

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

Nils Blümer

Institut für Physik, 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.*



Motivation: pseudogap, high- T_c superconductivity, antiferromagnetism

Challenge: spectra of Hubbard model in thermodynamic limit

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Results: unbiased PG spectra (continuous momentum resolution)

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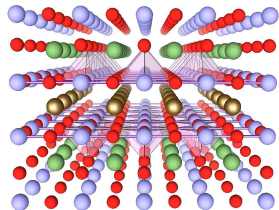
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Outlook: numerically exact multigrid DMFT+DQMC

Motivation: pseudogap physics in high- T_c cuprates

Layered cuprates: strongly correlated electron systems

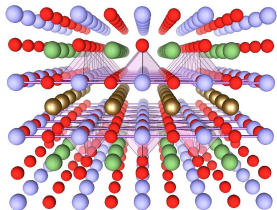


YBa₂Cu₃O₇ crystal structure

[Bobroff, Wikimedia Commons]

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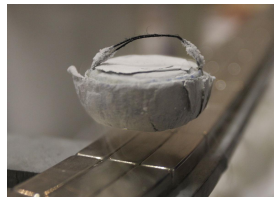


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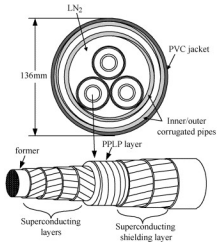
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All superconductors

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



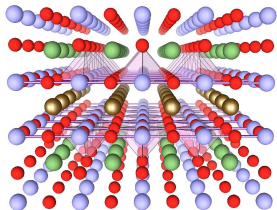
[Mühlpfordt, Wikipedia: Superconductivity]



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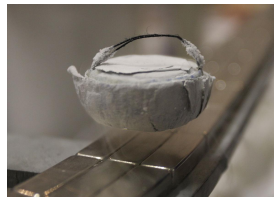


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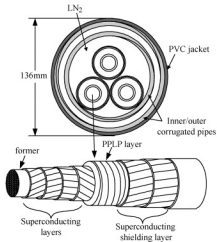
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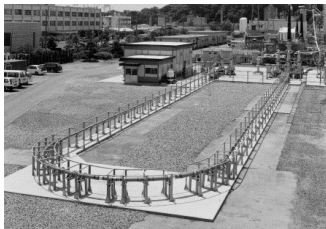
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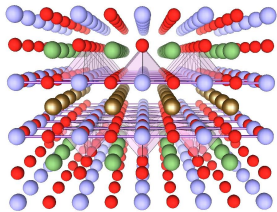


[Sumimoto - TEPCO test at Yokosuka]



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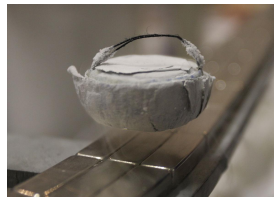


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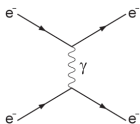
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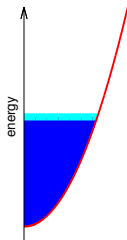


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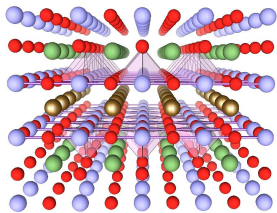
Electric resistance of **normal metals**:
electron-electron scattering + lattice
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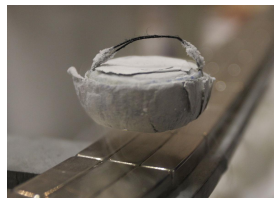


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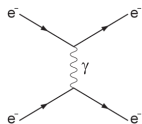
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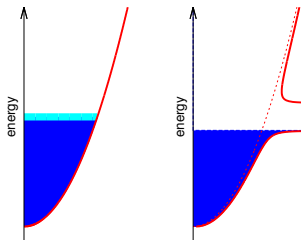
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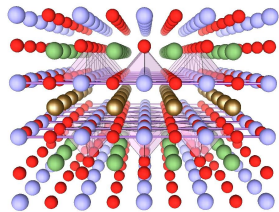
BCS state: isotropic full gap 2Δ



Motivation: pseudogap physics in high- T_c cuprates

Cuprate superconductors:

- planar structure
- ↪ quasi-2d electron systems
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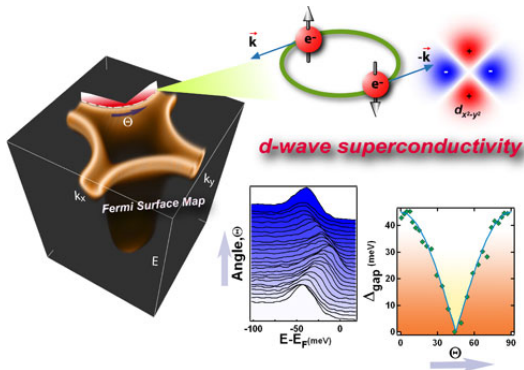


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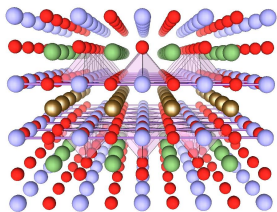
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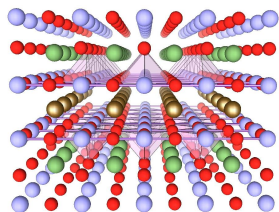


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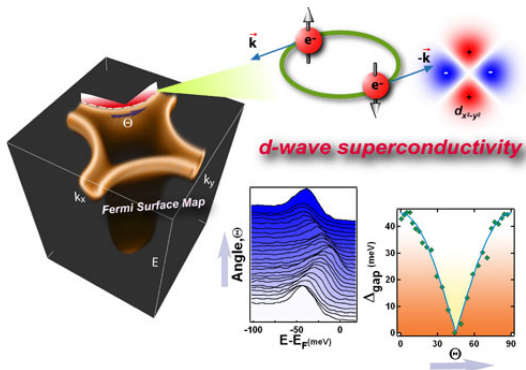
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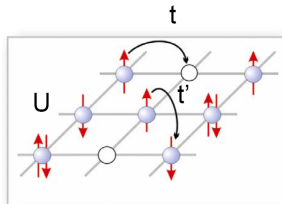


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Theory:
Hubbard model
on square lattice



Motivation: pseudogap physics in high- T_c cuprates

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

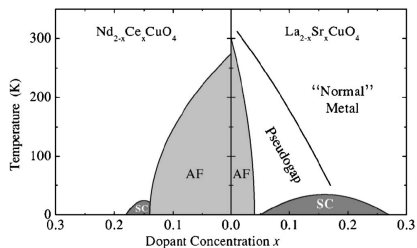


FIG. 1. Schematic phase diagram of high- T_c superconductors showing hole doping (right side) and electron doping (left side). From Damascelli *et al.*, 2003.

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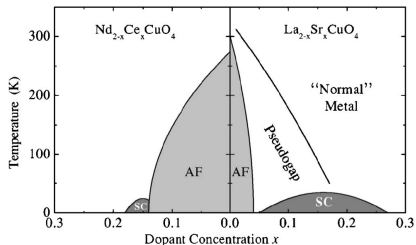


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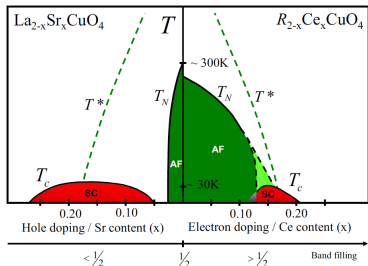


FIG. 2. (Color online) Joint phase diagram of the LSCO/NCCO material systems. The uncertainty regarding the extent of AF on the electron-doped side and its coexistence with superconductivity is shown by the dotted area. Maximum Néel

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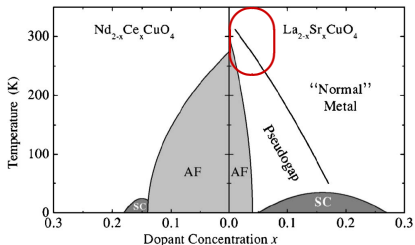


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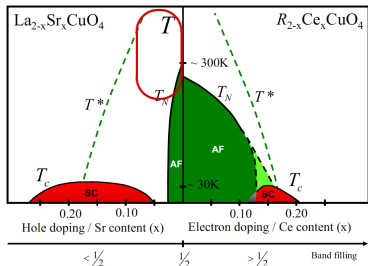


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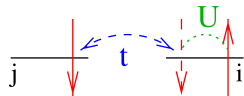
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Characteristic pseudogap temperature T^* near $x = 0$: at or far above T_N ?

