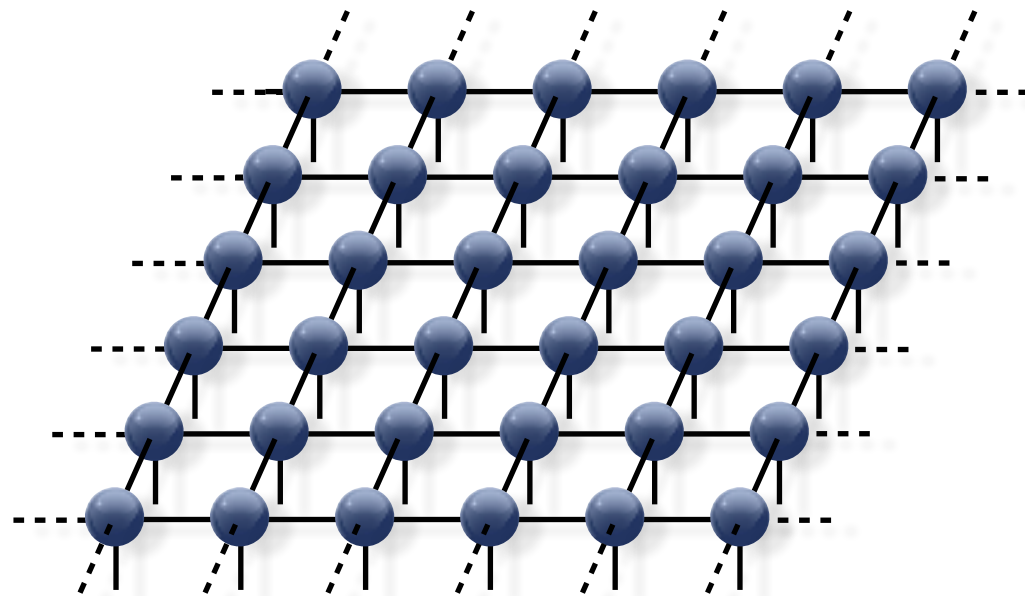


# Lecture III: fermionic tensor networks & simulations of the 2D Hubbard model & other recent progress

Philippe Corboz, Institute for Theoretical Physics, University of Amsterdam



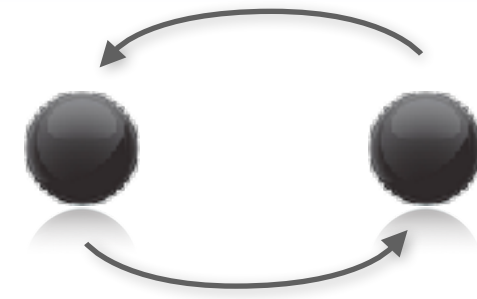


Steve White, 2005: *Perhaps the holy grail, reliable, accurate, and unbiased simulations of large 2D fermion clusters, is becoming within reach!*  
(*Journal Club for Condensed Matter Physics 2005*)

**BUT how can we simulate fermions with tensor networks in 2D???**

# Fermions with 2D tensor networks

**How to take fermionic statistics into account?**



$$\hat{c}_i \hat{c}_j = - \hat{c}_j \hat{c}_i$$

fermionic operators *anticommute*

## **Different formulations (but same fermionic ansatz):**

PC, Evenbly, Verstraete, Vidal (2009)

Kraus, Schuch, Verstraete, Cirac (2009)

Pineda, Barthel, Eisert (2009)

PC & Vidal (2009)

Barthel, Pineda, Eisert (2009)

Shi, Li, Zhao, Zhou (2009)

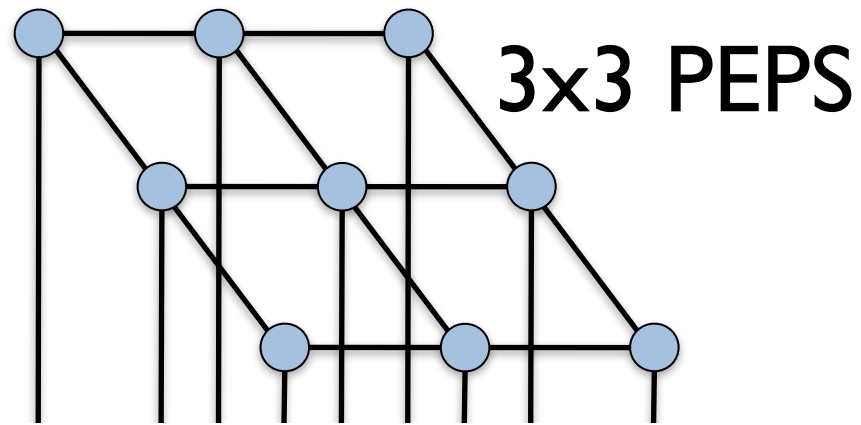
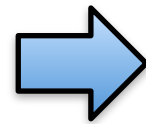
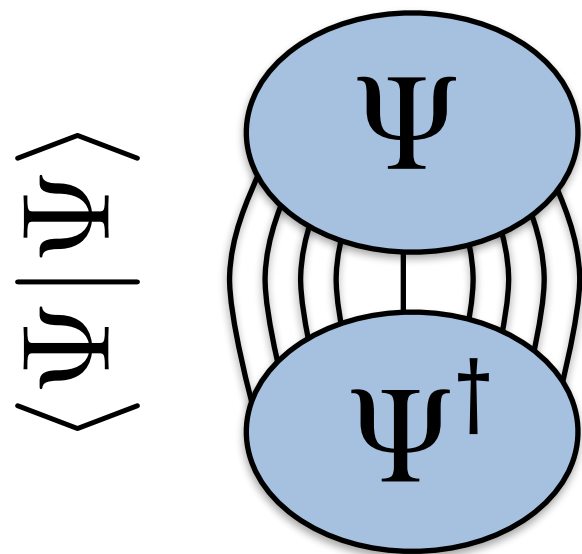
PC, Orus, Bauer, Vidal (2009)

Pizorn, Verstraete (2010)

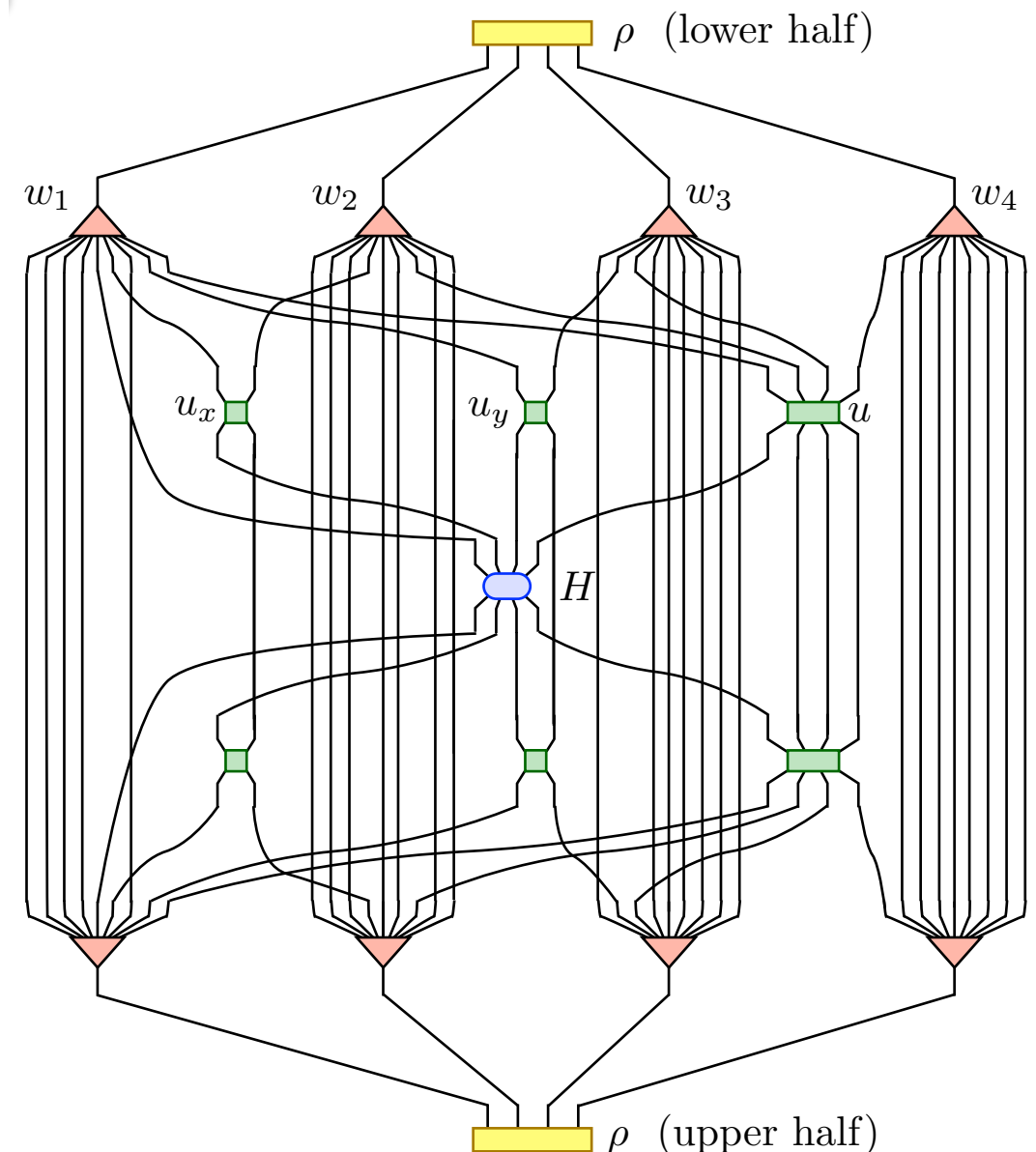
Gu, Verstraete, Wen (2010)

...

