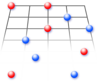
Numerically exact Quantum Monte Carlo Algorithms

for Impurity Problems

Nils Blümer

Institut für Physik, Johannes Gutenberg-Universität Mainz



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

FOR 1346
LDA+DMFT
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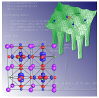

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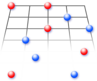
Momentum-dependent pseudogaps in the 2-d Hubbard model

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



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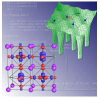

Outline

Motivation: pseudogap, high-T_c superconductivity, antiferromagnetism

Challenge: spectra of Hubbard model in thermodynamic limit

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maximum entropy method for analytic continuation

Results: unbiased pseudogap spectra (continuous **k** resolution)

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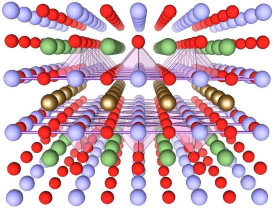
Outlook: numerically exact multigrid DMFT+DQMC

Motivation: pseudogap physics in high-T_c cuprates

Layered cuprates: strongly correlated electron systems



$YBa_2Cu_3O_7$ crystal structure

[Bobroff, Wikimedia Commons]

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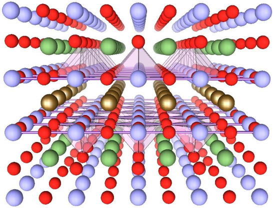

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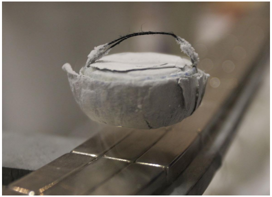
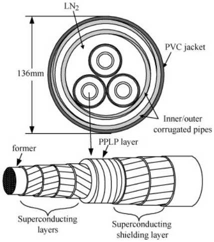
All superconductors

- expel (weak) magnetic fields
- have no electric resistance



[Mühlpfordt, Wikipedia: Superconductivity]



[Sumimoto HTS cable]

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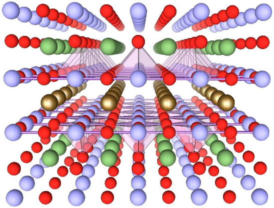

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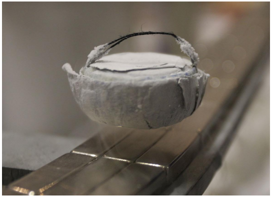

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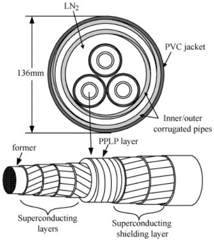

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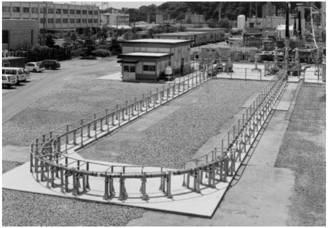

[Sumimoto - TEPCO test at Yokosuka]

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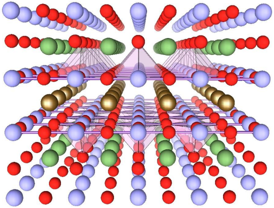

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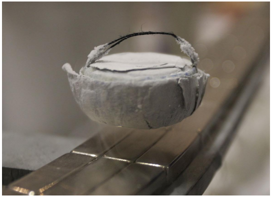
$\rightarrow$ charge excitation gap



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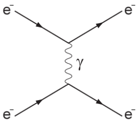


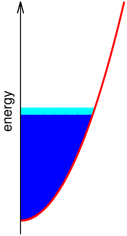
[Wikipedia]

Electric resistance of normal metals:

electron-electron scattering + lattice

[analogy: marathon through forest]

(only electrons near Fermi energy)



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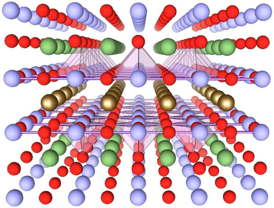

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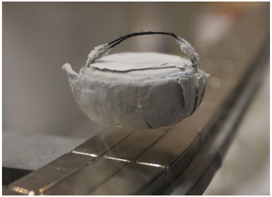

