High *Tc* superconductivity in the Hubbard model revisited

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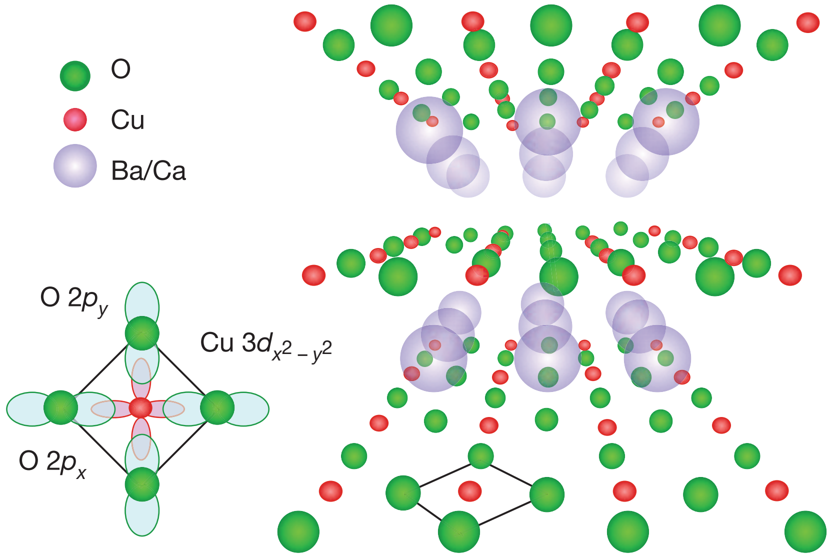
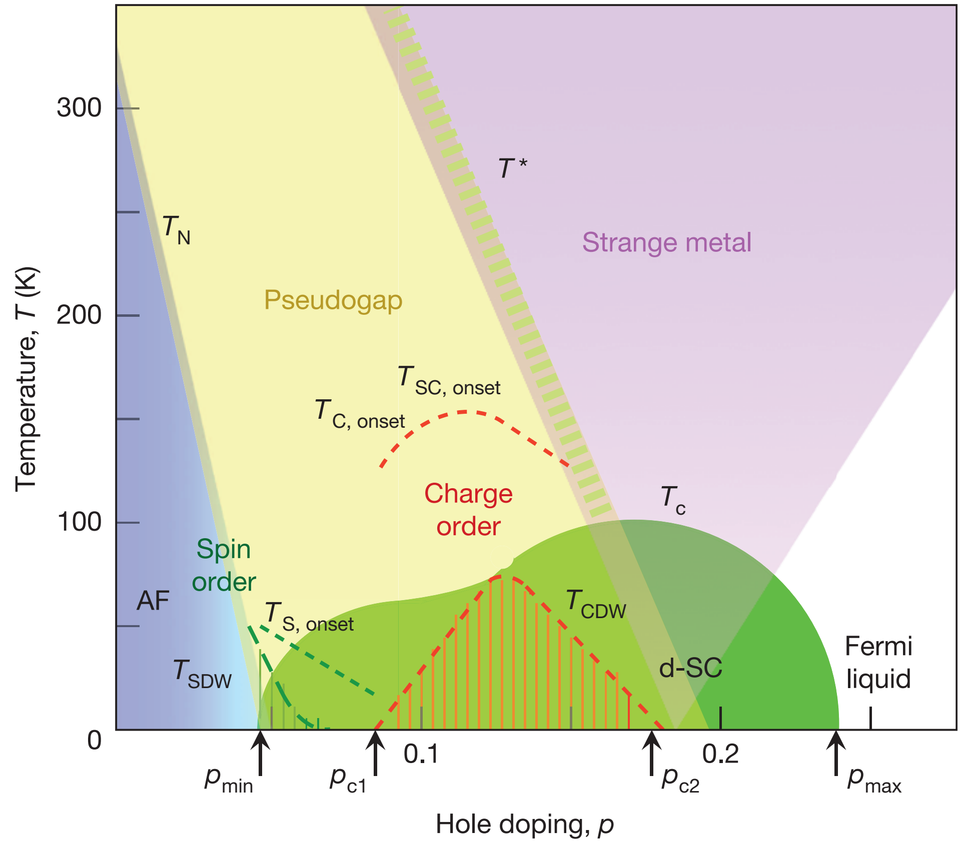
high-temperature superconductors



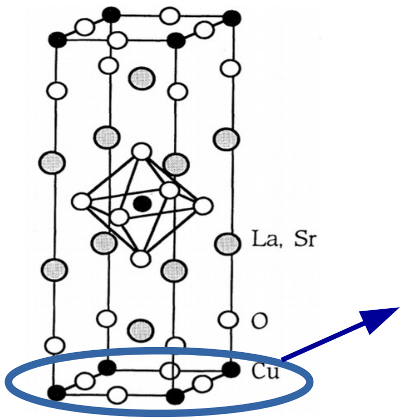


- typical structure
- generic phase diagram

(Keimer *et al.*, Nature 15)

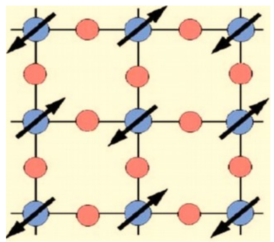
modeling high-Tc SCs

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



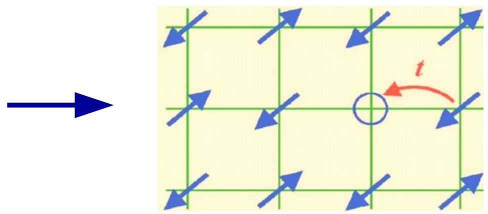
[RevModPhys.66.763]

Three-band



[RevModPhys.78.17]

Single-band



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?