# Crossings in 2D tensor networks



Example network  
of the 2D MERA



Crossings appear when  
projecting the 3D  
network onto 2D!

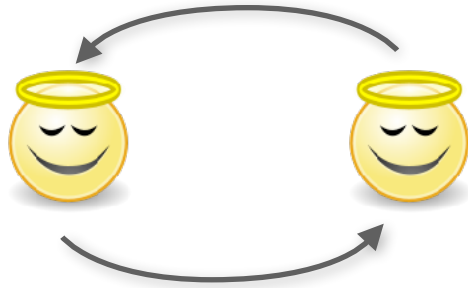




**Bosons**

vs

**Fermions**

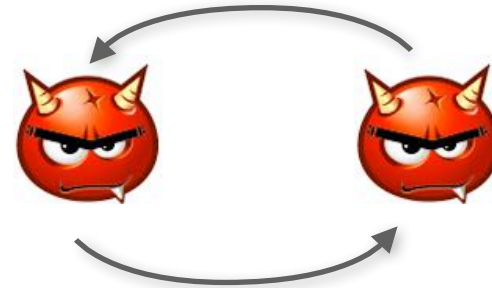


$$\Psi_B(x_1, x_2) = \Psi_B(x_2, x_1)$$

**symmetric!**

$$\hat{b}_i \hat{b}_j = \hat{b}_j \hat{b}_i$$

operators **commute**



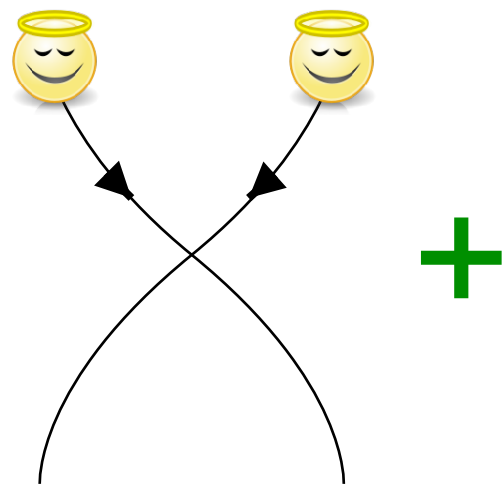
$$\Psi_F(x_1, x_2) = -\Psi_F(x_2, x_1)$$

**antisymmetric!**

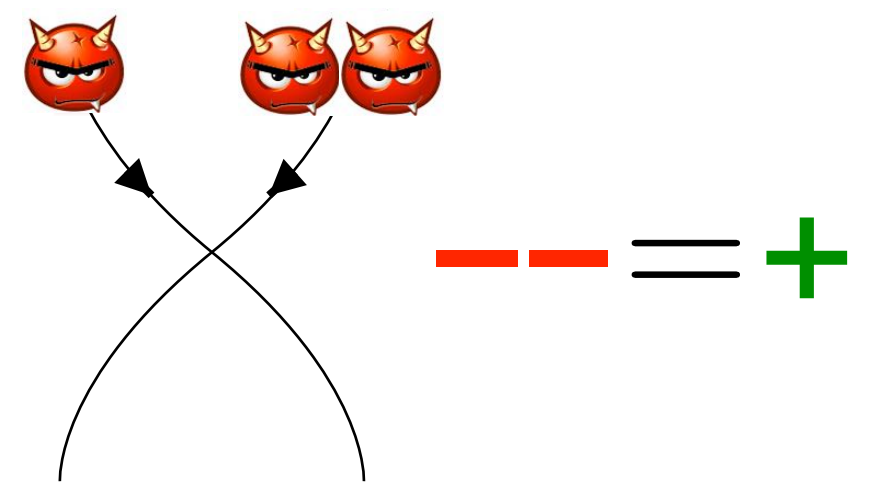
$$\hat{c}_i \hat{c}_j = -\hat{c}_j \hat{c}_i$$

operators **anticommute**

Crossings  
in a tensor  
network



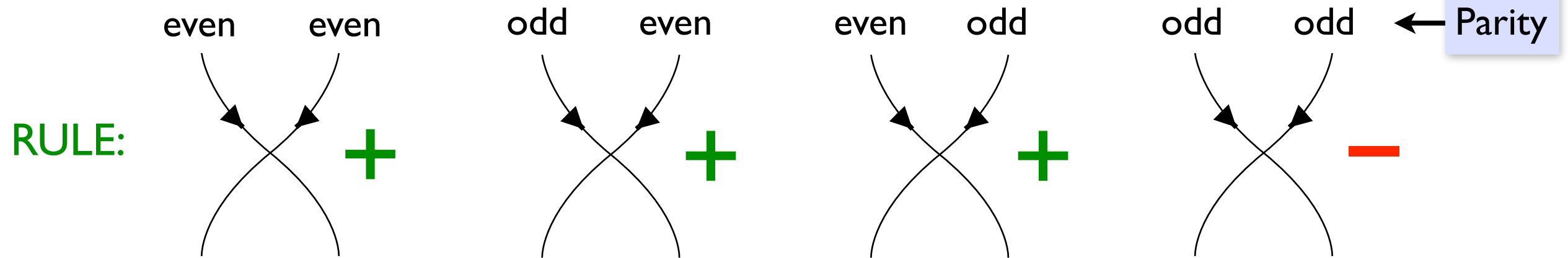
ignore crossings



**take care!**

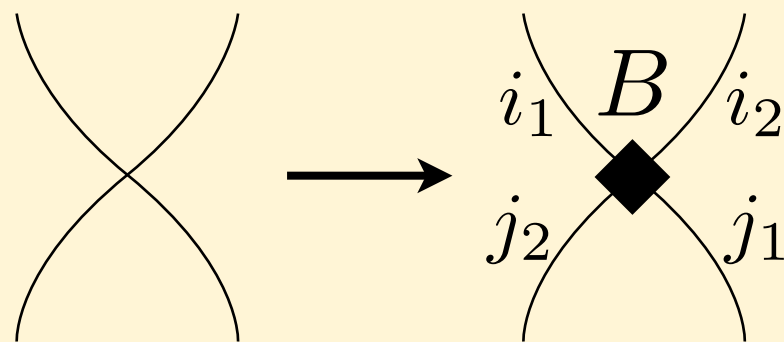
# The swap tensor

# Fermions



Parity  $P$  of a state:  $\begin{cases} P = +1 & \text{(even parity), even number of particles} \\ P = -1 & \text{(odd parity), odd number of particles} \end{cases}$

Replace crossing by **swap tensor**



$$B_{j_2 j_1}^{i_1 i_2} = \delta_{i_1, j_1} \delta_{i_2, j_2} S(P(i_1), P(i_2))$$

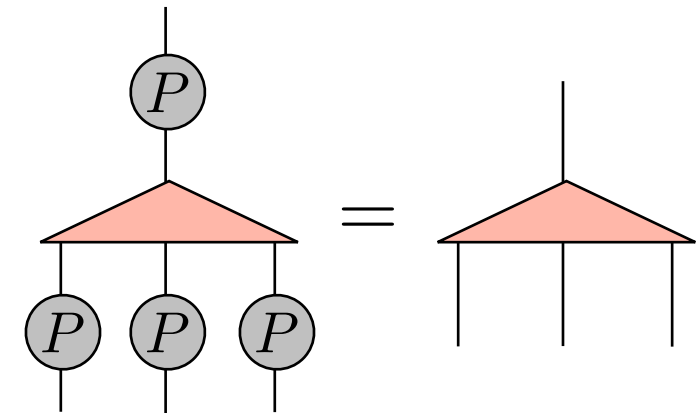
$$S(P(i_1), P(i_2)) = \begin{cases} -1 & \text{if } P(i_1) = P(i_2) = -1 \\ +1 & \text{otherwise} \end{cases}$$

