Kinks in the dispersion relation of strongly correlated electrons

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Collaboration

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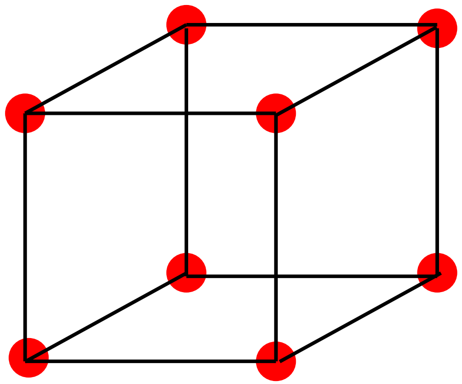
Support from SFB 484

Outline

- Kinks in the dispersion relations
- Origin of kinks in strongly correlated electrons
  - DMFT solution
  - Physical picture
- Predictions: energy scales and examples of kinks
  - Estimation of energy scale
  - Bethe DOS
  - Hypercubic DOS
  - $SrVO_3$
  - HTC and pd systems
- Conclusions and outlooks

Standard model of quantum many-body system



emergent particles

quasiparticle

quasihole

holon

spinon

plasmon

magnon

phonon

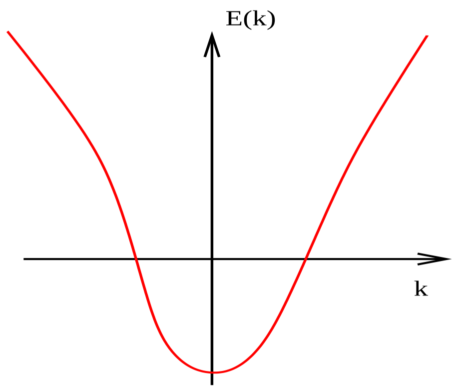
polariton

exciton

anyon

g-on

...



