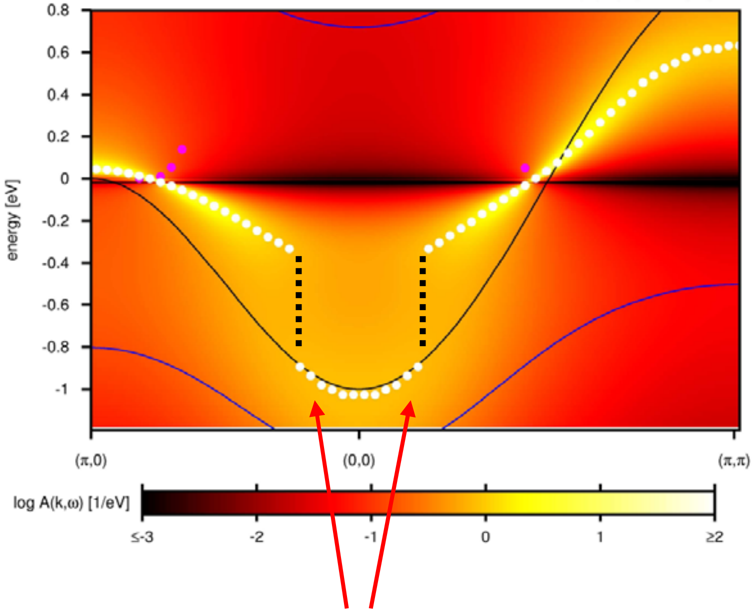
Graf *et al.* (2006)
Graf, Gweon, Lanzara (2006)

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

U=8t, n=0.79

Byczuk, Kollar (2009, unpublished)





"Waterfalls"

Dispersion jumps from central peak to lower Hubbard band

see also Held, Yang (2009, unpublished)

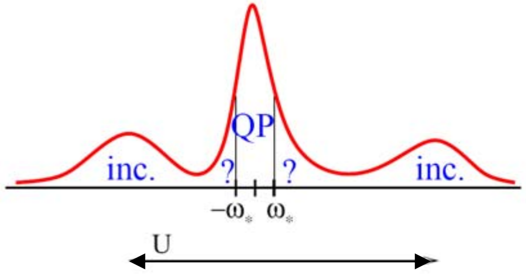
Conclusions

1. Kinks in the electronic dispersion

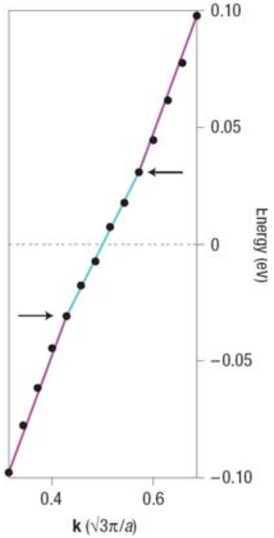
- Purely electronic mechanism
- Generic for strong correlations
- 3-peak spectral function A(ω) sufficient
- New energy scale

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

  inside central peak
- FL regime terminates at ω_*
- Robust mechanism based on local physics
- Does not rule out other kinks



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



2. Waterfalls in the electronic dispersion

- Dispersion jumps from central peak to LHB