Thomas Pruschke
Institut für Theoretische Physik
Universität Göttingen

Cluster Extensions to the Dynamical Mean-Field Theory

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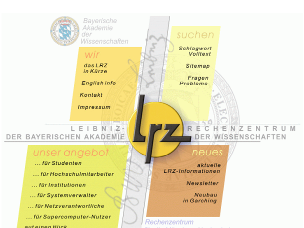

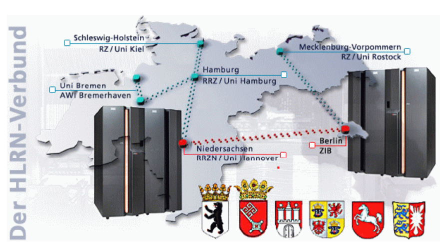

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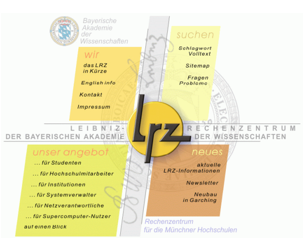

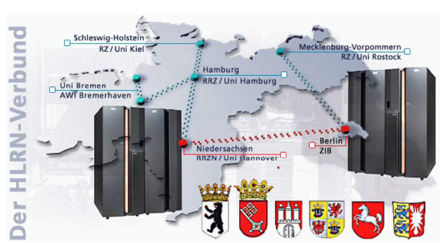

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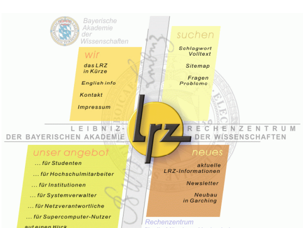

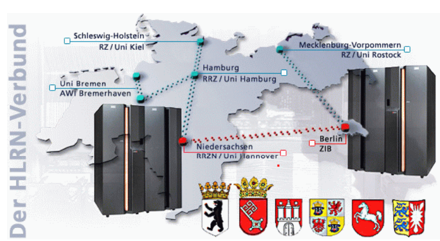

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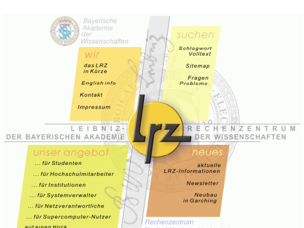

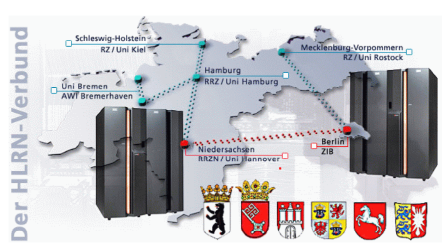

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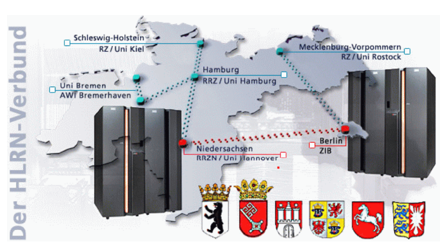
Collaborators:
Th. Maier, M. Jarrell



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Standard model for e.g. TMO: One band Hubbard model

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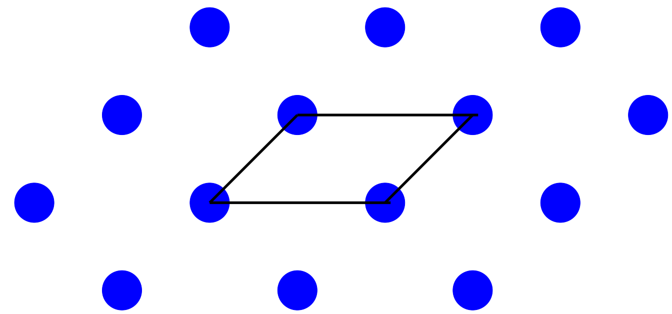
- Simplest possible lattice



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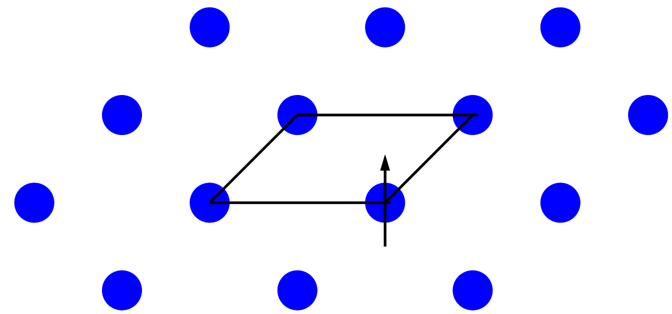

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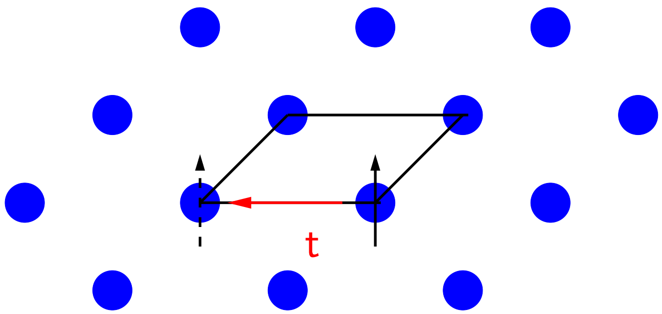

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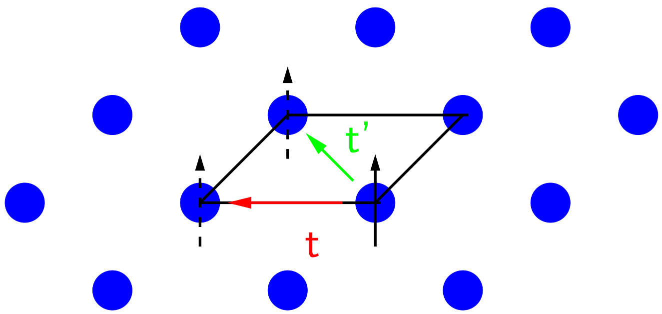

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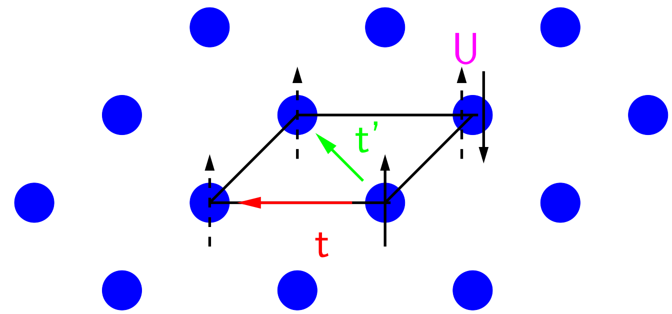

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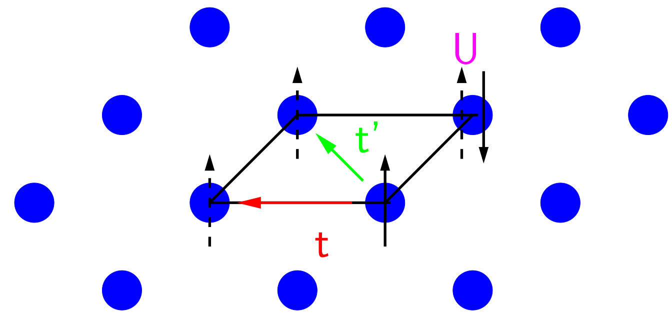

$$H = \sum_{ij,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Dispersion: $\epsilon_{\mathbf{k}} = \epsilon_0 - 2t(\cos k_x + \cos k_y) - 4t'\,(\cos k_x \cos k_y - 1)$

Typical parameters: $t \approx 0.25$eV, $t'/t \approx -0.2$

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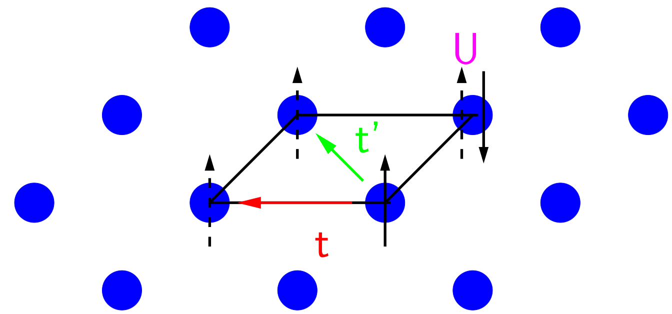

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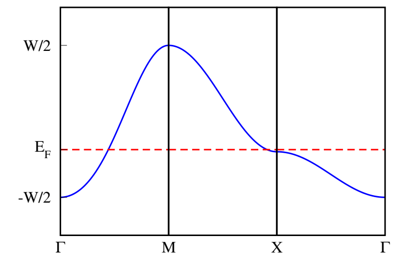

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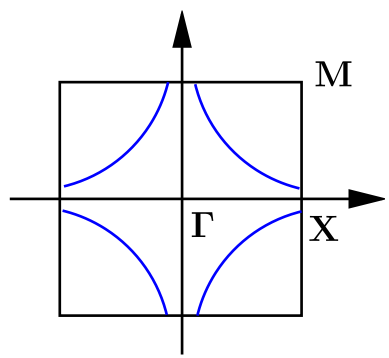

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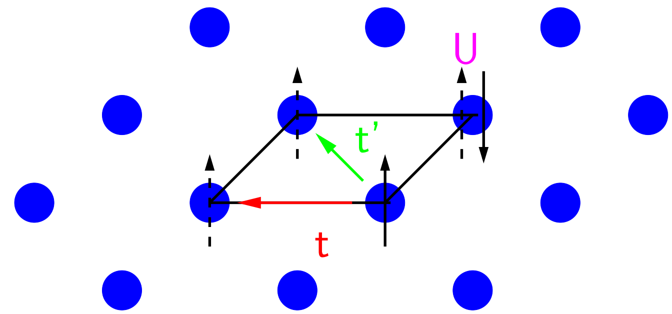

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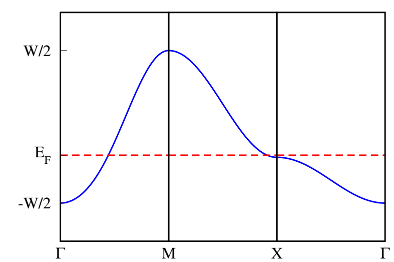

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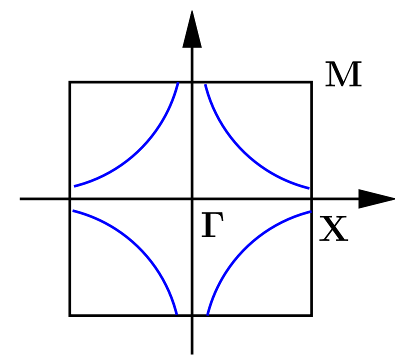

Intermediate coupling Regime

Standard techniques

Exact Diagonalization Quantum Monte-Carlo	Properties of finite systems (ED: $N < 20$, QMC: $N < 100$)
Density-Matrix RenormalizationGroup	Ground state and dynamics for $D = 1$
Dynamical Mean-Field Theory	Approach to local properties
RenormalizationGroup	Low-energy properties
Perturbation Theory	Resummation of sub-classes of diagrams (FLEX)
Variational wave functions	Ground state properties

