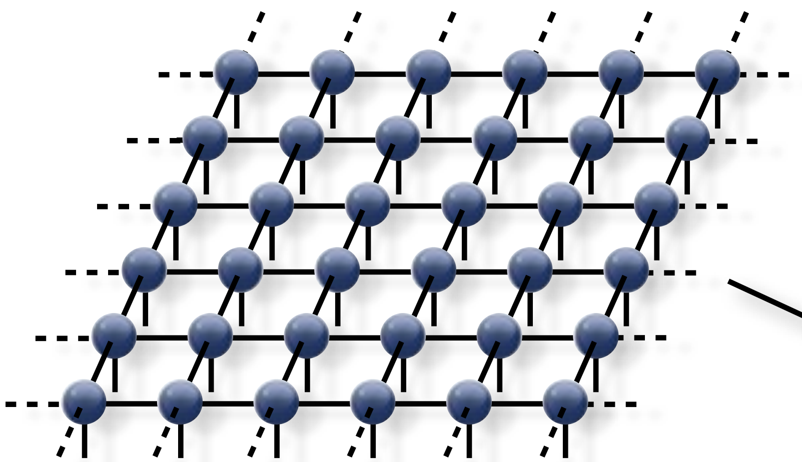
Stripe order in the 2D Hubbard model

Philippe Corboz, Institute for Theoretical Physics, University of Amsterdam

Boxiao Zheng, Chia-Min Chung, PC, Georg Ehlers, Ming-Pu Qin, Reinhard Noack,
Hao Shi, Steven White, Shiwei Zhang, Garnet Chan, arXiv:1701.00054



iPEPS
tensor network ansatz

+ DMRG + AFQMC + DMET

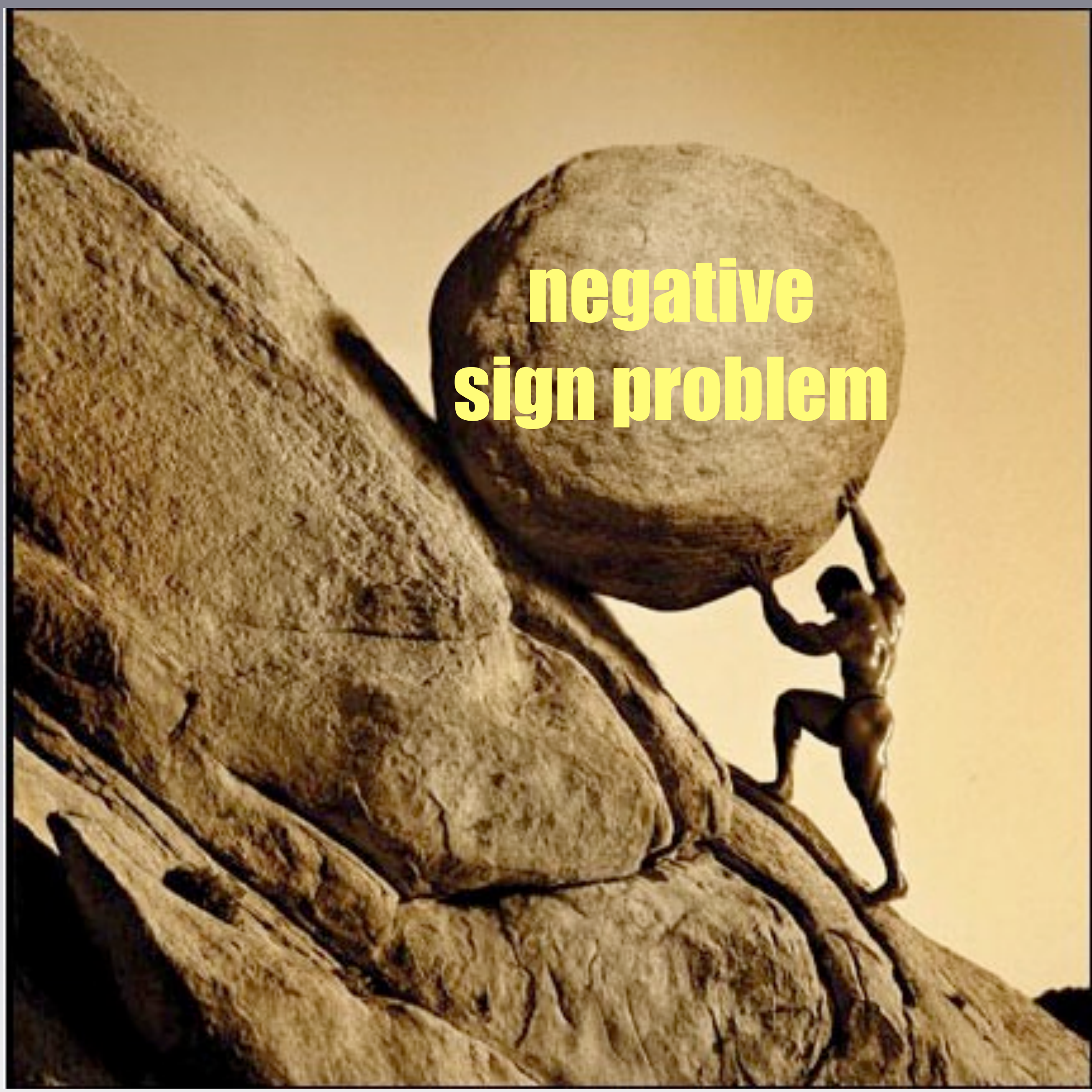
$U/t = 8$

$\delta = 1/8$

Ground state:
Stripe state

Solve the 2D Hubbard model $\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + h.c. + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$

★ *Phase diagram? Is it the relevant model for high-T_c superconductivity (cuprates)?*



Many powerful and promising methods, e.g.:

- DMFT / DCA
- Diagrammatic Monte Carlo
- Tensor network algorithms
- Density Matrix Embedding Theory
- Fixed-node Monte Carlo
- Series expansion
- Variational Monte Carlo
- Coupled-cluster methods
- Auxiliary-field QMC
- Functional renormalization group
- ... and more ...

Main candidate ground states for U/t~8, $\delta\sim 1/8$

or in the *t-J* model (effective model)

Uniform d-wave superconducting state

Yokoyama & Shiba, JPSJ 57 (1988)
Gros, PRB 38 (1988)
Dagotto et al, PRB 49 (1994)
S. Sorella, et al., PRL 88 (2002)
Maier et al., PRL 95 (2005)
Senechal et al. PRL 94 (2005)
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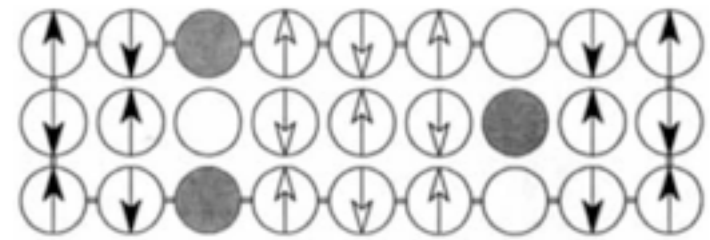
Aichhorn et al., PRB 74 (2006)
Lugas, et al. PRB 74 (2006)
Aimi & Imada, JPSJ 76 (2007)
Yokoyama, Ogata & Tanaka: JPSJ 75 (2006)
Yokoyama, et al. JPSJ 73 (2004)
Eichenberger & Baeriswyl, PRB 76 (2007)
Macridin, Jarrell, Maier, PRB 74 (2006)
Hu, Becca & Sorella, PRB 85 (2012)
Gull, Parcollet, Millis, PRL 110 (2013)
Misawa & Imada, PRB 90 (2014)
... and many more ...

VS

Stripe state
modulated spin/charge
w. or w/o coexisting SC



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Theory:

Poilblanc & Rice, PRB **39** (1989)
Zaanen & Gunnarsson, PRB **40** (1989)
Machida, Physica **158C** (1989)
Schulz, J. Phys. **50** (1989)
Emery, Kivelson & Tranquada PNAS **96** (1999)
White & Scalapino, PRL **80** (1998)
White & Scalapino, PRB **60** (1999)
Himeda, Kato & Ogata, PRL **88** (2002)
Kivelson, Bindloss, Fradkin, Oganesyan,
Tranquada, Kapitulnik & Howald, RMP **75** ('03)
Berg, Fradkin, Kim, Kivelson, Oganesyan,
Tranquada & Zhang PRL **99** (2007)
Chou, Fukushima & Lee, PRB **78** (2008)
Yang, Chen, Rice, Sigrist & Zhang, NJP **11** (2009)
Berg, Fradkin, Kivelson & Tranquada, NJP **11** ('09)
Berg, Fradkin & Kivelson, PRB **79** (2009)
Vojta, Adv. Phys. **58** (2009)
Fradkin & Kivelson, Nature Physics **8** (2012)
... and many more ...

Main candidate ground states for U/t~8, δ~1/8

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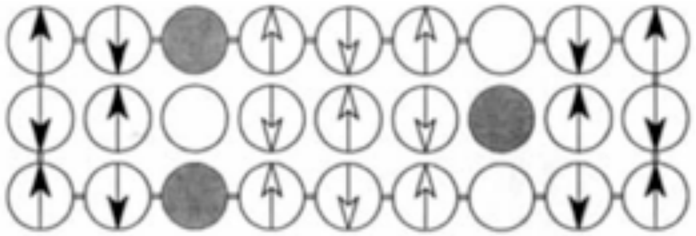

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White & Scalapino, PRB 60 (1999)
Himeda, Kato & Ogata, PRL 88 (2002)
White & Scalapino, PRL 91 (2003)
Hager, Wellein, Jeckelmann, Fehske, PRB 71 (2005)
Raczkowski, et al. PRB 76 (2007)
Chou, Fukushima & Lee, PRB 78 (2008)
Chang & Zhang, PRL 104 (2010)
Corboz, White, Vidal & Troyer, PRB 84 (2011)
Corboz, Rice & Troyer, PRL 113 (2014)
Zheng, Chan, PRB 93 (2016)
Zhao, Ido, Morita & Imada, arXiv:1703.03537 (2017)
... and many more ...

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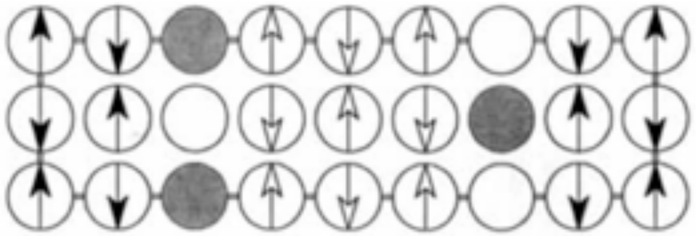
or in the *t-J* model (effective model)

Uniform d-wave superconducting state

VS

Stripe state
modulated spin/charge
w. or w/o coexisting SC



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... and ma

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? Which is the true ground state **?**

Goal: get conclusive answer for U/t=8, δ=1/8 using iPEPS, DMRG, AFQMC, DMET

2D Hubbard benchmark paper:
Simons collaboration on Many Electron Problem: J. P. F. LeBlanc, et al., PRX 5 (2015).

