# Kinks in the dispersion of strongly correlated electrons

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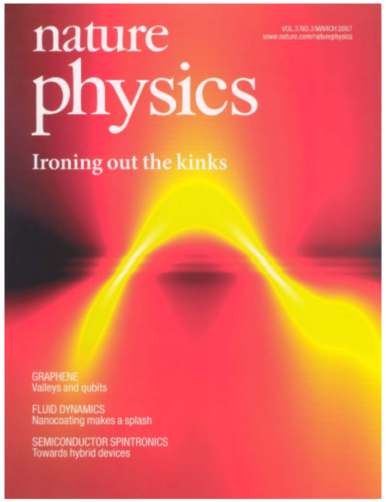


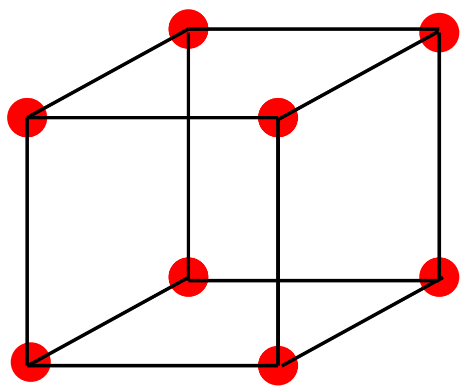

K. Byczuk, M. Kollar, K. Held, Y.-F. Yang, I.A. Nekrasov, Th. Pruschke, D. Vollhardt
Nature Physics **3**, 168 (2007)

# Collaboration

- M. Kollar, D. Vollhardt, Augsburg, Germany
- K. Held, Y.-F. Yang, Stuttgart, Germany
- I. Nekrasov, Ekaterinburg, Russia
- T. Pruschke, Göttingen, Germany

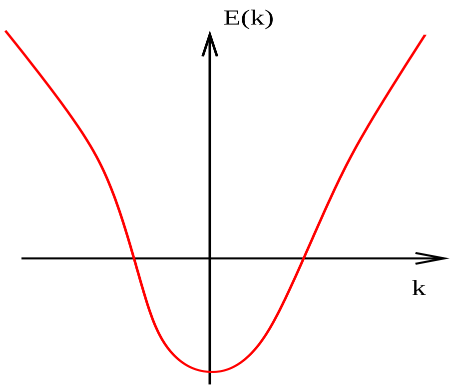
Support from SFB 484

# Standard model of quantum many-body system



emergent particles

quasiparticle
quasihole
holon
spinon
plasmon
magnon
phonon
polariton
exciton
anyon
g-on
...




(i) well defined dispersion relation $E(\mathbf{k})$

(ii) long (infinite) life-time $\tau$

(iii) proper set of quantum numbers

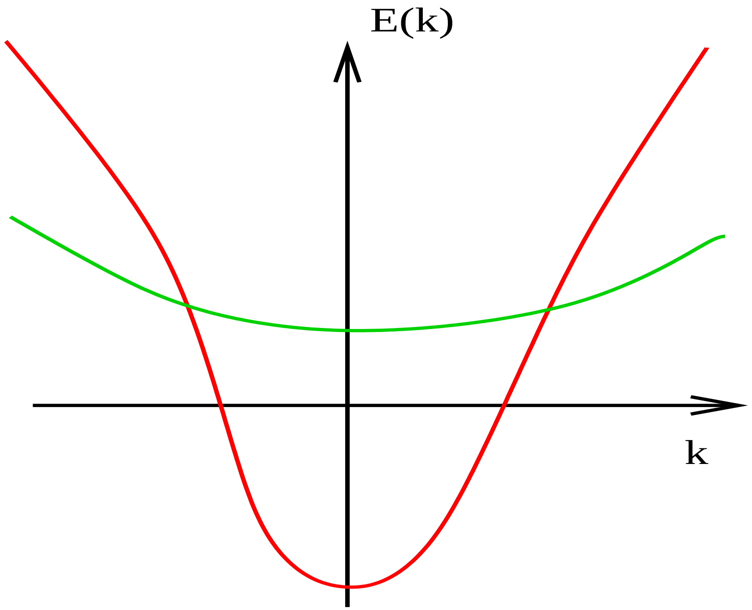
(iv) statistics

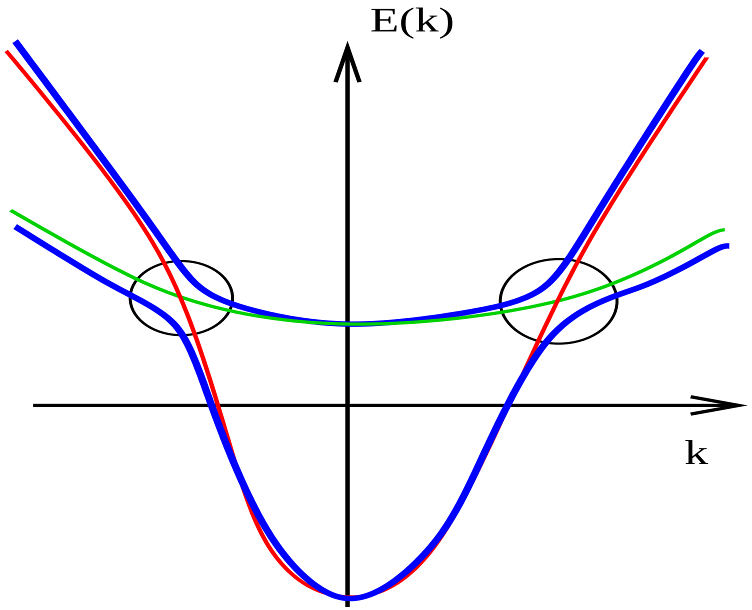
# Dispersions and kinks

Coupling/hybridization $\hat{V}$ between different particles/modes

$$\langle \Psi | \hat{V} | \Phi \rangle \neq 0$$

anticrossing, lifting degeneracy, ...