Successful approach for qualitative properties: DMFT

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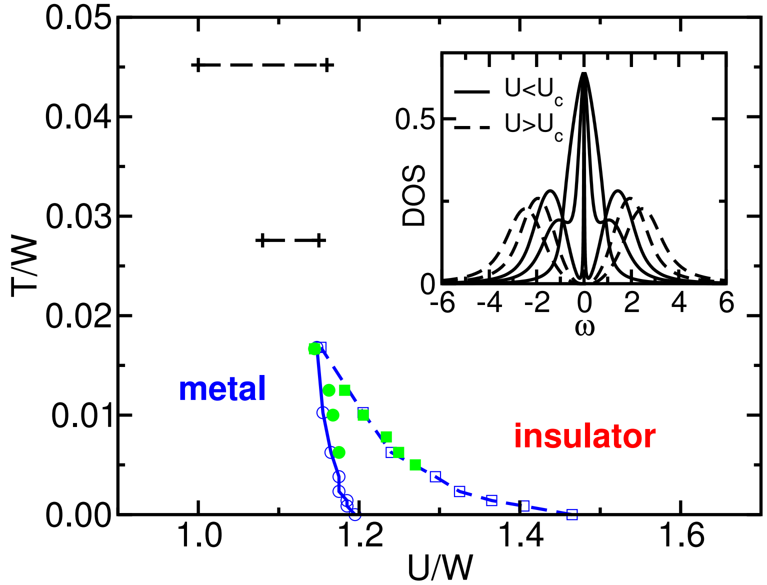
Georges et al., RMP '96, Bulla et al.,PRL '99 & PRB '01

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



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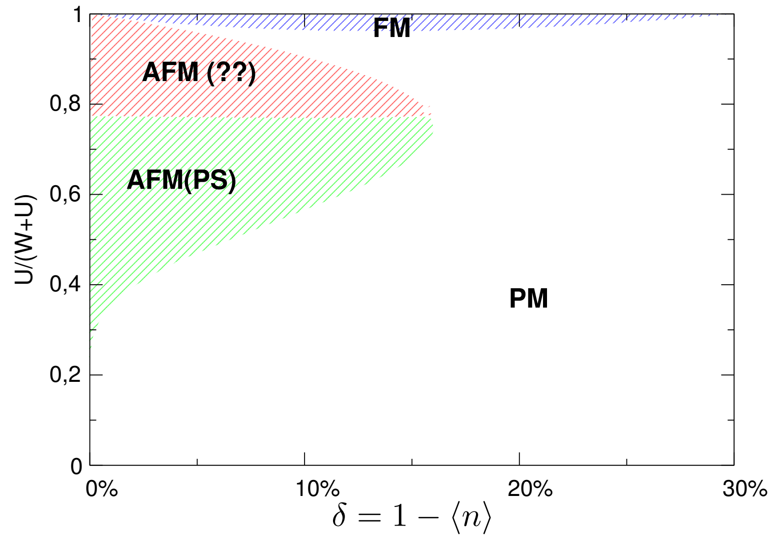
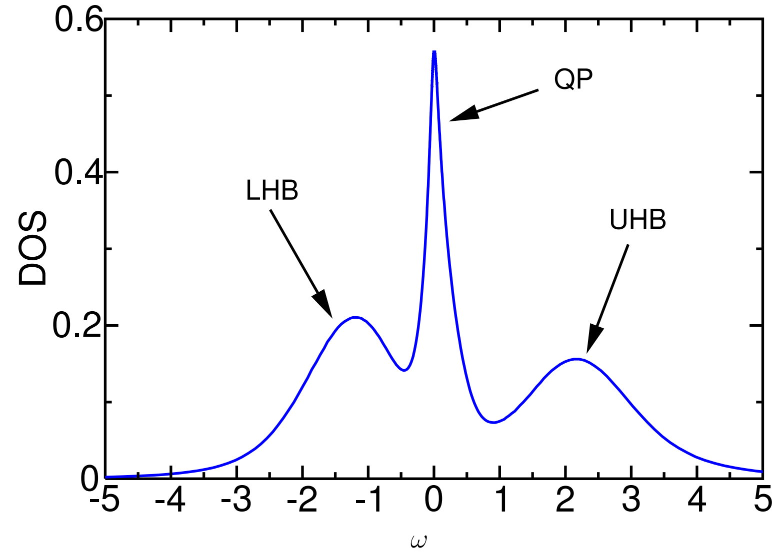
- Magnetism (AFM & FM)

Zitzler et al., EPJ '02



Successful approach for qualitative properties: DMFT

TP et al., PRB '93



- Metal-insulator transition for $\langle n \rangle = 1$
- Magnetism (AFM & FM)
- Correlated metal for $\langle n \rangle < 1$

Problems:

☛ No dependency on dimensionality of system — wrong for $D = 1$

☛ Fermi liquid ubiquitous

☛ No phases with non-local order parameter — e.g. d-wave sc

Idea: Try to combine ED, QMC and (D)MFT

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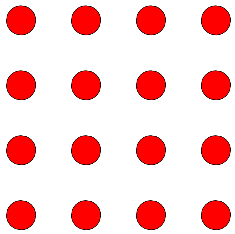
FiniteSystemSimulations



- ✔ Numerical exact
- ✔ Local & non-local dynamics
- ✘ Thermodynamic limit

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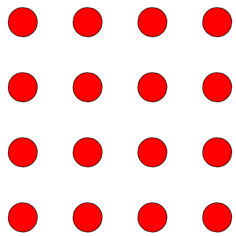

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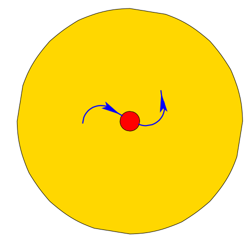

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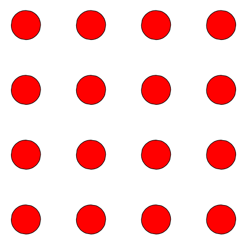

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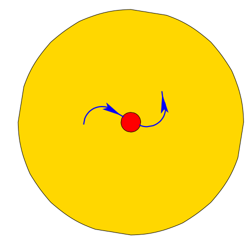

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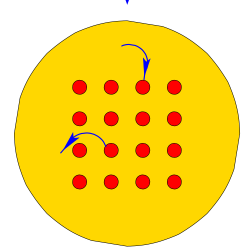
Combination:
Cluster MFT



Hettler, TP et al., PRB **58**, 7475('98)
Lichtenstein *et al.*, PRB **62**, R9283 ('00)
Kotliar *et al.* PRL **87**, 186401 ('01)
Maier *et al.*, RMP ('05).

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General scheme in all cluster MFT:

- Take into account short-ranged correlations exactly
- Neglect long-ranged correlations

➥ Example DCA: Reduce k-space resolution to $\Delta K = 2\pi/L$.

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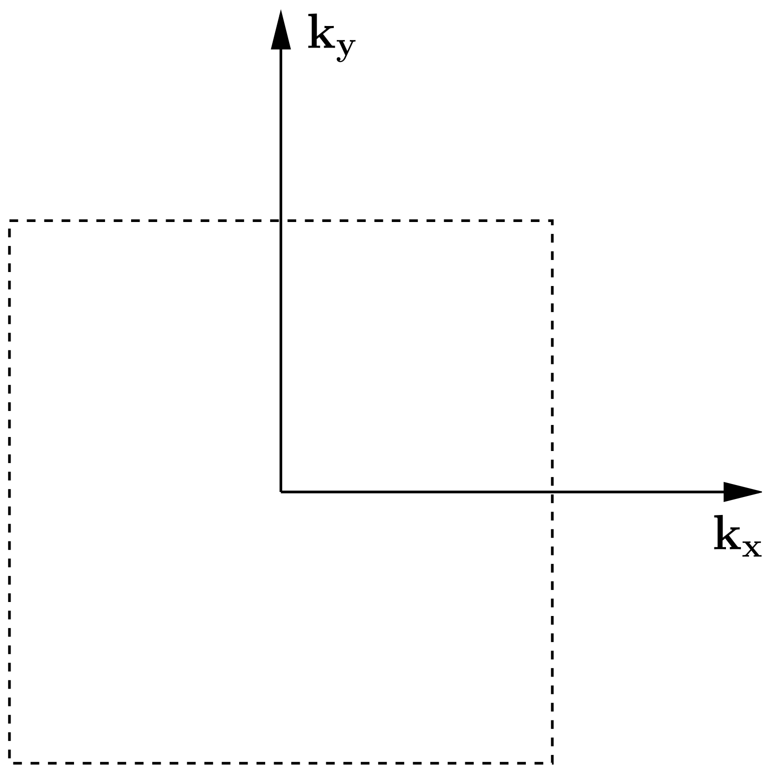

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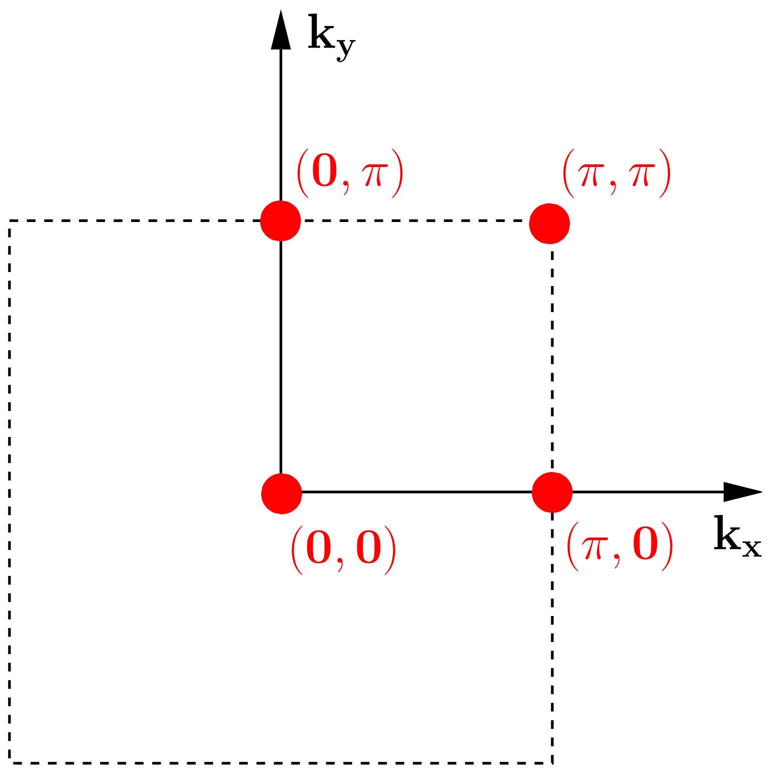

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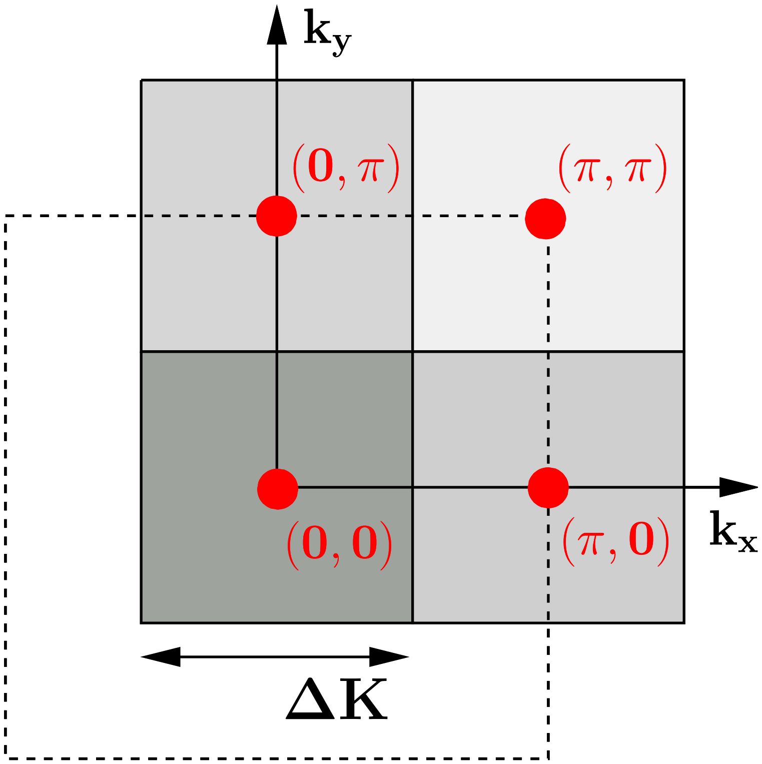

