Poor man´s explanation of kinks
in strongly correlated electron systems

Karsten Held (TU Wien)

ISSP Tokyo, June 27th 2014

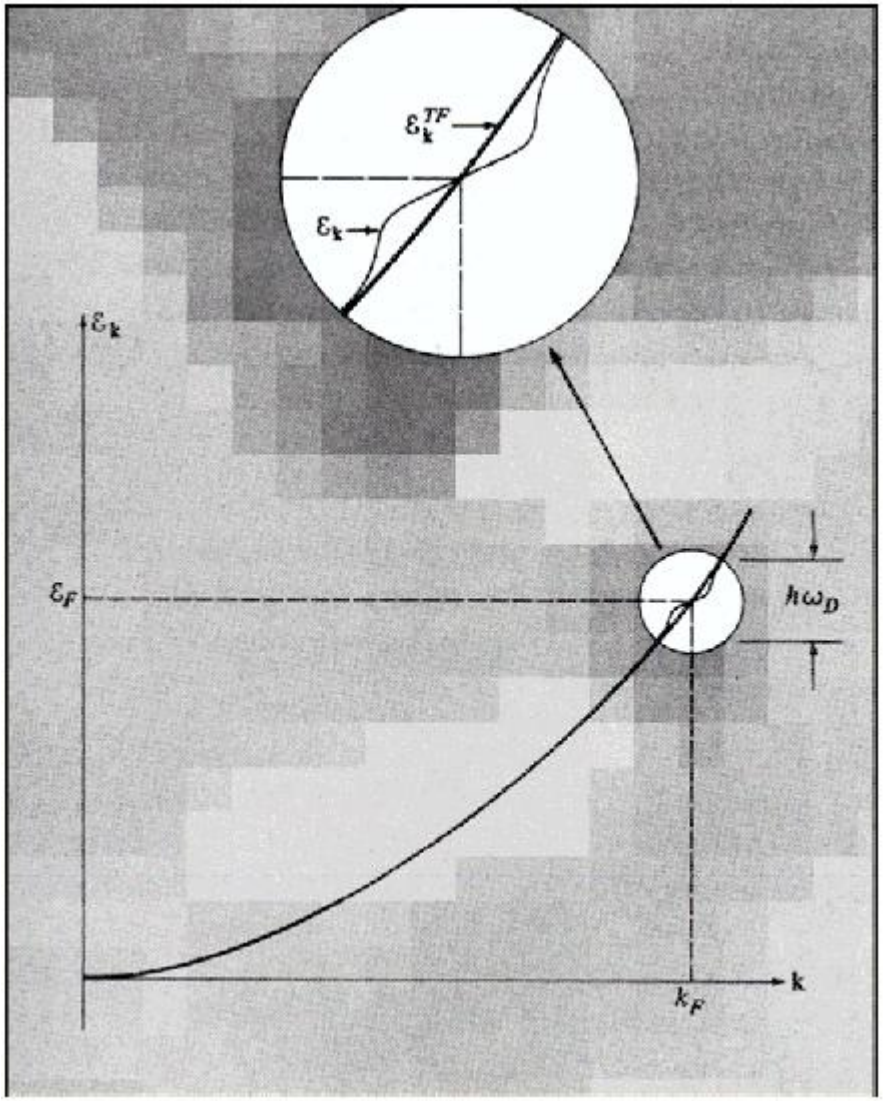
- **Kinks are everywhere**
- **Kinks are generic in SCES**
- **Kinks in SCES can be explained by Kondo effect**

Kinks in textbooks

Electron-phonon coupling
(or any boson)

→ kink in *E(k)*

Which boson?
phonon? paramagnon?