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

(ii) long (infinite) life-time τ

(iii) proper set of quantum numbers

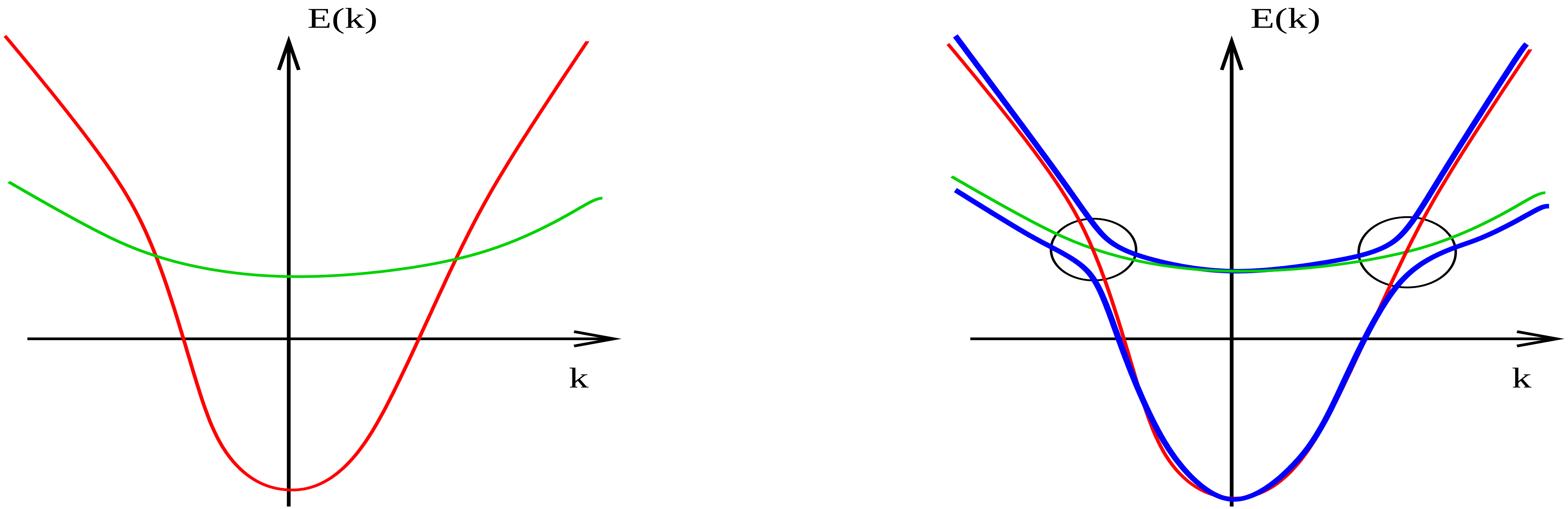
(iv) statistics

Dispersions and kinks

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

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

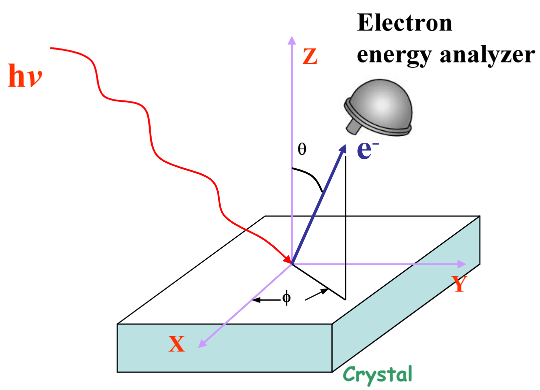
anticrossing, lifting degeneracy, ...

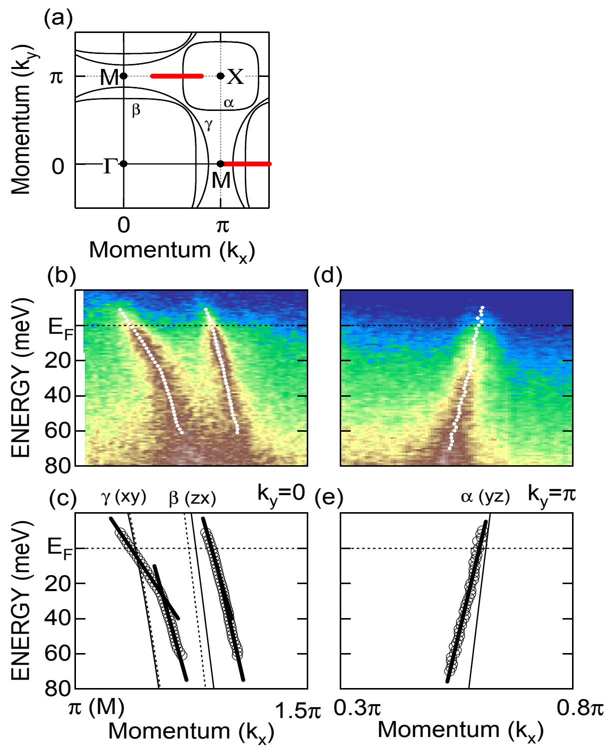


Df. **kinks are sudden slope changes in the dispersion relations**

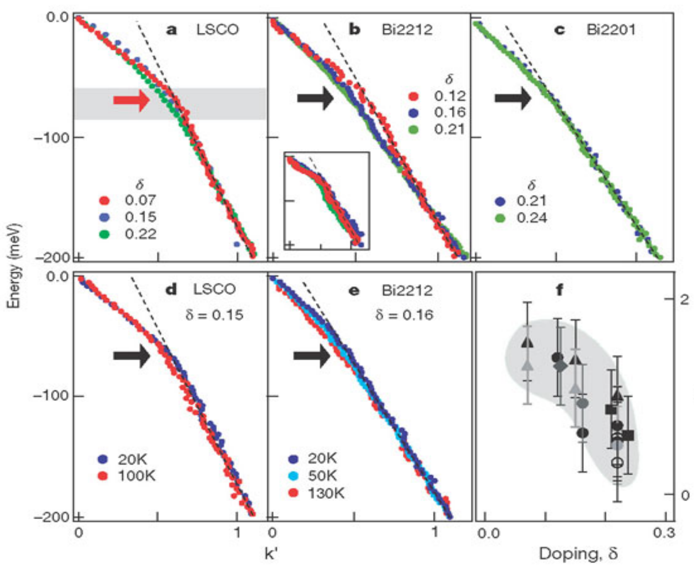
they provide information on different modes and their coupling

