What does it take for a Hubbard model to show *d*-wave superconductivity?

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MCQST

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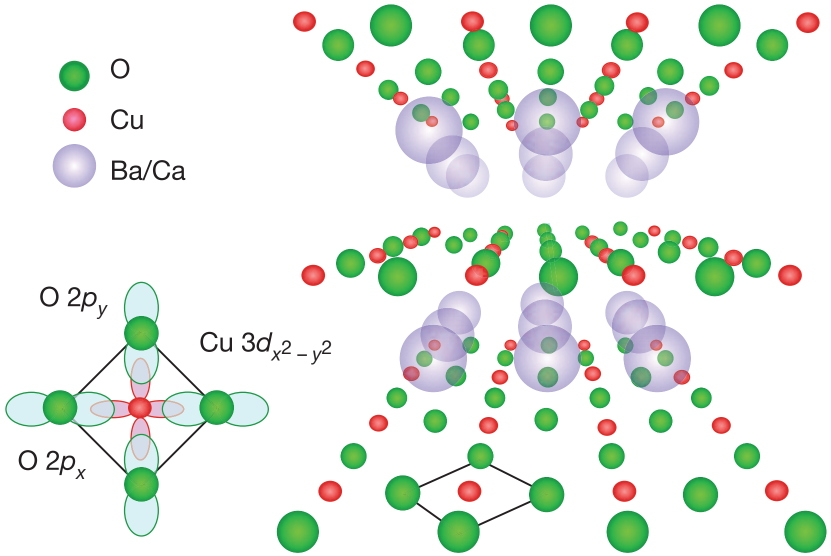
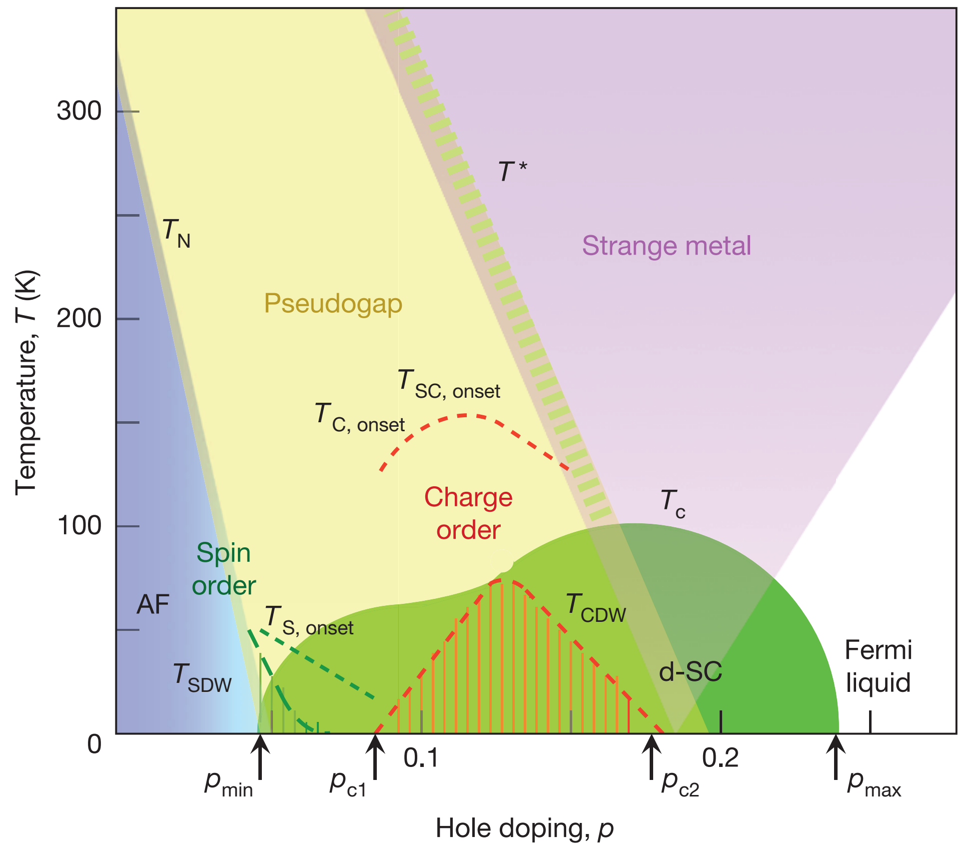
high-temperature superconductors



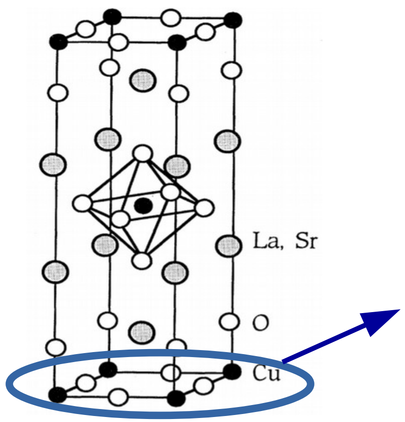


- typical structure
- generic phase diagram

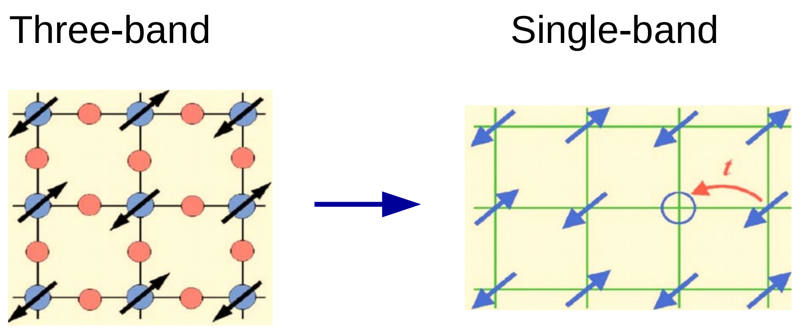
(Keimer *et al.*, Nature 15)

modeling high-Tc SCs

- „complete“ description unfeasible and probably uninformative
- modeling to capture essential concepts and mechanism
- „a theory should be as simple as possible, but not simpler“



[RevModPhys.66.763]



[RevModPhys.78.17]

single-band Hubbard model:
square lattice, hole doping, nearest neighbor hopping, on-site repulsion

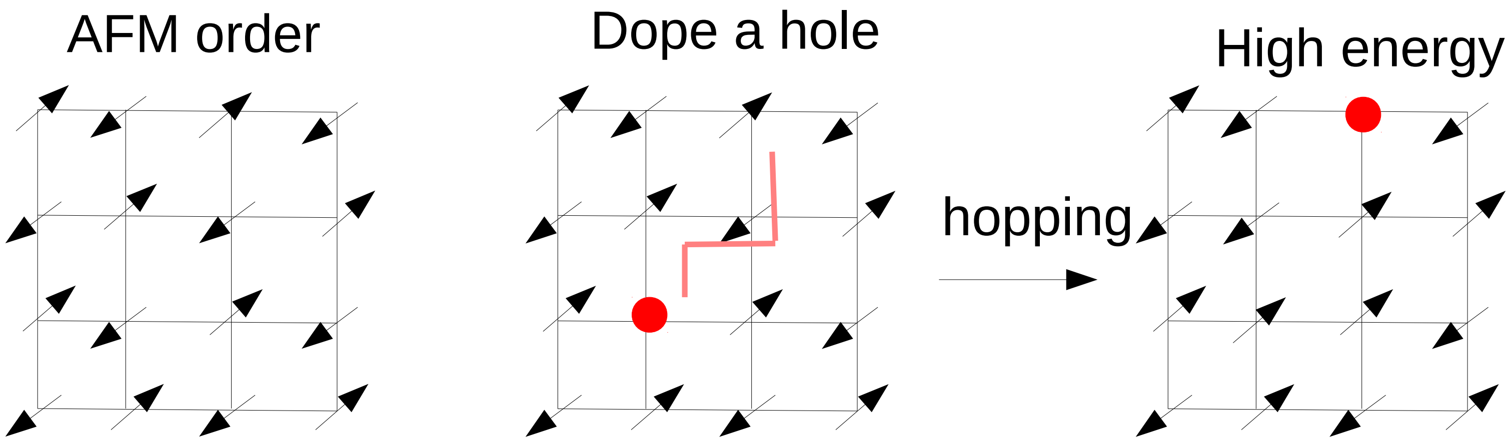
$$\hat{H} = -t \sum_{\langle ij \rangle \sigma} \left(\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \hat{c}^{\dagger}_{j\sigma} \hat{c}_{i\sigma} \right) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

too simple?

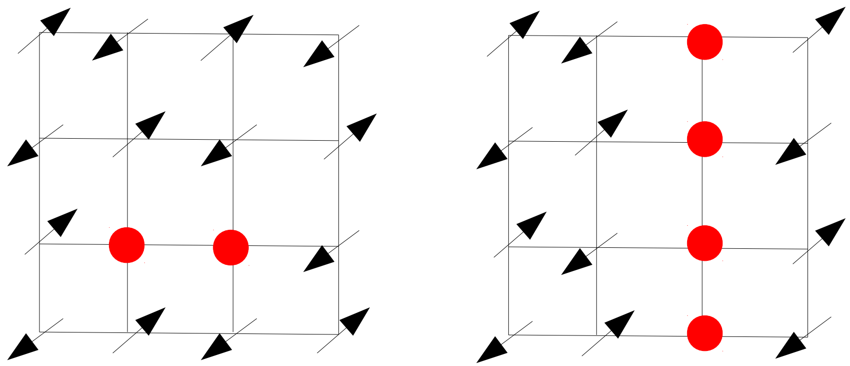
$$\hat{H} = -t \sum_{\langle ij \rangle \sigma} \left(\hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + \hat{c}^\dagger_{j\sigma} \hat{c}_{i\sigma} \right) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

- antiferromagnetism?
- pseudogap behavior? previous talks!
- in this talk: at *T*=0
  - presence of stripes?
  - presence of power-law *d*-wave superconducting correlations? („superconducting order“)
- „complexification“ of Hubbard model
  - *t’*=0: no next-nearest neighbor hopping
  - *t’* non-zero
- ultracold atom experiments cannot do $t' \neq 0$

naive picture of stripes & SC



- competition of hopping and interaction (AFM)
- lowering of energy by
  - correlated (pair) hopping (forming SC at low T)
  - stripe formation:
    high hole density
    low magnetic moment



cooperation or competition?

enormous amount of studies …

What is the ground state under doping?

uniform d-wave superconductor

[Gros, et al., PRB 38, 931 (1988)]

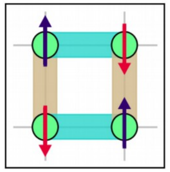
[Halboth, et al., PRL 85, 5162 (2000)]

[Maier, et al., PRL 95, 237001 (2005)]

[Sénéchal, et al., PRL 94, 156404 (2005)]

[Gull, et al., PRL 110, 216405 (2013)]

……...and a lot of more!

