Momentum-dependent pseudogaps in the half-filled 2d Hubbard model

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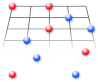
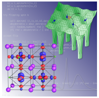
JOHANNES GUTENBERG UNIVERSITÄT MAINZ

[D. Rost, E. V. Gorelik, F. Assaad, N. Blümer, arXiv:1205.6788]



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

FOR 1346
LDA+DMFT
Augsburg *et al.*



Outline

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History: pseudogap in unfrustrated half-filled Hubbard model

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Unbiased PG spectra at high-symmetry points

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Full momentum resolution along high-symmetry lines

PG characteristic temperature T^*

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PG characteristic temperature T^*

Numerically exact multigrid DMFT+DQMC

Motivation I: nonlocal AF signatures in $d = 2$ at finite T?

RAPID COMMUNICATIONS

PHYSICAL REVIEW A **85**, 061602(R) (2012)

Universal probes for antiferromagnetic correlations and entropy in cold fermions on optical lattices

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[2]*Instituto de Fisica, Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brazil*
[3]*Department of Physics, University of California, Davis, California 95616, USA*
[4]*University of Wuppertal, Wuppertal, Germany*

(Received 18 May 2011; revised manuscript received 20 March 2012; published 7 June 2012)

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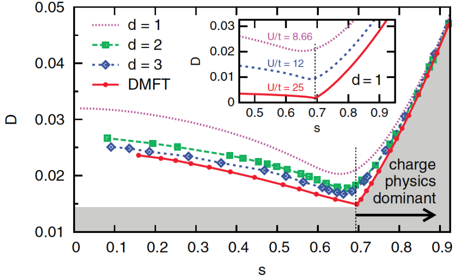

FIG. 2. (Color online) Hypercubic lattice at strong coupling: Double occupancy vs entropy. In all cases, the minimum of the double occupancy corresponds to $s^* \approx \ln(2)$ (dotted line). The shaded area indicates the nonmagnetic contribution to D. Inset: $D(s)$ in $d = 1$ for various interactions.

Double occupancy looks as if AF order sets in at $s \lesssim \ln(2)$ (Heisenberg regime), even in dimension $d \leq 2$!

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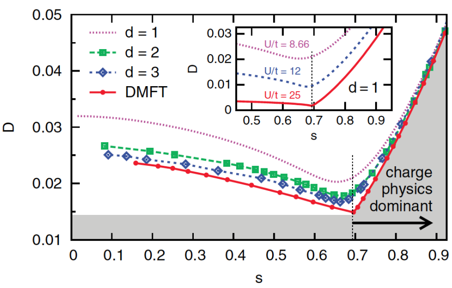

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Double occupancy looks as if AF order sets in at $s \lesssim \ln(2)$ (Heisenberg regime), even in dimension $d \leq 2$!

- AF sigs at weak coupling?
- less local observable: $A(\omega)$

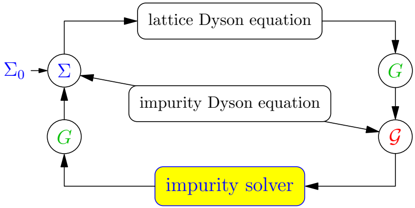
Motivation II: exact (unbiased) DMFT+DQMC implementation

PHYSICAL REVIEW E **81**, 056703 (2010)

Cluster solver for dynamical mean-field theory with linear scaling in inverse temperature

E. Khatami,[1,2] C. R. Lee,[3] Z. J. Bai,[4] R. T. Scalettar,[5] and M. Jarrell[2]
[1]*Department of Physics, University of Cincinnati, Cincinnati, Ohio 45221, USA*
[2]*Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803, USA*
[3]*Computer Science Department, National Tsing Hua University, Taiwan*
[4]*Computer Science Department, University of California, Davis, California 95616, USA*
[5]*Physics Department, University of California, Davis, California 95616, USA*
(Received 8 April 2009; revised manuscript received 20 January 2010; published 12 May 2010)

DMFT: better impurity solver?



Standard: direct QMC impurity solvers (Hirsch-Fye, CT-QMC) - cost $\propto T^{-3}$

Khatami et al: solve auxiliary Hamiltonian by DQMC (instead of ED) - cost $\propto T^{-1}$

Proposal: eliminate Trotter (+ FS?) error from BSS Green function $\rightsquigarrow$ exact solver

Motivation III: pseudogap physics in high-T_c cuprates

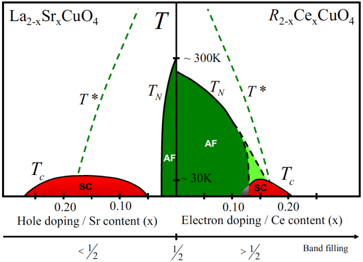


FIG. 2. (Color online) Joint phase diagram of the LSCO/NCCO material systems. The uncertainty regarding the extent of AF on the electron-doped side and its coexistence with superconductivity is shown by the dotted area. Maximum Néel

[Armitage et al., RMP (2010)]

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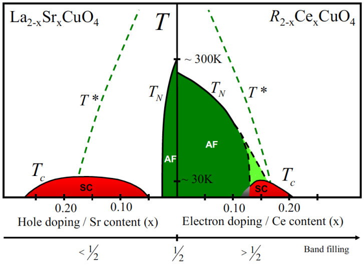

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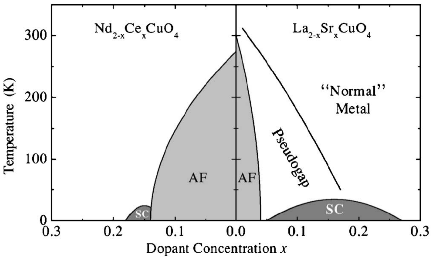

FIG. 1. Schematic phase diagram of high-T_c superconductors showing hole doping (right side) and electron doping (left side). From Damascelli *et al.*, 2003.

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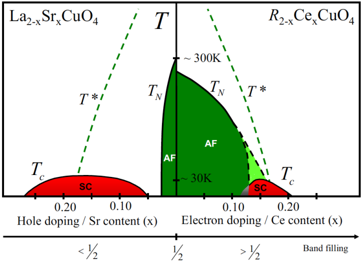

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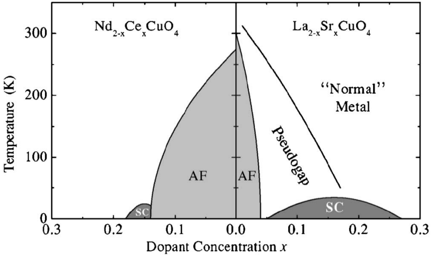

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Origin/nature of pseudogap: preformed sc pairs, competing phenomenon (AF)?

