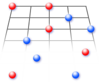
Momentum-dependent pseudogaps in the half-filled 2-d Hubbard model - an unbiased QMC study

Nils Blümer

Institut für Physik, Johannes Gutenberg-Universität Mainz

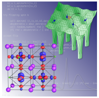
JOHANNES GUTENBERG UNIVERSITÄT MAINZ

[D. Rost, E. V. Gorelik, F. Assaad, N. Blümer, Phys. Rev. B **86**, 155109 (2012)]



TR 49: *Condensed matter systems with variable many-body interactions*
Frankfurt / Kaiserslautern / Mainz

FOR 1346
LDA+DMFT
Augsburg *et al.*



Outline

Motivation: pseudogap, high-T_c superconductivity, antiferromagnetism

Challenge: spectra of $2d$ Hubbard model in thermodynamic limit

Outline

Motivation: pseudogap, high-T_c superconductivity, antiferromagnetism

Challenge: spectra of $2d$ Hubbard model in thermodynamic limit

Approach: determinantal QMC, Trotter+FS extrapolations, MEM

Results: unbiased PG spectra (continuous momentum resolution)

Outline

Motivation: pseudogap, high-T_c superconductivity, antiferromagnetism

Challenge: spectra of 2d Hubbard model in thermodynamic limit

Approach: determinantal QMC, Trotter+FS extrapolations, MEM

Results: unbiased PG spectra (continuous momentum resolution)

Outlook: multigrid DMFT+DQMC

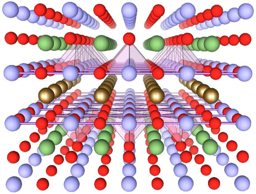
[D. Rost, F. Assaad, N. Blümer, arXiv:1303.2004]

Daniel Rost
Univ. Mainz

Motivation: pseudogap physics in high-T_c cuprates

Cuprate superconductors:

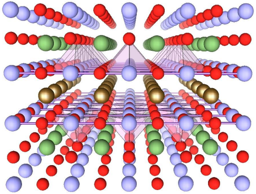
- planar structure $\rightsquigarrow$ quasi-2d electron systems



Motivation: pseudogap physics in high-T_c cuprates

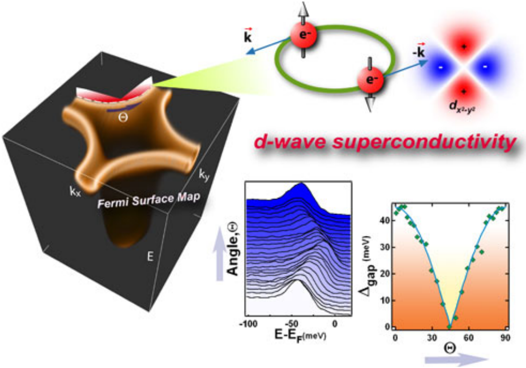
Cuprate superconductors:

- planar structure $\rightsquigarrow$ quasi-2d electron systems



- *d*-wave pair function

$\rightsquigarrow$ excitation gap has nodes
(and "antinodes")



[Shen group, Stanford University]

Experiment: "pseudogap" above T_c
(towards AF regions near half filling)

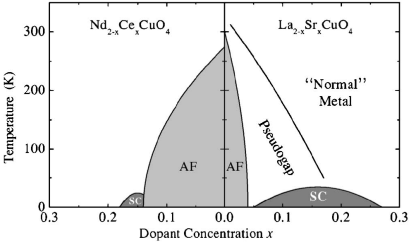


FIG. 1. Schematic phase diagram of high-T_c superconductors showing hole doping (right side) and electron doping (left side). From Damascelli *et al.*, 2003.

[Lee et al., RMP (2006)]

Motivation: pseudogap physics in high-T_c cuprates

Experiment: "pseudogap" above T_c
(towards AF regions near half filling)

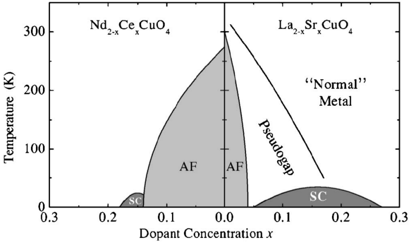


FIG. 1. Schematic phase diagram of high-T_c superconductors showing hole doping (right side) and electron doping (left side). From Damascelli *et al.*, 2003.

[Lee et al., RMP (2006)]

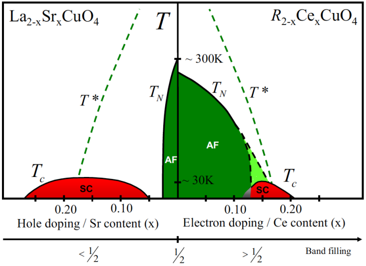


FIG. 2. (Color online) Joint phase diagram of the LSCO/NCCO material systems. The uncertainty regarding the extent of AF on the electron-doped side and its coexistence with superconductivity is shown by the dotted area. Maximum Néel

[Armitage et al., RMP (2010)]

Origin/nature of pseudogap: preformed sc pairs, competing phenomenon (AF)?