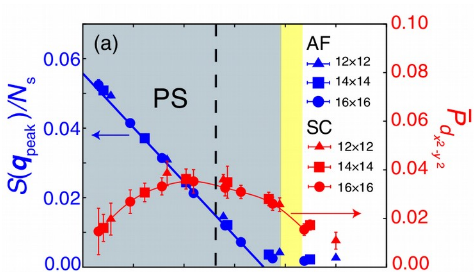


phase separation

[Misawa, et al., PRB 90, 115137 (2014)]

[Otsuki, et al., PRB 90, 235132 (2014)]

……...and a lot of more!



new orders: CDW+SDW

[Zaanen, et al., PRB 40, 7391 (1989)]

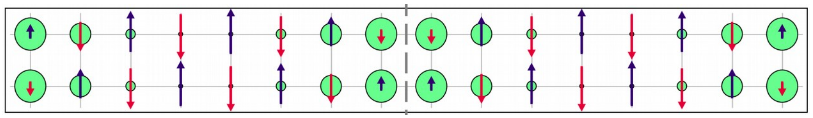
[Poilblanc, et al., PRB 39, 9749 (1989)]

[White, et al., PRL 91, 136403 (2003)]

[Hager, et al., PRB 71, 075108 (2005)]

[Chang et al., PRL 104, 116402 (2010)]

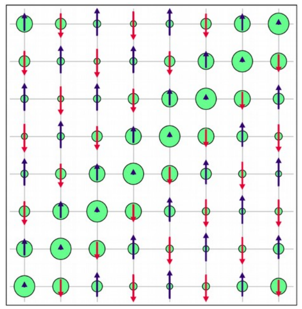
……...and a lot of more!



[Raczkowski, et al., Phys. Stat. Sol. 376 (2003)]

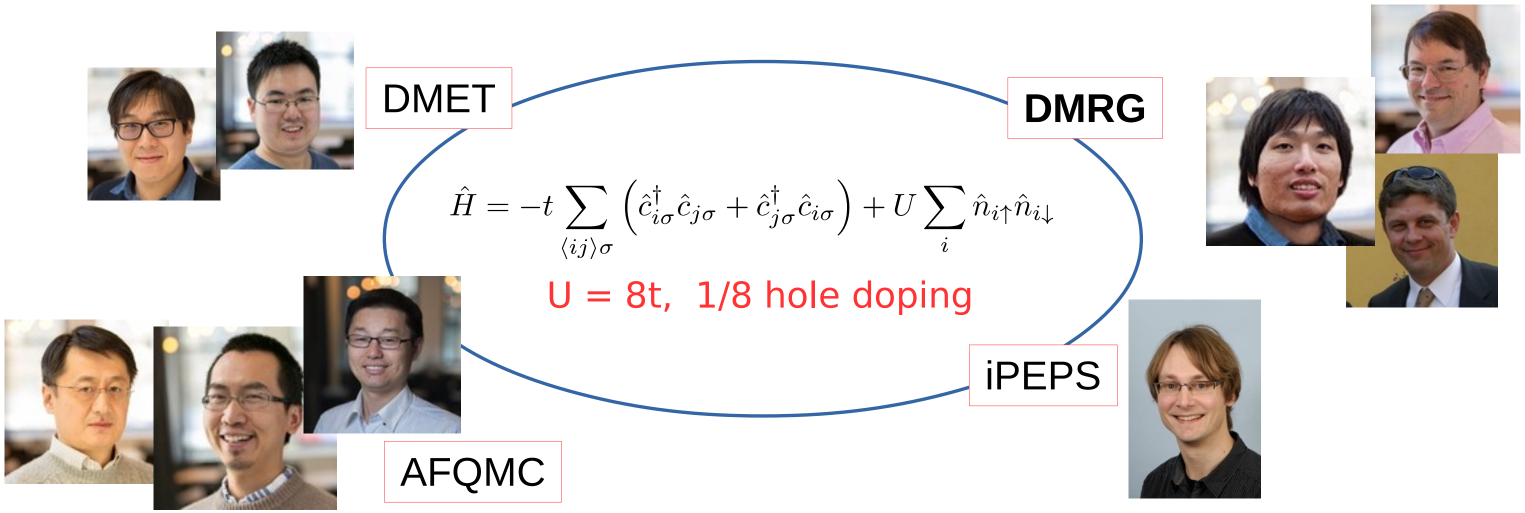
[Miyazaki, et al., J. Phys. Soc. Jpn. 73, 1643 (2004)]

……...and a lot of more!



back to the drawing board: t'=0

- each numerical method has its own methodological shortcomings
- believe only results where methods mutually support each other



(Zheng, Chung *et al.*, Science 358, 1155 (2017))

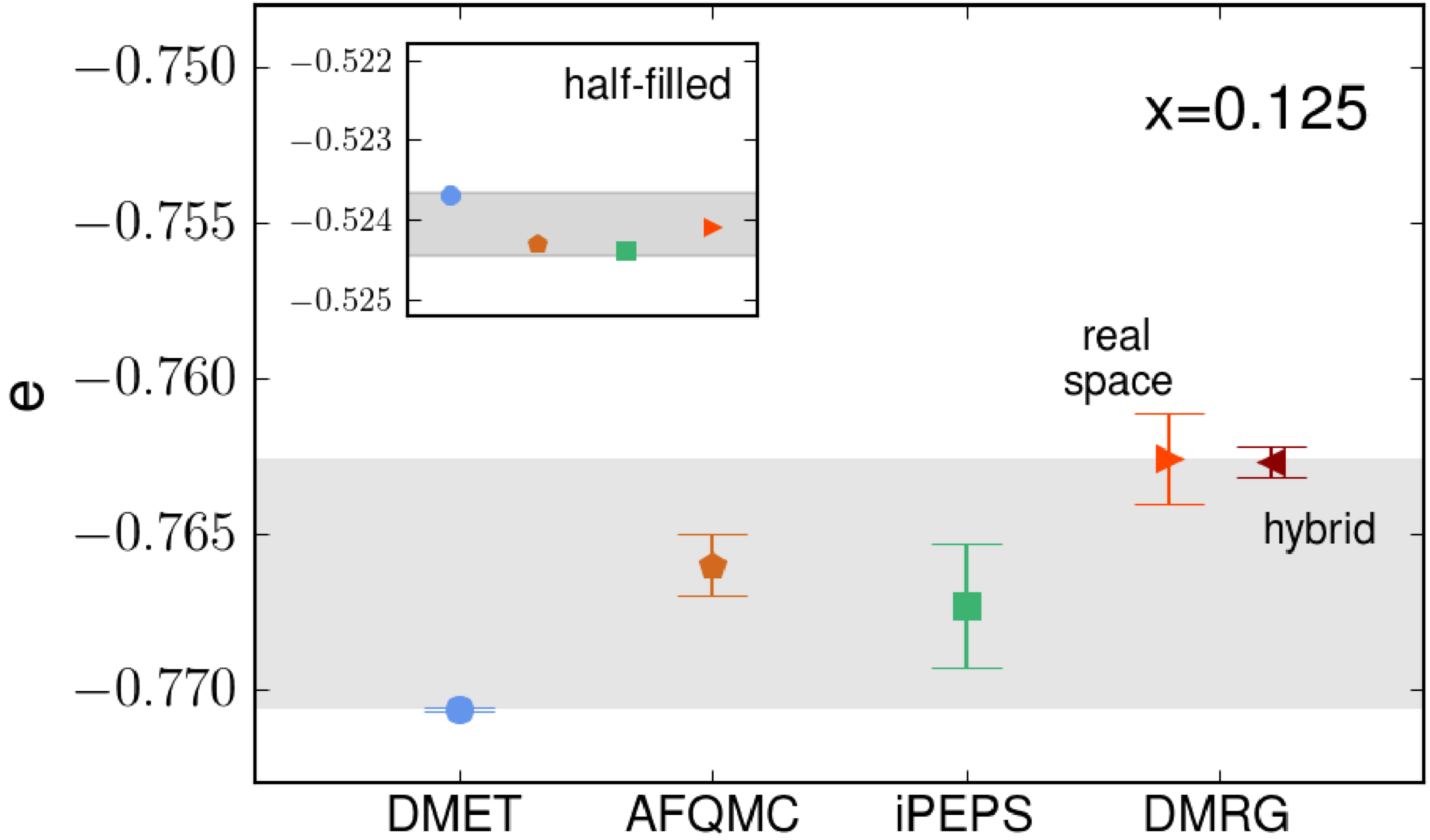
Simons Collaboration on the Many Electron Problem

methods overview

	variational	size	entanglement	preferred U/t	uncontrolled error
AFQMC	NO	finite	NO	small	constraint error
DMET	NO	∞	YES	small	cluster size
DMRG	YES	finite	YES	large	cylinder width
iPEPS	YES	∞	YES	large	cluster size

