Self-energy parametrization for the 2D Hubbard Model

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with

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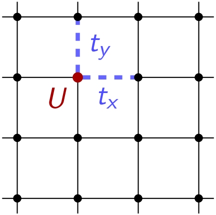
Motivation

Hubbard model for the 2d square lattice

$$H = -\sum_{<i,j>,\sigma} t_{ij}(c^\dagger_{i,\sigma} c_{j,\sigma} + \text{h.c.}) + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$



- not exactly solvable for $d > 1$
- finite-size clusters: **q**uantum **M**onte **C**arlo simulation $(d = 2, 3)$
- mean-field: **d**ynamical **m**ean-**f**ield **t**heory

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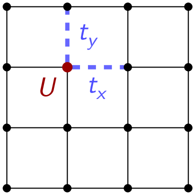

QMC

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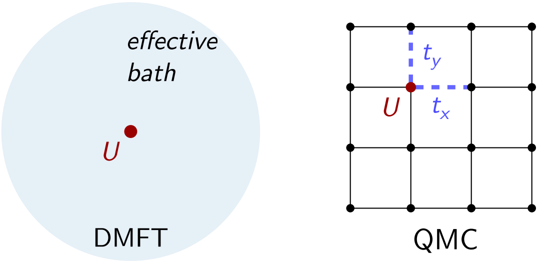

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Motivation

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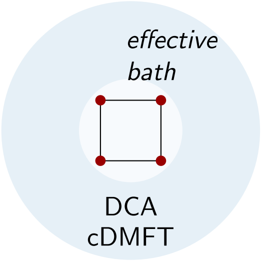
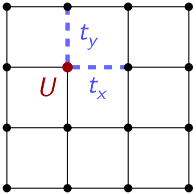
$$H = -\sum_{<i,j>,\sigma} t_{ij}(c^{\dagger}_{i,\sigma}c_{j,\sigma} + \text{h.c.}) + U\sum_{i} n_{i,\uparrow}n_{i,\downarrow}$$





QMC

- not exactly solvable for $d > 1$
- finite-size clusters: **q**uantum **M**onte **C**arlo simulation $(d = 2, 3)$
- mean-field: **d**ynamical **m**ean-**f**ield **t**heory + extensions $(d = 2)$

Motivation

$$G_\sigma(\mathbf{k},\omega) = \frac{1}{\omega - \varepsilon_{\mathbf{k}} + \mu - \Sigma_\sigma(\mathbf{k},\omega)}$$

DMFT ↙

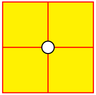
$\Sigma(\mathbf{k},\omega) \to \Sigma(\omega)$

Motivation

$$G_\sigma(\mathbf{k},\omega) = \frac{1}{\omega - \varepsilon_{\mathbf{k}} + \mu - \Sigma_\sigma(\mathbf{k},\omega)}$$

DMFT

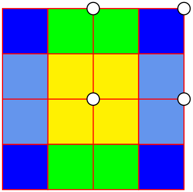
$$\Sigma(\mathbf{k},\omega) \to \Sigma(\omega)$$



DCA

$$\Sigma(\mathbf{k},\omega) \to \Sigma_{\mathrm{DCA}}(\mathbf{K},\omega)$$

for 4-16 **K**-points



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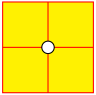

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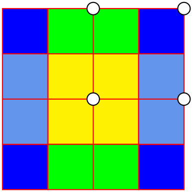


finite-size cluster

$\Sigma(\mathbf{k},\omega) \to \Sigma_{\text{QMC}}(\mathbf{K},\omega)$

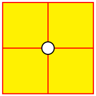
up to 256 **K**-points

Motivation

$$G_\sigma(\mathbf{k},\omega) = \frac{1}{\omega - \varepsilon_{\mathbf{k}} + \mu - \Sigma_\sigma(\mathbf{k},\omega)}$$

DMFT

$$\Sigma(\mathbf{k},\omega) \to \Sigma(\omega)$$



DCA

$$\Sigma(\mathbf{k},\omega) \to \Sigma_{\mathrm{DCA}}(\mathbf{K},\omega)$$

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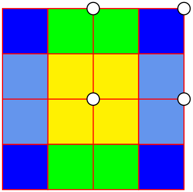


finite-size cluster

$$\Sigma(\mathbf{k},\omega) \to \Sigma_{\mathrm{QMC}}(\mathbf{K},\omega)$$

up to 256 **K**-points

we use QMC

Motivation

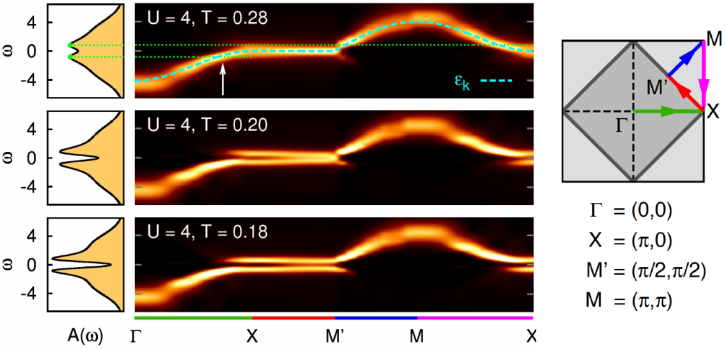
pseudogap physics: nonlocal correlations along the Fermi edge