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

Motivation III: pseudogap physics in high-T_c cuprates

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

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arXiv:1207.2490v1

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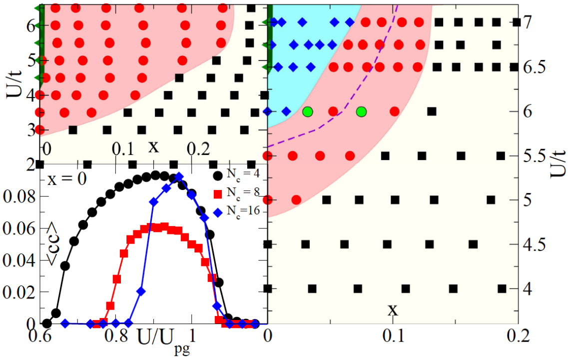


Figure 1: **Superconducting phase diagram of the two-dimensional Hubbard model** in plane of interaction strength U and carrier concentration x computed using the 8-site (right panel) and 4-site (left upper panel) DCA dynamical mean field approximation at temperature $T = t/40$ with $t'/t = 0$. Dashed 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 2d 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

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

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

Daniel Rost
Univ. Mainz

Elena Gorelik
Univ. Mainz

Fakher Assaad
Univ. Würzburg

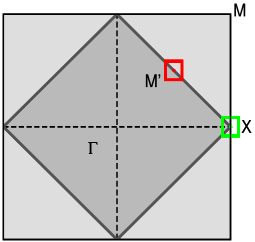
Nils Blümer
Univ. Mainz

Pseudogap in half-filled Hubbard model - brief history I

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

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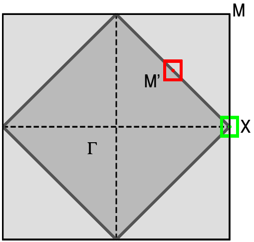

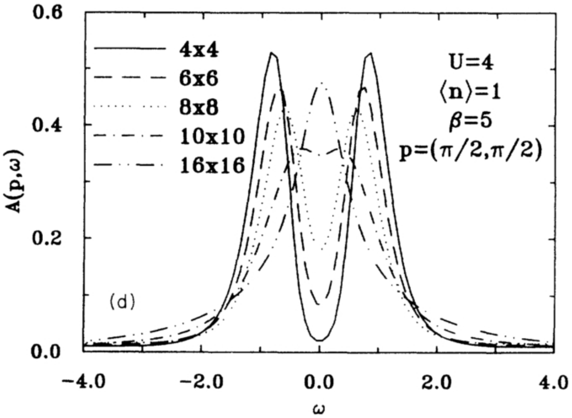

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DQMC [White, PRB (1992)]: PG pure FS effect

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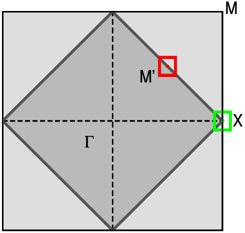

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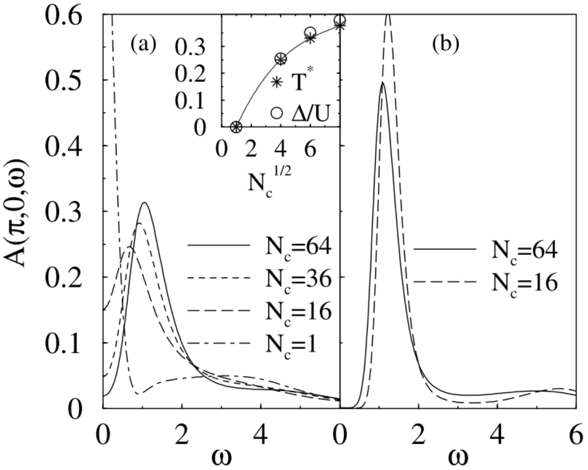
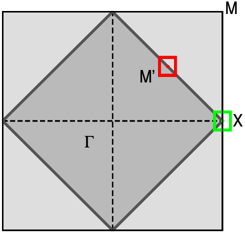


DCA + DQMC under/overest. PG [Huscroft et al. (2001)]

Pseudogap in half-filled Hubbard model - brief history II

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



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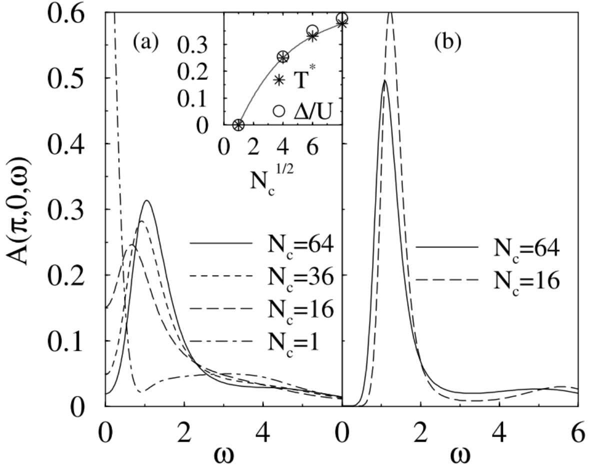
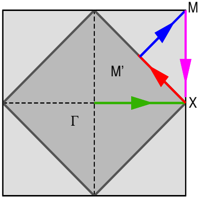


DCA + DQMC under/overest. PG [Huscroft et al. (2001)]

Goal: first exact (unbiased) DQMC spectra in thermodynamic limit

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")

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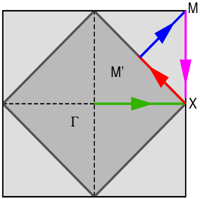

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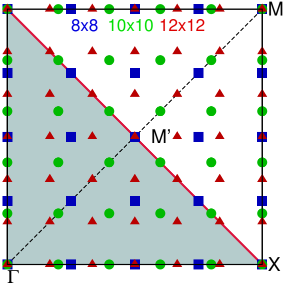
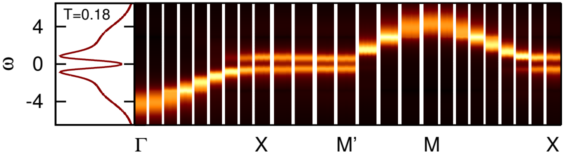