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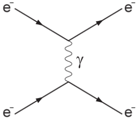

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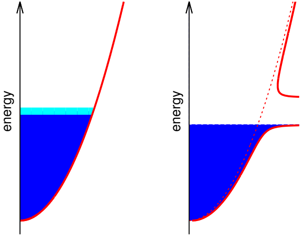
BCS state: isotropic full gap 2Δ



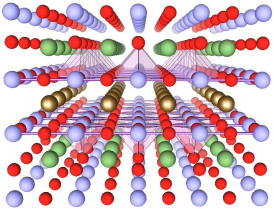
Motivation: pseudogap physics in high-T_c cuprates

Cuprate superconductors:

- planar structure

$\rightsquigarrow$ quasi-2d electron systems

(Cu-O planes)



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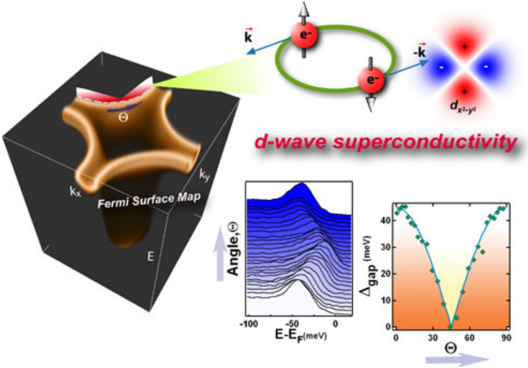
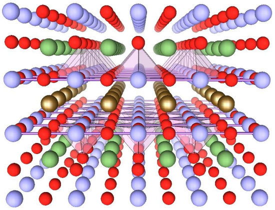
$\rightsquigarrow$ excitation gap has nodes (and "antinodes")



[Shen group, Stanford University]



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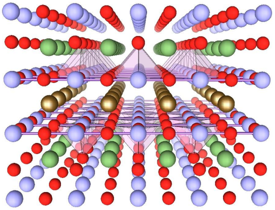

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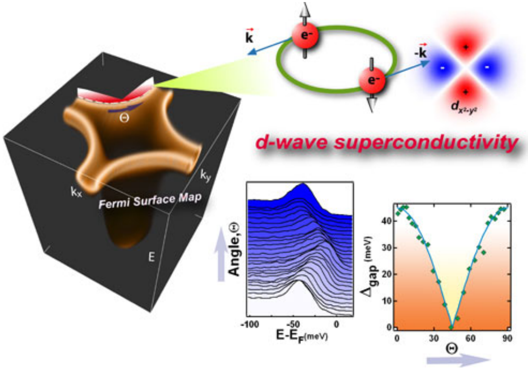

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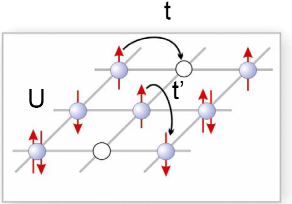
Theory:

Hubbard model

on square lattice

[on-site interaction U]



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

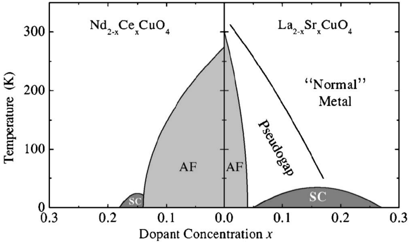

FIG. 1. Schematic phase diagram of high-T_c superconductors showing hole doping (right side) and electron doping (left side). From Damascelli *et al.*, 2003.

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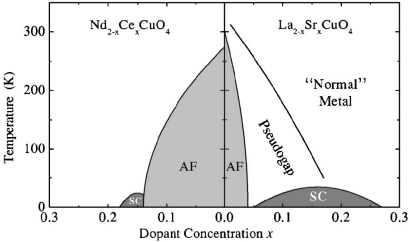

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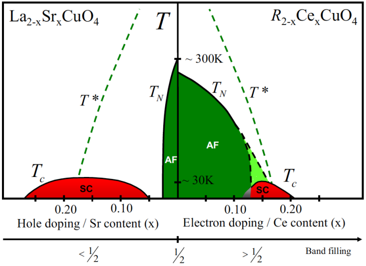