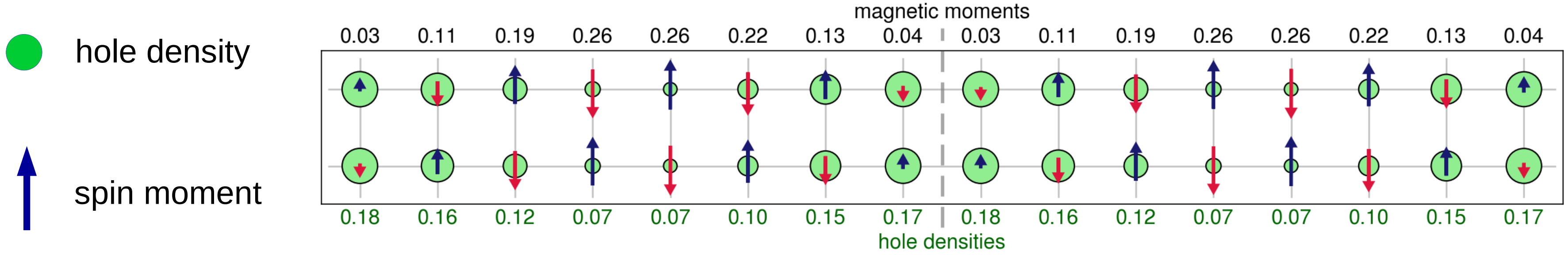
(Zheng, Chung *et al.*, Science 358, 1155 (2017))

ground state energies at doping 1/8

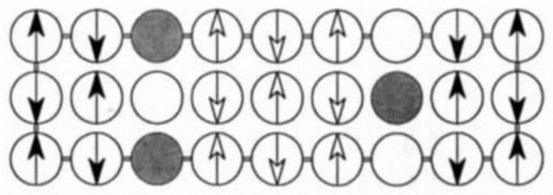


(Zheng, Chung *et al.*, Science 358, 1155 (2017))

stripe phase as ground state

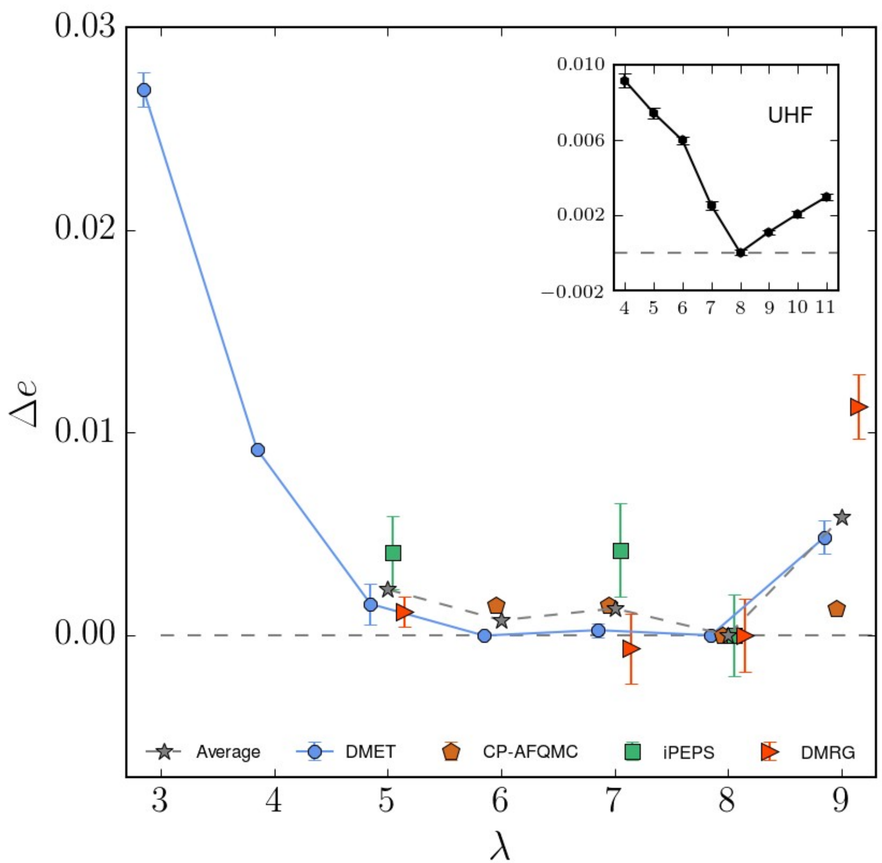


experiment: $\lambda = 4$ (half-filled stripe)



$La_{2-x}Sr_xCuO_4$

[Tranquada, Nature 375, 15 (1995)]



simulations:
almost degenerate stripes $\lambda = 5...8$

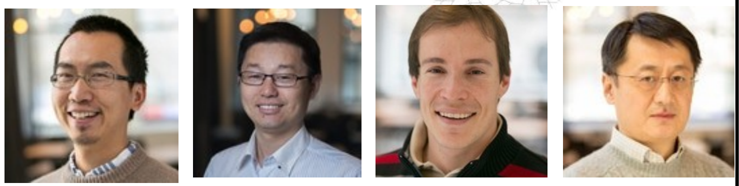
pure *d*-wave quite a bit higher in energy

„pure“ (t'=0) Hubbard model

- so far: focus on stripe order
- *d*-wave pairing order?
- superconducting correlations exist (power laws…)?
  - Yes:
    [Andrew S. Darmawan, et al., Phys. Rev. B 98, 205132 (2018)]
    [Vanhala, et al., PRB 97, 075112 (2018)]
    [Zhao, et al., PRB 96, 085103 (2017)]
    ...many more
  - No:
    [S. Zhang, et al., Phys. Rev. Lett. 78, 4486 (1997)]
    [M. Guerrero, et al., Phys. Rev. B 59, 1706 (1999)]
    [C. T. Shih, et al., Phys. Rev. Lett. 81, 1294 (1998)]
- stripes and SC: cooperation or competition?

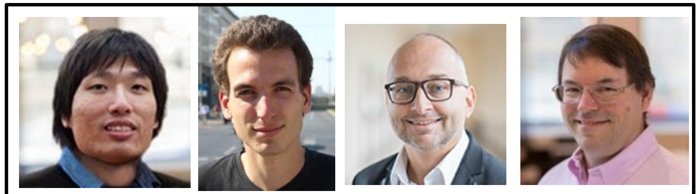
Simons Collaboration on the Many Electron Problem

AFQMC



Mingpu Qin H. Shi E. Vitali S. Zhang

DMRG



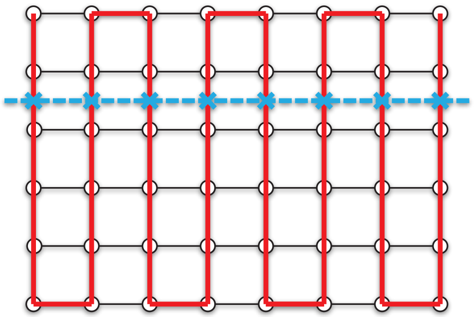
C.-M. Chung C. Hubig U. Schollwöck S.R. White

- AFQMC meets DMRG

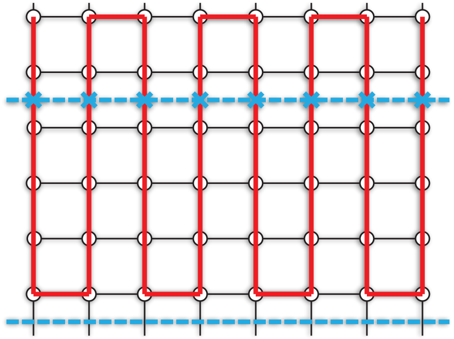
Qin, Chung, …, US, White, Zhang, arXiv:1910.08931

DMRG/MPS in two dimensions

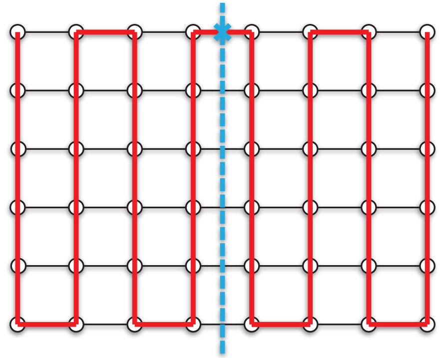
- map 2D lattice to 1D (vertical) „snake“ with long-ranged interactions



vertically OBC



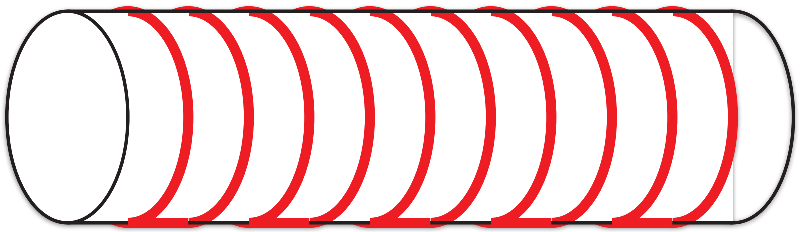
vertically PBC: extra cost!



$$\boxed{\begin{array}{l} S \sim \log_2 D \\ \to D \sim 2^L \end{array}}$$

- horizontally: ansatz obeys area law: easy axis, long at linear cost
- vertically: ansatz violates area law: hard axis, long at exponential cost
- consider long cylinders of **small** circumference c: mixed BC

circumference c



length L

AFQMC

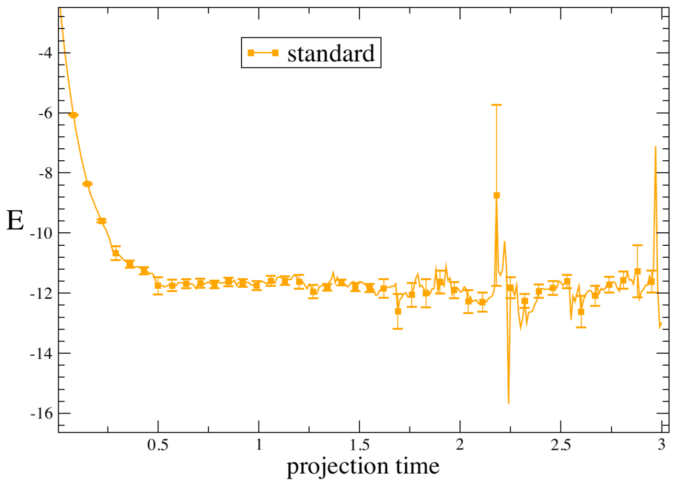
- ground state by imaginary time evolution of trial state

$$\frac{\langle 0|O|0\rangle}{\langle 0|0\rangle} = \lim_{\beta\to\infty} \frac{\langle \psi_T|\mathrm{e}^{-\beta H} O \mathrm{e}^{-\beta H}|\psi_T\rangle}{\langle \psi_T|\mathrm{e}^{-\beta 2H}|\psi_T\rangle}$$ using Slater determinants

