Kinks in the dispersion relations of strongly correlated fermions

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dedicated to prof. Jozef Spałek

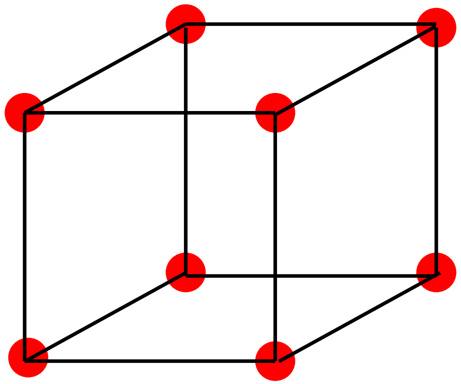
on the occasion of his 60th birthday

Collaboration

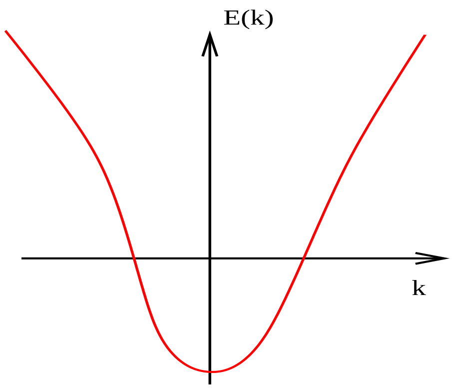
- M. Kollar, D. Vollhardt, Augsburg, Germany
- K. Held, Y.-F. Yang, Stuttgart, Germany
- I. Nekrasov, Ekaterinburg, Russia
- T. Pruschke, Göttingen, Germany

