Center for
Electronic Correlations and Magnetism
University of Augsburg

# Isosbestic Points and Kinks: Fingerprints of Electronic Correlations

Conference celebrating
Elihu Abrahams‘ 80th Birthday;
Rutgers University, April 20, 2007

**Dieter Vollhardt**

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*"Localization and Interactions in Impure Metals";* Aspen, July 1981
Elihu Abrahams, Patrick Lee


*Heavy Fermions and Valence Fluctuations/Glassy Dynamics;* Aspen, July 1985

Phil Anderson


*Heavy Fermions and Valence Fluctuations/Glassy Dynamics;* Aspen, July 1985
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Phil Anderson

*Strongly Correlated Electron Systems;* Aspen, July 1988
Ravin Bhatt, Steve Kivelson


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*Strongly Correlated Electron Systems;* Aspen, July 1988
Ravin Bhatt, Steve Kivelson

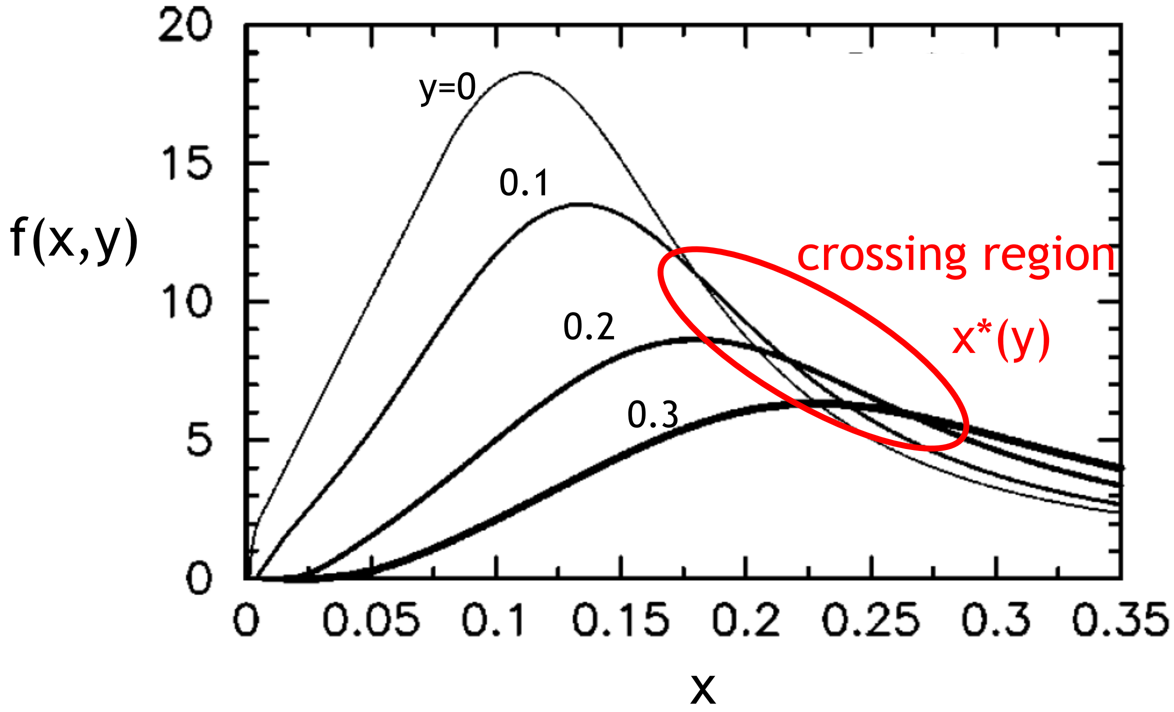
# Outline:

- Isosbestic points
- Kinks in the electronic dispersion

Characteristic energies/temperatures
due to electronic correlations

# I. Sharp crossing ("isosbestic") points

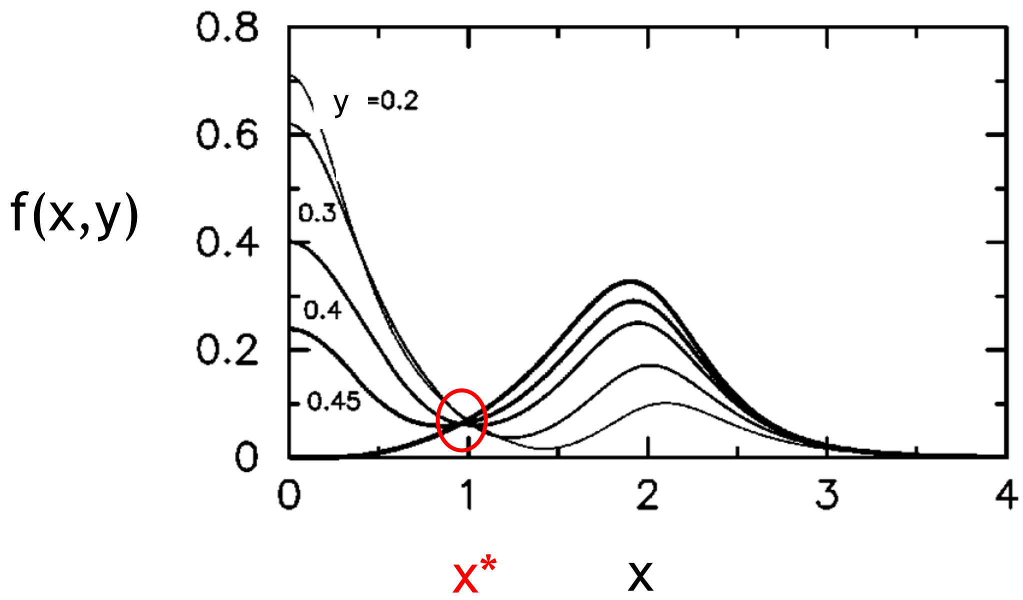
Eckstein, Kollar, DV (2007)




$$\left.\frac{\partial f(x,y)}{\partial y}\right|_{x^*(y)} = 0$$

# I. Sharp crossing ("isosbestic") points

Eckstein, Kollar, DV (2007)




$$\left.\frac{\partial f(x,y)}{\partial y}\right|_{x^*(y)} = 0\,,$$ x*(y) = const → sharp crossing *point*

"isosbestic" point

What do they tell us?

# 1) Isosbestic points in chemistry

Scheibe (1937)

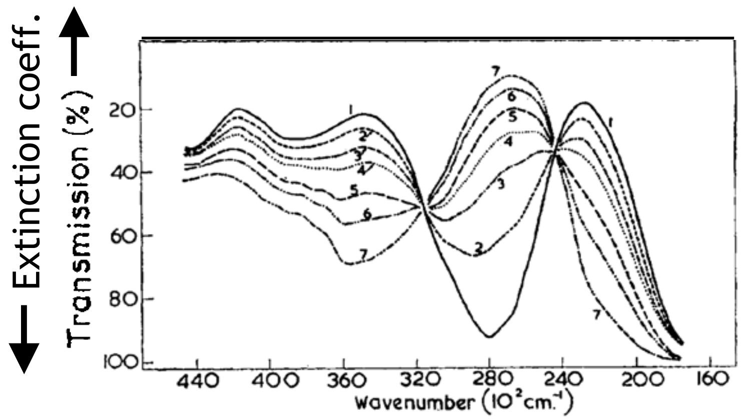
Cohen and Fischer (1962)

Isosbestic point: “Specific wavelength at which two (or more) chemical species have the same extinction coefficient.”