Ashcroft, Mermin, Solid State Physics '76

Kinks everywhere

in cuprates

in graphene

in tungsten

in platinum (110)

and everywhere …

- Mo (110) — Valla et al.'99
- Fe (110) — Schäfer et al.'04
- Na_xCoO_2 — Jin et al. '05
- Sr_2RuO_4 — Iwasawa et al.'04

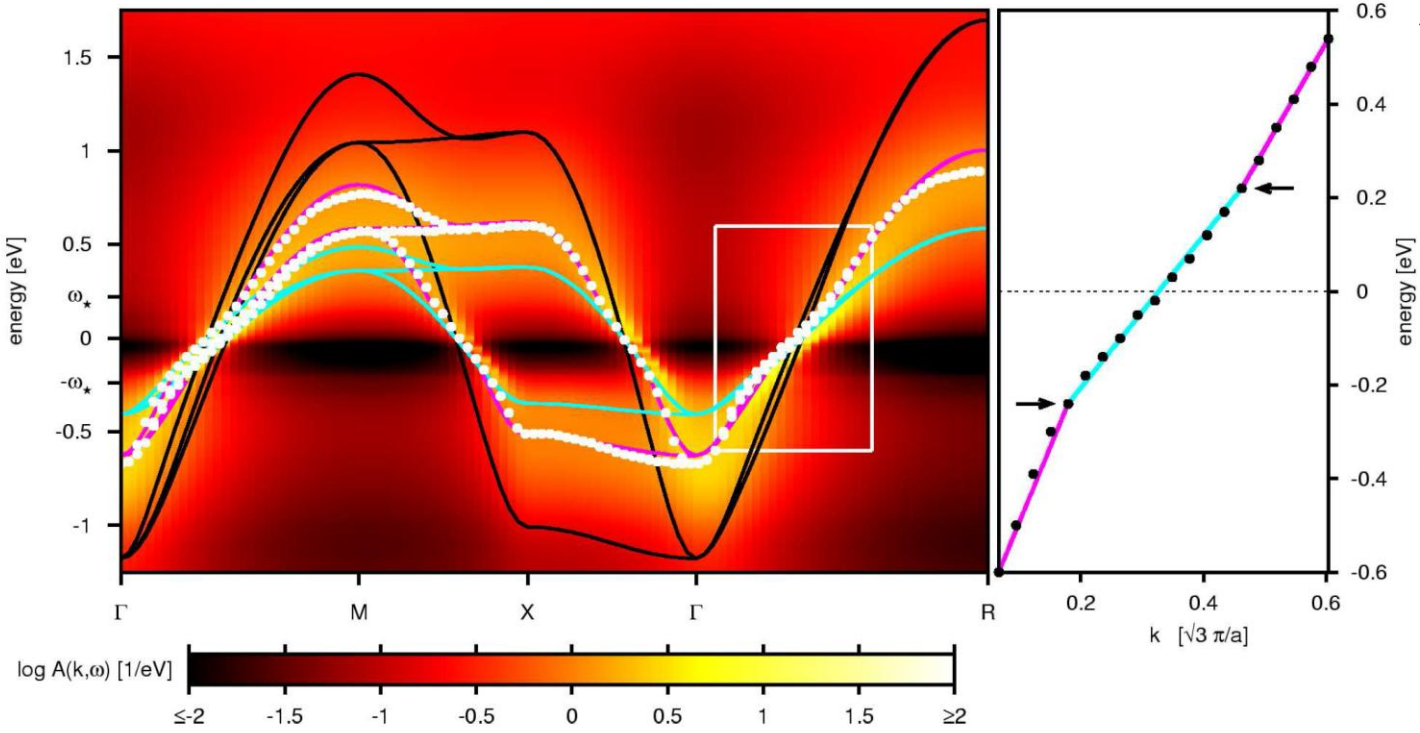
$La_{2-x}Sr_{1+x}Mn_2O_7$ — Sun et al.'05

…

Kinks in SCES (generic, no bosons)