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 τ

(iii) proper set of quantum numbers

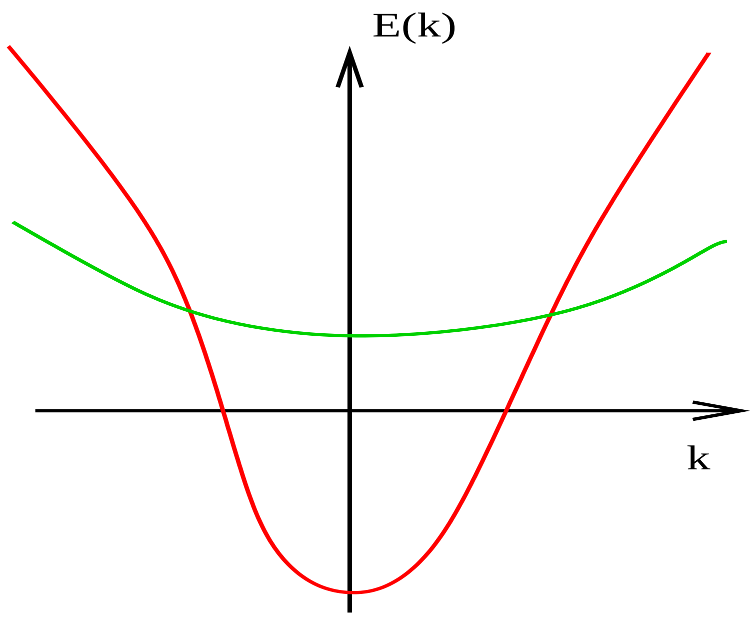
(iv) statistics

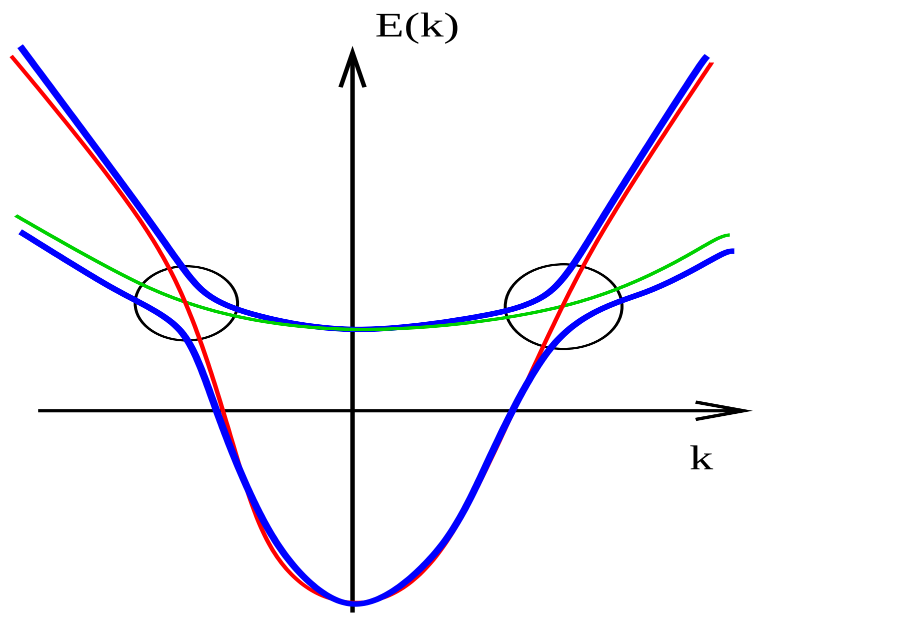
Dispersions and kinks

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

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

anticrossing, lifting degeneracy, ...