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

- (too) many features!
- in this talk: at *T*=0
  - presence of stripes?
  - presence of power-law *d*-wave superconducting correlations? („superconducting order“)
- two step „complexification“ of Hubbard model
  - *t*'=0: no next-nearest neighbor hopping
  - *t*' non-zero
  - ultracold atom quantum simulation challenge: $t' \neq 0$

enormous amount of studies …

What is the ground state under doping?

uniform d-wave superconductor

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

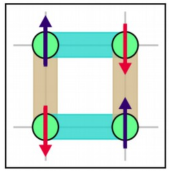
[Halboth, et al., PRL 85, 5162 (2000)]

[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!

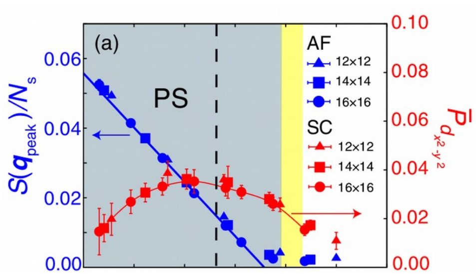


phase separation

[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)]

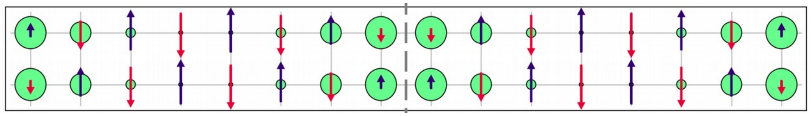
[Poilblanc, et al., PRB 39, 9749 (1989)]

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

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

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

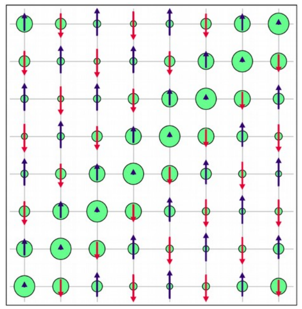
……...and a lot of more!



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

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

……...and a lot of more!

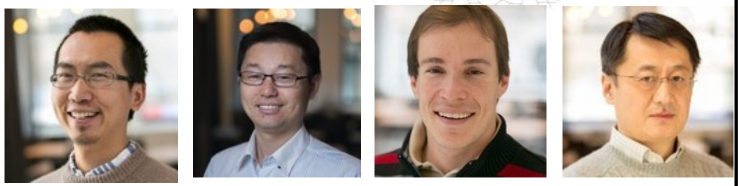


„pure“ (t'=0) Hubbard model

- many-electron collaboration: 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?

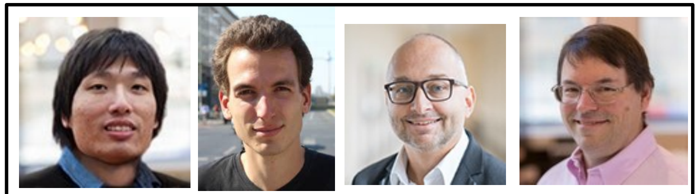
Simons Collaboration on the Many Electron Problem

AFQMC



Mingpu Qin H. Shi E. Vitali S. Zhang

DMRG



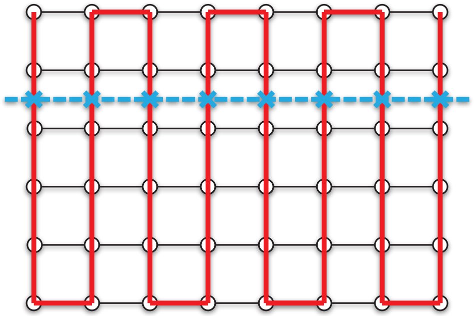
C.-M. Chung C. Hubig U. Schollwöck S.R. White

- AFQMC meets DMRG

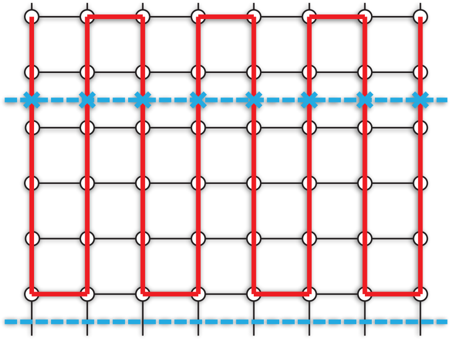
Qin, Chung, …, US, White, Zhang, PRX 10, 031016 (2020)

DMRG/MPS in two dimensions

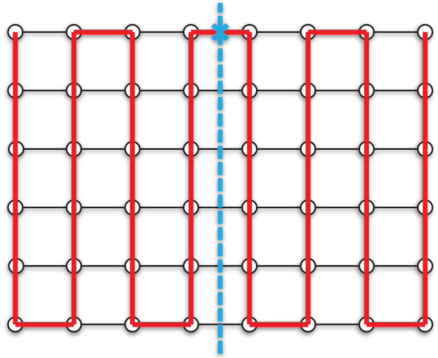
- map 2D lattice to 1D (vertical) „snake" with long-ranged interactions



vertically OBC



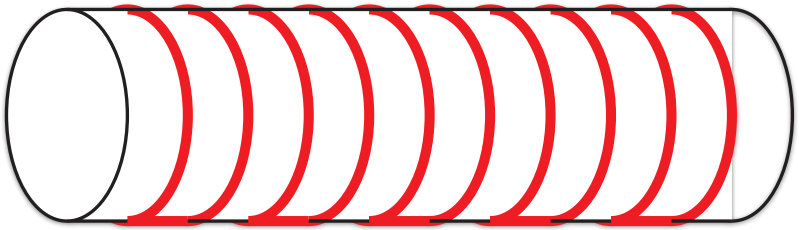
vertically PBC: extra cost!