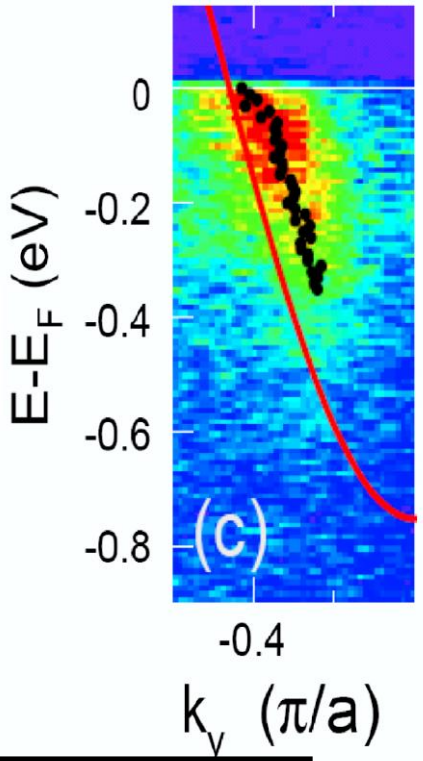
Kinks in $SrVO_3$: LDA+DMFT

Nekrasov et al. PRB'06



experiment

Fujimori et al.'06, Aizahi et al.PRL'12



two renormalization factors

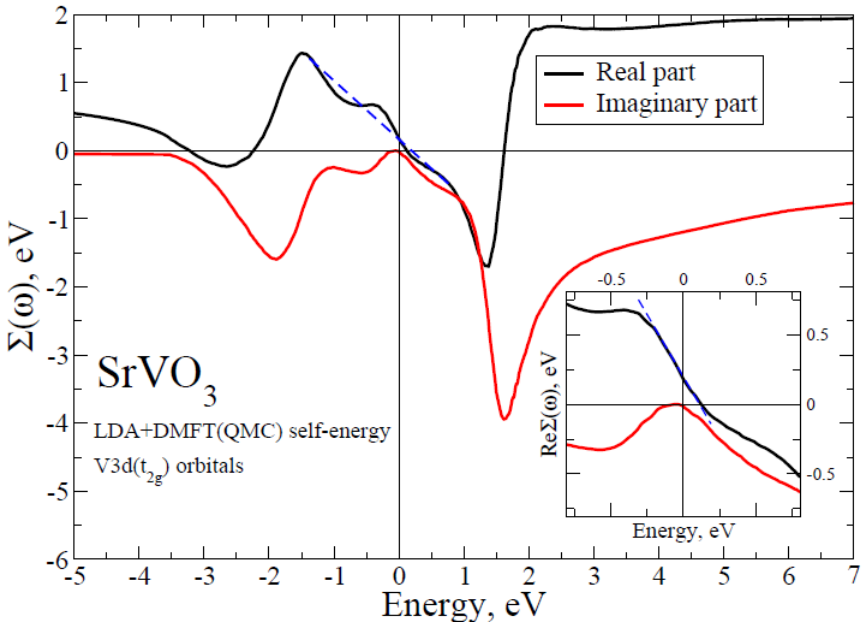
Fermi-liquid regime: $E_{\mathbf{k}} = Z_{\mathrm{FL}}\epsilon_{\mathbf{k}}$ $\quad |E_{\mathbf{k}}| < \omega_*$

Beyond FL regime: $E_{\mathbf{k}} = Z_{\mathrm{CP}}\epsilon_{\mathbf{k}} \pm c$ $\quad |E_{\mathbf{k}}| > \omega_*$

Kinks in SCES (generic, no bosons)