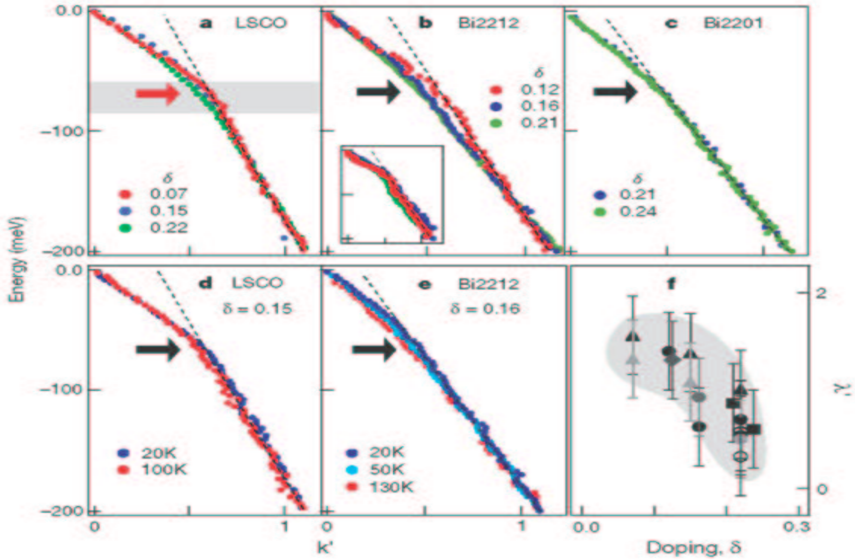


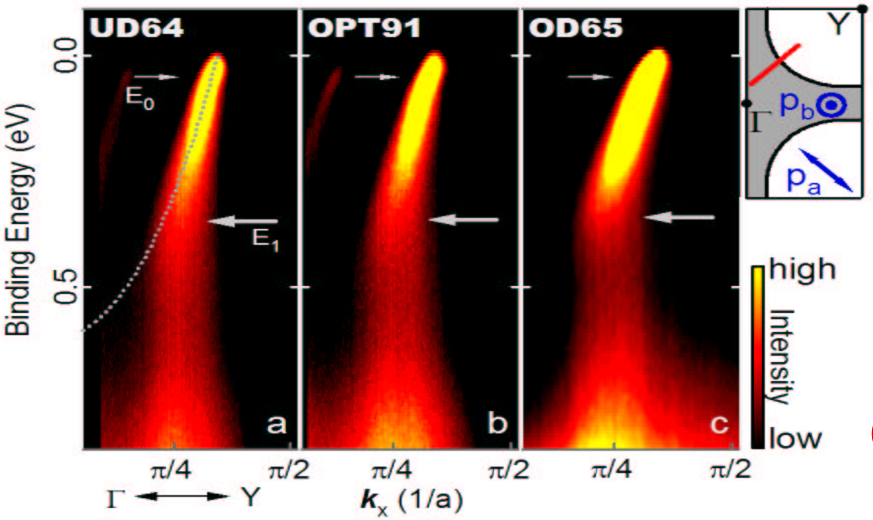


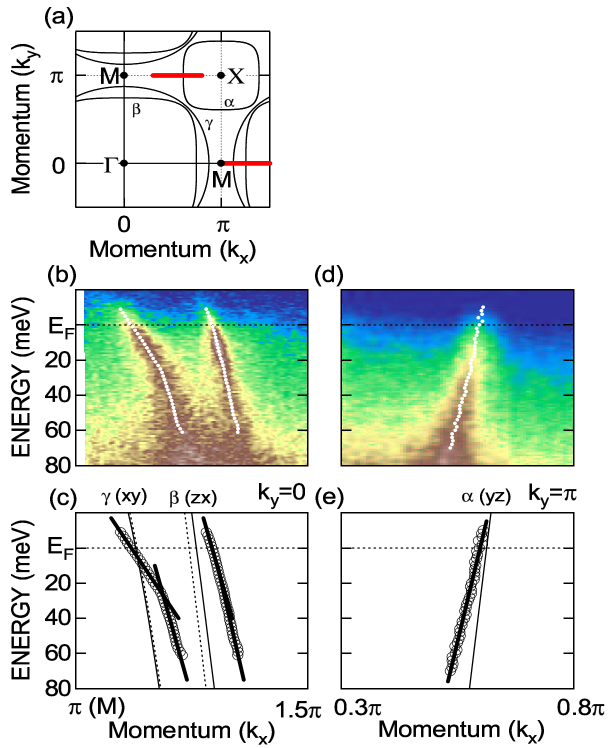
Df. kinks are abrupt slope changes in the dispersion relations