Motivation: pseudogap physics in high-T_c cuprates

Experiment: "pseudogap" above T_c
(towards AF regions near half filling)

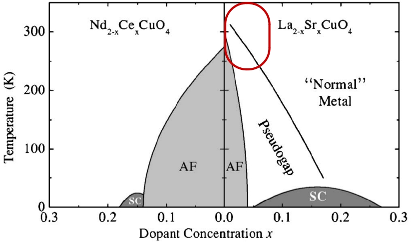


FIG. 1. Schematic phase diagram of high-T_c superconductors showing hole doping (right side) and electron doping (left side). From Damascelli *et al.*, 2003.

[Lee et al., RMP (2006)]

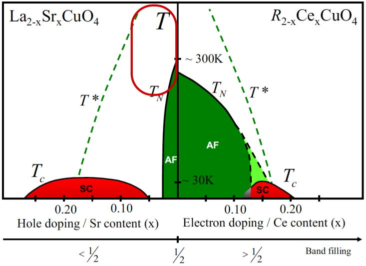


FIG. 2. (Color online) Joint phase diagram of the LSCO/ NCCO material systems. The uncertainty regarding the extent of AF on the electron-doped side and its coexistence with superconductivity is shown by the dotted area. Maximum Néel

[Armitage et al., RMP (2010)]

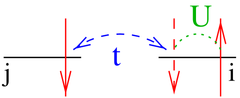
Origin/nature of pseudogap: preformed sc pairs, competing phenomenon (AF)?

Characteristic pseudogap temperature T^* near $x = 0$: at or far above T_N?

Computational approaches for Hubbard-type models

Target: Hubbard model on infinite lattice

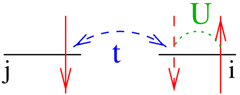
$$\hat{H} = \sum_{(i,j),\sigma} t_{ij}\,(\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + \text{h.c.}) + U \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$



Computational approaches for Hubbard-type models

Target: Hubbard model on infinite lattice

$$\hat{H} = \sum_{(i,j),\sigma} t_{ij} \, (\hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + \text{h.c.}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

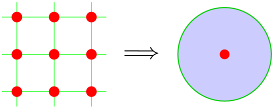


1) Special limits/cases

- Perturbation theory ($U \ll t$ or $t \ll U$)
- Bethe Ansatz, DMRG ($t_x \gg t_y, t_z \rightsquigarrow d = 1$)

2) Approximate mapping

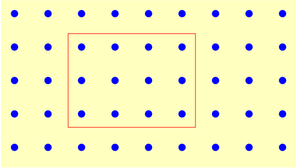
Dynamical mean-field theory



+ extensions (DCA, CDMFT)

need impurity/cluster solver

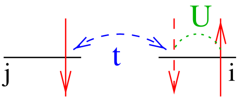
3) Treat finite clusters



ED, determinantal QMC

Computational approaches for Hubbard-type models

Target: Hubbard model on infinite lattice



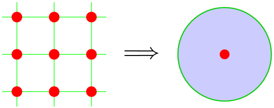
$$\hat{H} = \sum_{(i,j),\sigma} t_{ij} \left(\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \text{h.c.}\right) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

1) Special limits/cases

- Perturbation theory ($U \ll t$ or $t \ll U$)
- Bethe Ansatz, DMRG ($t_x \gg t_y, t_z \rightsquigarrow d = 1$)

2) Approximate mapping

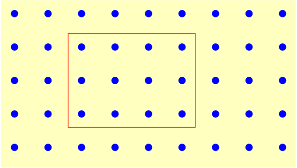
Dynamical mean-field theory



+ extensions (DCA, CDMFT)

need impurity/cluster solver

3) Treat finite clusters



ED, determinantal QMC

Challenges:

(a) Compute exact imaginary-time Green functions for large clusters ($\leq 16 \times 16$)

(b) Perform analytic continuation $\rightsquigarrow$ unbiased spectral functions

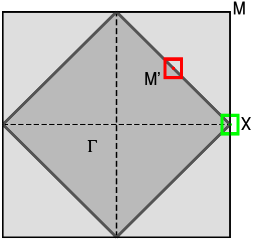
(c) Extrapolate to the thermodynamic limit

Pseudogap in half-filled Hubbard model - a finite-size artifact?

Unfrustrated model: particle-hole symmetry at $n = 1$

$$\hat{H} = -t \sum_{\langle ij \rangle, \sigma} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

Interesting: momenta $\mathbf{k}$ with $\varepsilon_{\mathbf{k}} = 0$ (i.e. noninteracting Fermi surface)



"antinode" $\mathbf{X} = (\pi, 0)$

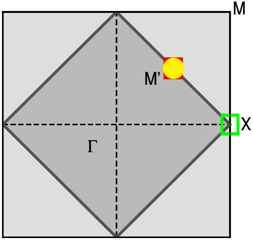
"node" $\mathbf{M}' = (\pi/2, \pi/2)$

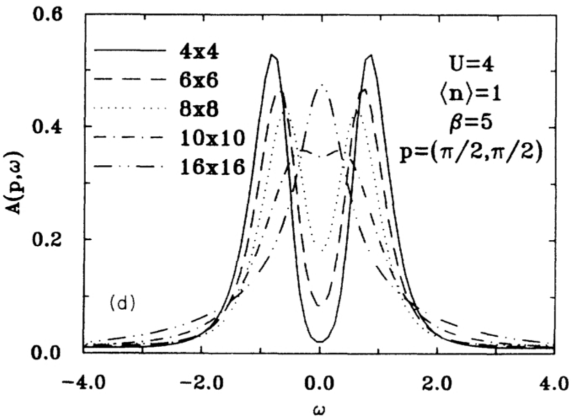
Pseudogap in half-filled Hubbard model - a finite-size artifact?