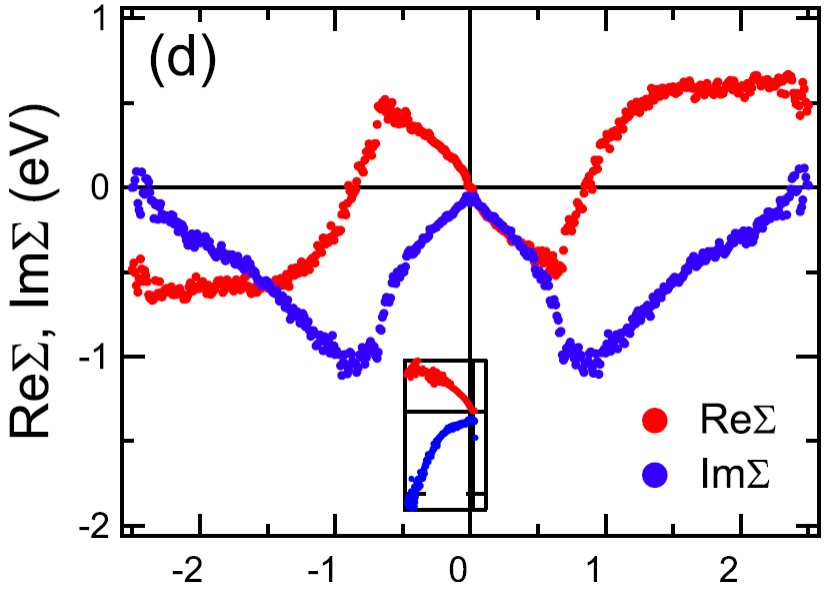
Kinks in $SrVO_3$: LDA+DMFT

Nekrasov et al. PRB'06



experiment

Aizaki et al.PRL'12



$E_k = e_k + \Sigma(E_k)$

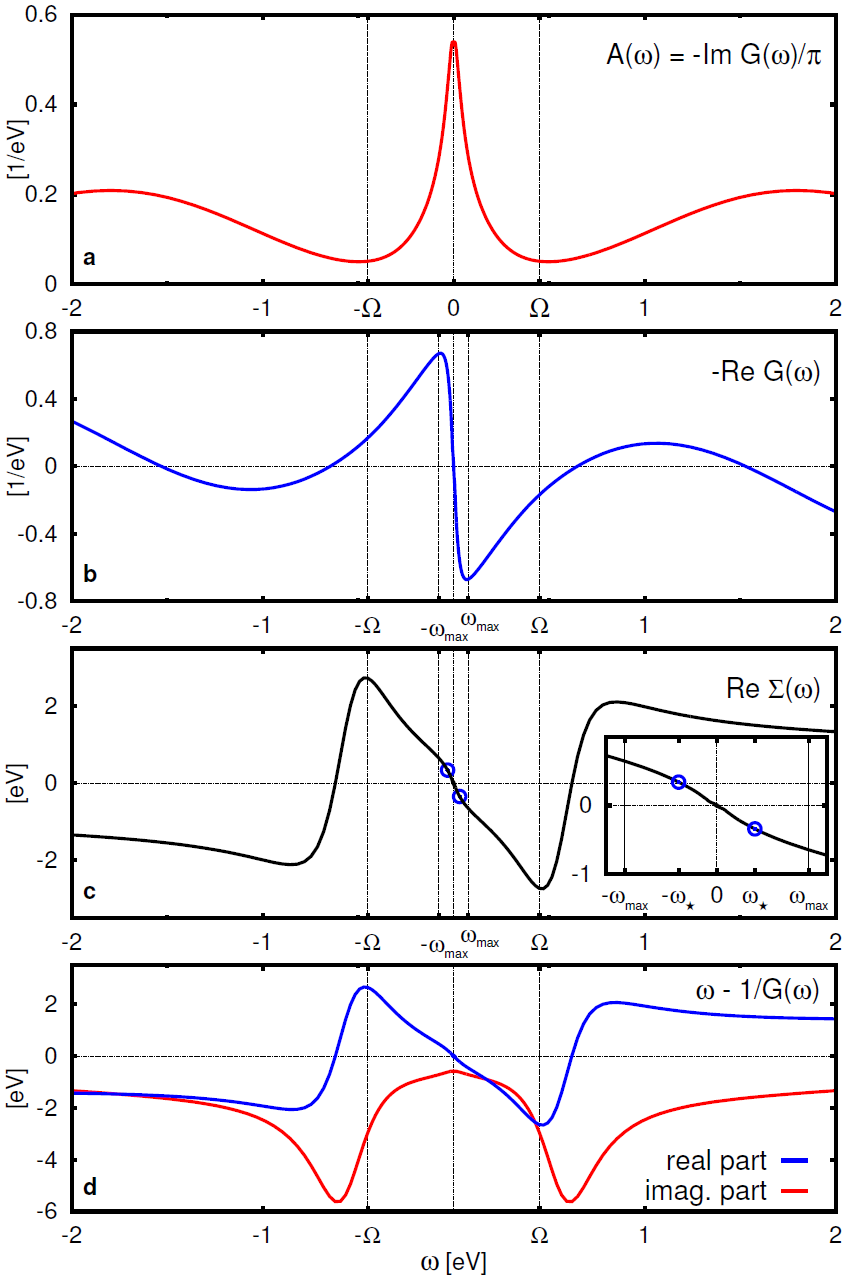
$Z = (1 - d\Sigma(\omega)/d\omega)^{-1}$

two renormalization factors

Fermi-liquid regime: $E_{\mathbf{k}} = Z_{\mathrm{FL}}\epsilon_{\mathbf{k}}$ $\quad |E_{\mathbf{k}}| < \omega_*$