- evolution requires quadratic Hamiltonian: Hubbard-Stratonovich!

$$\mathrm{e}^{-\Delta_\tau U n_\uparrow n_\downarrow} = \mathrm{e}^{-\Delta_\tau U (n_\uparrow + n_\downarrow - 1)} \sum_{\boxed{x=\pm 1}} \frac{1}{2} \mathrm{e}^{\gamma x (n_\uparrow + n_\downarrow - 1)}$$

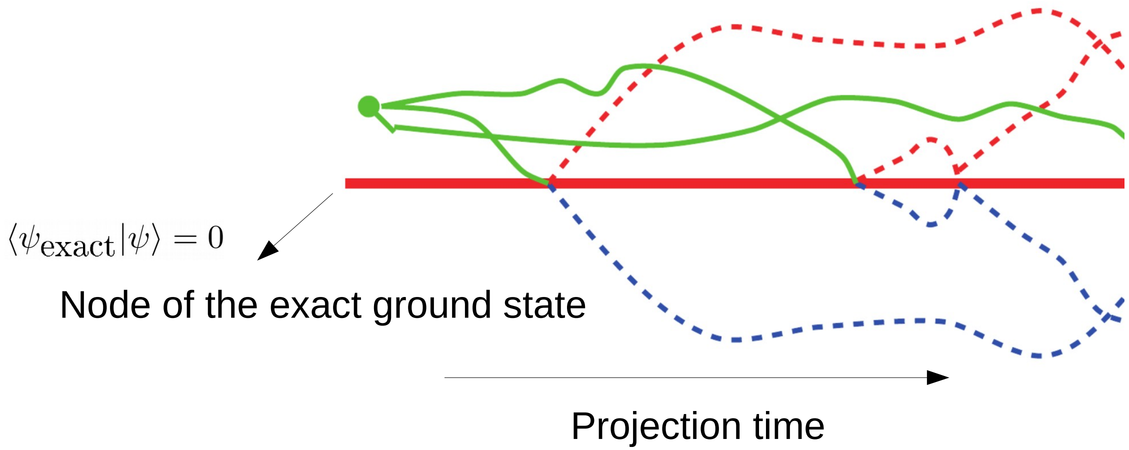
- auxiliary fields are sampled stochastically: quantum Monte Carlo!



4 x 4, n = 0.875, U = 8

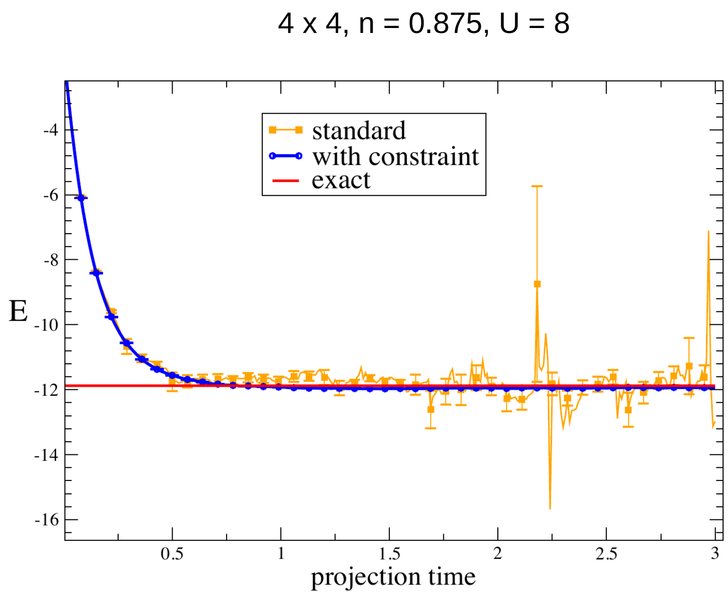
- **sign problem!!!**

constrained path-AFQMC



- sign problem:
  exact analytical cancellation
  not captured by sampling

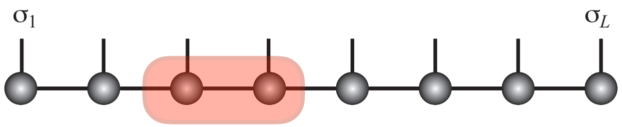
- keep only the positive-weight paths (constrained path)
- approximate nodal structure by trial wave function

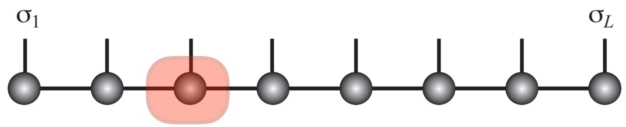


Zhang, Carlson, Gubernatis, PRL 1995

algorithmic improvements and checks

- single-site DMRG: approximately 4x more efficient





  - convergence to true state — Hubig, McCulloch, US, Wolf, PRB 2015
  - error monitoring: two-site variance — Hubig, Haegeman, US, PRB 2018

- CP-AFQMC
  - BCS-type trial wave function — Vitali, Rosenberg, Zhang, PRA 2019
  - OP from total energy calculations

- our strategy
  - quasiexact DMRG results on cylinders up to width 6 check AFQMC
  - AFQMC then taken to the “thermodynamic limit“

what we measure

- apply bulk (global) pairing field and observe pairing response

$$\hat{\Delta}_{ij} \equiv (\hat{c}_{i\uparrow}\hat{c}_{j\downarrow} - \hat{c}_{i\downarrow}\hat{c}_{j\uparrow})/\sqrt{2}$$

nearest-neighbor pairing

$$\Delta_{ij} = \langle \hat{\Delta}_{ij} + \hat{\Delta}^{\dagger}_{ij} \rangle / 2$$

pairing order parameter

$$H_p = -\sum_{\langle ij \rangle} h_p^{ij} \frac{1}{2} \left(\hat{\Delta}_{ij} + \hat{\Delta}^{\dagger}_{ij} \right)$$

bulk pairing field taken to zero

- apply boundary (edge) pairing field and observe decay of pairing in bulk

$$H_p = -\sum_{\langle ij \rangle} h_p^{ij} \frac{1}{2} \left(\hat{\Delta}_{ij} + \hat{\Delta}^{\dagger}_{ij} \right)$$

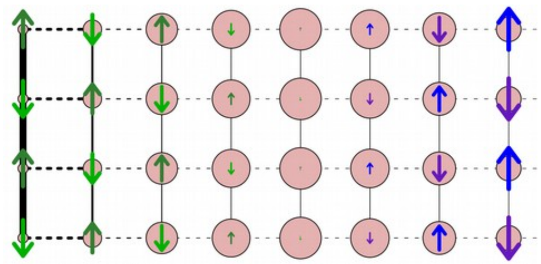
only on edge

- calculate decay of pair-pair correlations

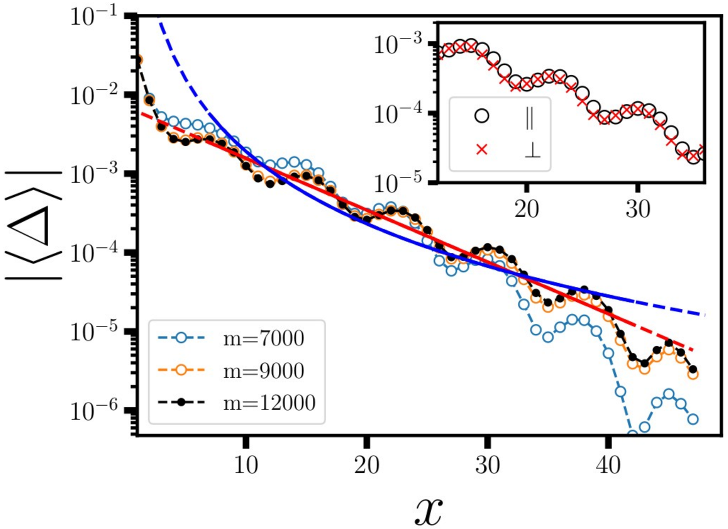
$$P_{i'j',ij} = \langle \hat{\Delta}^{\dagger}_{i'j'} \hat{\Delta}_{ij} \rangle$$

bulk decay and correlation decay

- edge pairing field



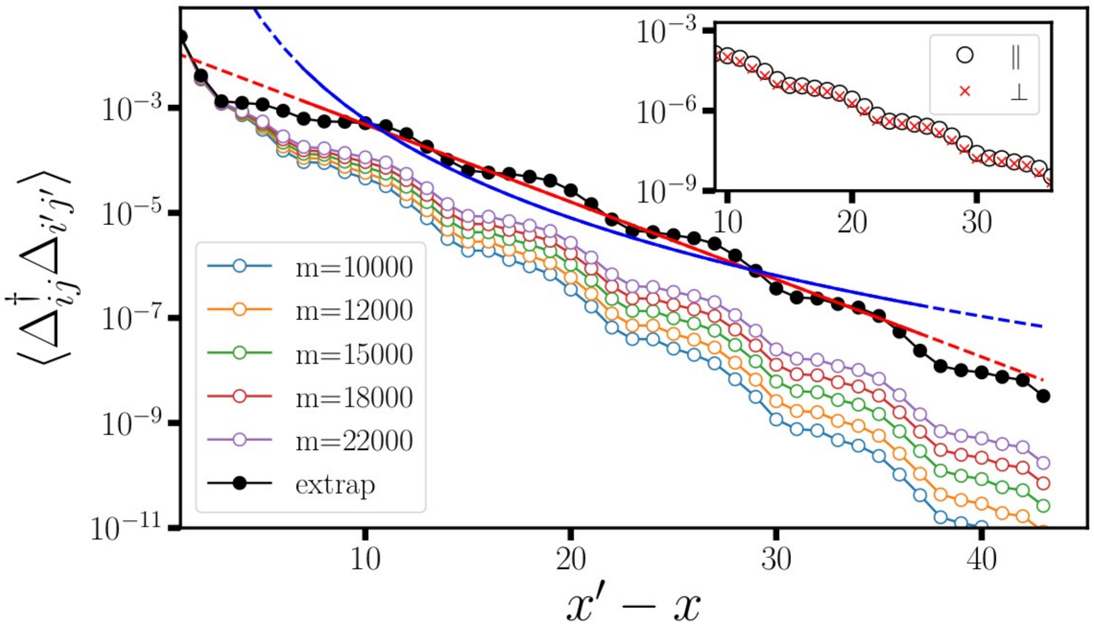
48x4



$$\hat{\Delta}_{ij} \equiv (\hat{c}_{i\uparrow}\hat{c}_{j\downarrow} - \hat{c}_{i\downarrow}\hat{c}_{j\uparrow})/\sqrt{2}$$