Outline

- *Overview of methods*
  - ✦ DMRG & **iPEPS**
  - ✦ DMET & auxiliary field QMC
  - ✦ Strengths & weaknesses
- *Results*
  - ✦ iPEPS results for U/t=8, δ=1/8
  - ✦ Comparison with other methods
  - ✦ Comparison with U/t=6, U/t=12 (δ=1/8)
- *Conclusion*
  - ✦ Main results & outlook
- *Related topic: SU(N) Hubbard models*

Tensor network ansatz for a wave function

Lattice: 1 2 3 4 5 6

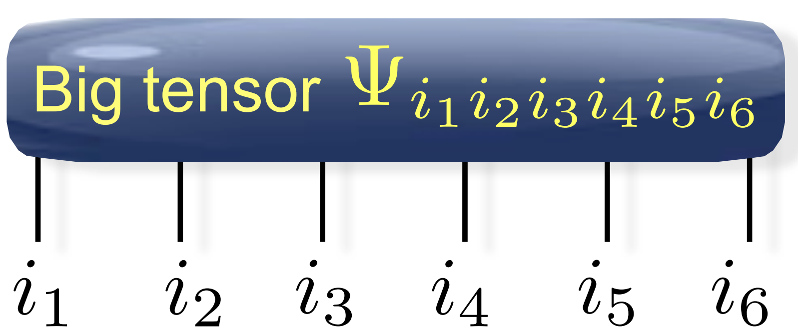
2 basis states per site: $\{|\uparrow\rangle, |\downarrow\rangle\}$

2^6 basis states

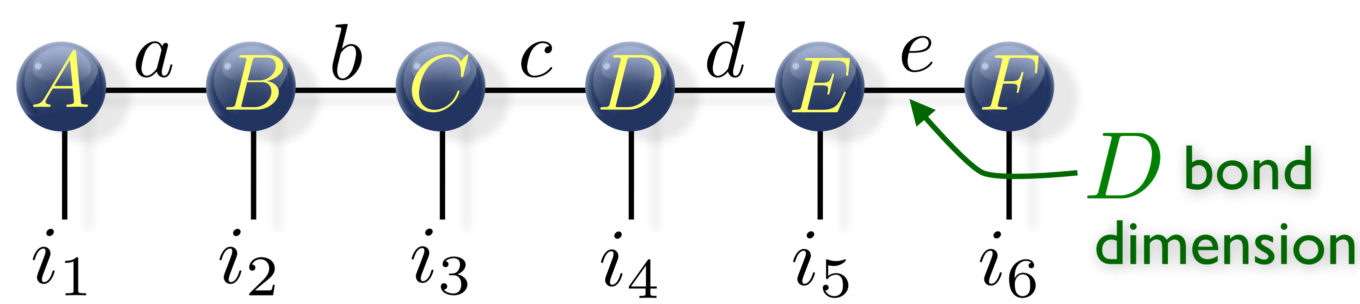
2^6 coefficients

State: $|\Psi\rangle = \sum_{i_1 i_2 i_3 i_4 i_5 i_6} \Psi_{i_1 i_2 i_3 i_4 i_5 i_6} |i_1 \otimes i_2 \otimes i_3 \otimes i_4 \otimes i_5 \otimes i_6\rangle$

Tensor/multidimensional array



Tensor network: matrix product state (**MPS**)

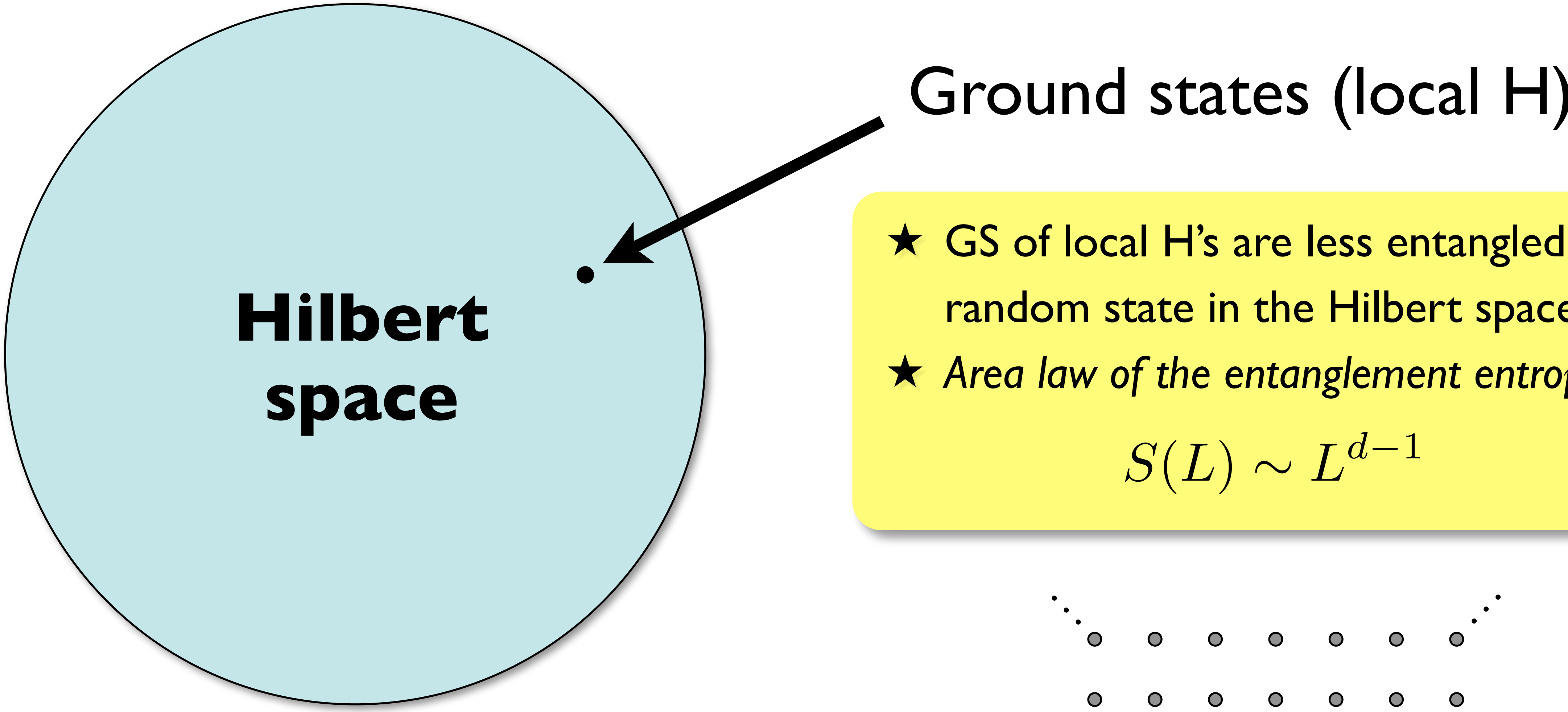


$$\Psi_{i_1 i_2 i_3 i_4 i_5 i_6} \approx \sum_{abcde} A^{a}_{i_1} B^{ab}_{i_2} C^{bc}_{i_3} D^{cd}_{i_4} E^{de}_{i_5} F^{e}_{i_6} = \tilde{\Psi}_{i_1 i_2 i_3 i_4 i_5 i_6}$$

exp(N) many numbers **vs** poly(D,N) numbers

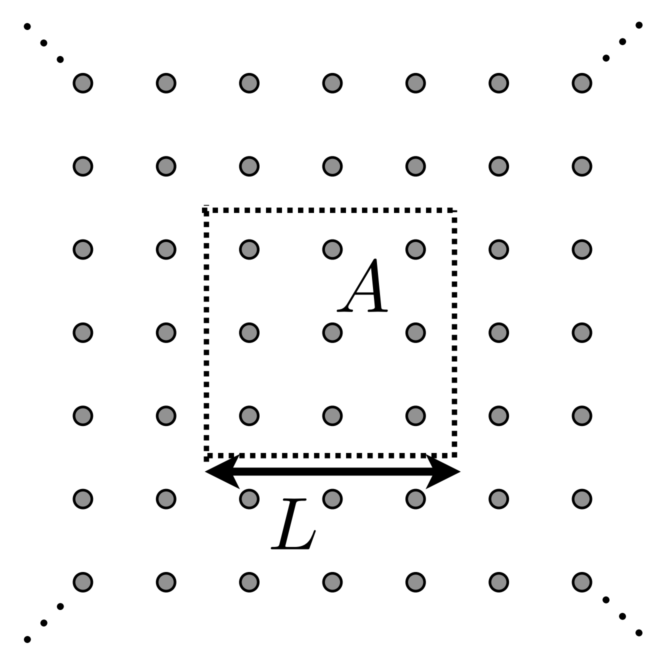
Efficient representation!

“Corner” of the Hilbert space



- ★ GS of local H’s are less entangled than a random state in the Hilbert space
- ★ *Area law of the entanglement entropy*

$$S(L) \sim L^{d-1}$$

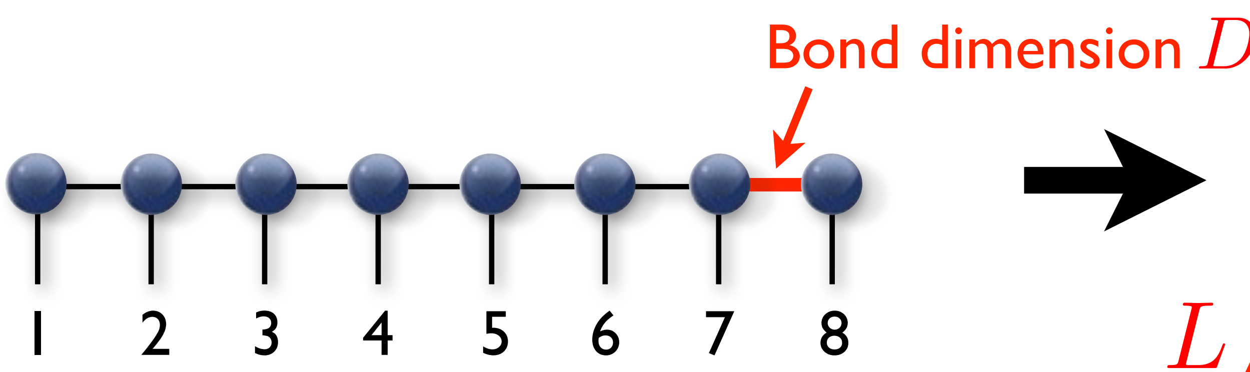


MPS & PEPS

1D

MPS

Matrix-product state
(underlying ansatz of DMRG)



Physical indices (lattices sites)

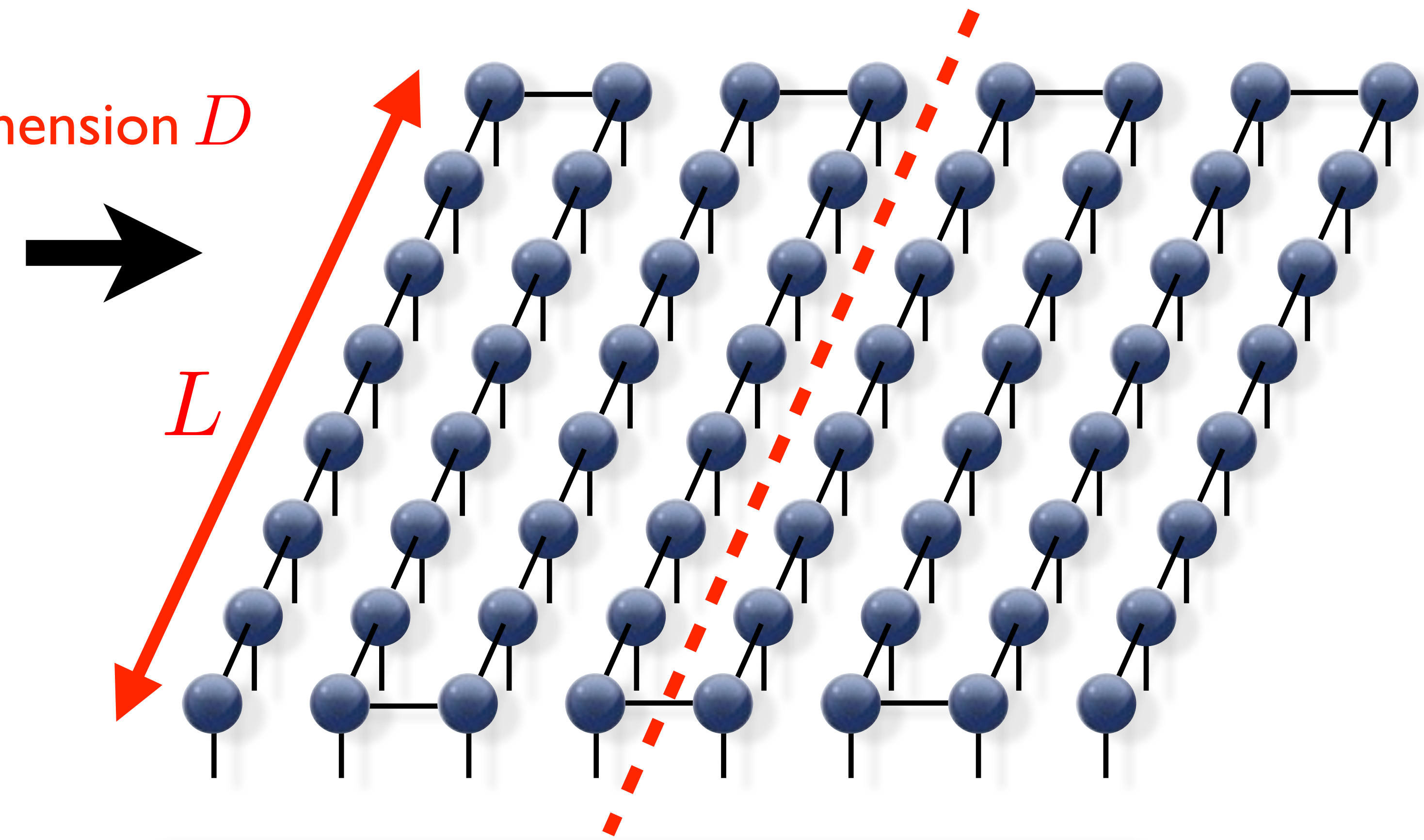
S. R. White, PRL 69, 2863 (1992)

Fannes et al., CMP 144, 443 (1992)

Östlund, Rommer, PRL 75, 3537 (1995)

2D

Snake MPS



Computational cost:

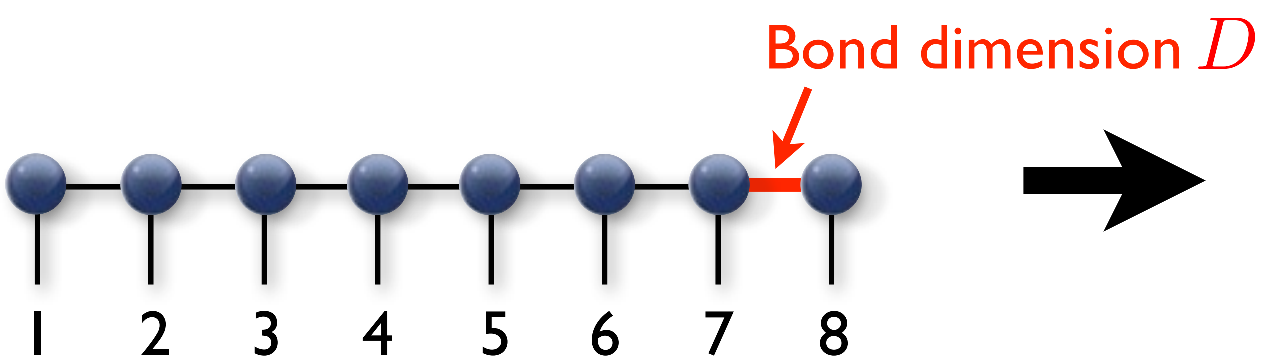
$$\propto \exp(L)$$

MPS & PEPS

1D

MPS

Matrix-product state
(underlying ansatz of DMRG)

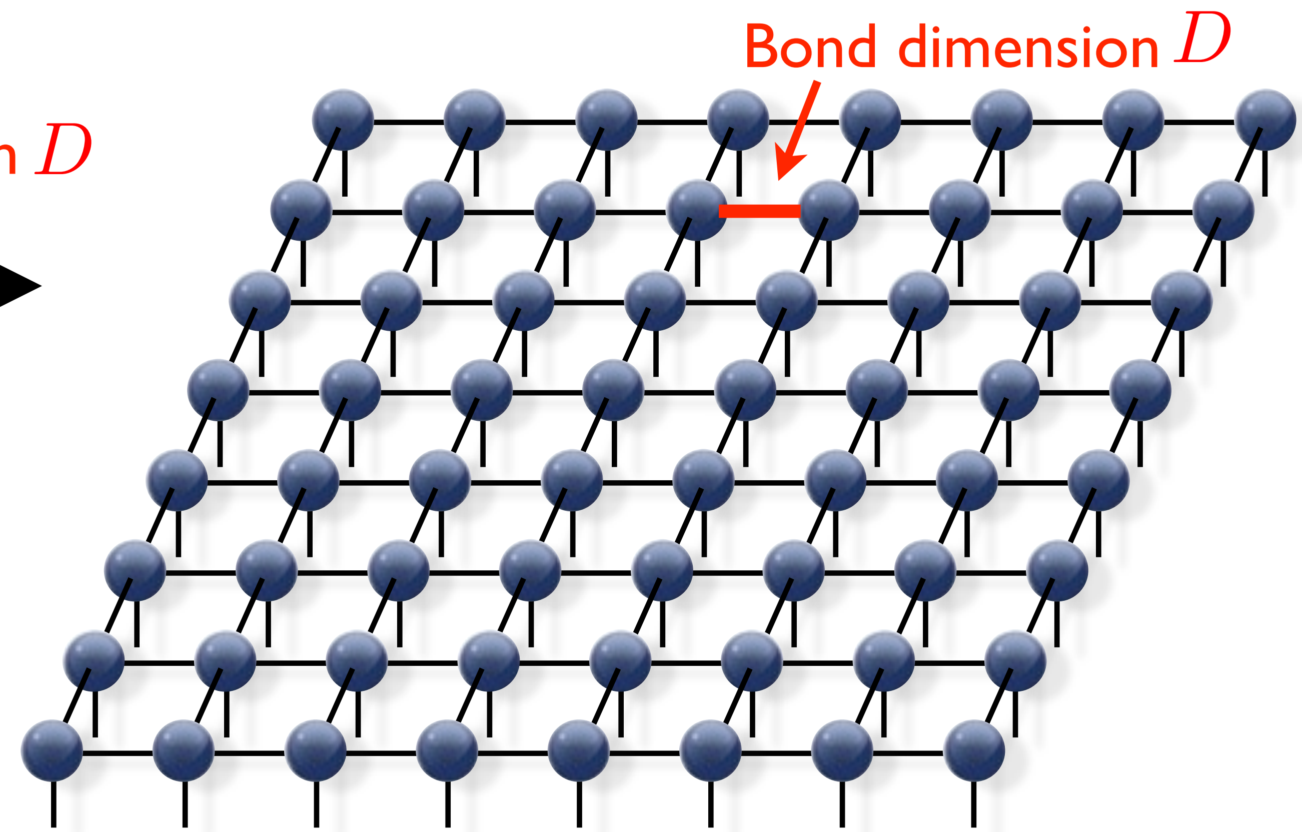


Physical indices (lattices sites)

2D

PEPS (TPS)

projected entangled-pair state
(tensor product state)



Computational cost:

$$\propto poly(L, D)$$

and Gendiar,

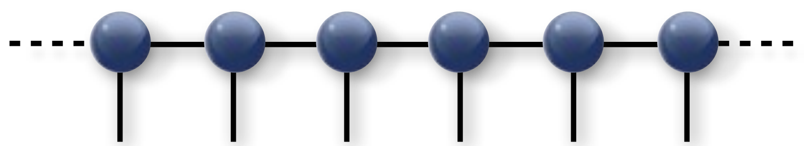
-mat/0401115

Infinite PEPS (iPEPS)

1D

iMPS

infinite matrix-product state

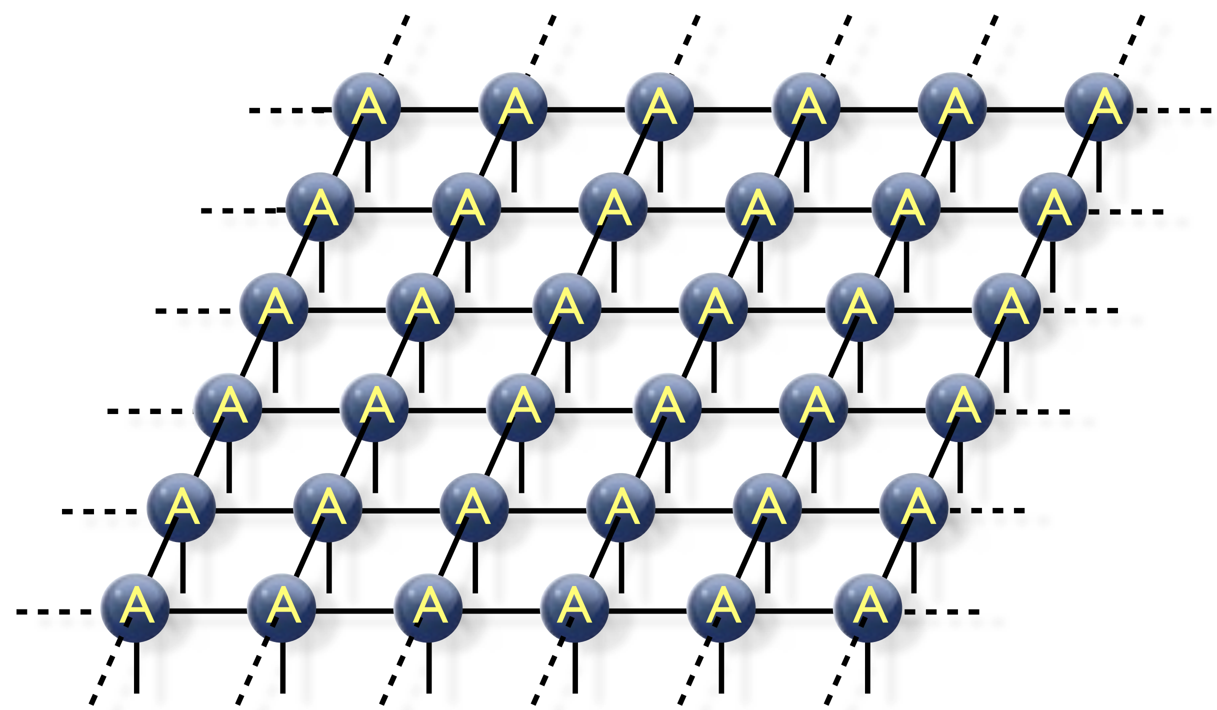


→

2D

iPEPS

infinite projected entangled-pair state



Jordan, Orus, Vidal, Verstraete, Cirac, PRL (2008)

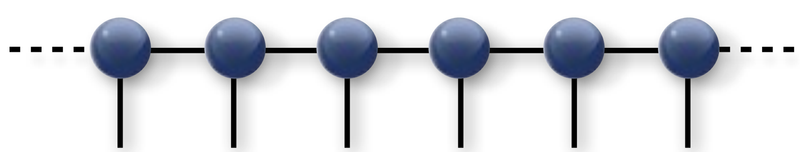
★ Work directly in the thermodynamic limit:
No finite size and boundary effects!

iPEPS with arbitrary unit cells

1D

iMPS

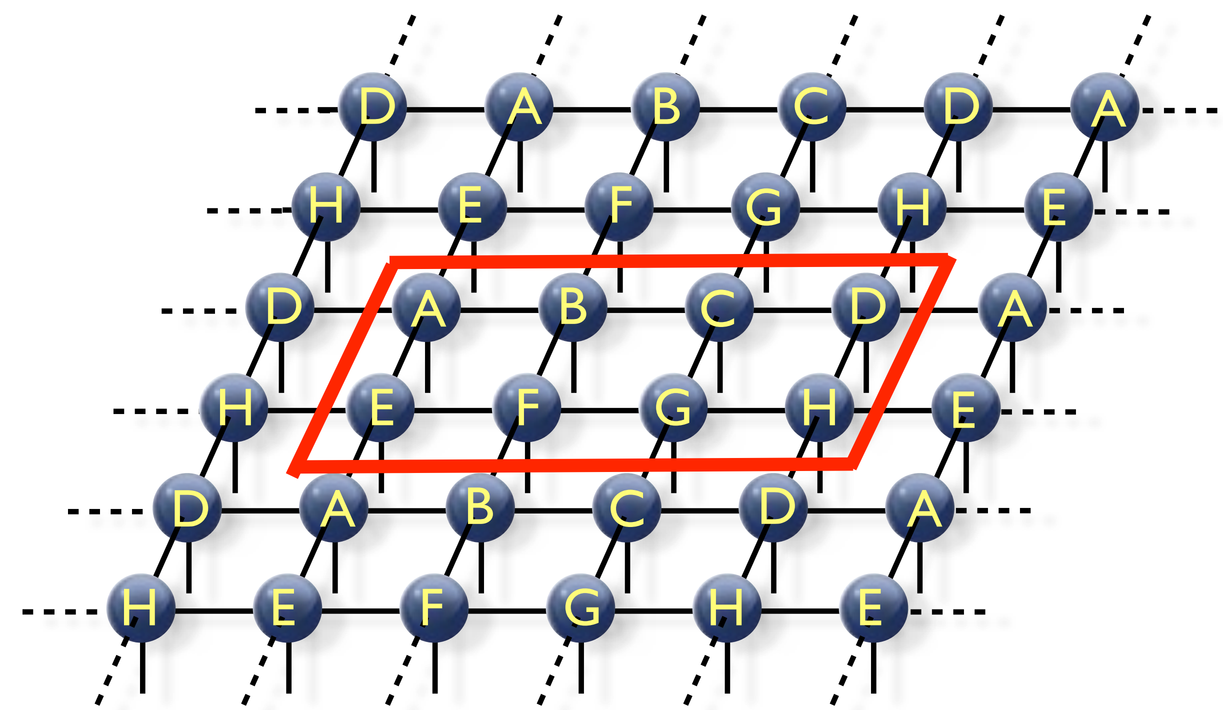
infinite matrix-product state



2D

iPEPS

with arbitrary unit cell of tensors



here: 4x2 unit cell

PC, White, Vidal, Troyer, PRB **84** (2011)

- ★ Run simulations with different unit cell sizes
- ★ Different (meta-stable) states can be realized
- ★ Systematically compare variational energies

Overview of methods

- **DMRG**: Matrix product states on cylinders (real-space & hybrid approach)
  - ✓ very accurate for cylinders up to a certain width (L=6)
  - \- finite size error due to finite width

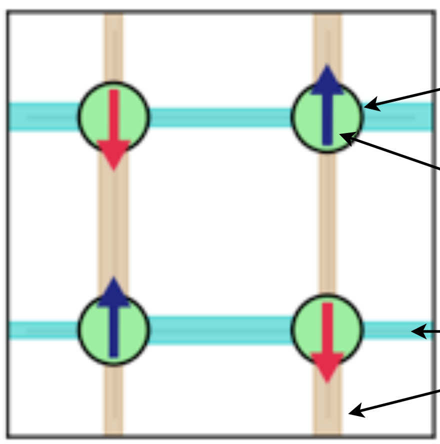
- **iPEPS**: 2D tensor network ansatz in the thermodynamic limit
  - ✓ no finite size effects & systematic improvement with bond dimension D
  - – need extrapolation in D