FS effects shift physical quantities and lead to incommensurate **k** grids

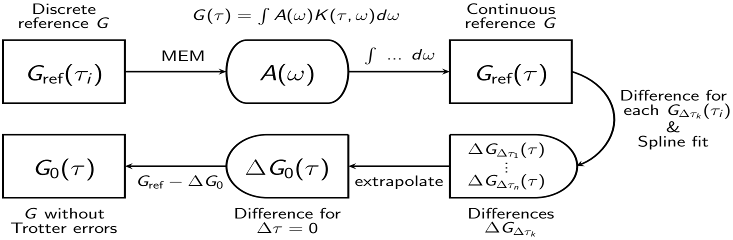
$\Rightarrow$ not every **k**-point is accessible

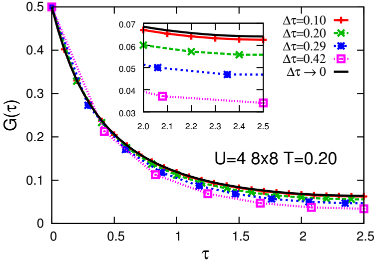
$\Rightarrow$ pointwise extrapolation rarely possible

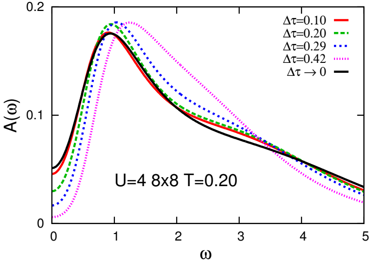


16 x 16

Elimination of Trotter errors







- Extrapolated G yields valid, consistent spectra!
- $\Delta\tau = 0.1$ “good enough”

Elimination of finite size effects: high-symmetry points

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

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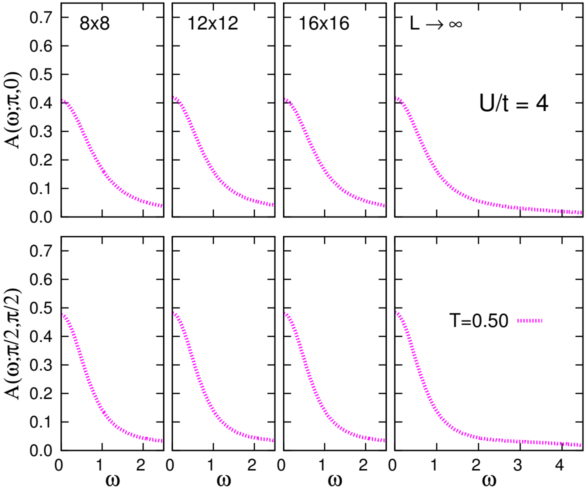

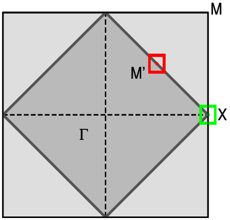

$$\mathbf{X} = (\pi, 0)$$
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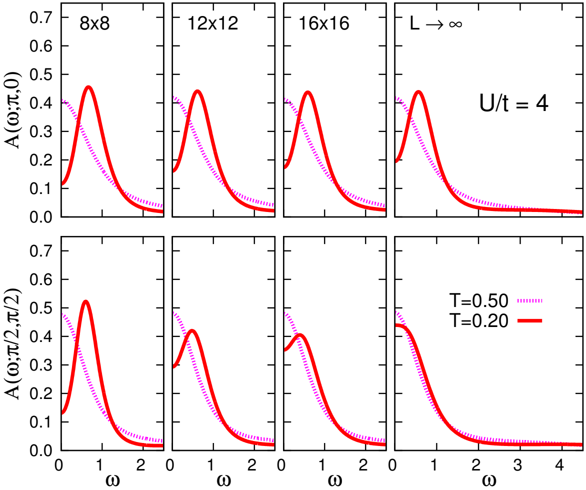

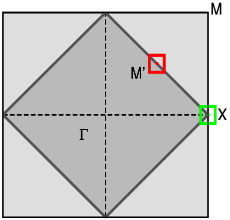

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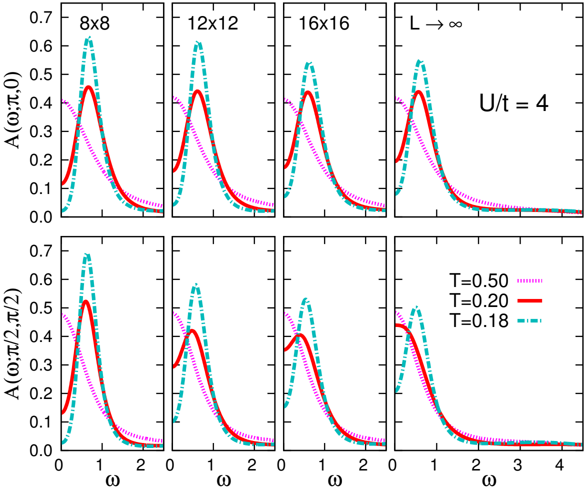

At weak coupling ($U/t = 4$):

pseudogap remains in thermodynamic limit

d-wave type anisotropy grows with lattice size

Pseudogap strength versus temperature?

Scalar measure of pseudogap strength: $r_{\mathbf{k}} \equiv 1 - A_{\mathbf{k}}(\omega = 0) / \max_{\omega} A_{\mathbf{k}}(\omega)$

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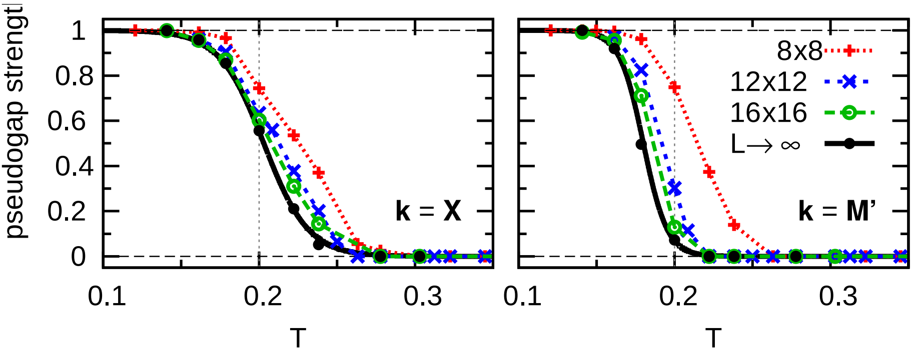