Computational approaches for Hubbard-type models

Target: Hubbard model on infinite lattice

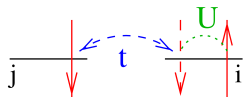
$$\hat{H} = \sum_{(i,j),\sigma} t_{ij} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{h.c.}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$



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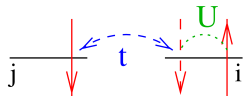
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- Perturbation theory
($U \ll t$ or $t \ll U$)
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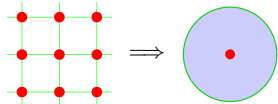


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Dynamical mean-field theory



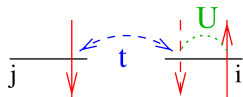
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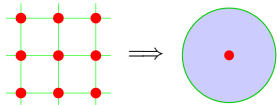


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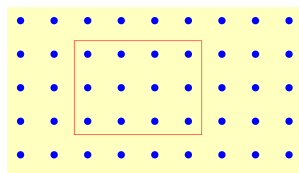
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3) Treat finite clusters

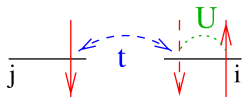


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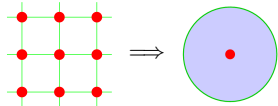


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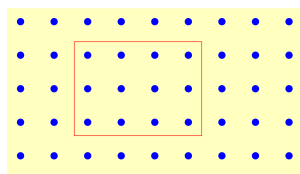
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Challenges:

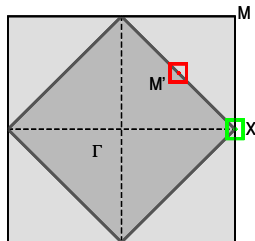
- Compute **exact imaginary-time Green functions** for large clusters ($\leq 16 \times 16$)
- Perform analytic continuation \rightsquigarrow **unbiased spectral functions**
- Extrapolate to the **thermodynamic limit**

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

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

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



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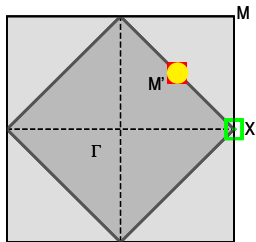
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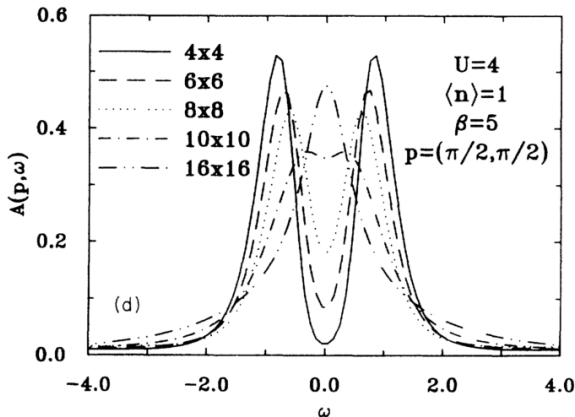
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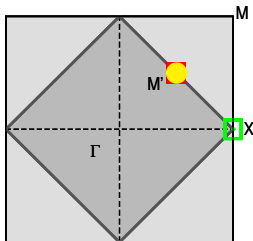
DQMC [White, PRB (1992)]: PG pure FS effect