Momentum-dependent pseudogaps in the half-filled two-dimensional Hubbard model

D. Rost,[1] E. V. Gorelik,[1] F. Assaad,[2] and N. Blümer[1]

[1] *Institute of Physics, Johannes Gutenberg University, Mainz, Germany*
[2] *Institute of Theoretical Physics and Astrophysics, University of Würzburg, Würzburg, Germany*

(Dated: October 3, 2012)



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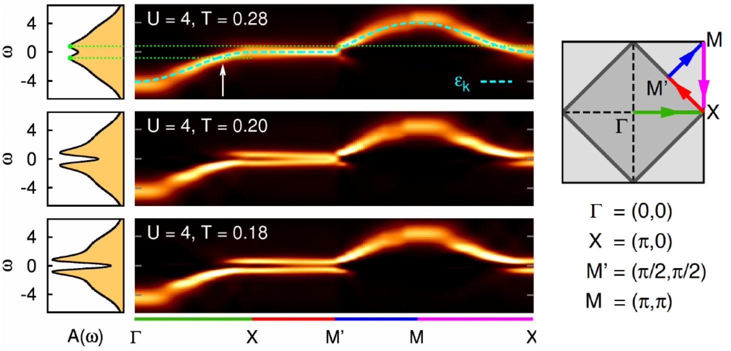


Full **k**-space structure? Self-energy?

Outline

1. the self-energy for low frequencies
2. the self-energy for the full-frequency regime
3. Temperature dependence
4. Conclusions & outlook

Outline

1. the self-energy for low frequencies
   - → **k**-space structure
   - → parametrization
2. the self-energy for the full-frequency regime
   - → **k**-space structure
   - → parametrization
3. Temperature dependence
4. Conclusions & outlook

Σ for low frequencies

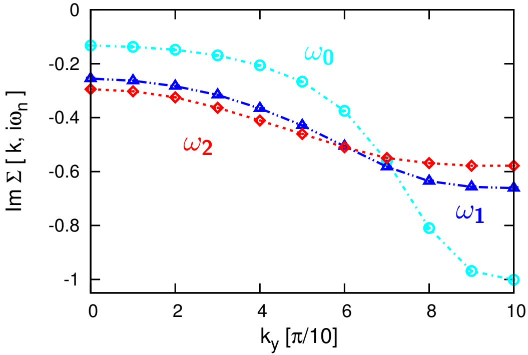
$\rightarrow$ **k**-space structure

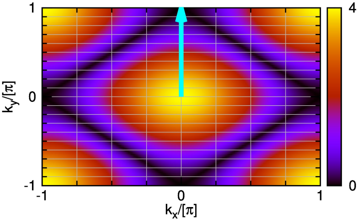
$\rightarrow$ parametrization

k-structure of Σ

$U = 4t$
$\beta t = 5.6$
$L = 8 \times 20$
$\Delta\tau = 0.1$

Im $\Sigma(\mathbf{k}, i\omega_n)$ vs. path in the Brillouin zone:





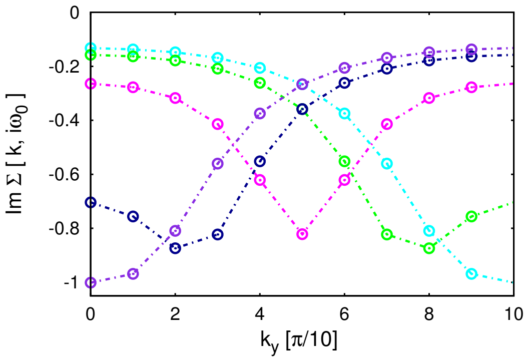
→ Strong variations across the Brillouin zone

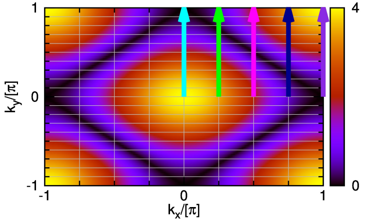
in the low-frequency region!

k-structure of Σ

dependence on all **k**-points of the Brillouin zone

$$U = 4t$$
$$\beta t = 5.6$$
$$L = 8 \times 20$$
$$\Delta\tau = 0.1$$





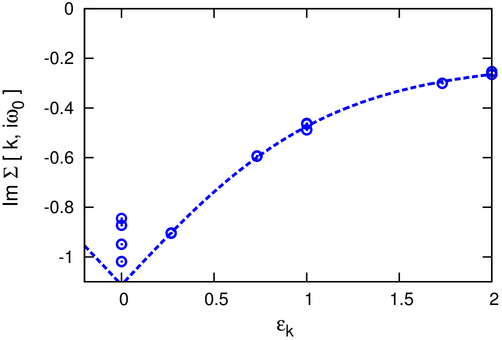
→ Variations are not smooth along generic directions!

→ Global structure of the momentum dependence?

