SMR.1667 - 6

Summer School and Miniconference on
Dynamical Mean-Field Theory for Correlated Electrons:
Applications to Real Materials, Extensions and Perspectives
25 July - 3 August, 2005

Approximate Treatments and Cluster Extensions III

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Cluster Extensions to the DMFT systems

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1. Motivation: Why need a cluster MFT?

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2. Realizations: DCA and CDMFT

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3. Selected results for DCA

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2. Realizations: DCA and CDMFT
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4. Summary

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Cluster Extensions to the DMFT

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2. Realizations: DCA and CDMFT
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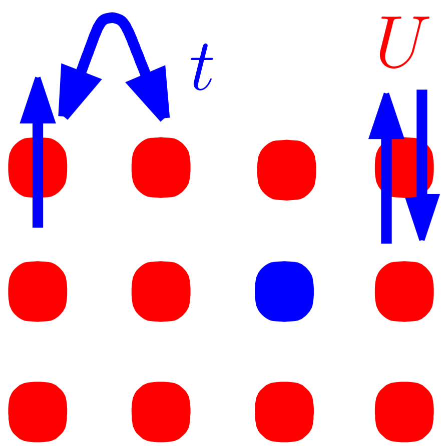
DMFT in a nutshell



$$H = \sum_{\langle i,j\rangle\sigma} t_{ij} d^\dagger_{i\sigma} d_{j\sigma} + \frac{U}{2}\sum_{i\sigma} n_{i\sigma} n_{i\bar{\sigma}}$$

non-local and dynamical

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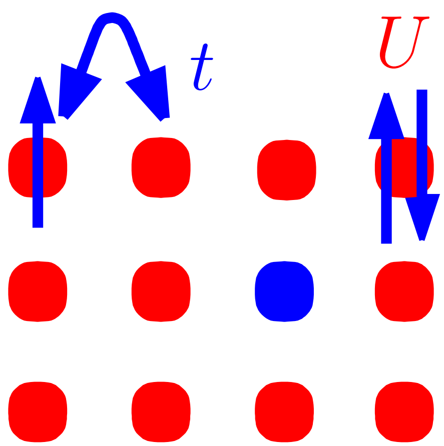
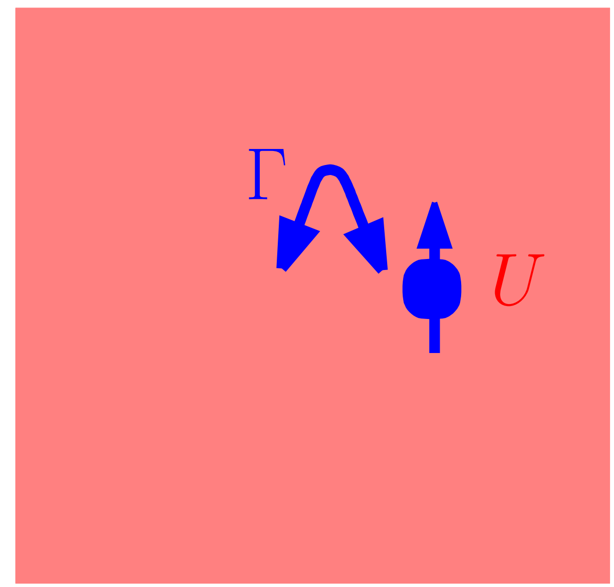


$$\Sigma(\vec{k}, z) \longrightarrow \Sigma(z)$$



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non-local and dynamical

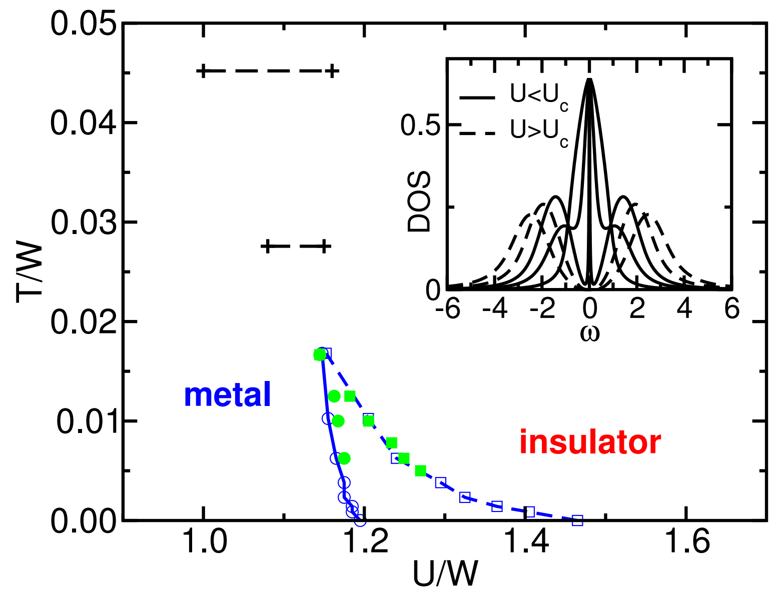
$$H_{\text{DMFT}} = H_{\text{Bath}} + H_U + H_{\text{Hyb}}$$

local and dynamical

Georges et al., RMP '96, Bulla et al.,PRL '99 & PRB '01

Key results from DMFT:

- Metal-insulator transition for $\langle n \rangle = 1$



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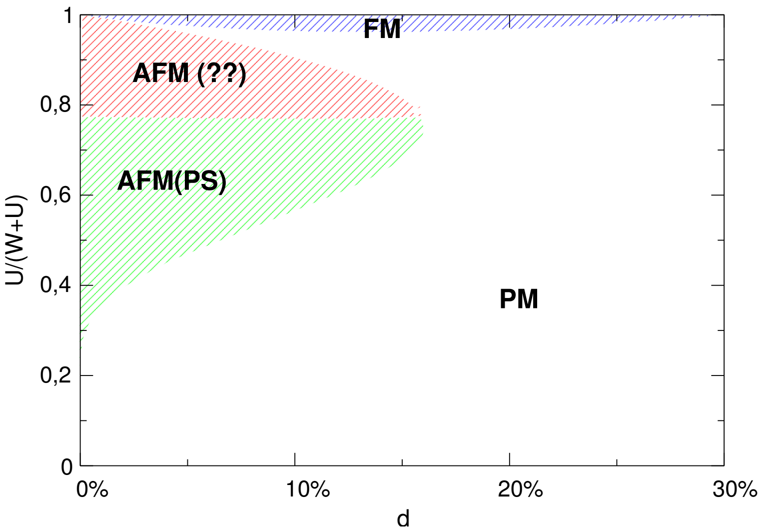
Zitzler et al., EPJ '02



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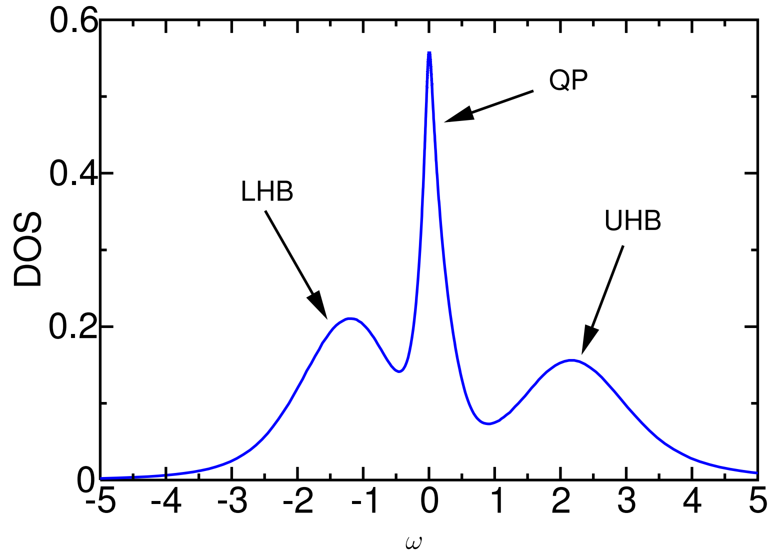

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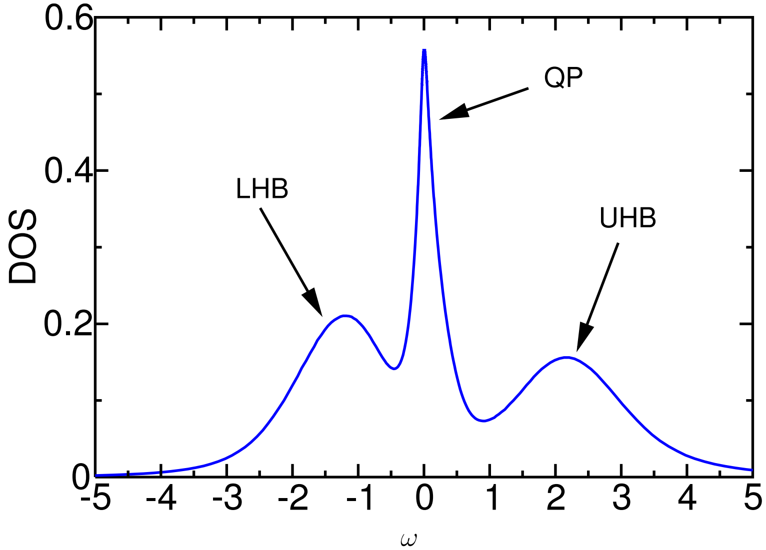

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✔ Thermondynamically consistent

✔ Non-trivial single-particle dynamics

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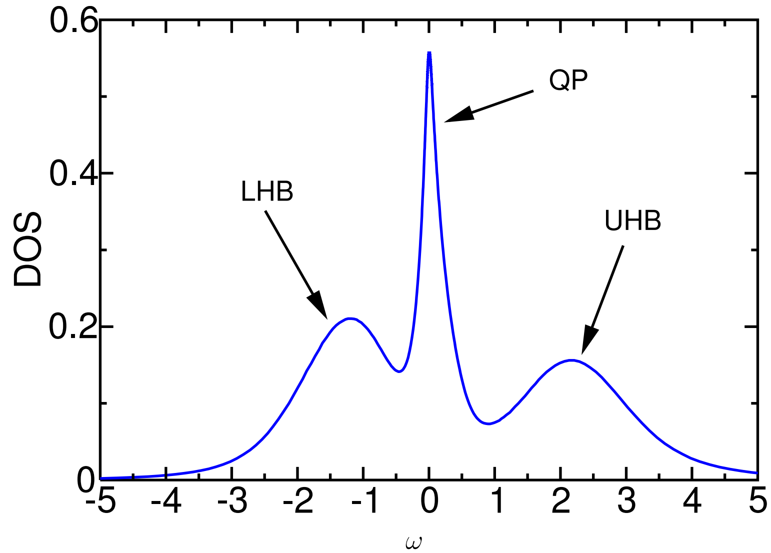

✔ Thermondynamically consistent

✔ Non-trivial single-particle dynamics

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✘ Only local dynamics & OPs

✘ Insensitiv to dimensionality

✘ Violation of Nernst's theorem

Where can and will DMFT go wrong?