FIG. 2. (Color online) Joint phase diagram of the LSCO/NCCO material systems. The uncertainty regarding the extent of AF on the electron-doped side and its coexistence with superconductivity is shown by the dotted area. Maximum Néel

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

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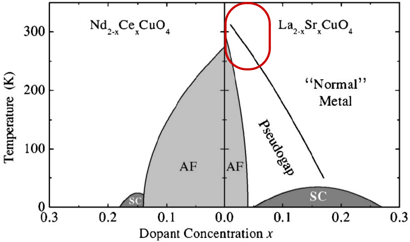

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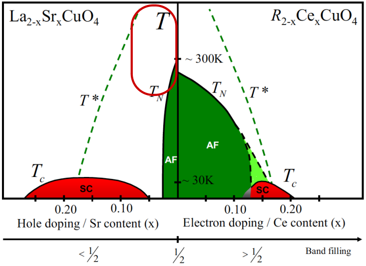

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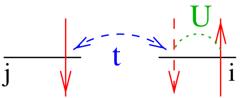
Characteristic pseudogap temperature T^* near $x = 0$: at or far above T_N?

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

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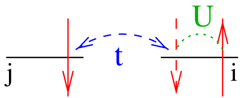

1) Special limits/cases

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

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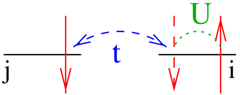

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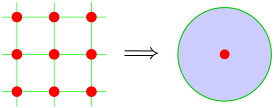
Dynamical mean-field theory



+ extensions (DCA, CDMFT)

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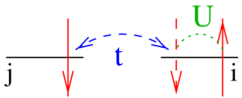

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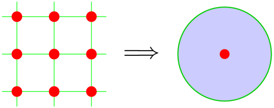

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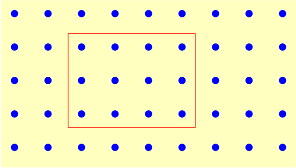

ED, determinantal QMC

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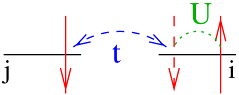

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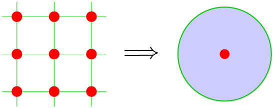

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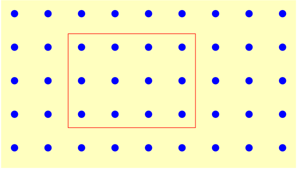


ED, determinantal QMC

Challenges:

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

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

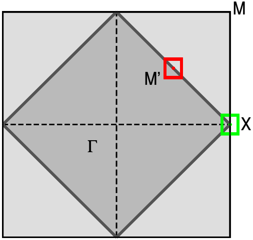
(c) Extrapolate to the thermodynamic limit

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)



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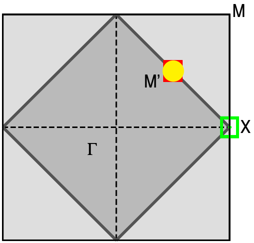

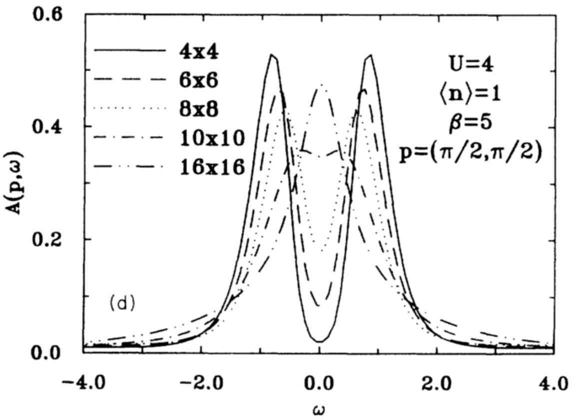

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DQMC [White, PRB (1992)]: PG pure FS effect

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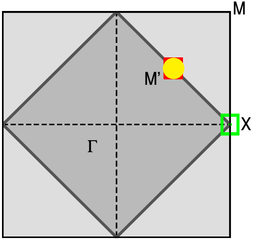