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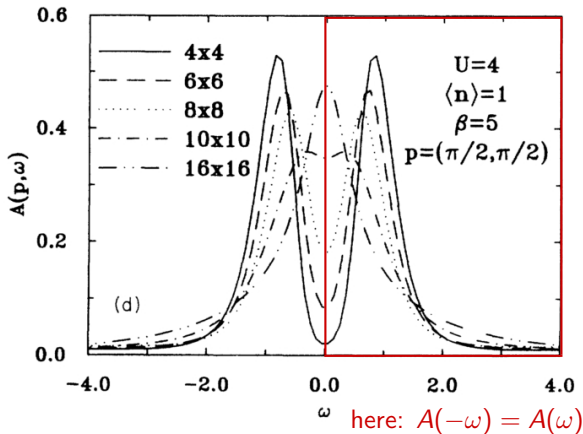
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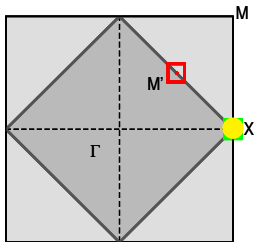
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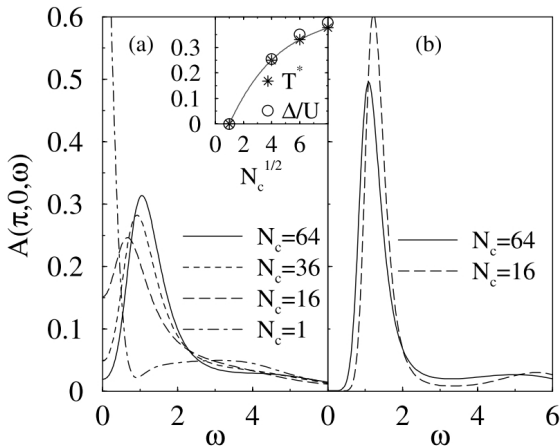
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DCA + DQMC under/overest. PG [Huscroft et al. (2001)]

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

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

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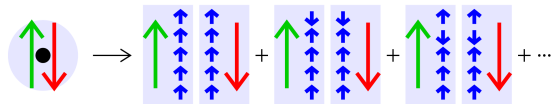
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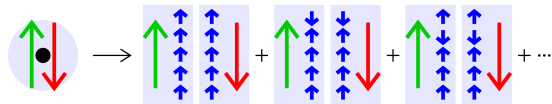
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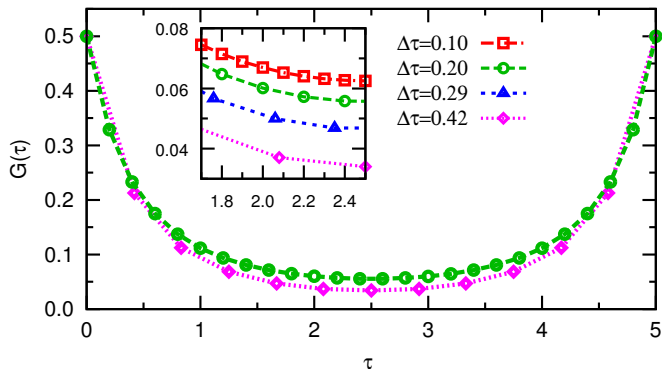
(iv) MC importance sampling over auxiliary Ising field $\{s\}$: $2^{N\Lambda}$ configurations

Sources of errors (for given cluster size):

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

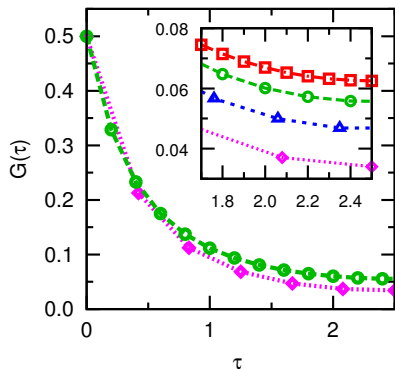
Impact of Trotter error on imaginary-time Green function + spectra

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



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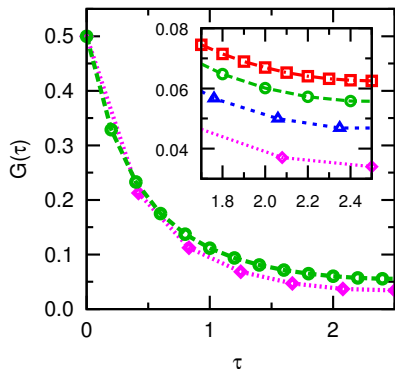
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\rightsquigarrow point-wise extrapolation impossible!