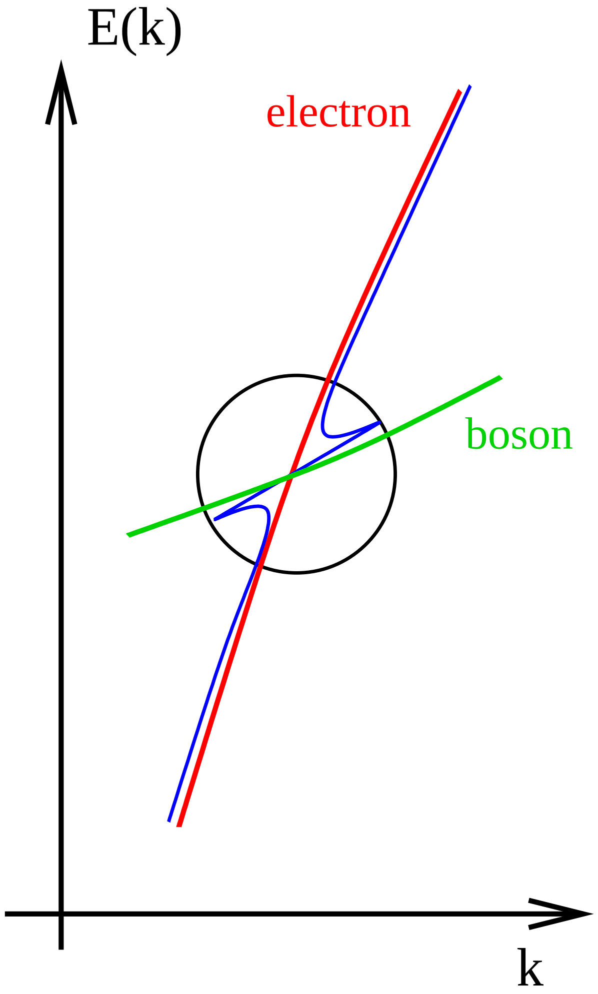



**Df. kinks are abrupt slope changes in the dispersion relations**

## Provide information on modes and couplings

# Dispersions and kinks - coupling to bosons




energy of a kink is related to energy of a bosonic fluctuation

# Dispersion of correlated electrons

One-particle spectral function - excitations at $\mathbf{k}$ and $\omega$

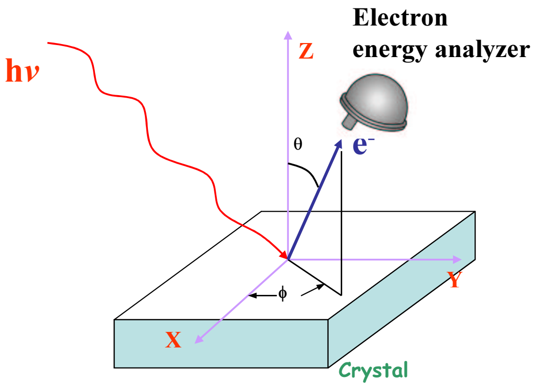
$$A(\mathbf{k},\omega) = -\frac{1}{\pi}\mathrm{Im}\frac{1}{\omega+\mu-\epsilon_{\mathbf{k}}-\Sigma(\mathbf{k},\omega)}$$

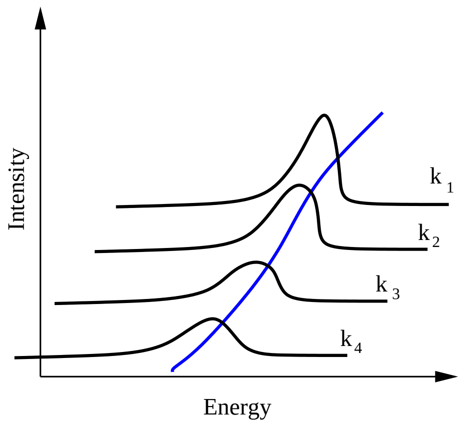
Dispersion relation $E_{\mathbf{k}}$

$$E_{\mathbf{k}} = \{\omega \text{ where } A(\mathbf{k},\omega) = \max\}$$

Dispersion relation is experimentally measured

# Angular Resolved Photoemission Spectroscopy

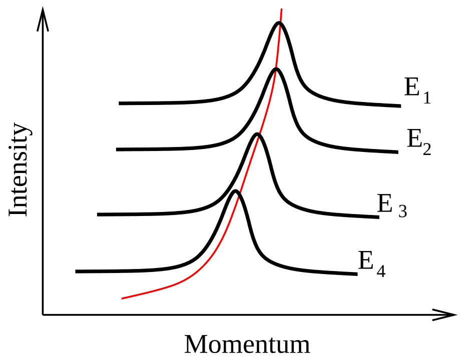



energy distribution curve (EDC)

$$k_x = k\cos\phi$$
$$k_y = k\sin\phi$$

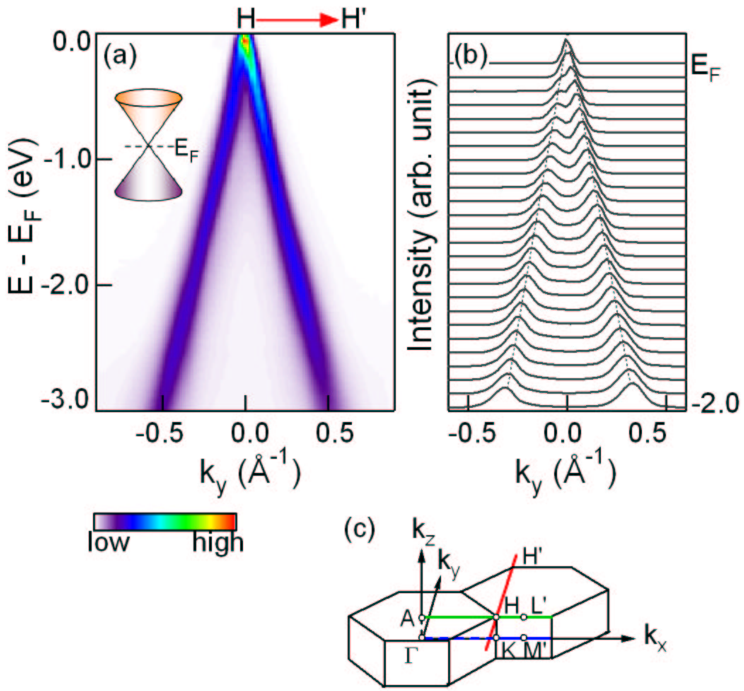
$$E = k^2/2m$$




energy resolution 1meV

momentum distribution curve (MDC)