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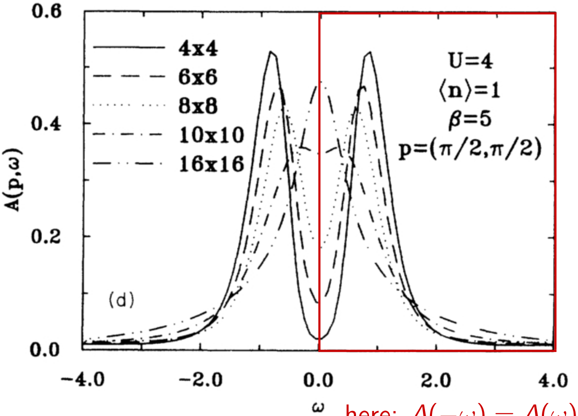


here: $A(-\omega) = A(\omega)$

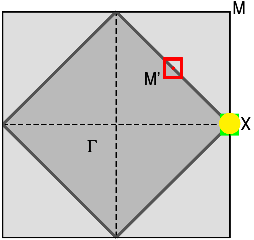
DQMC [White, PRB (1992)]: PG pure FS effect

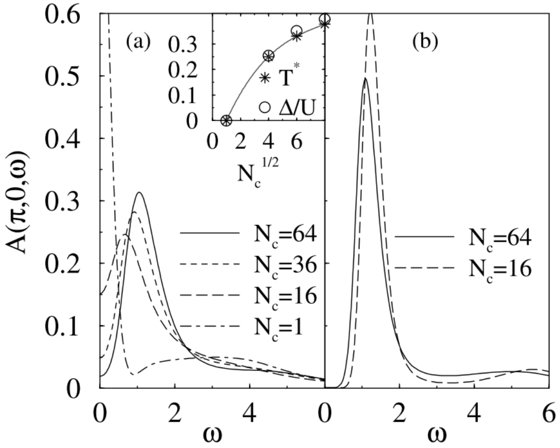
Pseudogap in half-filled Hubbard model - a finite-size artifact?

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)]

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

Goal: thermal expectation values of observables $\hat{A}$:

$$\langle\hat{A}\rangle = Z^{-1}\,\mathrm{Tr}\big[\hat{A}\,e^{-\beta\hat{H}}\big];\quad Z = \mathrm{Tr}\big[e^{-\beta\hat{H}}\big];\quad \beta = (k_B T)^{-1}$$

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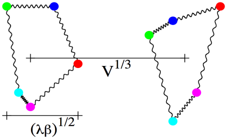

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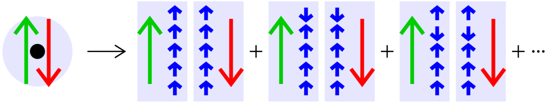

Wick theorem:

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

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

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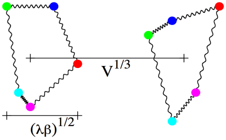

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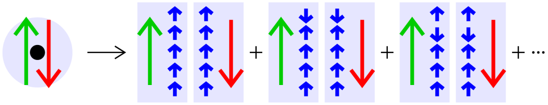

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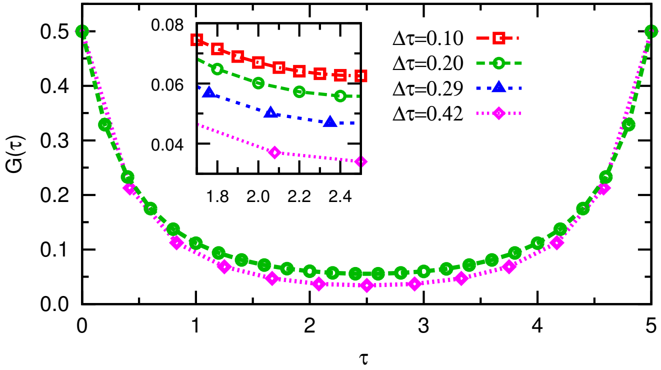
Sources of errors (for given cluster size):

- statistical error [from MC sampling, (iv)]
- systematic error [from Trotter decoupling, (ii)]

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



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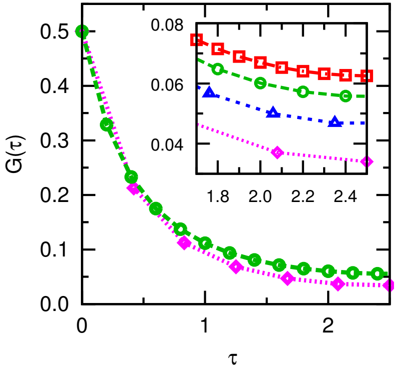

$\rightsquigarrow$ point-wise extrapolation impossible!