Beyond FL regime: $E_{\mathbf{k}} = Z_{\mathrm{CP}}\epsilon_{\mathbf{k}} \pm c$ $\quad |E_{\mathbf{k}}| > \omega_*$

Mathematical explanation of kinks



3 peak strucutre in Im G(ω)

Kramers-Kronig

max |Re G(ω)|

$\Sigma(\omega)=\omega-1/G(\omega)-t^2G(\omega)+\ldots$

$\omega-1/G(\omega)$

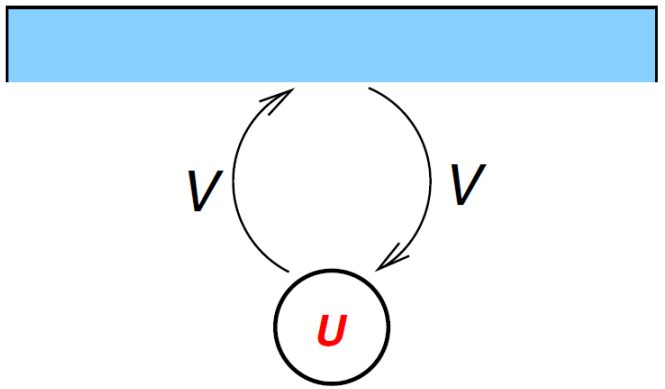
Z_{CP} and Z_{FL}

Byczuk et al. Nat.Phys'07

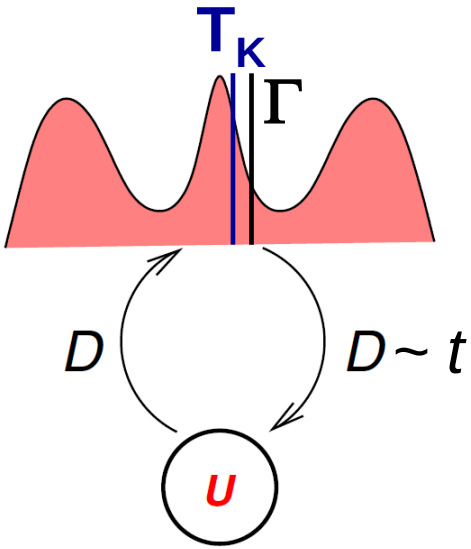
But what is the physical origin?

Kinks in SCES

Held, Peters, Toschi PRL'13



(usual) impurity model



correlated lattice model

no kink in Σ(ω)

kink in Σ(ω) and ARPES

one energy scale:
- **T_K= width of central peak**

two energy scales
- **kink energy = T_K**
- **width of central peak Γ**

Poor man's scaling

Anderson'70

$$dJ(\mathcal{D})/d\ln\mathcal{D} = -2\rho(\mathcal{D})J^2(\mathcal{D})$$

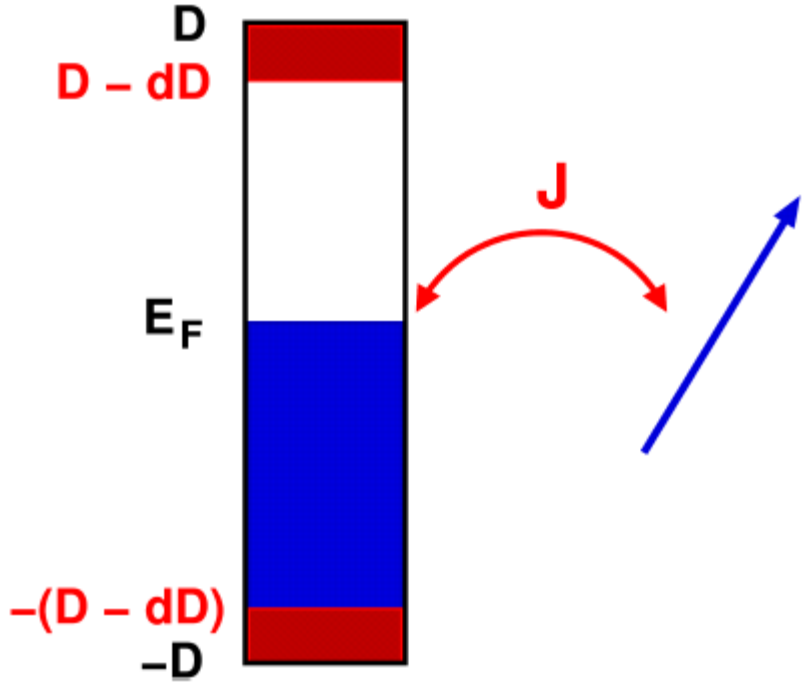
Flat wide band

$$\rho(\mathcal{D}) = \rho_0$$

$$\mathcal{D}e^{-1/(J(\mathcal{D})\rho_0)} = \mathcal{D}_0 e^{-1/(J(\mathcal{D}_0)\rho_0)} = const. \equiv T_K$$