Example:

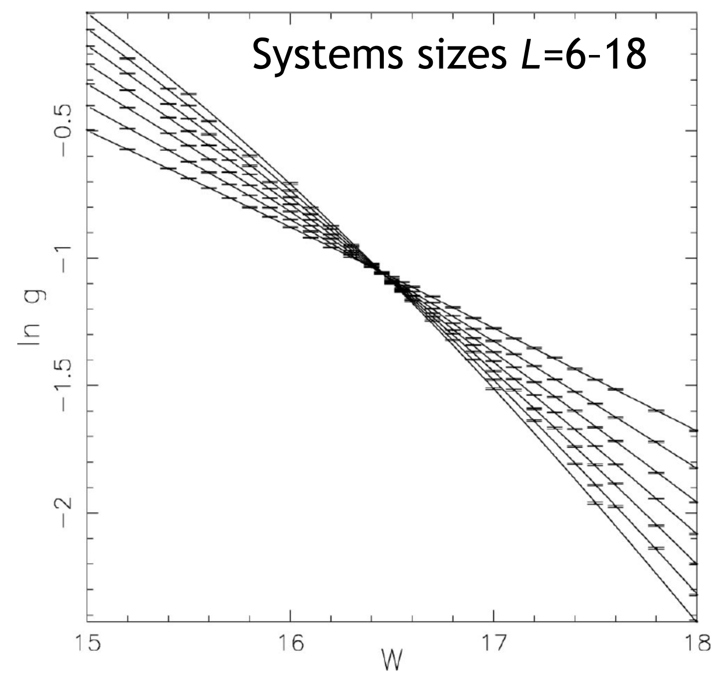
Solution of components A, B with concentrations $n_A$, $n_B$

A: 1,4-naphtaquinone diphenylhydrazone
B: 4-dimethylaminoazobenzene




**Isosbestic**: from Greek *isos* “equal” + *sbestos*, verbal adj. from *sbennynai* “to quench, extinguish” = “**equal attenuance**”

# 2) Sharp crossing points in critical phenomena

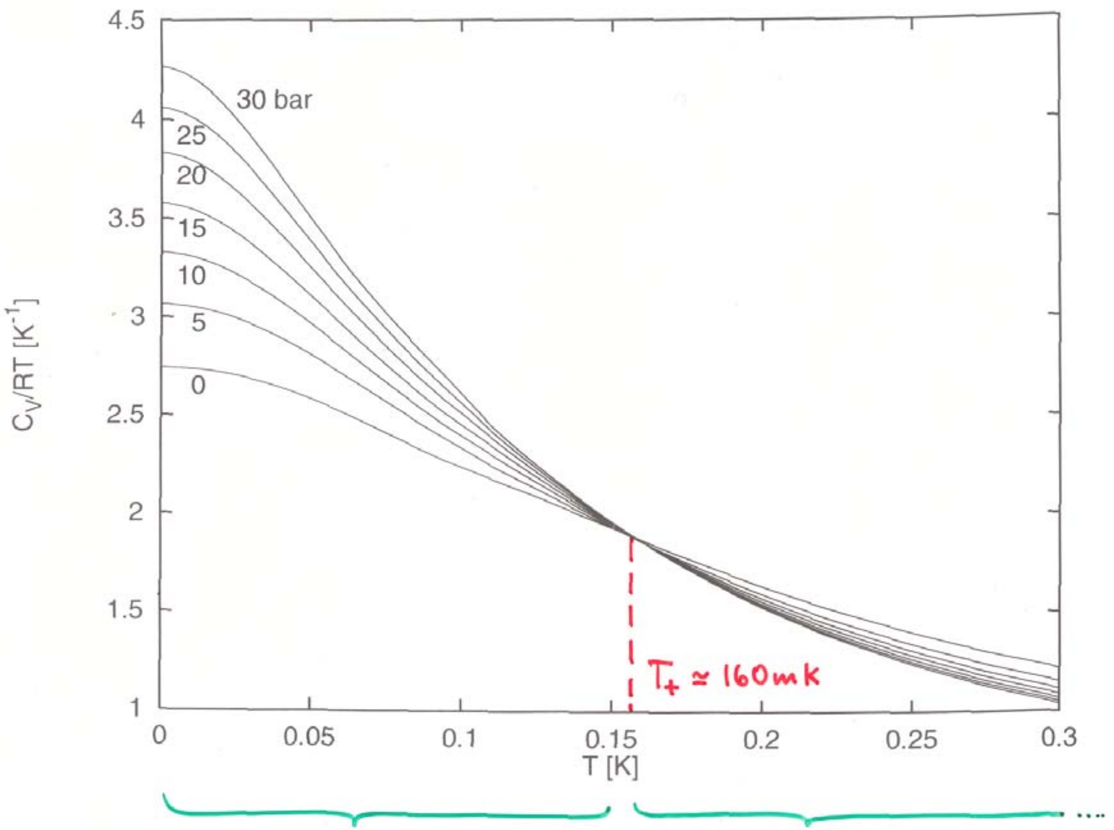



Slevin *et al.* (2003)

Conductance distribution near the Anderson localization transition

# 3) Sharp crossing points in the specific heat of Fermi systems

$^3He$

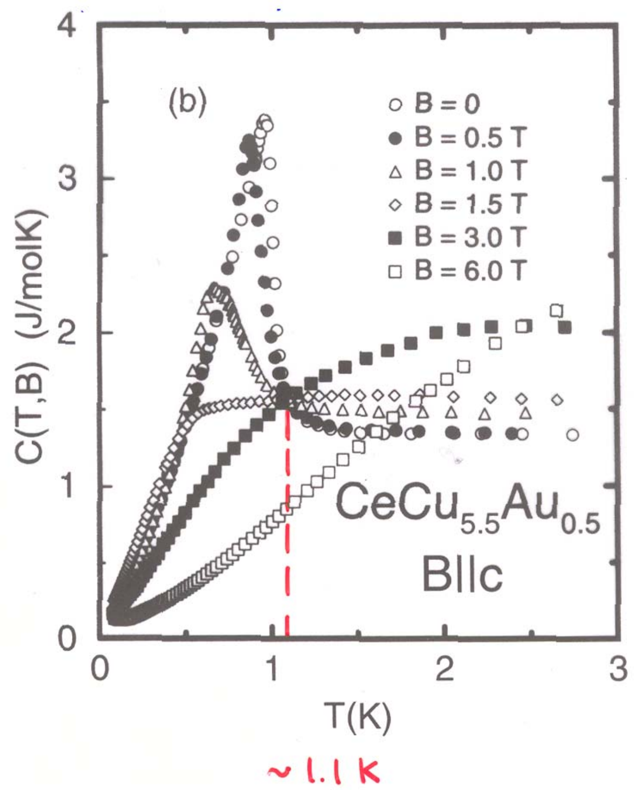



Greywall (1983)

$$\frac{\partial C}{\partial P} > 0 \qquad = 0 \qquad < 0$$

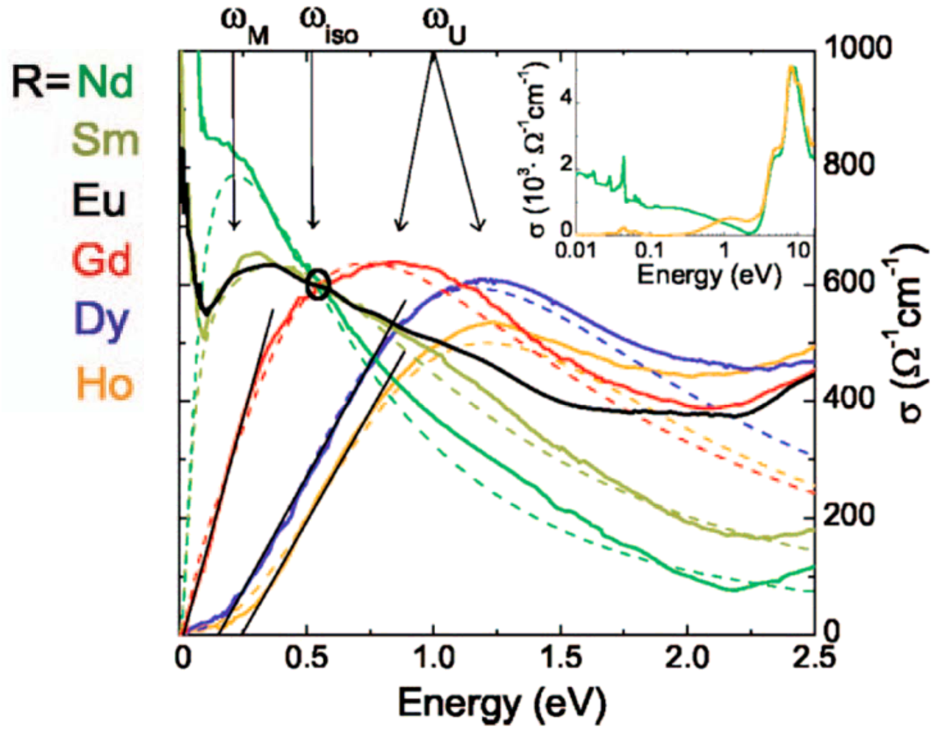
# 3) Sharp crossing points in the specific heat of Fermi systems