Simple example: Old acquaintance Hubbard model in $D = 2$, at $\langle n \rangle = 1$

Expected physics:

- Ground state antiferromagnetic insulator for all $U > 0$
- Mermin-Wagner: No long-range order for $T > 0$
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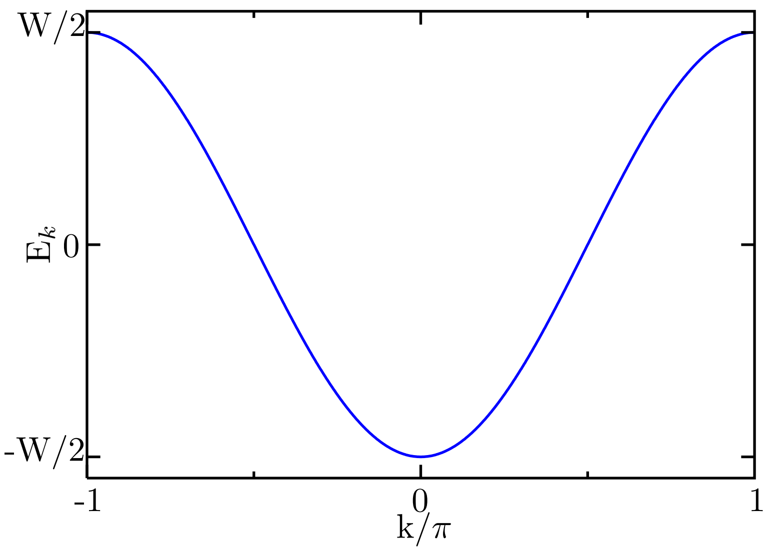
Answer from DMFT:

- Antiferromagnetic insulator for all $U > 0$ and $T < T_N$, $T_N(U) > 0$
- No order-parameter fluctuations as $T \gtrsim T_N$ (“spin-waves”)

DMFT: Long-range AF order



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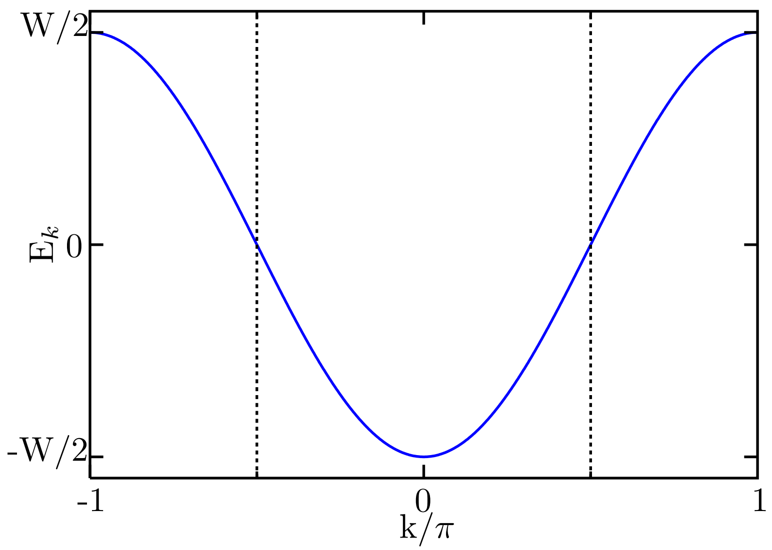

broken translational symmetry

$\Rightarrow$ reduced Brillouin zone

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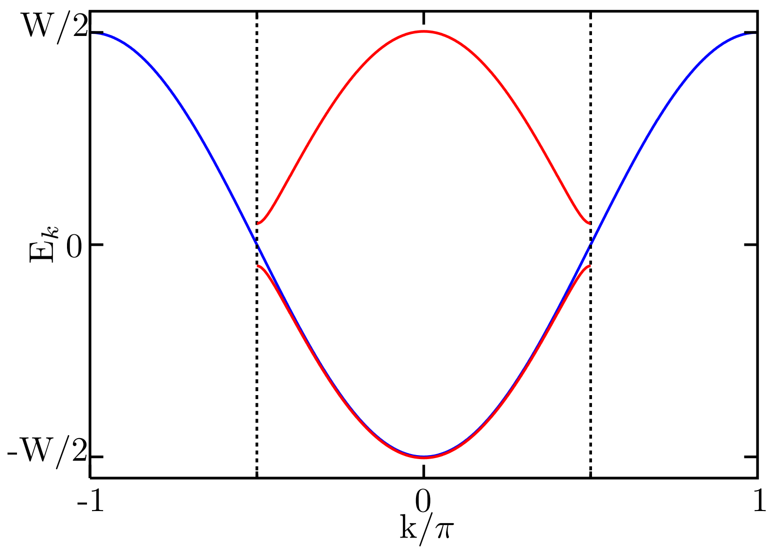

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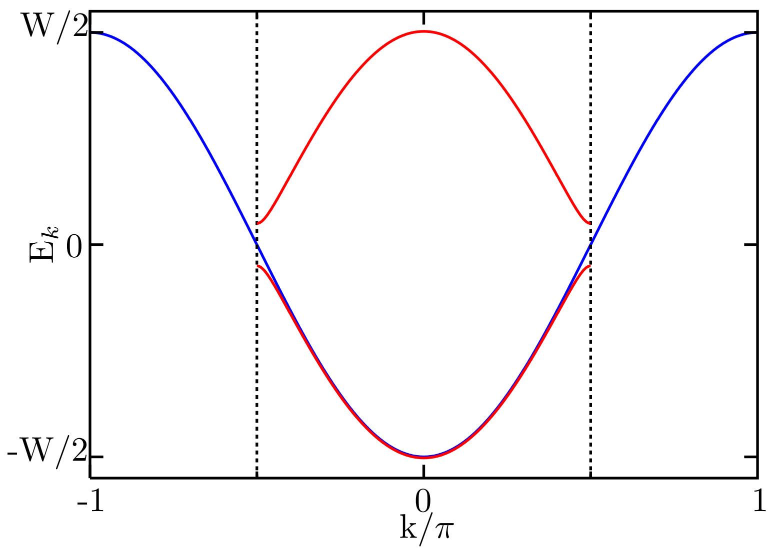
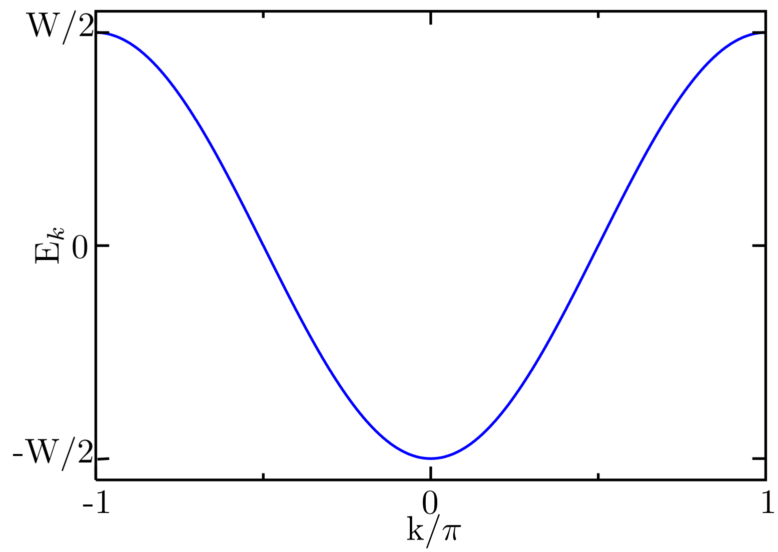


True system: OP fluctuations



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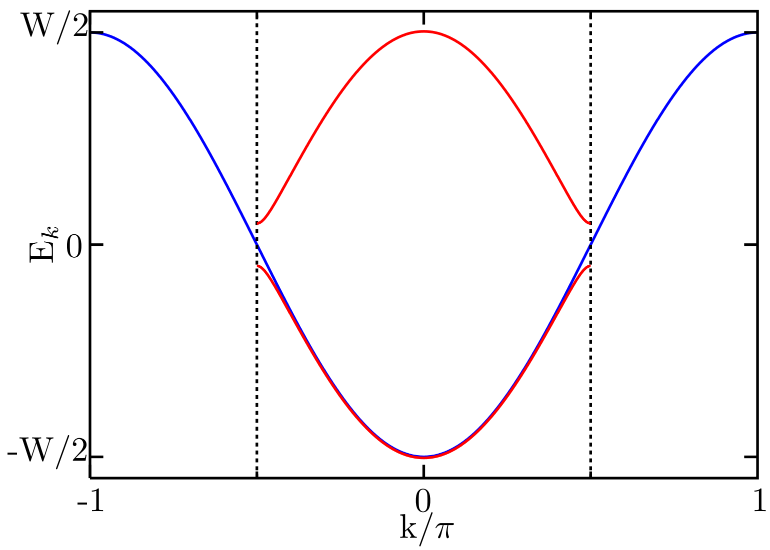

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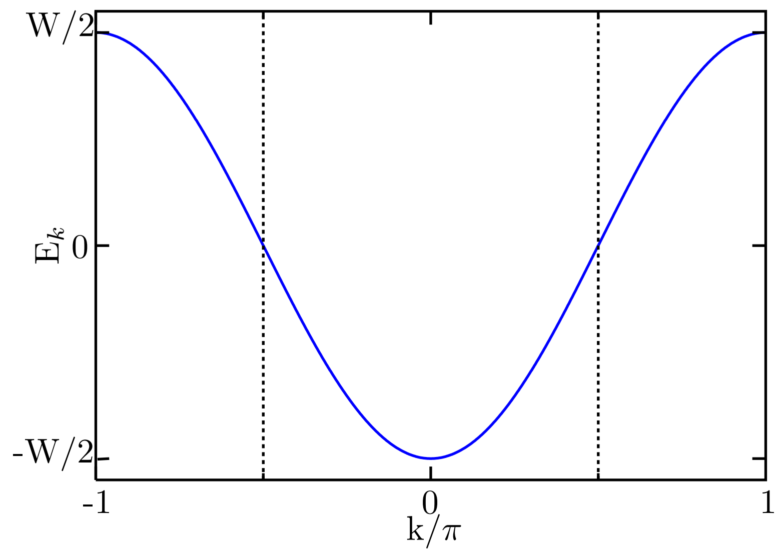

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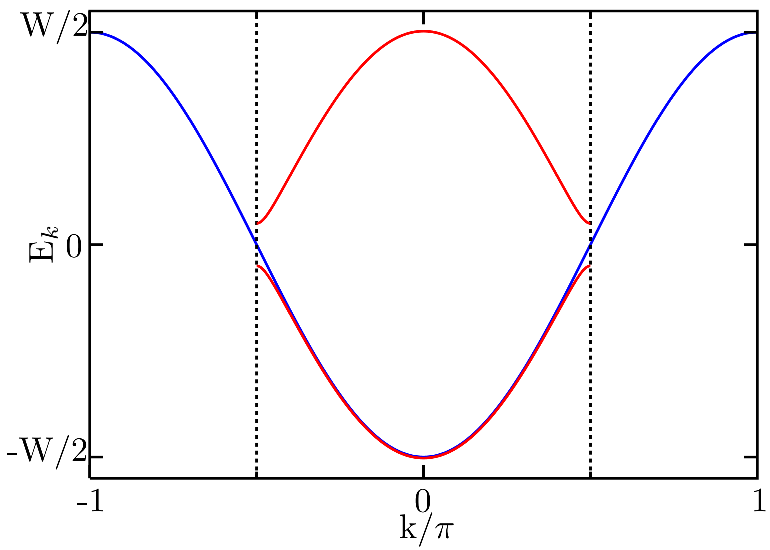

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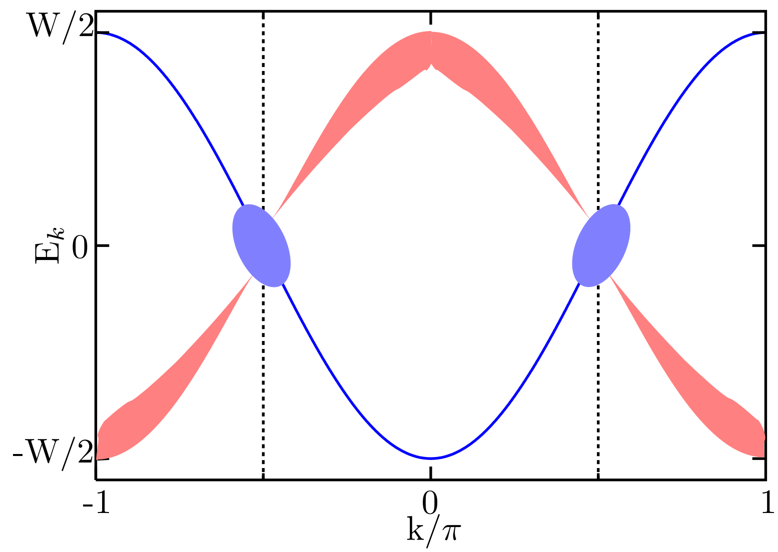

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But dynamical short-ranged order:

Shadow bands, pseudo gaps, . . .