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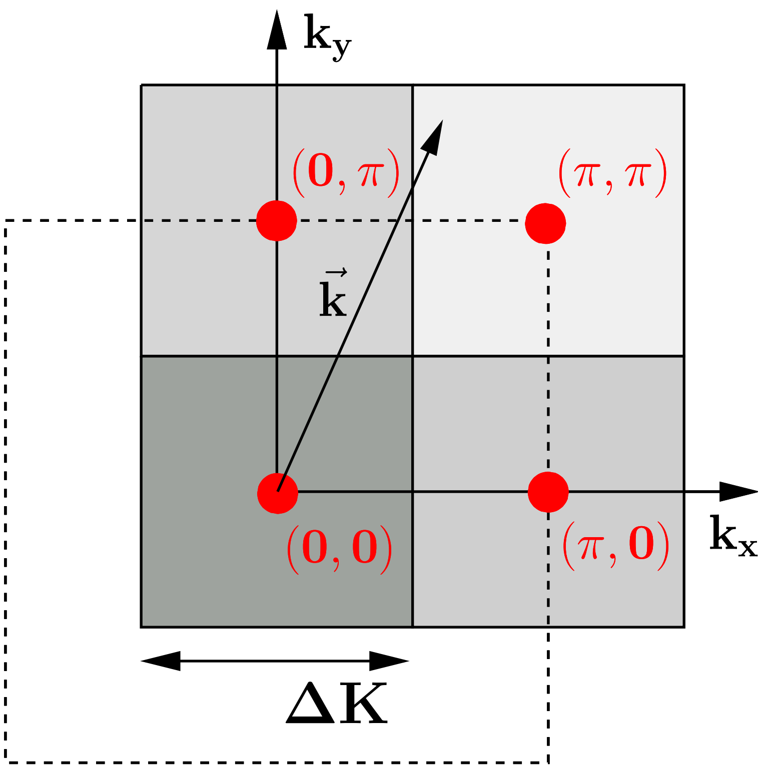

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  $\Sigma(\vec{k}, z)$

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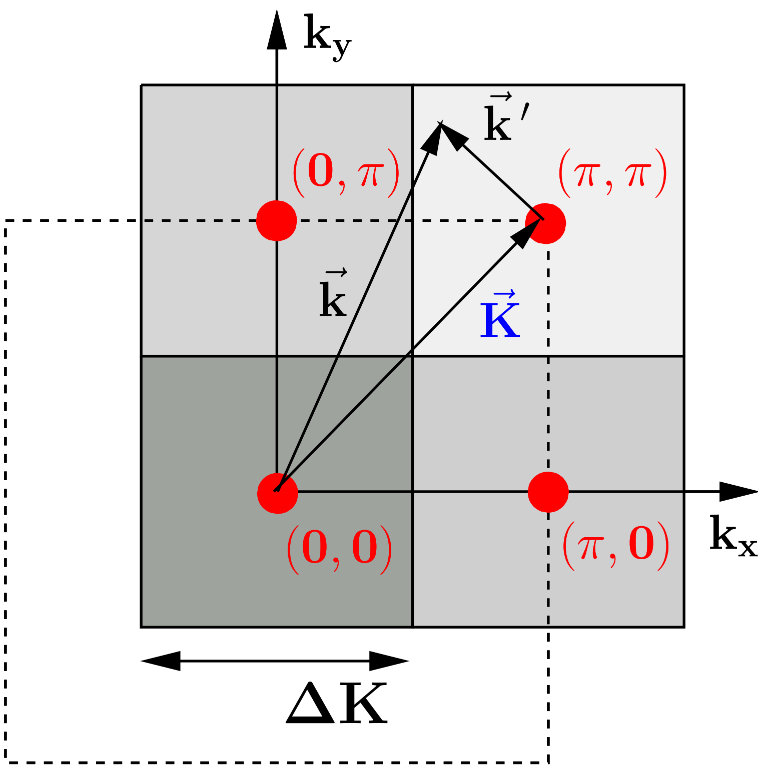

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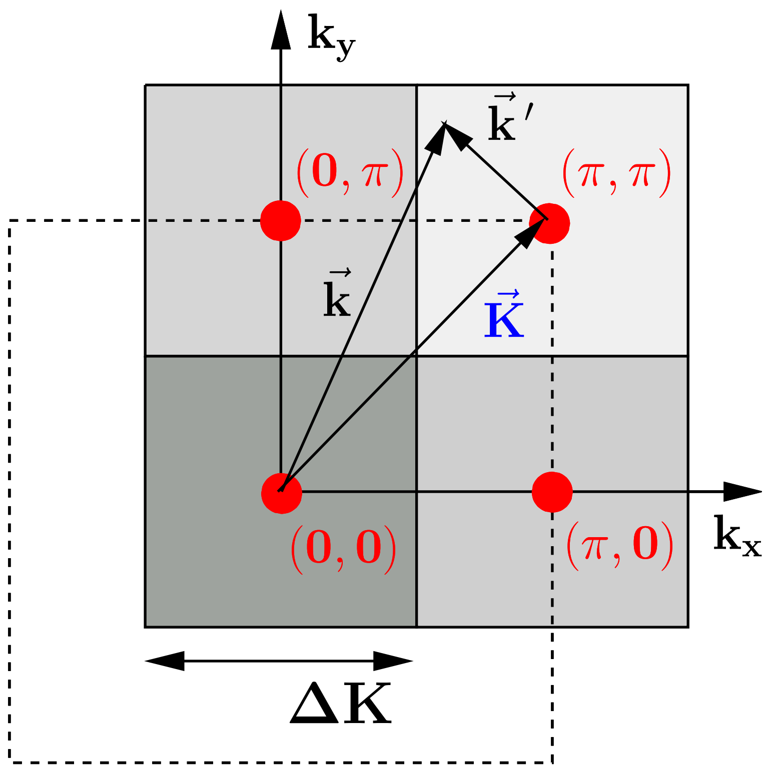

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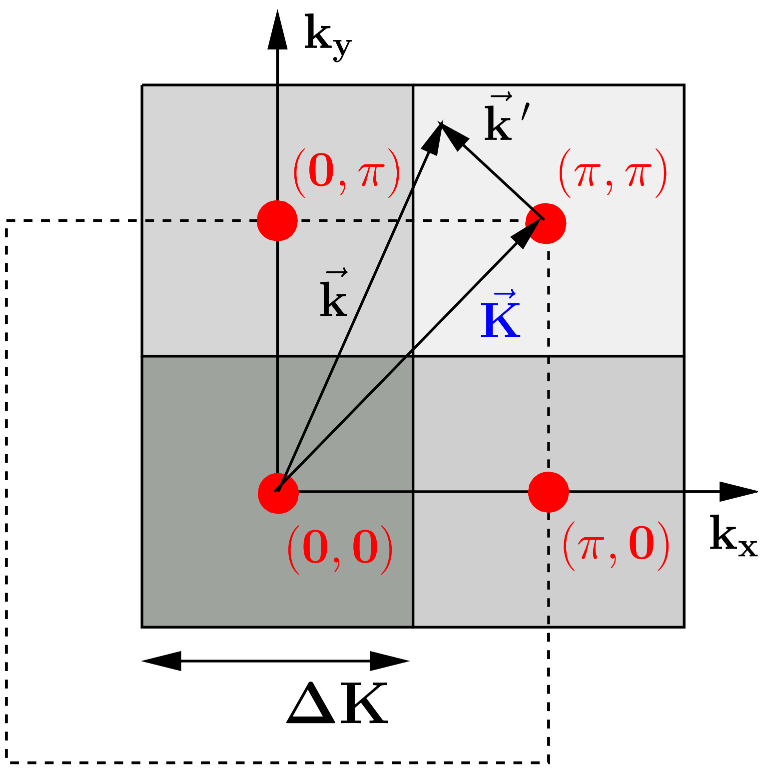

- Choose N_c cluster points $\mathbf{K}$:

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

- coarse graining:

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

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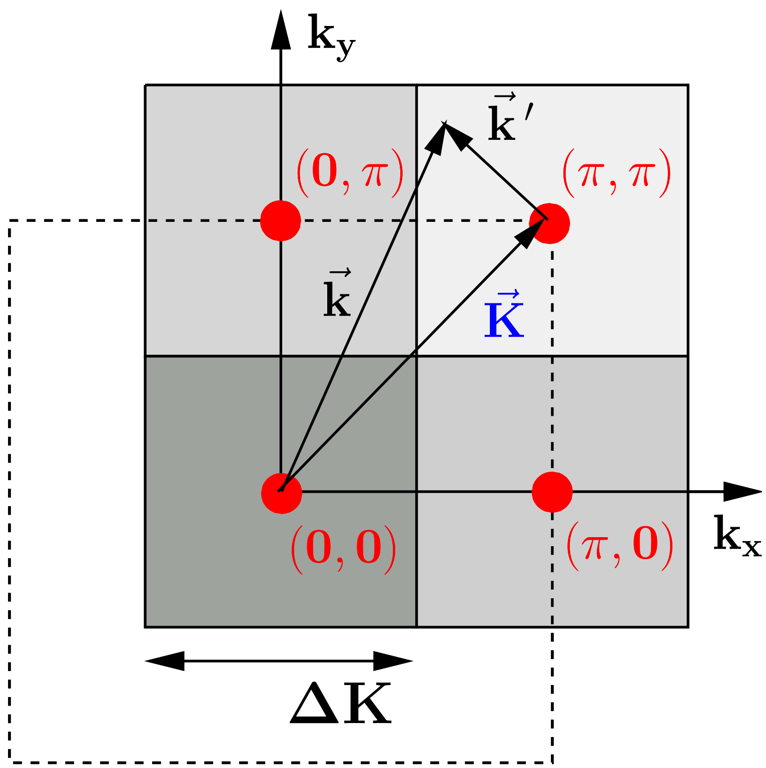

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- effective periodic cluster model

Maier *et al.*, RMP '05

Practical implementation:

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

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

↓

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

Practical implementation:

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

Initial 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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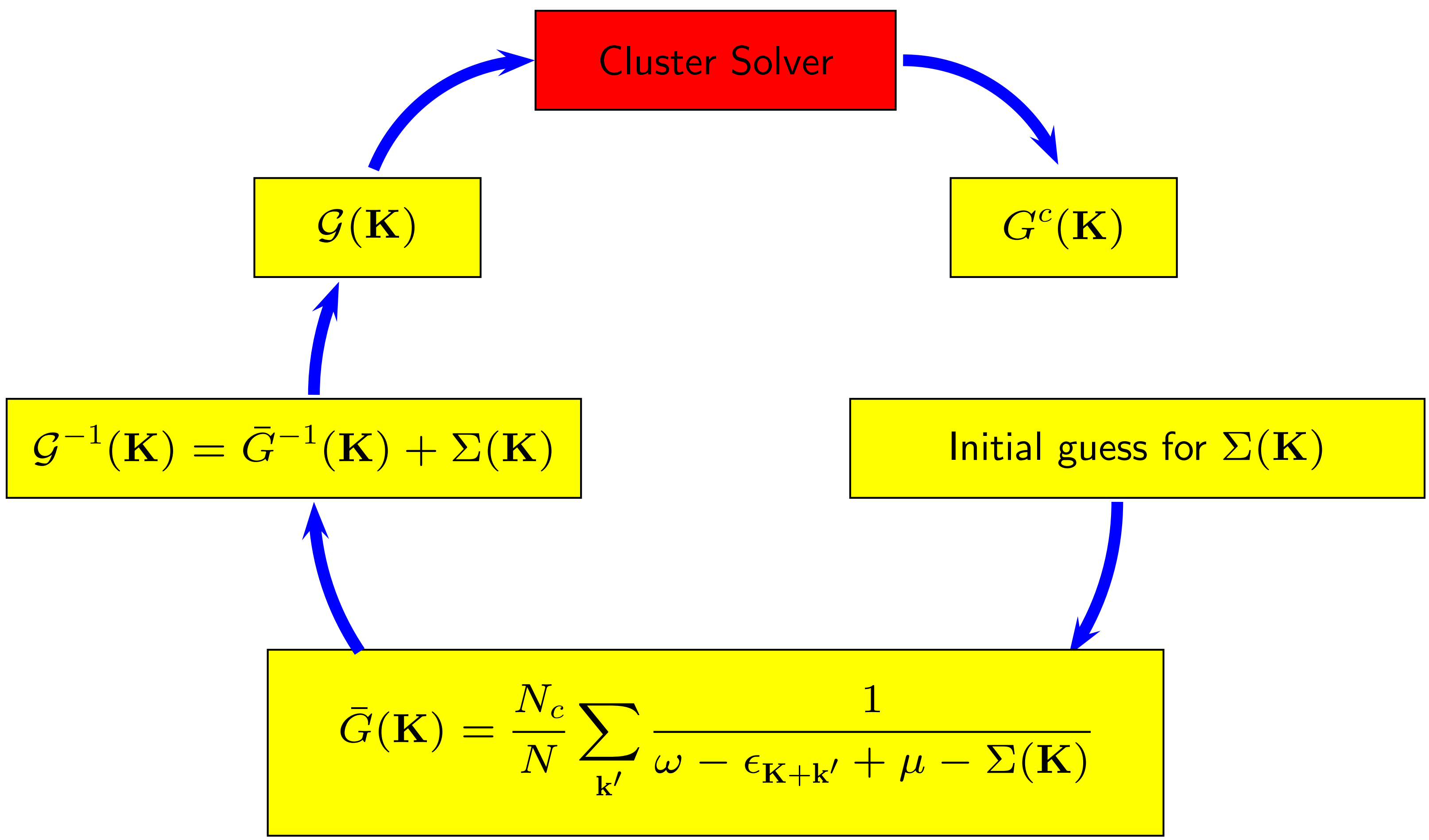

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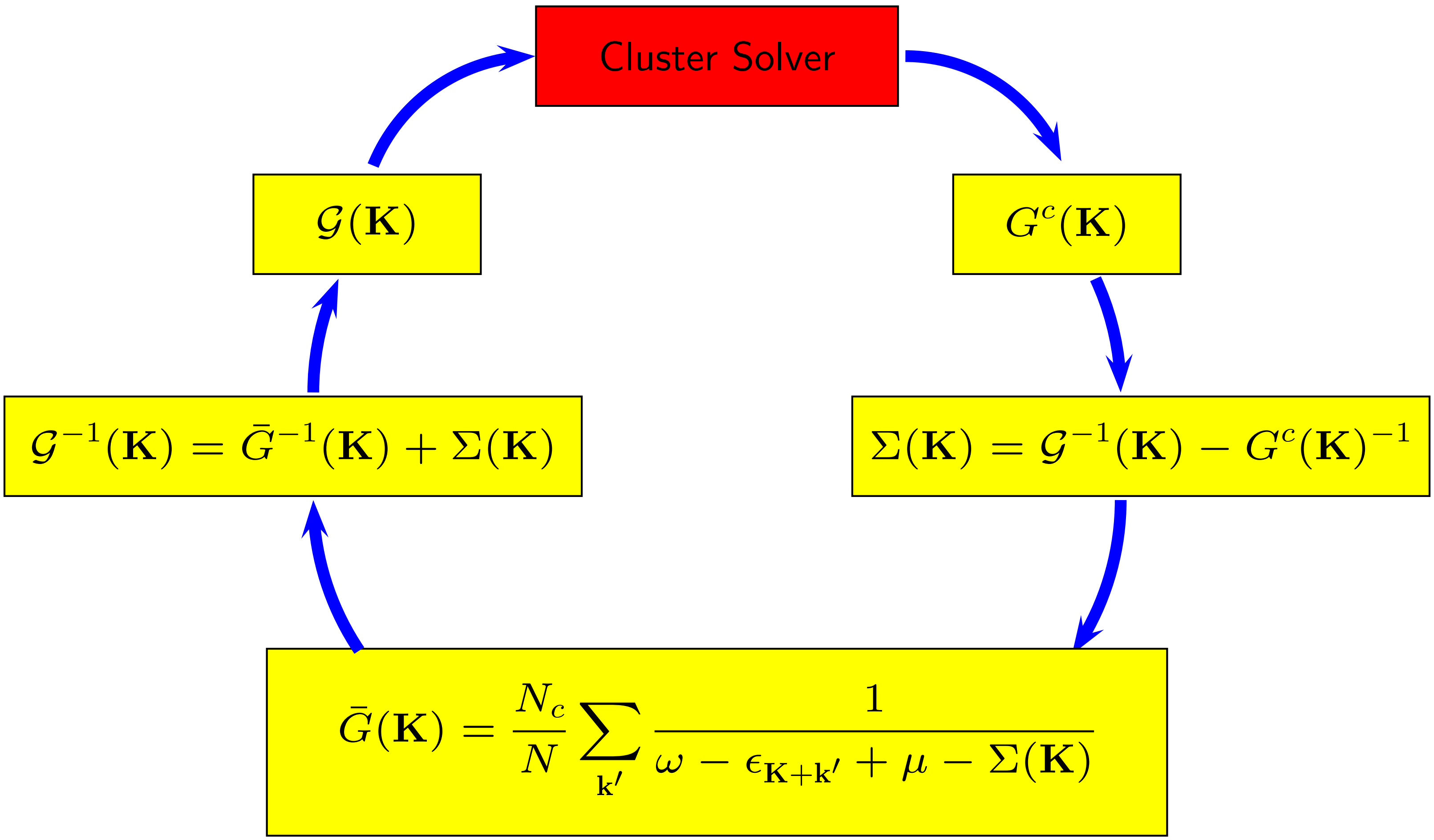

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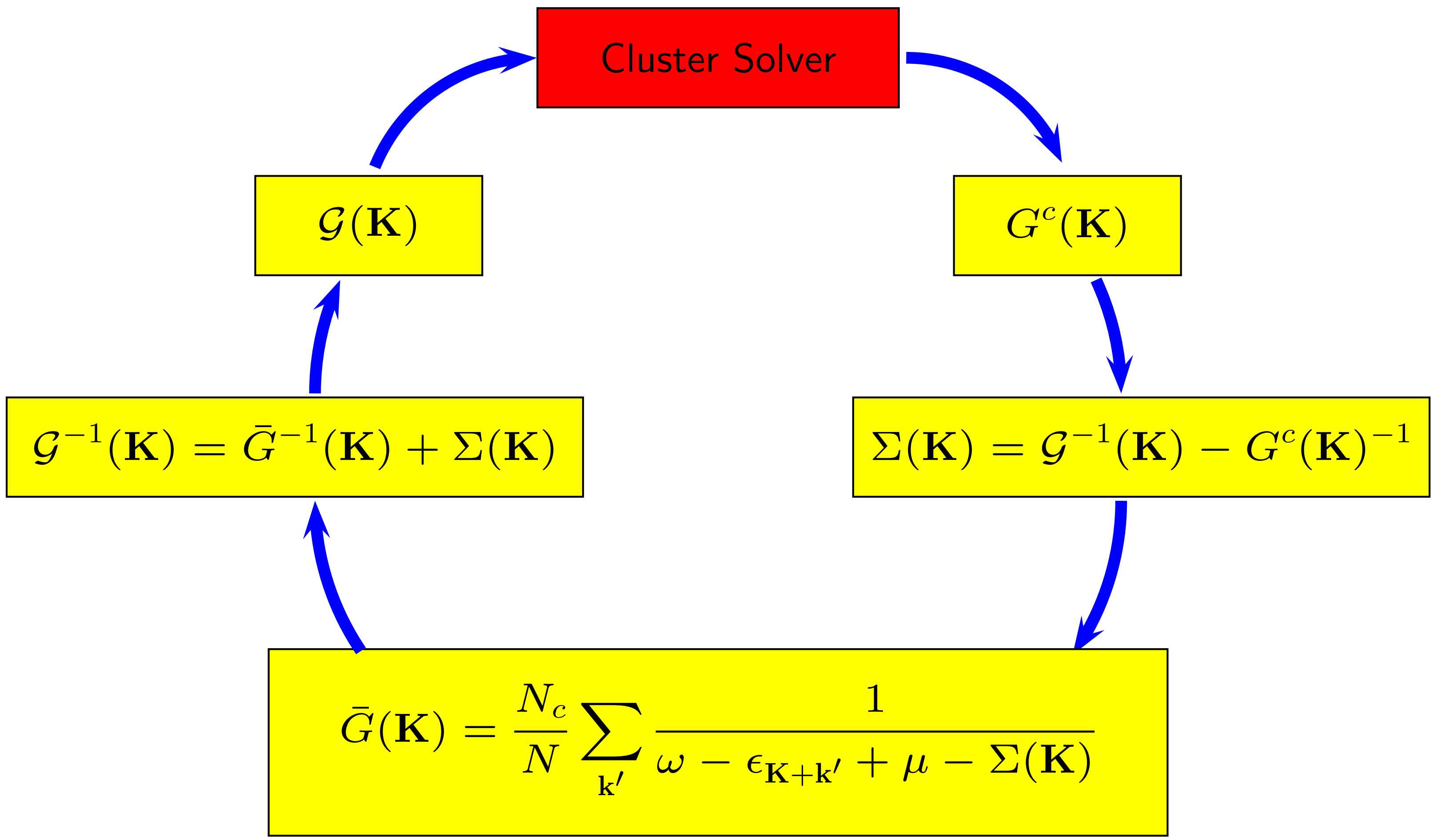


Exact limits: $N_c = 1 \;\Rightarrow$ DMFT, $N_c = N \;\Rightarrow$ exact

Other realizations:

- Define cluster in real space

  Lichtenstein *et al.*, PRB '00; Kotliar *et al.* PRL '01

- Neglect self-consistency

  cluster perturbation-theory

  Gros & Valenti, Ann. der Physik '94; Sénéchal *et al.*, PRL '00

Unifying framework:

- Self-energy functional theory

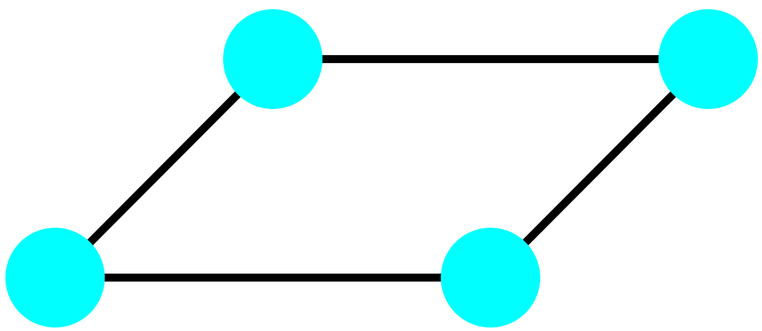
  Potthoff, EPJ '03; Dahnken *et al.*, '03