# Parity symmetry

- Fermionic systems exhibit **parity symmetry!**  $[\hat{H}, \hat{P}] = 0$

- Choose all tensors to be **parity preserving!**

$$T_{i_1 i_2 \dots i_M} = 0 \quad \text{if } P(i_1)P(i_2) \dots P(i_M) \neq 1$$



- Decomposing local Hilbert spaces into even and odd parity sectors

$$\mathbb{V} = \underbrace{\mathbb{V}(+) \oplus}_{\text{even}} \underbrace{\mathbb{V}(-)}_{\text{odd}}$$

- Label state by a composite index

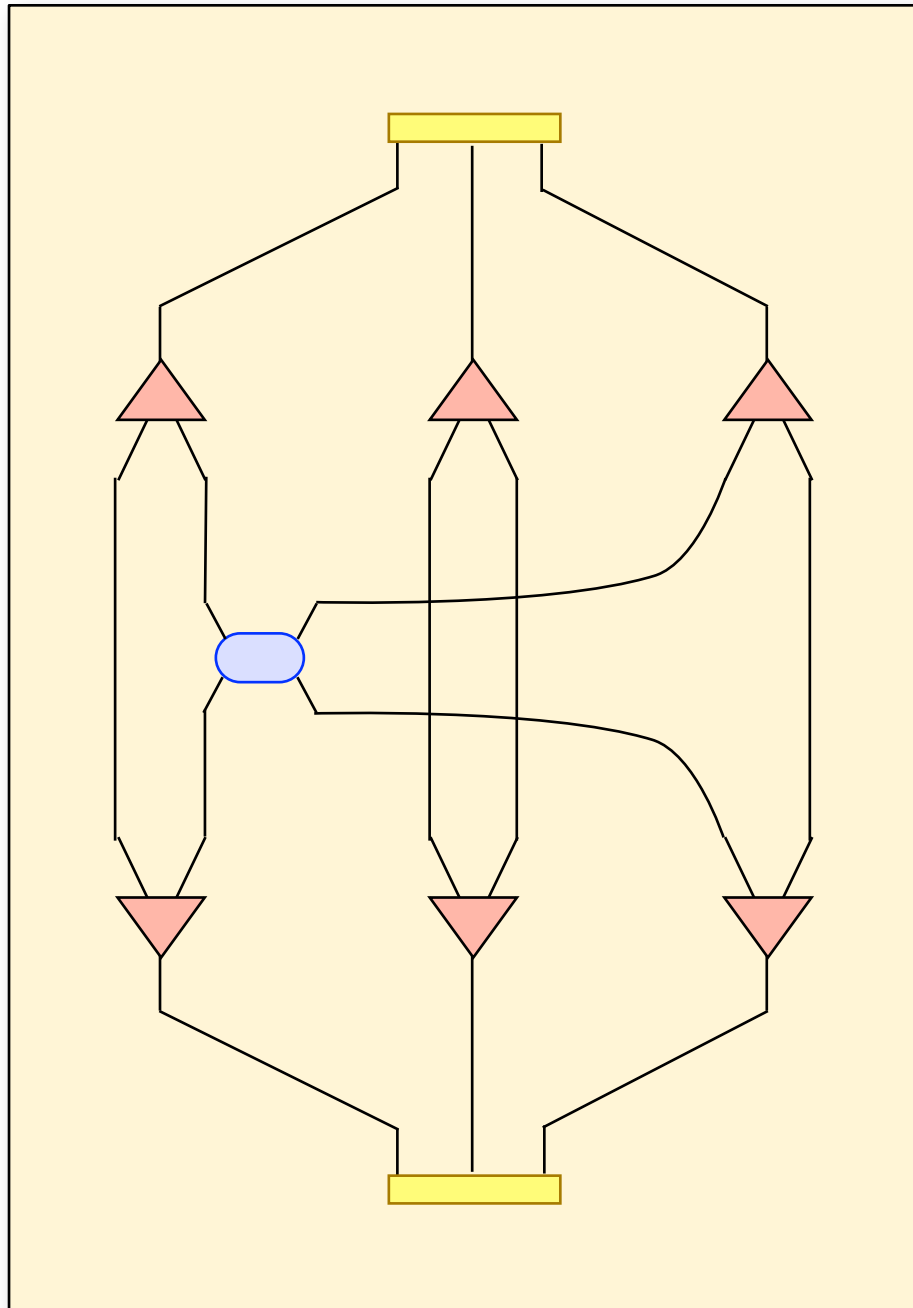
$$i = (p, \alpha_p)$$

parity sector  $\swarrow$   $\nwarrow$  enumerate states in parity sector  $p$   
 $\downarrow$   $\nearrow$

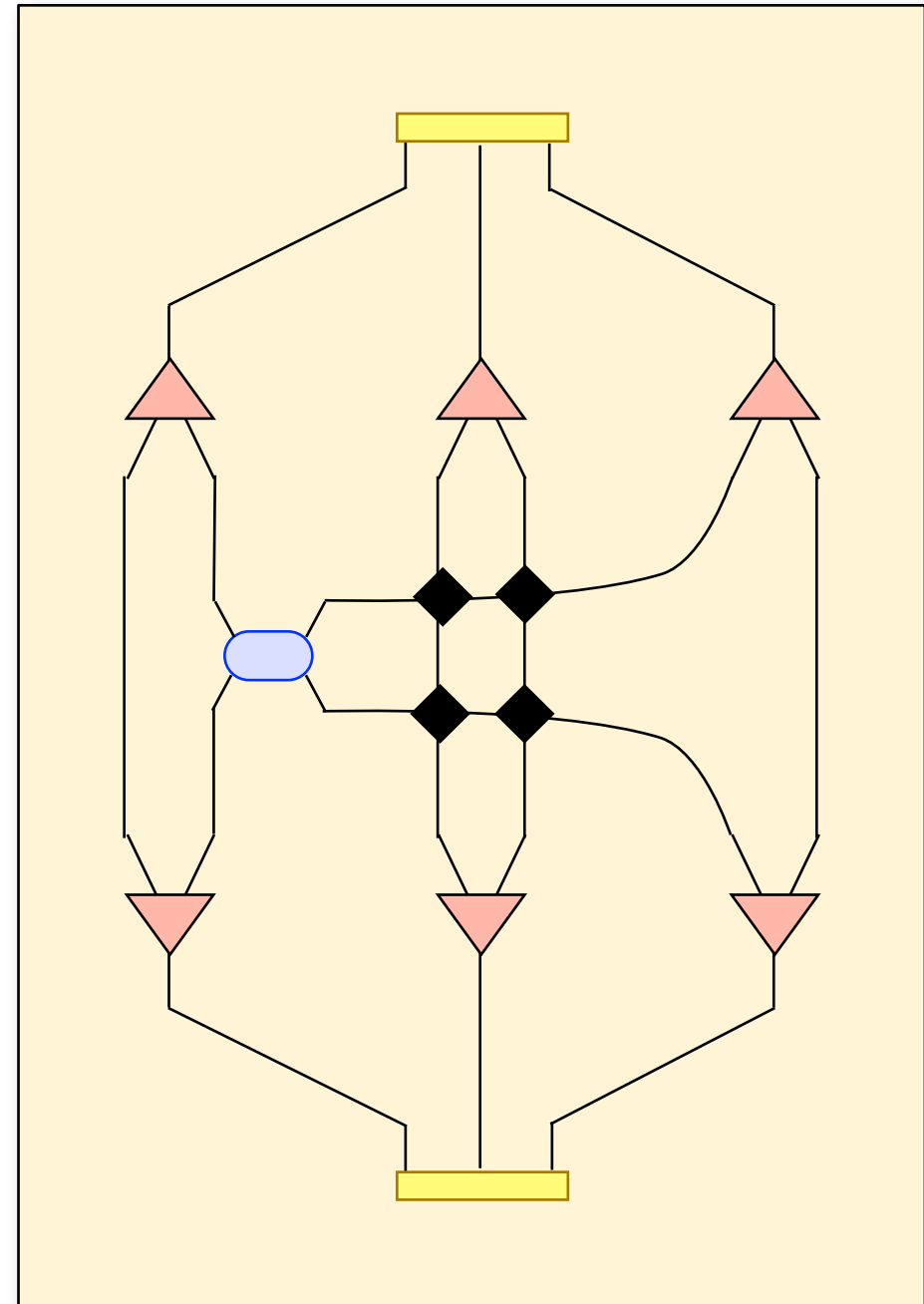
- ➡ tensor with a block structure (similar to a block diagonal matrix)
- ➡ Easy identification of the parity of a state!
- ➡ Important for efficiency