Unfrustrated model: particle-hole symmetry at $n = 1$

$$\hat{H} = -t \sum_{\langle ij \rangle, \sigma} \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

Interesting: momenta $\mathbf{k}$ with $\varepsilon_{\mathbf{k}} = 0$ (i.e. noninteracting Fermi surface)





"antinode" $\mathbf{X} = (\pi, 0)$

"node" $\mathbf{M}' = (\pi/2, \pi/2)$

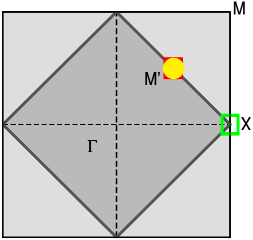
DQMC [White, PRB (1992)]: PG pure FS effect

Pseudogap in half-filled Hubbard model - a finite-size artifact?

Unfrustrated model: particle-hole symmetry at $n = 1$

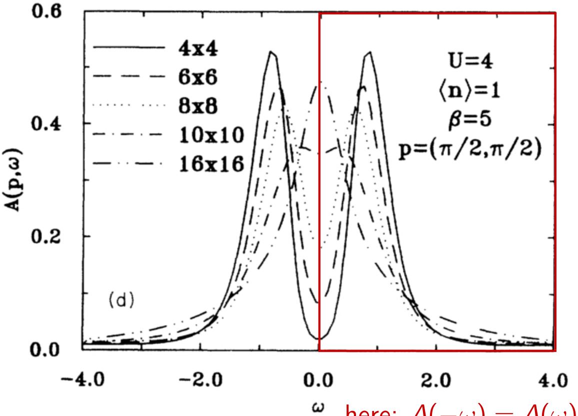
$$\hat{H} = -t \sum_{\langle ij \rangle, \sigma} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

Interesting: momenta $\mathbf{k}$ with $\varepsilon_{\mathbf{k}} = 0$ (i.e. noninteracting Fermi surface)



"antinode" $\mathbf{X} = (\pi, 0)$

"node" $\mathbf{M}' = (\pi/2, \pi/2)$



here: $A(-\omega) = A(\omega)$

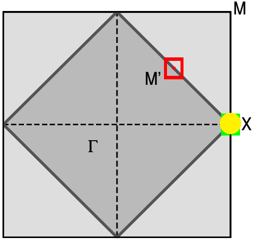
DQMC [White, PRB (1992)]: PG pure FS effect

Pseudogap in half-filled Hubbard model - a finite-size artifact?

Unfrustrated model: particle-hole symmetry at $n = 1$

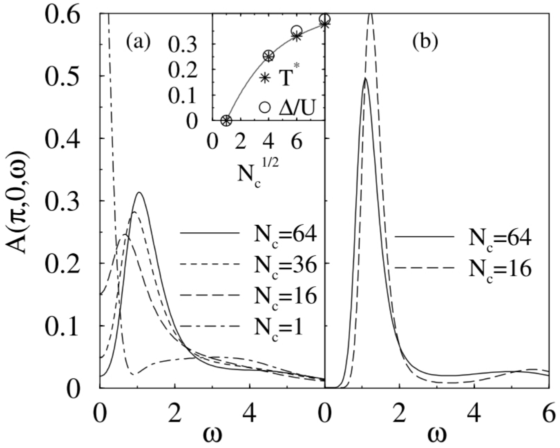
$$\hat{H} = -t \sum_{\langle ij\rangle,\sigma} \hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + U \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$

Interesting: momenta $\mathbf{k}$ with $\varepsilon_{\mathbf{k}} = 0$ (i.e. noninteracting Fermi surface)



“antinode” $\mathbf{X} = (\pi, 0)$

“node” $\mathbf{M}' = (\pi/2, \pi/2)$



DCA + DQMC under/overest. PG [Huscroft et al. (2001)]

Finite-size effects in current DCA studies of pseudogap physics

arXiv:1207.2490v1

Superconductivity and the Pseudogap in the two-dimensional Hubbard model

Emanuel Gull,[12*] Olivier Parcollet,[3] Andrew J. Millis[2]

[1]Max Planck Institut für Physik komplexer Systeme, Dresden, Germany
[2]Department of Physics, Columbia University, New York, NY, USA
[3]Institut de Physique Théorique, CEA, IPhT, CNRS, URA 2306, F-91191 Gif-sur-Yvette, France

Superconductivity and the Pseudogap in the two-dimensional Hubbard model

Emanuel Gull,[12*] Olivier Parcollet,[3] Andrew J. Millis[2]