Examples of kinks in ARPES





Sr_2RuO_4, cond-mat/0508312



Kinks seen experimentally between 20-300 meV

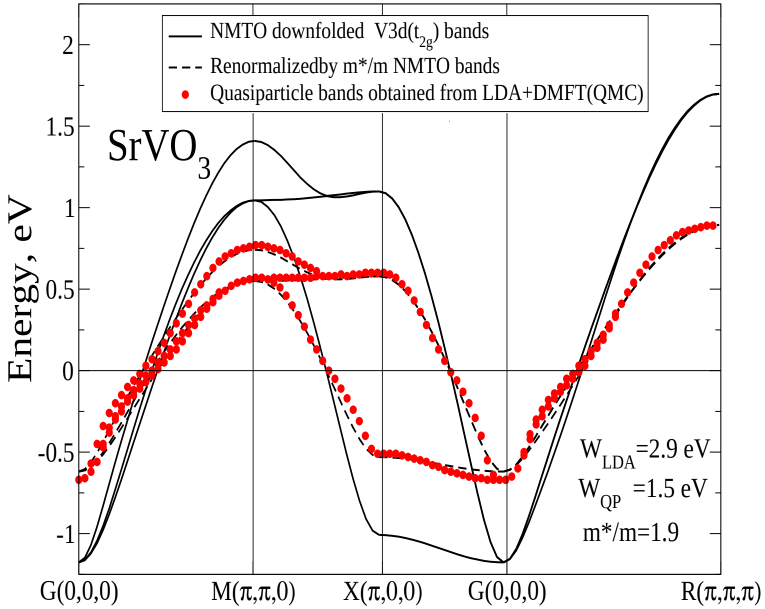
Origin: phonos, spin fluctuations, often not known