# Example

Bosonic tensor network



Fermionic tensor network



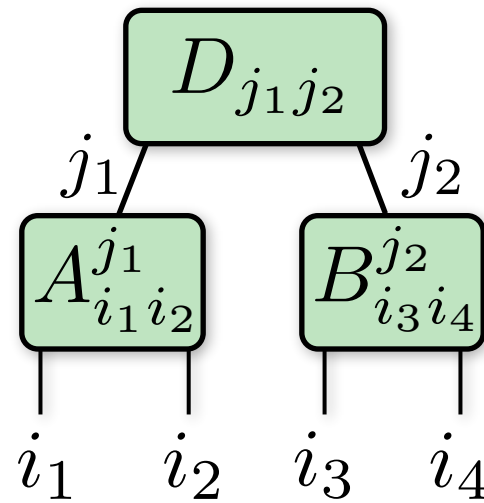
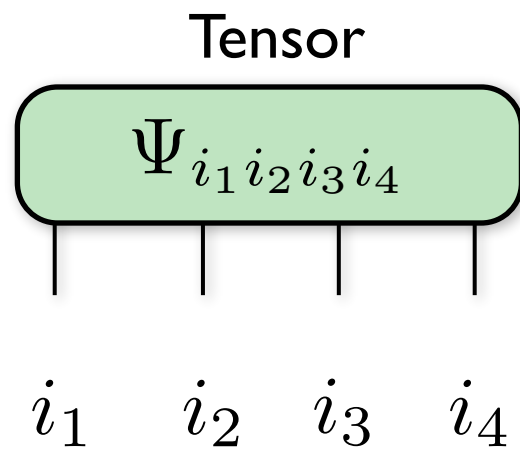
# Fermionic “operator networks”

State of 4 site system

$$|\Psi\rangle = \sum_{i_1 i_2 i_3 i_4} \Psi_{i_1 i_2 i_3 i_4} |i_1 i_2 i_3 i_4\rangle$$

$\{|0\rangle, |1\rangle\}$

Bosons

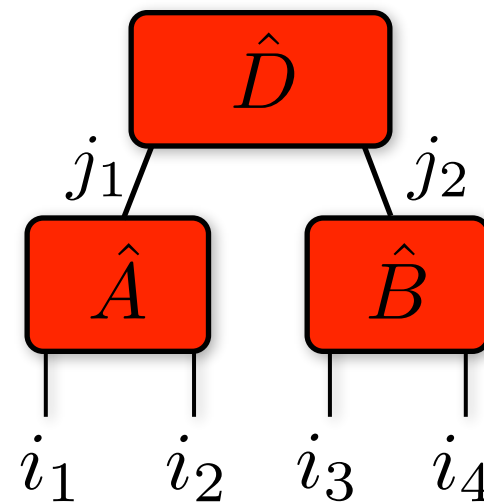
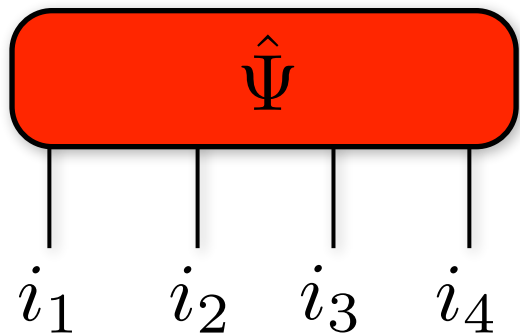


**bosonic  
tensor  
network**

Contract

Fermions

Tensor + fermionic ops



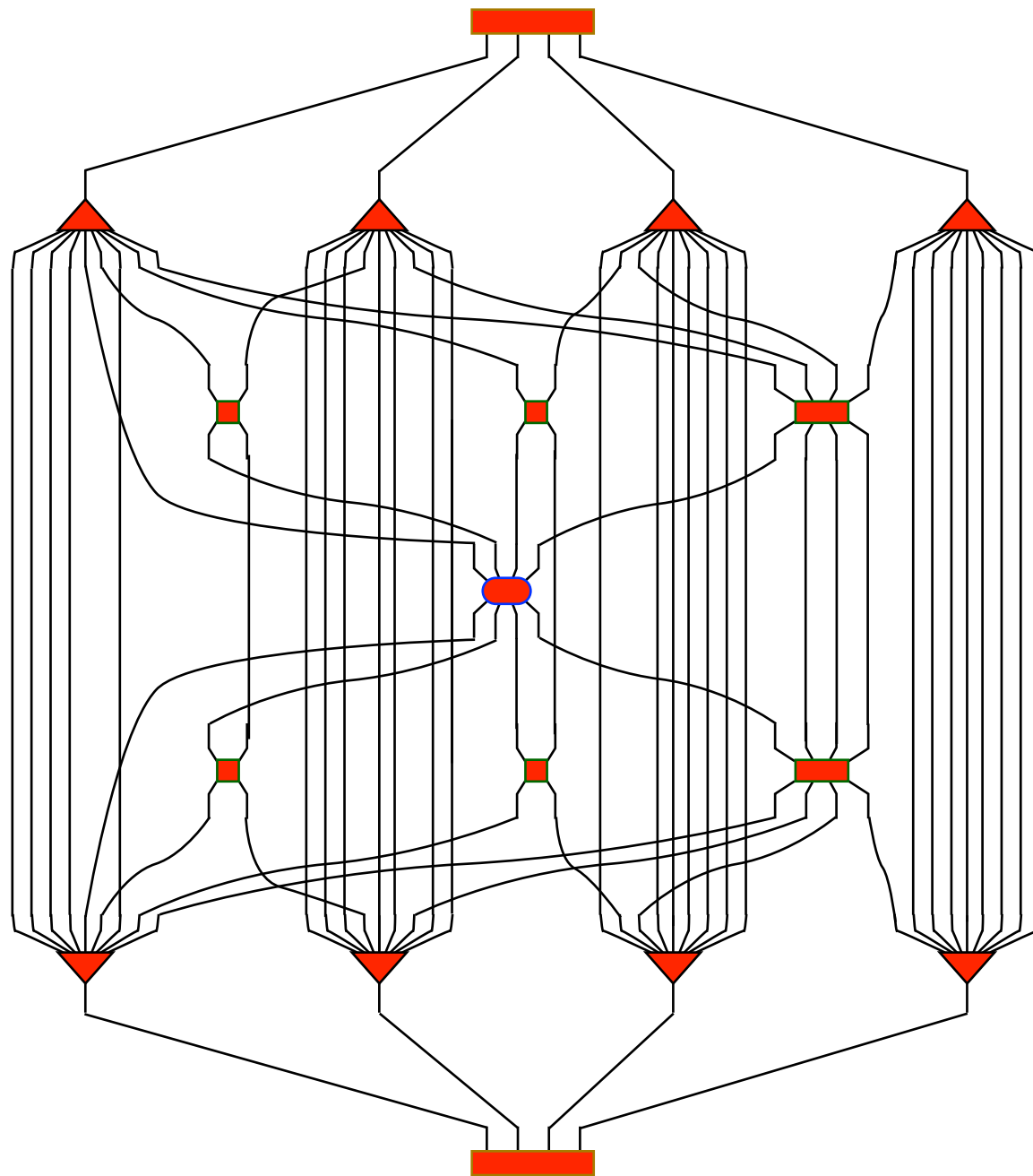
**fermionic  
operator  
network**

Contract  
+  
operator  
calculus

$$\hat{A} = A_{i_1 i_2}^{j_1} |i_1 i_2\rangle \langle j_1| = A_{i_1 i_2}^{j_1} \hat{c}_1^{\dagger i_1} \hat{c}_2^{\dagger i_2} |0\rangle \langle 0| \hat{c}_1^{j_1}$$