they provide information on different modes and their coupling

Examples of kinks in ARPES







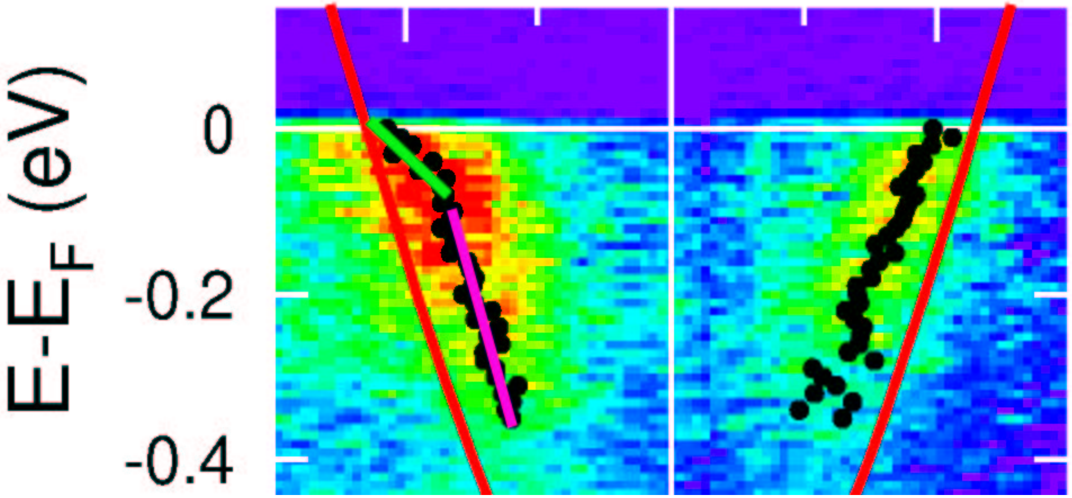
Sr_2RuO_4, cond-mat/0508312

Kinks seen experimentally between 20-800 meV

Origin: phonos, spin fluctuations, often not known

different HTC systems, cond-mat/0604284, cond-mat/0607319

More examples of kinks in ARPES



$SrVO_3$, cond-mat/0504075

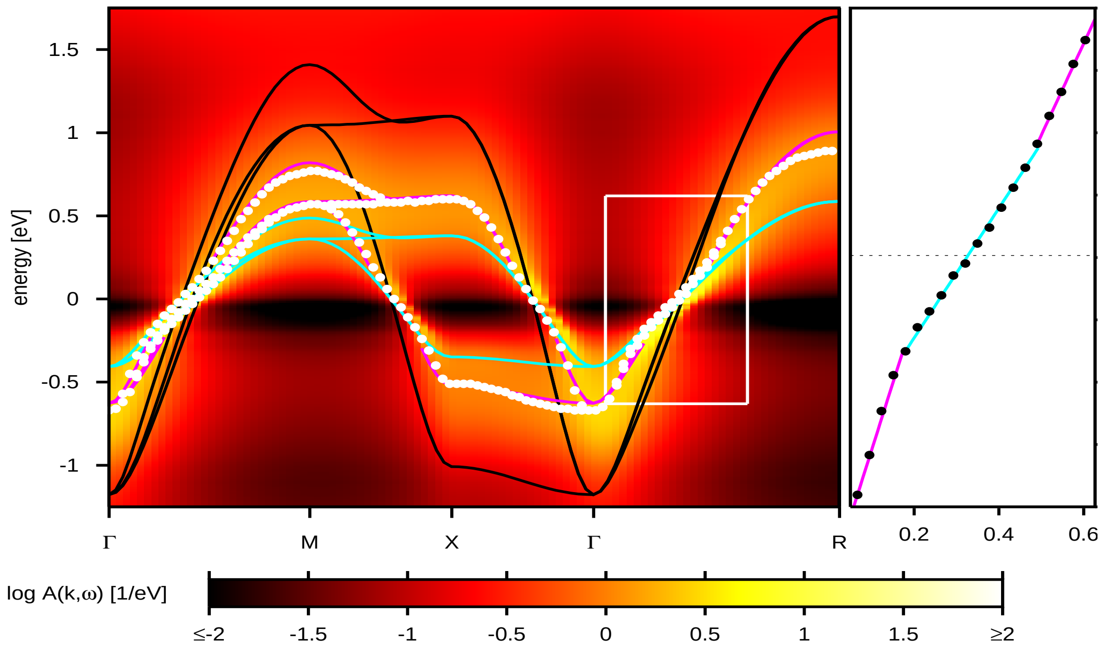
Kinks seen experimentally at 150 meV

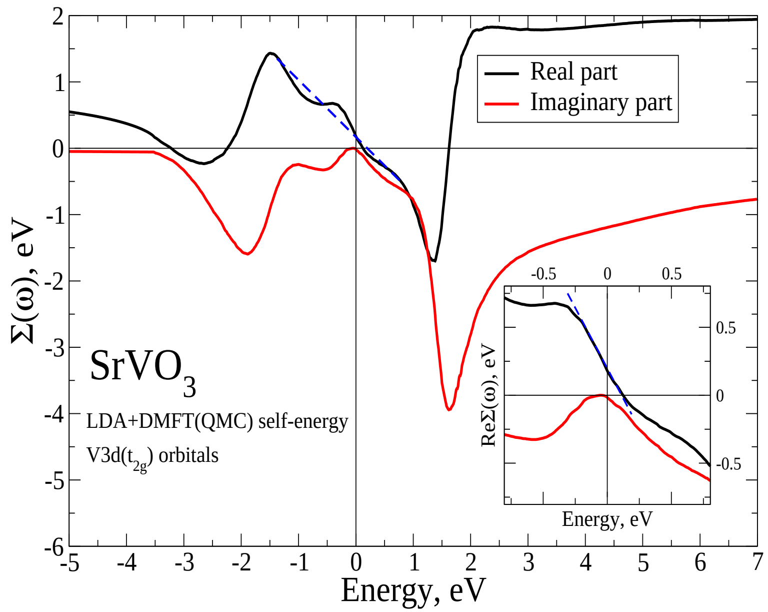
Pure electronic origin?

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)