## Heavy fermion systems




Schlager, Schröder, Welsch, v. Löhneysen (1993)

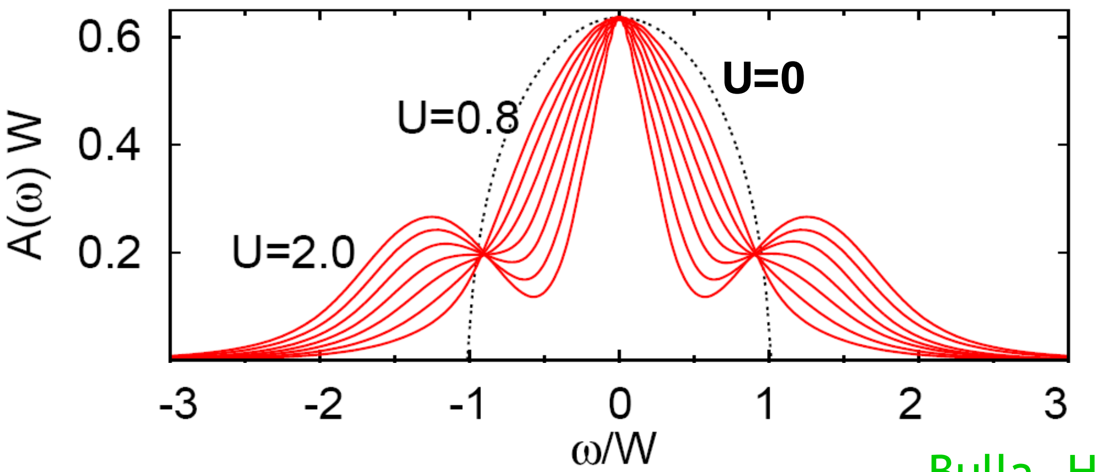
# 4) Sharp crossing points in the dynamical conductivity




$T$=10 K spectra of the $R_2Mo_2O_7$ family

Kezsmarki *et al.* (2006)

# 5) Sharp crossing points in the spectral function




Hubbard model,
n=1, T=0,
Bethe-DOS,
DMFT(NRG)

Bulla, Hewson, Pruschke (1998)

# Sharp crossing ("isosbestic") points:

Width of crossing regime?

DV (1997)

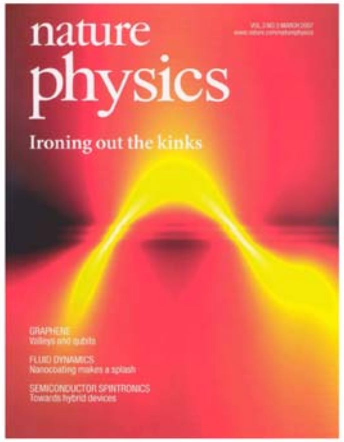
Eckstein, Kollar, DV (2007)

Sharp: - Linear superposition of two quantitites,
- Two-fluid model
- Scaling behavior

Approximate:
- Smallness of a susceptibility, e.g., compressibility
- Existence of a small parameter (1/Z)
- Shape of band edges of spectral function

# II. Kinks in the electronic dispersion

a) Kinks

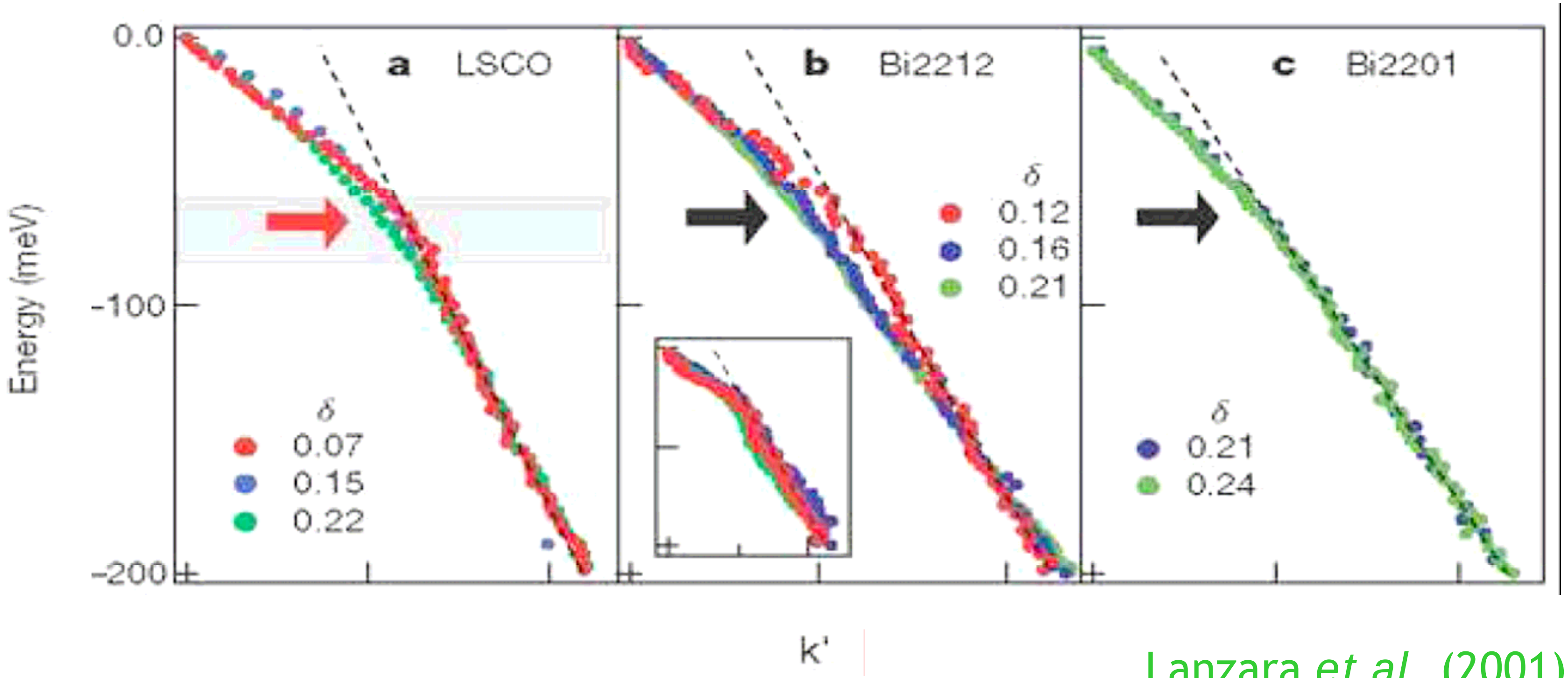



Byczuk, Kollar, Held, Yang, Nekrasov, Pruschke, DV; **Nature Phys.** (2007)

b) Waterfalls

# Kinks: High-$T_c$ cuprates

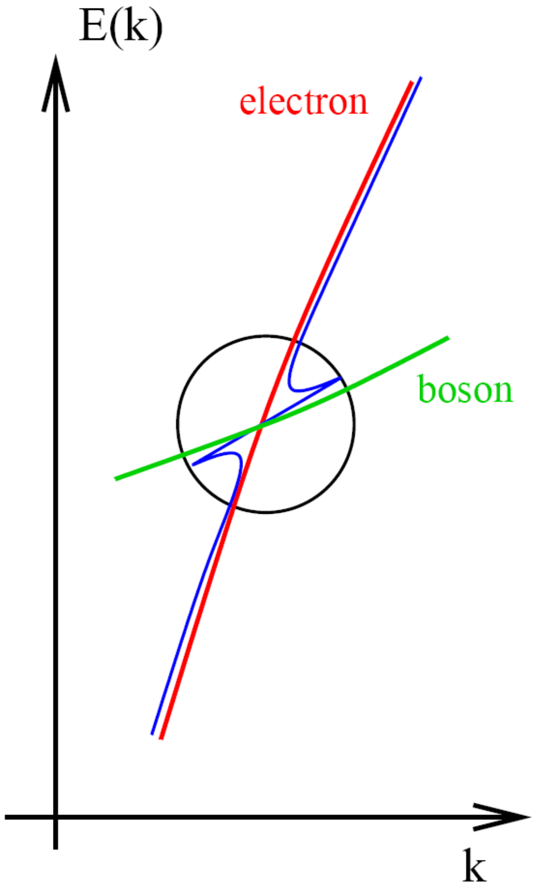
Valla *et al.* (1999)
Bogdanov et al. (2000)