- pair-pair correlations (no field)

48x6

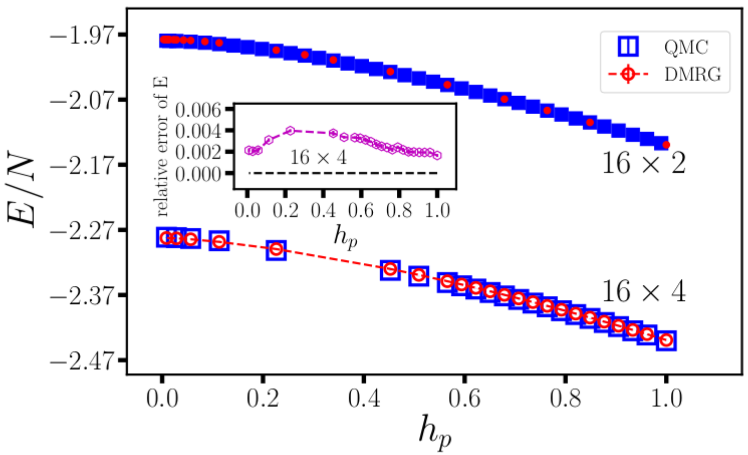


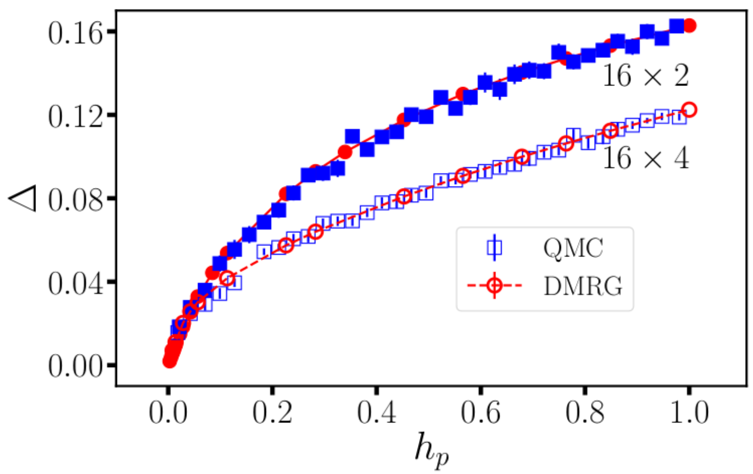
$$\langle \hat{\Delta}^\dagger_{i'j'} \hat{\Delta}_{ij} \rangle$$

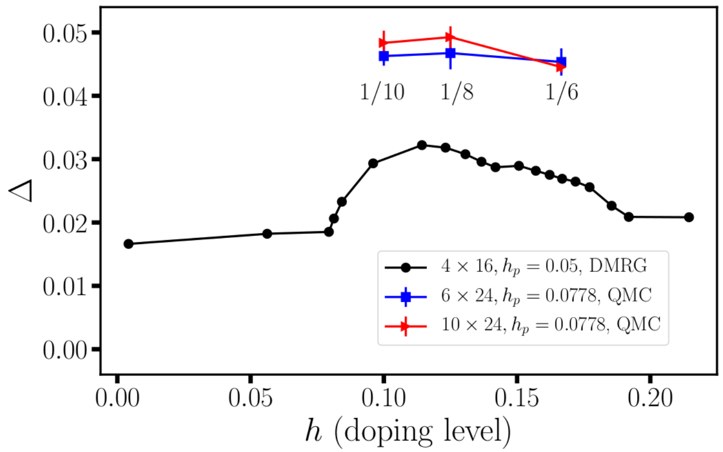
up to 70,000 DMRG states
(SU(2) reps vs. U(1))

bulk pairing field: AFQMC/DMRG

- ground state energies of cylinders with applied pairing fields
- pairing correlator via Hellmann-Feynman theorem (derivative)



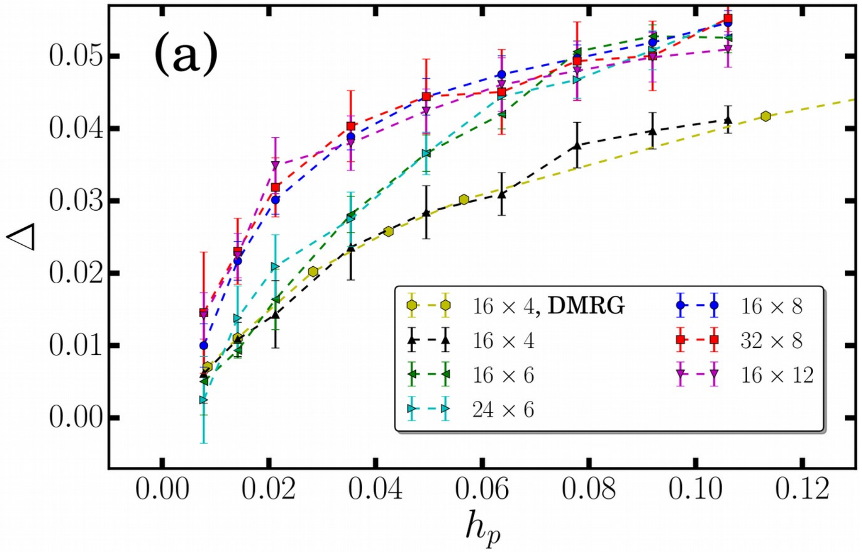




- response to pairing field strongest around doping 1/8

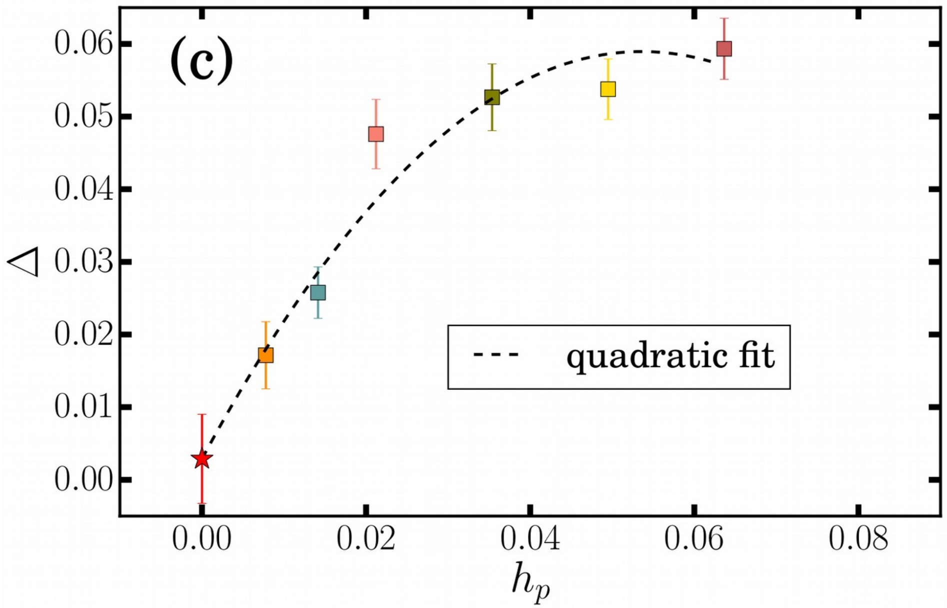
bulk pairing fields

finite sizes



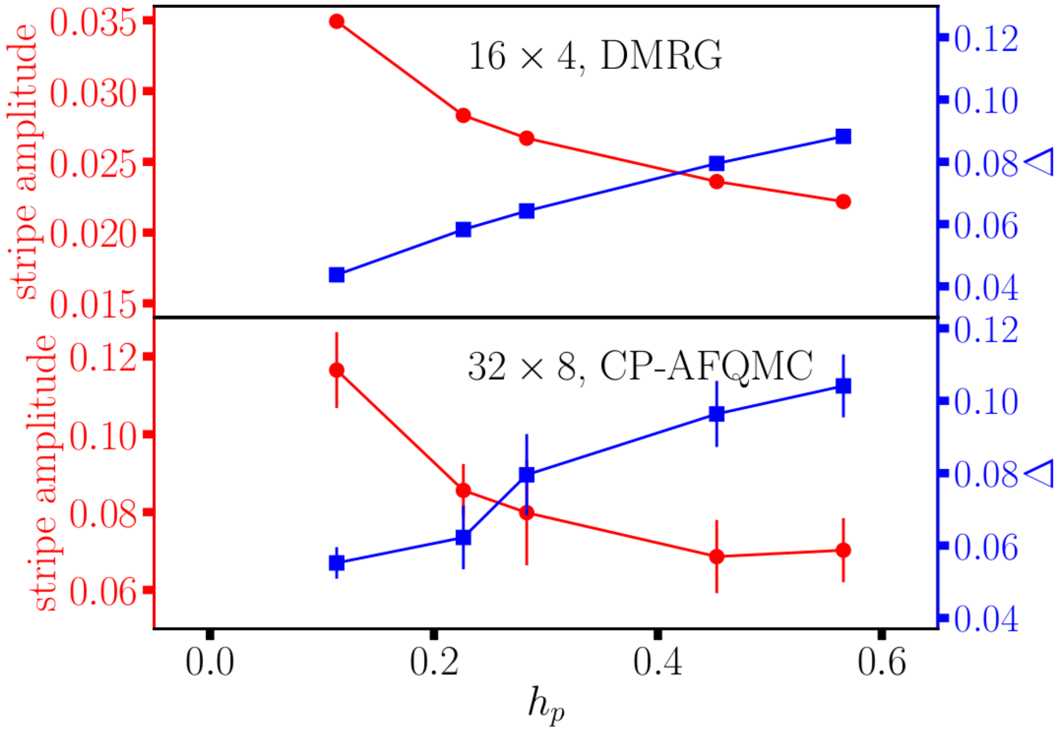
- order of extrapolations matters
  - for each pairing field, take TD limit
  - then take field to zero