# Fermionic “operator network”

**Use anticommutation rules to evaluate fermionic operator network:**

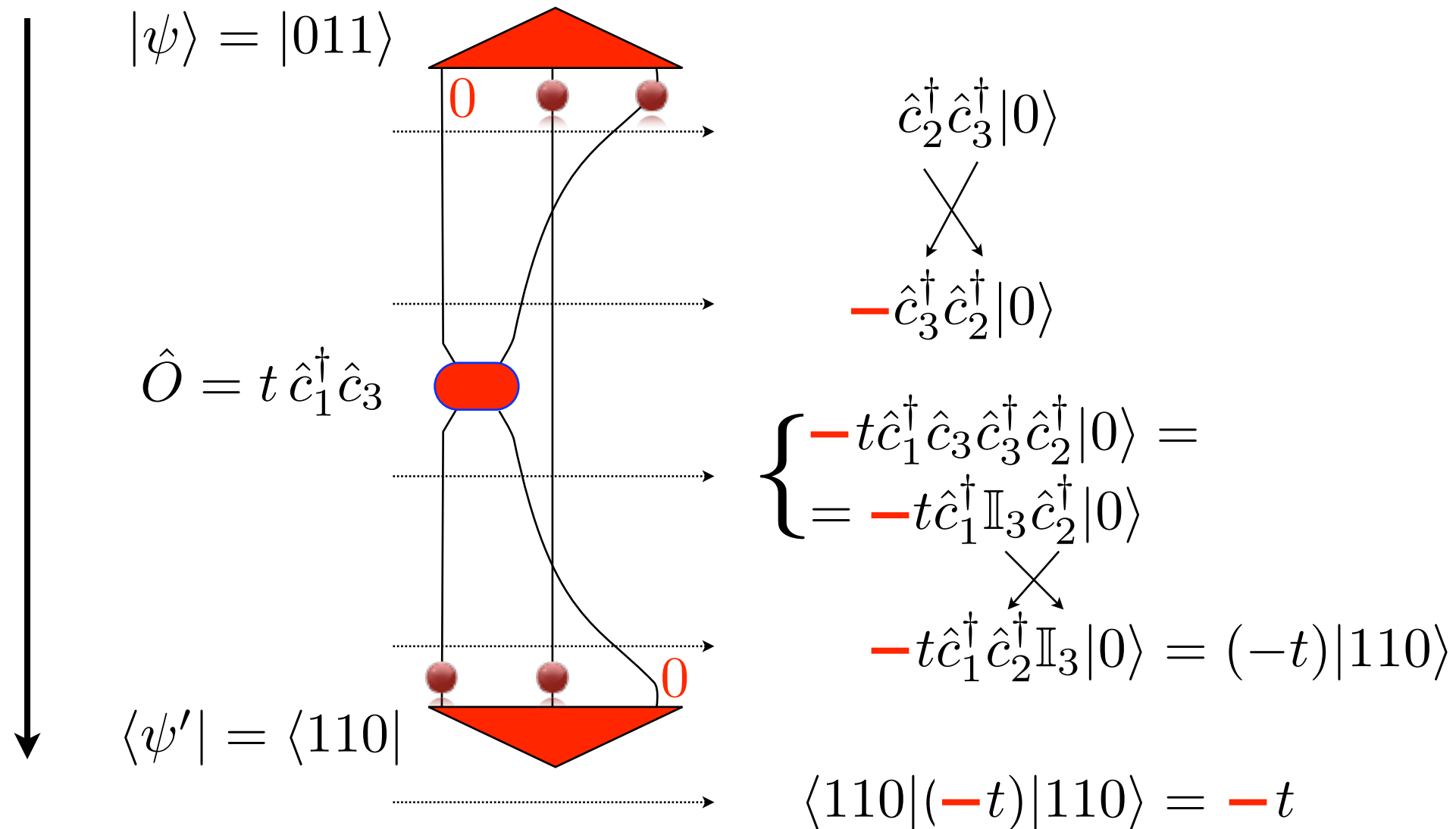


**Solution:**  
Map it to a tensor network by replacing crossings by swap tensors



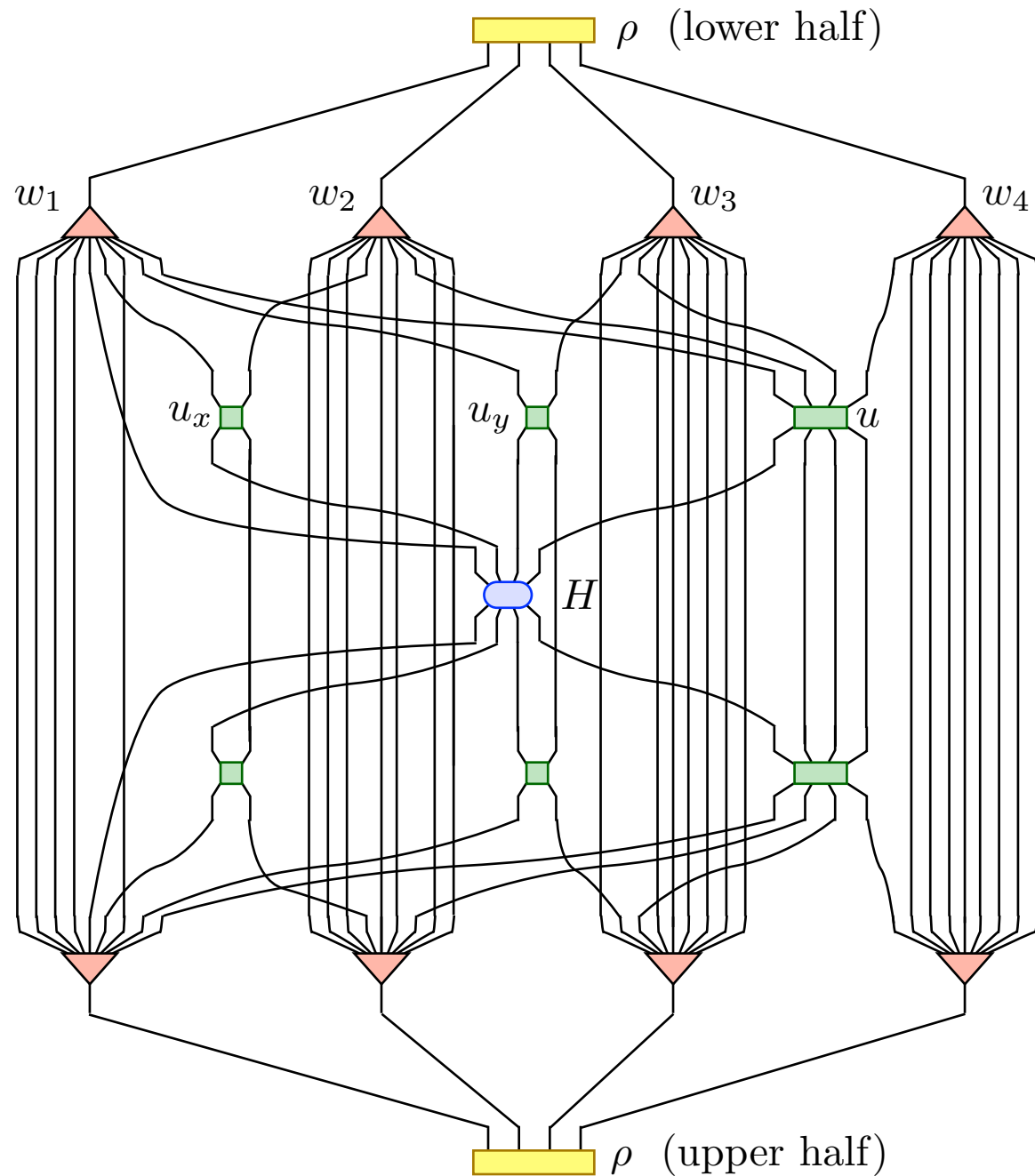
# Example

A simple example:  $\langle \psi' | \hat{O} | \psi \rangle$ ,  $\hat{O} = t \hat{c}_1^\dagger \hat{c}_3$



➡ All involved anticommutations to evaluate a fermionic operator network are represented by a crossing

# Cost of fermionic tensor networks??



First thought:

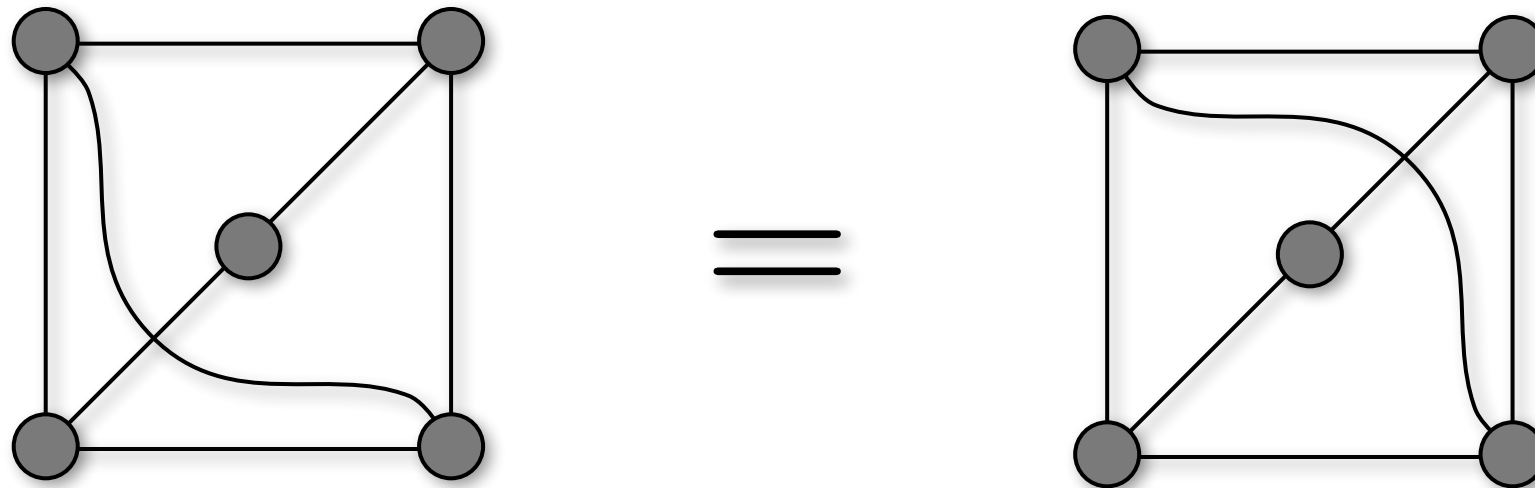
Many crossings  $\rightarrow$  many more tensors