Kampf & Schrieffer ’89

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Cluster Extensions to the DMFT

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- DMFT $+$ local two-particle dynamics — EDMFT, Si et al. '96

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- DMFT + phenomenological two-particle dynamics — Nekrassov et al. '05

  ✔ Pseudo-gap in DOS
  ✔ True $\vec{k}$-dependence
  ✘ No true microscopic foundation

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Relax $\Sigma(\vec{k},z) \longrightarrow \Sigma(z)$ to

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with $N_c > 1$ points $\vec{K} \in 1.$ BZ

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DCA, Hettler et al. '98

Use "molecule" formed by

$N_c > 1$ sites $\vec{R}_J$ for DMFT

$\Sigma_{ij}(z) \longrightarrow \Sigma_{IJ}(z)$

CDMFT, Kotliar et al. '01

Realization of DCA:

- Reduce resolution in $\vec{k}$-space

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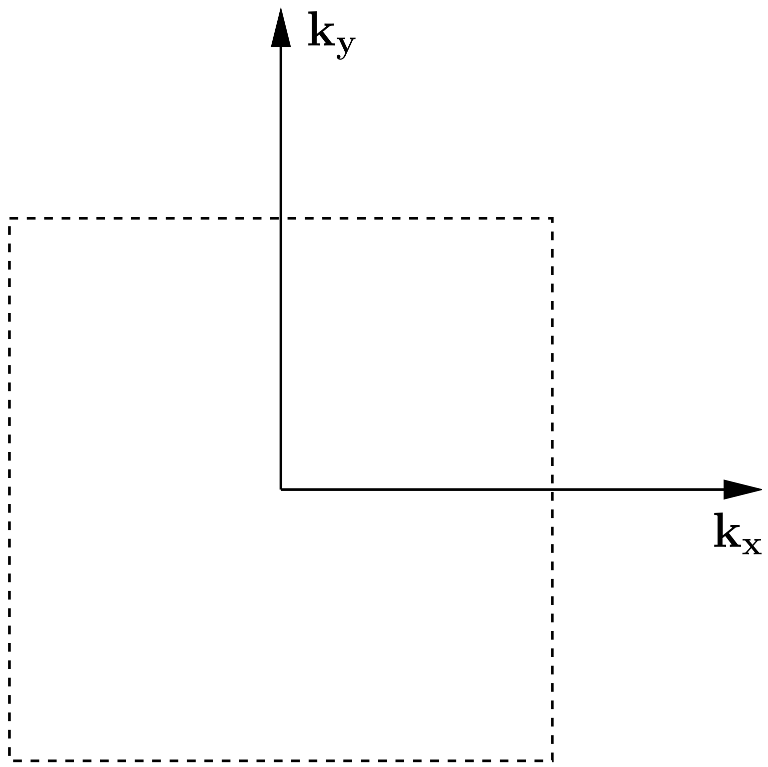

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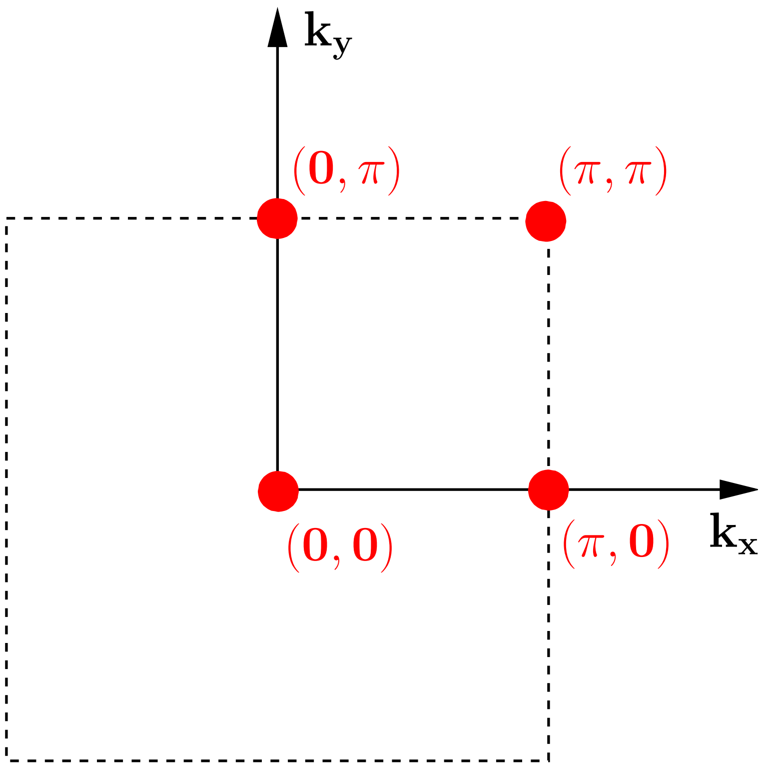

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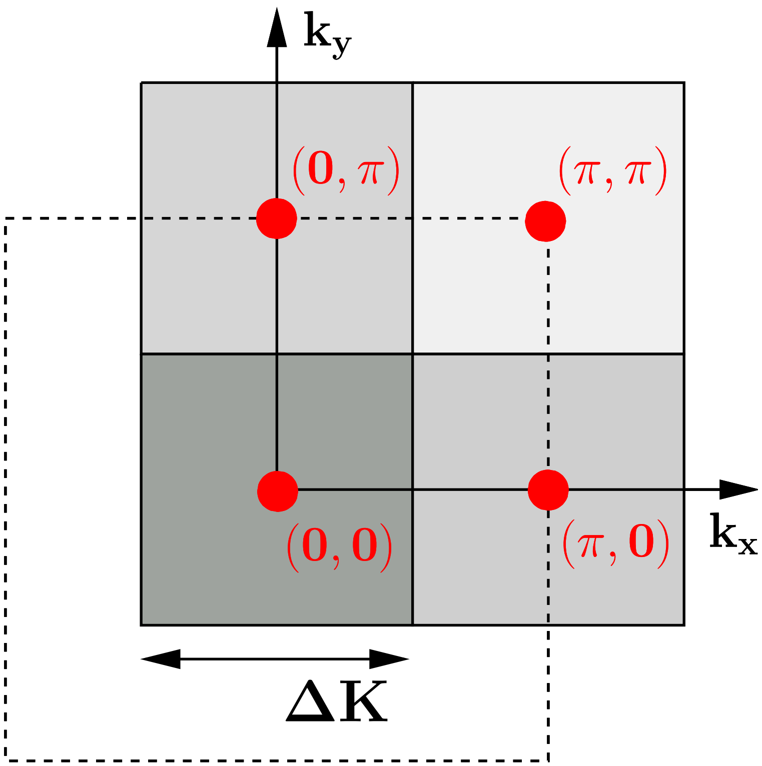

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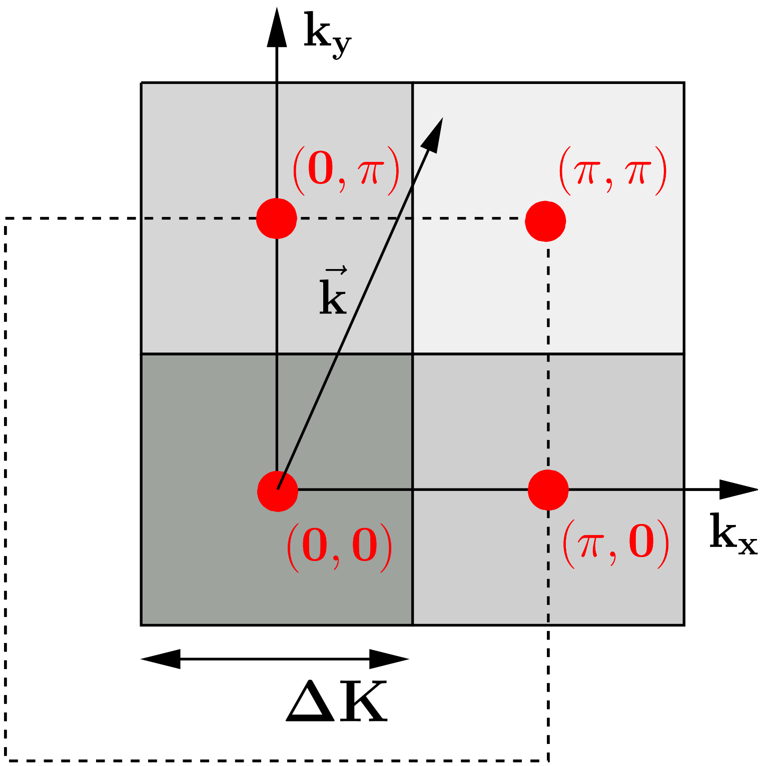

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  $\Sigma(\vec{k}, z)$

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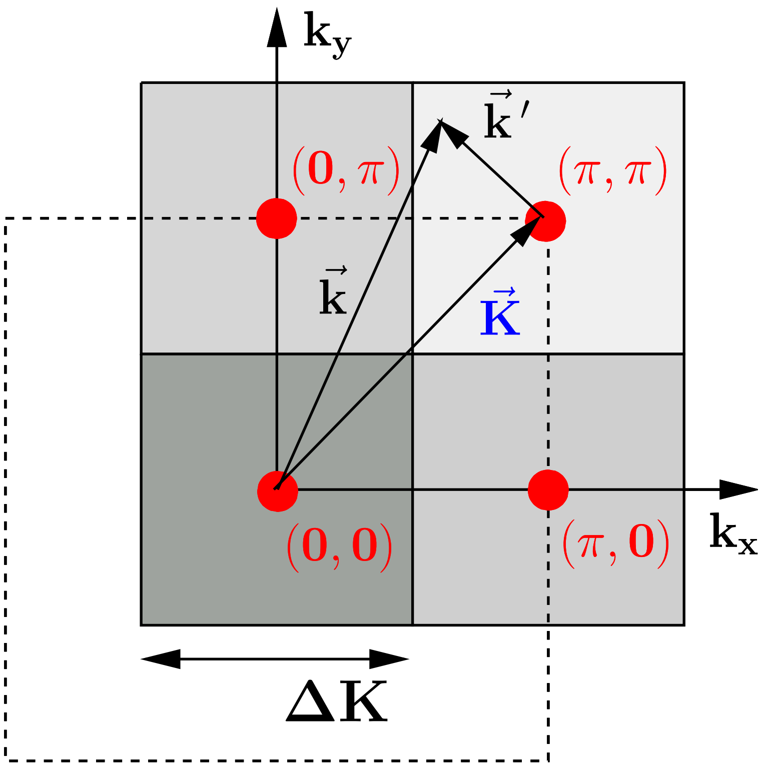

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$$\Sigma(\vec{k}, z) = \Sigma(\vec{K} + \vec{k}', z)$$

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Realization of DCA:

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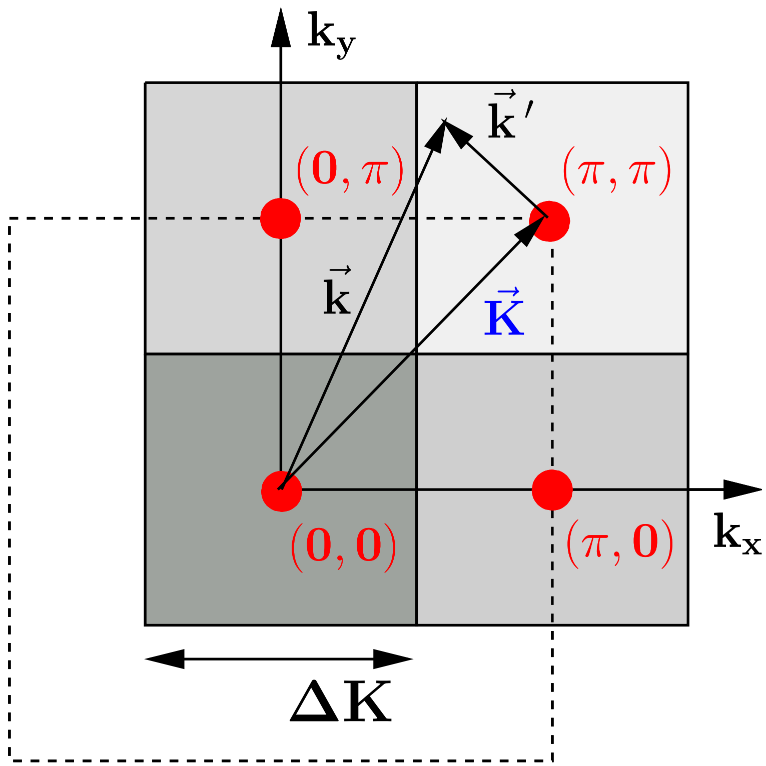