Kondo model

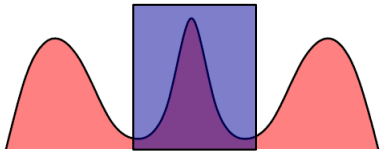
$$H = \sum_{k\sigma} \varepsilon_k n_{k\sigma} + J \vec{s}_0 \vec{S}$$



Poor man's scaling

Held, Peters, Toschi PRL'13

$$dJ(\mathcal{D})/d\ln\mathcal{D} = -2\rho(\mathcal{D})J^2(\mathcal{D})$$



correlated bath ~ Lorentzian $\rho(\mathcal{D}) = \rho_0\Gamma^2/(\mathcal{D}^2+\Gamma^2)$

$$\frac{\mathcal{D}^2}{\mathcal{D}^2+\Gamma^2}\, e^{-1/[J(\mathcal{D})\rho_0]} = \text{const.}$$

$T_K\,(J\to\infty) = \sqrt{\eta/(1-\eta)}\,\Gamma \quad \text{with} \quad \eta = e^{-1/[J(\mathcal{D}_0)\rho_0]} < 1$

two energy scales $T_K\,(J\to\infty) < \Gamma$

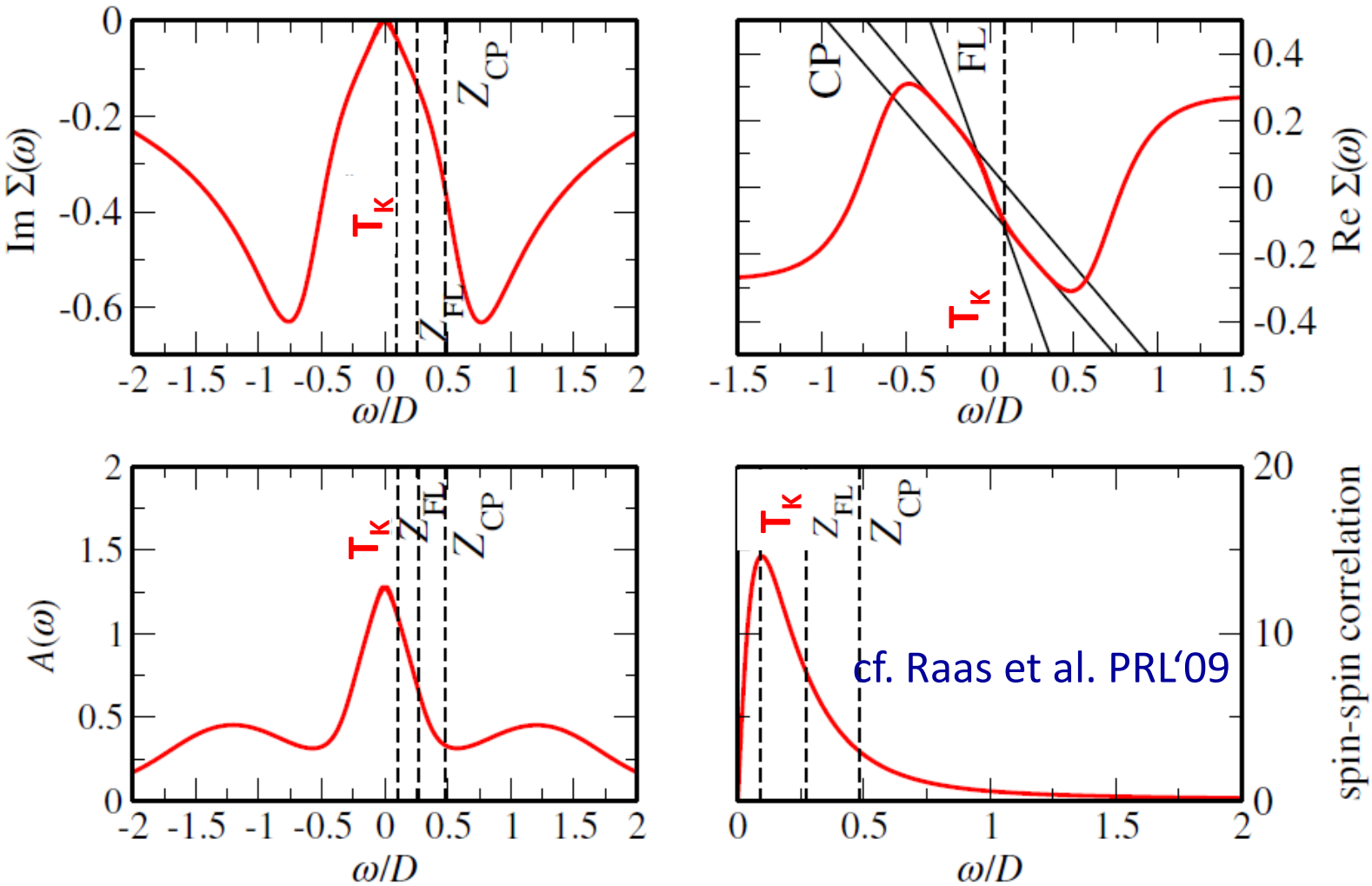
Kinks in SCES Hubbard model (DMFT)