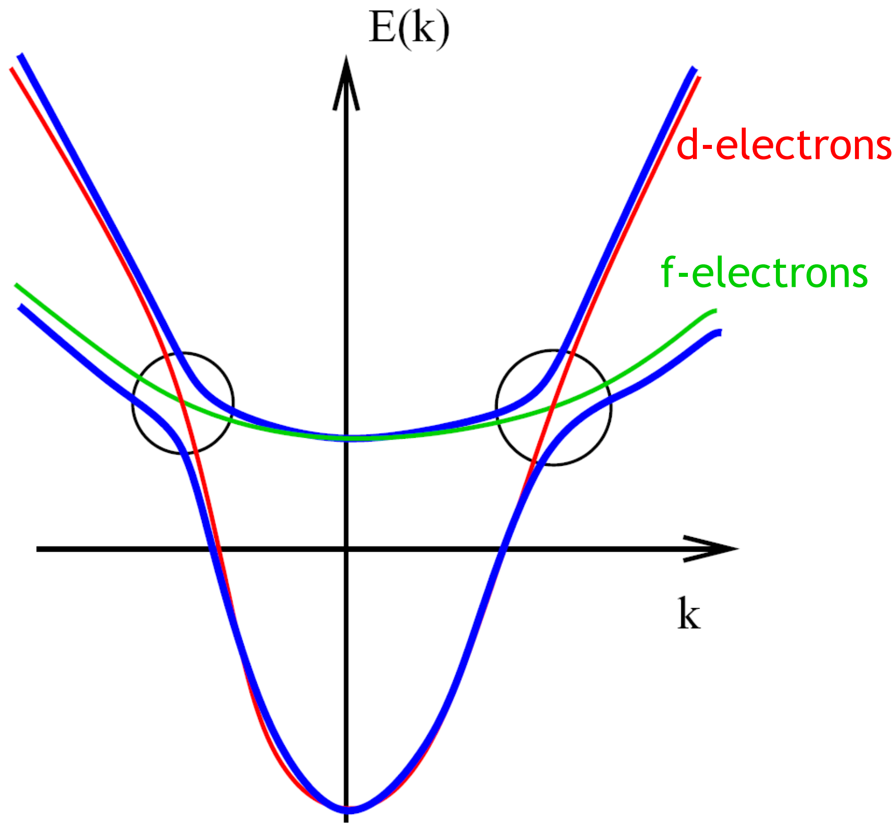



Lanzara *et al.* (2001)

- Kinks at $\omega_*$ = 40-70 meV
- Coupling of electrons to phonons or spin fluctuations ?
- Coulomb interaction ?

Manske *et al.* (2001)
Kordyuk *et al.* (2004)
Randeria *et al.* (2004)
Kakehashi, Fulde (2005)



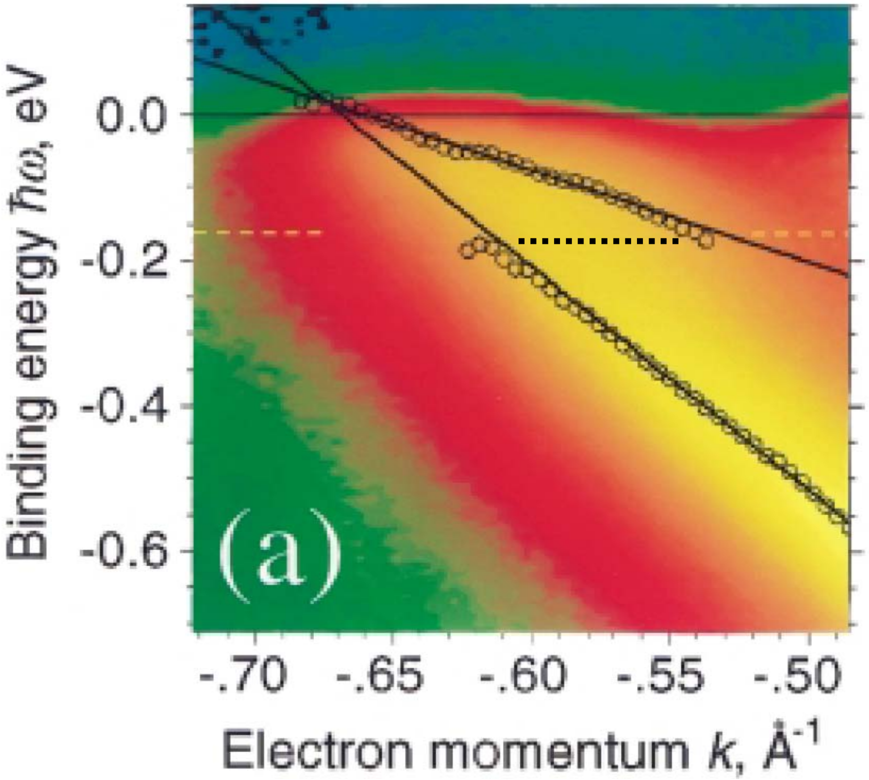




Kinks due to
electron-boson coupling

Kinks due to
electron-electron hybridization

# Kinks: Metal surfaces

Tungsten



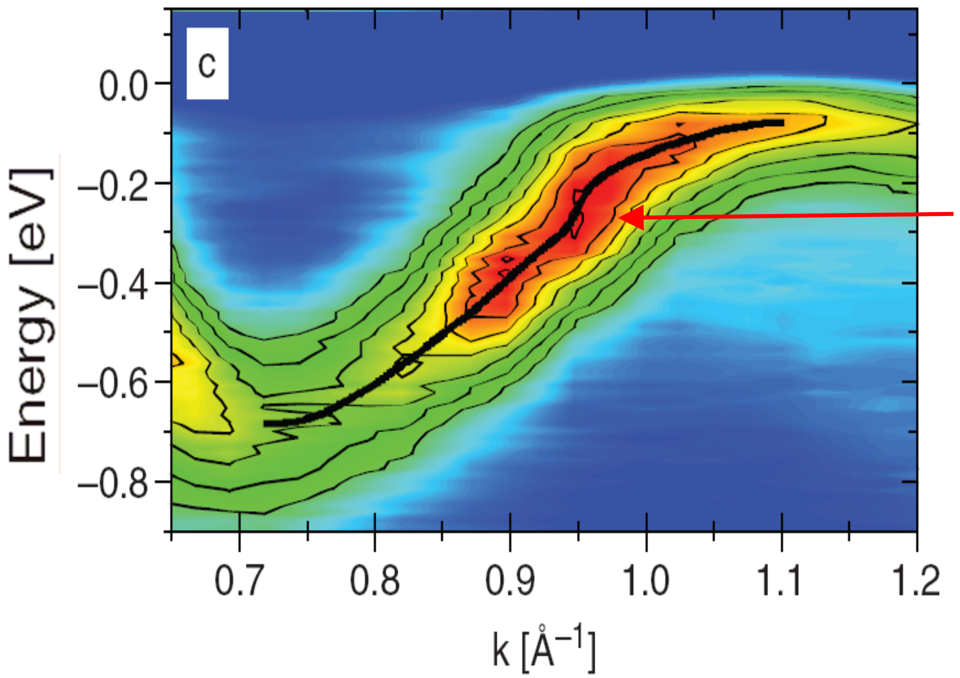

ω* = 160 meV:
Surface phonon

Rotenberg *et al.* (2000)