General problem:

- Reconstruct full k-dependence from coarse-grained self-energy

  e.g. DCA: interpolate $\Sigma(K, z) \longrightarrow \Sigma(k, z)$

Schematic structure of effective cluster:



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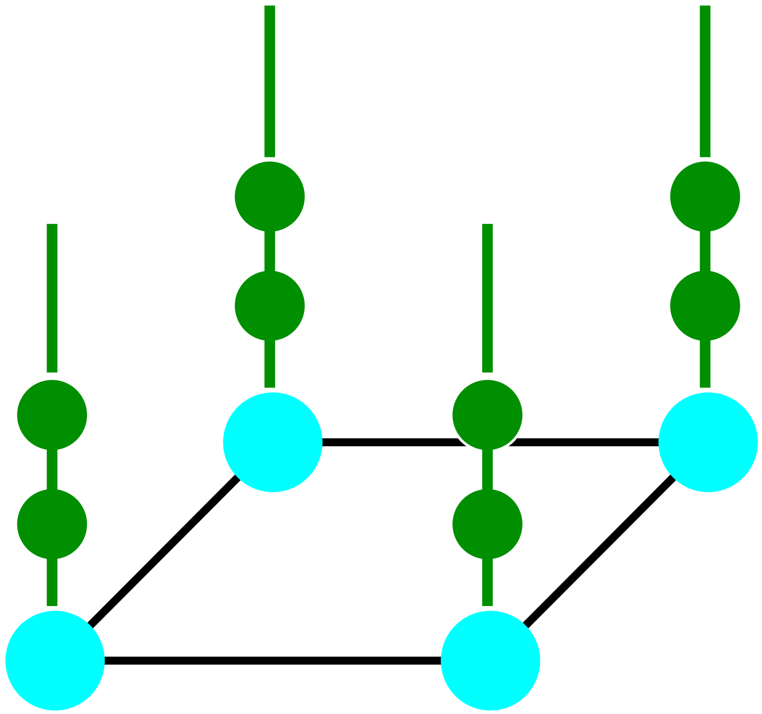

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➥ infinitely many degrees of freedom (noninteracting)

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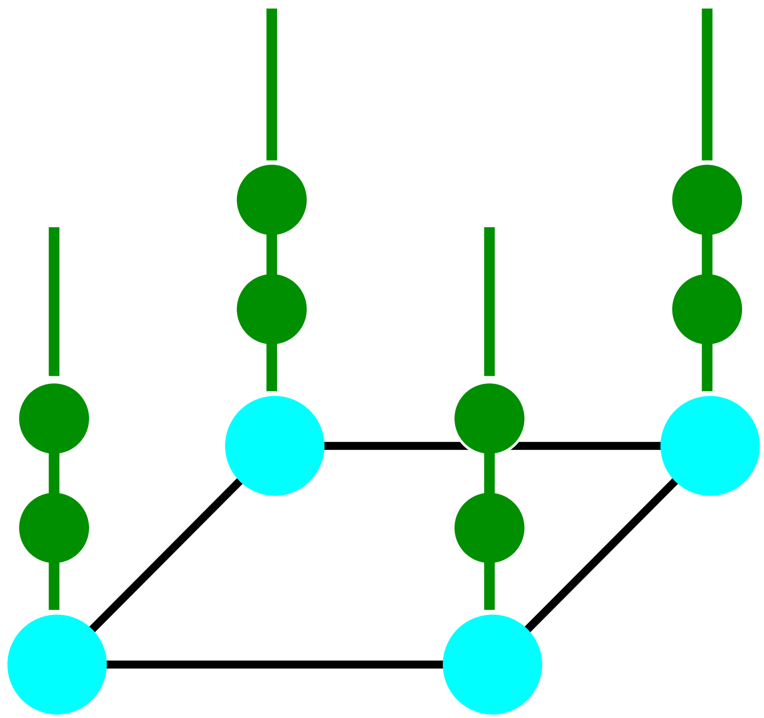

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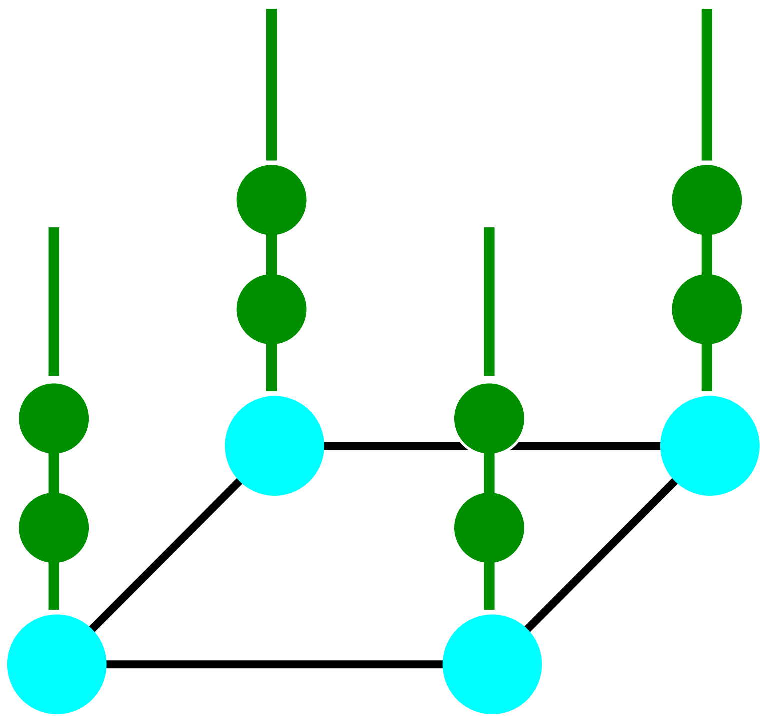
☛ Method of choice:
Hirsch-Fye QMC

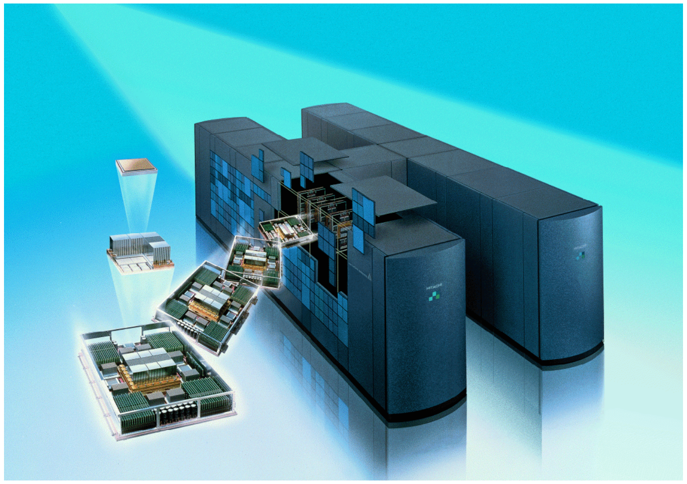
Schematic structure of effective cluster:



❏ Dynamical mean-field:

➥ infinitely many degrees of freedom (noninteracting)

☛ Method of choice:
Hirsch-Fye QMC



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Cluster Extensions to the Dynamical Mean-Field Theory

2D Hubbard Modell: $N_c = 1$ vs. $N_c > 1$ $(t' = 0)$

Maier, TP *et al.*, EPJ B **13** ('00)

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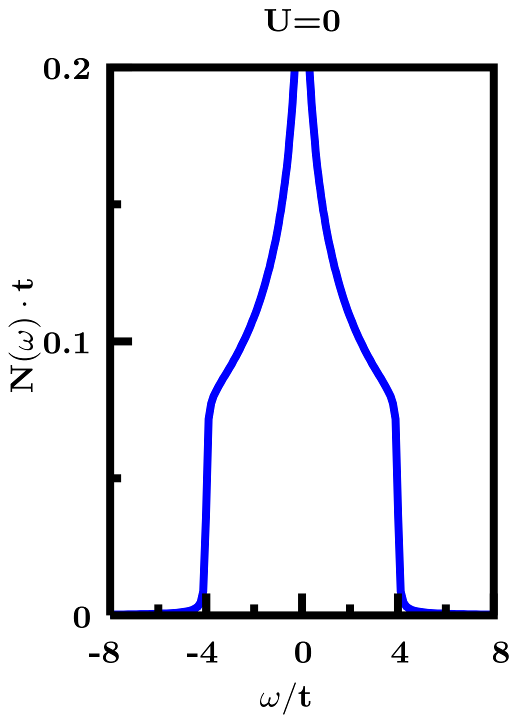

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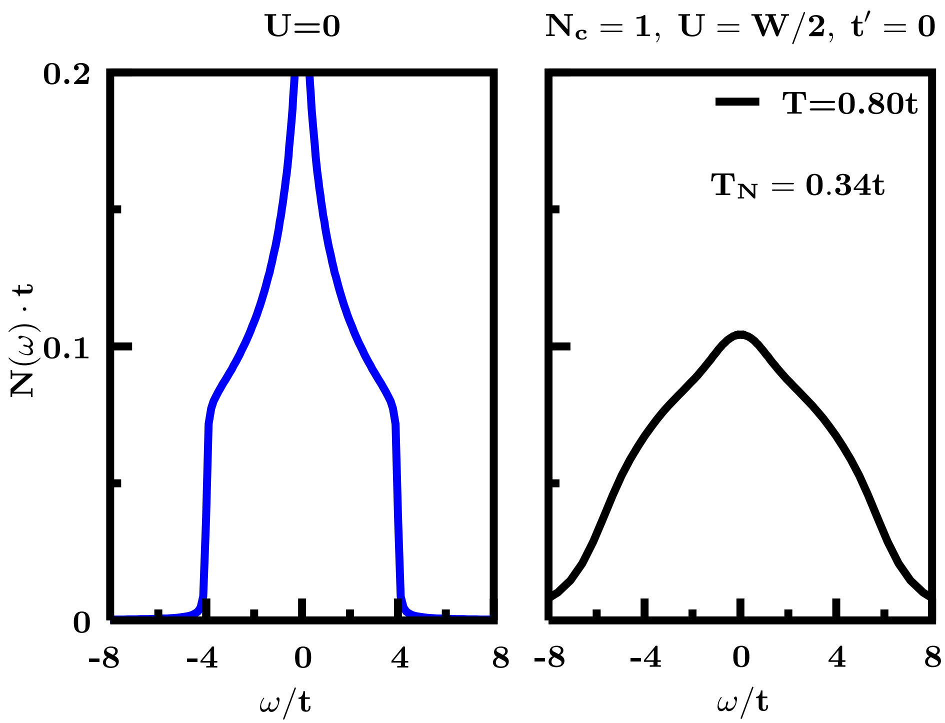