Hubbard model U=2D

Held, Peters, Toschi PRL'13

$T_K = 0.21\Gamma$ (poor man)

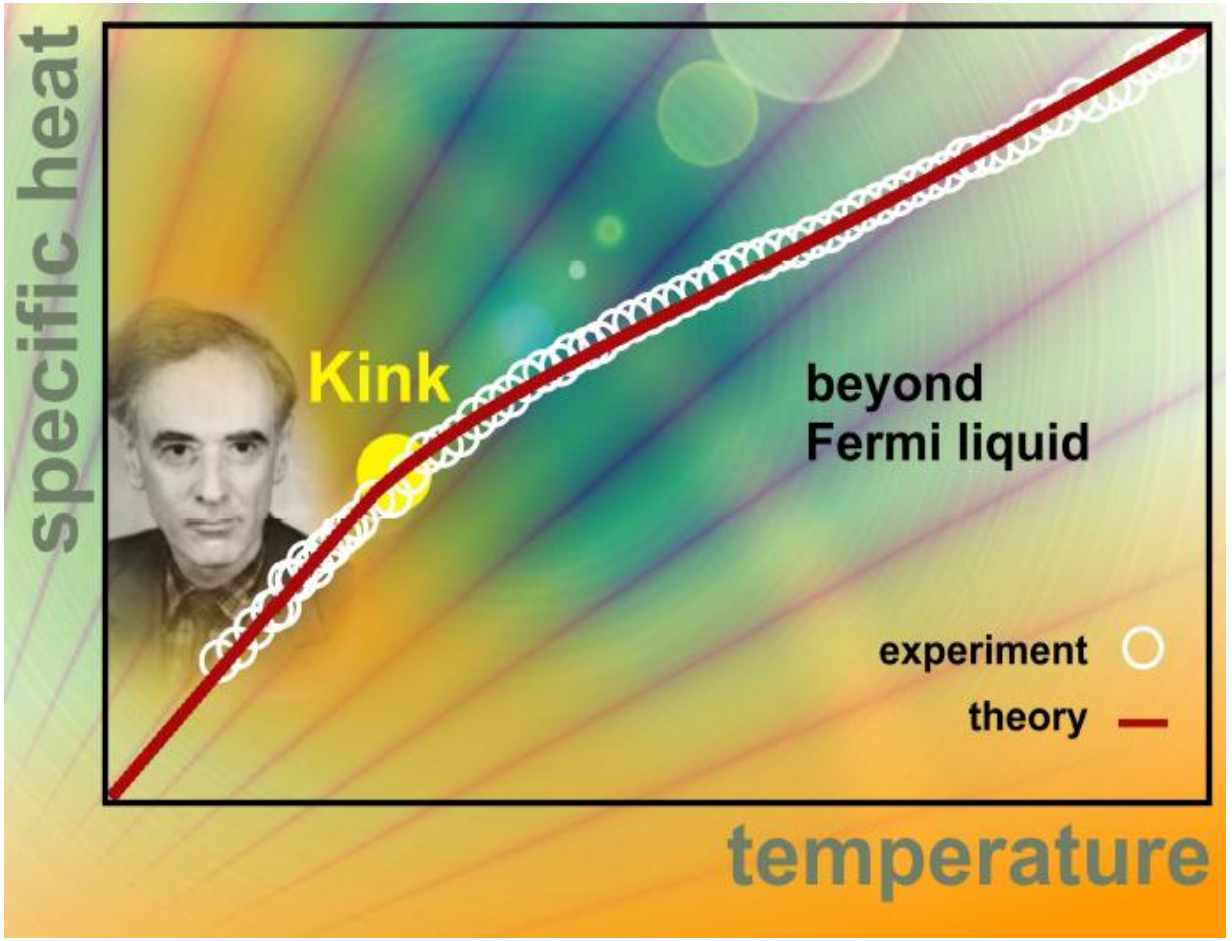
$\sim 0.21\Gamma$ (NRG)