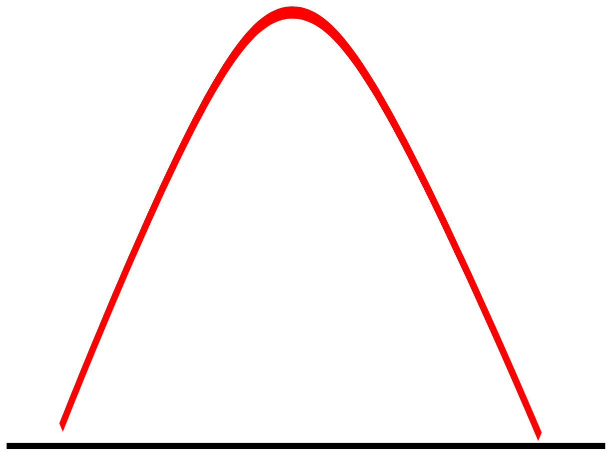


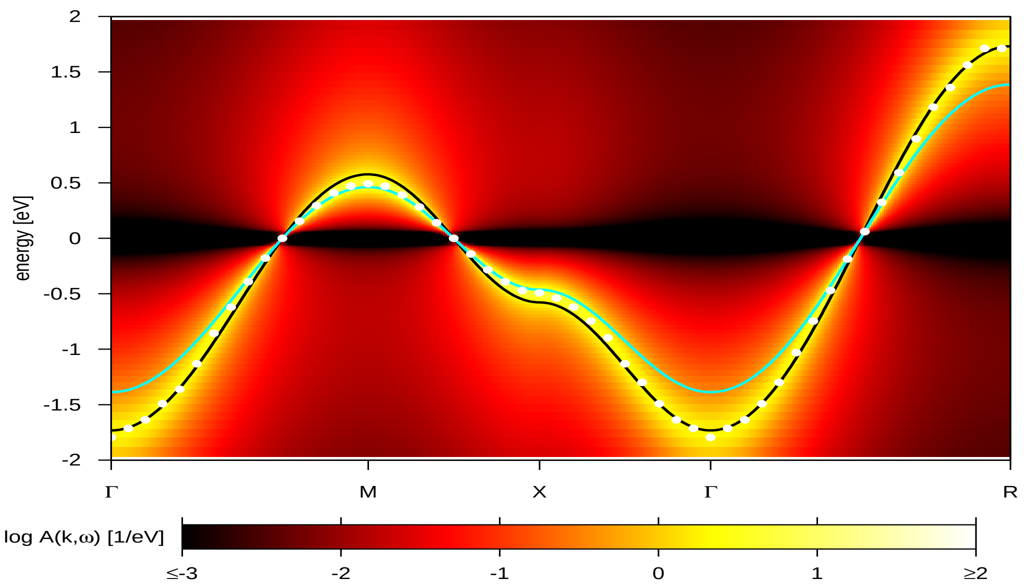


$$G_{\mathbf{k}}(\omega) = \frac{1}{\omega+\mu-\epsilon_{\mathbf{k}}-\Sigma(\omega)} \quad \rightarrow E_{\mathbf{k}} + \mu - \epsilon_{\mathbf{k}} - \mathrm{Re}\Sigma(E_{\mathbf{k}}) = 0$$

Not found in SIAM with simple hybridization function! → DMFT self-consistency effect