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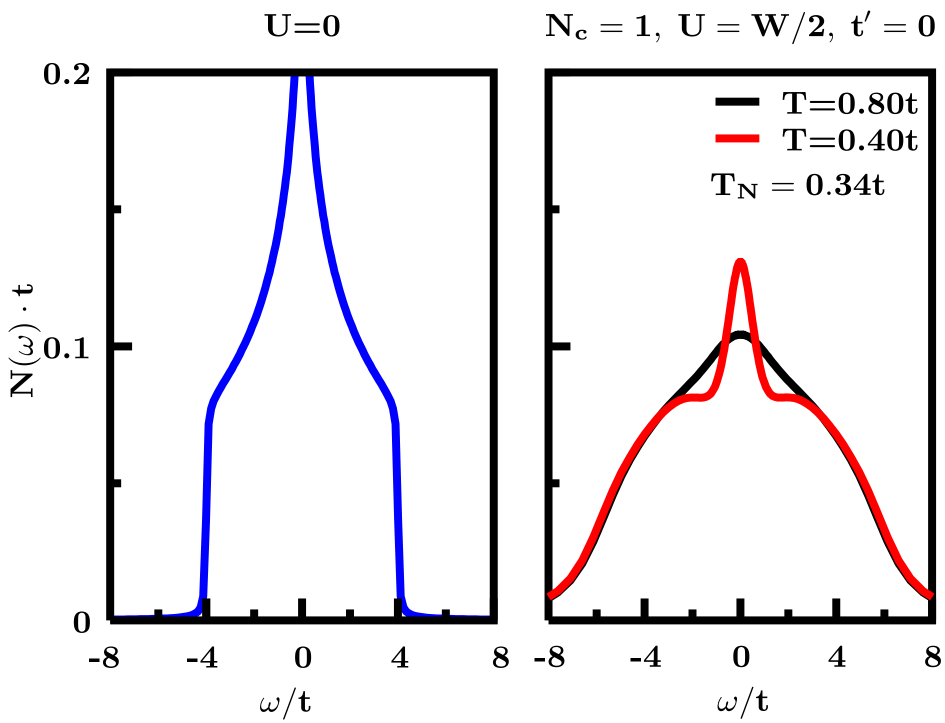

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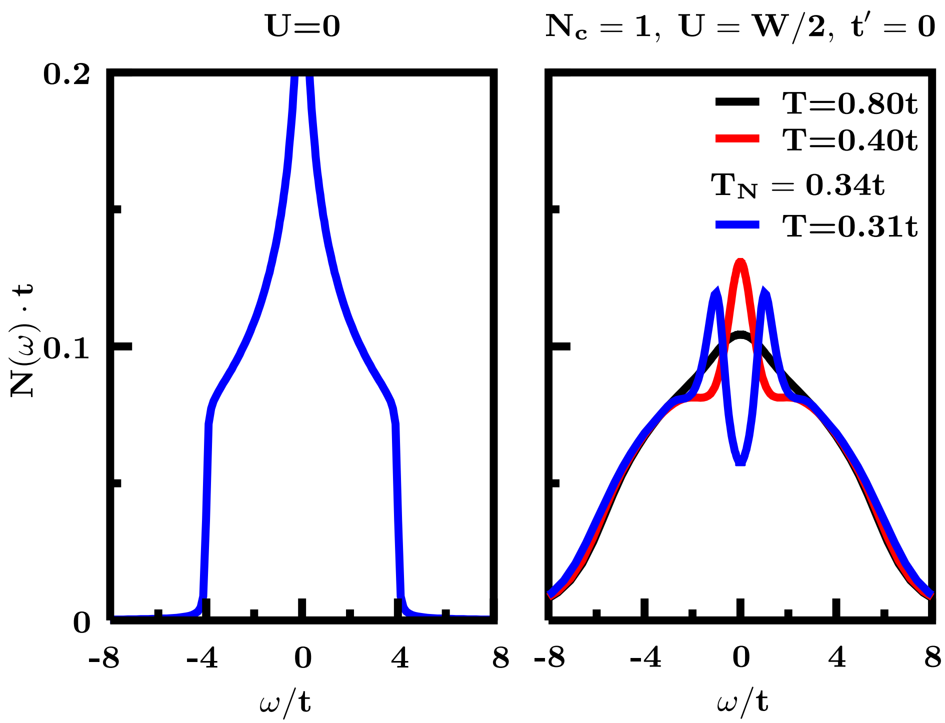

$N_c = 1$:

➥ No precursor of AF

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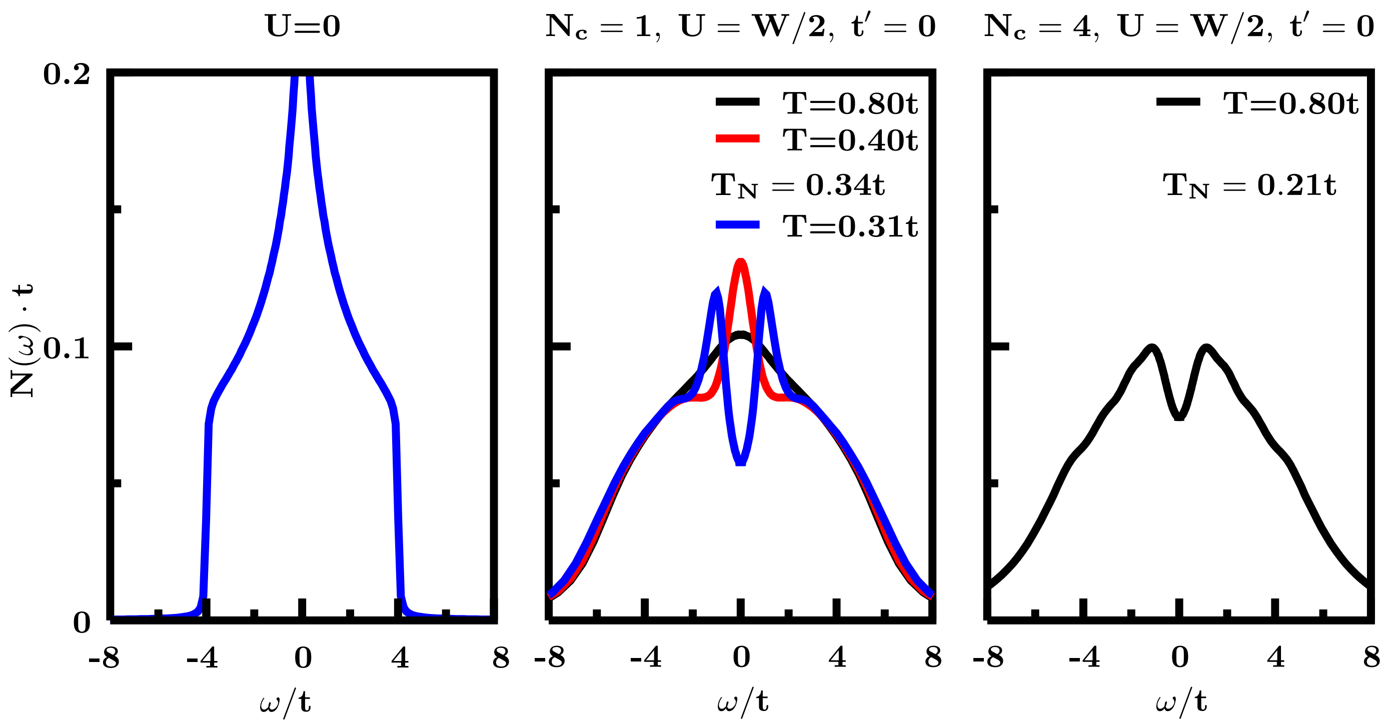

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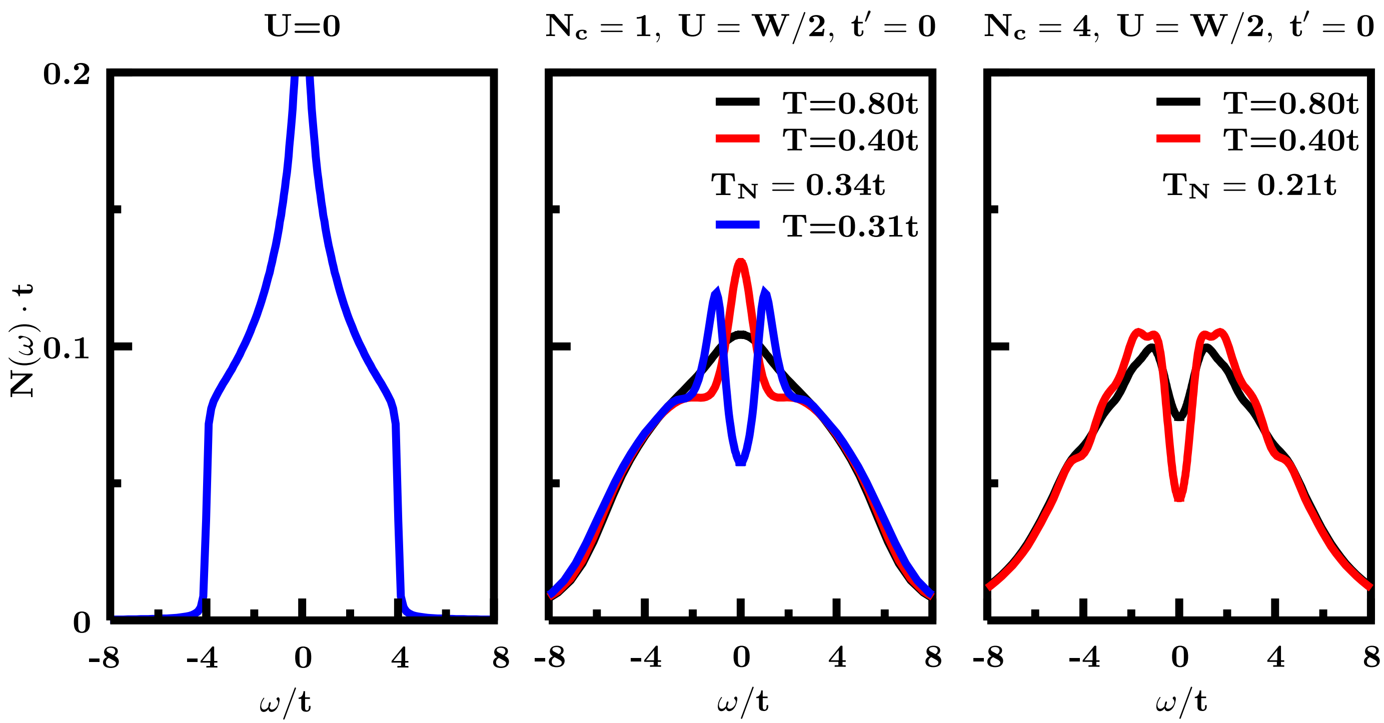