$$S \sim \log_2 D \\ \rightarrow D \sim 2^L$$

- 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

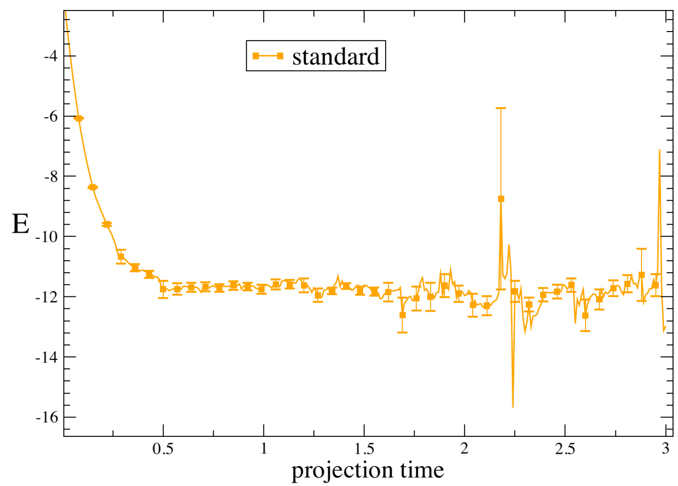
- ground state by imaginary time evolution of trial state

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

- evolution requires quadratic Hamiltonian: Hubbard-Stratonovich!

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

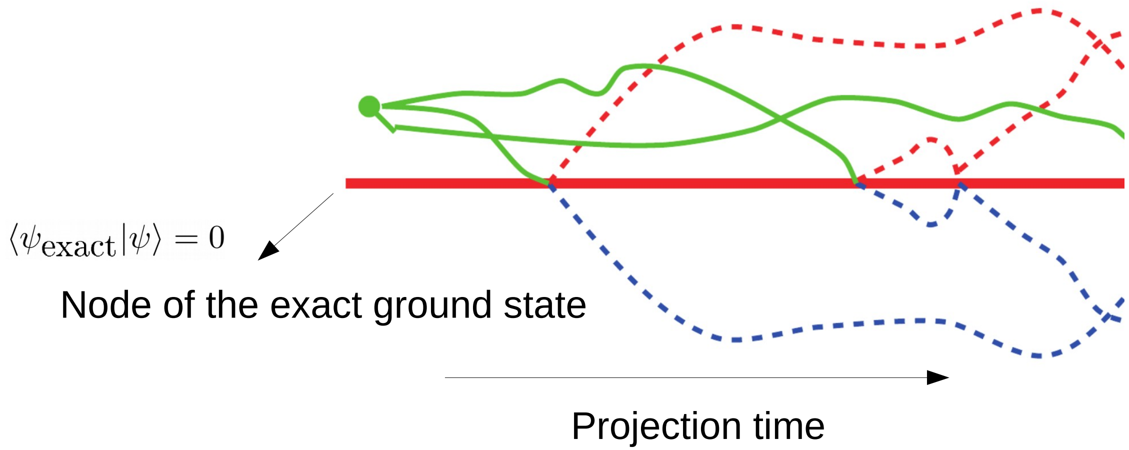
- auxiliary fields are sampled stochastically: quantum Monte Carlo!



4 x 4, n = 0.875, U = 8

- **sign problem!!!**

constrained path-AFQMC

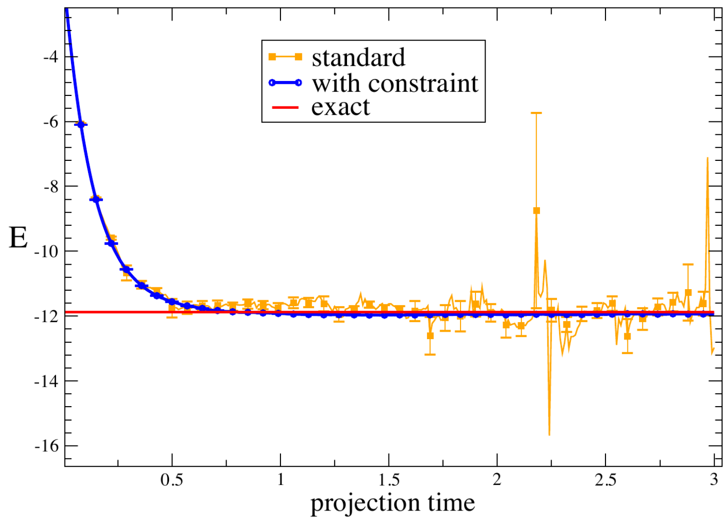


- sign problem:
  exact analytical cancellation
  not captured by sampling

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

Zhang, Carlson, Gubernatis, PRL 1995

4 x 4, n = 0.875, U = 8



what we measure

- apply bulk (global) *d*-wave 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 OP

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

bulk pairing field taken to zero

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

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

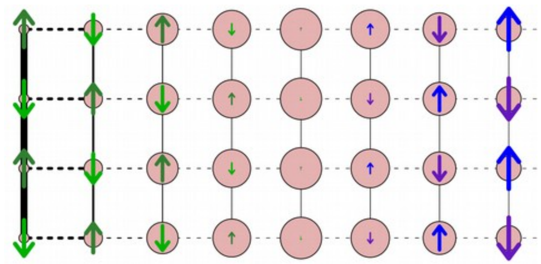
only on edge

- calculate decay of pair-pair correlations

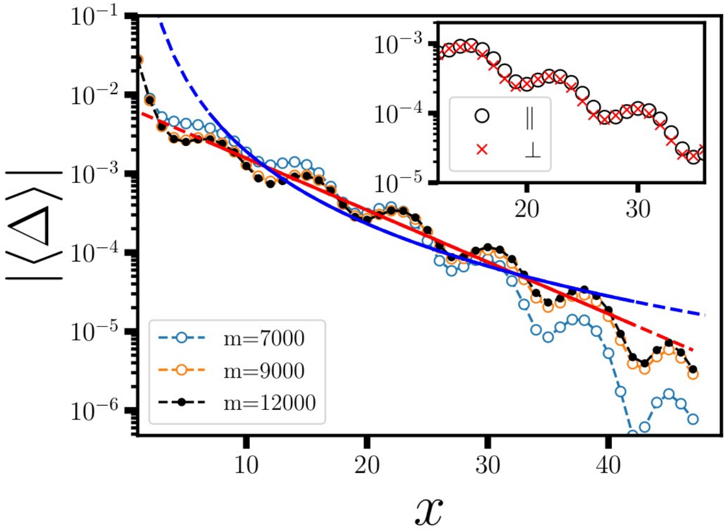
$$P_{i'j',ij} = \langle \hat{\Delta}^{\dagger}_{i'j'} \hat{\Delta}_{ij} \rangle$$