Kinks in the specific heat

Toschi, Capone, Castellani, Held PRL'09

LiV_2O_4:
first d-electron heavy fermion system

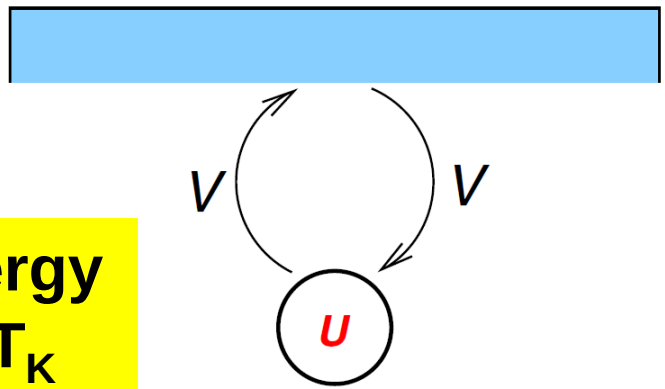


Conclusion

If your ARPES resolution is good enough, chances are high to see a kink

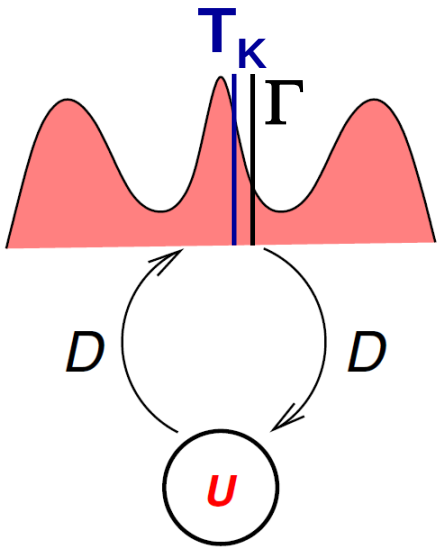
→ **origin I: phonons (or other bosons)**

→ **origin II: Kondo effect in lattice SCES**



(usual) impurity model

one energy scale T_K



correlated lattice model

two energy scales Γ,T_K & kink at T_K

Thanks…

Discovery by serendipity in LDA+DMFT for $SrVO_3$
I.A. Nekrasov, K. Held, G. Keller, D. E. Kondakov, T. Pruschke, M. Kollar, O.K. Andersen, V. I. Anisimov, D. Vollhardt,
Phys. Rev. B 73, 155112 (2006).

Mathematical explanation of kinks
K. Byczuk, M. Kollar, K. Held, Y.-F. Yang, I. A. Nekrasov, T. Pruschke, D. Vollhardt,
Nat. Phys. 3, 168 (2007).

(Physical) Poor man's explanation of kinks
K. Held, R. Peters, A. Toschi
Phys. Rev. Lett. 110, 246402 (2013)

Kinks in specific heat C_V
A. Toschi, M. Capone, C. Castellani, K. Held,
Phys. Rev. Lett. 102, 076402 (2009).

European Research Council
Established by the European Commission