$\varepsilon_{\mathbf{k}}$-structure of Σ

$U = 4t$
$\beta t = 5.6$
$L = 12 \times 12$
$\Delta\tau = 0.1$

Im $\Sigma(\mathbf{k}, i\omega_0)$ vs. $\varepsilon_{\mathbf{k}}$:



collapse of all data points for $\varepsilon_{\mathbf{k}} \neq 0$:

$$\Sigma(\mathbf{k}, i\omega_0) \to \Sigma(\varepsilon_{\mathbf{k}}, i\omega_0)$$

→ scalar dependence

→ allows for parametization

$\varepsilon_{\mathbf{k}}$-structure of Σ

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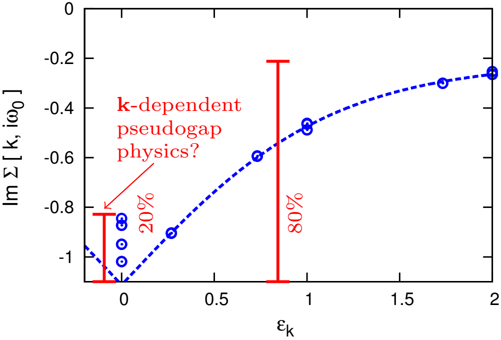

collapse of all data points for $\varepsilon_{\mathbf{k}} \neq 0$:

$$\Sigma(\mathbf{k}, i\omega_0) \rightarrow \Sigma(\varepsilon_{\mathbf{k}}, i\omega_0)$$

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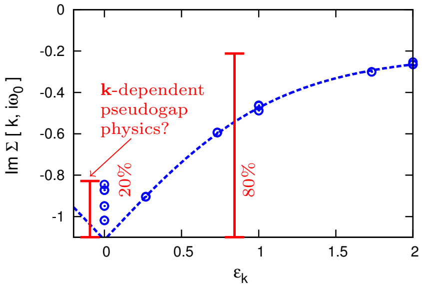
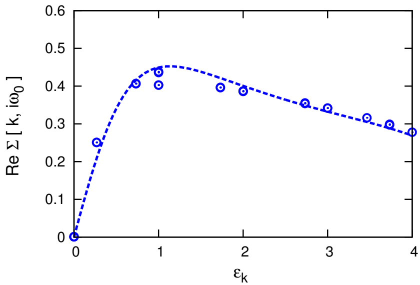
$\rightarrow$ allows for parametization

ε_k-structure of Σ

Im $\Sigma(\mathbf{k}, i\omega_0)$ vs. $\varepsilon_\mathbf{k}$:



Re $\Sigma(\mathbf{k}, i\omega_0)$ vs. $\varepsilon_\mathbf{k}$:



for $\varepsilon_\mathbf{k} \neq 0$:

$$\Sigma(\mathbf{k}, i\omega_n) \rightarrow \Sigma(\varepsilon_\mathbf{k}, i\omega_n)$$

$\rightarrow$ comparable results also for the real part

$$U = 4t$$
$$\beta t = 5.6$$
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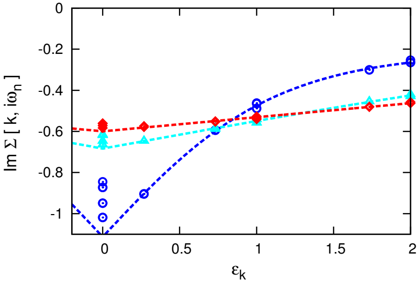
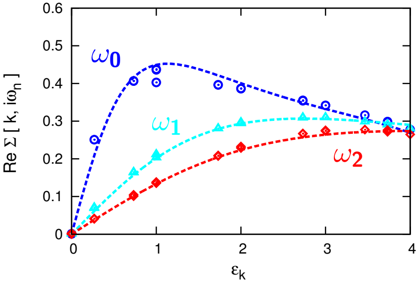
$\varepsilon_{\mathbf{k}}$-structure of Σ

Im $\Sigma(\mathbf{k}, i\omega_n)$ vs. $\varepsilon_{\mathbf{k}}$:



Re $\Sigma(\mathbf{k}, i\omega_n)$ vs. $\varepsilon_{\mathbf{k}}$:



for $\varepsilon_{\mathbf{k}} \neq 0$:

$$\Sigma(\mathbf{k}, i\omega_n) \rightarrow \Sigma(\varepsilon_{\mathbf{k}}, i\omega_n)$$

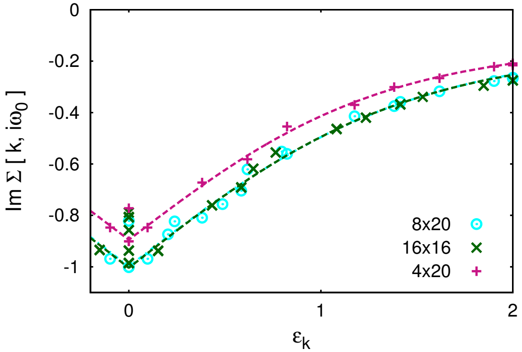
$\rightarrow$ comparable results also for the real part and higher frequencies

$$U = 4t$$
$$\beta t = 5.6$$
$$L = 12 \times 12$$
$$\Delta\tau = 0.1$$

Finite-size effects

$U = 4t$
$\beta t = 5.6$
$\Delta\tau = 0.1$

$\mathrm{Im}\, \Sigma\left(\mathbf{k}, i\omega_0\right)$ vs. $\varepsilon_{\mathbf{k}}$:



collapse of all data points for $\varepsilon_{\mathbf{k}} \neq 0$:

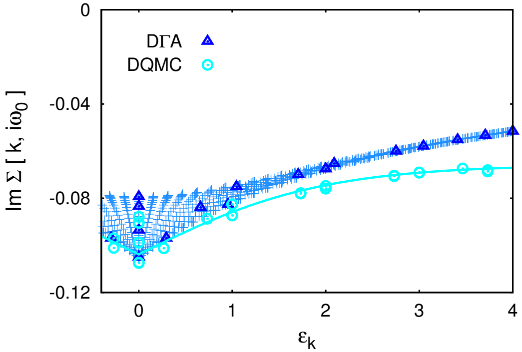
$$\Sigma\left(\mathbf{k}, i\omega_n\right) \rightarrow \Sigma\left(\varepsilon_{\mathbf{k}}, i\omega_n\right)$$

$\rightarrow$ Deviations from global fit curves smaller than finite-size effects and independent of lattice geometry!