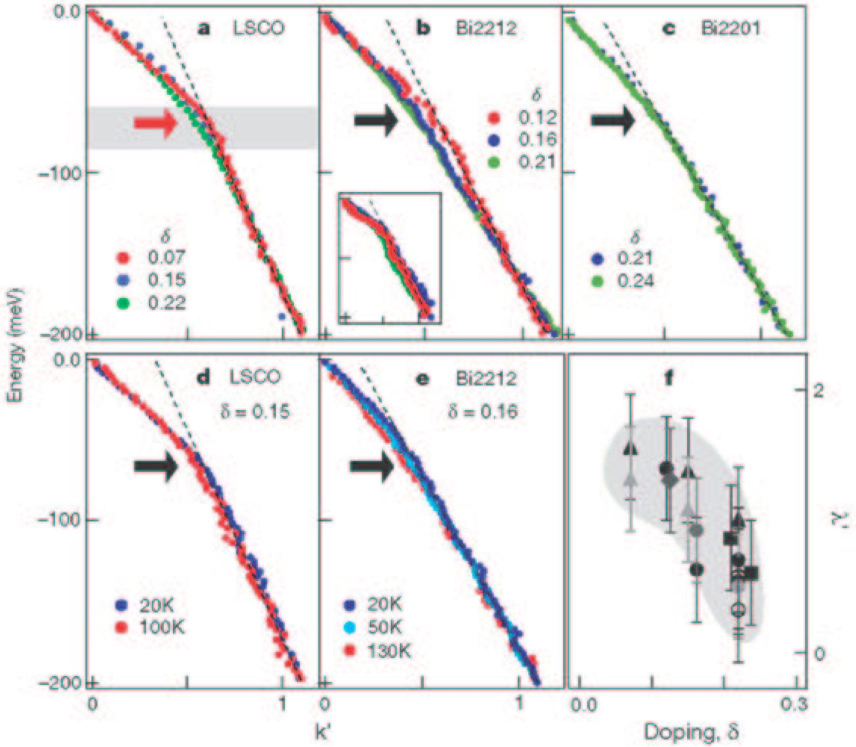
# ARPES and graphene




Dirac linear dispersion relation for graphene

cond-mat/0608069

# Kinks in HTC

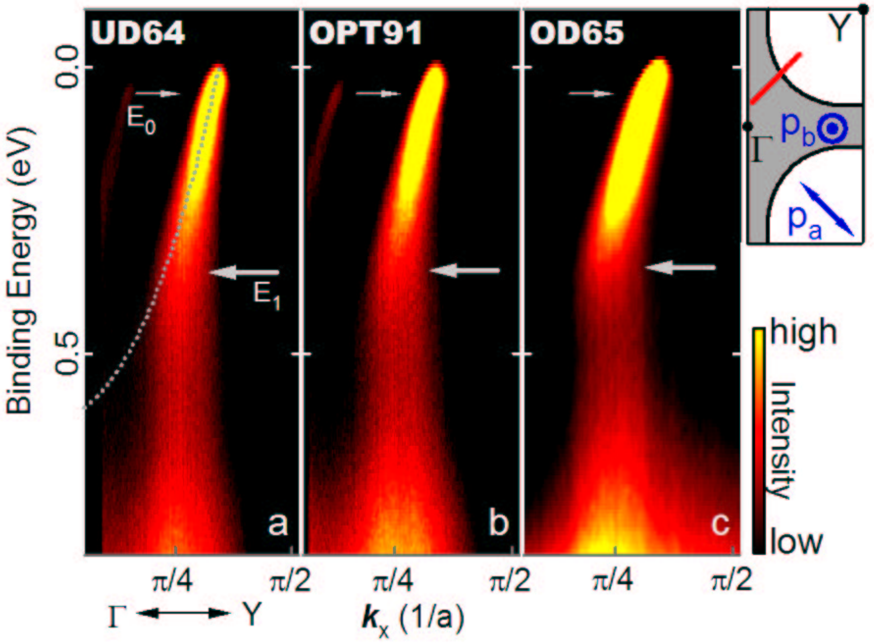



cond-mat/0604284

Kinks at $40 - 70$meV

electron-phonon or electron-spin fluctuations coupling

# “Waterfalls” in HTC

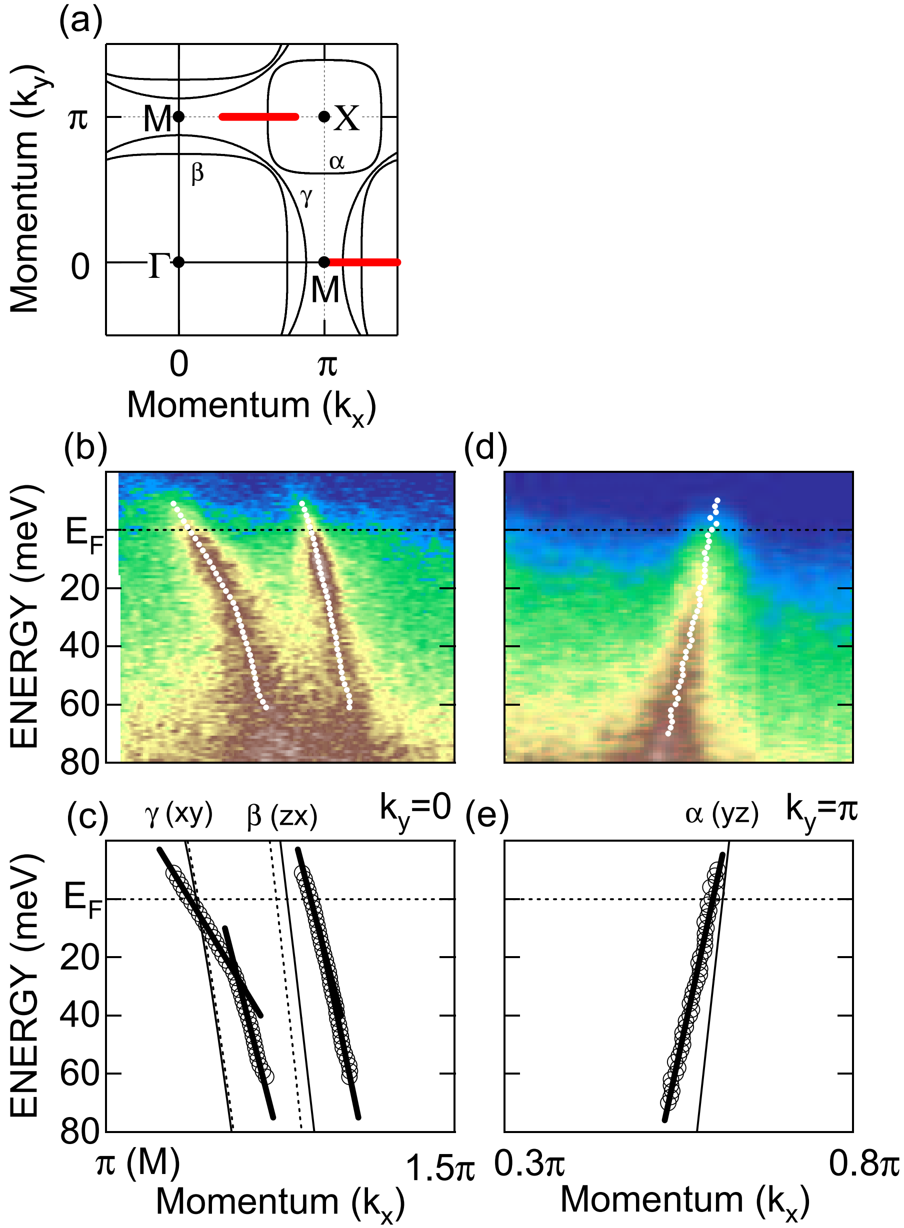



different HTC systems, cond-mat/0607319

Kinks seen experimentally between 300-800 meV

Origin: phonos, spin fluctuations, not known yet