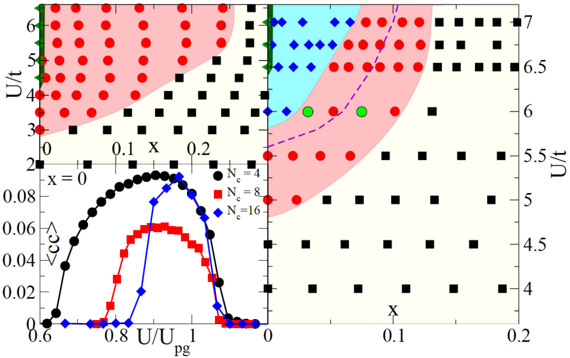


Figure 1: **Superconducting phase diagram of the two-dimensional Hubbard model** in plane of interaction strength U and carrier concentration x computed using the 8-site (right panel) and 4-site (left upper panel) DCA dynamical mean field approximation at temperature $T = t/40$ with $t'/t = 0$. Dashed line: location of the normal state pseudogap onset. Circles (red and light green) and red shading indicates the superconducting region, squares (black) and no shading the

Unfrustrated 2*d* Hubbard model ($t' = 0$): sc at half filling???

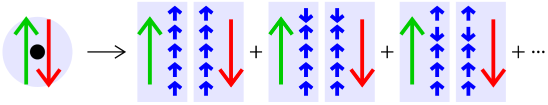
Enormous FS effects in DCA (4 / 8 sites)!

N	4	8	16
U_{pg}	4.2	5.6	3

Given: Hamiltonian $\hat{H} = \hat{T} + \hat{V}$

(i) Trotter decoupling $e^{-\beta(\hat{T}+\hat{V})} \approx \left[e^{-\Delta\tau\hat{T}} e^{-\Delta\tau\hat{V}}\right]^{\Lambda}$; $\beta = \Lambda\,\Delta\tau$

(ii) Hubbard-Stratonovich transformation



Wick theorem:

$$Z = \sum_{\{s_{il}\}} \det M_{\uparrow}^{\{s\}} \det M_{\downarrow}^{\{s\}}$$

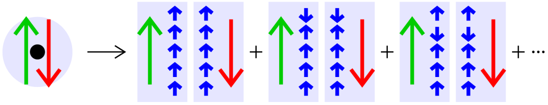
(iii) MC importance sampling over auxiliary Ising field $\{s\}$: $2^{N\Lambda}$ configurations

Determinantal QMC algorithm [Blankenbecler, Scalapino, Sugar, 1981]

Given: Hamiltonian $\hat{H} = \hat{T} + \hat{V}$

(i) Trotter decoupling $e^{-\beta(\hat{T}+\hat{V})} \approx \left[e^{-\Delta\tau\hat{T}} e^{-\Delta\tau\hat{V}}\right]^{\Lambda}$; $\beta = \Lambda\,\Delta\tau$

(ii) Hubbard-Stratonovich transformation



Wick theorem:

$$Z = \sum_{\{s_{il}\}} \det M_{\uparrow}^{\{s\}} \det M_{\downarrow}^{\{s\}}$$

(iii) MC importance sampling over auxiliary Ising field $\{s\}$: $2^{N\Lambda}$ configurations

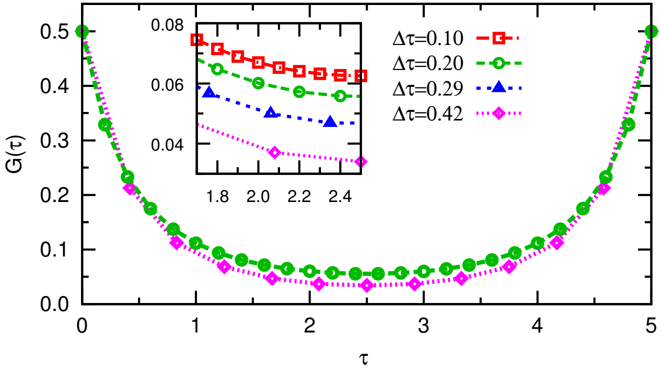
Sources of errors (for given cluster size):

- statistical error [from MC sampling, (iii)]
- systematic error [from Trotter decoupling, (i)]

Computational effort $\propto N^3\Lambda \propto N^3\beta$

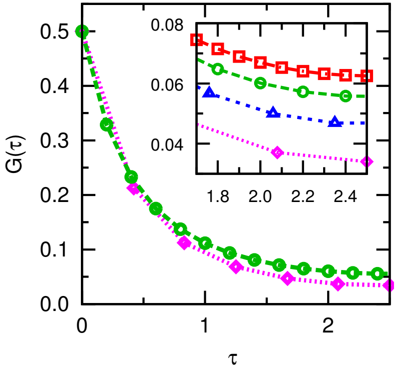
Impact of Trotter error on imaginary-time Green function + spectra

Trotter discretization $\Delta\tau$ determines: (i) bias in shape of $G(\tau)$ and (ii) grid in τ



Impact of Trotter error on imaginary-time Green function + spectra

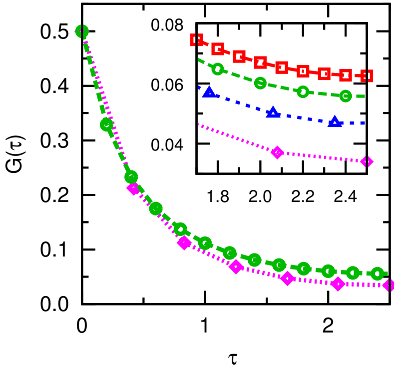
Trotter discretization $\Delta\tau$ determines: (i) bias in shape of $G(\tau)$ and (ii) grid in τ



$\rightsquigarrow$ point-wise extrapolation impossible!