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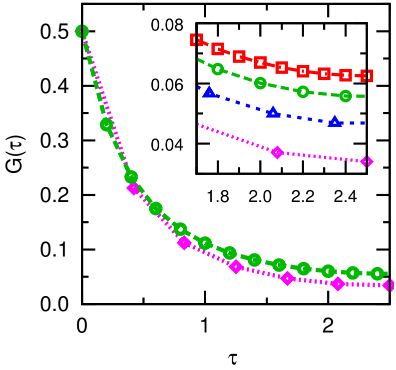

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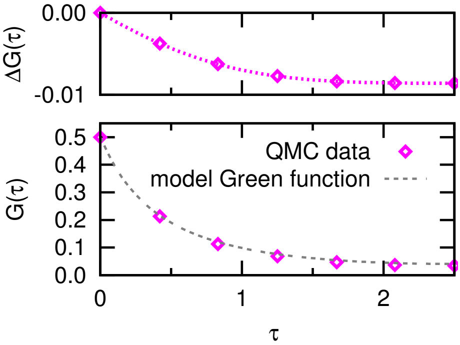
Idea:
- generate cont. model Green function (correct curvature at boundaries)
- fit difference with natural cubic spline



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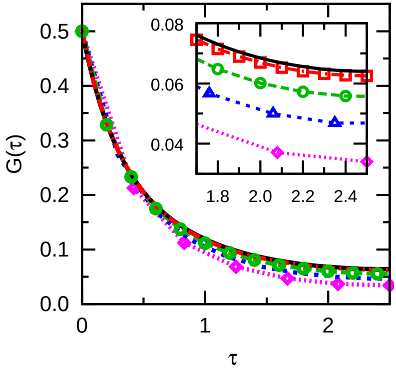

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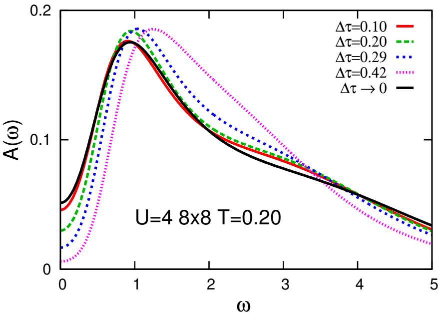
- least-squares extrapolation in $\Delta\tau^2$



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

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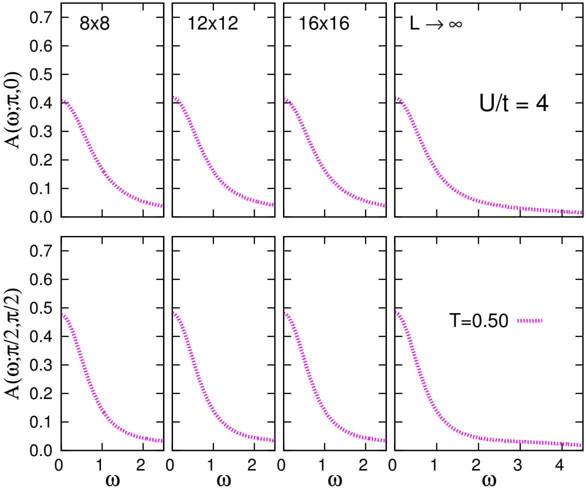