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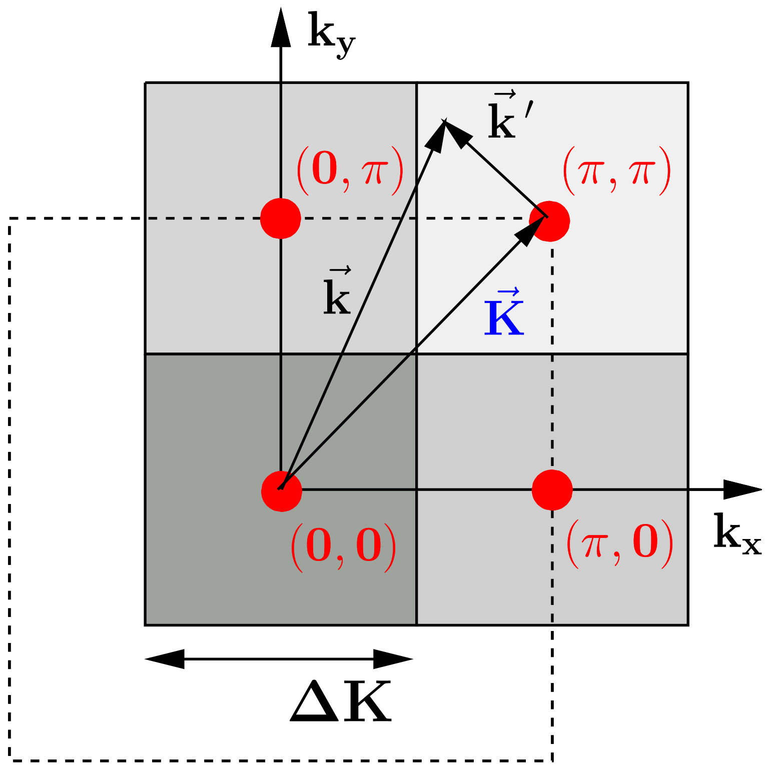

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- Perform coarse graining:

$$\bar{G}(\vec{K},z) = \frac{N_c}{N}\sum_{\vec{k}'}\frac{1}{z+\mu-\epsilon_{\vec{K}+\vec{k}'}-\Sigma(\vec{K},z)}$$

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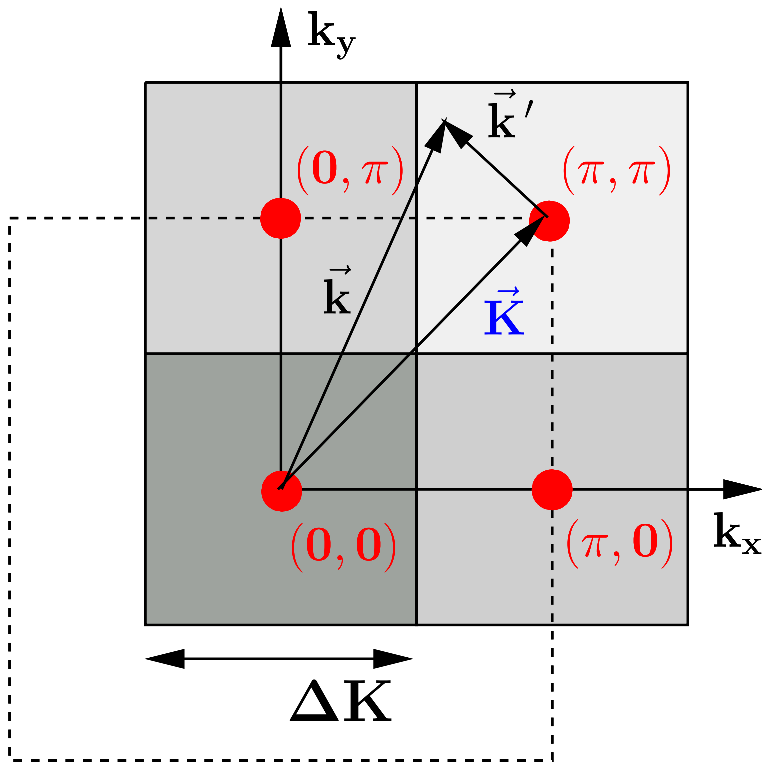

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❑ effective model on periodic cluster

Realization of CDMFT:

- Build clusters in real space

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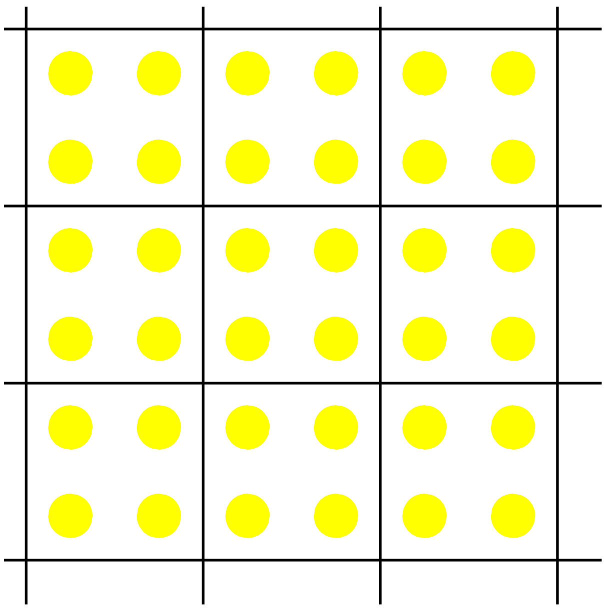

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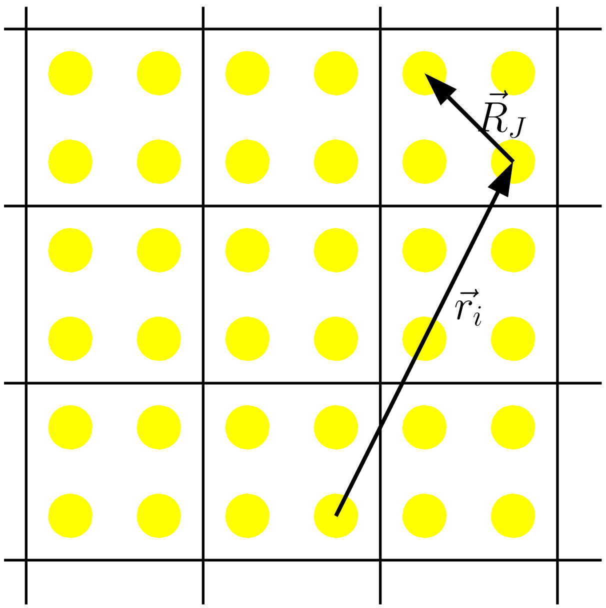

- Choose cluster with $N_c \times N_c$ points $\vec{R}_J$

- Break up

$$[\mathbf{t}]_{ij} = [\mathbf{t}]_{IJ} + [\delta\mathbf{t}](\vec{r}_i - \vec{r}_j)$$

$$[\mathbf{\Sigma}(z)]_{ij} \approx [\mathbf{\Sigma}(z)]_{IJ}$$

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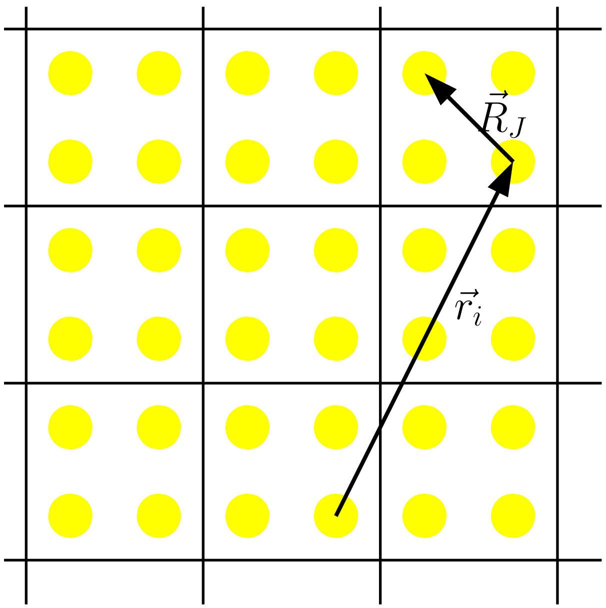

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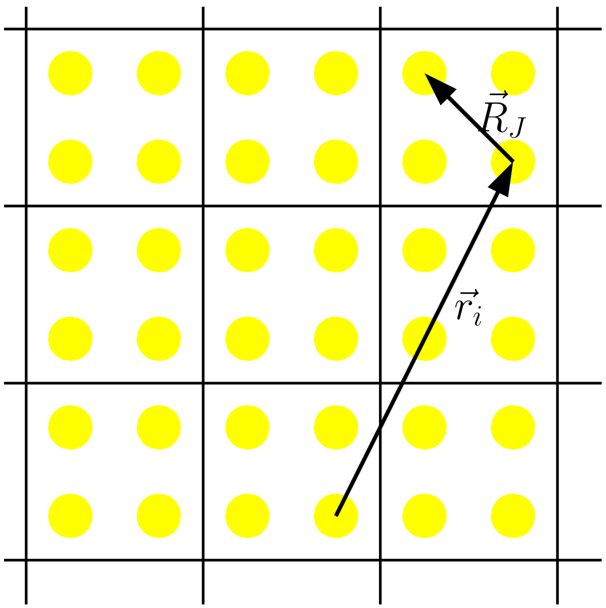

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- Effective model on open-boundary cluster

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Implementing the DCA algorithm:

similar for CDMFT with matrices

First guess for $\Sigma(\mathbf{K})$

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Implementing the DCA algorithm:

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First guess for $\Sigma(\mathbf{K})$

$$\bar{G}(\mathbf{K}) = \frac{N_c}{N} \sum_{\mathbf{k}'} \frac{1}{\omega - \epsilon_{\mathbf{K}+\mathbf{k}'} + \mu - \Sigma(\mathbf{K})}$$

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Implementing the DCA algorithm:

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$$\mathcal{G}^{-1}(\mathbf{K}) = \bar{G}^{-1}(\mathbf{K}) + \Sigma(\mathbf{K})$$