Comparison with DΓA

$U = 2t$
$\beta t = 2$
$\Delta\tau = 0.1$

Im $\Sigma(\mathbf{k}, i\omega_0)$ vs. $\varepsilon_\mathbf{k}$:



collapse of all data points for $\varepsilon_\mathbf{k} \neq 0$:

$$\Sigma(\mathbf{k}, i\omega_n) \rightarrow \Sigma(\varepsilon_\mathbf{k}, i\omega_n)$$

→ bias of QMC for a more insulating solution w.r.t DΓA

→ higher **k**-resolution of DΓA:
spread also apart from Fermi edge

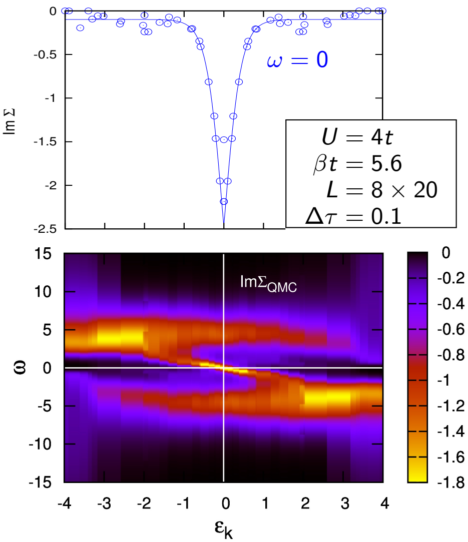
Σ for the full-frequency regime

$\rightarrow$ **k**-space structure

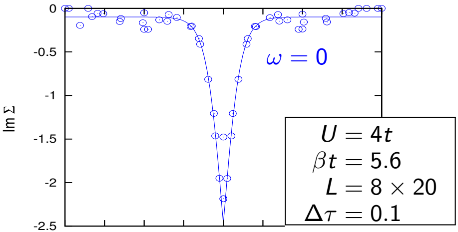
$\rightarrow$ parametrization

$(\omega, \varepsilon_{\mathbf{k}})$-structure of Σ

Im $\Sigma(\mathbf{k}, \omega)$ vs. $\varepsilon_{\mathbf{k}}$, ω:

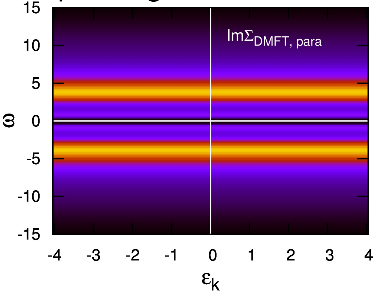


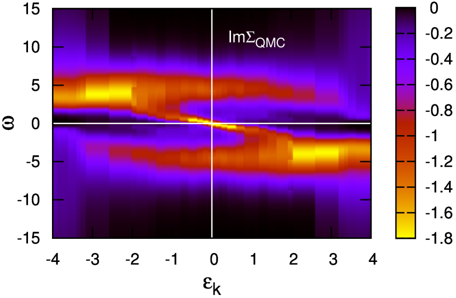
$(\omega, \varepsilon_{\mathbf{k}})$-structure of Σ



$\text{Im}\,\Sigma\,(\mathbf{k},\omega)$ vs. $\varepsilon_{\mathbf{k}}$, ω:

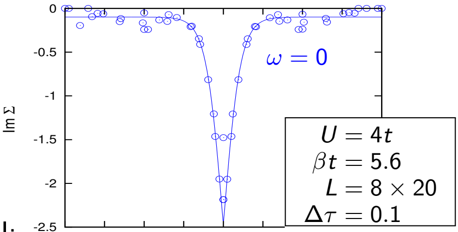
paramagnetic DMFT:





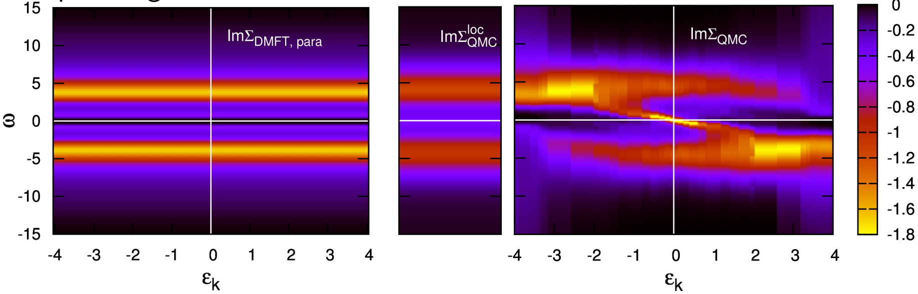
$(\omega, \varepsilon_{\mathbf{k}})$-structure of Σ

$$\text{Im}\Sigma_{\text{loc}} = {}^1\!/_{N_k} \sum_k \Sigma(\mathbf{k}, \omega)$$