$\rightarrow$  **larger computational cost??**

**NO!**

**Same computational cost**

# The “jump” move

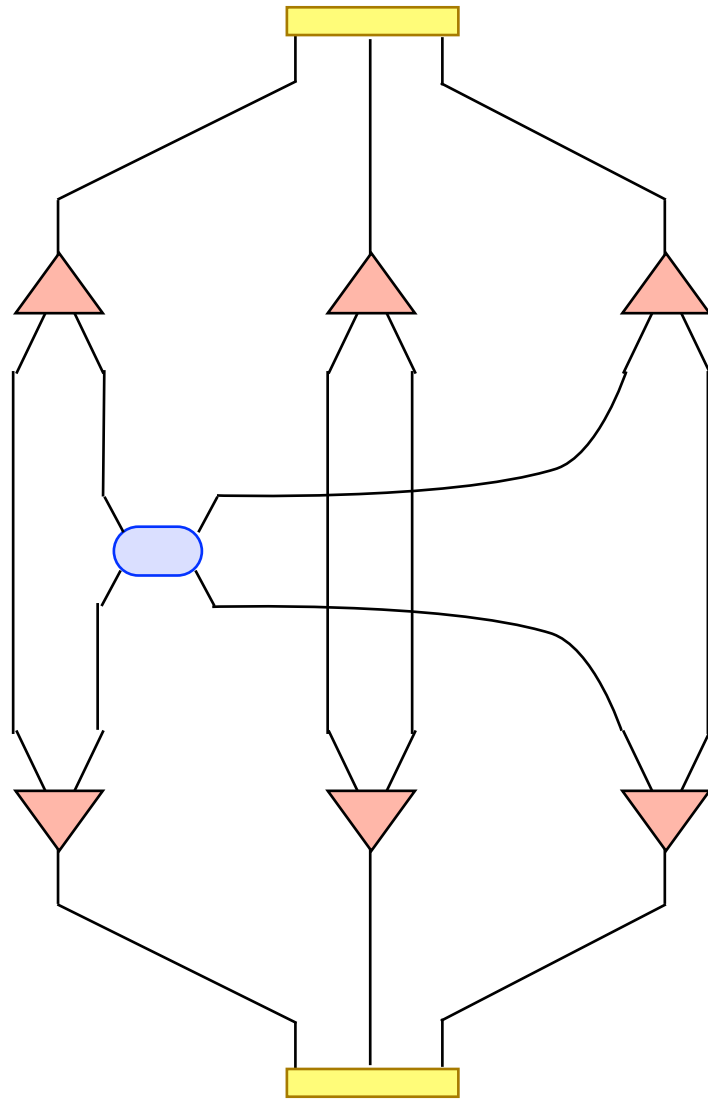


- Jumps over tensors leave the tensor network **invariant**
- Follows form parity preserving tensors

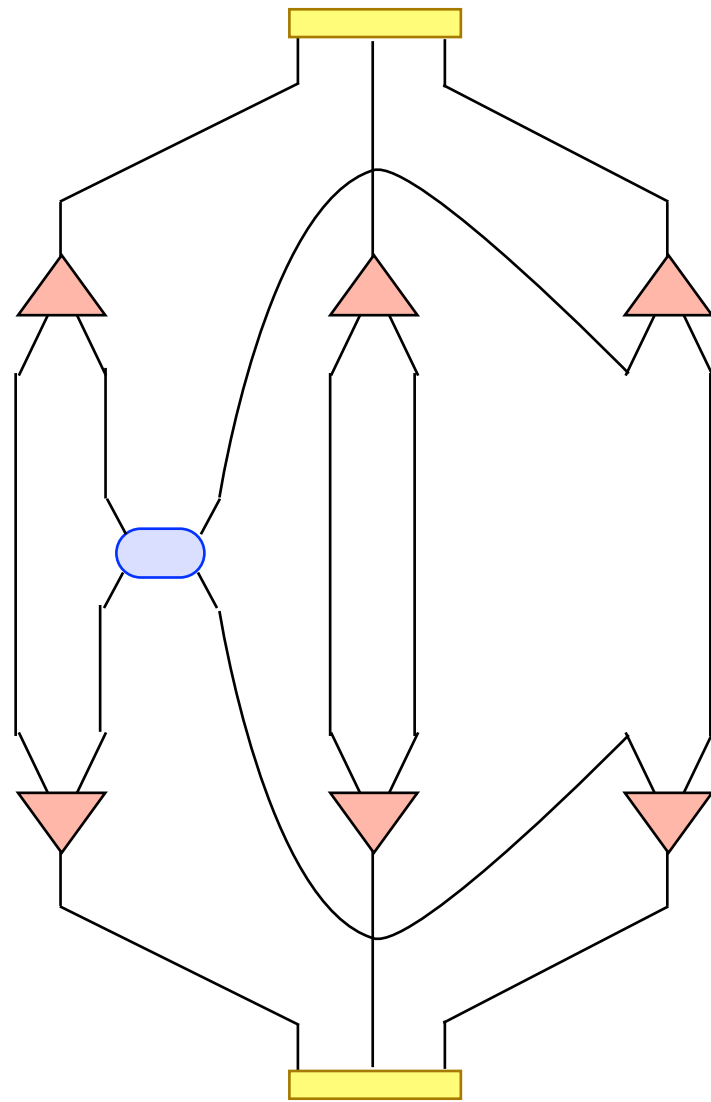
$$[\hat{T}, \hat{c}_k] = 0, \quad \text{if } k \notin \text{sup}[\hat{T}]$$

- Allows us to simplify the tensor network
- Final cost of contraction is the same as in a bosonic tensor network