- **DMET**: Density matrix embedding theory
  - Idea: map lattice model onto cluster-impurity problem (cluster embedded in a set of bath sites) which is solved in a self-consistent way
  - ✓ no finite size effects
  - – error due to finite cluster size

- **AFQMC**: Auxiliary-field quantum Monte Carlo
  - Idea: Obtain ground state through imaginary time evolution, using Trotter decomposition + Hubbard-Stratonovich decoupling of interaction term. Use trial state to circumvent the sign problem (constrained path approximation)
  - ✓ Exact at half filling (no sign problem) & large systems possible
  - – Error from choice of trial state

iPEPS: main competing states (U/t=8, δ=1/8)

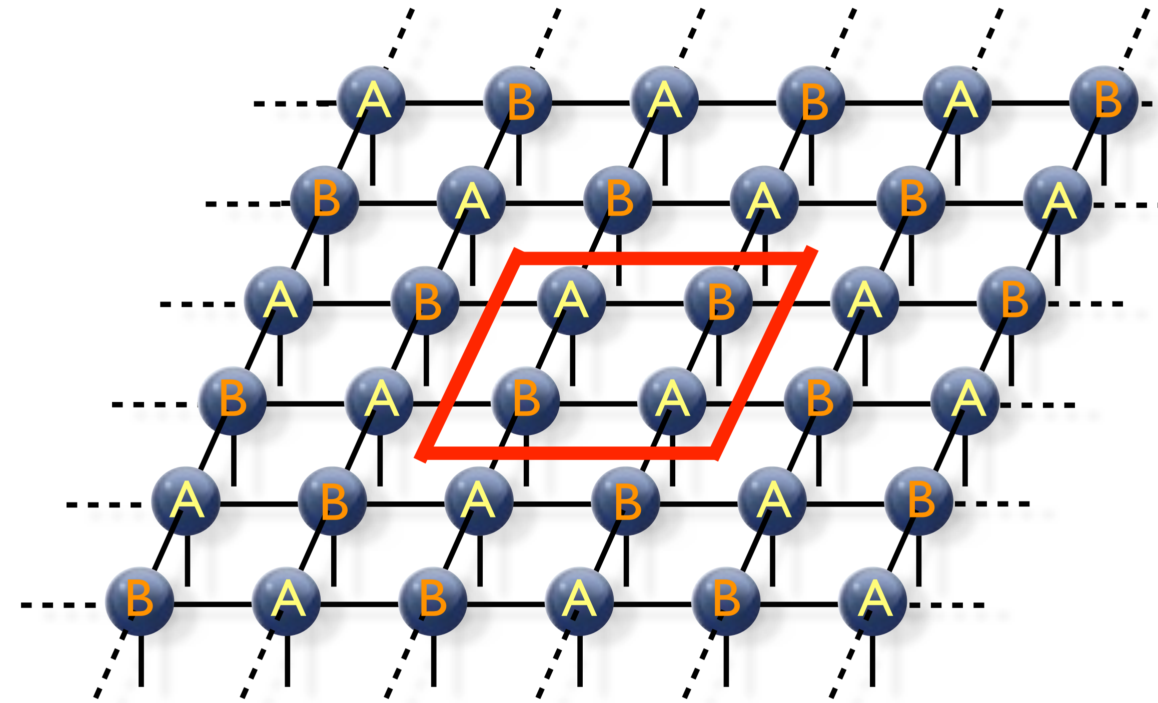
Uniform d-wave SC state (+ AF order)



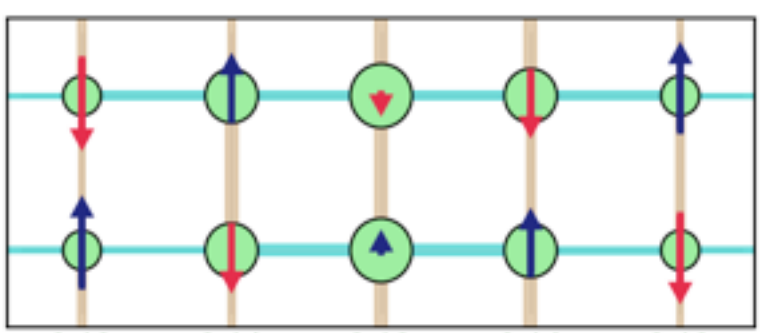
δ_i hole density

m_i magnetic moment

Δ_{ij} nearest-neighbor singlet pairing amplitude



Period λ=5 (W5 stripe)



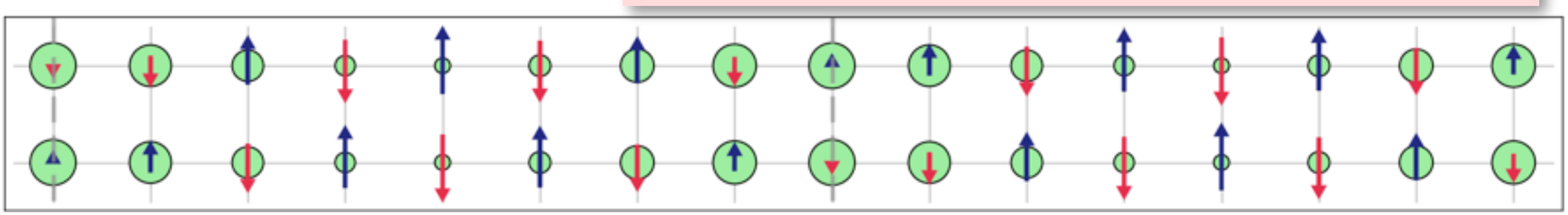
★ Modulation in the charge, AF, and SC order

★ “Site-centered” stripe

★ π-phase shift in the AF order

Period λ=8 (W8 stripe)

★ Superconductivity suppressed (1 hole per unit length)



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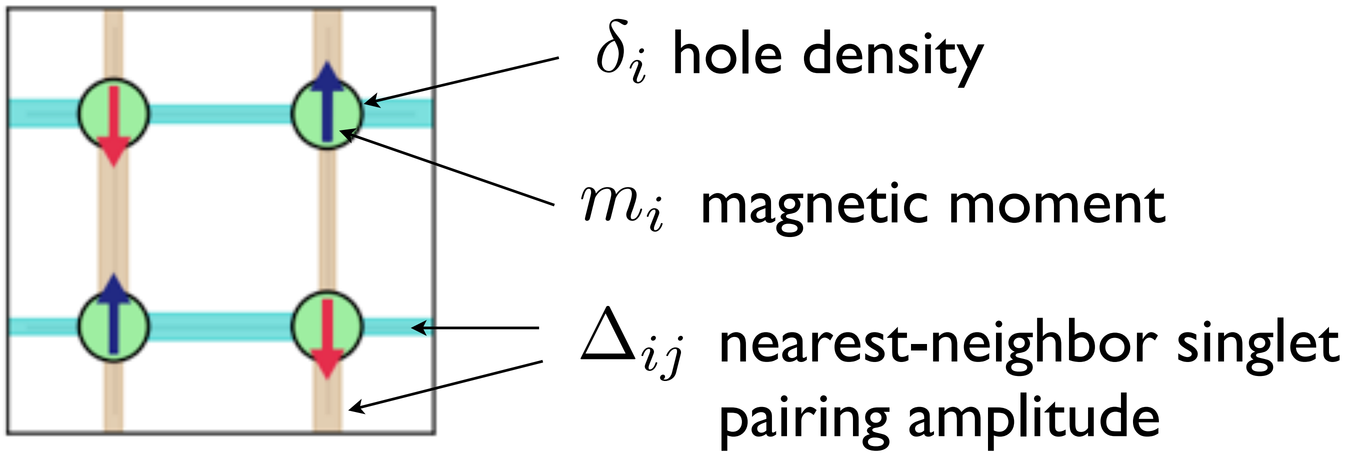
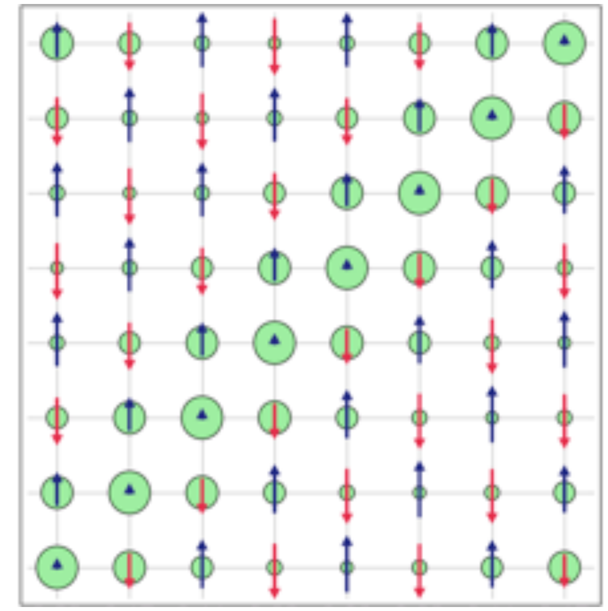


Diagonal stripe (16x16 cell)



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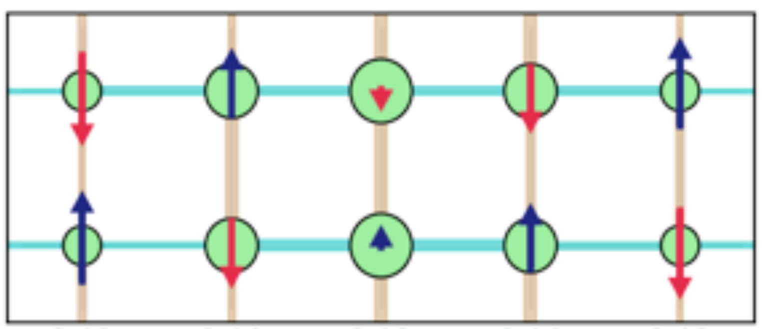

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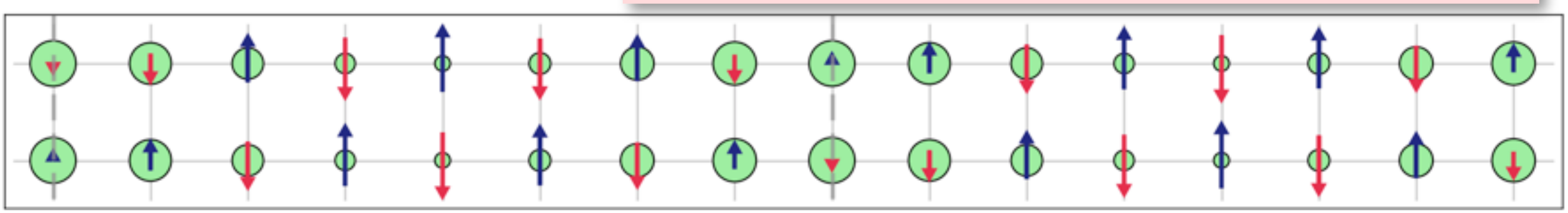
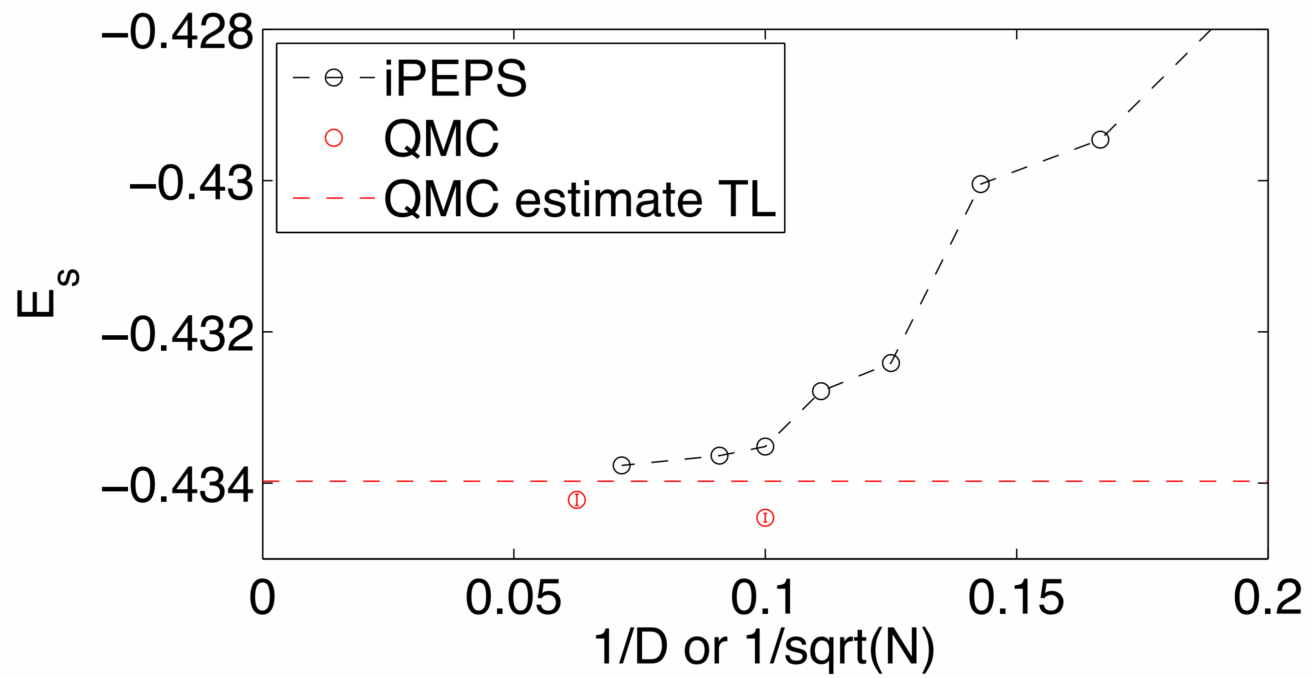