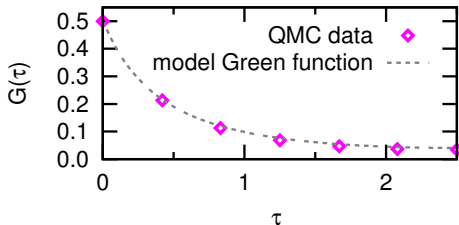
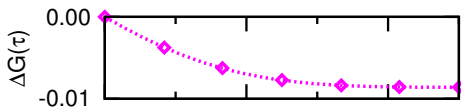
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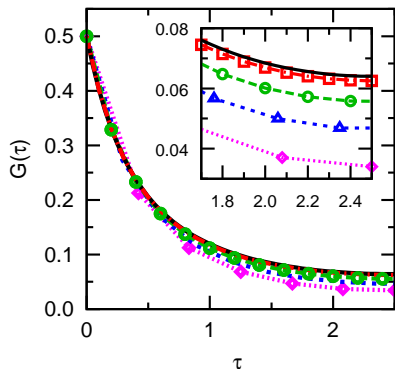
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- Idea:
- generate **cont. model Green function** (correct curvature at boundaries)
 - fit difference with **natural cubic spline**



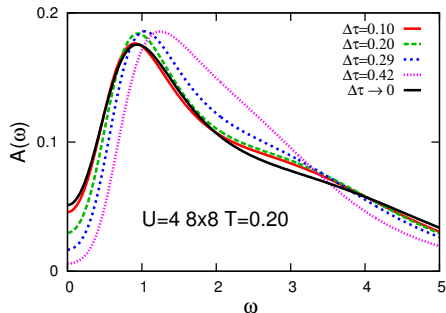
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- Idea:
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 - least-squares extrapolation in $\Delta\tau^2$



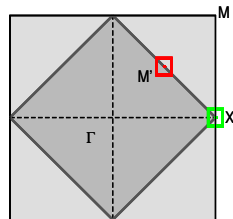
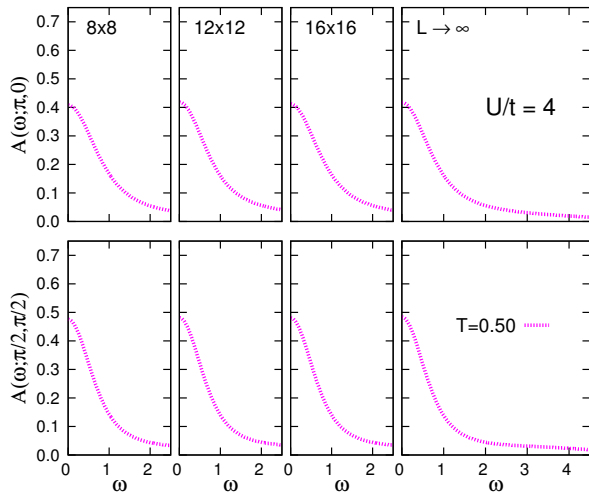
Multigrid DQMC eliminates Trotter errors reliably
 \rightsquigarrow unbiased spectra!

Elimination of finite size effects: high-symmetry points

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

Elimination of finite size effects: high-symmetry points

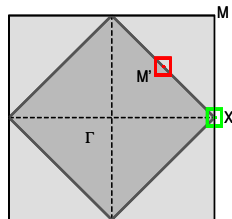
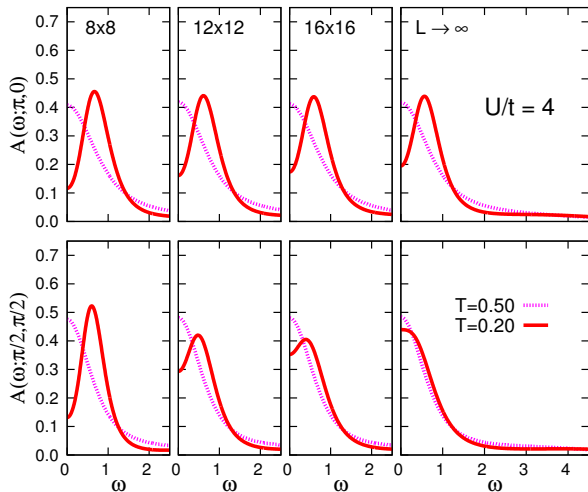
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$$\mathbf{X} = (\pi, 0)$$
$$\mathbf{M}' = (\pi/2, \pi/2)$$