Kink due to electron-phonon coupling

# Kinks: Metal surfaces

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



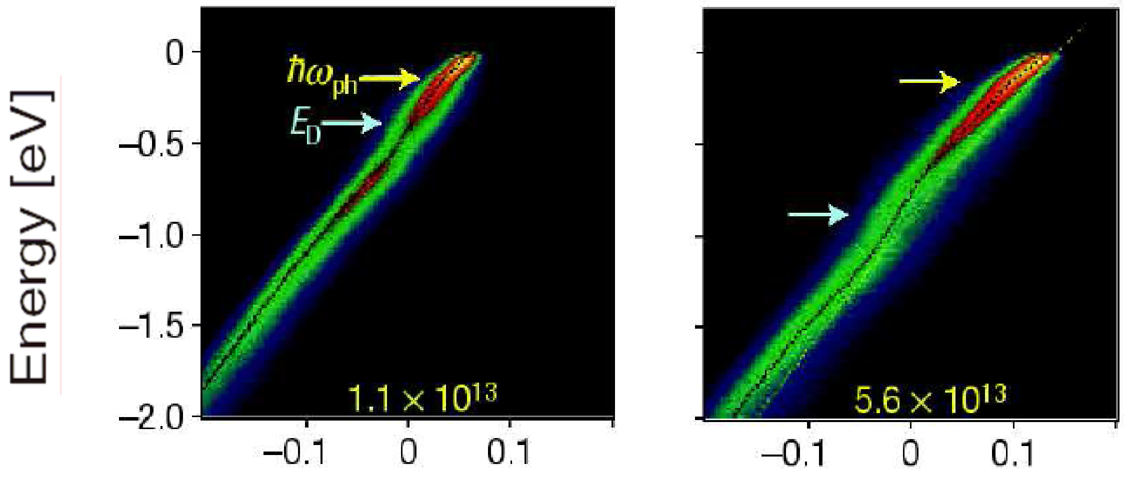

300meV: too high for phonons

Menzel *et al.* (2005)

Kinks due to coupling of electrons to what?

# Kinks: Graphene

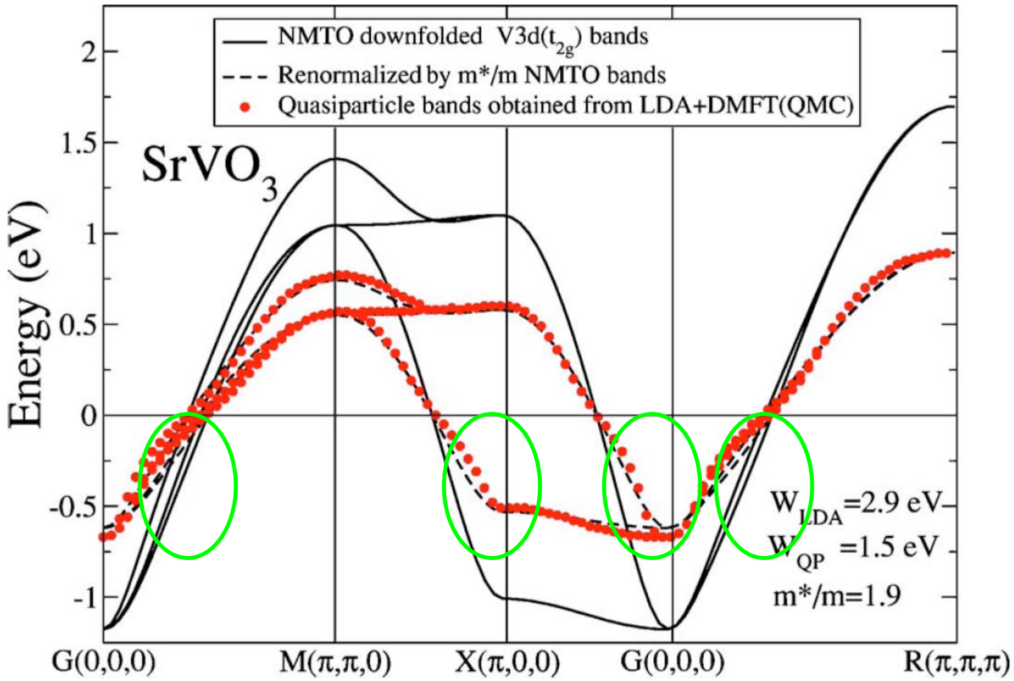
Doping by potassium adsorption



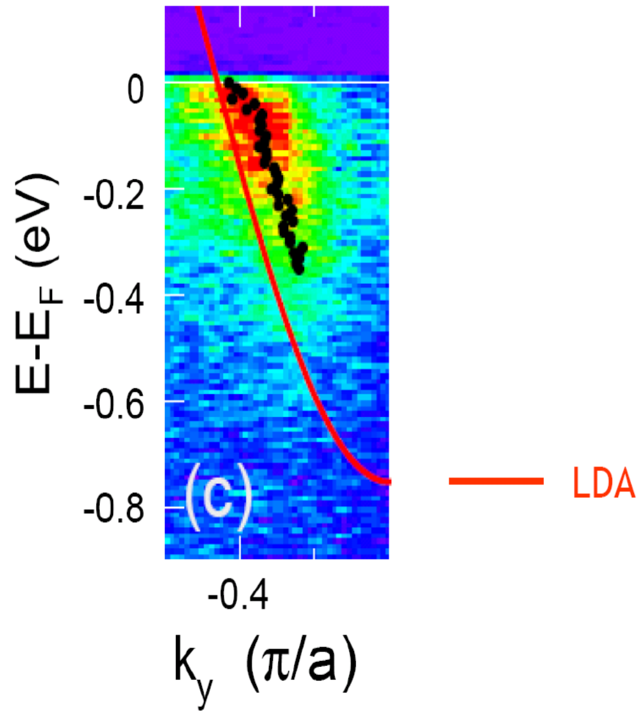

Bostwick *et al.* (2007)

- “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 ?

# Purely electronic mechanism for kinks: Strong correlations




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




Yoshida *et al.* (2005)