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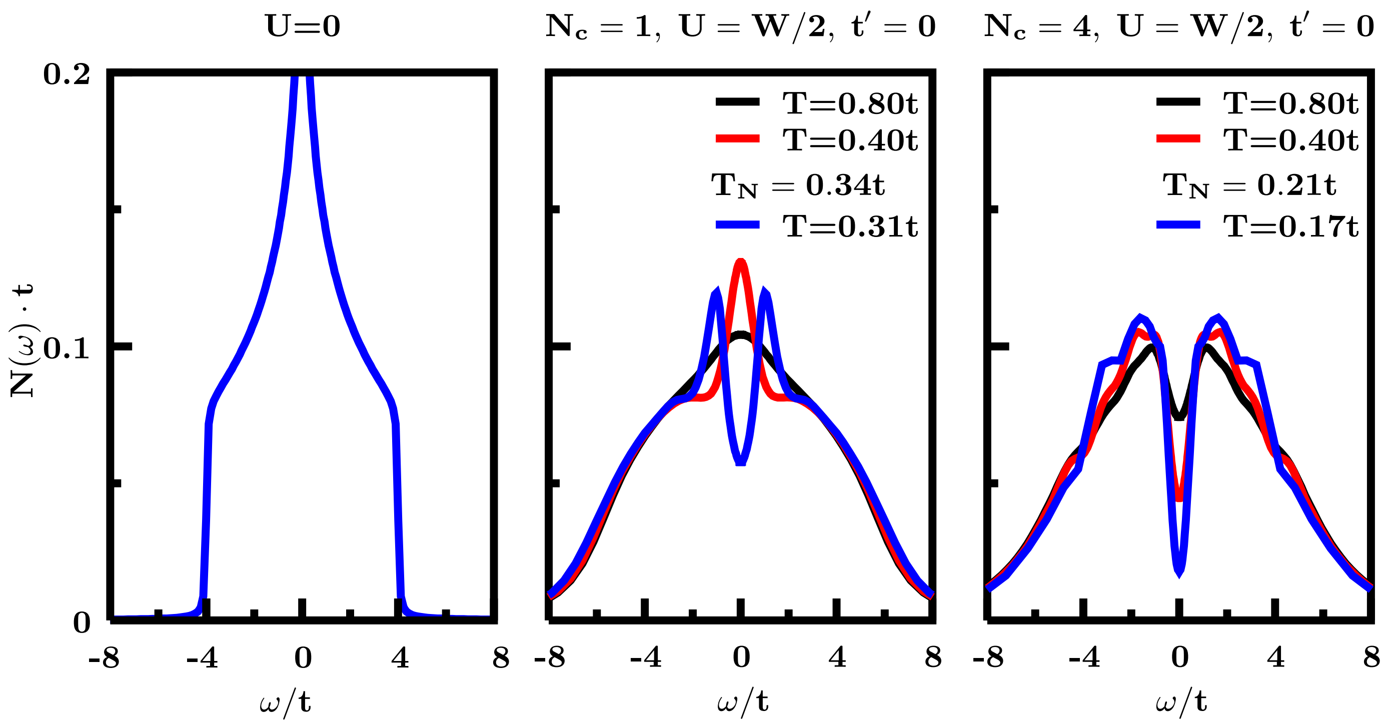


$N_c = 1$:

➥ No precursor of AF

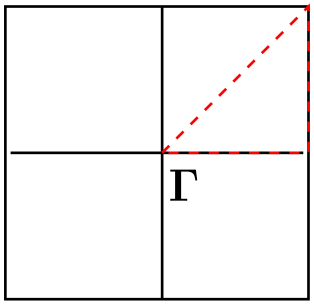
$N_c = 4$:

➥ pseudo gap in paramagnet

Spectral functions

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

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

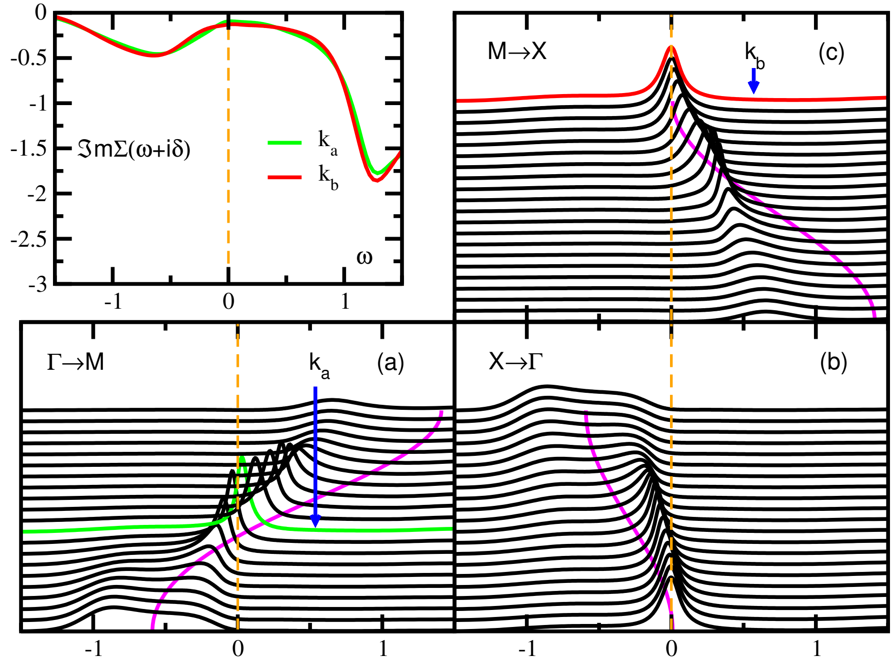


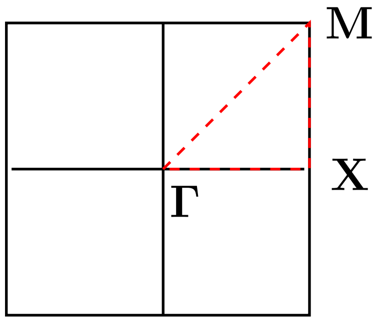
Spectral functions

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

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

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





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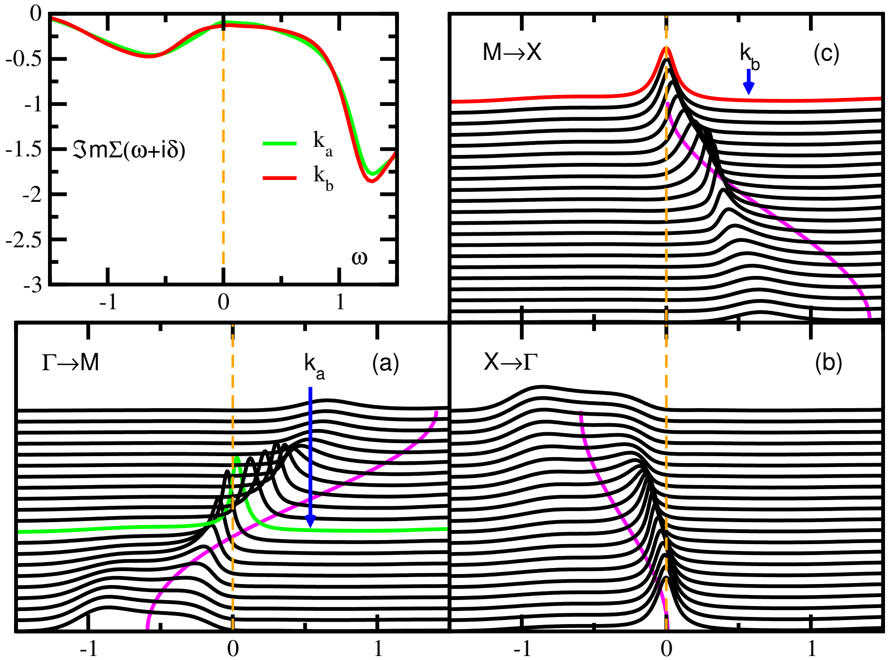
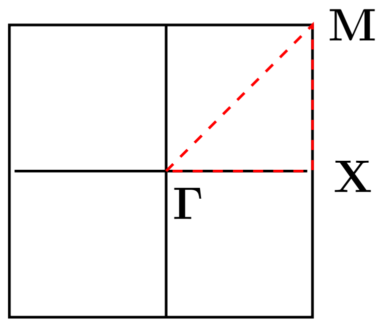


- ❑ well defined quasi particles
- ❑ weak $\vec{k}$-dependence of $\Sigma(\vec{k}, \omega)$



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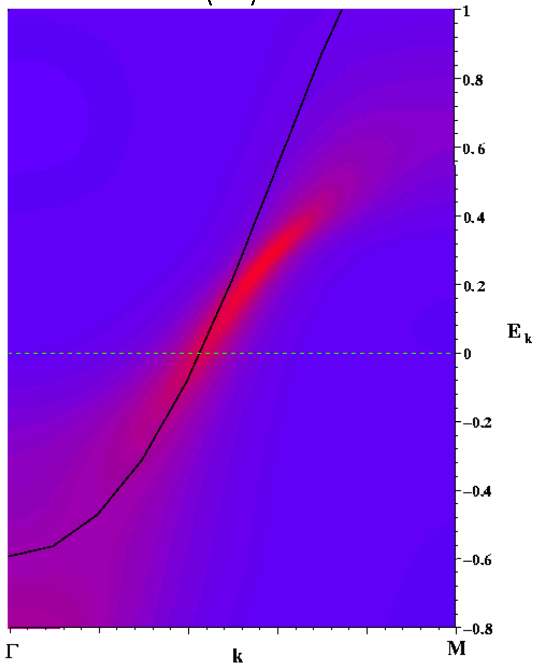
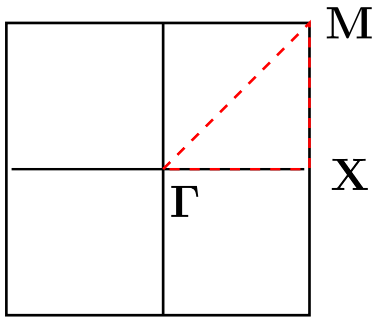


- well defined quasi particles
- weak $\vec{k}$-dependence of $\Sigma(\vec{k}, \omega)$
- reduced quasi-particle bandwidth



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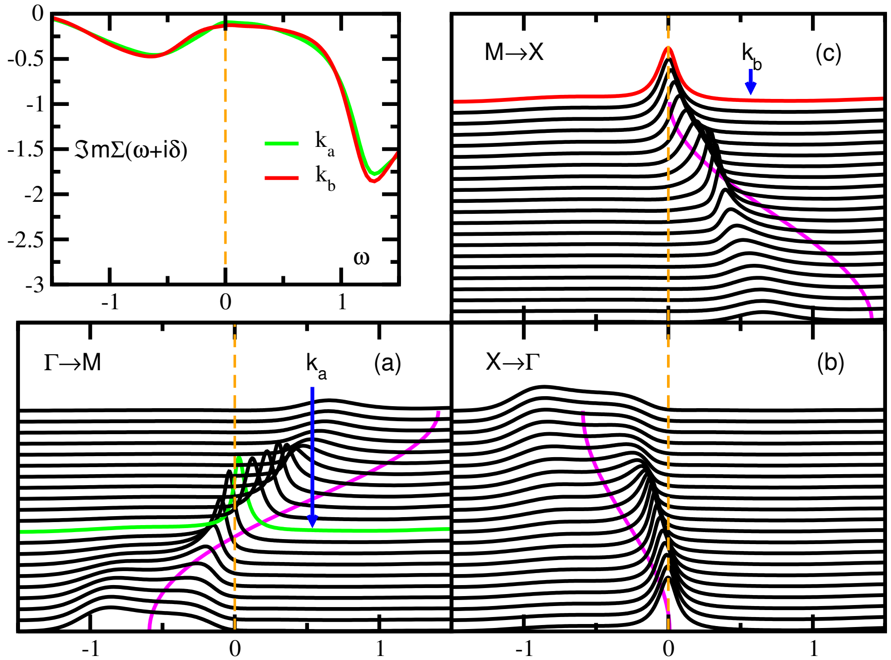

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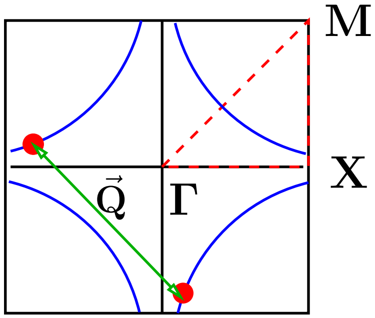