bulk decay and correlation decay

- edge pairing field



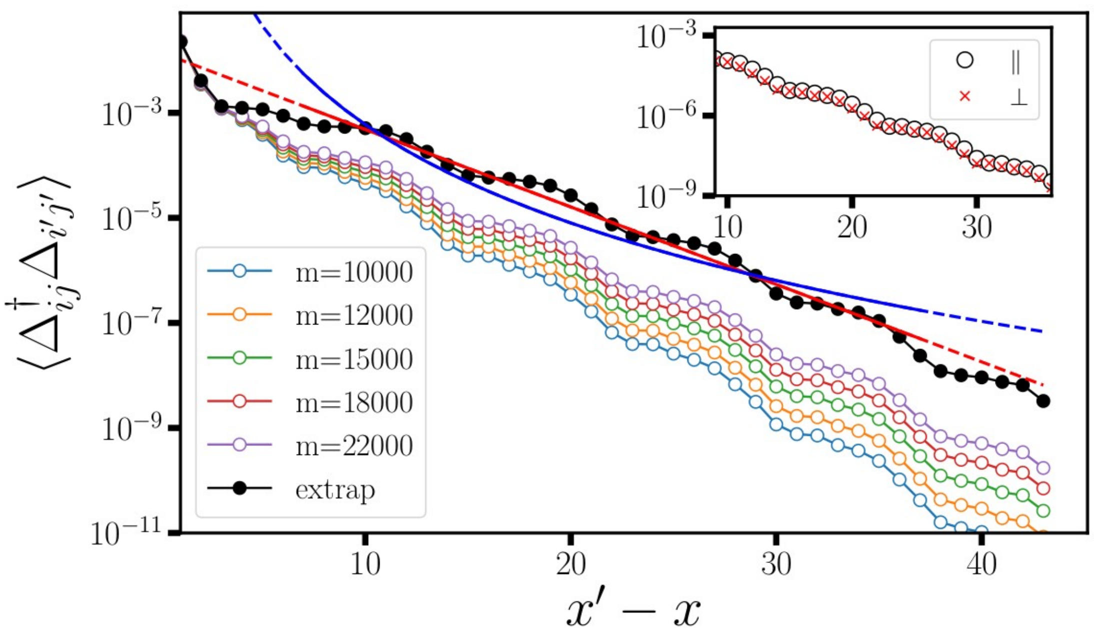
48x4



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

- pair-pair correlations (no field)
- U=8, doping 1/8

48x6

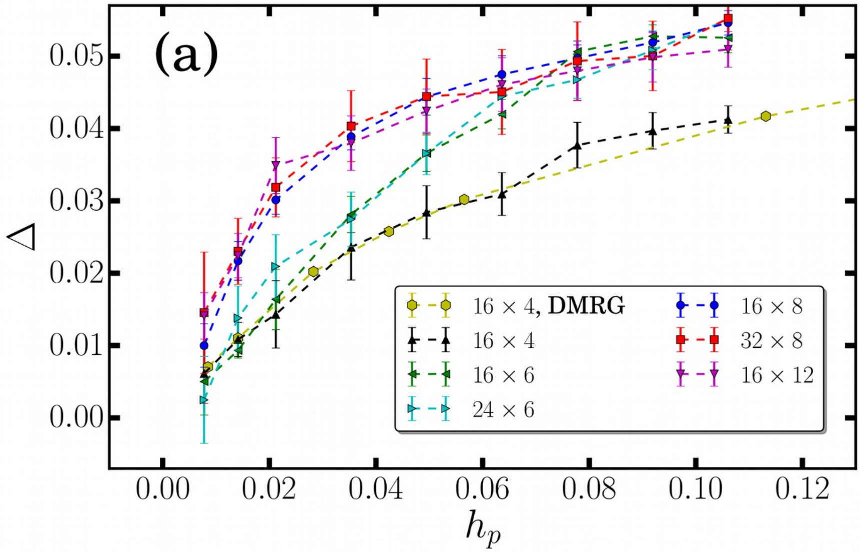


$\langle\hat{\Delta}^{\dagger}_{i'j'}\hat{\Delta}_{ij}\rangle$

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

bulk pairing fields

finite sizes

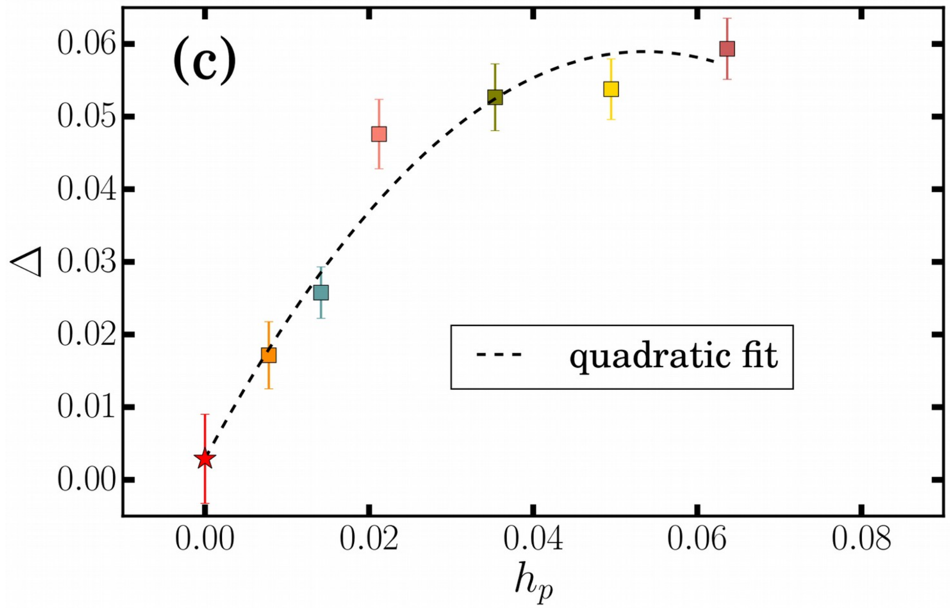


- order of extrapolations matters