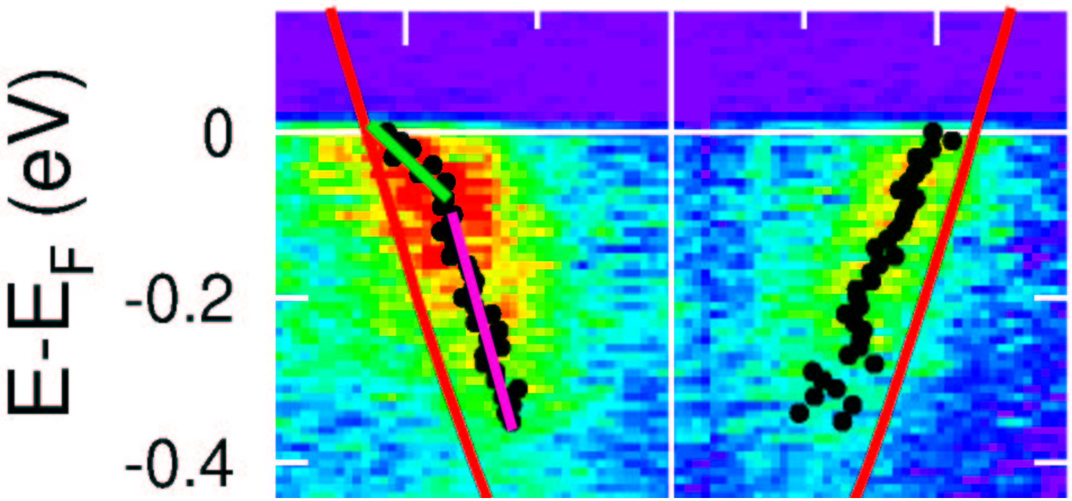
# Kinks orbital selective




Kink at 30meV in $\gamma$-band only

$Sr_2RuO_4$, cond-mat/0508312

# More examples of kinks in ARPES




$SrVO_3$, cond-mat/0504075

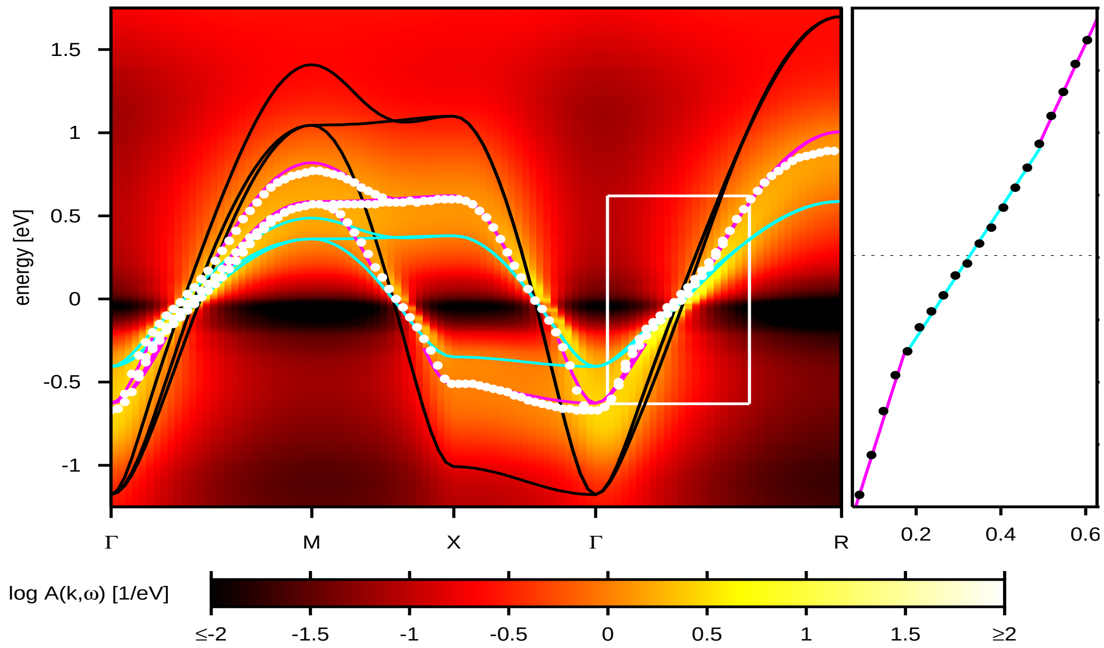
Kinks seen experimentally at 150 meV

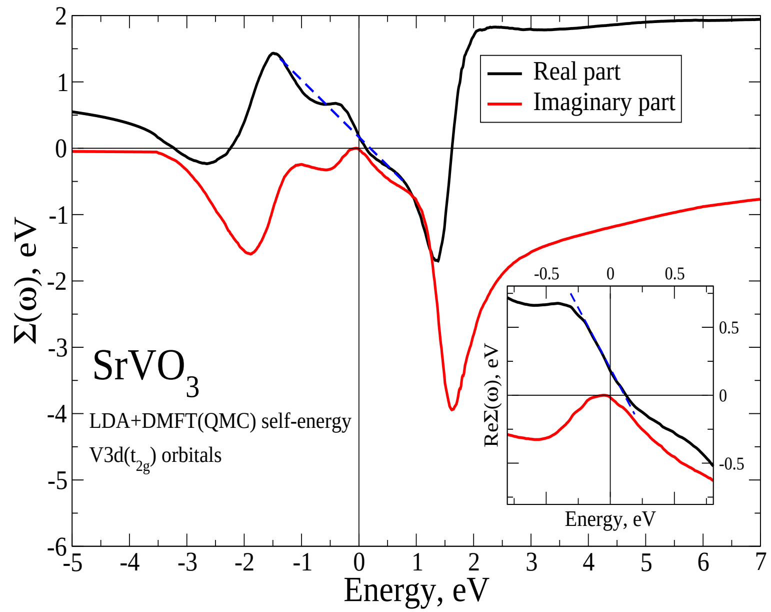
Pure electronic origin?

# Kinks in LDA+DMFT study of $SrVO_3$

plain band model with local correlations, no other bosons, ... but kinks!