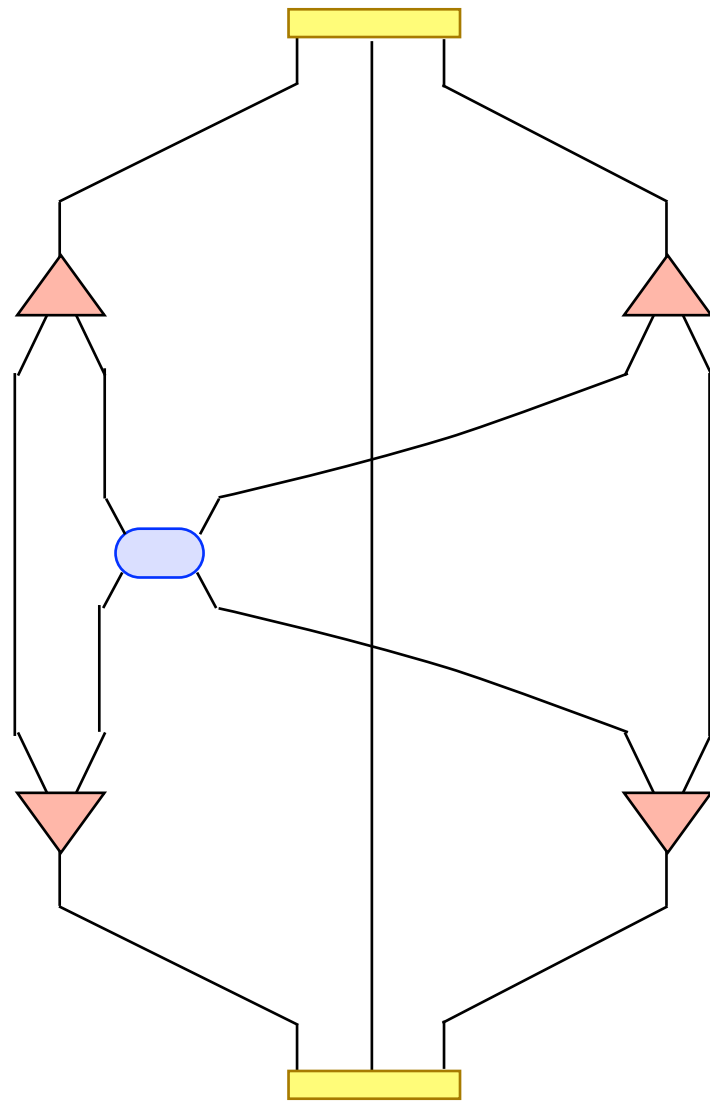
# Example of the “jump” move



# Example of the “jump” move

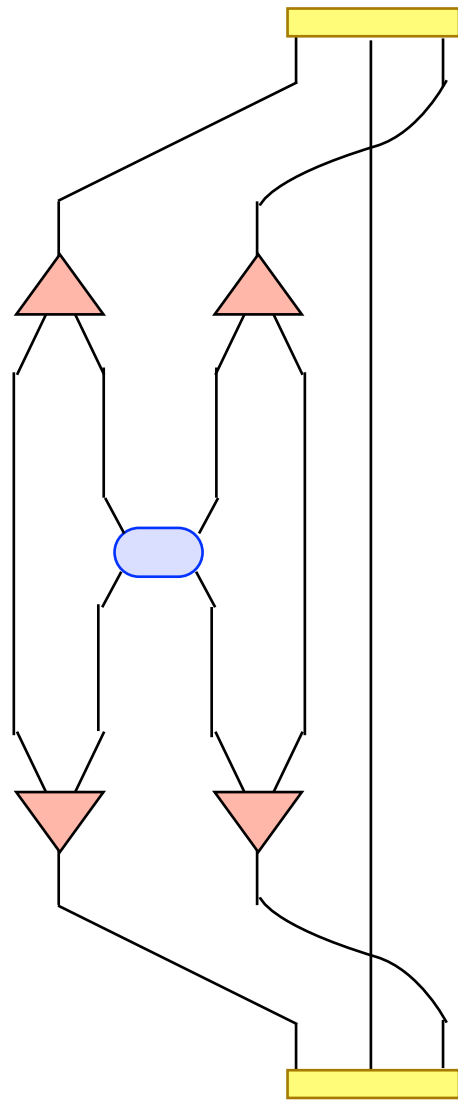


# Example of the “jump” move

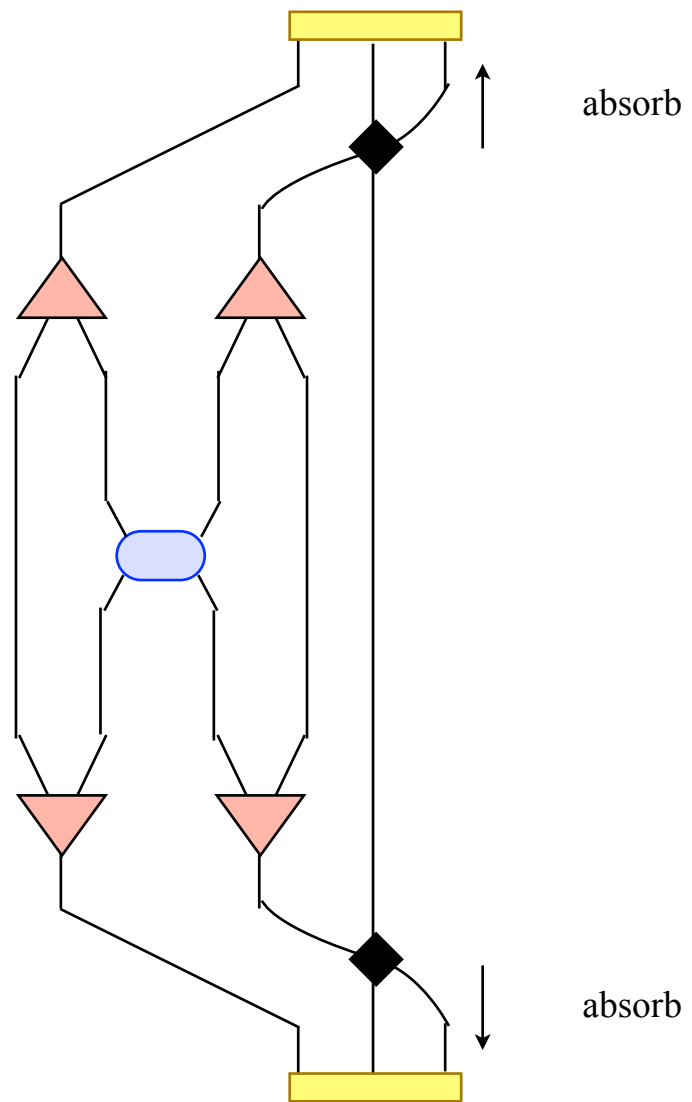




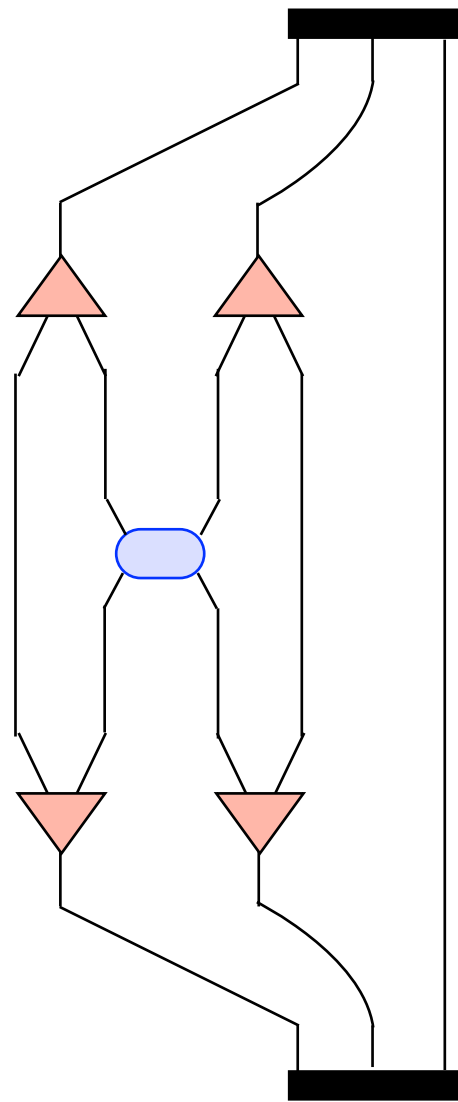
# Example of the “jump” move



# Example of the “jump” move



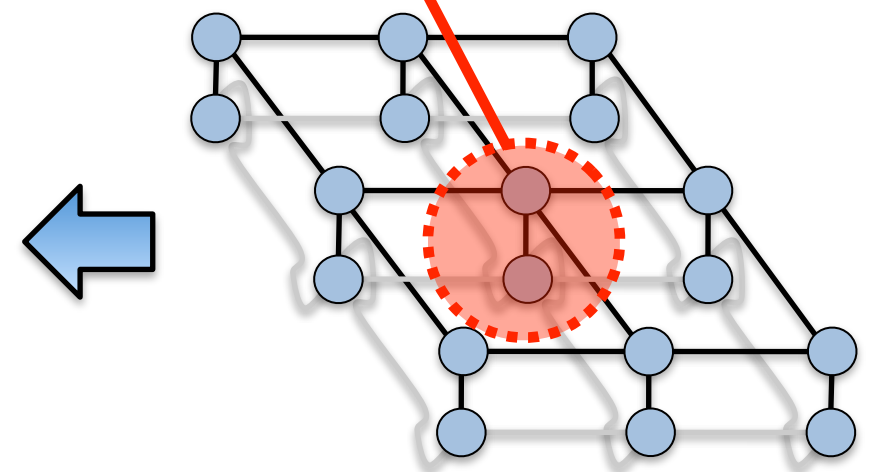
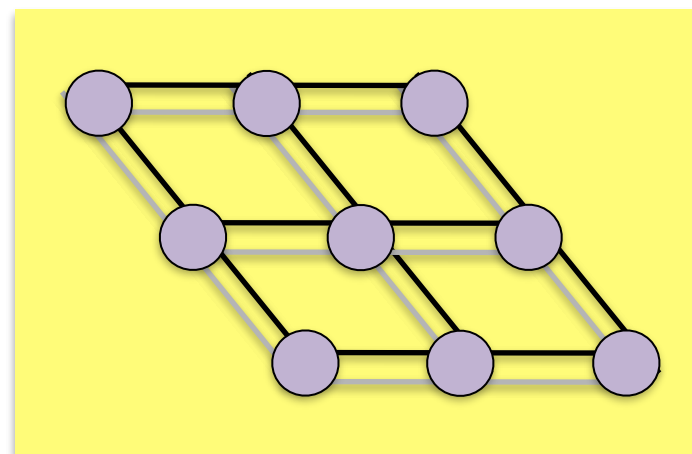