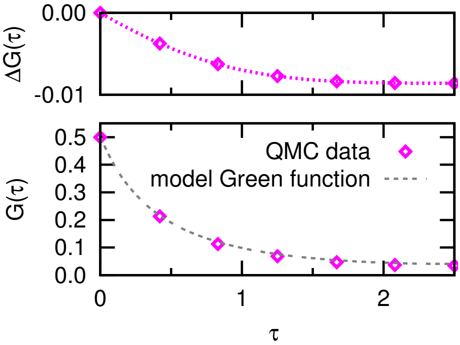
Impact of Trotter error on imaginary-time Green function + spectra

Trotter discretization $\Delta\tau$ determines: (i) bias in shape of $G(\tau)$ and (ii) grid in τ



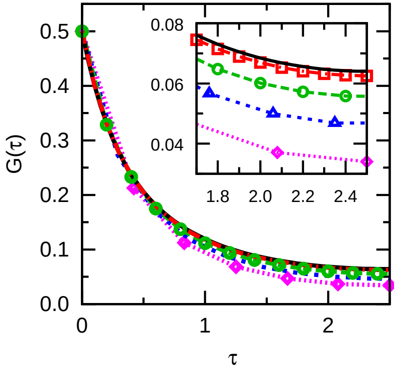
$\rightsquigarrow$ point-wise extrapolation impossible!

Idea:
- generate cont. model Green function (correct curvature at boundaries)
- fit difference with natural cubic spline



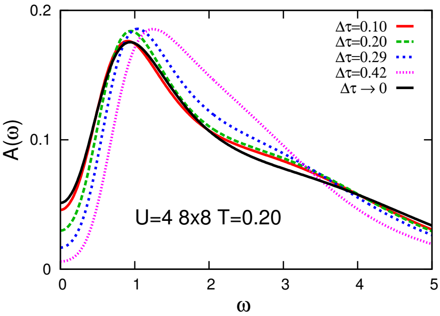
Impact of Trotter error on imaginary-time Green function + spectra

Trotter discretization $\Delta\tau$ determines: (i) bias in shape of $G(\tau)$ and (ii) grid in τ



$\rightsquigarrow$ point-wise extrapolation impossible!

Idea:
- generate cont. model Green function (correct curvature at boundaries)
- fit difference with natural cubic spline
- least-squares extrapolation in $\Delta\tau^2$



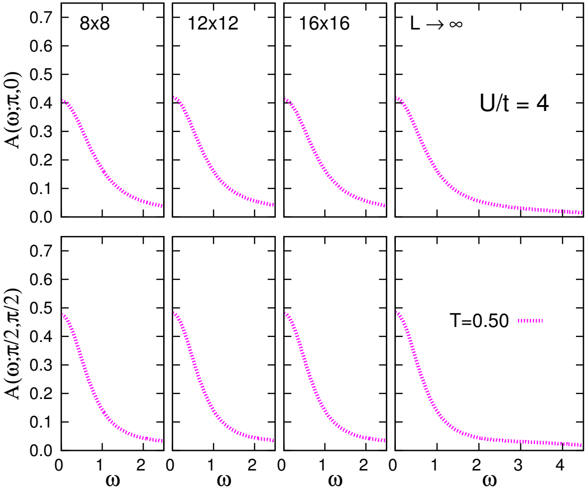
Multigrid DQMC eliminates Trotter errors reliably
$\rightsquigarrow$ unbiased spectra!

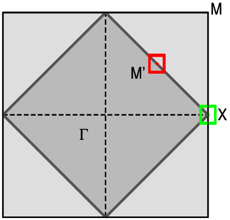
Elimination of finite size effects: high-symmetry points