Weakly correlated system

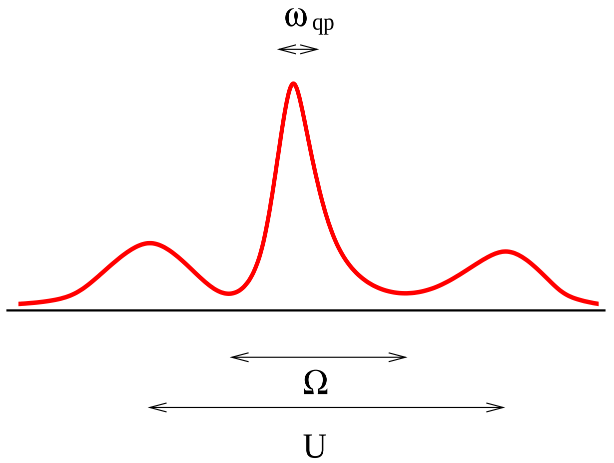


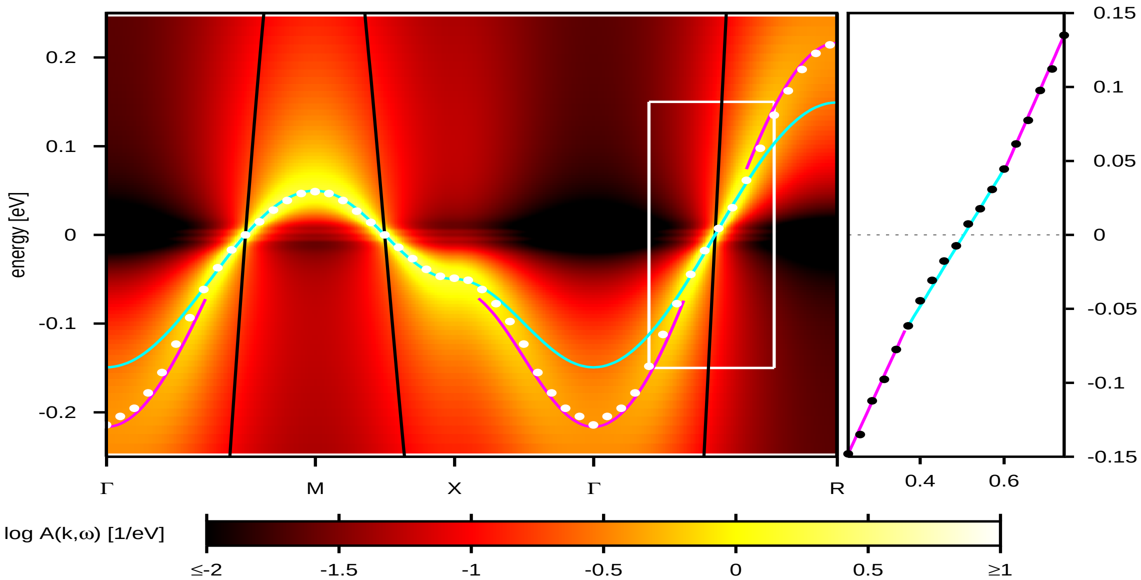


Fermi liquid $Z_{FL} \lesssim 1$: $E_{\mathbf{k}} = Z_{FL}\epsilon_{\mathbf{k}}$ for $|E_{\mathbf{k}}| < \omega_*$

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

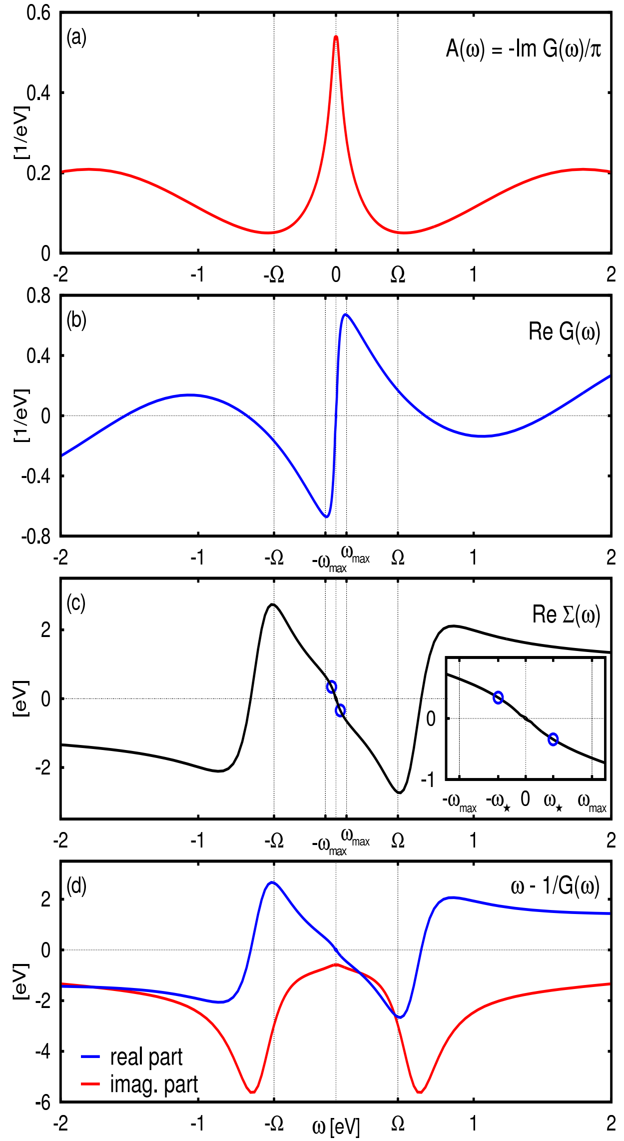
Different renormalization $Z_{CP} \ll 1$: $E_{\mathbf{k}} = Z_{CP}\epsilon_{\mathbf{k}} \pm c$ for $|E_{\mathbf{k}}| > \omega_*$

Mathematical explanation of kinks within DMFT

DMFT self-consistency condition

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

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



Microscopic predictions - summary

- 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
- ω_* 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 are generic feature of strongly correlated systems