  - for each pairing field, take TD limit
  - then take field to zero

- U=8, doping 1/8

- no pairing order survives

thermodynamic limit



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

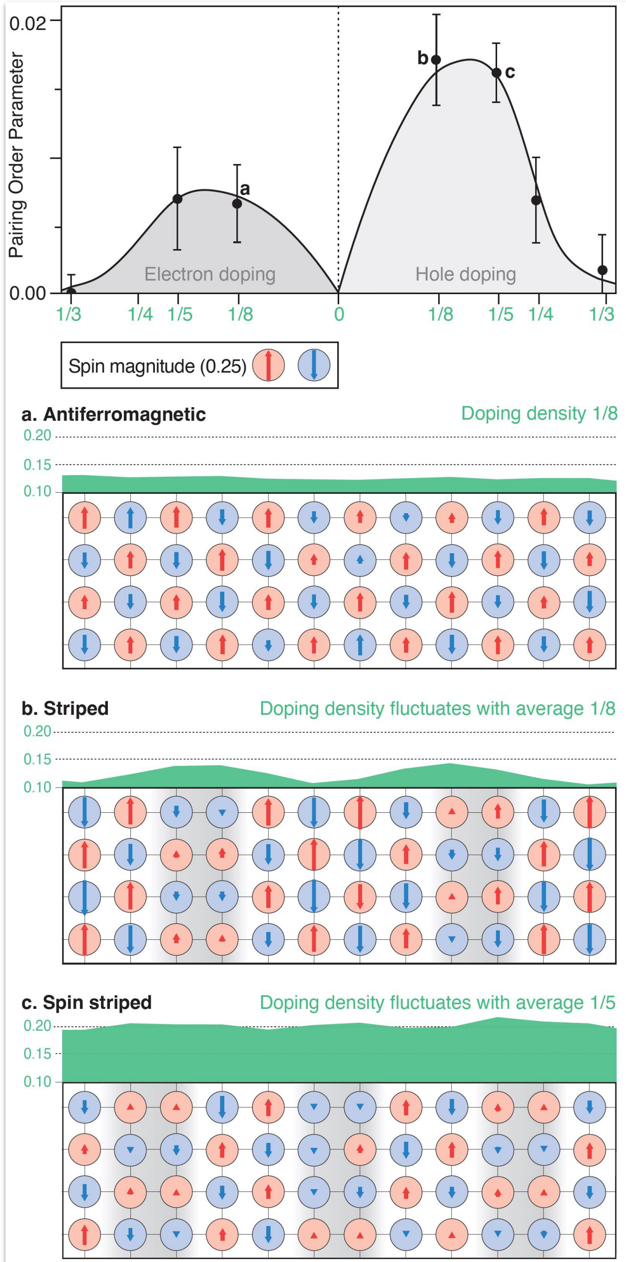
switching on *t*'

- electronic structure suggests weak negative *t*' (roughly -0.2)
- do we find superconductivity now?

Hao Xu, Chia-Min Chung, Mingpu Qin,
Uli Schollwöck, Steve White, Shiwei Zhang,
2303.08376

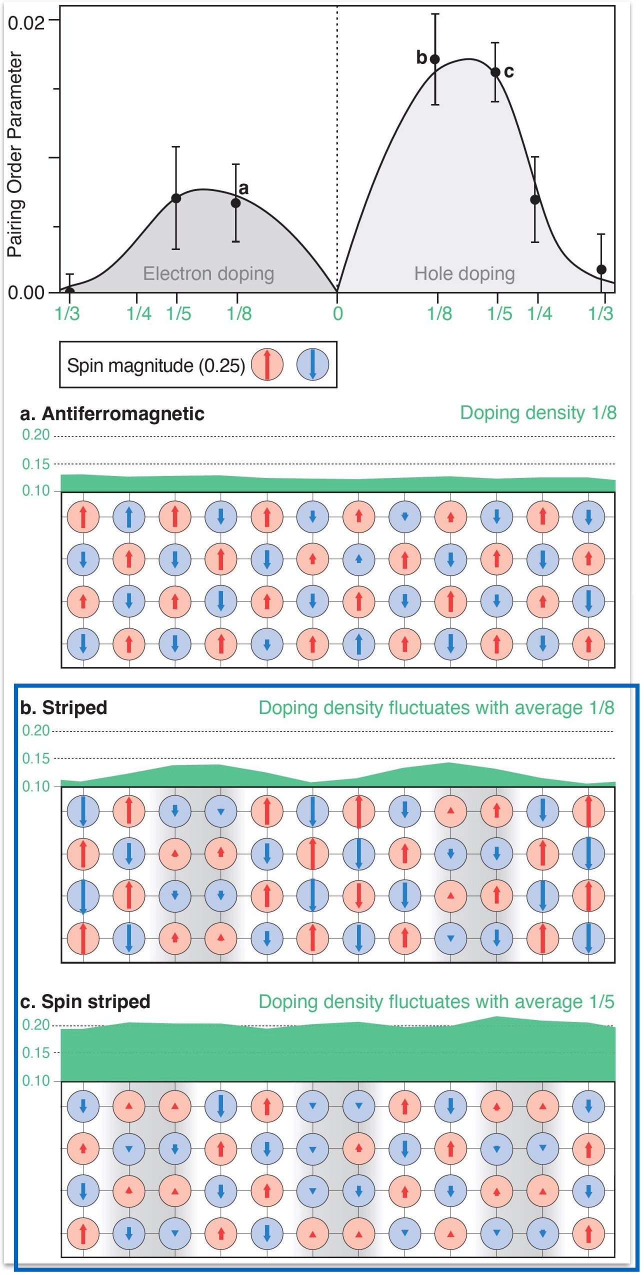
overview: „phase diagram"