At high-symmetry points: local FS extrapolation possible for each τ

Elimination of finite size effects: high-symmetry points

At high-symmetry points: local FS extrapolation possible for each τ

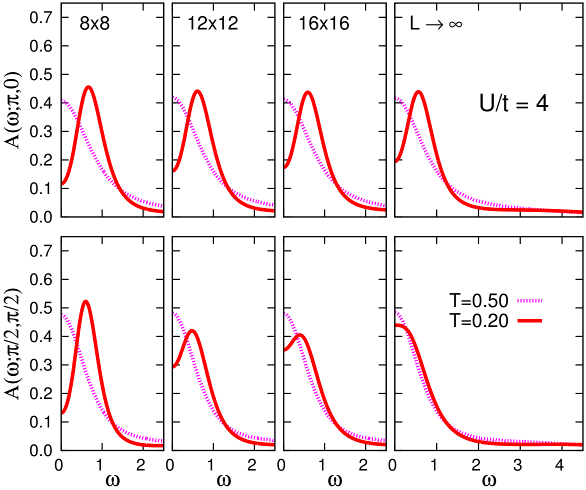


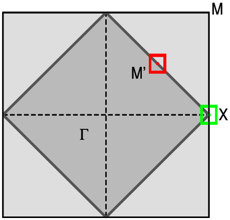


$$\mathbf{X} = (\pi, 0)$$
$$\mathbf{M}' = (\pi/2, \pi/2)$$

Elimination of finite size effects: high-symmetry points

At high-symmetry points: local FS extrapolation possible for each τ

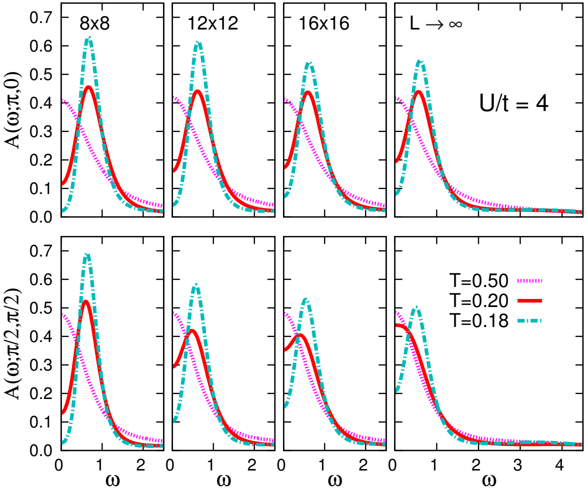




$$\mathbf{X} = (\pi, 0)$$
$$\mathbf{M}' = (\pi/2, \pi/2)$$

Elimination of finite size effects: high-symmetry points

At high-symmetry points: local FS extrapolation possible for each τ

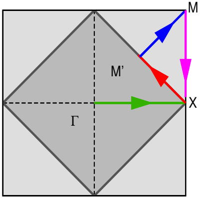


At weak coupling ($U/t = 4$):

pseudogap remains in thermodynamic limit

d-wave type anisotropy grows with lattice size

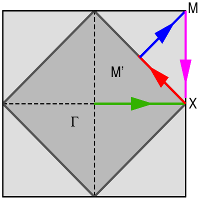
Goal: unbiased spectra ($\Delta\tau \to 0$, $N \to \infty$) along high-symmetry lines



Wanted: spectral function with continuous momentum resolution along high-symmetry lines through BZ

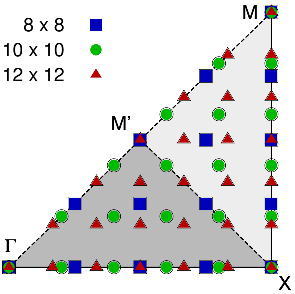
Special path: Fermi surface included ("beyond DMFT")

Goal: unbiased spectra ($\Delta\tau \to 0$, $N \to \infty$) along high-symmetry lines



Wanted: spectral function with continuous momentum resolution along high-symmetry lines through BZ

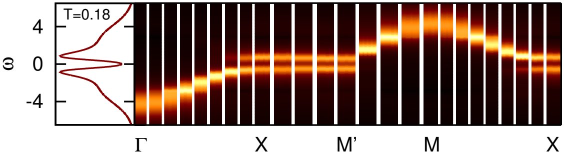
Special path: Fermi surface included ("beyond DMFT")



FS effects shift physical quantities and lead to incommensurate **k** grids

⇒ not every **k**-point is accessible

⇒ pointwise extrapolation rarely possible

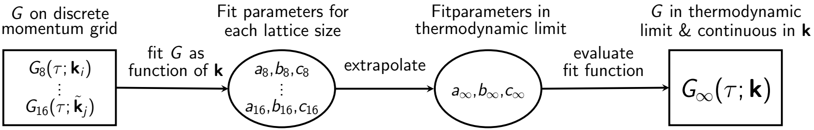


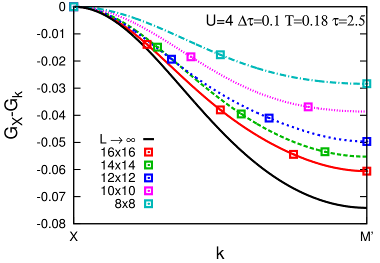
16 x 16

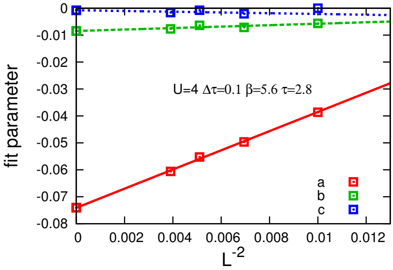
Elimination of finite size effects: high-symmetry lines