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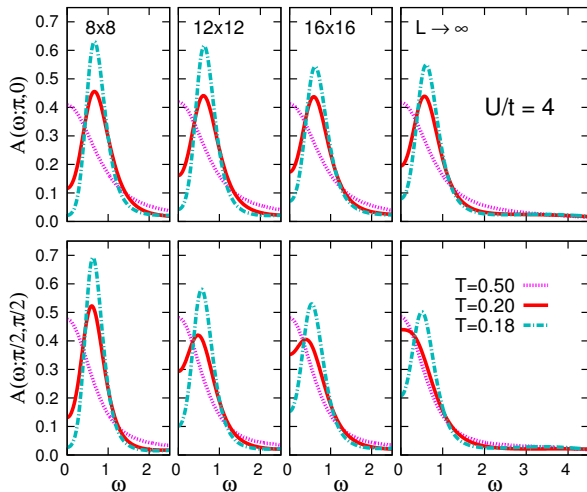
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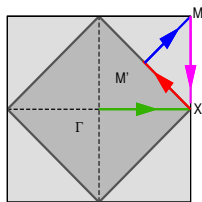


At weak coupling
($U/t = 4$):

pseudogap remains in
thermodynamic limit

d-wave type
anisotropy grows with
lattice size

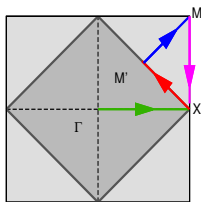
Goal: unbiased spectra ($\Delta\tau \rightarrow 0, N \rightarrow \infty$) along high-symmetry lines



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

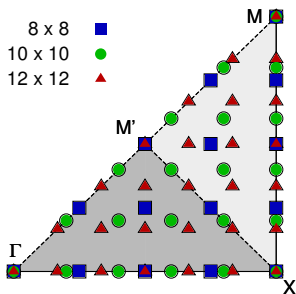
Special path: Fermi surface included (“beyond DMFT”)

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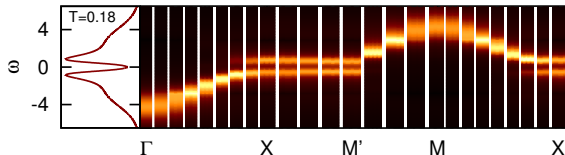
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FS effects shift physical quantities and lead to incommensurate **k** grids

⇒ not every **k**-point is accessible

⇒ pointwise extrapolation rarely possible

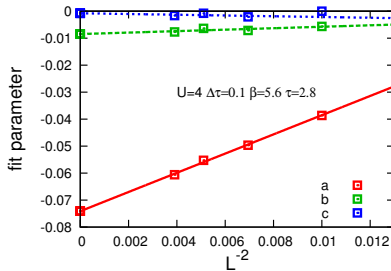
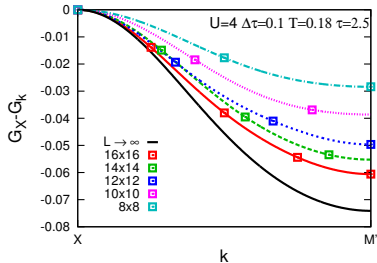
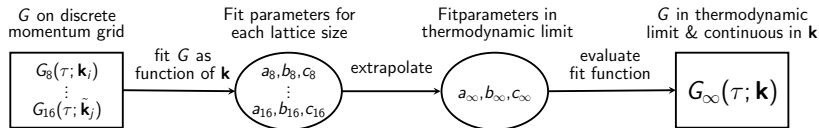