PG opens first at antinodal point **X**; $r_{\mathbf{X}} \gtrsim 0.5$ triggers PG at nodal point M'

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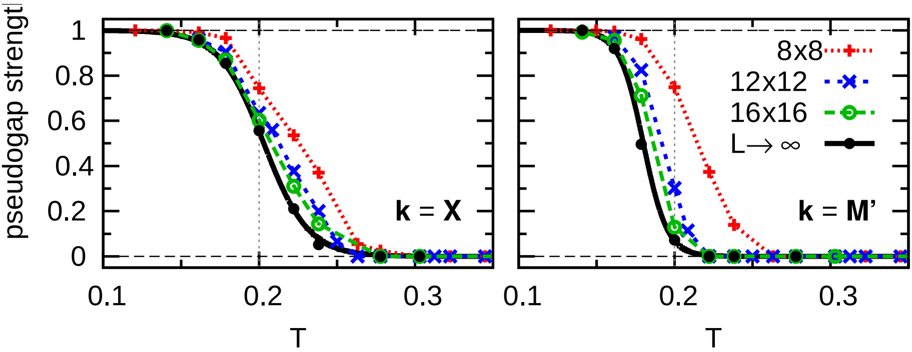

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Precision of scalar measure $r_{\mathbf{k}}$ limited by MEM

Test of maximum entropy procedure: local vs. **k**-summed spectra

$G(\tau) \equiv G_{ii}(\tau) = \frac{1}{N}\sum_{\mathbf{k}} G_{\mathbf{k}}(\tau); \quad G(\tau) = -\int_{-\infty}^{\infty} d\omega A(\omega) \frac{e^{-\tau\omega}}{1+e^{-\beta\omega}}$

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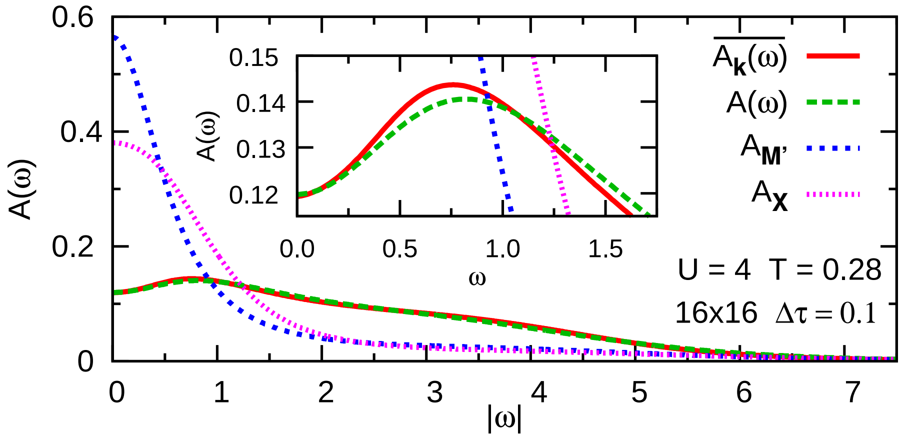
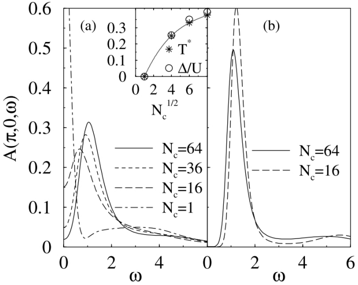


Perfect agreement: $A(\omega) \equiv A_{ii}(\omega) \stackrel{!}{=} \frac{1}{N}\sum_{\mathbf{k}} A_{\mathbf{k}}(\omega)$

Comparison with Huscroft results at $\mathbf{k} = (\pi, 0)$



Huscroft et al. (2001):
FS-DQMC overestimates gap
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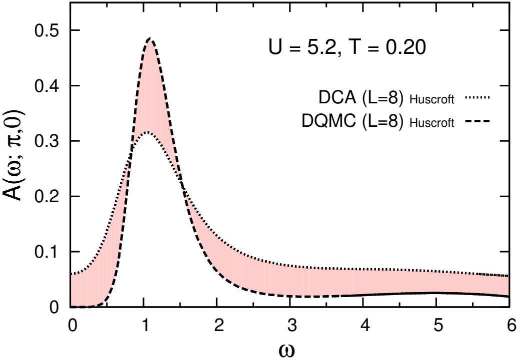

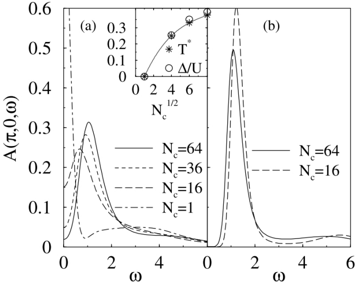

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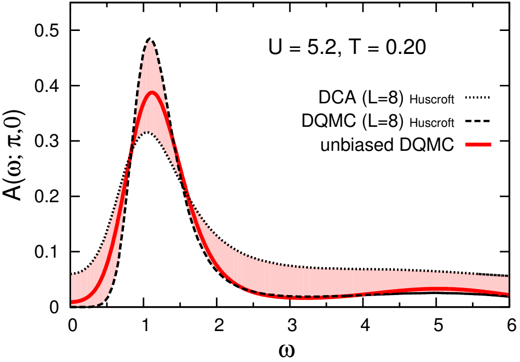

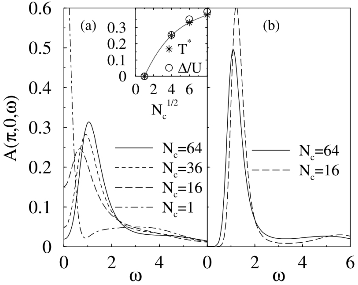

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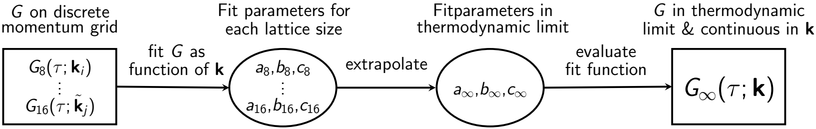
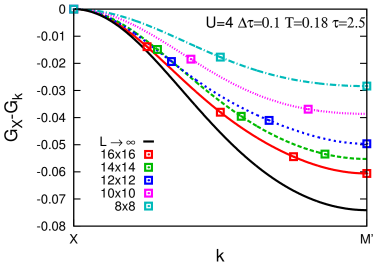
Result fulfills expectation:
unbiased spectrum is found between
FS-DQMC and DCA result!