At high-symmetry points: local FS extrapolation possible for each τ

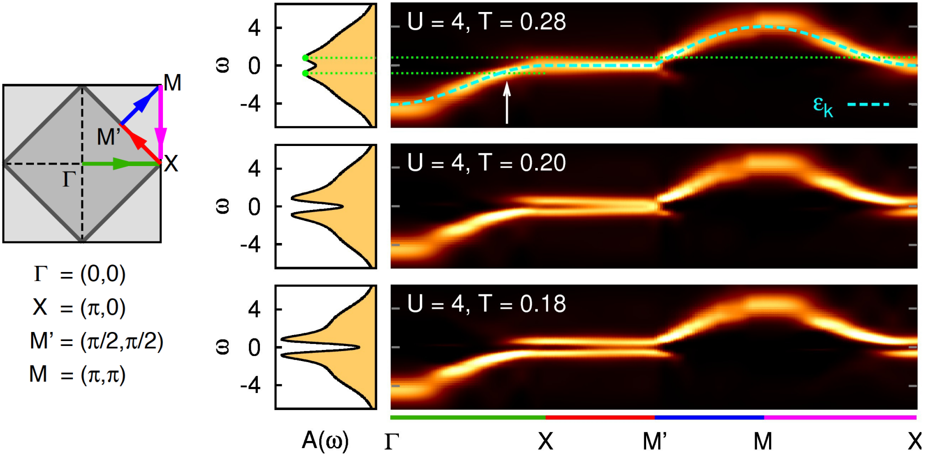
Better: global Fourier fits along high-symmetry lines $\rightsquigarrow$ continuous **k**-resolution







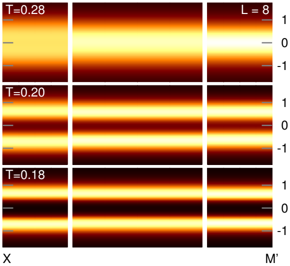
Spectral function for square lattice at weak coupling ($U/t = 4$)



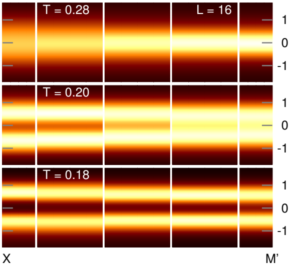
First unbiased spectra in thermodynamic limit (from DQMC and MEM)!

Finite-range AF opens pseudogap; **k** dependence (beyond DMFT) at $X \to M'$

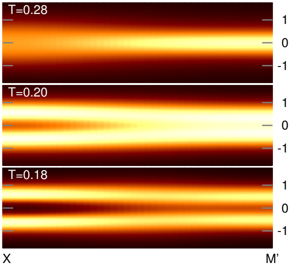
Anisotropy along the fermi edge (U/t=4)



8 x 8



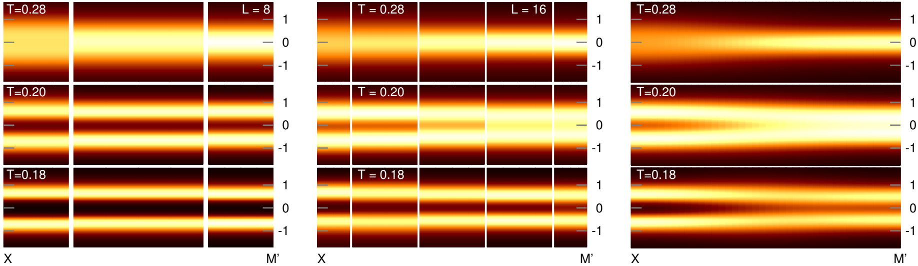
16 x 16



thermodynamic limit

Momentum resolution of FS-extrapolated spectra impossible to reach by brute force!

Anisotropy along the fermi edge (U/t=4)



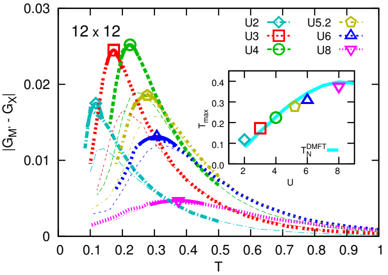
8 x 8 | 16 x 16 | thermodynamic limit

Momentum resolution of FS-extrapolated spectra impossible to reach by brute force!

Maximal momentum dependence $\rightsquigarrow T^*$:

- consistent with spectra
- agrees with DMFT critical temperature!

[D. Rost, E. V. Gorelik, F. Assaad, N. Blümer, Phys. Rev. B **86**, 155109 (2012)]



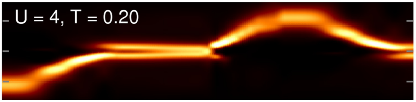
Summary

Trotter and FS errors eliminated from DQMC Green functions
(2d Hubbard model at $n = 1$, $U/t = 4$)

Summary

Trotter and FS errors eliminated from DQMC Green functions

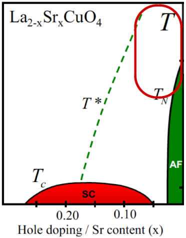
(2d Hubbard model at $n = 1$, $U/t = 4$)



$\rightsquigarrow$ unbiased spectra in thermodynamic limit with continuous momentum resolution

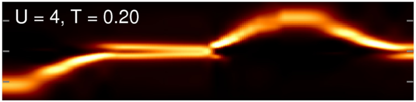
$\rightsquigarrow$ nodal-antinodal dichotomy of pseudogap (PG) fully resolved

$\rightsquigarrow$ PG opening at mean-field AF ordering temperature

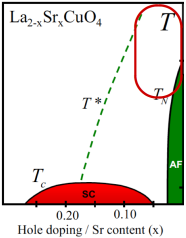


Summary

Trotter and FS errors eliminated from DQMC Green functions
(2d Hubbard model at $n = 1$, $U/t = 4$)