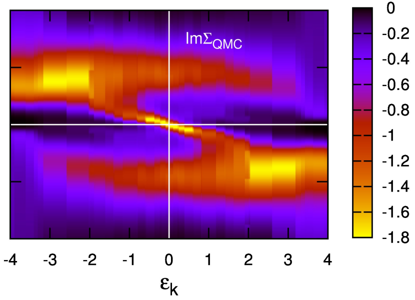


Im $\Sigma(\mathbf{k}, \omega)$ vs. $\varepsilon_{\mathbf{k}}$, ω:

paramagnetic DMFT: local:

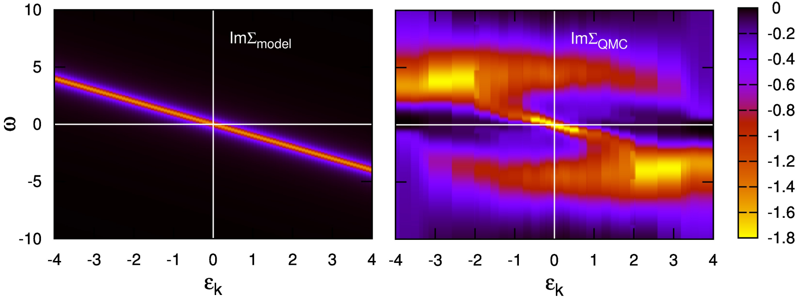


Modeling of Σ



3 main contributions for Σ:

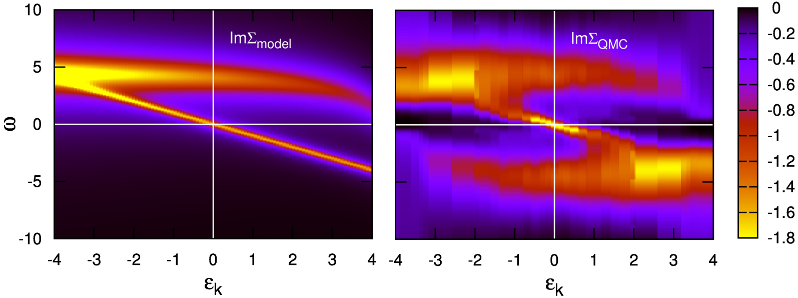
Modeling of Σ



3 main contributions for Σ:

$$\frac{m_1}{\omega + \epsilon + i d_1/2}$$

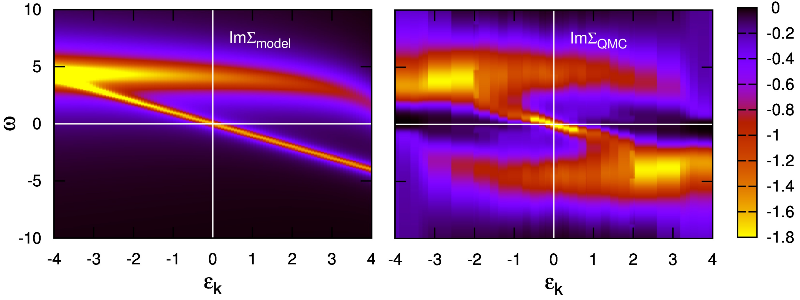
Modeling of Σ



3 main contributions for Σ:

$$\frac{m_1}{\omega + \epsilon + id_1/2} \qquad + \frac{m_2(\epsilon)}{\omega + h_1(\epsilon) + id_2/2}$$

Modeling of Σ



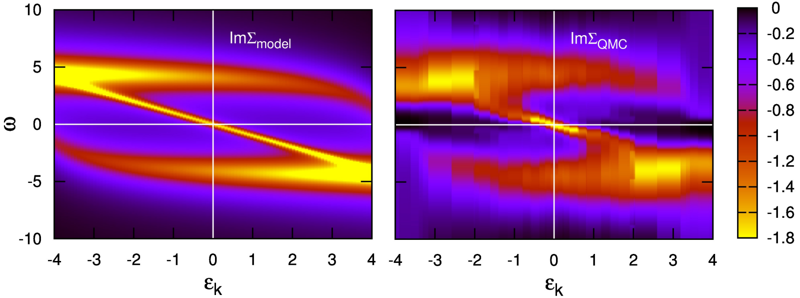
3 main contributions for Σ:

linear in ϵ

$$\frac{m_1}{\omega + \epsilon + id_1/2} \qquad + \frac{m_2(\epsilon)}{\omega + h_1(\epsilon) + id_2/2}$$

$\propto \quad \frac{4-x}{5-x}$

Modeling of Σ



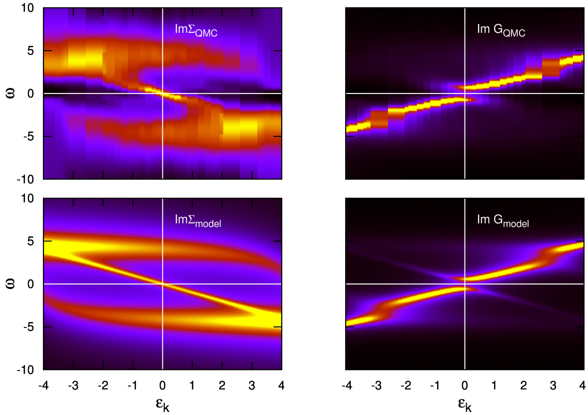
3 main contributions for Σ:

linear in $\pm\epsilon$

$$\frac{m_1}{\omega + \epsilon + i d_1/2} + \frac{m_2(\epsilon)}{\omega + h_1(\epsilon) + i d_2/2} - \frac{m_3(\epsilon)}{\omega + h_2(\epsilon) + i d_1/2}$$