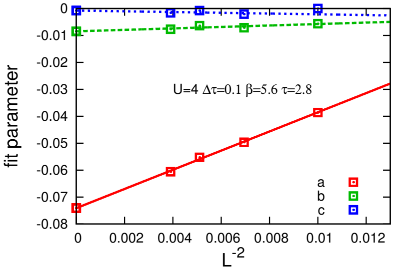
Elimination of finite size effects: high-symmetry lines

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

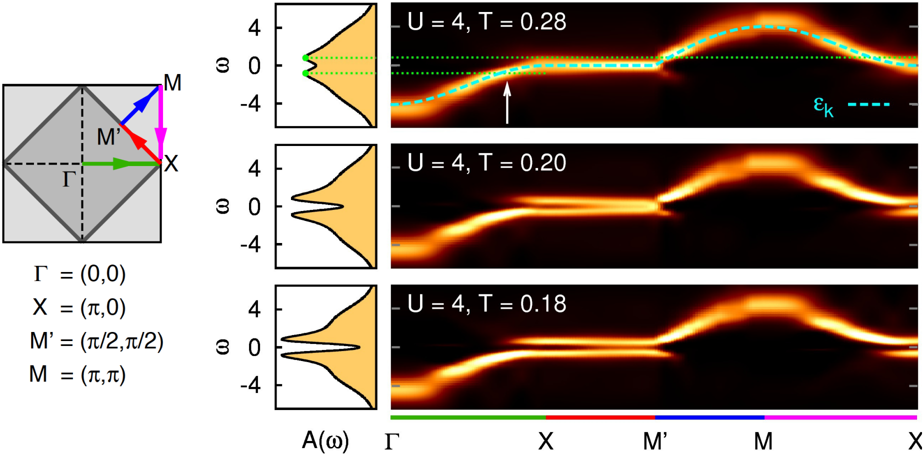
Better: global Fourier fits along high-symmetry lines $\rightsquigarrow$ continuous **k**-resolution







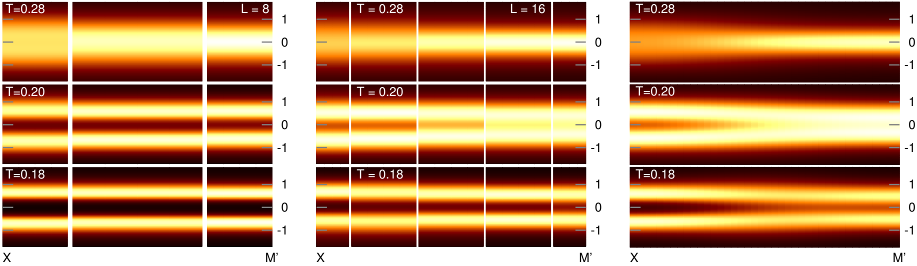
Spectral function for square lattice at weak coupling ($U/t = 4$)



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

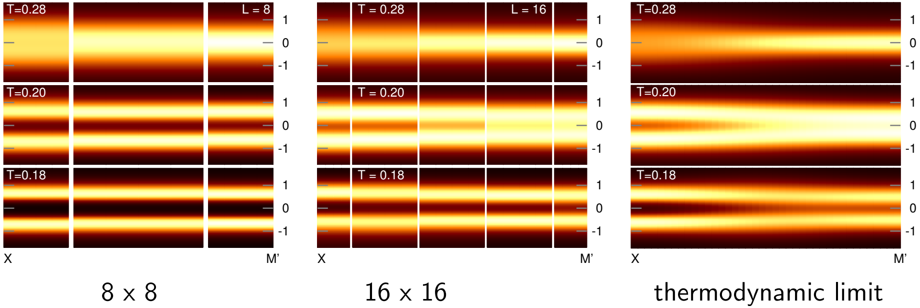
Finite-range AF opens pseudogap; **k** dependence (beyond DMFT) at $X \to M'$

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



8 x 8 | 16 x 16 | thermodynamic limit

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



Here: momentum dependence purely from nonlocal correlations (beyond DMFT)

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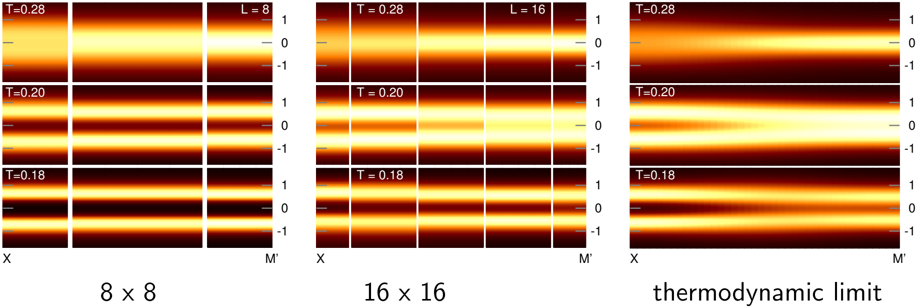
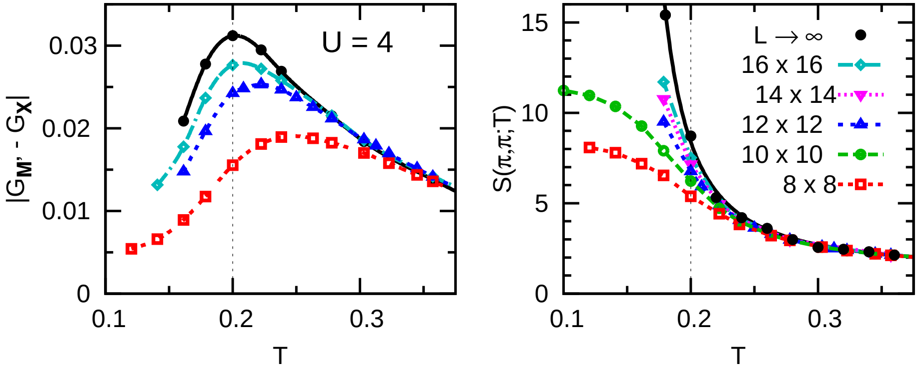


Here: momentum dependence purely from nonlocal correlations (beyond DMFT)

Momentum resolution of FS-extrapolated spectra far beyond brute force!