First guess for $\Sigma(\mathbf{K})$

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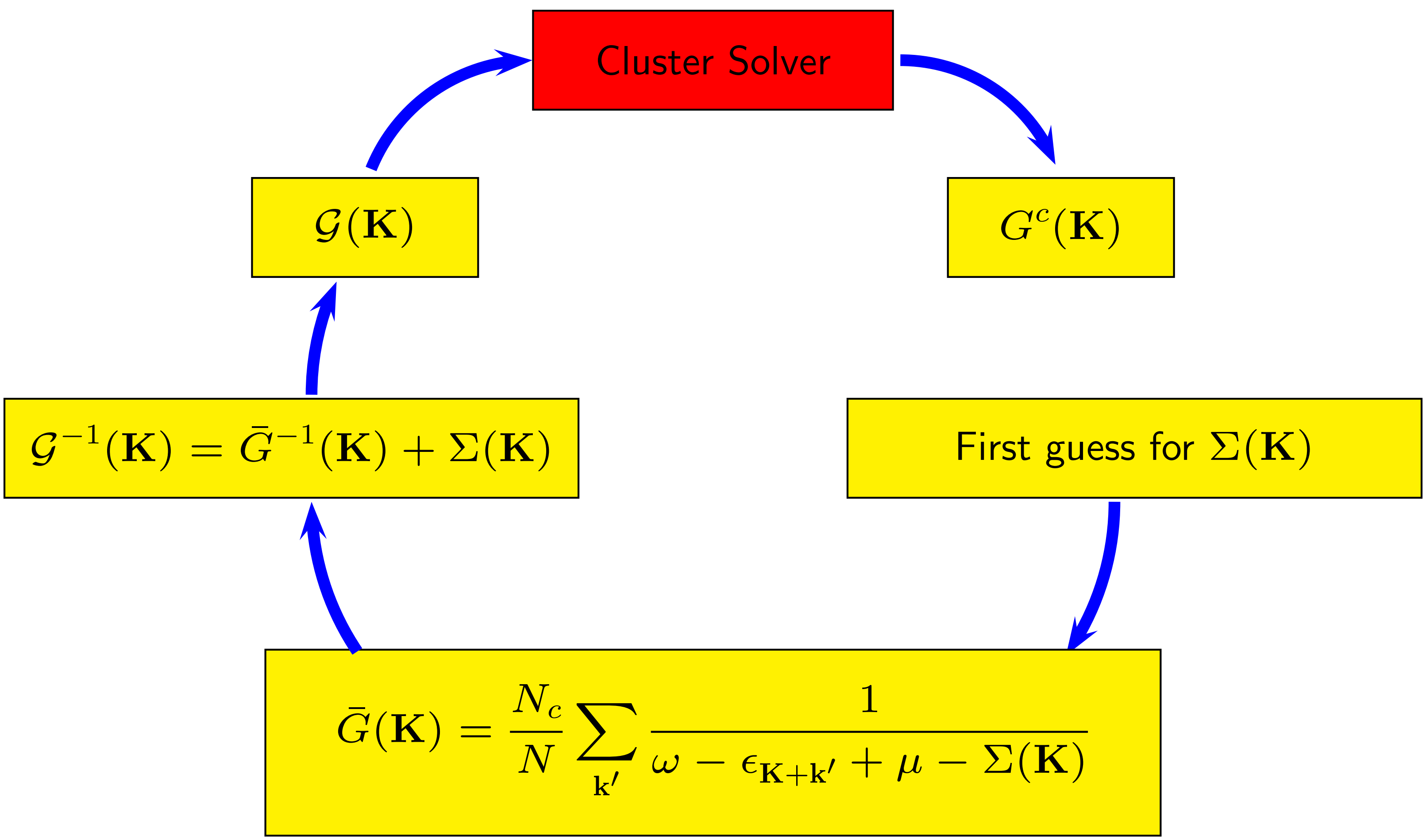

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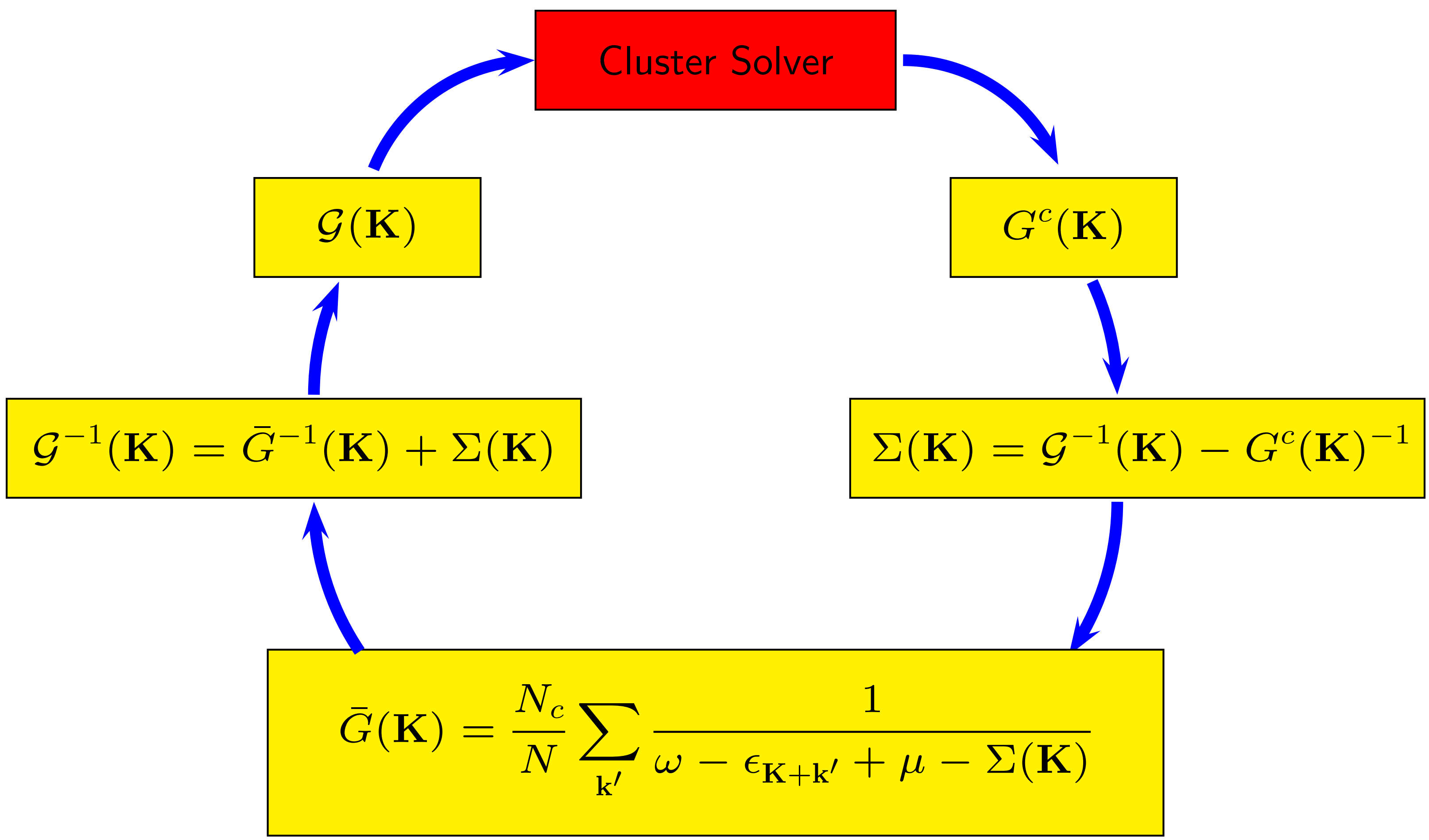

DCA and CDMFT seem to be nice schemes

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Structure of effective cluster

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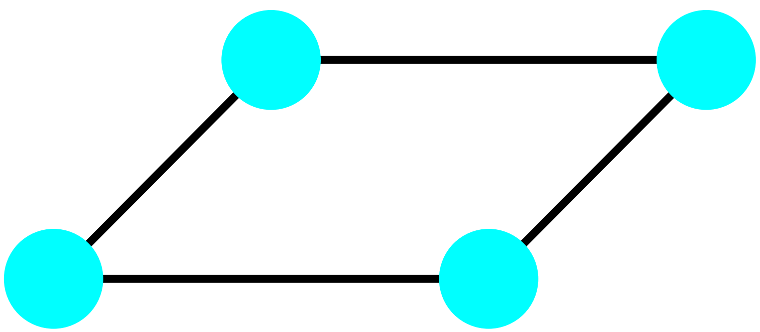

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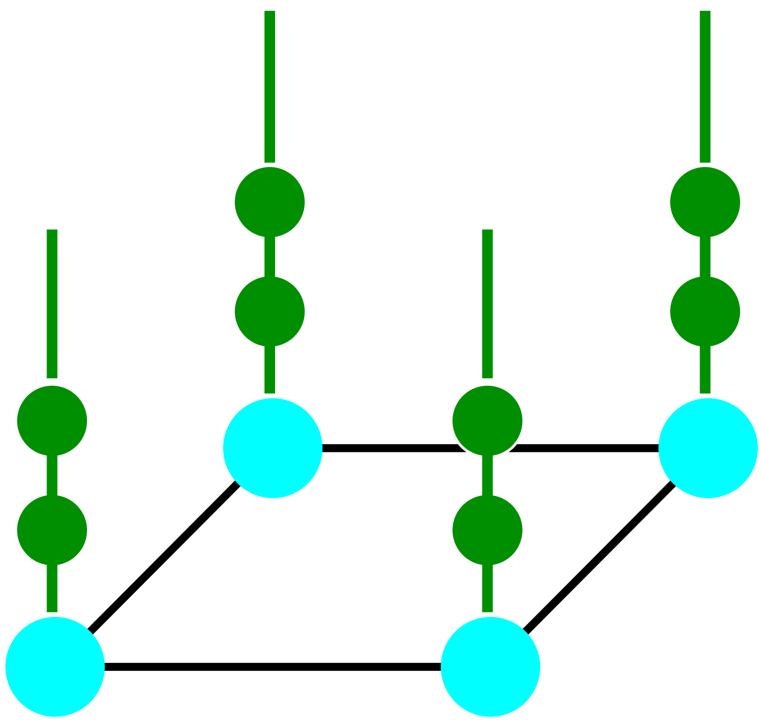

Structure of effective cluster

- ☛ N_c sites as in ED/QMC
- ➥ Well-developed techniques?
- ☛ "dyamical mean-field
- ☛ $O(N_c)$ semi-infinite chains
- ➥ Only Hirsch-Fye QMC left

Another potential problem:

- DCA gives $\Sigma(\vec{k}, z)$ only as "histogram" on the $\vec{K}$ values
  - ☛ Additional interpolation necessary
  - ☛ Reliability close to $\vec{k}_F$ and μ?

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General expectation:

"Smoothing" well-defined for smoothly $\vec{k}$-dependent $\Sigma(\vec{k},z)$

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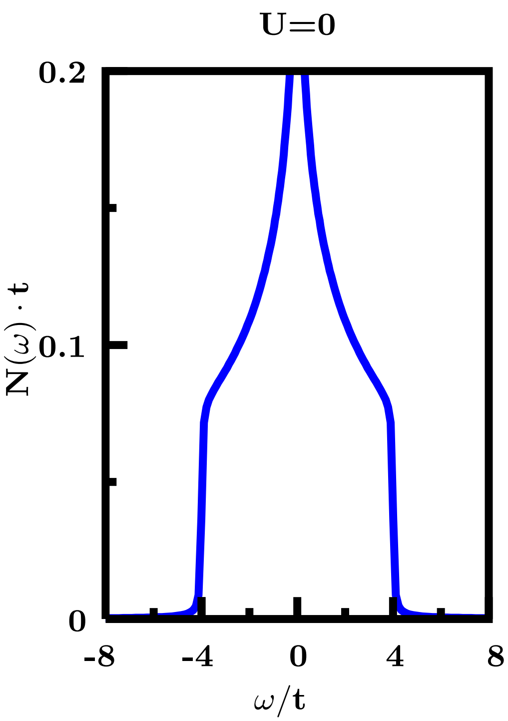
Cluster Extensions to the DMFT

Maier, TP *et al.*, EPJ B13 ('00)