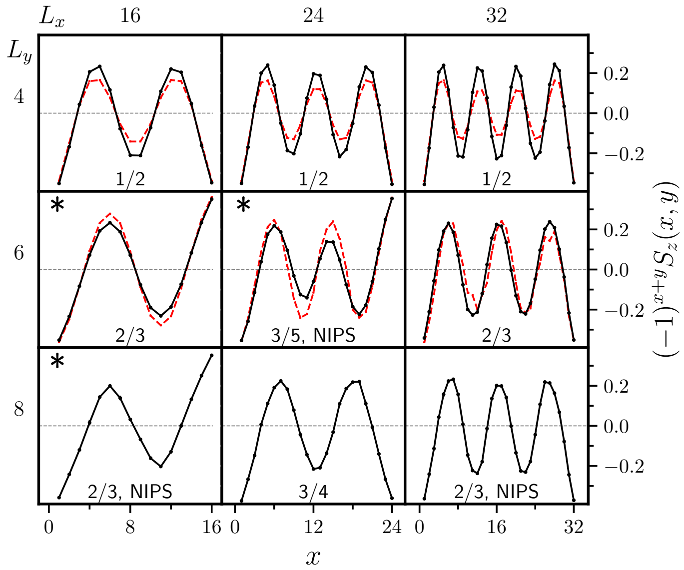
- U=8, t'=-0.2 physically
- variation of hole doping
  - t'=-0.2: hole doping
  - t'=0.2: electron doping (p-h!)
- mutual benchmarking DMRG - AFQMC
- pairing order parameter: response to pairing field extrapolated to
  - TD limit
  - zero pairing field

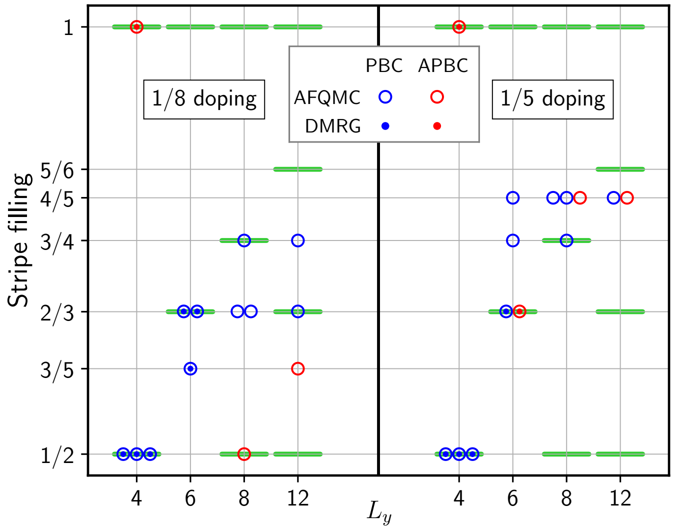


arXiv:2303.08376

holes: underdoped and overdoped



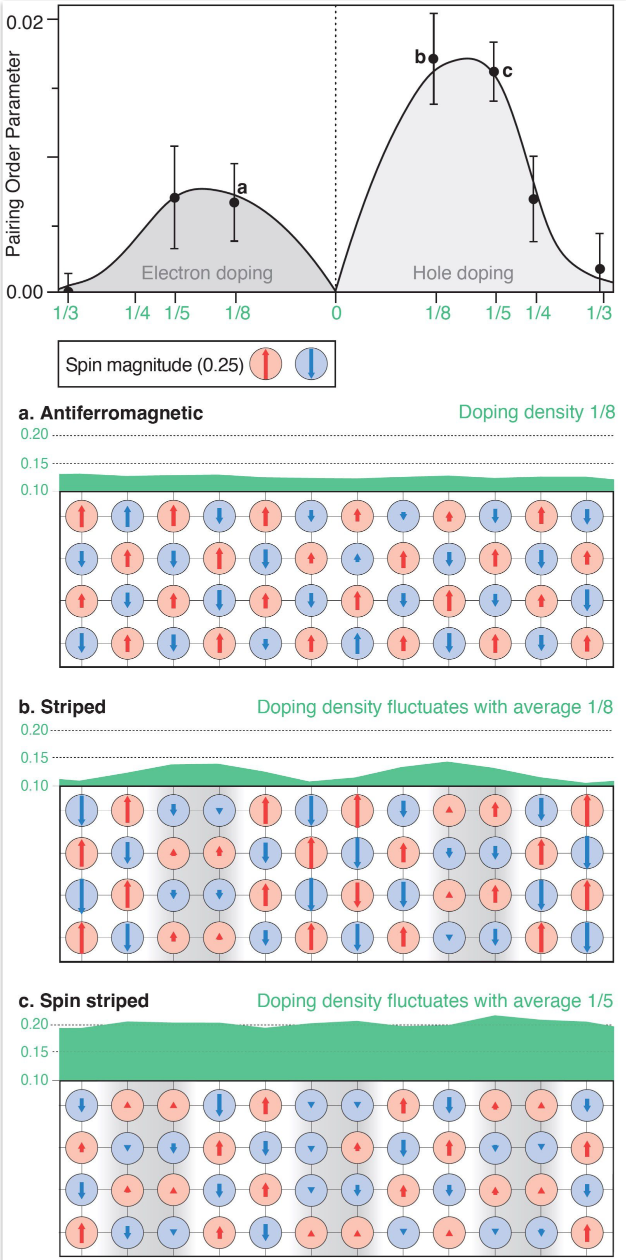




green: IPS

- stripe filling: $f = \delta\lambda_{\mathrm{SDW}}/2$
  hole (line) density
- hole pairs: $n_P = fL_y/2$
- many systems have non-integer pair stripes (NIPS)
- stripes fluctuating:
  mechanism for pair coherence?

what about the *t-t'-J* model?