I.A. Nekrasov *et al.*, cond-mat/0508313, PRB (2006)




$$G_{\mathbf{k}}(\omega) = \frac{1}{\omega + \mu - \epsilon_{\mathbf{k}} - \Sigma(\omega)} \quad \rightarrow E_{\mathbf{k}} + \mu - \epsilon_{\mathbf{k}} - \mathrm{Re}\Sigma(E_{\mathbf{k}}) = 0$$

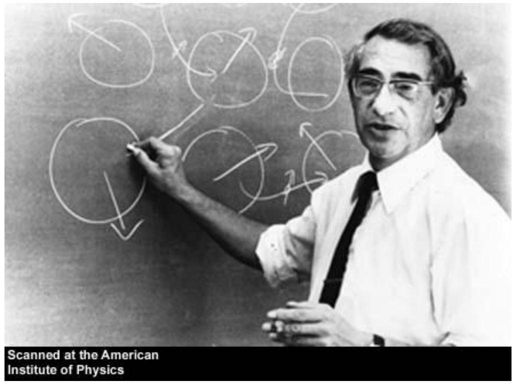
Not found in SIAM with simple hybridization function! $\rightarrow$ DMFT self-consistency effect

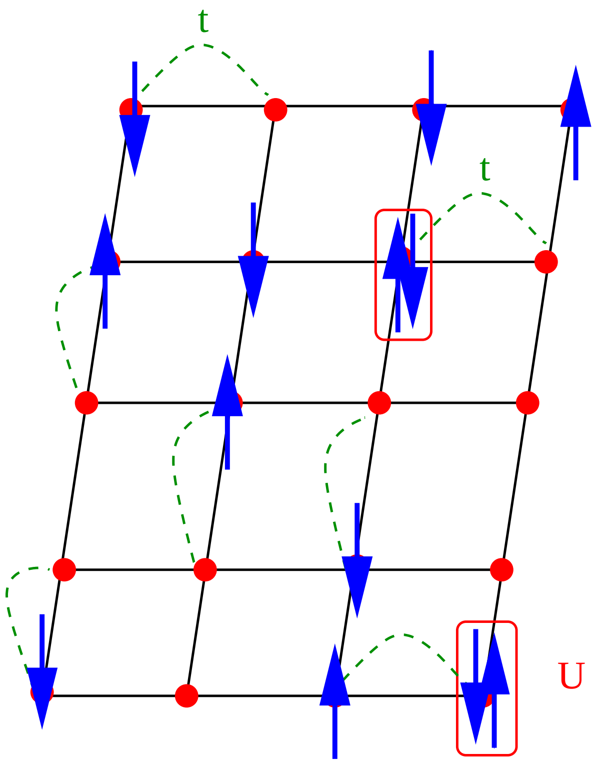
# New purely electronic mechanism

- in strongly correlated systems
- characteristic energy scale
- range of validity for Fermi liquid theory

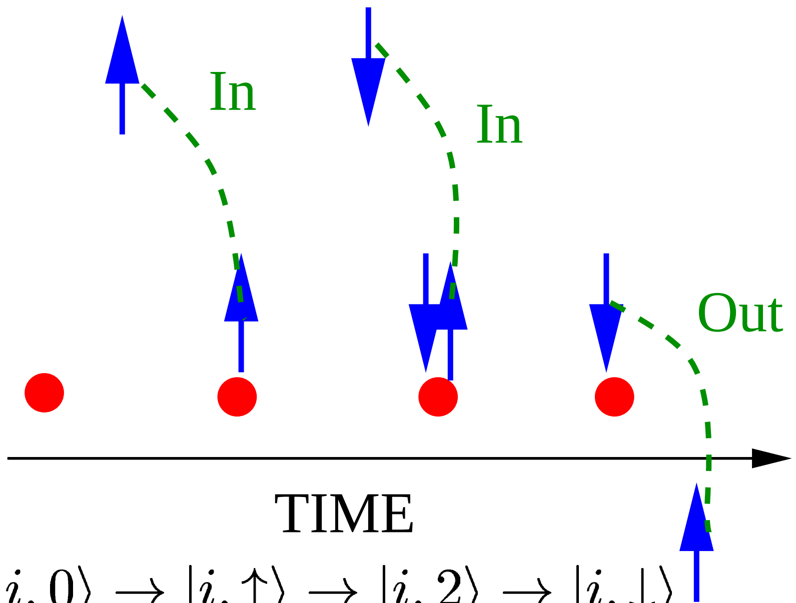
# Hubbard model for strongly correlated electrons

$$H = -\sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$




Local Hubbard physics




$$|i,0\rangle \rightarrow |i,\uparrow\rangle \rightarrow |i,2\rangle \rightarrow |i,\downarrow\rangle$$

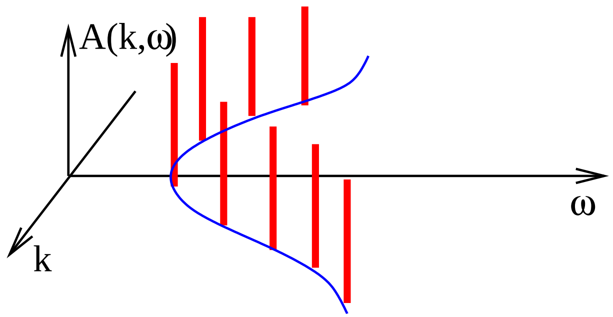
# All what we know about Hubbard model

Solved in $U = 0$ limit (non-interacting limit)

$$G_\sigma(\mathbf{k},\omega) = \frac{1}{\omega + \mu - \epsilon_\mathbf{k}}$$

Dispersion relation

$$\epsilon_\mathbf{k} = \sum_{j(i)} t_{ij} e^{i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)}$$

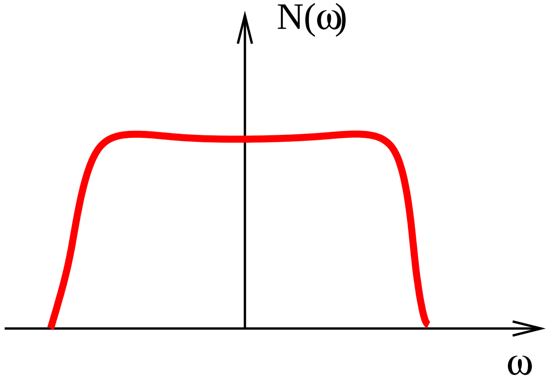



Spectral function - one-particle excitations

$$A_\sigma(\mathbf{k},\omega) \equiv -\frac{1}{\pi}\mathrm{Im}G(\mathbf{k},\omega) = \delta(\omega + \mu - \epsilon_\mathbf{k})$$

Density of states (DOS) - thermodynamics

$$N_\sigma(\omega) \equiv \sum_\mathbf{k} A(\mathbf{k},\omega) = \sum_\mathbf{k} \delta(\omega + \mu - \epsilon_\mathbf{k})$$



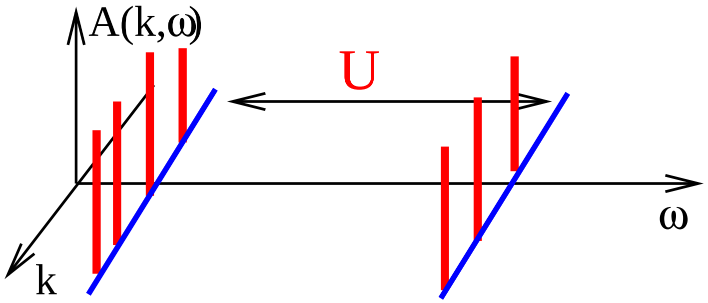
# All what we know about Hubbard model

Solved in $t = 0$ limit (atomic limit)

$$G_\sigma(\mathbf{k},\omega) = \frac{1 - n_{-\sigma}}{\omega + \mu} + \frac{n_{-\sigma}}{\omega + \mu - U} = \frac{1}{\omega + \mu - \Sigma_\sigma(\omega)}$$