16 x 16

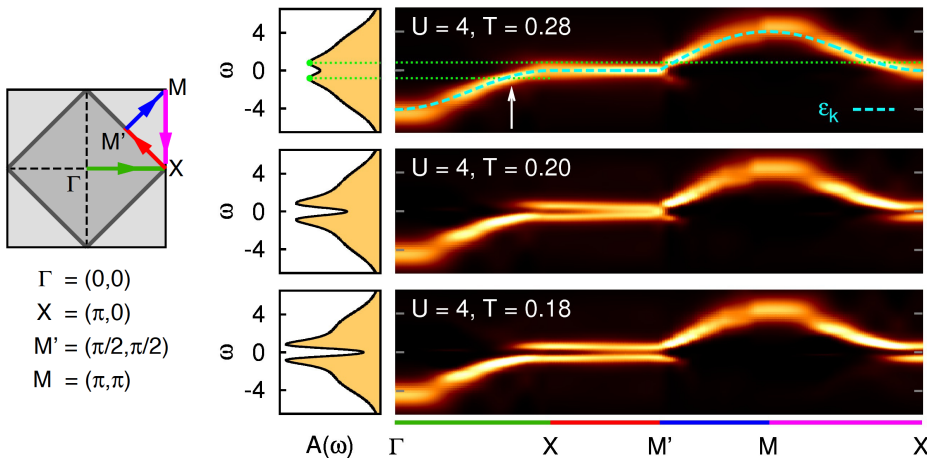
Elimination of finite size effects: high-symmetry lines

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

Better: global Fourier fits along high-symmetry lines \rightsquigarrow continuous \mathbf{k} -resolution



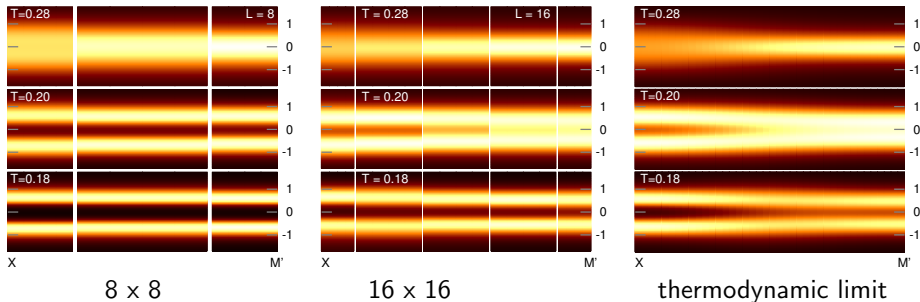
Spectral function for square lattice at weak coupling ($U/t = 4$)



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

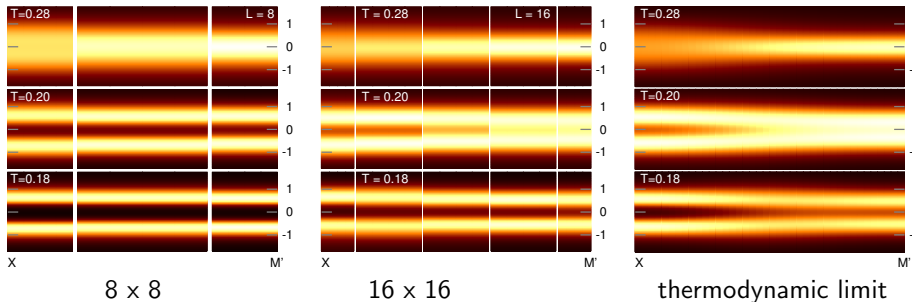
Finite-range AF opens **pseudogap**; \mathbf{k} dependence (**beyond DMFT**) at $X \rightarrow M'$

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



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

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

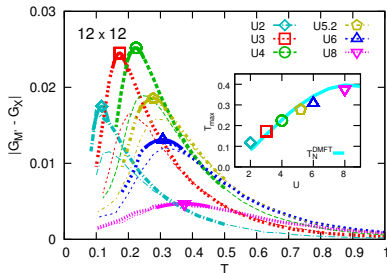


Momentum resolution of FS-extrapolated spectra impossible to reach by brute force!

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
benchmark for approximate methods (DCA)

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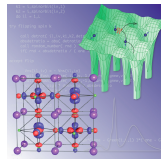
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- Extension to finite doping and/or frustration
 - Application as impurity solver for (cellular) DMFT
 - ↪ linear (instead of cubic) scaling in β



DFG research
unit 1346