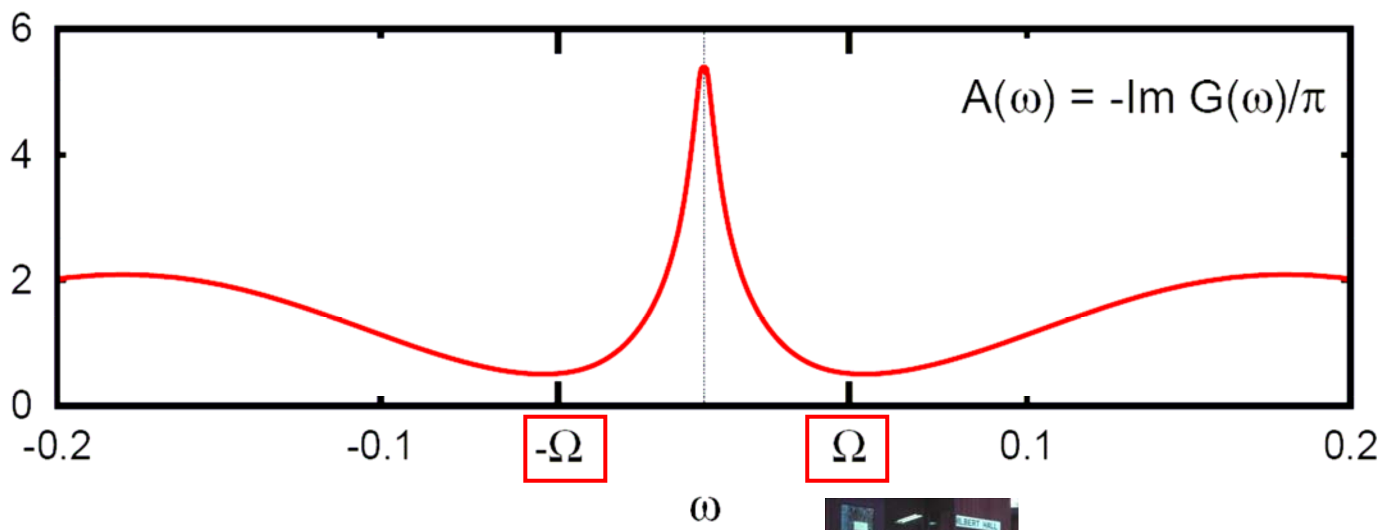
Kinks at $\omega_* \approx 100$ meV

Renormalization of LDA-bands by self-energy

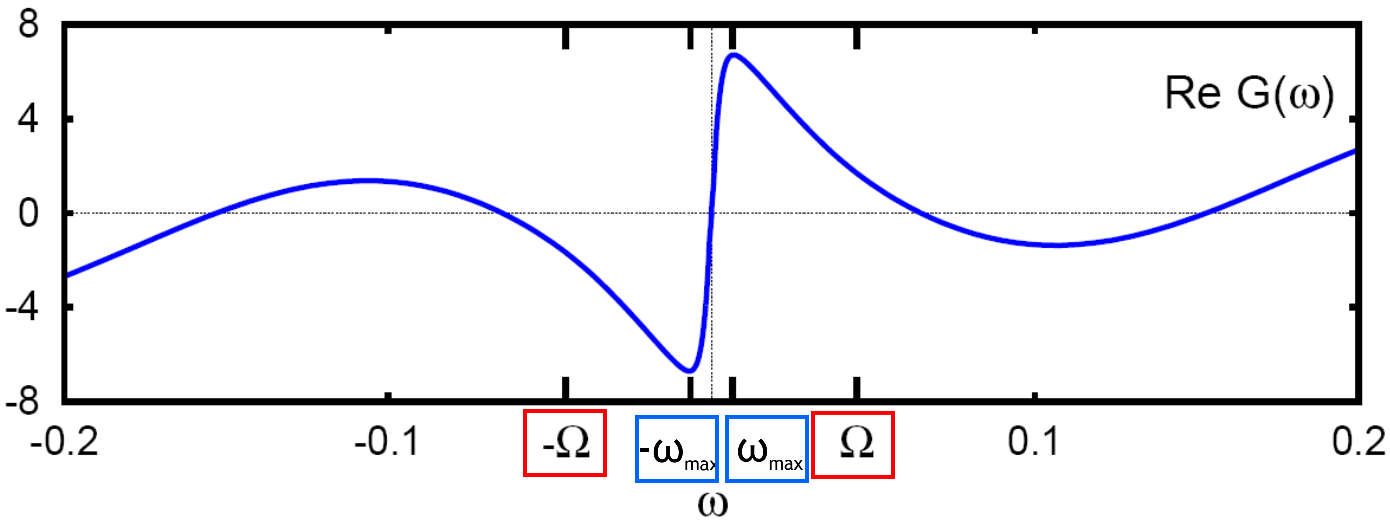
Kinks at $|\omega_*| \approx 200$ meV

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

# Strongly correlated paramagnetic metal




⇓ KK

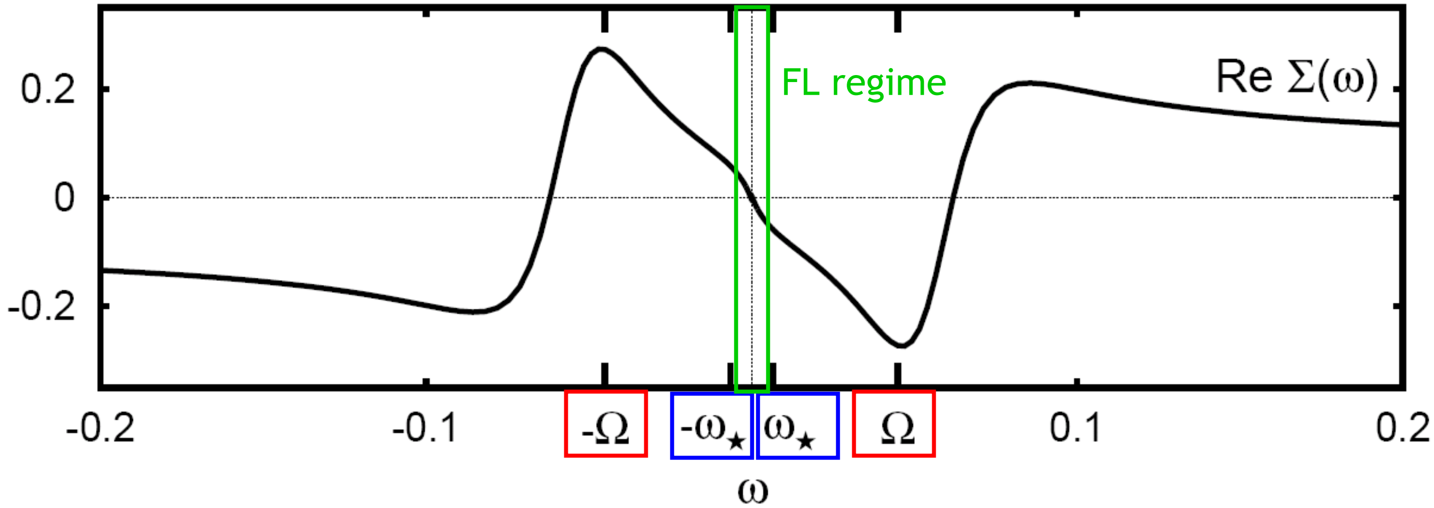



New energy scale ?

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)

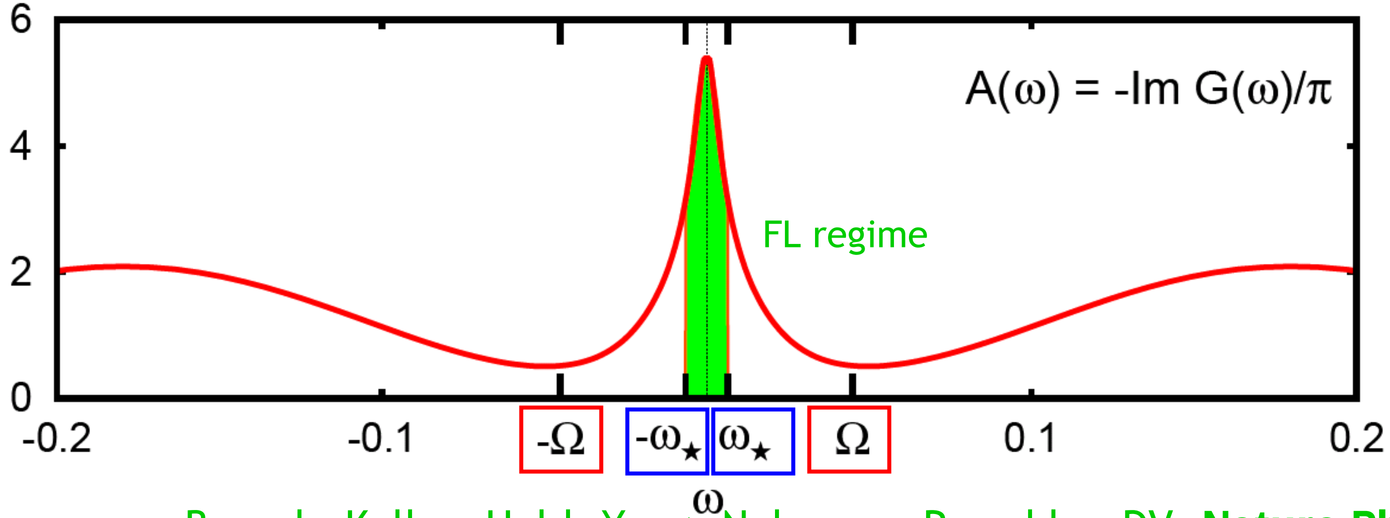



Fermi liquid regime restricted to

$|\omega| \leq \omega_* \propto Z_{FL}$

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

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




Electronic dispersion *outside* Fermi liquid regime?