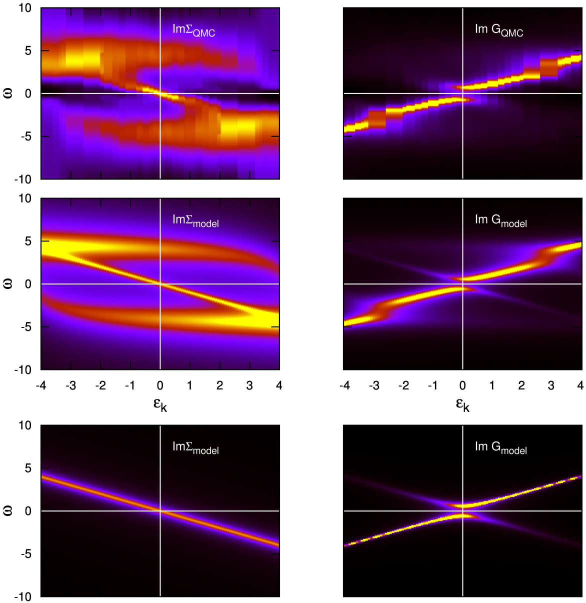
$\propto \pm \frac{4 \mp x}{5 \mp x}$

Analysis of Σ



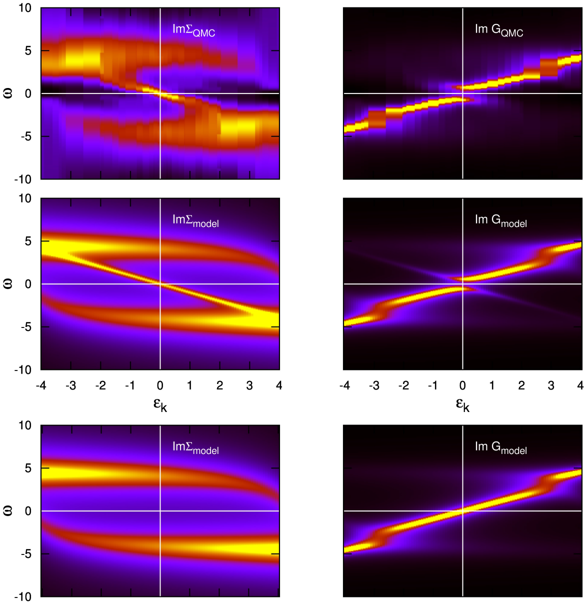
- representation Σ reproduces main features of spectral function
- allows rough analysis:

Analysis of Σ



- representation Σ reproduces main features of spectral function
- allows rough analysis:
  - characteristic AF effect → broadened δ-function
  - but no resolution of k-dependent pseudogap

Analysis of Σ



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- characteristic AF effect $\rightarrow$ broadened δ-function
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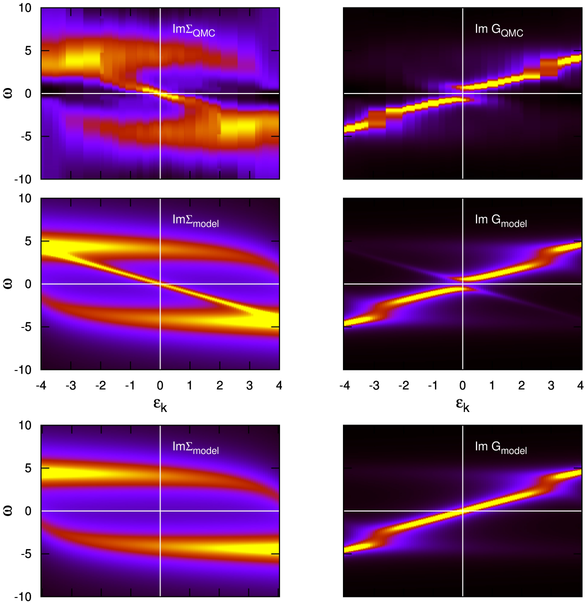


- representation Σ reproduces main features of spectral function
- allows rough analysis:

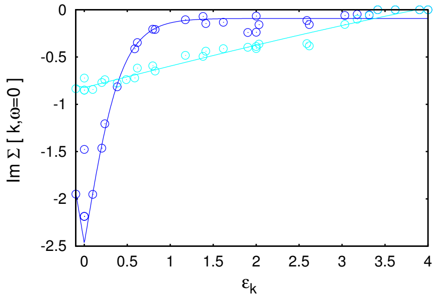
- characteristic AF effect → broadened δ-function
- but no resolution of k-dependent pseudogap

- finite-size dependent feature → specific to parameter set

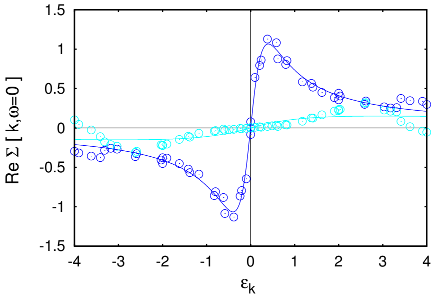
Temperature dependence

$\varepsilon_{\mathbf{k}}$-structure of Σ

Im $\Sigma(\mathbf{k}, \omega = 0)$ vs. $\varepsilon_{\mathbf{k}}$:



Re $\Sigma(\mathbf{k}, \omega = 0)$ vs. $\varepsilon_{\mathbf{k}}$:



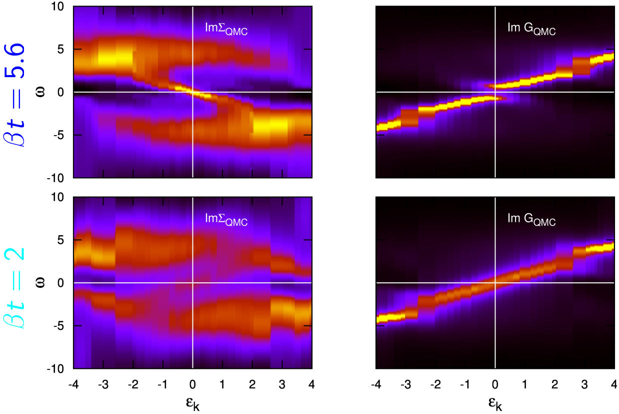
dependence on temperature:

$\rightarrow$ insulating / bad metallic behavior

$\beta t = 5.6$ $\quad$ $\beta t = 2.0$

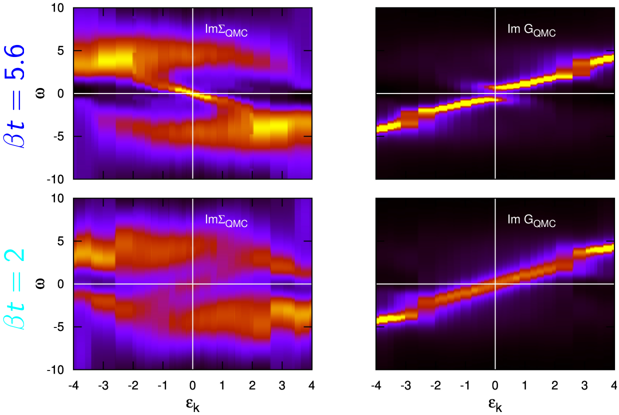
$U = 4t$
$L = 8 \times 20$
$\Delta\tau = 0.1$

Modeling of Σ



$$\Sigma(\epsilon, \omega, T\downarrow) = \frac{m_1}{\omega + \epsilon + i d_1/2} + \frac{m_2(\epsilon)}{\omega + h_1(\epsilon) + i d_2/2} + \frac{m_3(\epsilon)}{\omega + h_2(\epsilon) + i d_2/2}$$

Modeling of Σ



$$\Sigma(\epsilon, \omega, T\uparrow) = \frac{m_1}{\omega + \epsilon + i d_1/2}$$

$$\downarrow \; (+ \to -)$$

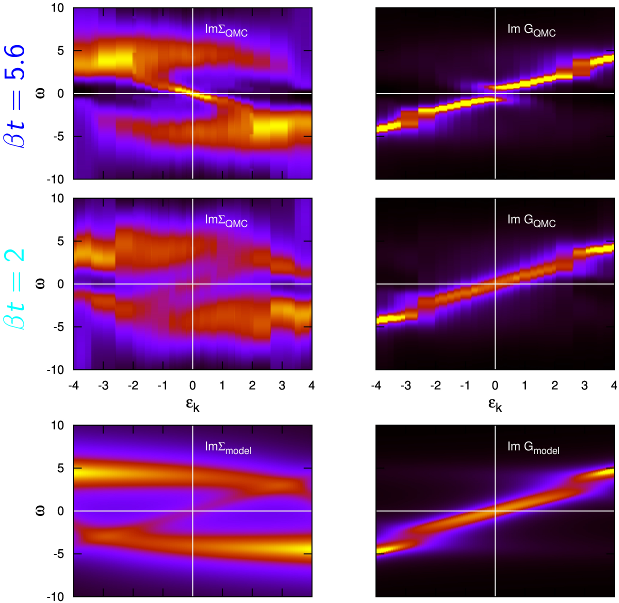
$$+ \frac{m_2(\epsilon)}{\omega + h_1(\epsilon) + i d_2/2}$$

$$+ \frac{m_3(\epsilon)}{\omega + h_2(\epsilon) + i d_2/2}$$

→ d_1 enlarged

→ m_1 reduced

Modeling of Σ



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$\downarrow$ $-$

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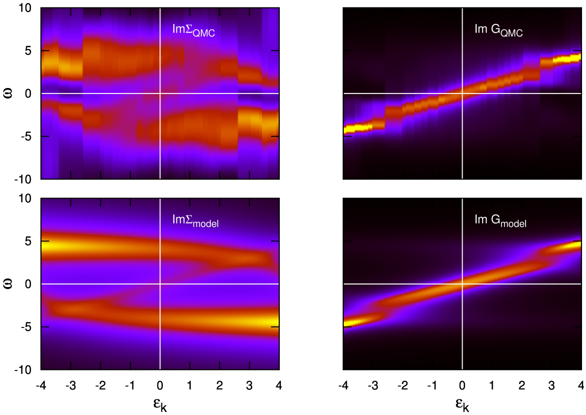
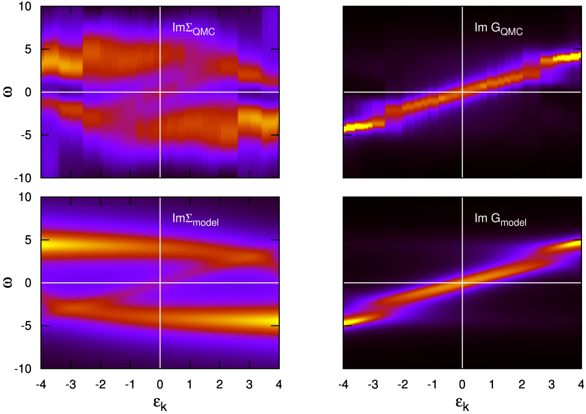
Analysis of Σ