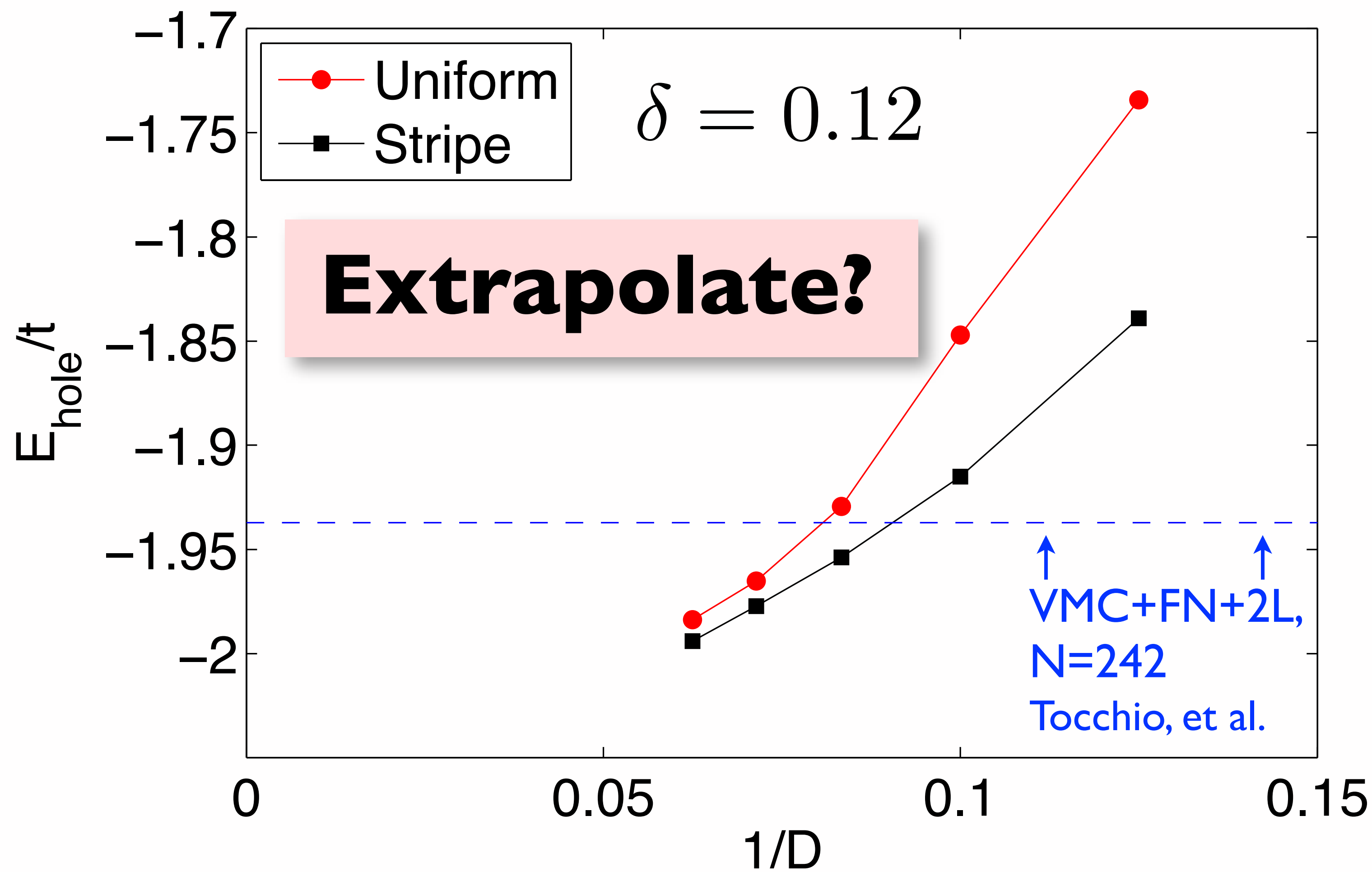
iPEPS: previous benchmarks (here: U/t=10)

Half-filled case (n=1):

- Relative error in the TL: O(**0.05%**)
  (D=14 without extrapolation!)
- QMC estimate by S. Sorella (unpublished)



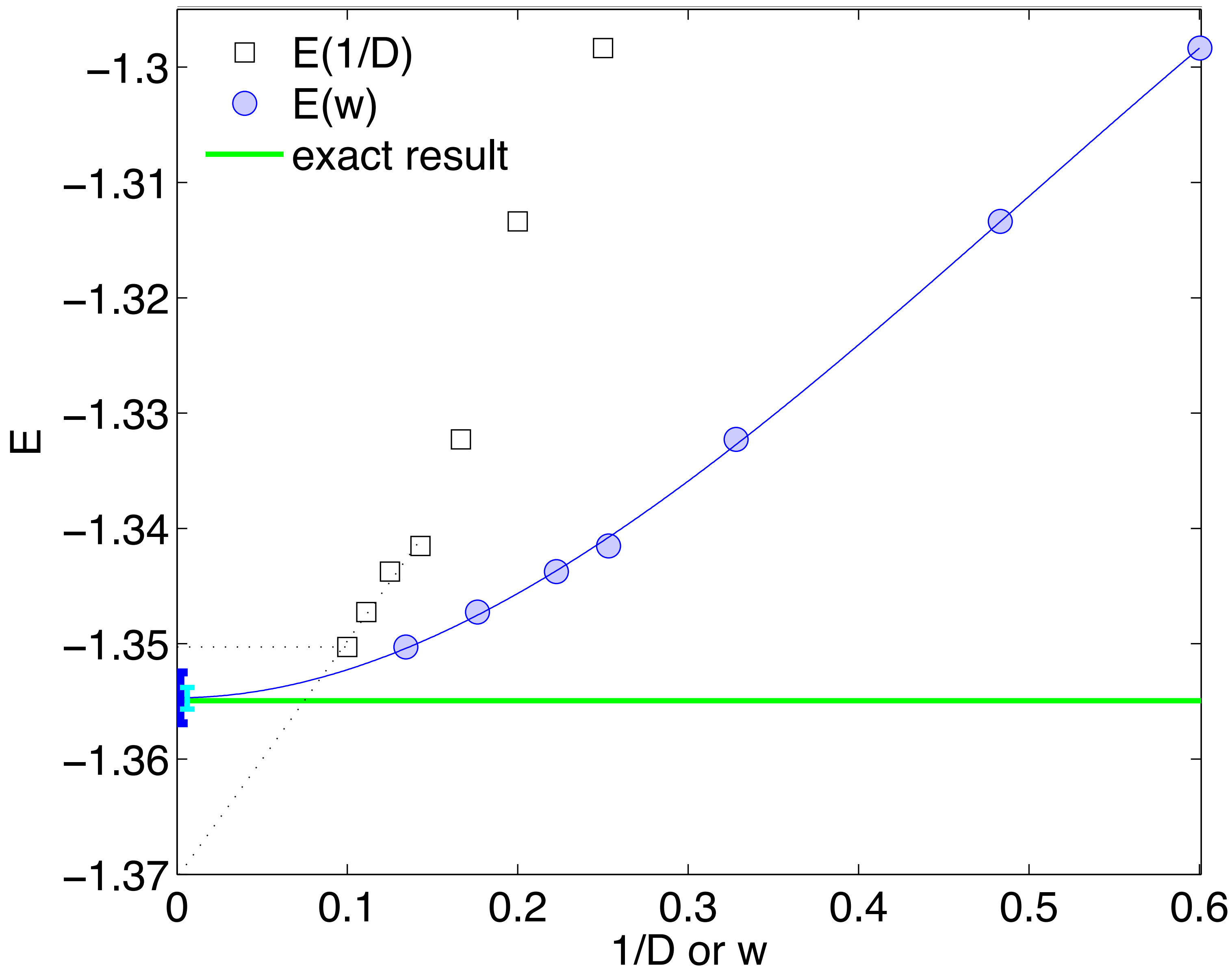
Doped case (n=0.88):



Improving energy extrapolations

PC, PRB **93** (2016)

Motivation: Need accurate energy extrapolation to determine the true ground state



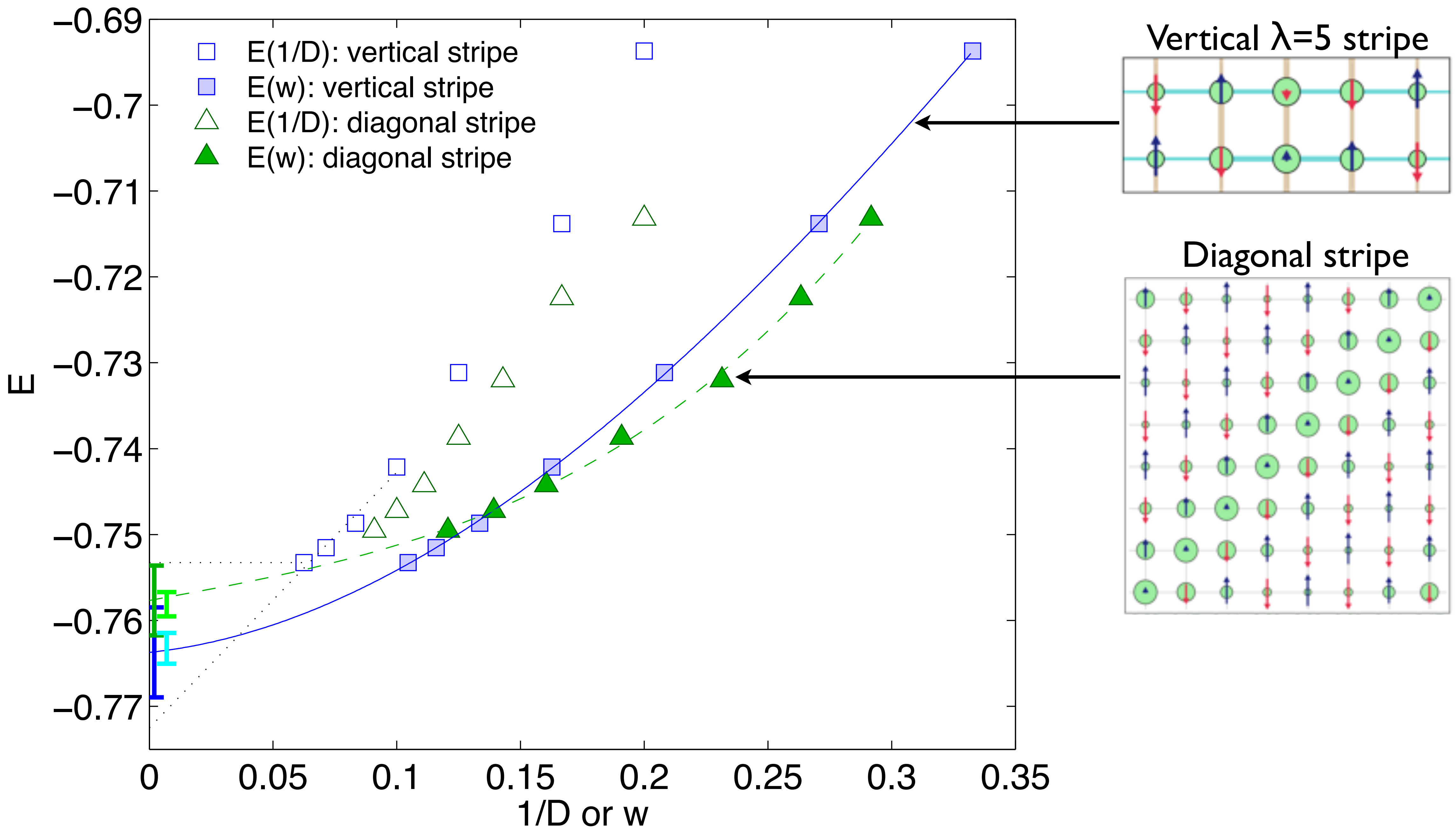
Bad estimate based on 1/D data!

Extrapolate in ***truncation error*** instead!