2D Hubbard model: $N_c = 1$ vs. $N_c > 1$



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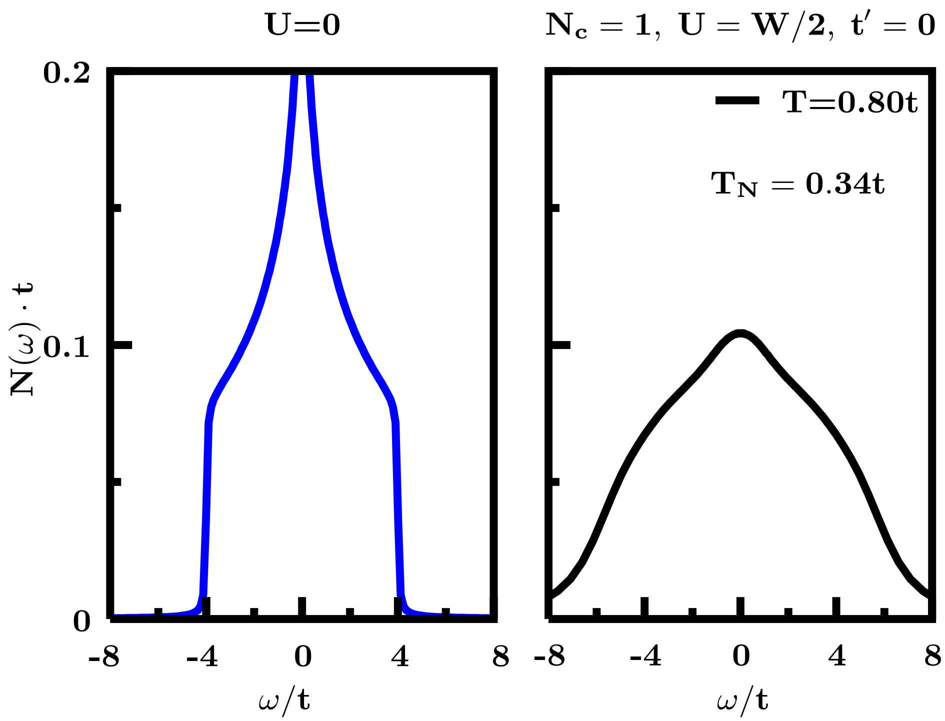

Maier, TP *et al.*, EPJ B13 ('00)

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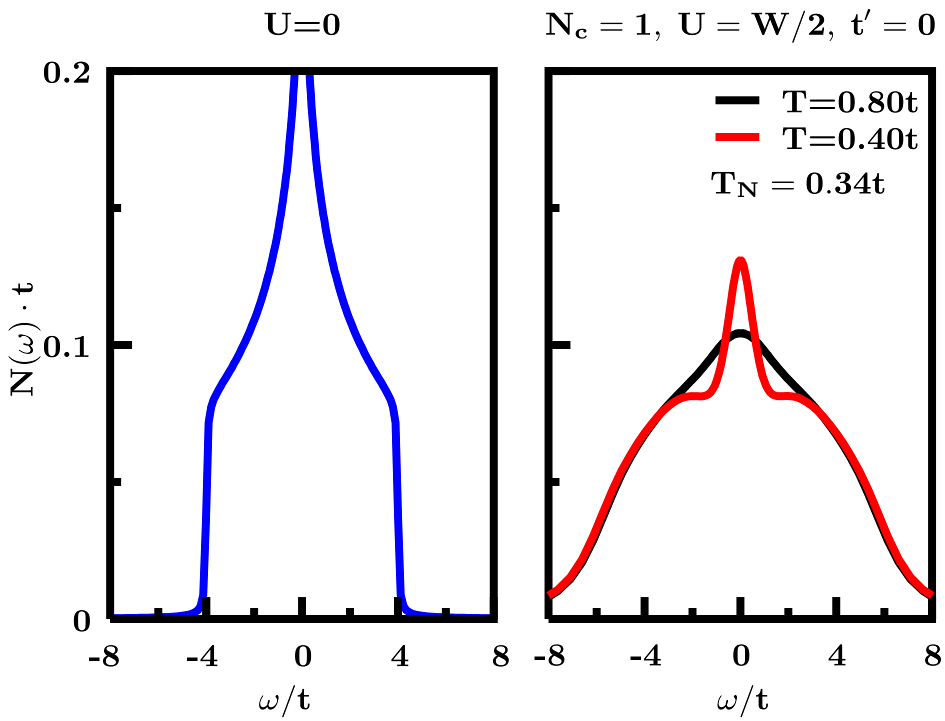

Maier, TP *et al.*, EPJ B13 ('00)

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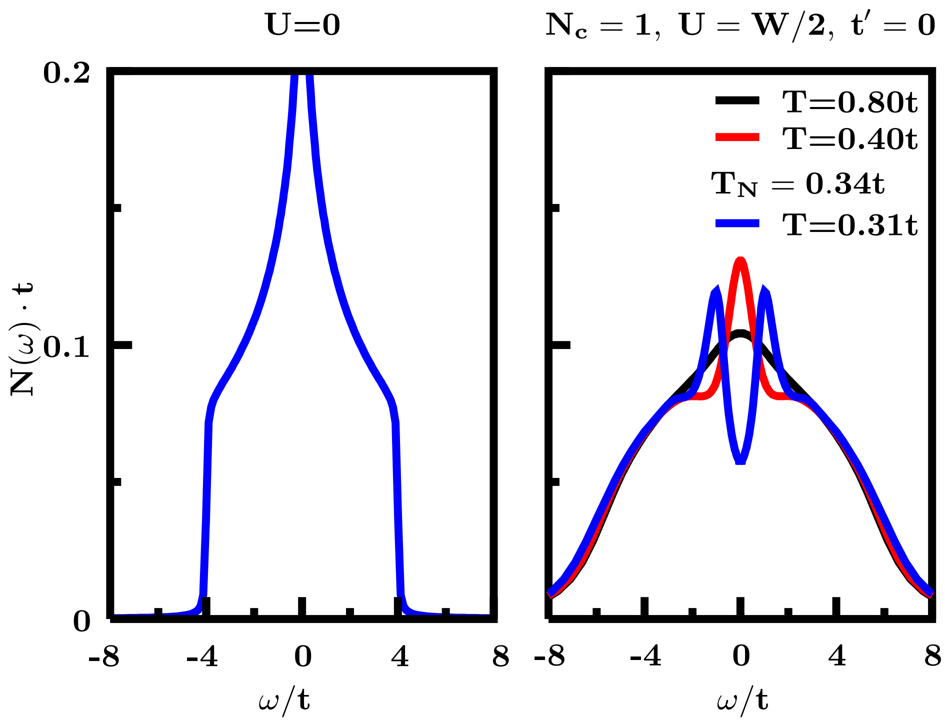

$N_c = 1$:

➥ No precursor of AF

Maier, TP *et al.*, EPJ B13 ('00)

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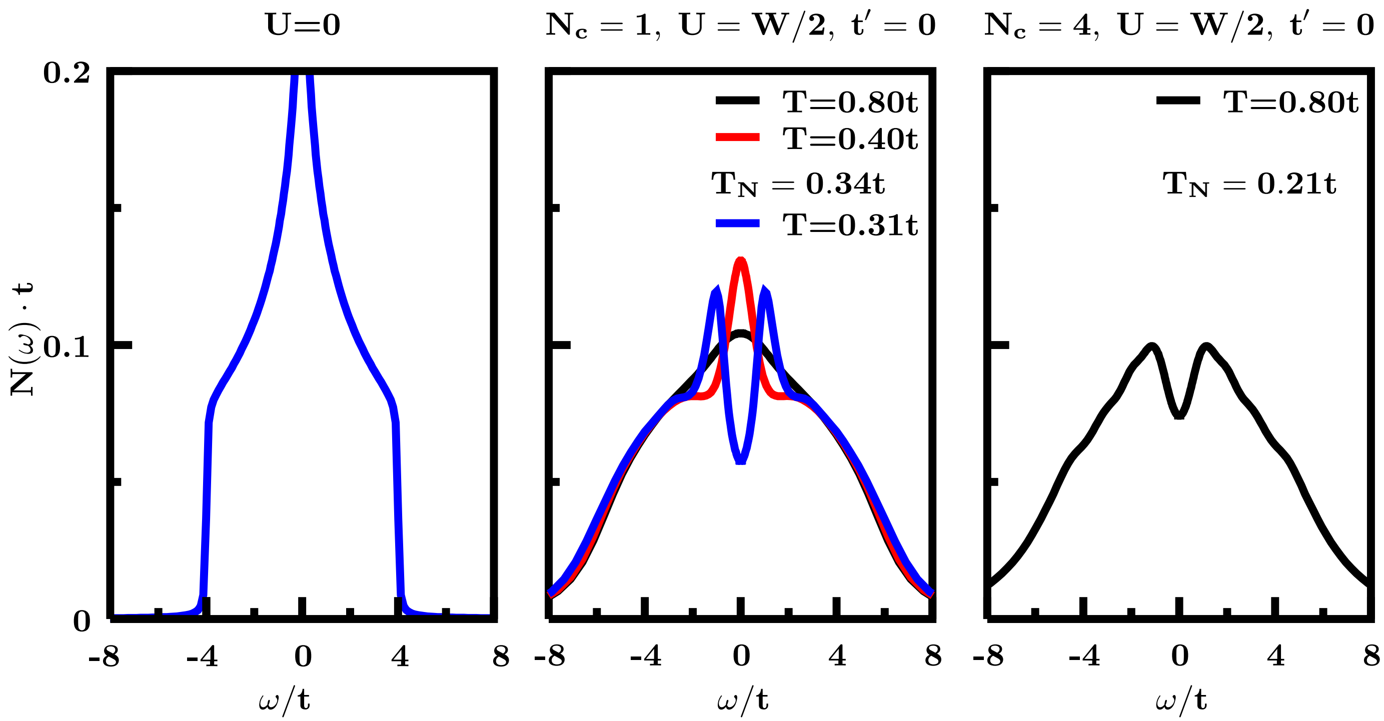

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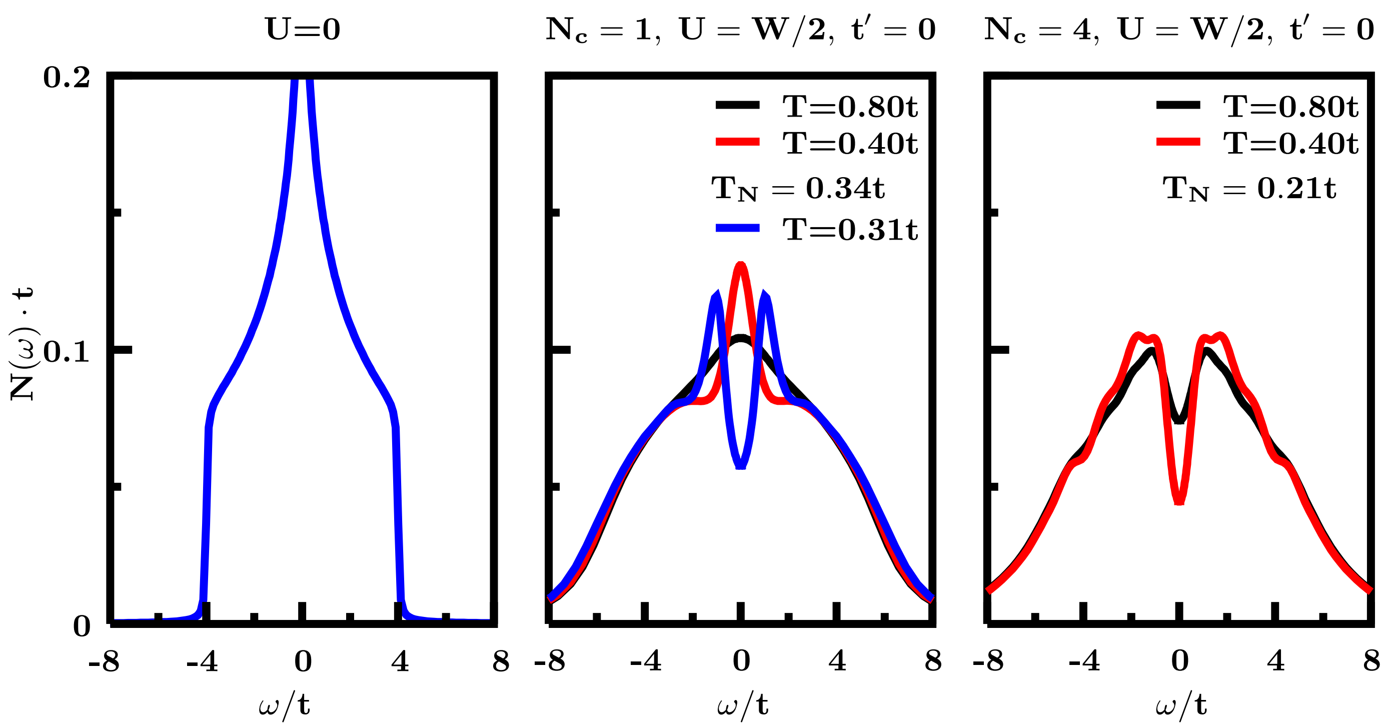