Scalar measure of momentum dependence

$$|G_1 - G_2| := \sqrt{\frac{1}{\beta}\int_0^\beta \left(G_1(\tau) - G_2(\tau)\right)^2 d\tau}$$



Momentum dependence maximal at pseudogap opening

Strong finite-size effects

Scalar measure of momentum dependence: weak/strong coupling?

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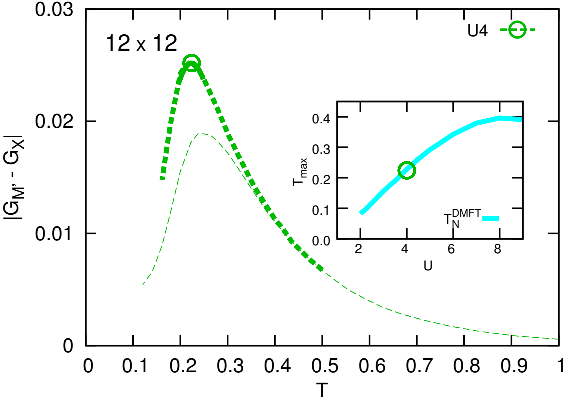

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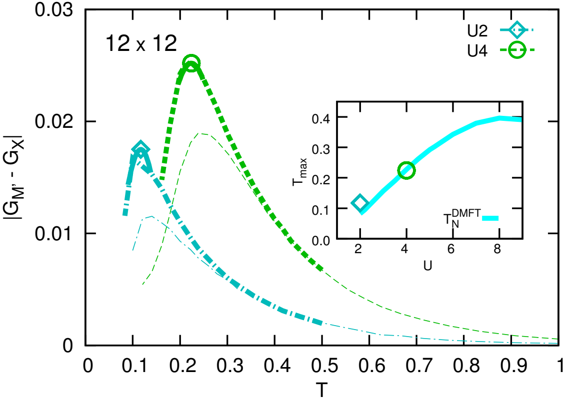

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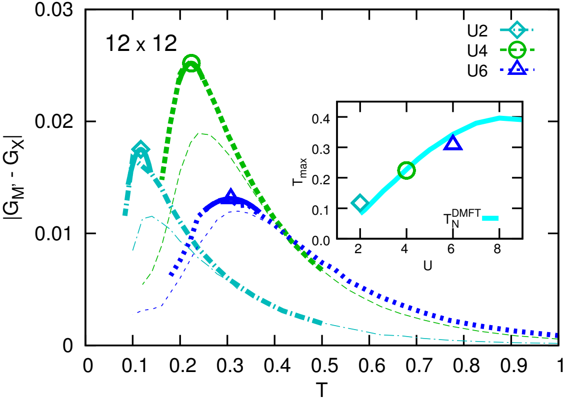

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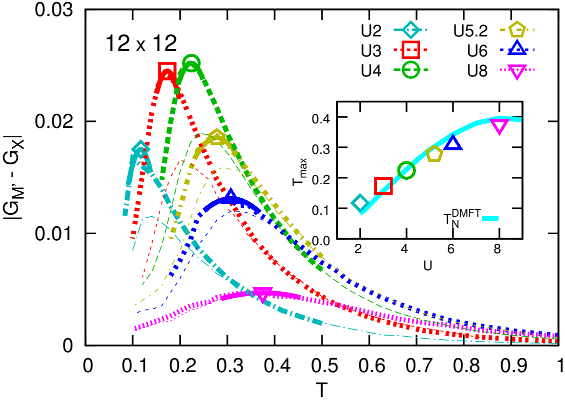


Maximal **k**-dependence defines T^*

T^* is consistent with pseudogap in the spectra

T^* coincides with mean-field (DMFT) critical temperature!

[arXiv:1201.5576v1: Gorelik, Rost, Paiva, Scalettar, Klümper, Blümer]

Numerically exact DMFT+DQMC method

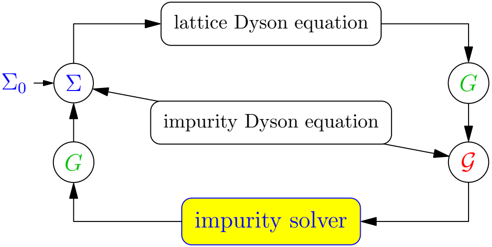
[D. Rost, F. Assaad, and N. Blümer]

Daniel Rost
Univ. Mainz

Fakher Assaad
Univ. Würzburg

Nils Blümer
Univ. Mainz

DMFT iteration scheme (direct impurity solver):
$\rightsquigarrow$ cost $\propto \beta^3$ (QMC)



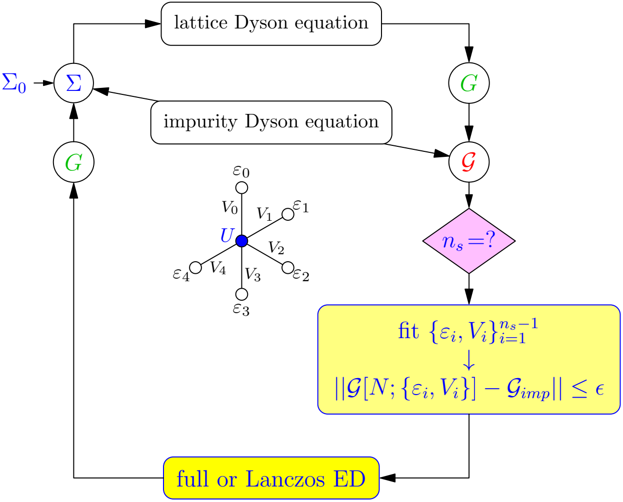
DMFT+DQMC: scheme and relation to ED

DMFT iteration scheme (direct impurity solver):

$\rightsquigarrow$ cost $\propto \beta^3$ (QMC)