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

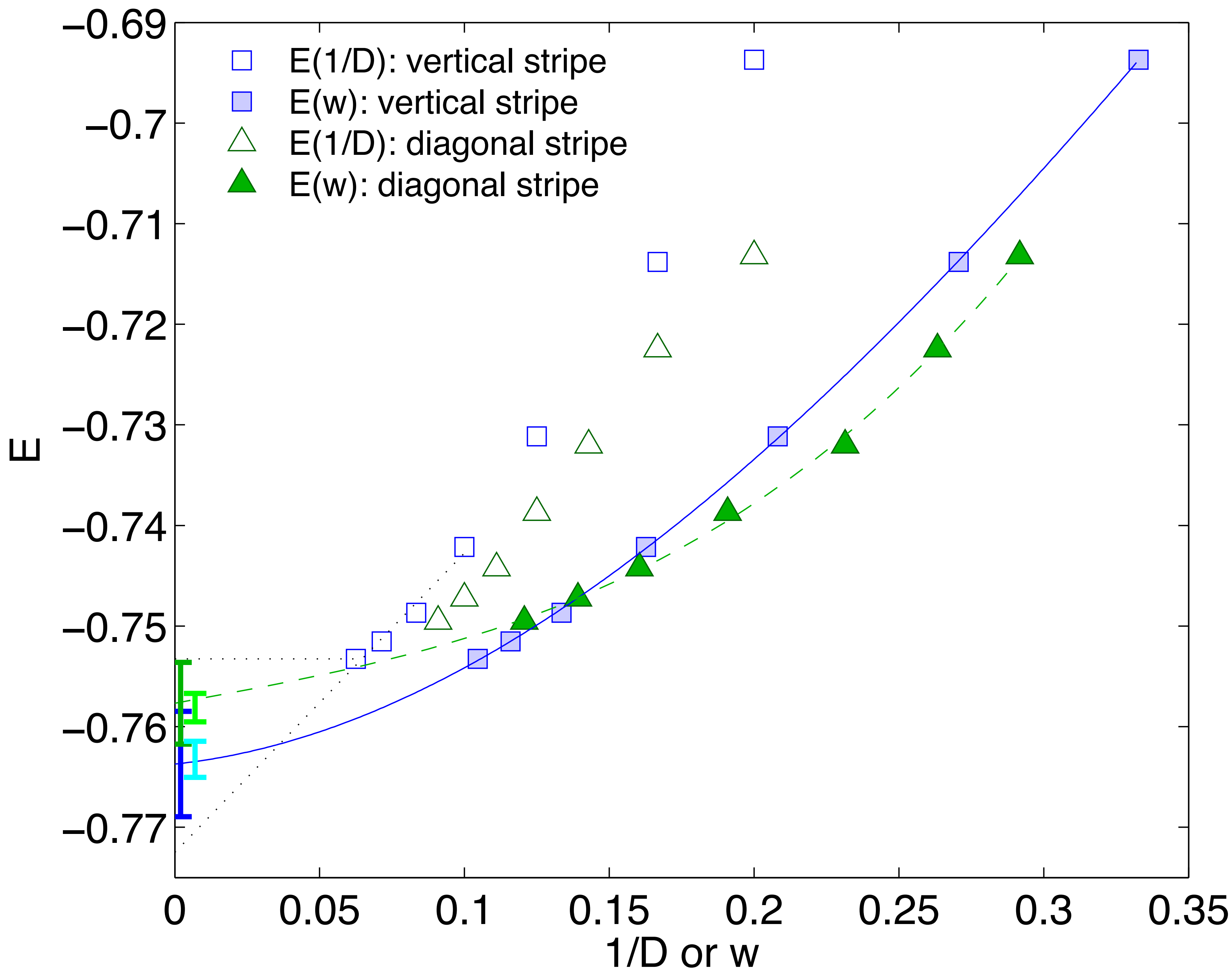
Example: vertical vs diagonal stripe, U/t=8, δ=1/8

PC, PRB **93** (2016)



Example: vertical vs diagonal stripe, U/t=8, δ=1/8

PC, PRB **93** (2016)

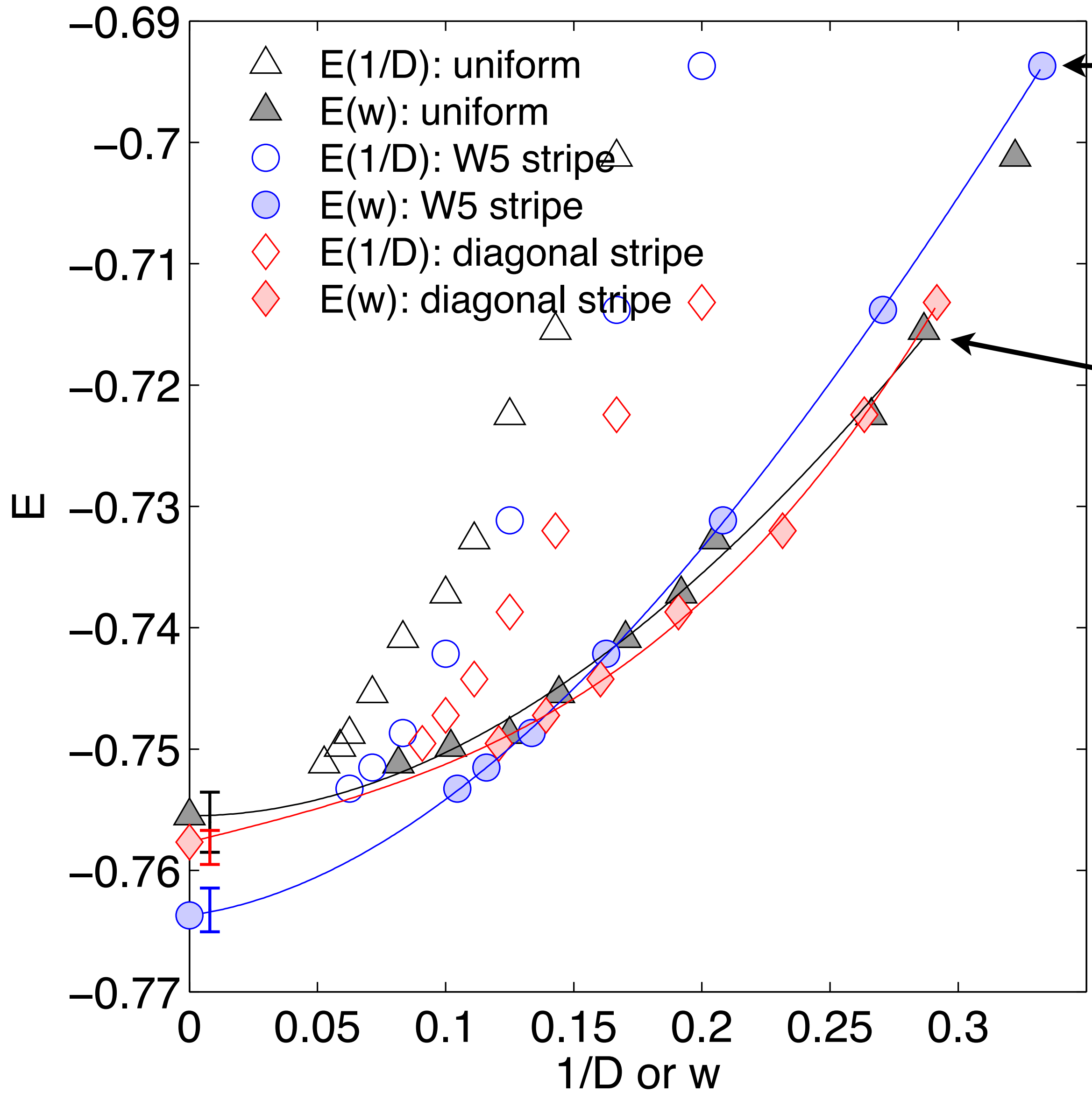


Vertical λ=5 stripe is **lower** than diagonal stripe

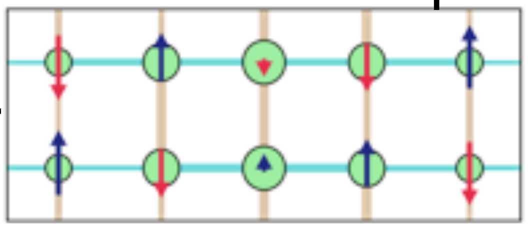
Extrapolation is CRUCIAL!!!

➔ Need to compare extrapolated energies of all competing states

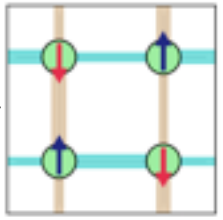
iPEPS: extrapolated energies



Vertical λ=5 stripe



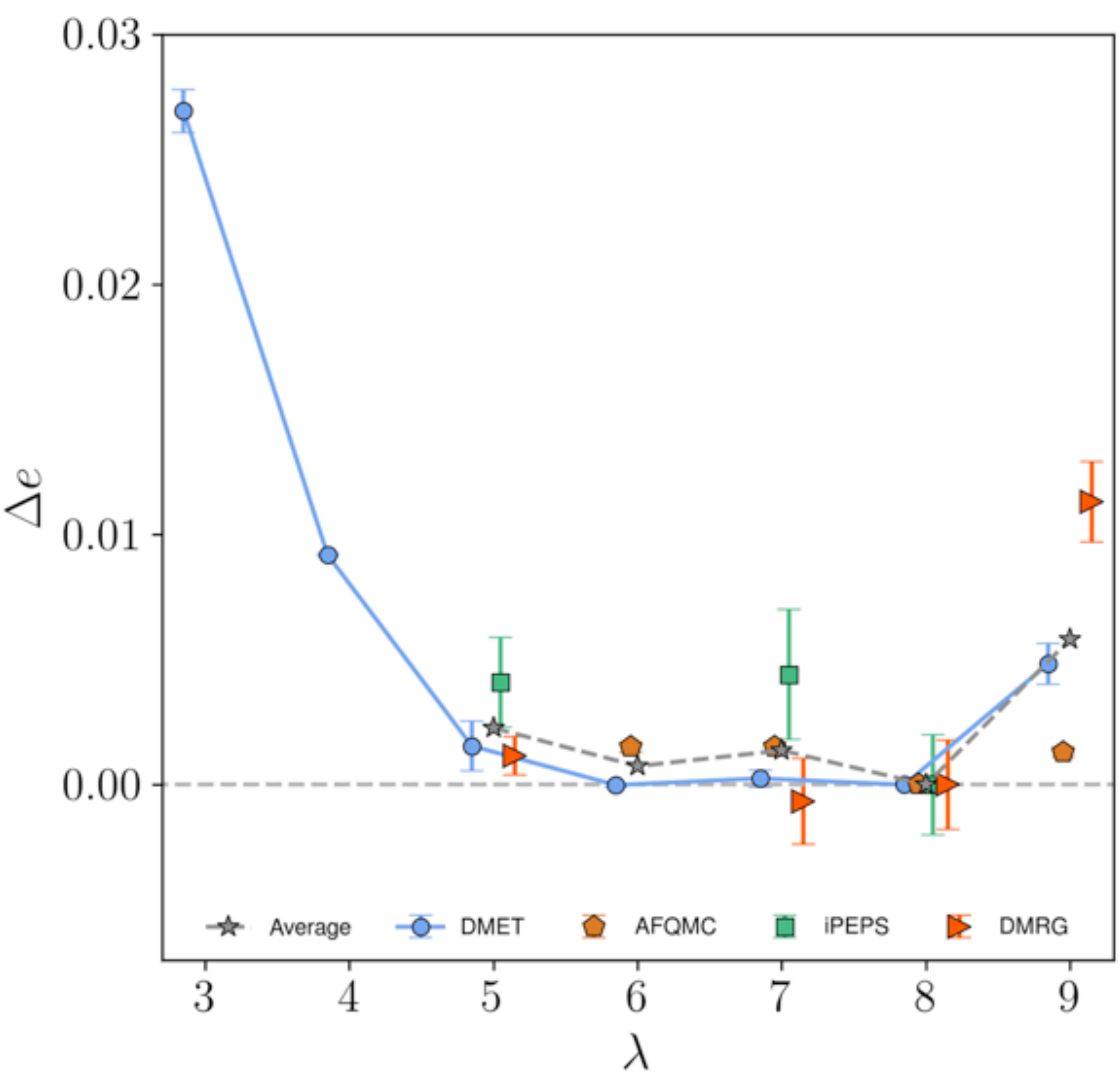
Uniform d-wave

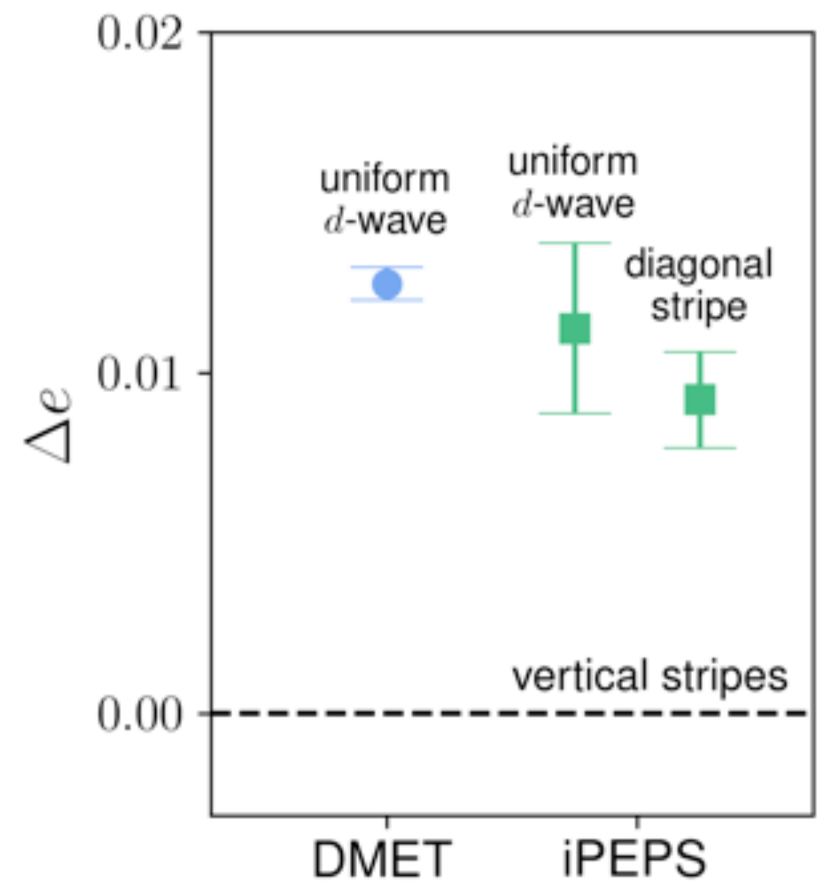


Stripe is lower than uniform state!