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

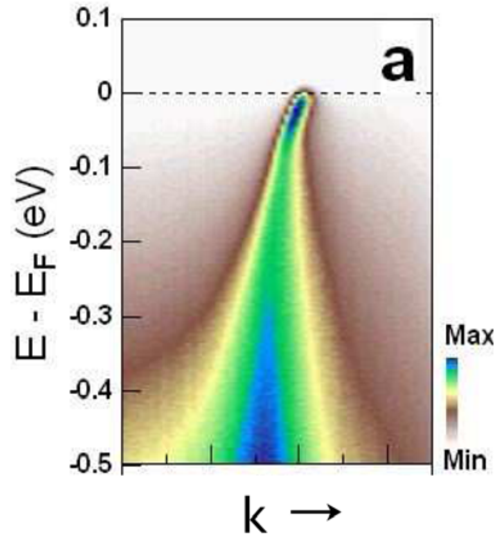
# Electronic dispersion

- Spectral function: $A(\mathbf{k},\omega) \propto \mathrm{Im}\dfrac{1}{\omega+\mu-\varepsilon_{\mathbf{k}}-\Sigma(\mathbf{k},\omega)}$

$$\propto \text{ \# excitations with } \mathbf{k},\omega$$

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

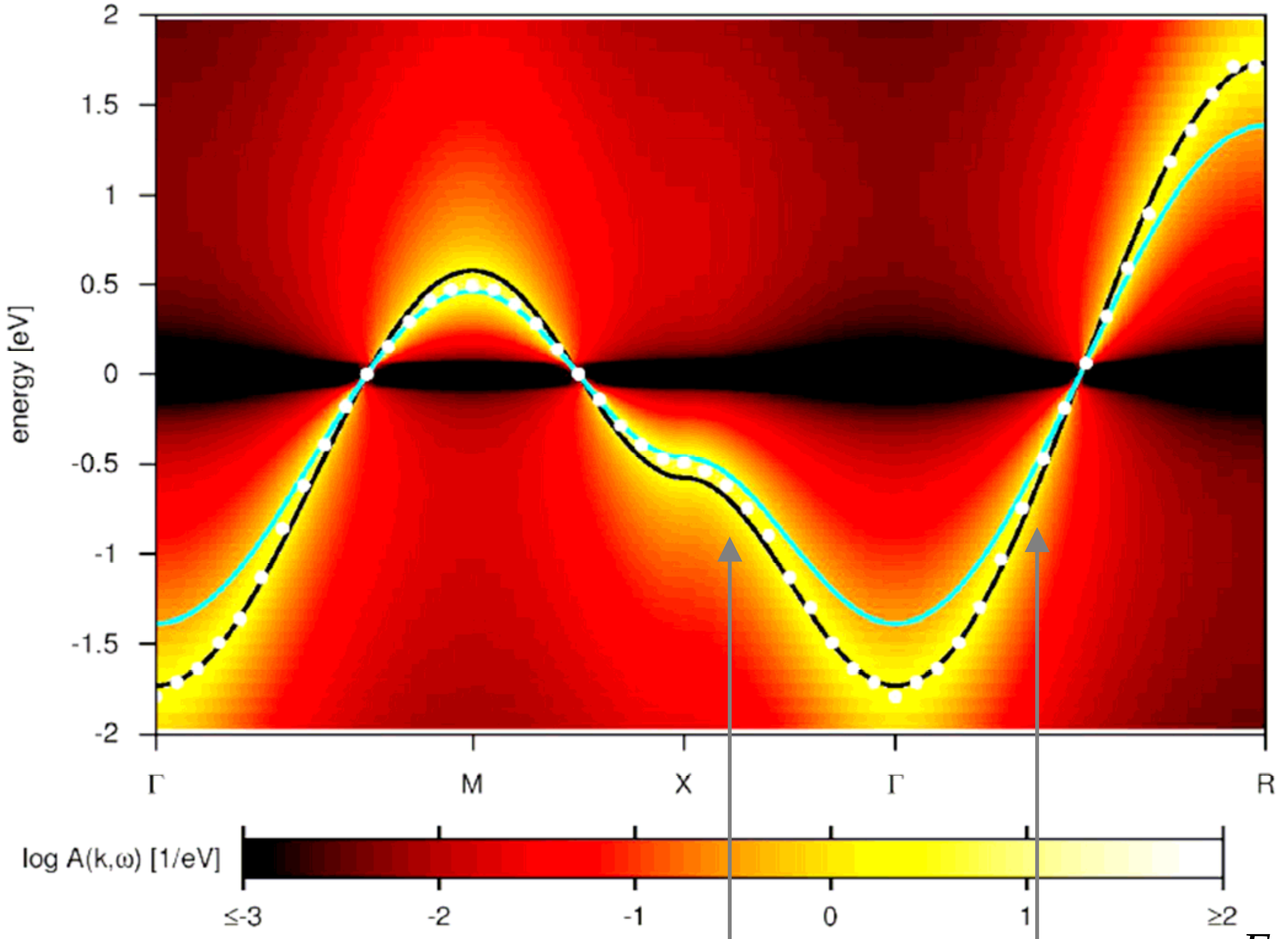
LSCO Zhou et al. (2006)