- *t-t'-J* model: large-*U* limit of Hubbard model

  Jiang, Scalapino, White PNAS (2021)
  Gong, Zhu, Sheng PRL (2021)
  Jiang, Kivelson, PRL (2021)
  Sheng group, 2304.03963 (2023)

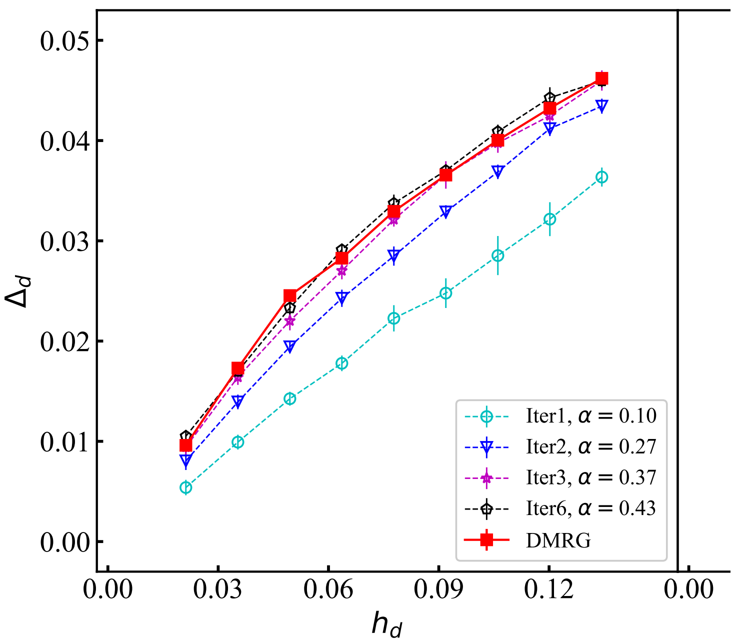
- electron-doped:
  d-wave SC, AFM background as in Hubbard

- hole-doped:
  stripes
  no superconductivity (perhaps weak??)

- stripe fluctuations too weak for SC
  because large *U*-limit??