➔ λ=8 stripe has lowest energy

Comparison with other methods





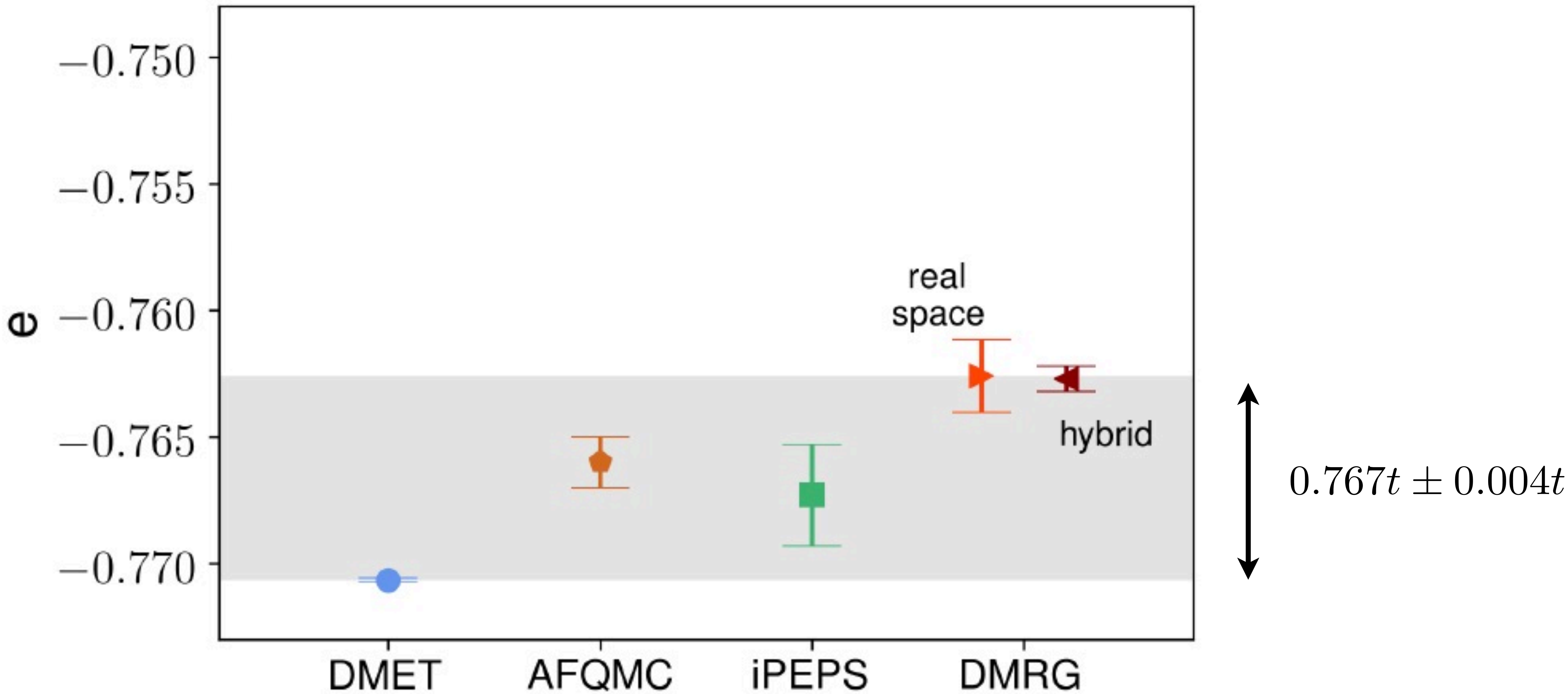
★ Uniform state: higher energy

★ λ=5...8: close in energy

★ λ=8 stripe: slightly lower

★ also compatible with fluctuating stripes

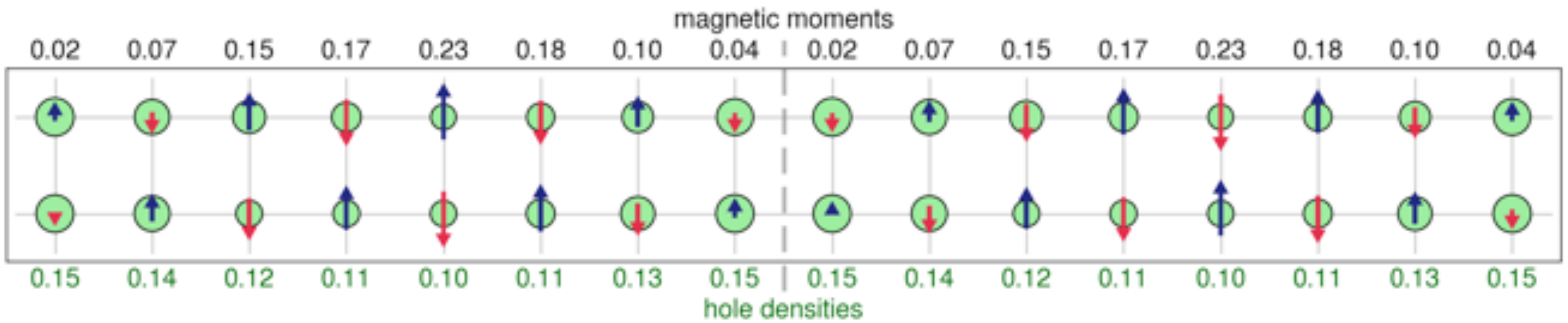
Energy of λ=8 stripe



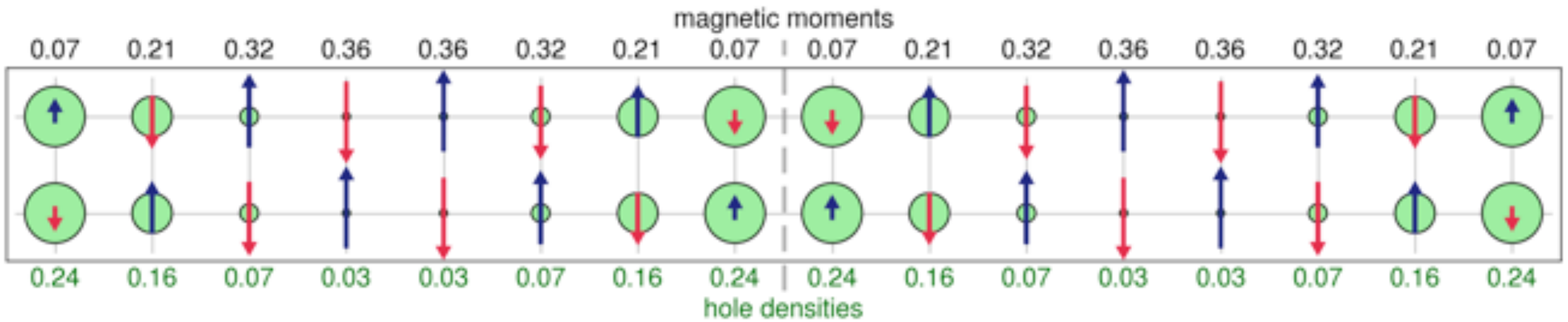
★ Close agreement between methods!

Comparison of λ=8 stripes

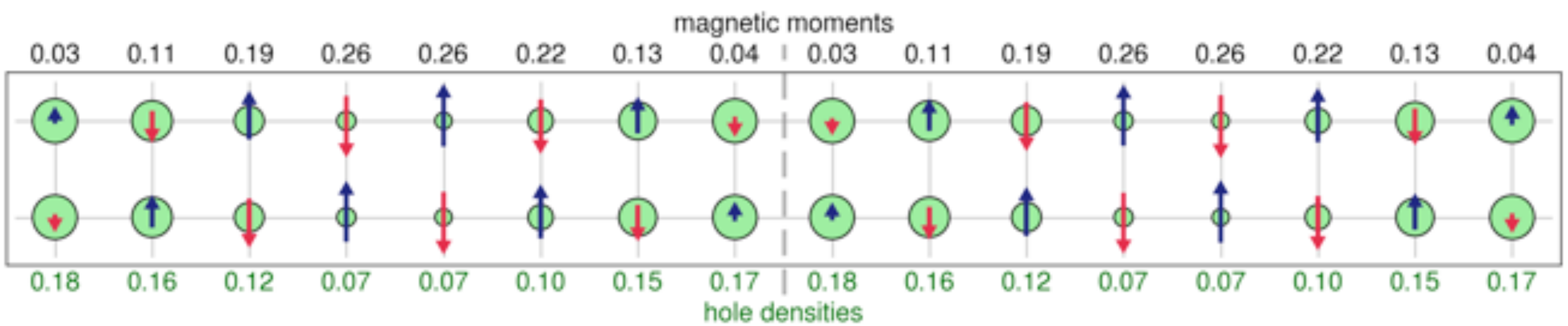
AFQMC:



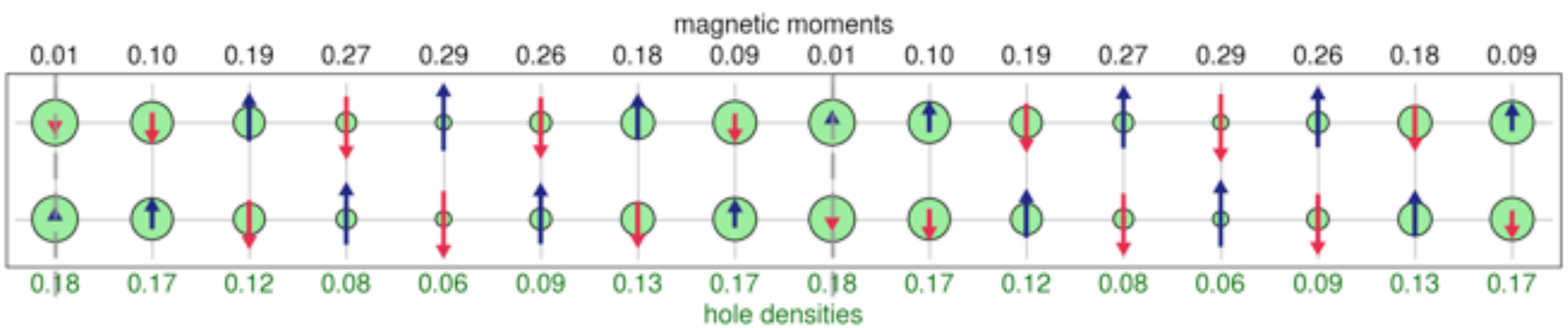
DMET:



DMRG:

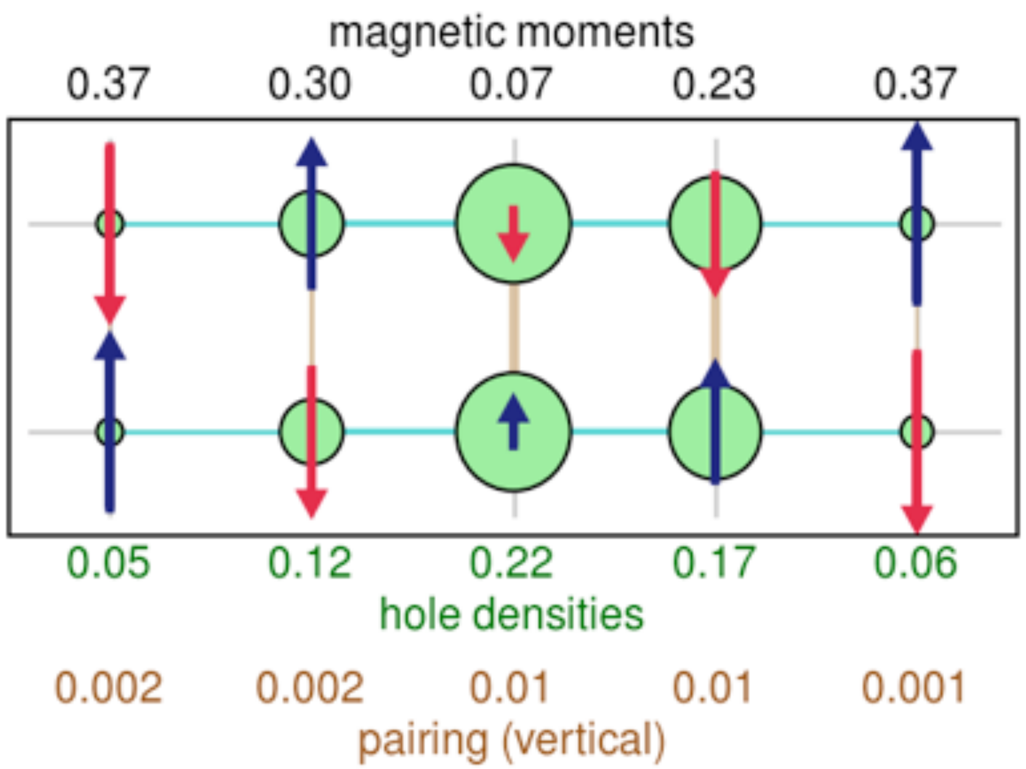


iPEPS:

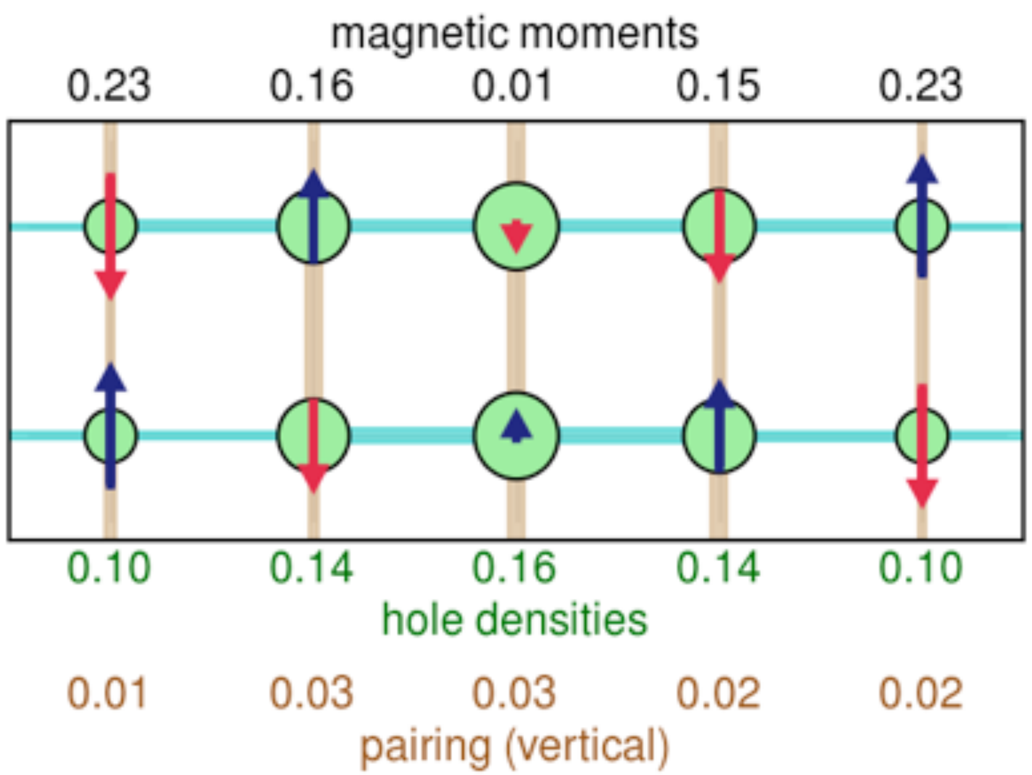


Comparison of λ=5 stripes

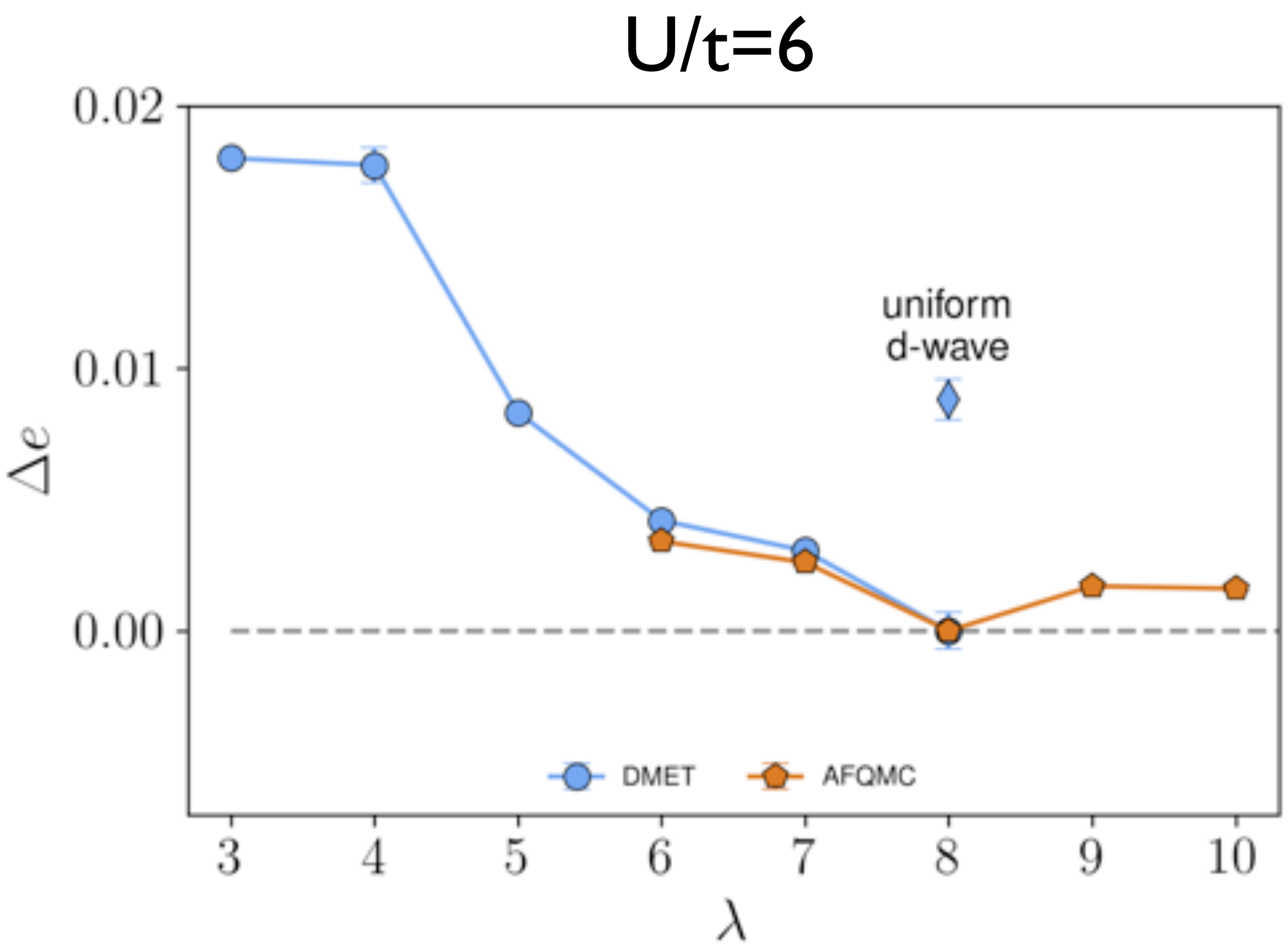
DMET:

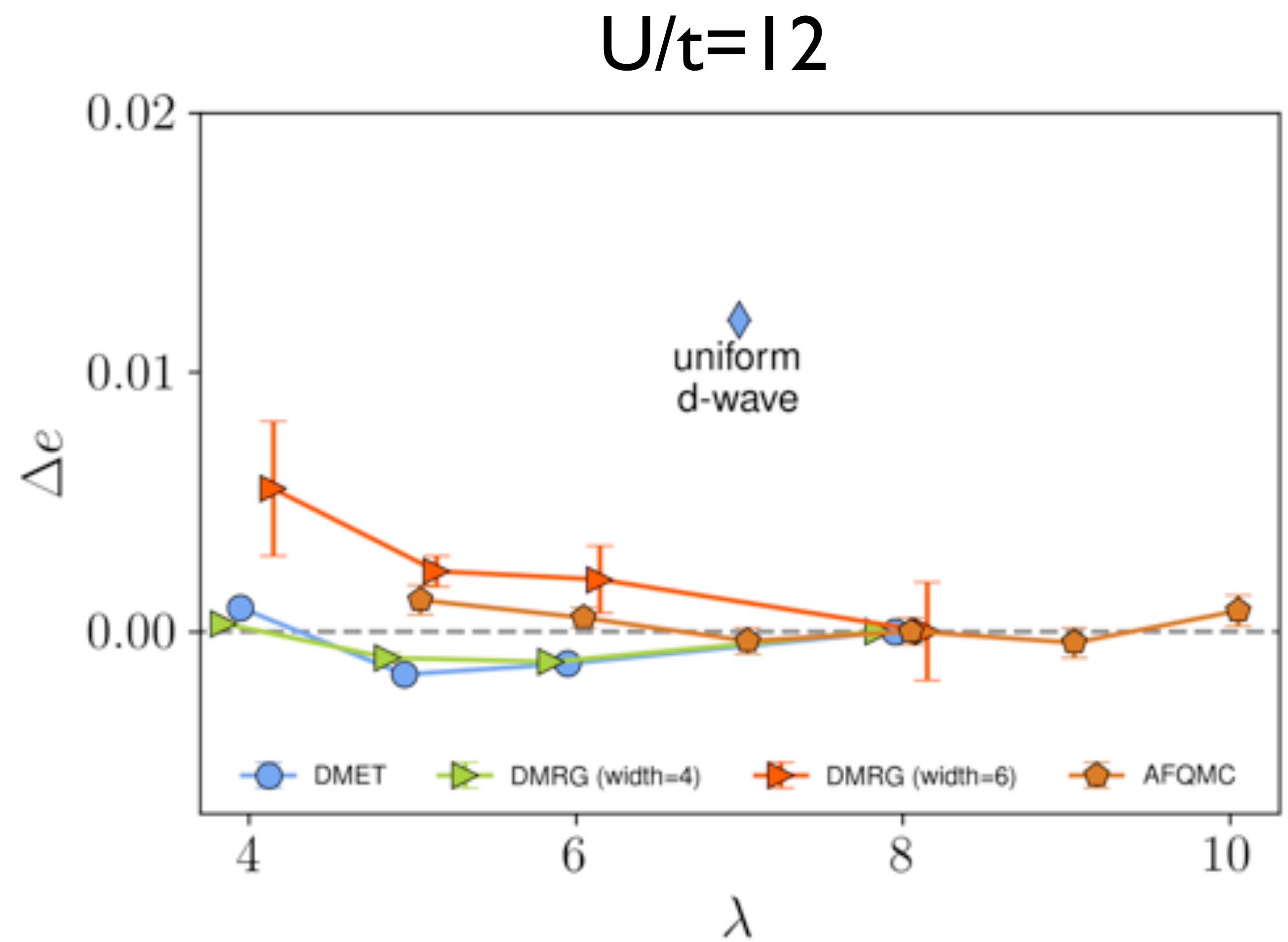


iPEPS:



Results: Other values of U/t





★ λ=8 stripe gets more stable

★ Stronger competition

★ Other wavelengths may get stabilized for larger U/t

★ Uniform state still higher

✓ *t-J* model (iPEPS): fully filled stripes (such as the λ=8 stripe) get favored with increasing J/t (i.e. decreasing U/t) PC, Rice & Troyer, PRL 113 (2014)

Summary

- Doped 2D Hubbard model exhibits many competing low energy states
- Stripes have lower energy than uniform d-wave state ($\delta=1/8$)
- $\lambda=8$ stripe lowest energy, with $\lambda=5$-7 stripes very close in energy (in contrast to $\lambda=4$ stripes in experiments)
- But: $\lambda=4$ may be easily stabilized in more realistic models of the cuprates
- Next: go beyond simple Hubbard model. Systematic study will help to get a better understanding of the competing phases

★ Close agreement between various methods!

★ Combined studies: promising route to solve challenging problems!

★ iPEPS: much room for improvement & many extensions