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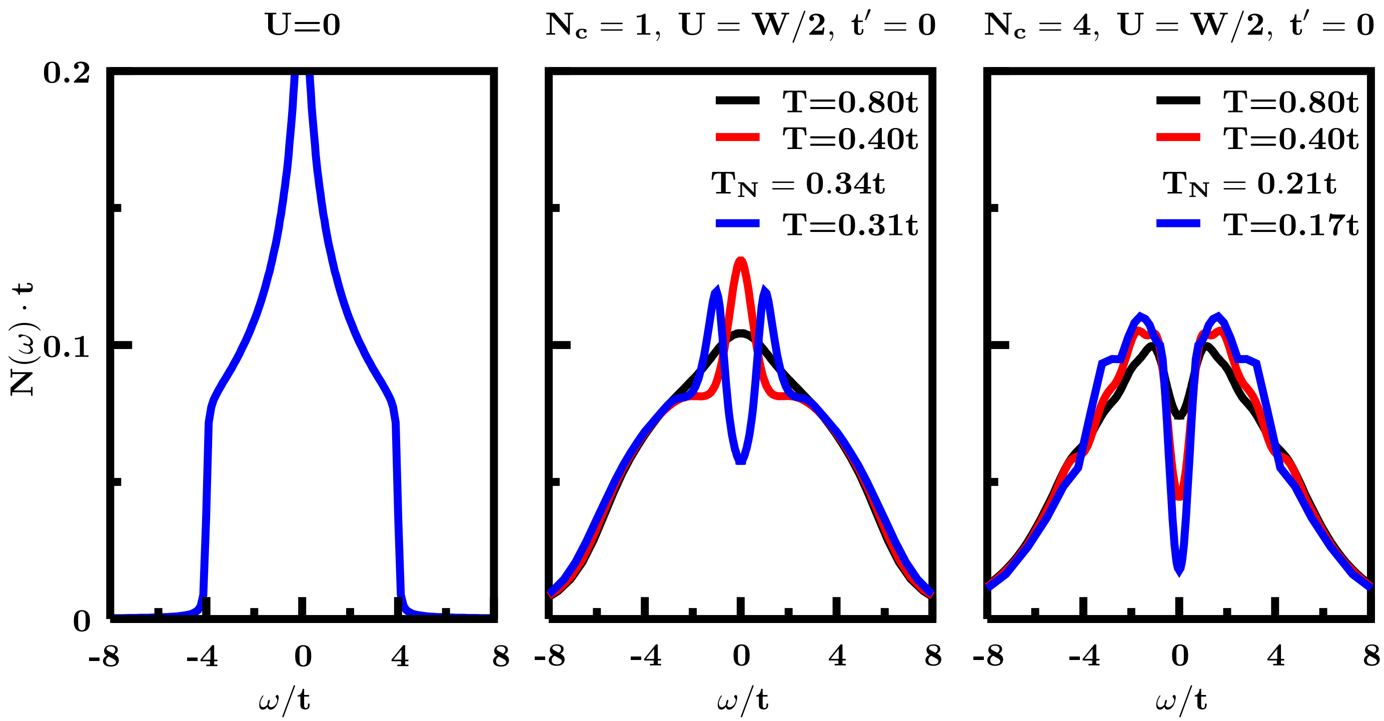


$N_c = 1$:

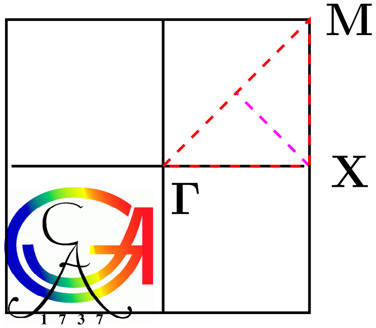
➥ No precursor of AF

$N_c = 4$:

➥ Pseudo gap in paramagnet

Maier, TP *et al.*, PRB **66** ('02)

$N_c = 16$, $U = W = 8t$, $t' = -0.2t$, $t = 0.25$eV



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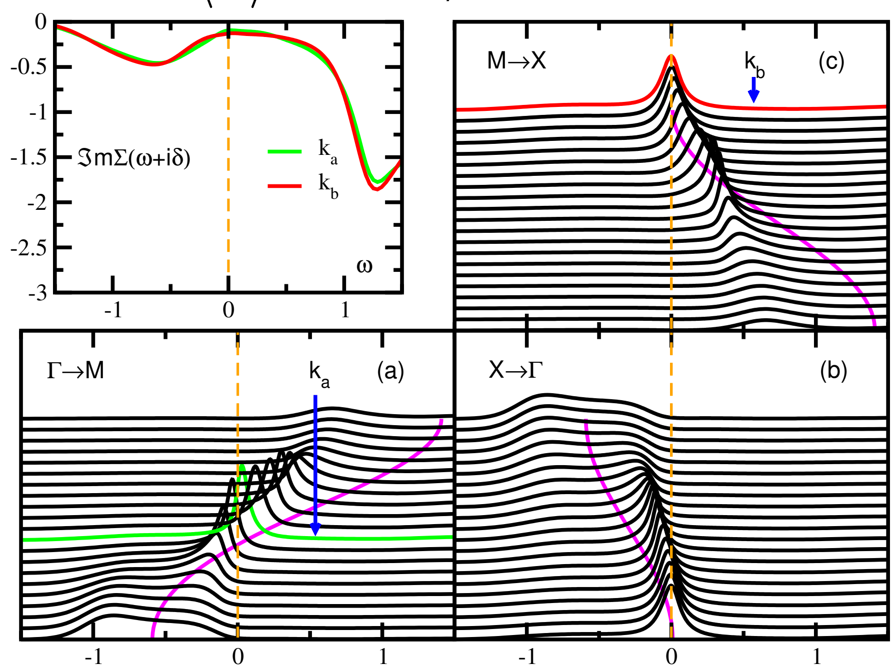
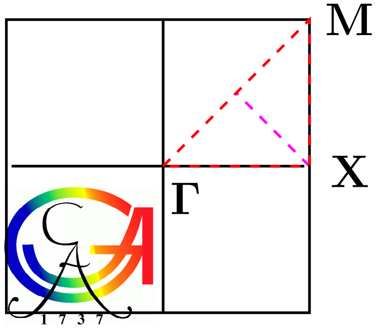
Maier, TP *et al.*, PRB **66** ('02)

$N_c = 16$, $U = W = 8t$, $t' = -0.2t$, $t = 0.25$eV

$\langle n \rangle = 0.80$, $T = 370$K



- ❑ Well defined quasi particles
- ❑ Weak $\vec{k}$-dependence of $\Sigma(\vec{k}, \omega)$



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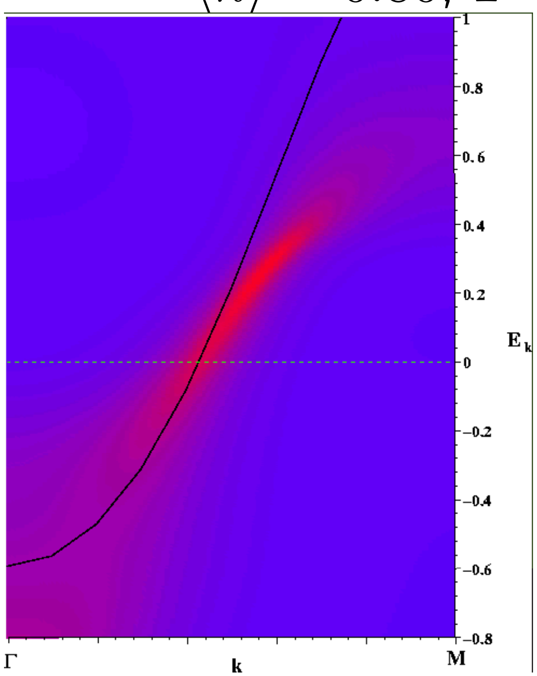

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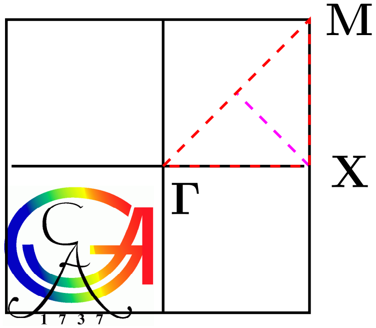

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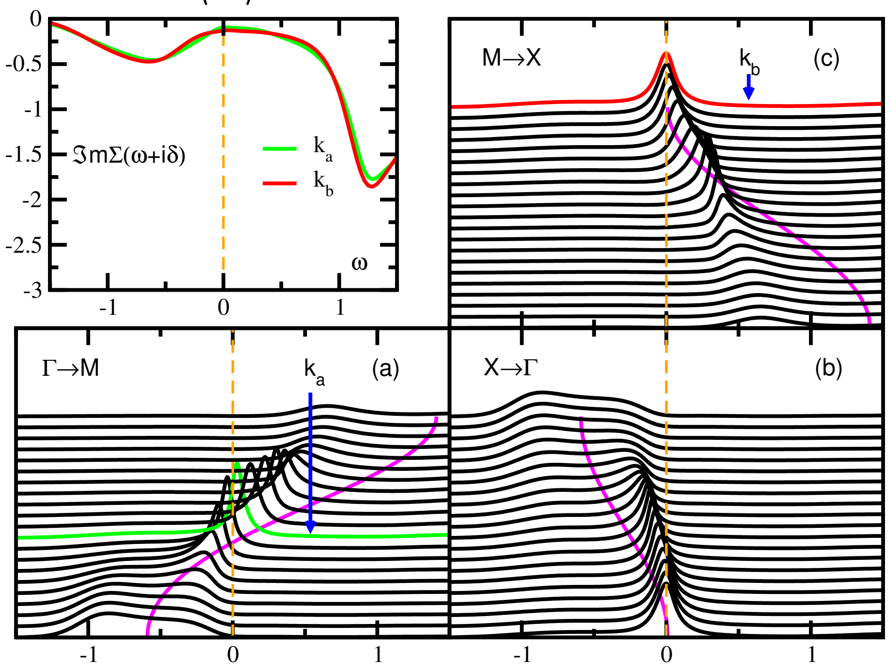
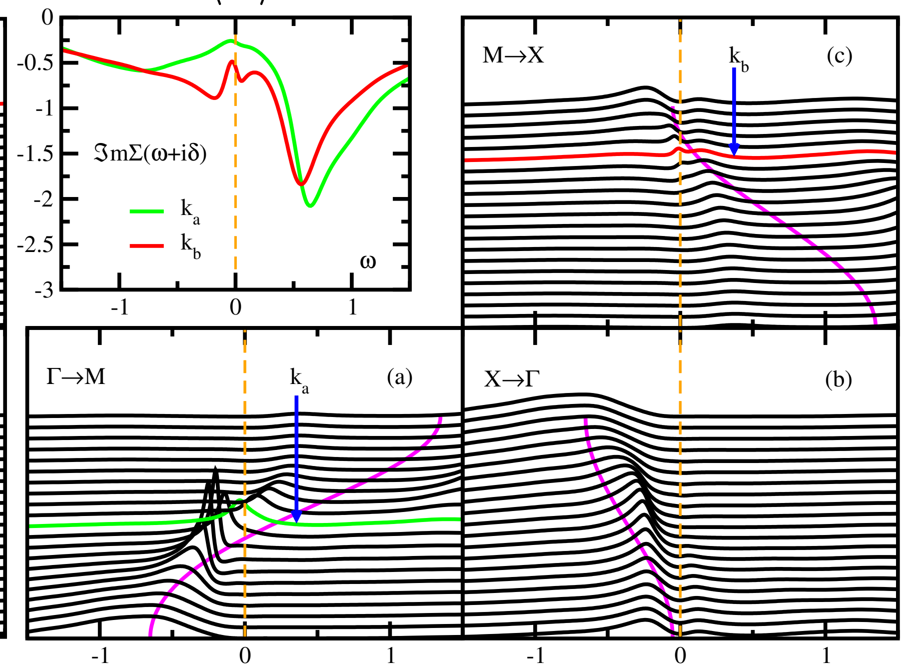
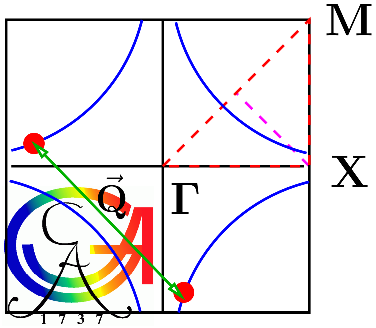