ED requires Hamiltonian representation, e.g. with star topology

$\rightsquigarrow$ cost exponential in n_s



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Khatami et al (2010): use determinantal QMC for Hamiltonian
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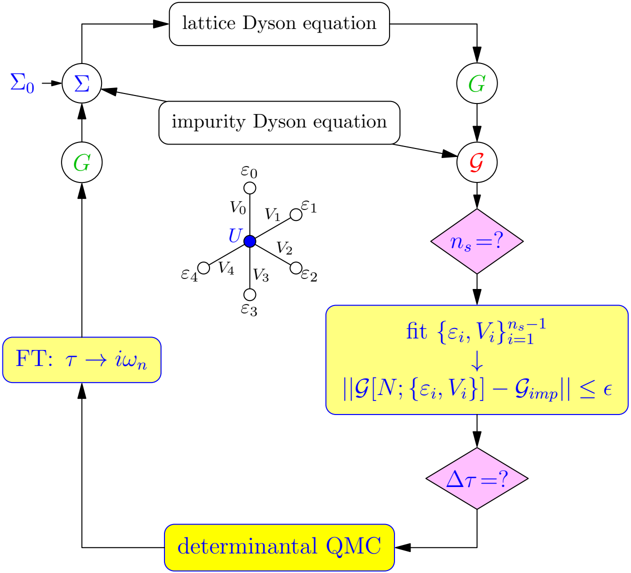

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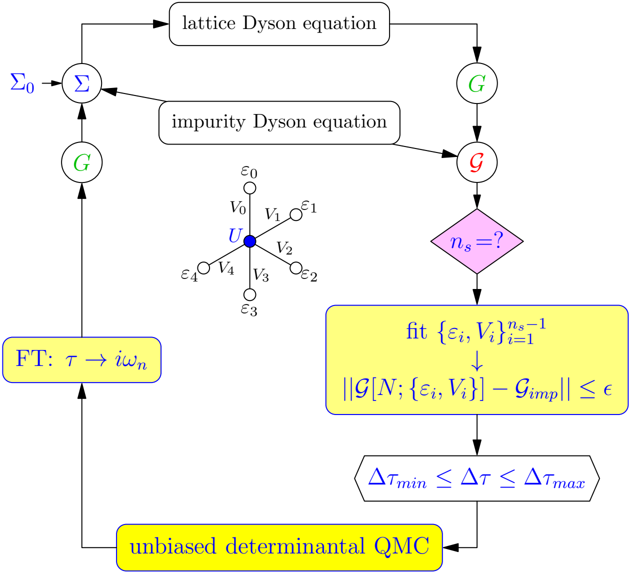
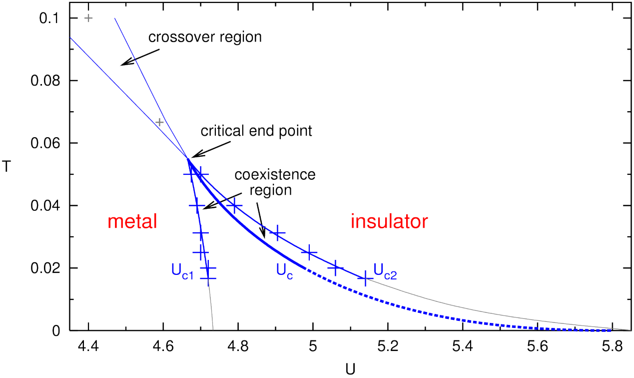
P8 (Mainz): eliminate discretization error(s)!



Mott metal-insulator transition within paramagnetic DMFT: reference



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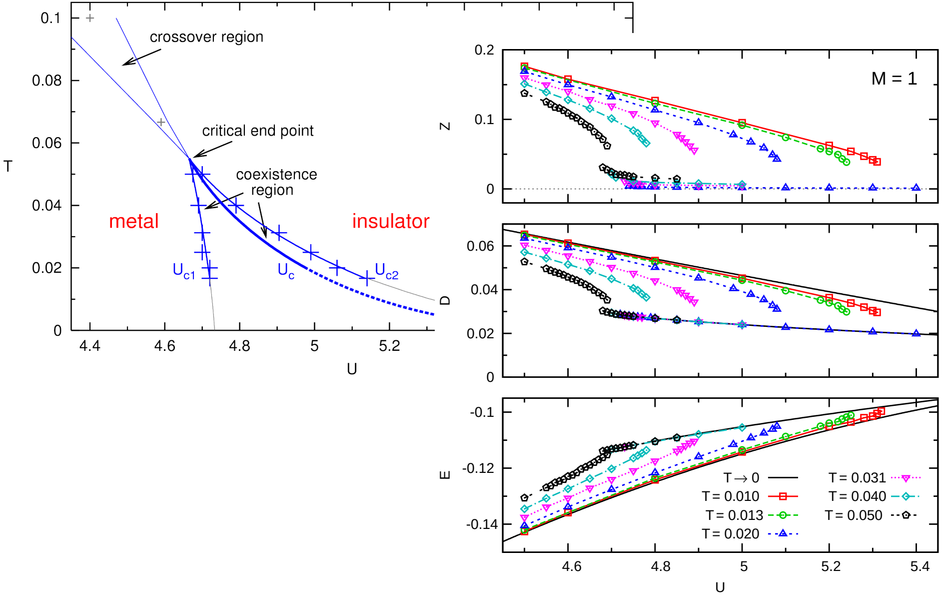
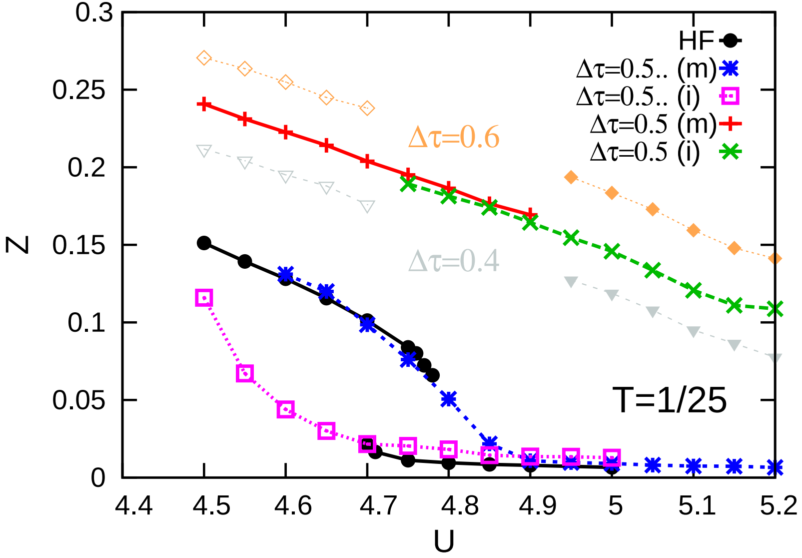
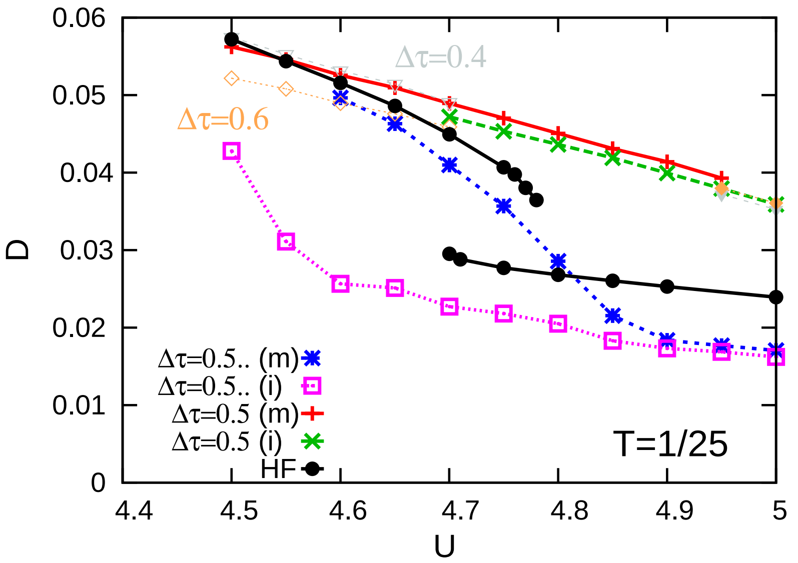