thermodynamic limit



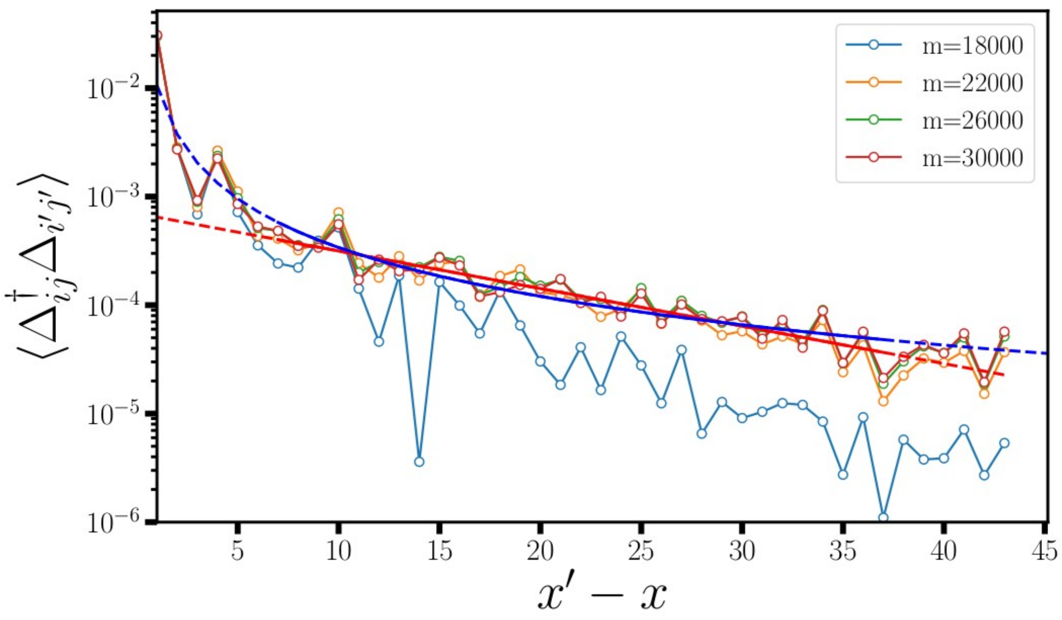
- no pairing order survives

stripe vs pairing: in competition



- stronger pairing due to pairing field suppresses stripe amplitude

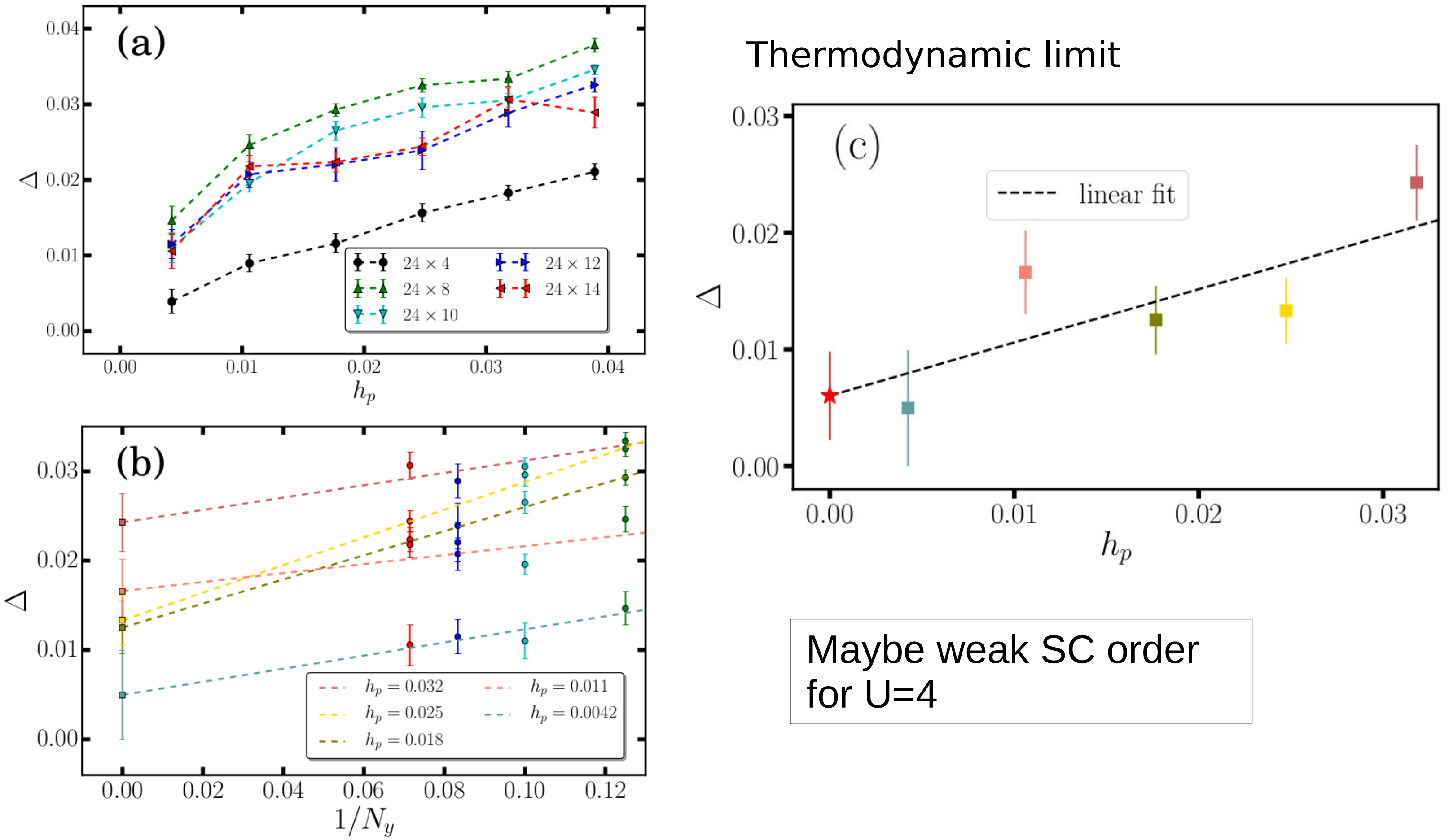
U=4, doping 1/8



- pair-pair correlation on 48x4 cylinder
- stripe order disappears (not shown)
- both exponential and power-law reasonable

U=4, doping 1/8

Thermodynamic limit



Maybe weak SC order for U=4

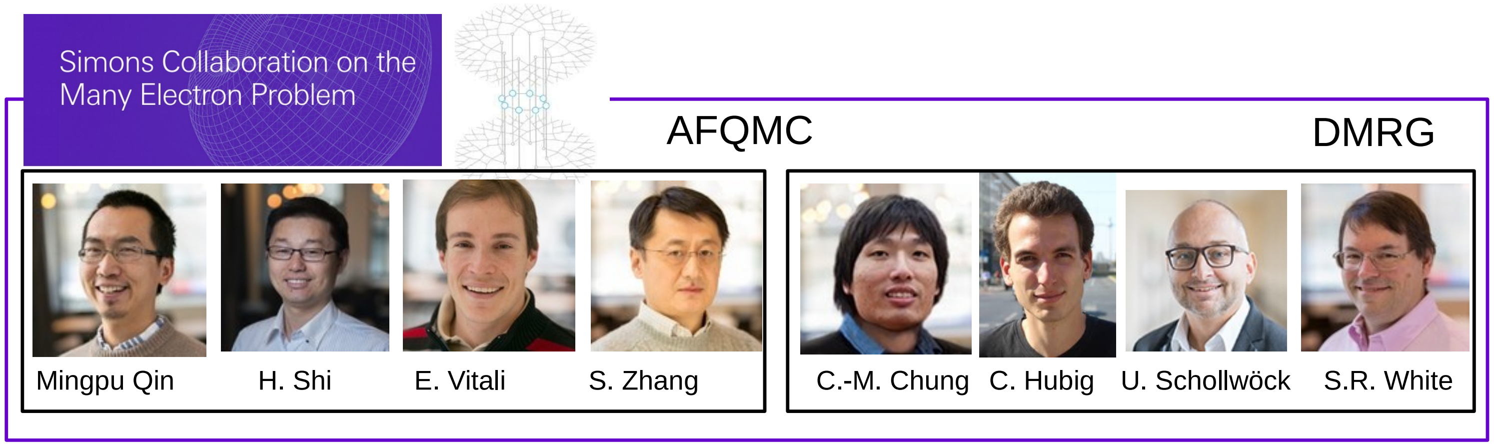
- bulk pairing fields

t'=0 summary

- U=8, doping 1/8:
  - period 8 stripes
  - *d*-wave pairing
  - no long-ranged superconductivity
- U=4, doping 1/6:
  - no stripes
  - possibly very weak superconductivity

switching on *t'*

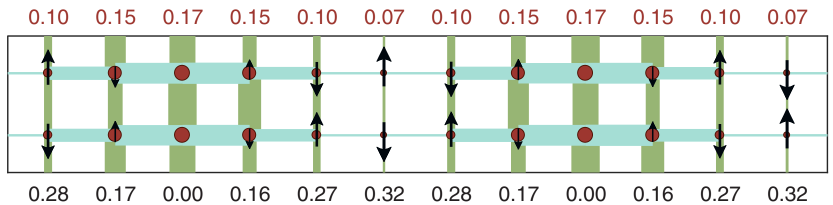
- electronic structure suggests weak negative *t'* (-0.2, -0.25, -0.33,…)
- does it generate power-law SC correlations?