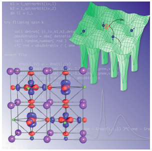
⇝ unbiased spectra in thermodynamic limit
with continuous momentum resolution



⇝ nodal-antinodal dichotomy of pseudogap (PG) fully resolved

⇝ PG opening at mean-field AF ordering temperature

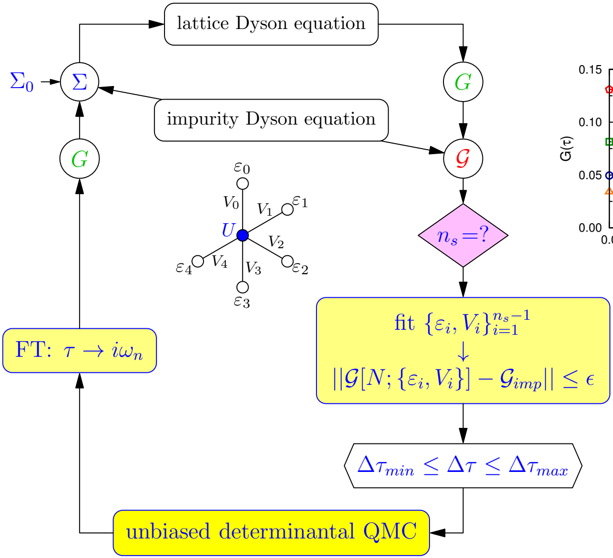
⇝ benchmark for approximate methods (DCA, DΓA)

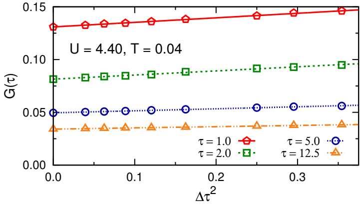


DFG research unit 1346

Outlook: • Application as impurity solver for (cellular) DMFT
⇝ linear (instead of cubic) scaling in β
[D. Rost, F. Assaad, N. Blümer, arXiv:1303.2004]

Multigrid DMFT+DQMC scheme

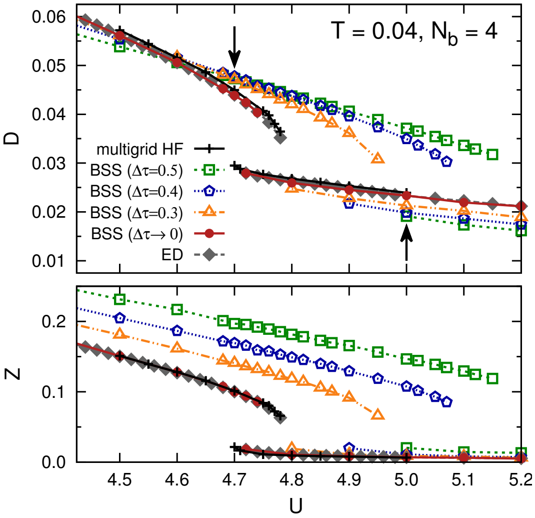


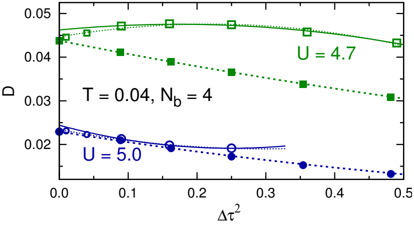


Use of determinantal QMC in DMFT context pioneered by Khatami et al (2010)⇝ cost $\propto \beta$

DMFT+ED/DQMC: impact and elimination of Trotter errors

Half-filled Hubbard model, Bethe DOS ($W = 4$)



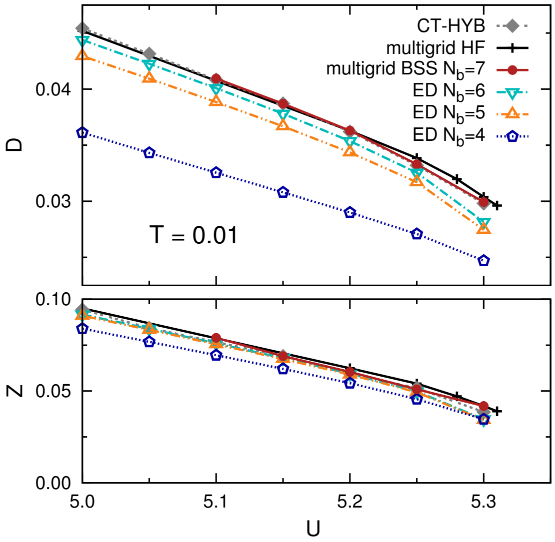


- Trotter bias → shift of coexistence region
- Regular $\Delta\tau$ dependence only in multigrid DMFT+BSS

First quasi-CT QMC impurity solver with linear scaling in β

[D. Rost, F. Assaad, N. Blümer, arXiv:1303.2004]

DMFT+ED/DQMC: impact of bath discretization



Half-filled Hubbard model, Bethe DOS ($W = 4$)

- Poor bath discretization leads to systematic discrepancies
- Lowering T requires more bath sites

$\rightarrow$ BSS-QMC much faster than ED