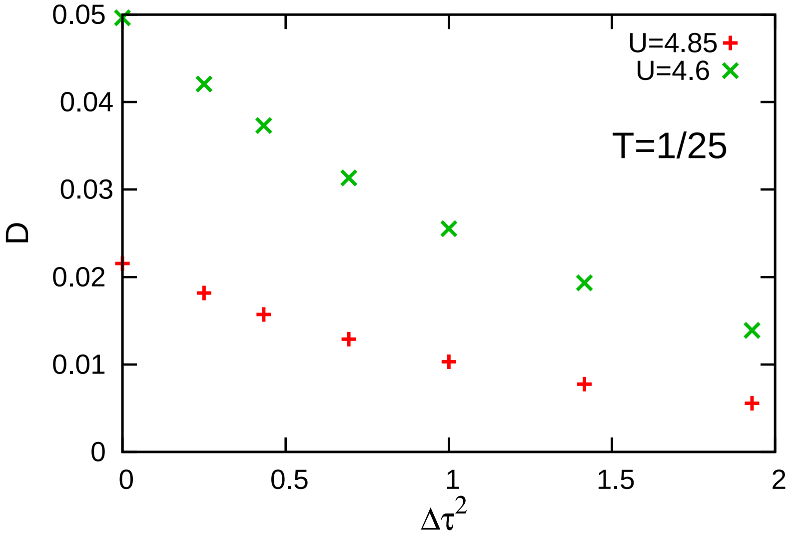
Mott metal-insulator transition within paramagnetic DMFT: QP weight



Mott metal-insulator transition within paramagnetic DMFT: *D*



Mott MIT within paramagnetic DMFT: extrapolation of D



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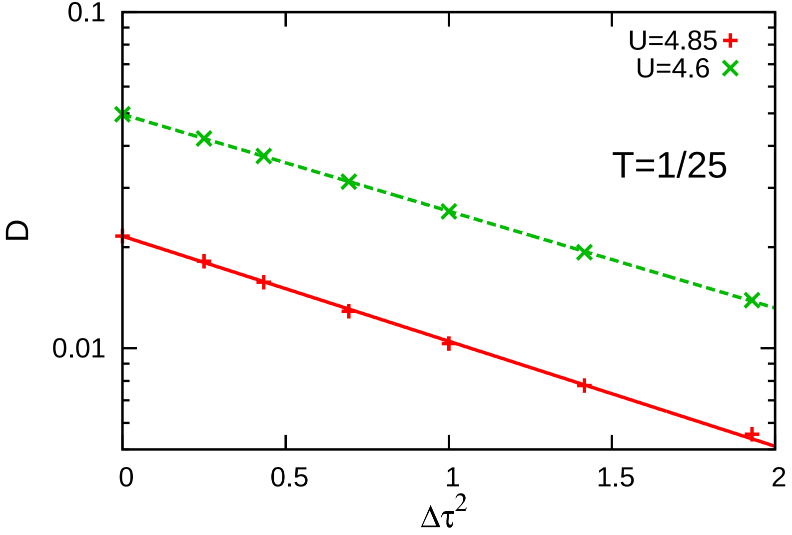
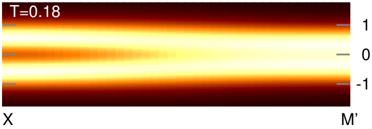


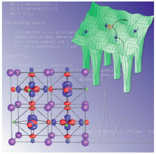
Summary

First unbiased spectra in thermodynamic limit

- by elimination of Trotter errors
- and extrapolating to the thermodynamic limit



- showed that occurrence of pseudogap is no FS effect
- clearly resolved **k**-dependence



FOR 1346

First unbiased spectra in thermodynamic limit

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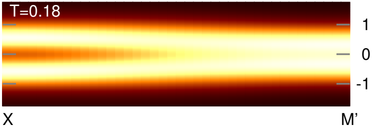
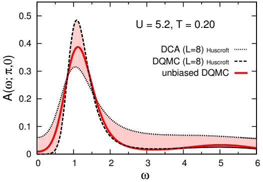
achieving consistency with previous results





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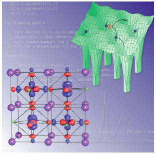

FOR 1346

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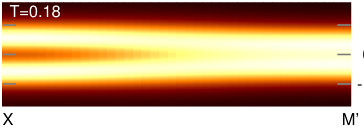

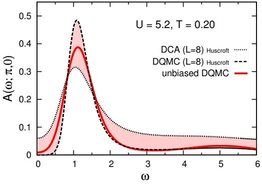

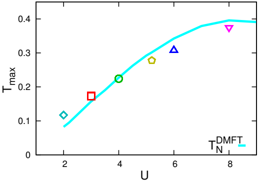

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- clearly resolved **k**-dependence
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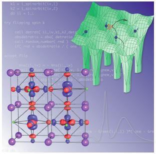
Outlook: Route to high-T_C for ultra cold fermions?



FOR 1346