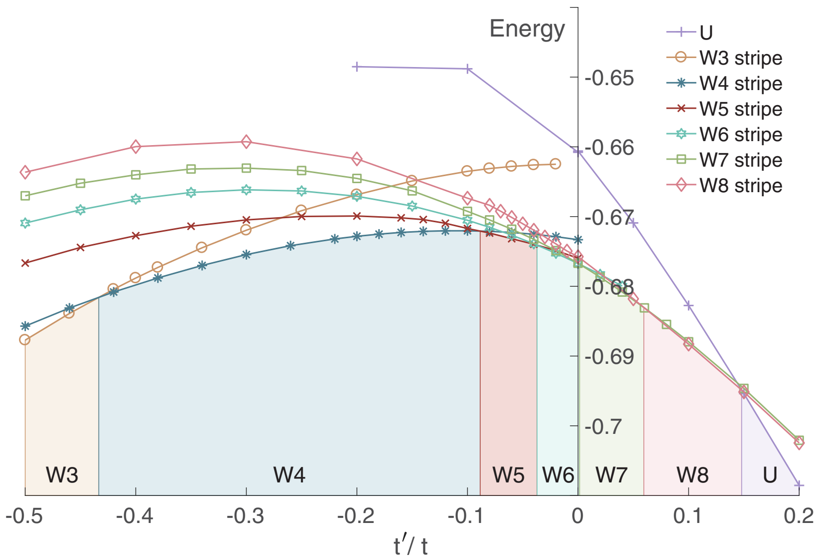
our DMRG/AFQMC results:
Qin, Chung, …, US, White, Zhang, work in progress …

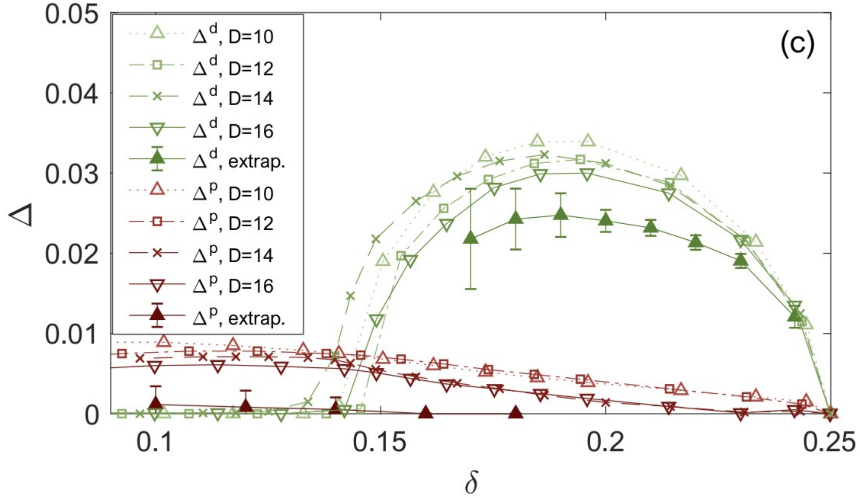
iPEPS at t'=-0.2

Ponsioen, Chung, Corboz, PRB 100, 195141 (2019)



- supercells embedded in TD limit
- bias results: stabilize different phases

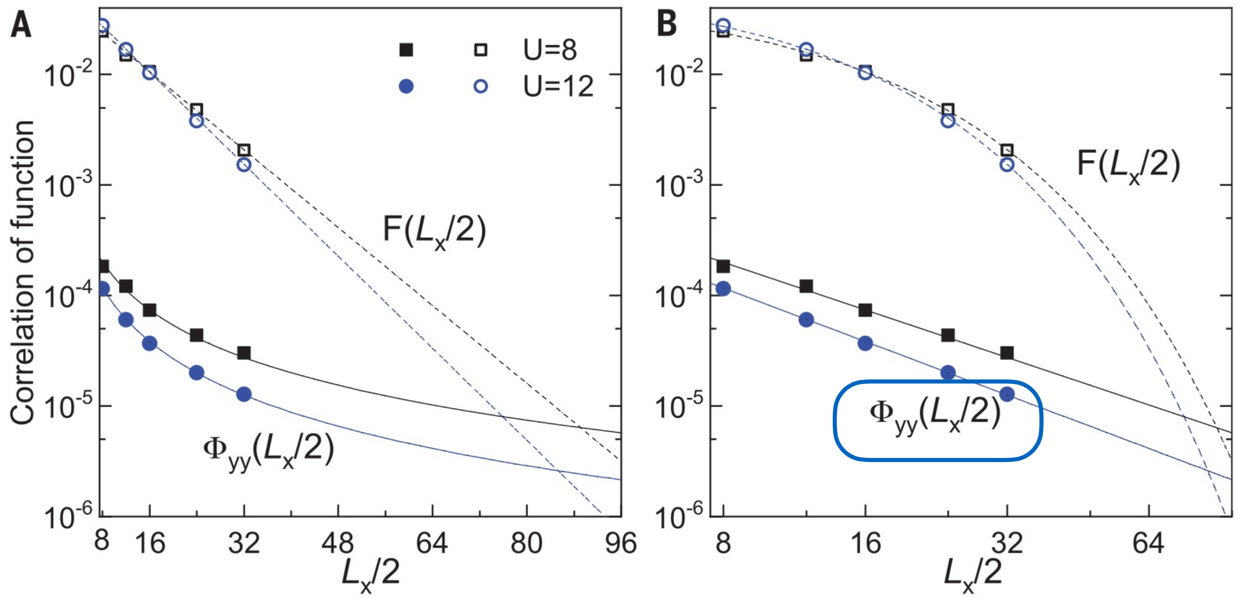




- period 4 stripes over wide range of t'
- U=10, doping 1/8
- d-wave pairing at doping > 0.14

DMRG on width-4 cylinders: t'=-0.25

Hong-Chen Jiang *et al.*, Science 365, 1424 (2019)

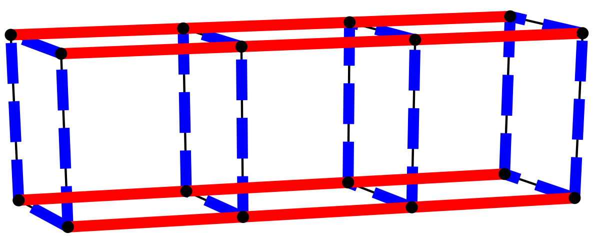


- *U*=8, *U*=12, doping 1/8
- period 4 stripes
- power-law decay of pair-pair correlations

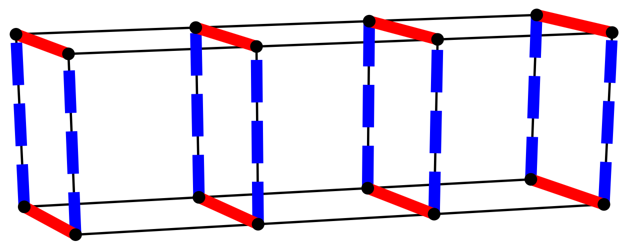
the special topology of width-4

White, Scalapino - late nineties …

- Orwell, *Animal Farm:* „Four legs good, two legs bad“
- really?



cylinder / surface *d*-wave
two-dimensional nature



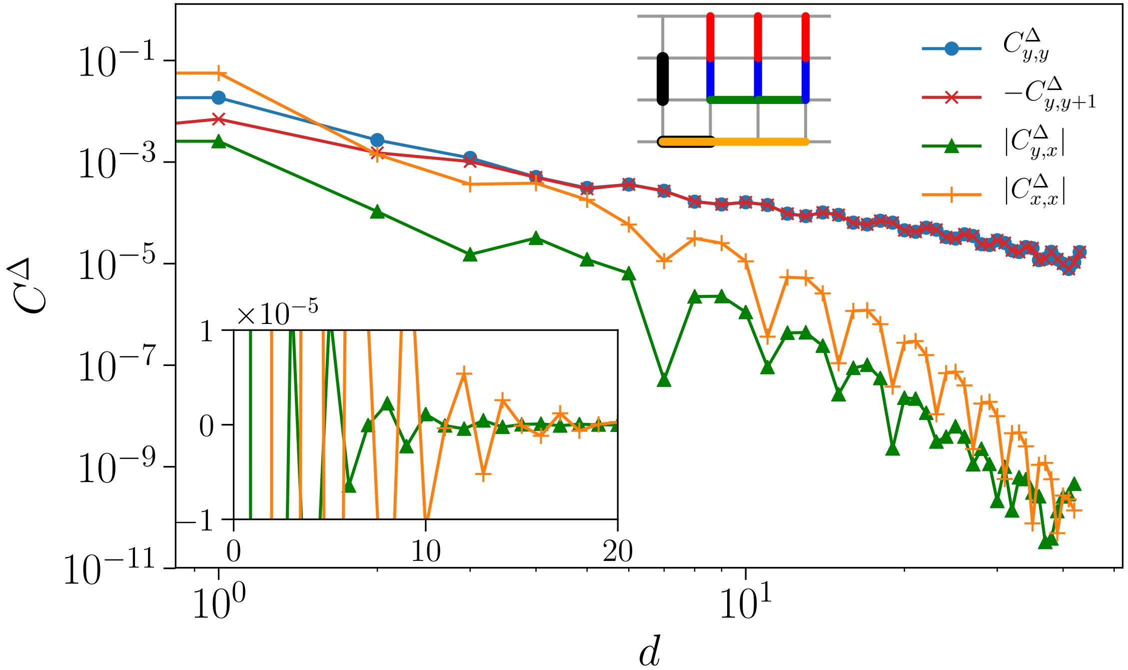
plaquette *d*-wave
one-dimensional nature

- two competing types of *d*-wave pairing correlations feasible
- only one of them relevant for the TD limit in 2D