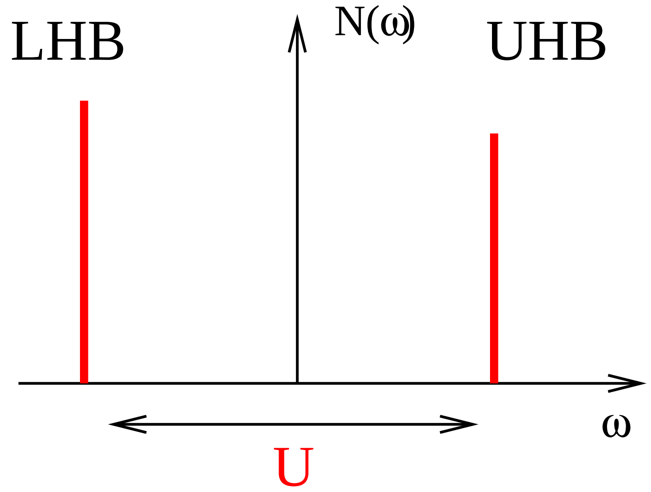
Real self-energy

$$\Sigma_\sigma(\omega) = n_\sigma U + \frac{n_{-\sigma}(1-n_{-\sigma})U^2}{\omega+\mu-(1-n_{-\sigma})U}$$



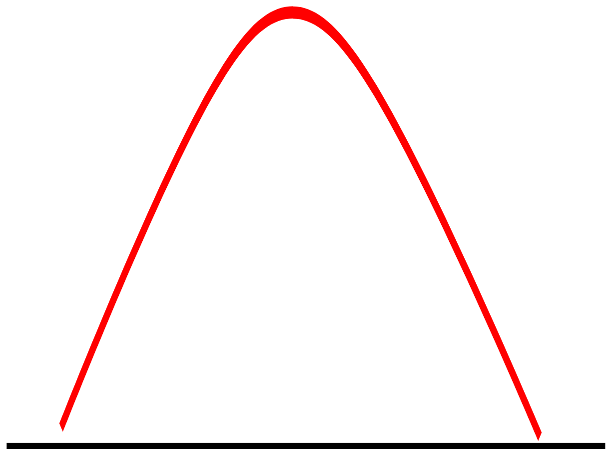

Spectral function

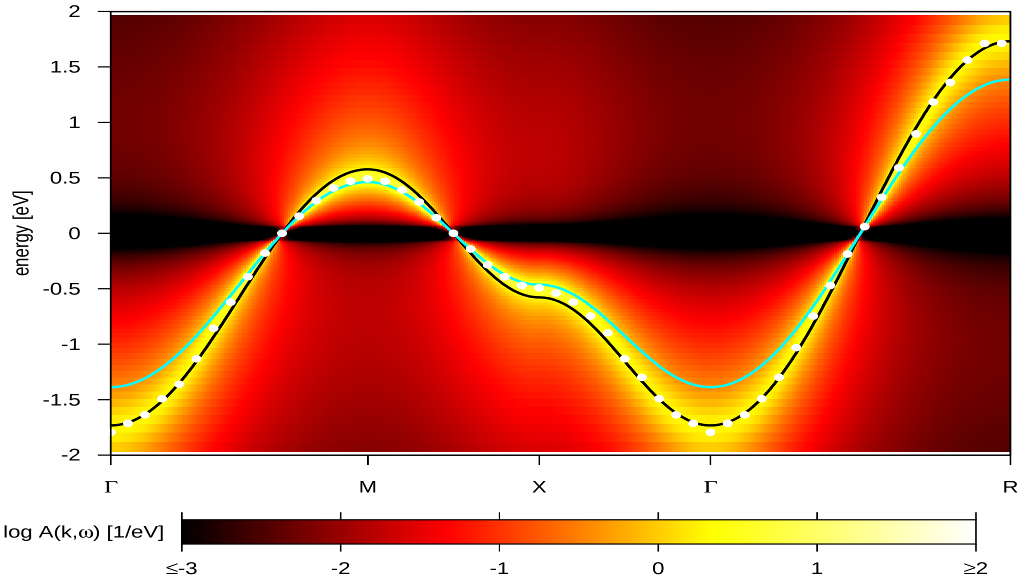
$$A_\sigma(\mathbf{k},\omega) = (1 - n_{-\sigma})\delta(\omega + \mu) + n_{-\sigma}\delta(\omega + \mu - U)$$