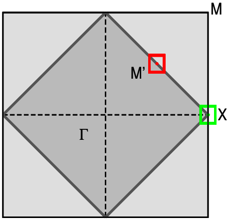

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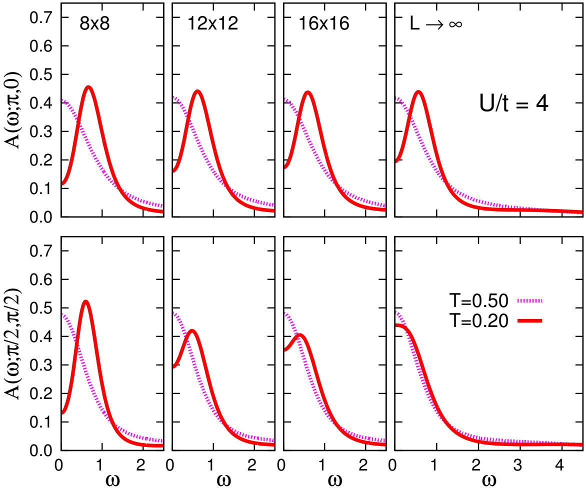

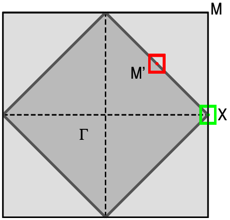

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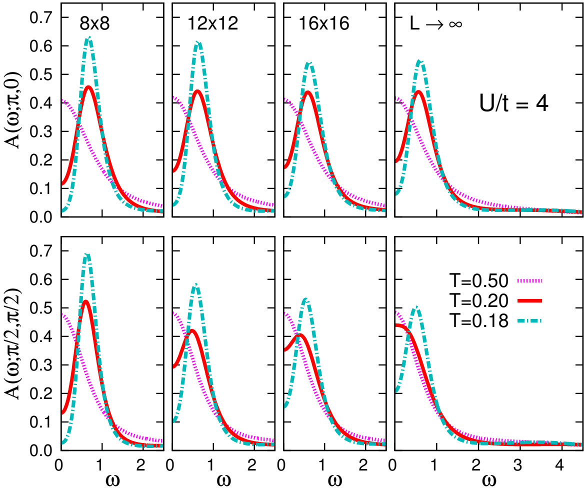
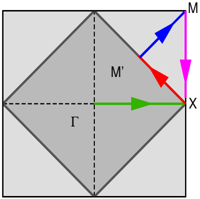


At weak coupling ($U/t = 4$):

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



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

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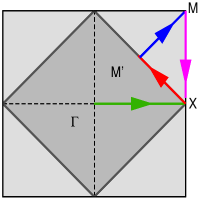

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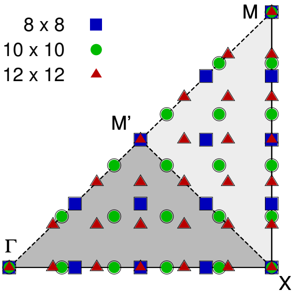
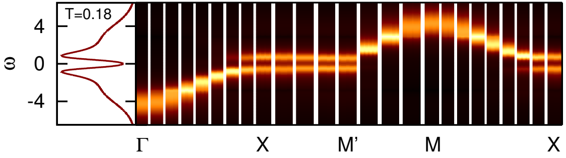


FS effects shift physical quantities and lead to incommensurate **k** grids

$\Rightarrow$ not every **k**-point is accessible

$\Rightarrow$ pointwise extrapolation rarely possible

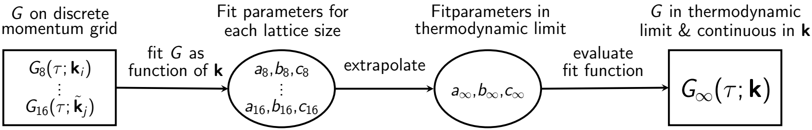


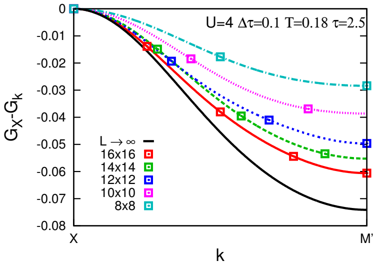
16 x 16

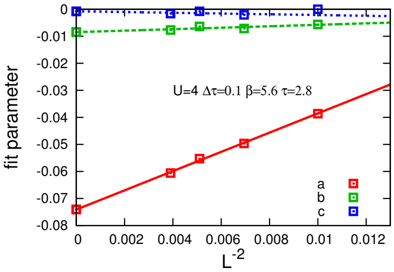
Elimination of finite size effects: high-symmetry lines