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

# $E_k$: Hubbard model, cubic lattice, DMFT(NRG)

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



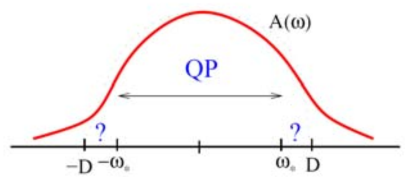

X-over

Fermi liquid dispersion

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

Non-interacting dispersion

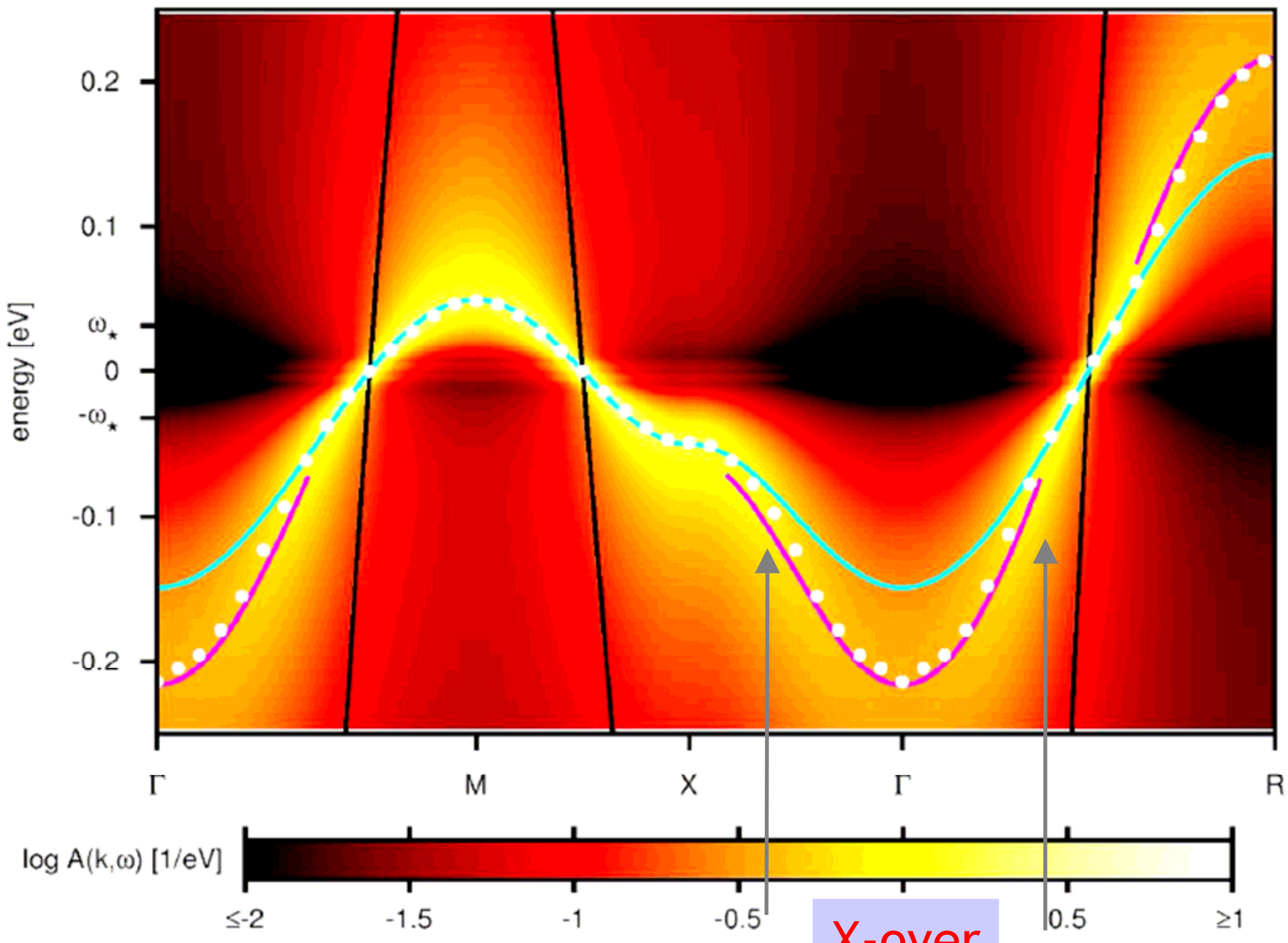
$$E_{\mathbf{k}}^0$$




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

# $E_k$: Hubbard model, cubic lattice, DMFT(NRG)

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

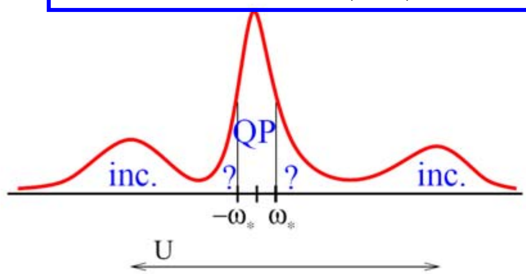



Non-interacting dispersion
$E_{\mathbf{k}}^0$

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

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

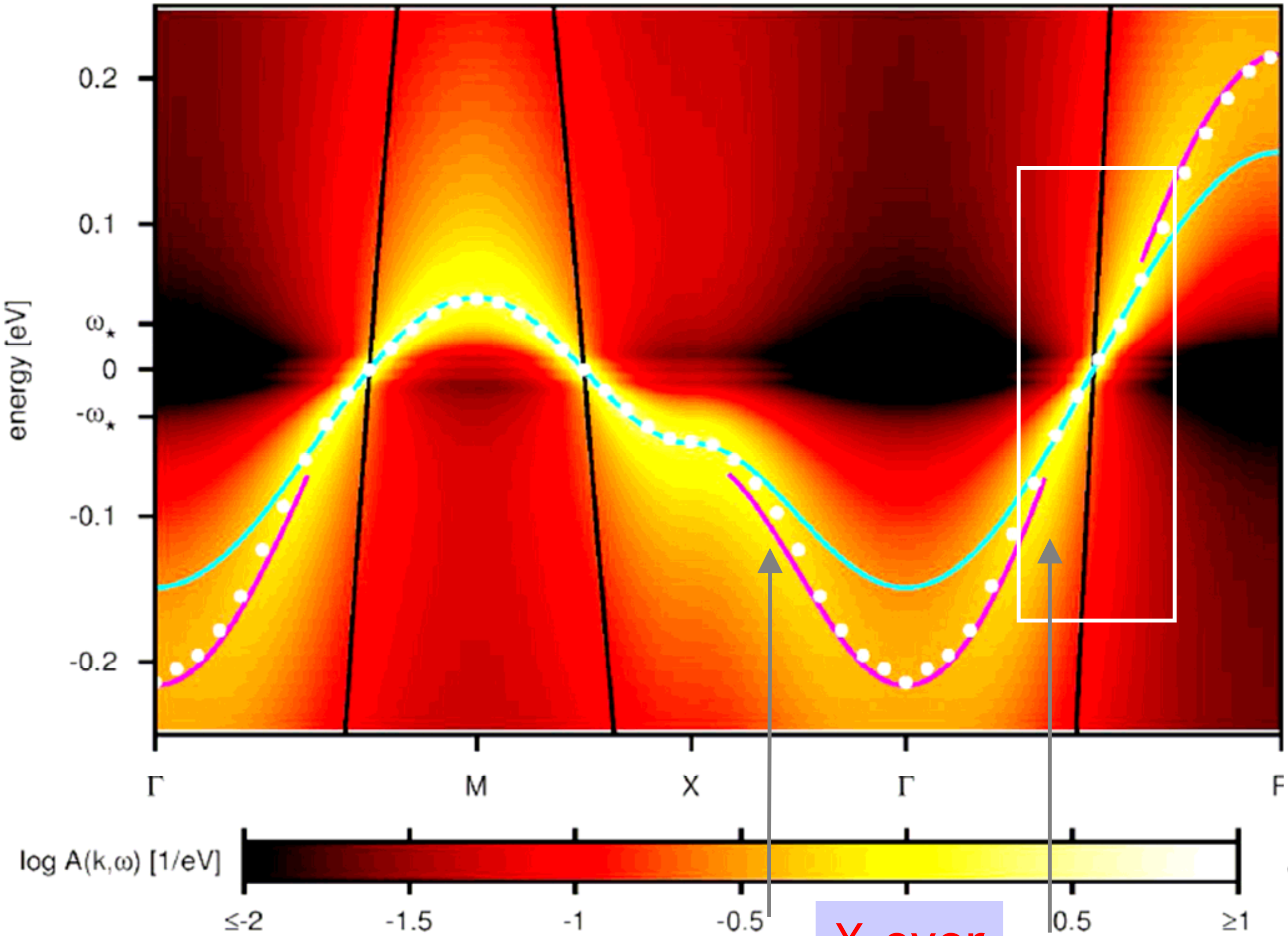
$$E_{\mathbf{k}} = \begin{cases} Z_{FL} E_{\mathbf{k}}^0 \ ; & |E_{\mathbf{k}}| \le \omega_* \\ Z' E_{\mathbf{k}}^0 + c \ ; & |E_{\mathbf{k}}| \ge \omega_* \ll U \end{cases}$$

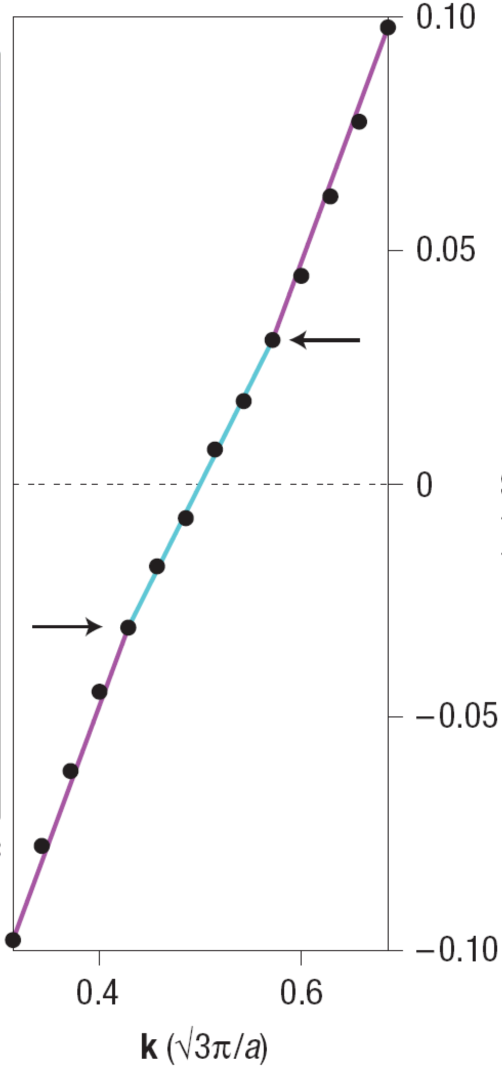



A(ω): three-peak structure
Z' = weight of central peak > $Z_{FL}$
= 0.135 (moderately correlated)

# $E_k$: Hubbard model, cubic lattice, DMFT(NRG)

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




X-over

→ Kinks

# Properties of the kinks

## E.g.: p-h symmetric case

- kink energy:

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

inside central peak

- intermediate-energy regime:

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

weight of central peak in $A(\omega)$

$\Rightarrow$ change in slope $Z'/Z_{\mathrm{FL}}$ independent of interaction strength

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

$\Rightarrow$ sharpness of kinks $\propto (Z_{\mathrm{FL}})^{-2}$

$\Rightarrow$ kinks get sharper with increasing interaction strength

# Conclusions

Kinks in the electronic dispersion

- generic for strongly correlated electrons
- purely electronic mechanism

- three-peak $A(\omega)$ sufficient
- new energy scale $\omega_\star$ inside central peak

- kinks at end of FL regime: $\omega_\star = Z_{\mathrm{FL}} \cdot$ (bare energy scale)
- intermediate-energy regime with $Z' > Z_{\mathrm{FL}}$

- robust mechanism based on local physics
- valid beyond DMFT


Happy
Birthday