result of **m**aximum **e**ntropy **m**ethod (MEM)

$$\Sigma(\epsilon, \omega, T\uparrow) \sim \frac{m_1}{\omega - \epsilon + id_1/2}$$

Analysis of Σ



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→ similar contribution in terms of a perturbative treatment

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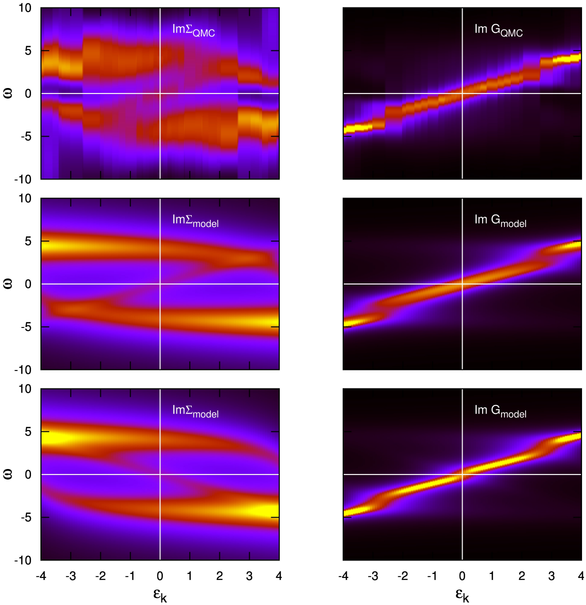
Analysis of Σ



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$$\Sigma(\epsilon, \omega, T\uparrow) \sim \frac{m_1}{\omega - \epsilon + i d_1/2}$$

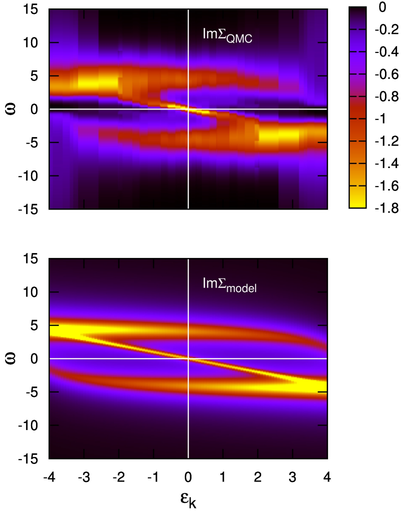
$$\Sigma(\epsilon, \omega, T\downarrow) \sim \frac{m_1}{\omega + \epsilon + i d_1/2}$$

Conclusions & outlook

Conclusions & outlook

- **method**
  - ∗ sharp **k**-space features - far beyond DCA ✓

- parametrization



Conclusions & outlook

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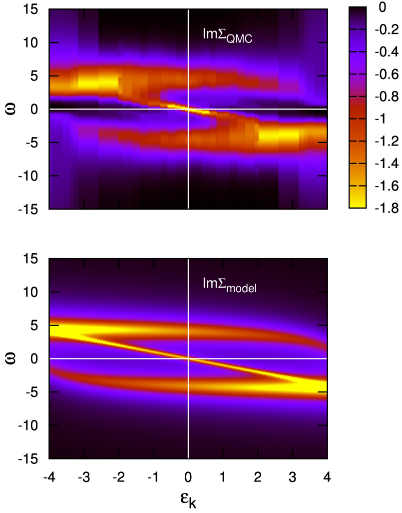

Conclusions & outlook

- **method**
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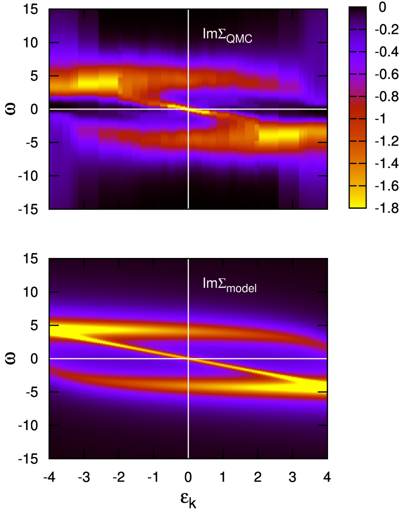
- **parametrization**
  - ∗ continuous representation in **k** ✓



Conclusions & outlook

- **method**
  - ∗ sharp **k**-space features - far beyond DCA ✓
  - ∗ explanations for $\delta(\omega + \varepsilon)$, contribution to Im Σ ?
- **parametrization**
  - ∗ continuous representation in **k** ✓
  - ∗ models allow for going beyond ✓
    - → case of half-filling
    - → isotropic case