$\langle n \rangle = 0.95$, $T = 370$K



- ❏ Well defined quasi particles
- ❏ Weak $\vec{k}$-dependence of $\Sigma(\vec{k}, \omega)$

- ❏ Strongly damped structures at X
- ❏ Strong $\vec{k}$-dependence of $\Sigma(\vec{k}, \omega)$



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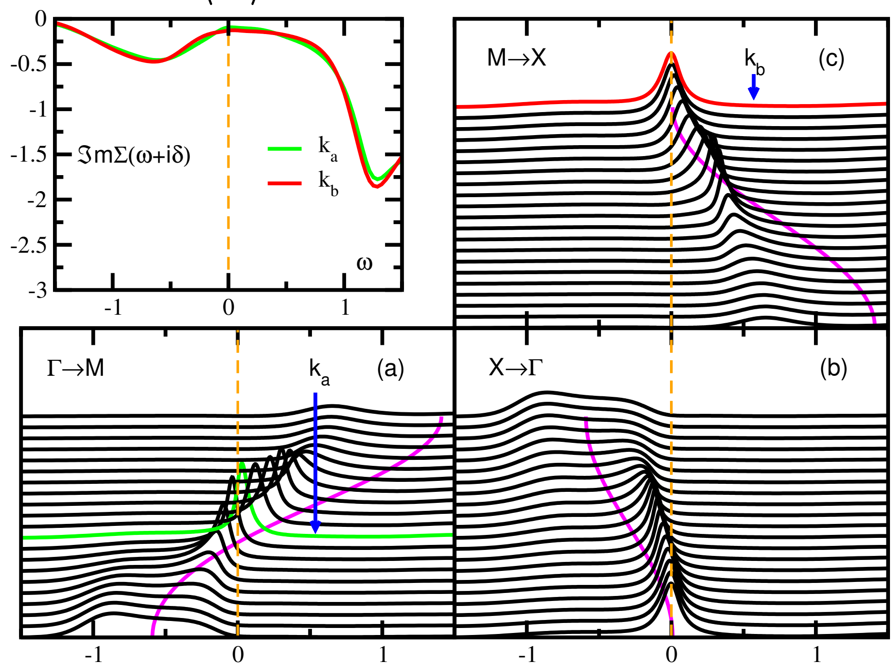
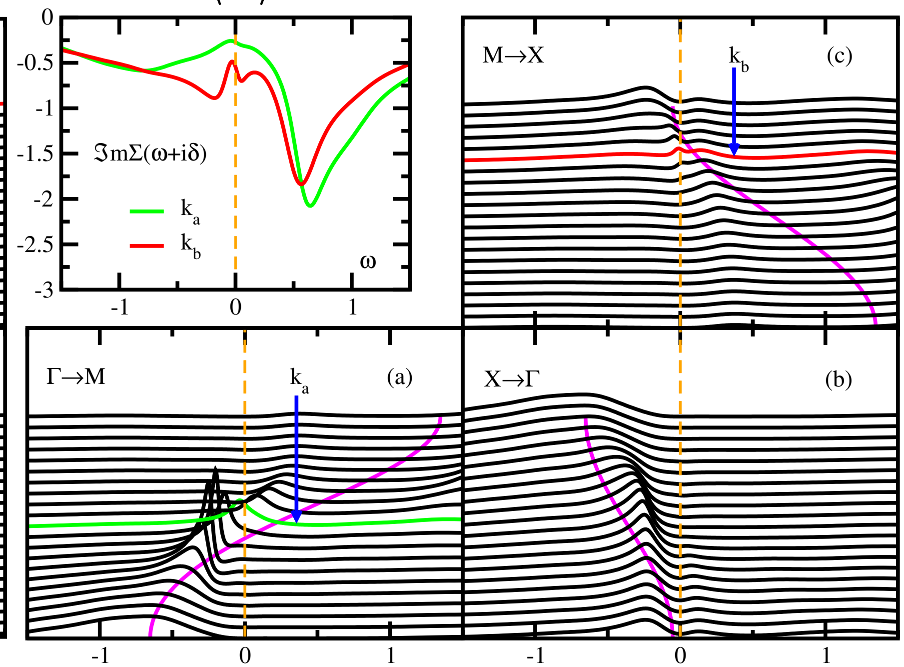
$N_c = 16,\ U = W = 8t,\ t' = -0.2t,\ t = 0.25\text{eV}$

$\langle n\rangle = 0.80,\ T = 370\text{K}$



$\langle n\rangle = 0.95,\ T = 370\text{K}$



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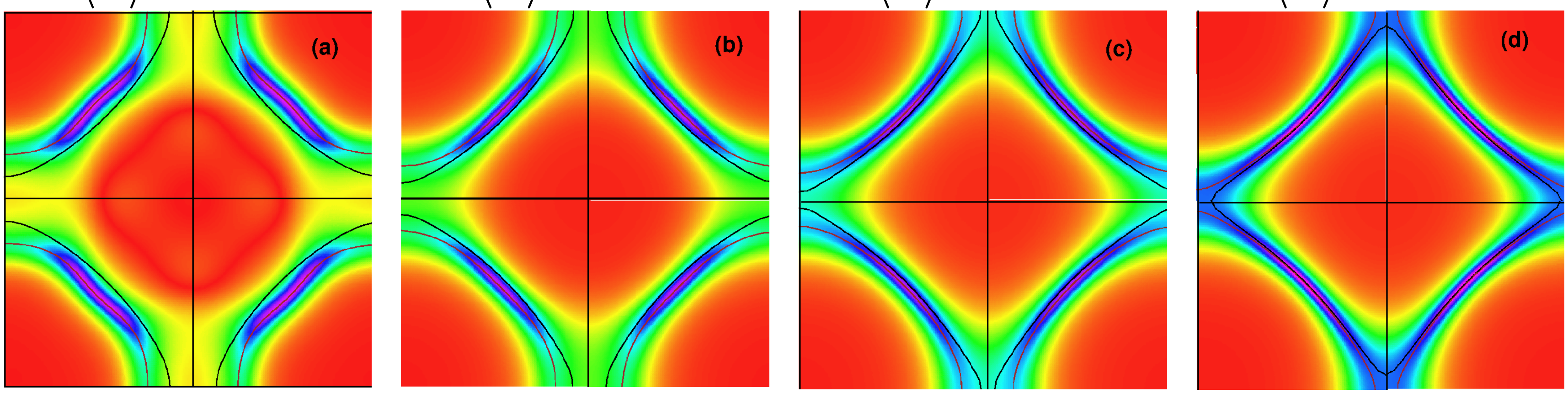
Maier, TP *et al.*, PRB **66** ('02)

$N_c = 16$, $U = W$, $t' = -0.2$, $T = 370$K

$\langle n \rangle = 0.95$ | $\langle n \rangle = 0.90$ | $\langle n \rangle = 0.85$ | $\langle n \rangle = 0.80$



$\langle n \rangle \gtrsim 0.9$

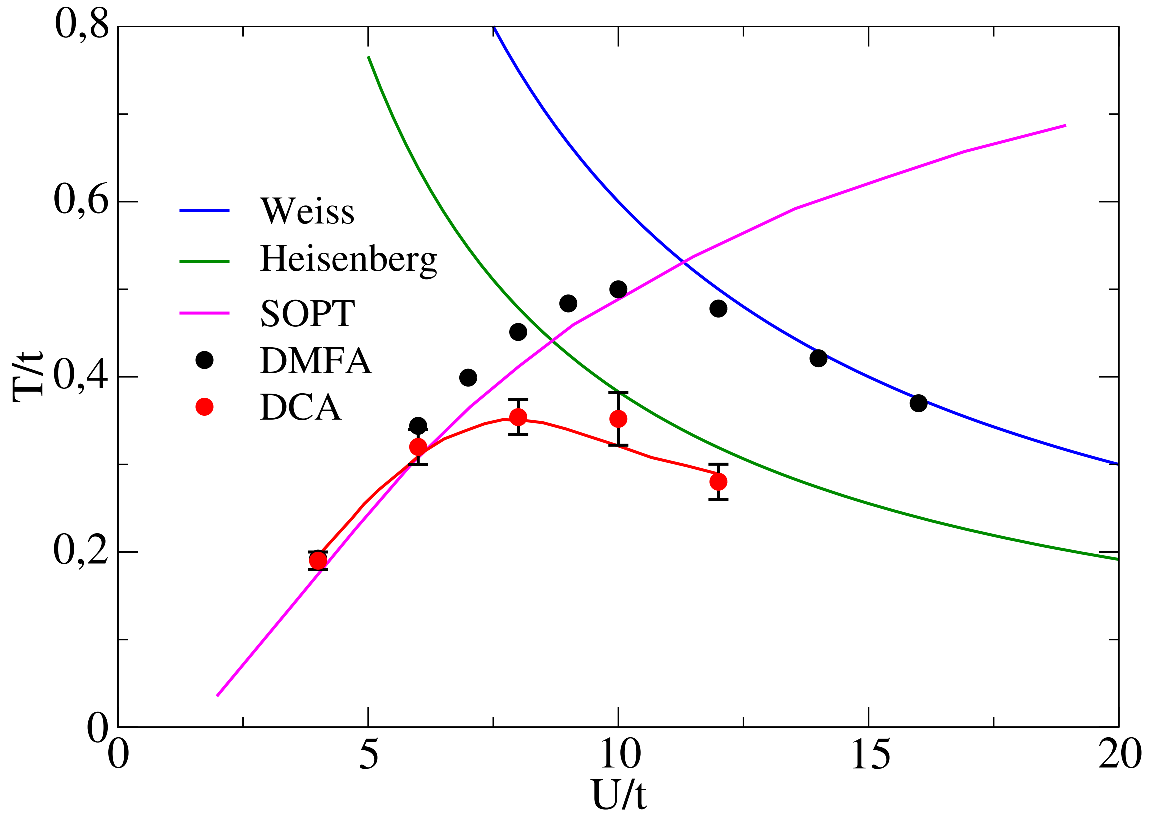
Small FS for $\langle n \rangle \to 1$
➥Luttinger's theorem violated

$\langle n \rangle \lesssim 0.9$

Large FS for $\langle n \rangle < 0.9$
➥Luttinger's theorem fulfilled

How does it perform for $D = 3$?

Kent et al. '05



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Cluster Extensions to the DMFT

1. Motivation: Why need a cluster MFT?
2. Realizations: DCA and CDMFT
3. Selected results for DCA
4. **Summary**

- Cluster extensions of DMFT:
  - ☛ Systematic inclusion of non-local correlations
  - ☛ Thermodynamic limit
  - ☛ Short-ranged correlations treated exactly
  - ☛ Long-ranged correlations mean-field like
  - ☛ Sensible results with acceptable computational effort

Further reading:

Th. Maier et al., cond-mat/0404055 (RMP in press)