Green function and self-energy are local,
i.e. $\mathbf{k}$ independent

# Weakly correlated system

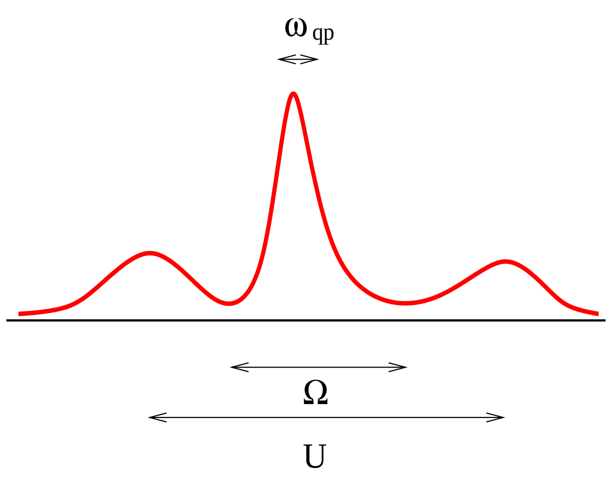


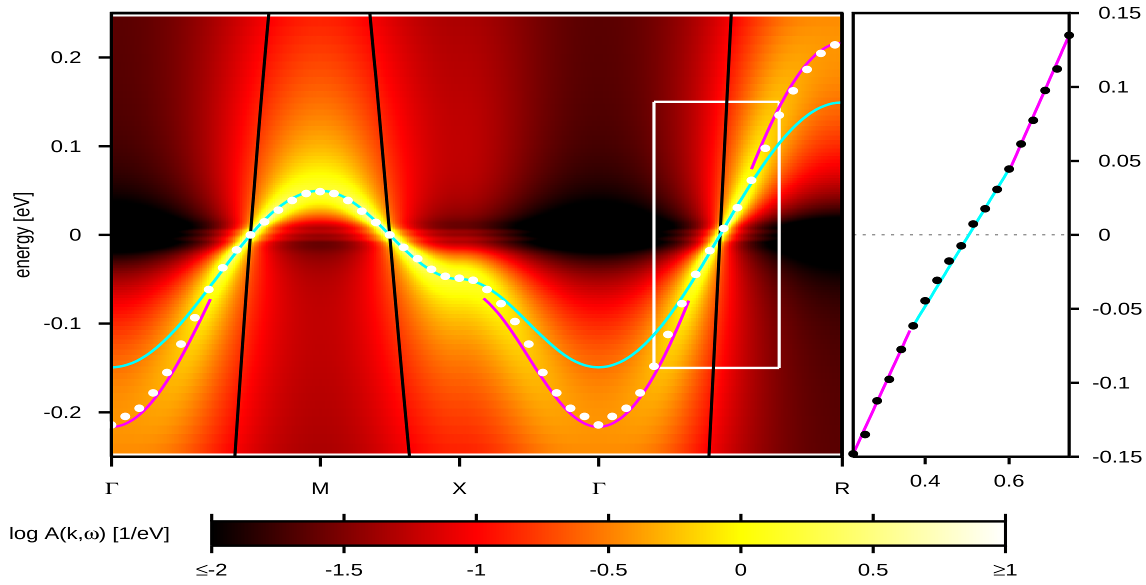



Fermi liquid $Z_{FL} \lesssim 1$: $E_{\mathbf{k}} = Z_{FL}\epsilon_{\mathbf{k}}$ for $|E_{\mathbf{k}}| < \omega_*$

$E_{\mathbf{k}} = \epsilon_{\mathbf{k}}$ for $|E_{\mathbf{k}}| > \omega_*$

# Kinks due to strong correlations




Fermi liquid $Z_{FL} \ll 1$: $E_{\mathbf{k}} = Z_{FL}\epsilon_{\mathbf{k}}$ for $|E_{\mathbf{k}}| < \omega_*$

Different renormalization $Z_{CP} \ll 1$: $E_{\mathbf{k}} = Z_{CP}\epsilon_{\mathbf{k}} \pm c$ for $|E_{\mathbf{k}}| > \omega_*$

# Mathematical explanation of kinks within DMFT

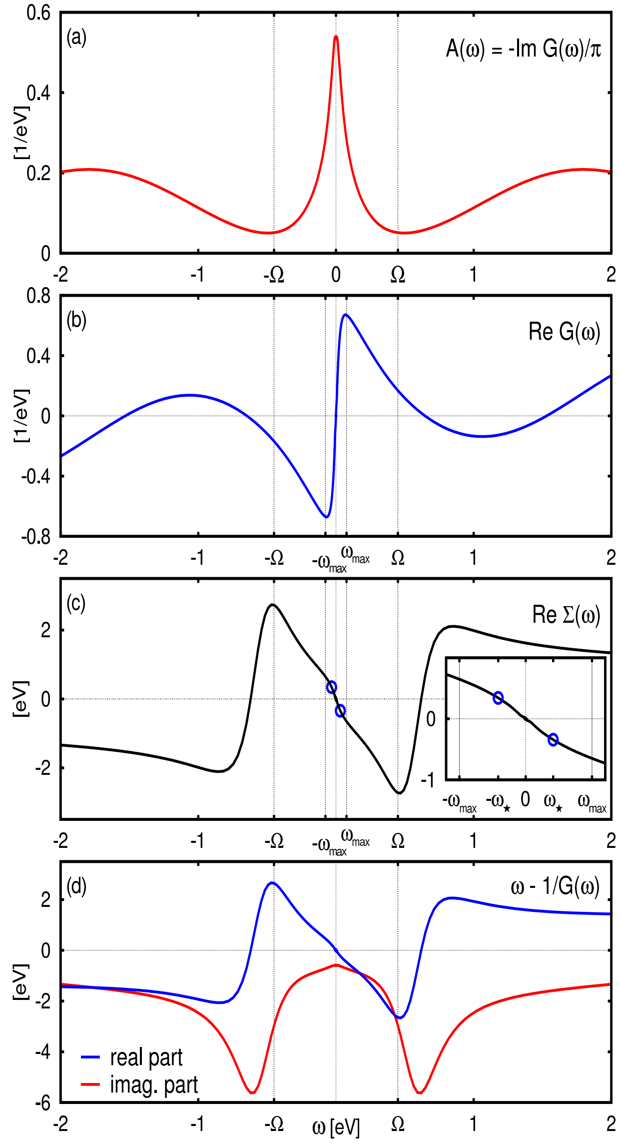
DMFT self-consistency condition

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

$$\Delta(G(\omega)) \approx (m_2 - m_1^2)G(\omega) + ...$$

Three-peak structure sufficient condition

Fermi-liquid for $|\omega| < \omega_* \sim Z_{FL}$



# Microscopic predictions

Starting from:

- $\epsilon_{\mathbf{k}}$ - bare dispersion relation

$$G_0(\omega) = \sum_{\mathbf{k}} \frac{1}{\omega - \epsilon_{\mathbf{k}}}$$

- $Z_{FL}$

we predict that:

# Microscopic predictions

- Kink position

$$\omega_* = 0.41 Z_{FL} \frac{\mathrm{Im} 1/G_0}{\mathrm{Re} G_0'/G_0^2}$$

- Intermediate energy regime

$$Z_{CP} = Z_{FL} \frac{1}{\mathrm{Re} G_0'/G_0^2}$$

- Change in the slope $Z_{FL}/Z_{CP}$ interaction independent
- Curvature of the kink $\sim Z_{FL}^2$
- Sharpness of the kink $\sim 1/Z_{FL}^2$
- Sharper for stronger $U$