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

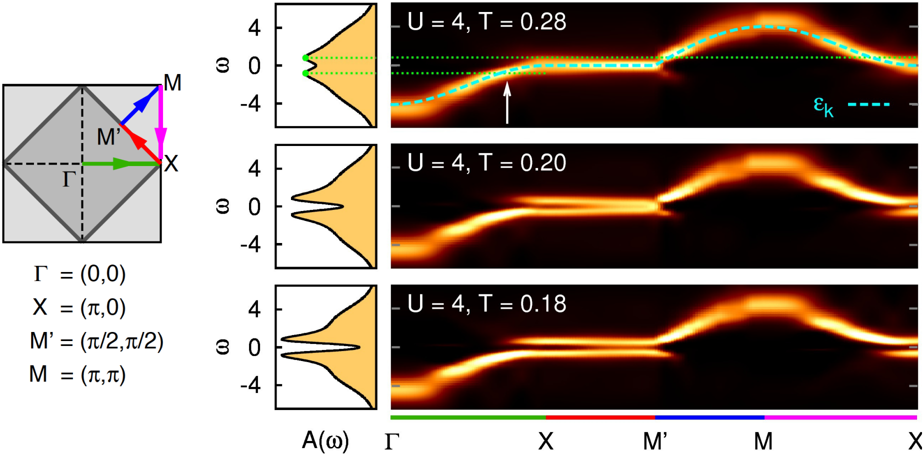
Better: global Fourier fits along high-symmetry lines $\rightsquigarrow$ continuous **k**-resolution







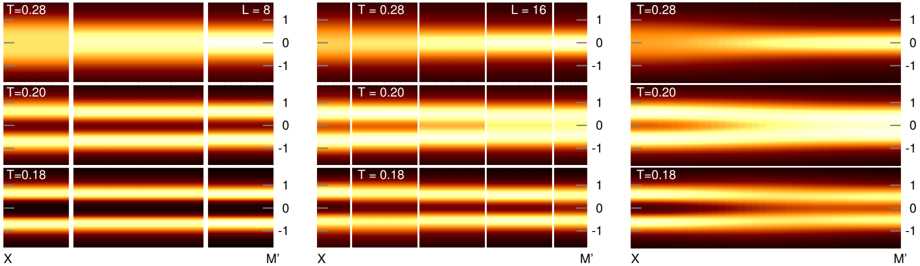
Spectral function for square lattice at weak coupling ($U/t = 4$)



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!

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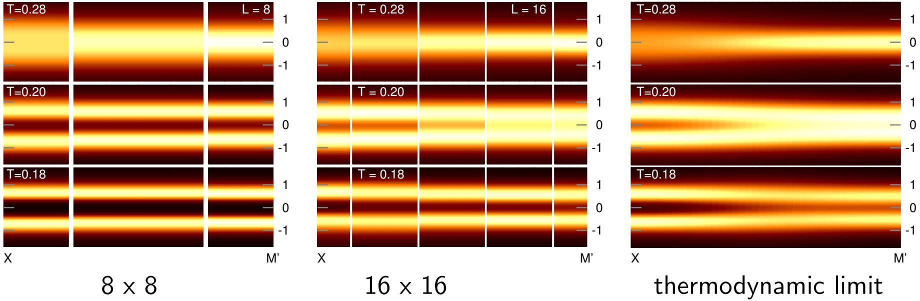
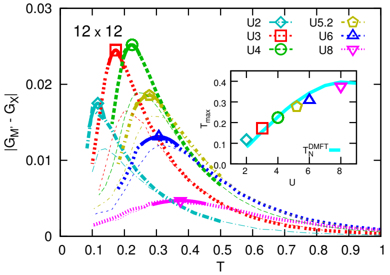


Momentum resolution of FS-extrapolated spectra impossible to reach by brute force!

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)]

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PG opening at mean-field AF ordering temperature

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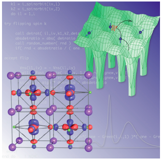
Outlook:
- Extension to finite doping and/or frustration
- Application as impurity solver for (cellular) DMFT

  $\rightsquigarrow$ linear (instead of cubic) scaling in β



DFG research unit 1346