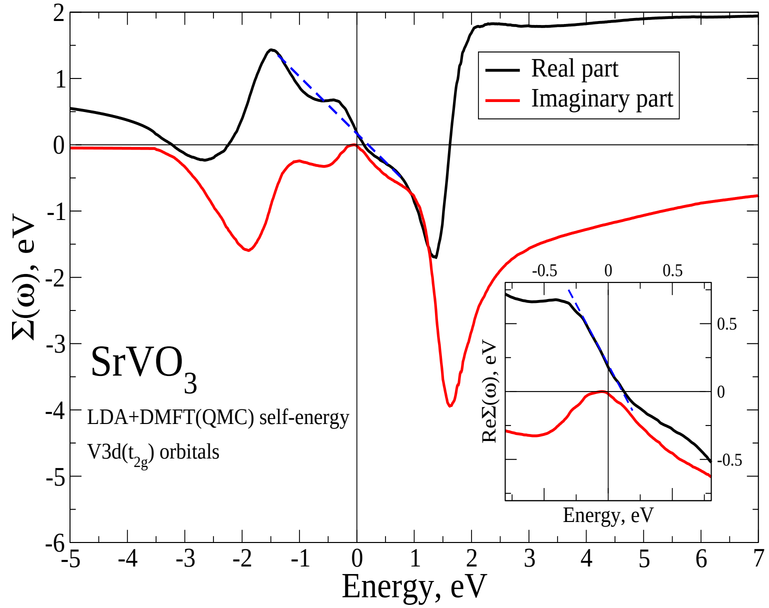
different HTC systems, cond-mat/0604284

Kinks in numerical DMFT solutions

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

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





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

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

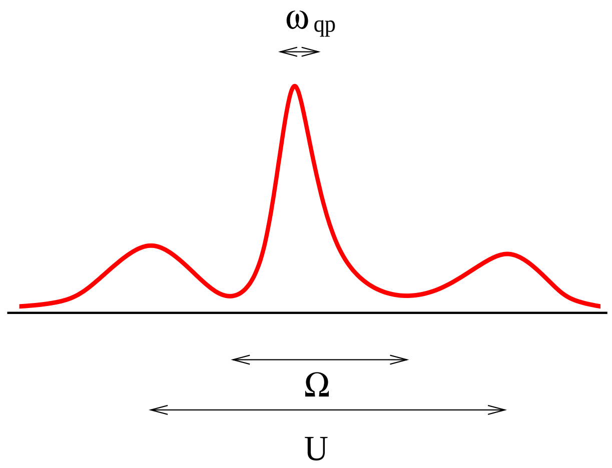
Origin of kinks within DMFT

Three peak structure is a sufficient condition to observe the kinks

- three separated energy scales

  1. ω_{qp} - quasiparticle width
  2. Ω - distance between dips
  3. U - distance between Hubbard satellites

$$\omega_{qp} \ll \Omega \ll U$$



- DMFT lattice self-consistency

$$\Sigma(\omega) = \omega + \mu - R[G(\omega)], \quad \text{inverse of} \quad G_0(\omega) = \int d\omega' \frac{N_0(\omega')}{\omega - \omega'}$$

Mathematical explanation of kinks within DMFT

Moment expansion for $R[G(\omega)]$

$$R[G(\omega)] = \frac{1}{G(\omega)} + m_1 + (m_2 - m_1^2)G(\omega) + (m_3 - 3m_2m_1 + 2m_1^3)G(\omega)^2 + ...$$

where $m_n = \int d\omega\, \omega^n N_0(\omega)$ the n-th moment of the DOS

DMFT self-consistency

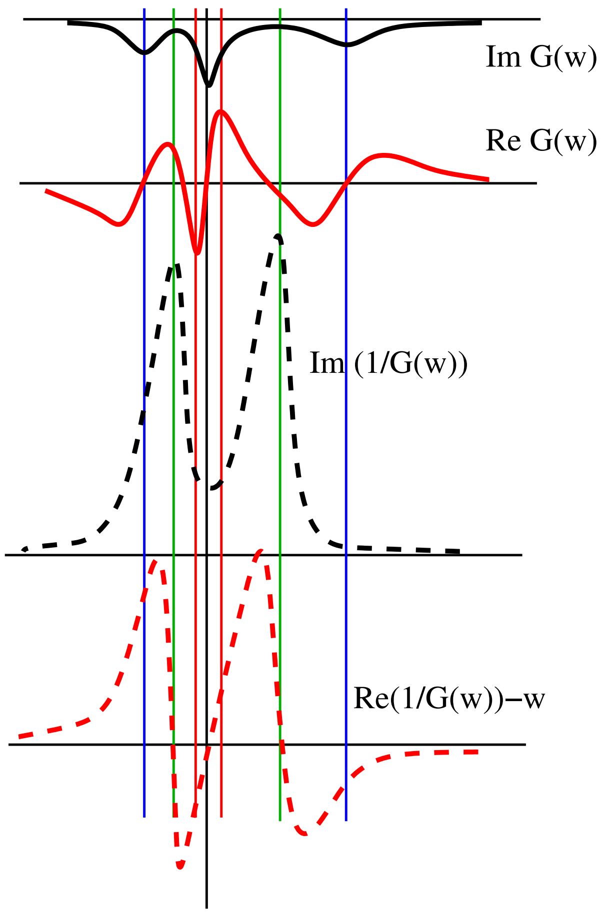
$$\Sigma(\omega) = \underbrace{\omega + \mu - \frac{1}{G(\omega)} + m_1}_{\omega+\tilde{\mu}-\frac{1}{G(\omega)}} - \underbrace{(m_2 - m_1^2)G(\omega) - (m_3 - 3m_2m_1 + 2m_1^3)G(\omega)^2 - ...}_{\Delta[G(\omega)]}$$