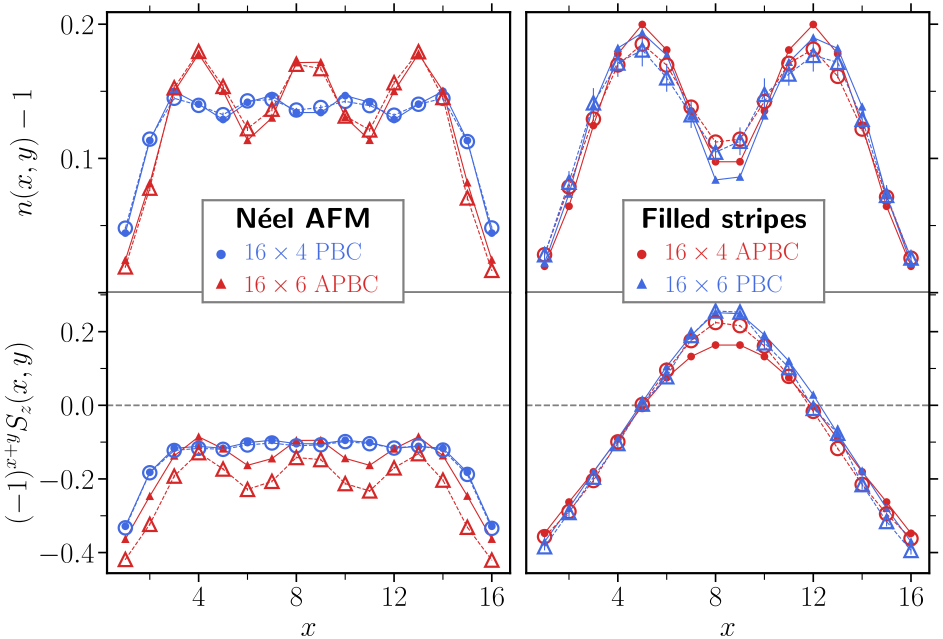
benchmarking: DMRG / AFQMC

hole-doping 1/4, 16 x 4 cylinders



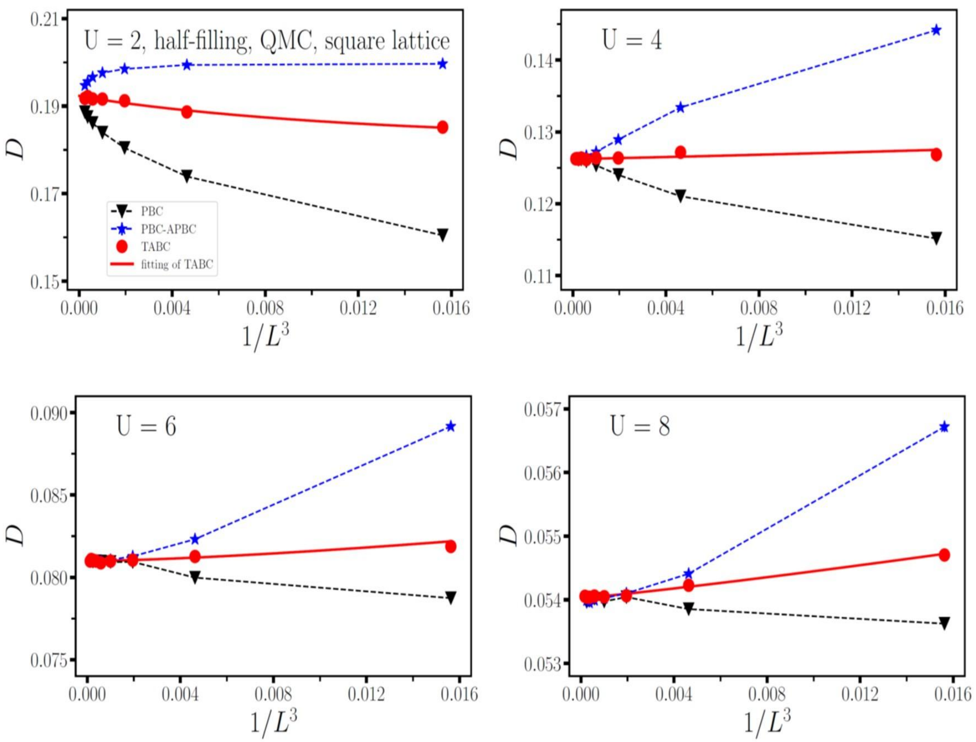
- start with bad trial wave function
- AFQMC optimizes it self-consistently; no fit parameter!
- then agreement with DMRG

electron-doping 1/8, 16 x 4 and x 6 cylinders



- mostly excellent agreement DMRG / AFQMC
- very strong and changing dependency on BCs: averaging over twisted BCs
- *t'*: more low-lying excited states, more sensitivity to BCs / size
- is this explanation of variety of results?

twist averaging: why?



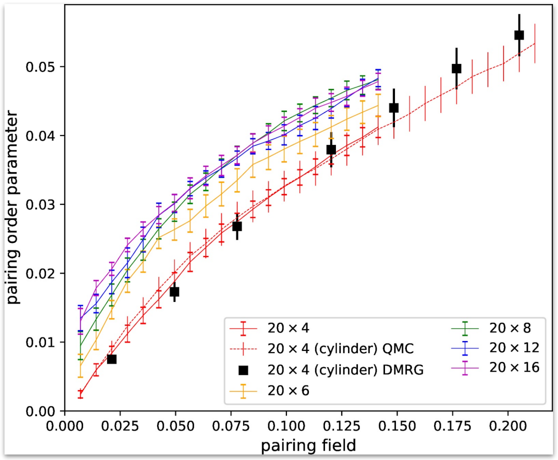
D: double occupancy

PBC, PBC/APBC, TABC

systems up to 20 x 20

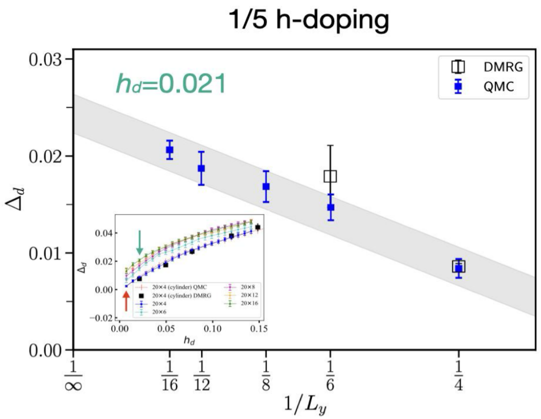
- half-filling: AFQMC without sign probem
- before twist: average: difficult and widely differing extrapolation
- after twist average: straightforward extrapolation in system size

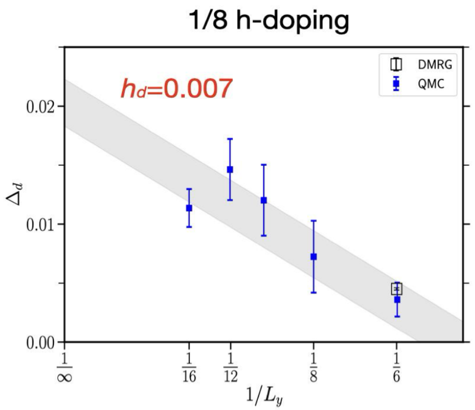
extrapolation of pairing order

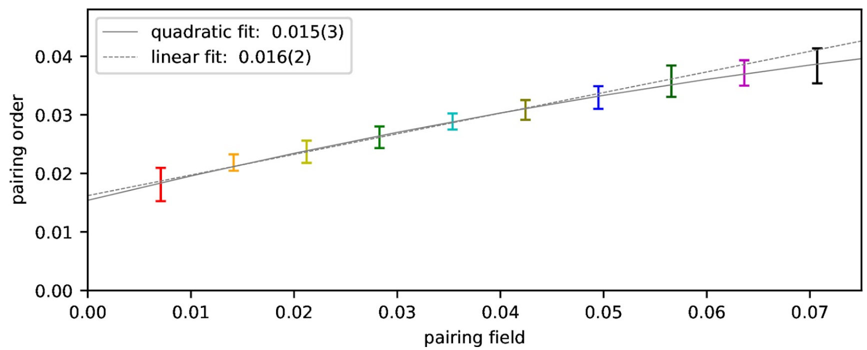


hole-doped (t'=-0.2), doping 1/5, twist-averaged (error bars!)

- good agreement DMRG / AFQMC
- DMRG cylinders too small for definite statement
- clear extrapolation in the AFQMC data
- non-zero pairing order!







conclusion

- adopt philosophy:
  only believe consistent results from several methods
- pure ($t'=0$) Hubbard ($U=8$, doping 1/8) shows period 8 [5…8] filled 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 often irrelevant
  - DMRG/AFQMC in excellent agreement
  - find *d*-wave SC, arguably related to strongly fluctuating stripes
  - very strong role of BCs, finite-size effects