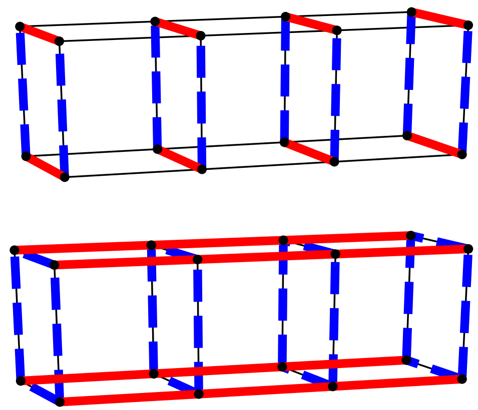
distinguishing *d*-wave correlations

(Chia-Min Chung, US, Steve White)

- U=8, t'=-0.25, doping 1/8
- decay of pair-pair correlations $\langle \Delta^\dagger_{i'j'} \Delta_{ij} \rangle$



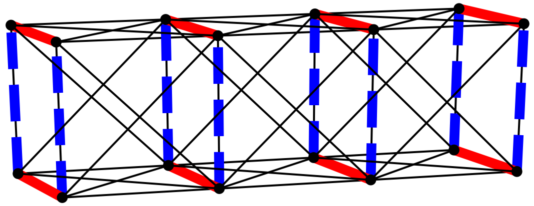
plaquette: power-law

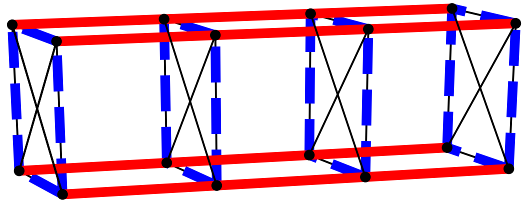


surface: exponential

- width-4 cylinder power-law decay one-dimensional effect …

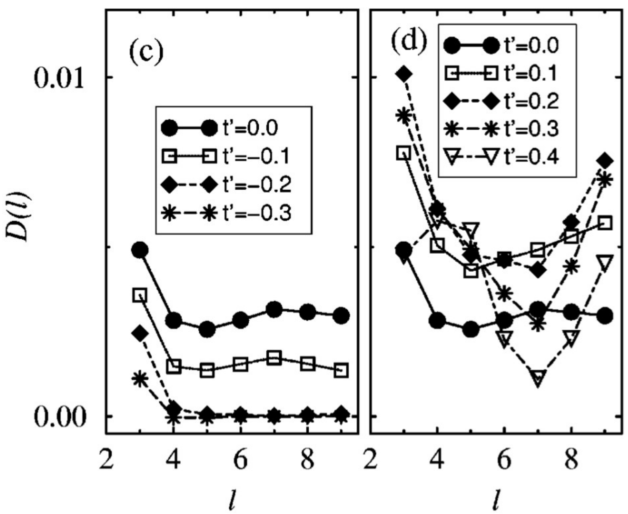
„asymmetry“ in t'<0

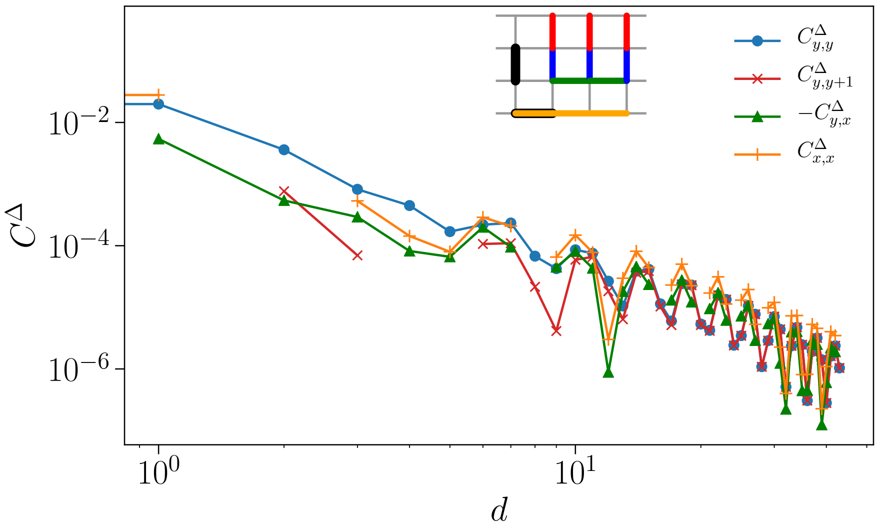




- t'<0(>0) suppresses (enhances) *d*-wave correlations
- t'<0 on stack plaquettes favors „surface“ SC

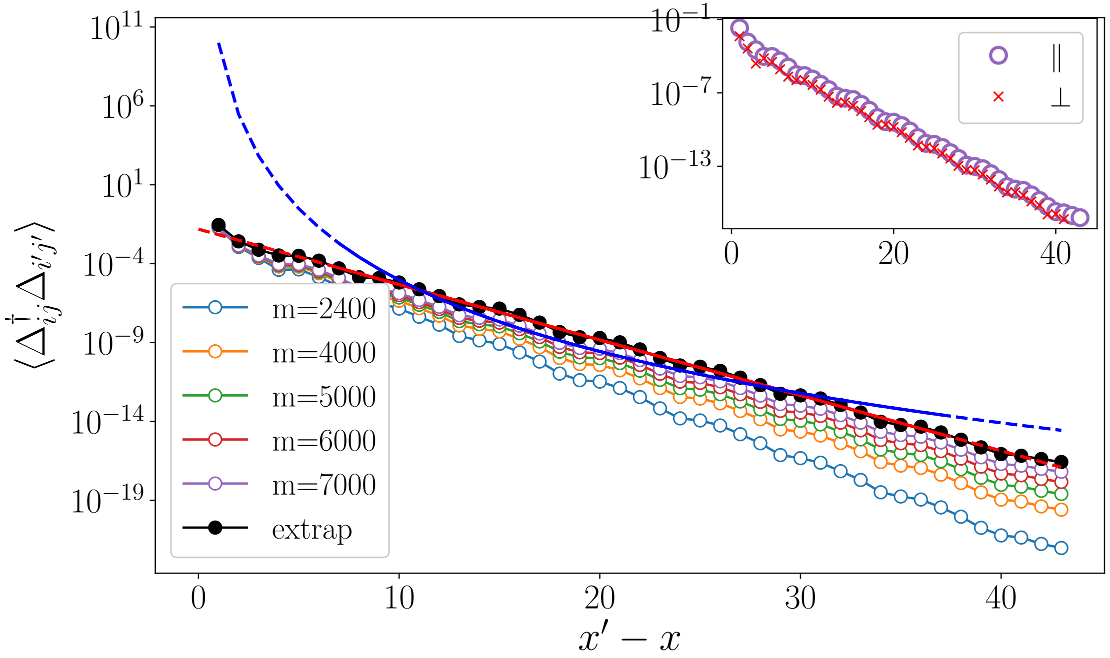
[Steven R. White, PRB.60.R753 (1999)]





width-6 cylinders

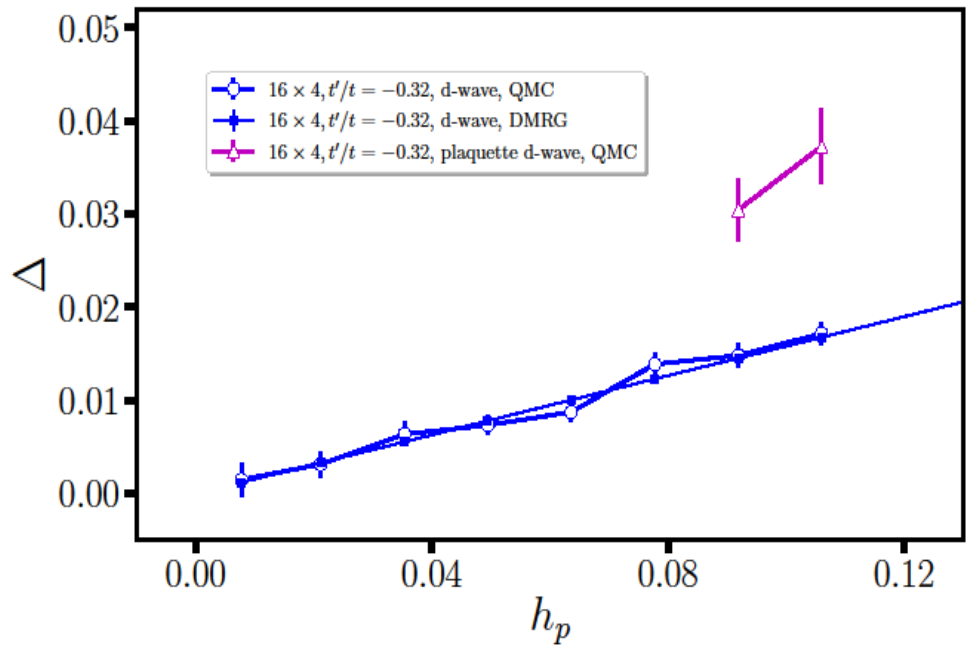
- Orwell, *Animal Farm* (adapted) „Six legs good, four legs bad"



- U=8, t'=-0.25, doping 1/8
- decay of pair-pair correlations $\langle \Delta^\dagger_{i'j'} \Delta_{ij} \rangle$ looks exponential

DMRG and AFQMC

- philosophy: only believe consistent results from several methods
- again, building the DMRG-AFQMC connection
  - four legs: excellent



response of pairing to pairing field

  - six legs: disagreement! currently exploring why … to be continued!

conclusion

- adopt philosophy:
  only believe consistent results from several methods
- pure (t'=0) Hubbard model shows period 8 [5…8] stripes
- pure (t'=0) Hubbard model does not show *d*-wave SC for experimentally relevant parameters
- seems insufficient model for high-Tc: cold atom experiments!

- switch on t'<0:
  - iPEPS finds period 4 stripes, pairing order (for larger doping)
  - DMRG results for width 4 cylinders probably irrelevant
  - DMRG/AFQMC comparisons not consistent so far