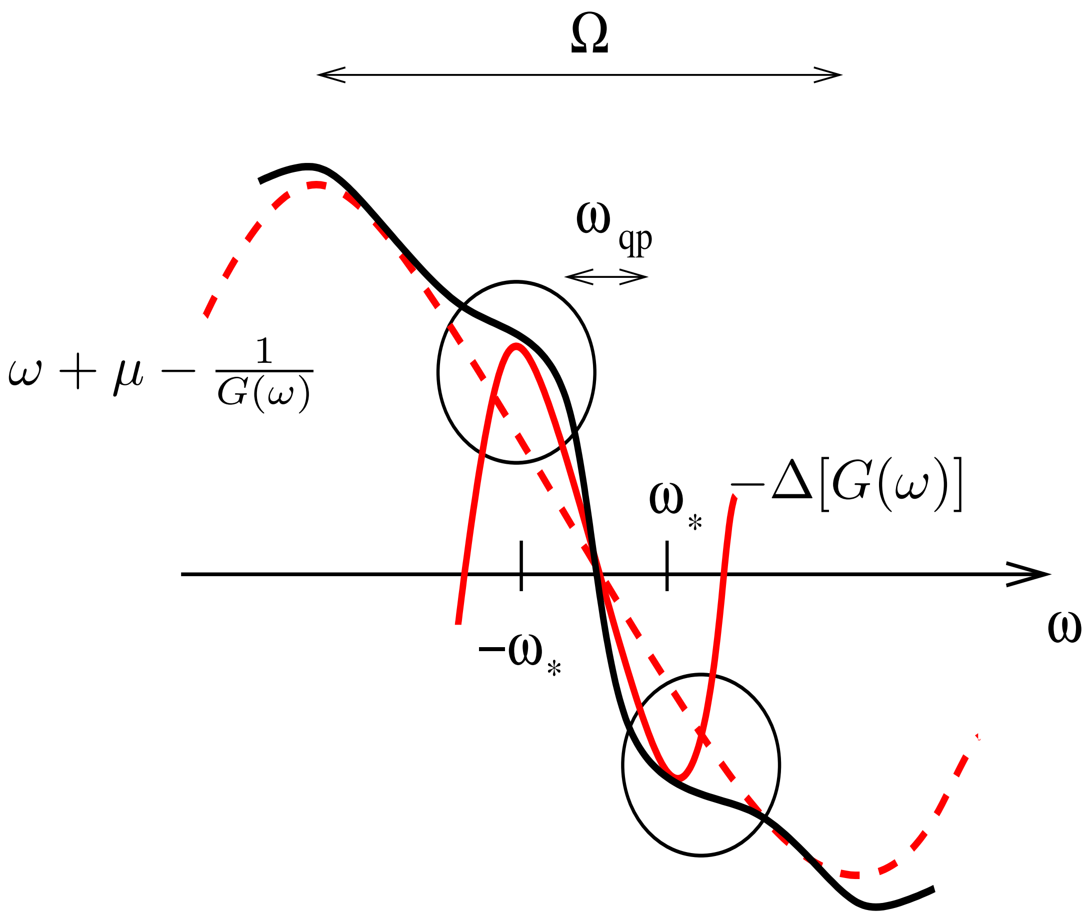
These two terms behave differently on the energy scale $|\omega| \lesssim \Omega$

$$\Sigma(\omega) = \omega + \mu - \frac{1}{G(\omega)} - \Delta[G(\omega)]$$

Mathematical explanation of kinks within DMFT

$$\Sigma(\omega) = \omega + \mu - \frac{1}{G(\omega)} - \Delta[G(\omega)]$$





contributions to $\mathrm{Re}\Sigma(\omega)$ and kinks at ω_*

Mathematical explanation - brief summary

When energy scales separate (three peak structure),

$$\omega_{qp} \ll \Omega \ll U,$$

the self-energy has two contributions:

$$\Sigma(\omega) = \omega + \mu - \frac{1}{G(\omega)} - \Delta[G(\omega)],$$

with two different behaviors:

- $\omega + \mu - \frac{1}{G(\omega)}$ is almost linear on the scale $|\omega| \lesssim \Omega$
- $\Delta[G(\omega)]$ is almost linear on the scale $|\omega| \lesssim \omega_{qp}$

energy scale ω_* of kinks is determined by slope changes in hybridization function $\Delta[G(\omega)]$

Beyond DMFT: DCA and further $N_c \to \infty$

When energy scales separate (three peak structure) at a given $\mathbf{K}$ point in BZ,

$$\omega_{qp}^{\mathbf{K}} \ll \Omega^{\mathbf{K}} \ll U,$$

the $\mathbf{K}$-resolved self-energy has two contributions:

$$\Sigma_{\mathbf{K}}(\omega) = \omega + \mu - \frac{1}{G_{\mathbf{K}}(\omega)} - \Delta[G_{\mathbf{K}}(\omega)],$$

with two different behaviors if close to Fermi surface:

- $\omega + \mu - \frac{1}{G_{\mathbf{K}}(\omega)}$ is almost linear on the scale $|\omega| \lesssim \Omega^{\mathbf{K}}$
- $\Delta[G_{\mathbf{K}}(\omega)]$ is almost linear on the scale $|\omega| \lesssim \omega_{qp}^{\mathbf{K}}$

Kinks are generic feature of strongly correlated metals with large spectral redistribution

Physical picture of the kink origin

$G_{\mathbf{k}}(\omega) = \frac{1}{\omega+\mu-\epsilon_{\mathbf{k}}-\Sigma(\omega)}$ with $\Sigma(\omega) = \omega + \mu - \frac{1}{G(\omega)} - \Delta[G(\omega)]$ leads to the dispersion relation $E_{\mathbf{k}}$ given by

$$\mathrm{Re}\left\{\frac{1}{G(E_{\mathbf{k}})} + \Delta[G(E_{\mathbf{k}})] - \epsilon_{\mathbf{k}}\right\} = 0$$

Approximate

$$\mathrm{Re}\left\{\frac{1}{G_{at}(E_{\mathbf{k}})} + \Delta[G_{qp}(E_{\mathbf{k}})] - \epsilon_{\mathbf{k}}\right\} = 0,$$

where

$$G_{at}(\omega) = \frac{1-n/2}{\omega+\mu+i\Gamma} + \frac{n/2}{\omega+\mu-U+i\Gamma} = \frac{1}{\omega+\mu+i\Gamma-\Sigma_{at}(\omega)}$$

and

$$G_{qp}(\omega) = \frac{Z^*}{\omega+\mu-\epsilon_{qp}+i\gamma}$$

with $\Delta[G(\omega)] = t^2 G(\omega)$.

Mapping onto three-level system

Eigen-value equation:

$$E_{\mathbf{k}} + \mu - U\frac{n}{2} - \epsilon_{\mathbf{k}} + i\Gamma - U^2 \frac{\frac{n}{2}(1-\frac{n}{2})}{E_{\mathbf{k}} + \mu - U(1-\frac{n}{2}) + i\Gamma} - \frac{Z^* t^2}{E_{\mathbf{k}} + \mu - \epsilon_{qp} + i\gamma} = 0$$

Equivalent three-level system Hamiltonian

$$H_{eff} = \begin{pmatrix} U(1-\frac{n}{2}) - \mu - i\Gamma & -U\sqrt{\frac{n}{2}(1-\frac{n}{2})} & 0 \\ -U\sqrt{\frac{n}{2}(1-\frac{n}{2})} & \epsilon_{\mathbf{k}} - \mu + U\frac{n}{2} - i\Gamma & -\sqrt{Z^*}t \\ 0 & -\sqrt{Z^*}t & \epsilon_{qp} - \mu - i\gamma \end{pmatrix}$$

and

$$\det(E_{\mathbf{k}} I - H_{eff}) = 0$$

gives the same spectrum.

Physical picture of the kink origin

Strong correlations leads to energy scale separation and formation effective three level system. Hybridization between three levels gives rise to kinks.