Spectral functions

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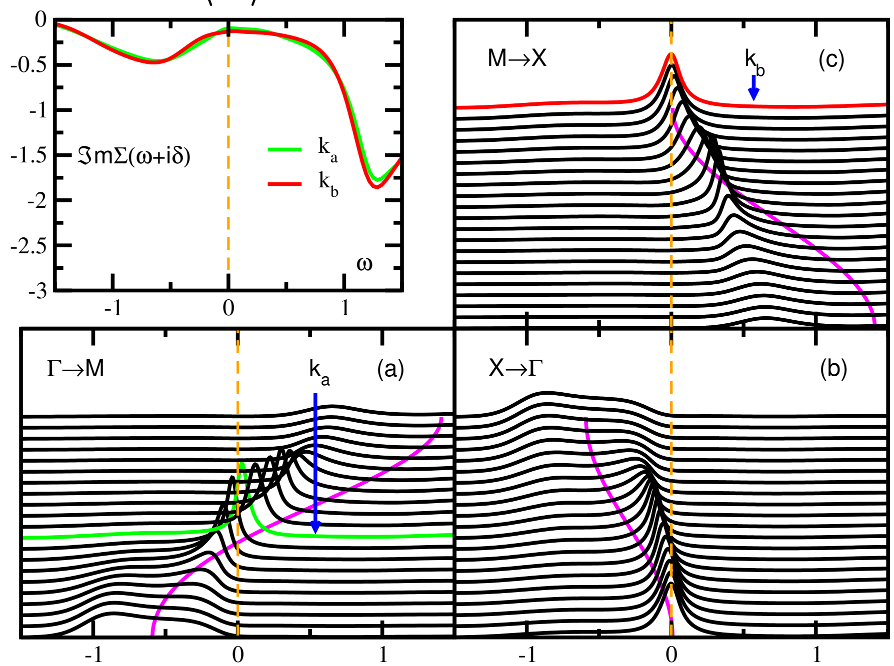
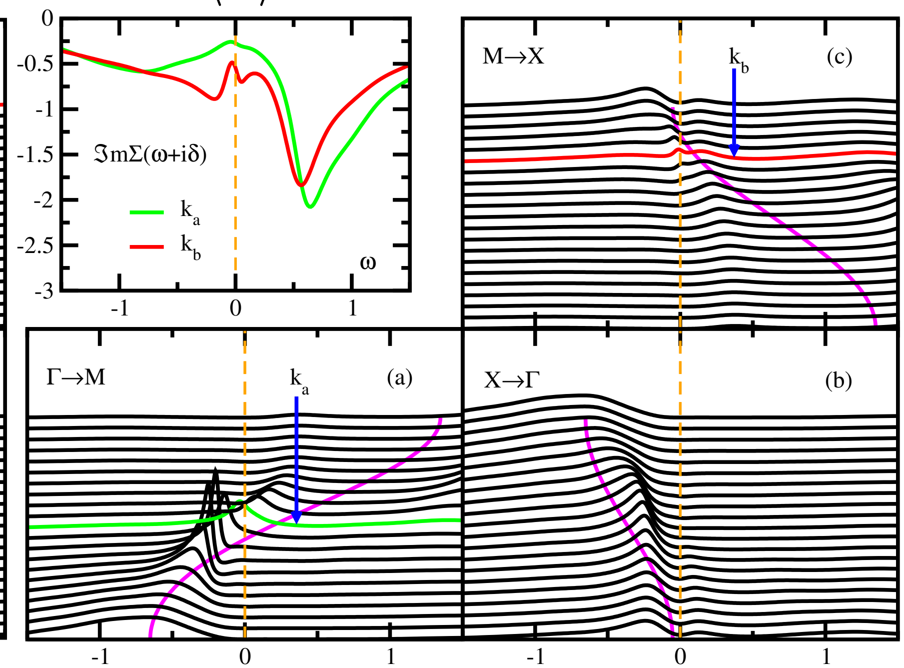
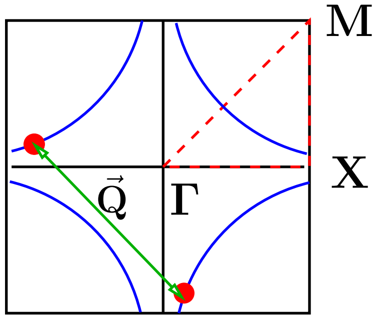


$\langle n \rangle = 0.95,\ T = 370\text{K}$



- ❑ well defined quasi particles
- ❑ weak $\vec{k}$-dependence of $\Sigma(\vec{k},\omega)$
- ❑ reduced quasi-particle bandwidth
- ❑ overdamping of structures near X



Spectral functions

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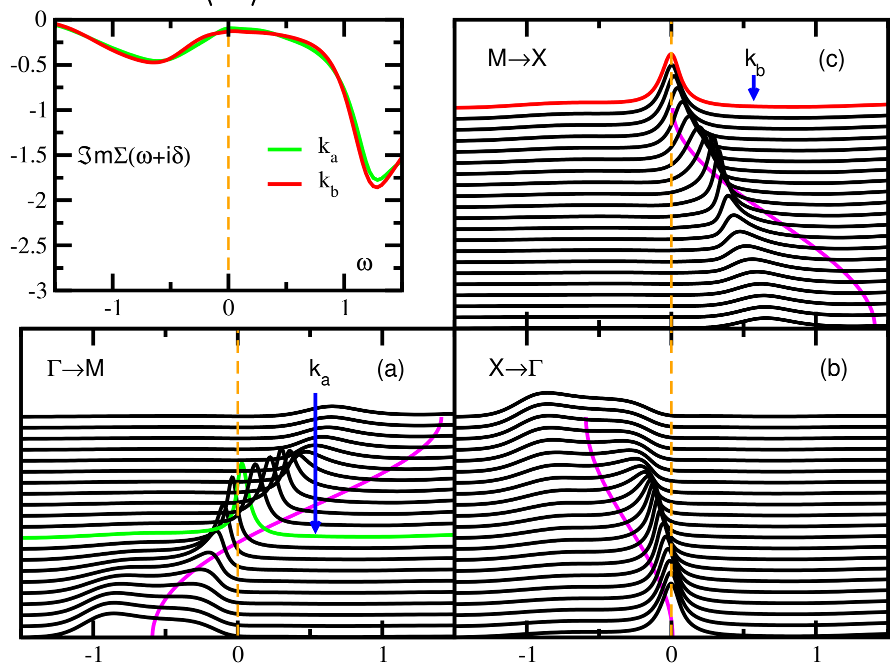

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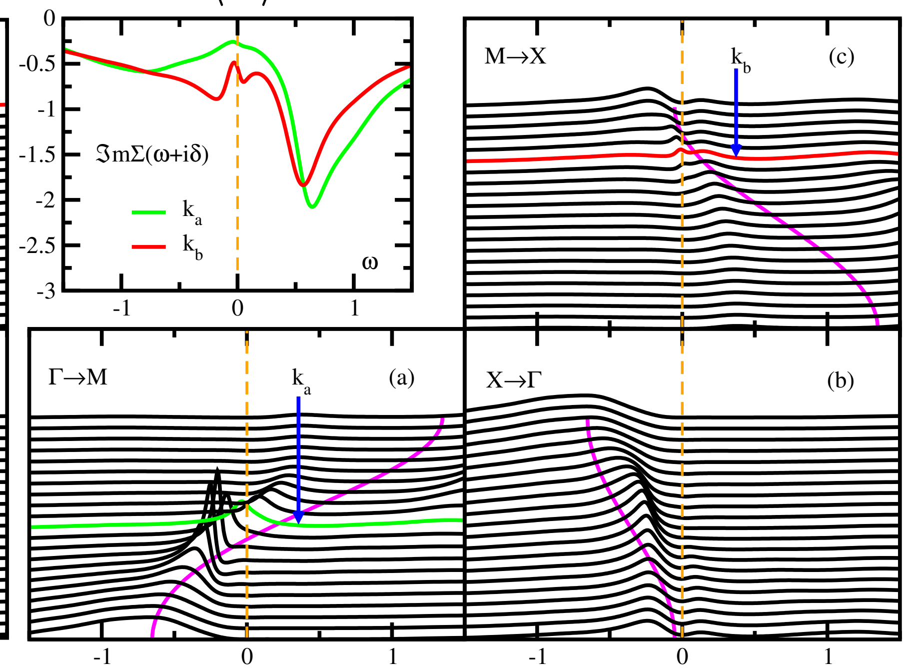


- ❏ well defined quasi particles
- ❏ weak $\vec{k}$-dependence of $\Sigma(\vec{k}, \omega)$
- ❏ reduced quasi-particle bandwidth

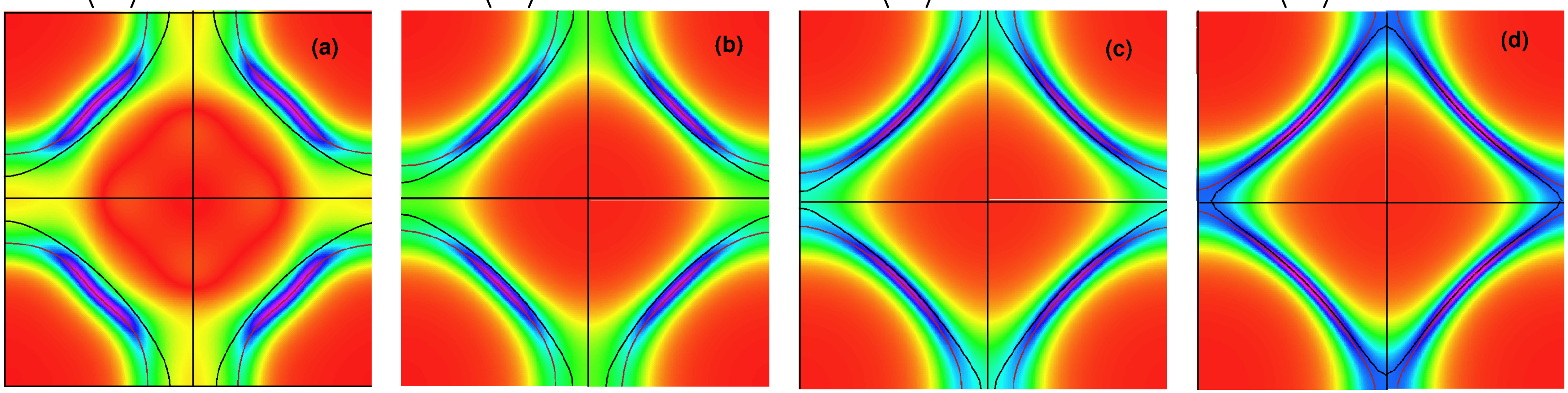
- ❏ overdamping of structures near X
- ❏ strong $\vec{k}$-dependence of $\Sigma(\vec{k}, \omega)$
- ❏ non-FL $\Sigma(\vec{k}, \omega)$ near X?

Fermi surface

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

$N_c = 16$, $U = W$, $t' = -0.2$, $T = 370\text{K}$

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



$\langle n \rangle \gtrsim 0.9$

Small FS for $\langle n \rangle \to 1$

➥Hole pockets?

$\langle n \rangle \lesssim 0.9$

Large FS for $\langle n \rangle < 0.9$

➥free-electron like FS

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Cluster Extensions to the Dynamical Mean-Field Theory

1. Why cluster methods?
2. Cluster extensions – DCA, CDMFT and Co.
3. Spectral functions from the DCA
4. **Summary**

Aspects of cluster MFT

- Interpolation between finite system simulations and DMFT
  - ☛ Thermodynamic limit for dynamics
  - ☛ Systematic inclusion of short- and mid-ranged correlations

- Sensible results
  - ☛ Reduction of transition temperatures
  - ☛ Fluctuation induced precursors of order in spectra
  - ☛ Nontrivial k-dependent renormalization of single-particle properties