# Outlook: possible origin of the "waterfalls"

"Waterfalls": kinks at $\omega_\star \approx$ 300-400 meV in cuprates

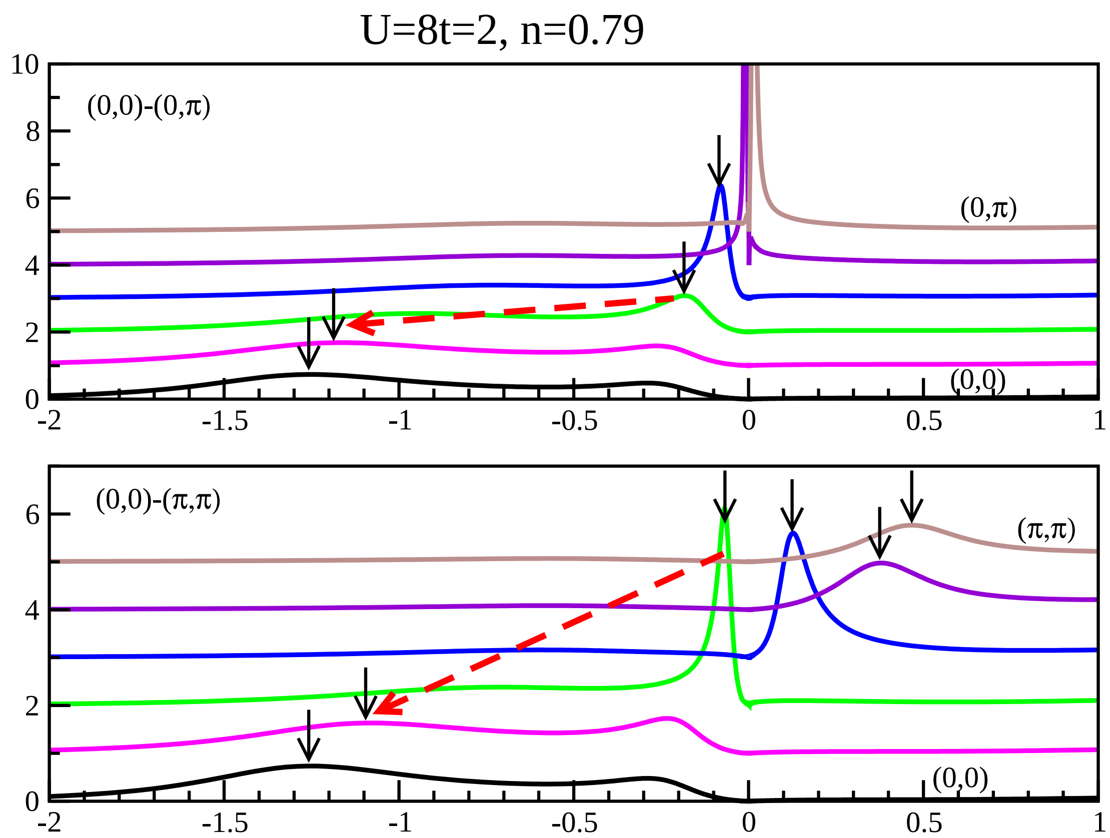
- crossover to Hubbard bands? Wang et al. (2006)
- $U \gg t \Rightarrow$ dispersion goes from central peak to Hubbard band

K. Byczuk, M. Kollar (unpublished)

$$\Sigma(\omega) = \Sigma_0 + \frac{\Sigma_1}{\omega} + O\left(\frac{1}{\omega^2}\right)$$

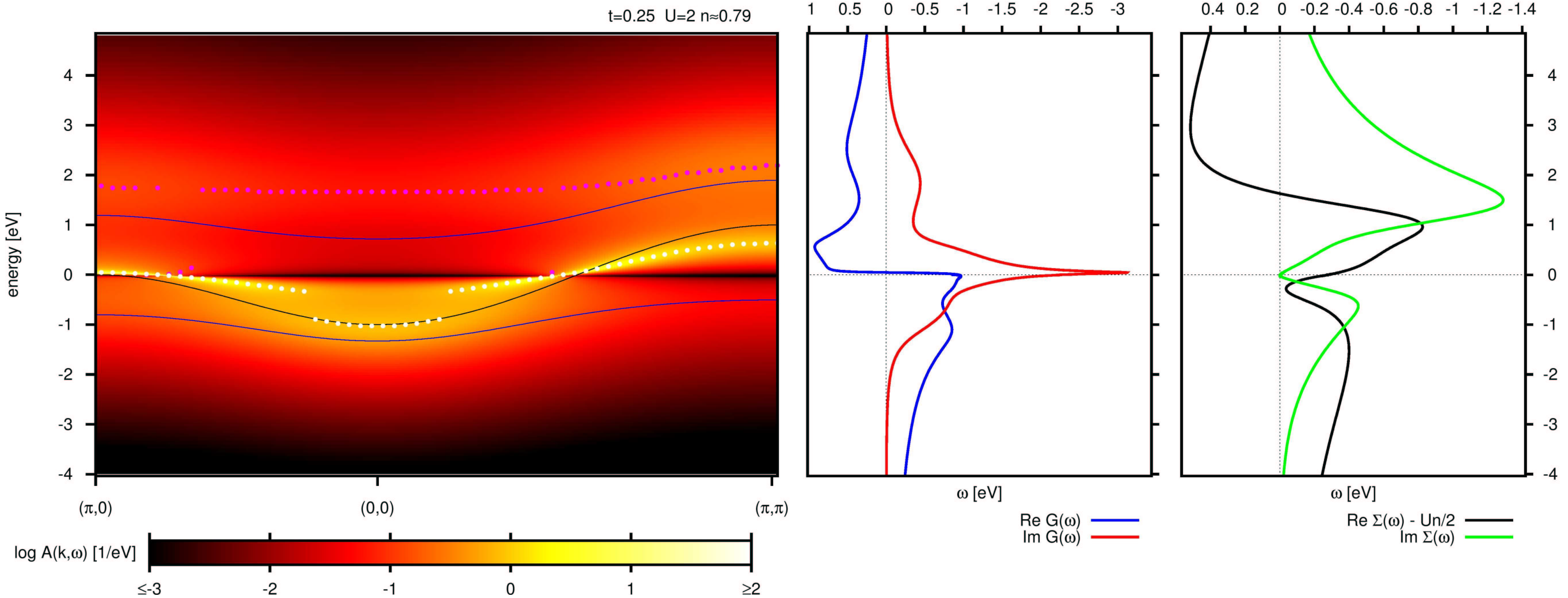
$$\Downarrow$$

$$E_{\boldsymbol{k}}^{\text{UHB,LHB}} \approx \frac{1}{2}\left[\epsilon_{\boldsymbol{k}} \pm \sqrt{\epsilon_{\boldsymbol{k}}^2 + cU^2}\right]$$



# Crossover to Hubbard bands

Hubbard model, square lattice, DMFT(NRG), $U = 8t$, $n = 0.79$




- ImΣ decays faster than ReΣ
- for large energies: $E_{\boldsymbol{k}}$ approaches $E_{\boldsymbol{k}}^{\text{UHB,LHB}}$
- waterfalls from central peak to LHB

K. Byczuk, M. Kollar (unpublished)
Y.-F. Yang, K. Held (unpublished)

# Conclusions

- Strong correlations (three peak spectral function) a sufficient condition for electronic kinks

- Energy scale for electronic kinks $\omega_* = Z_{FL} D$ determined by Fermi-liquid renormalization and bare (LDA) density of states

- $\omega_*$ sets the energy scale for Fermi-liquid regime where $E_{\mathbf{k}} = Z_{FL}\epsilon_{\mathbf{k}}$ for $|E_{\mathbf{k}}| < \omega_*$

- Beyond Fermi-liquid regime the dispersion is still renormalized and useful $E_{\mathbf{k}} = Z_{CP}\epsilon_{\mathbf{k}} \pm c$ for $|E_{\mathbf{k}}| > \omega_*$ where the offset $c$ and $Z_{CP}$ determined by $Z_{FL}$ and $D$

- Electronic kinks are within cluster extension of DMFT (DCA) $\Sigma_{\mathbf{K}}(\omega) = \omega - \frac{1}{G_{\mathbf{K}}(\omega)} - \Delta(G_{\mathbf{K}}(\omega))$

- Electronic kinks and waterfalls are generic feature of strongly correlated systems