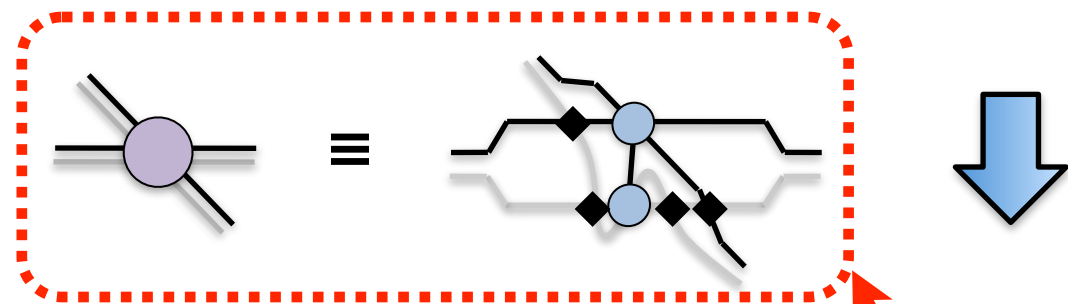
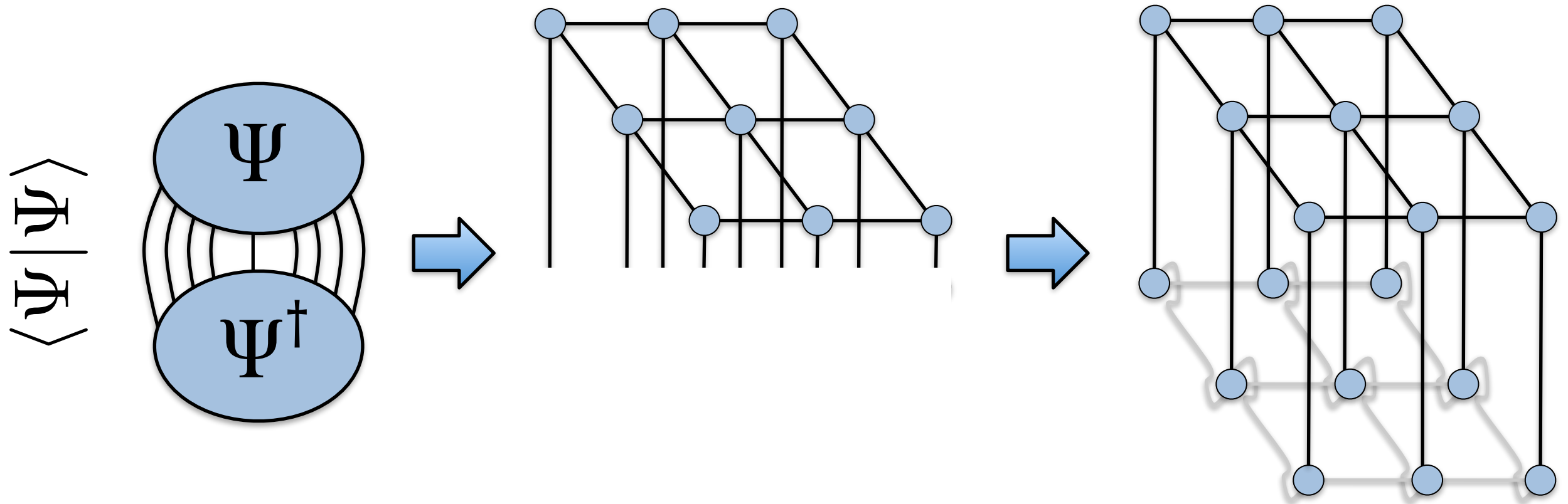
# Example of the “jump” move



now  
contract as usual!

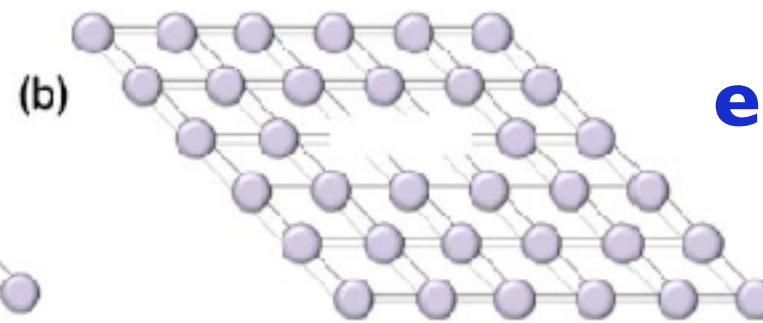
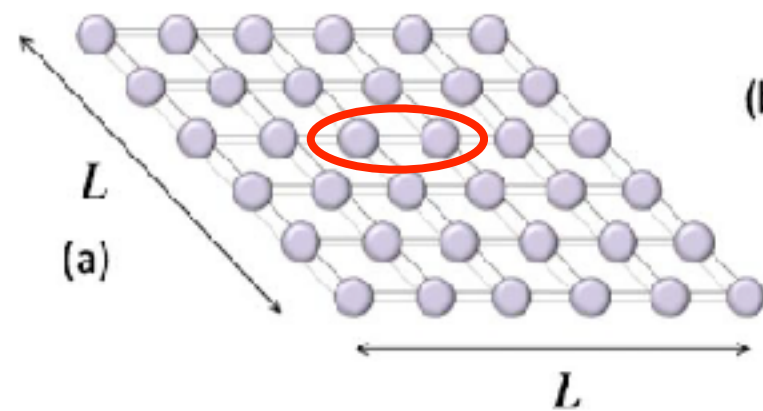
- ▶ **Possible to automatize:  
add swap whenever legs  
of tensors are permuted**

# Fermionic (i)PEPS



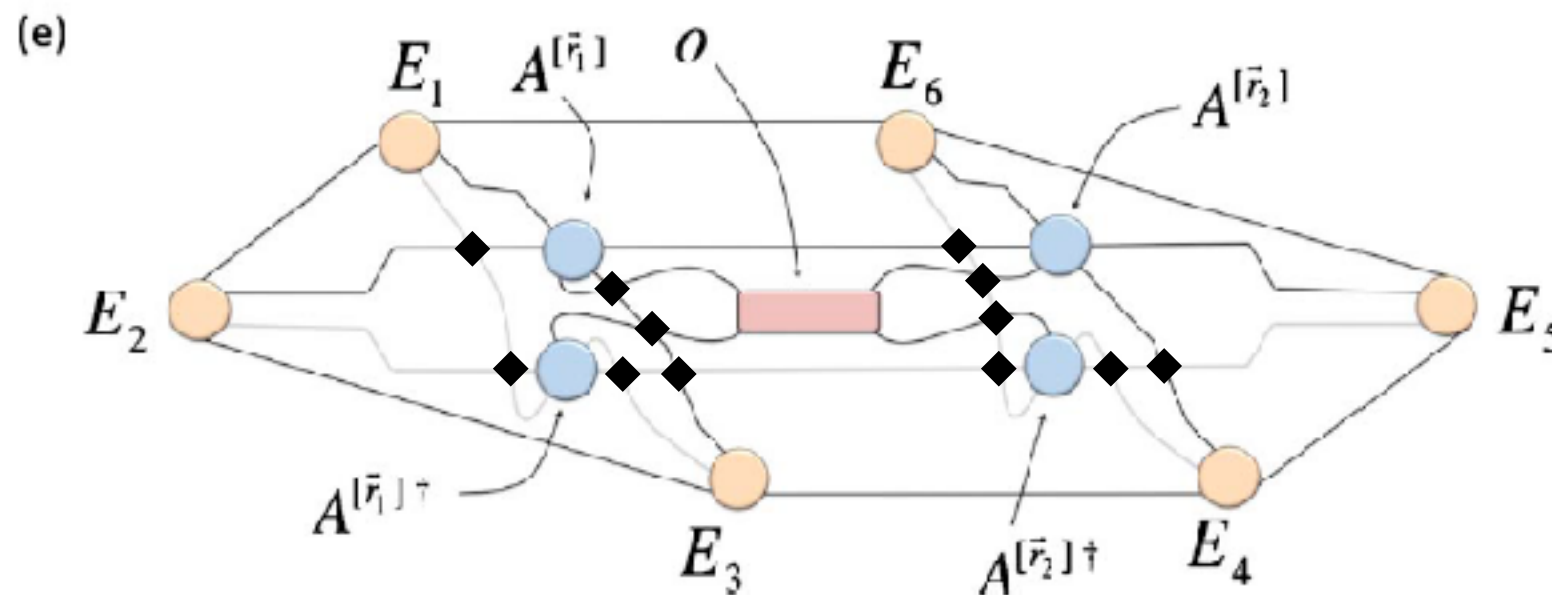
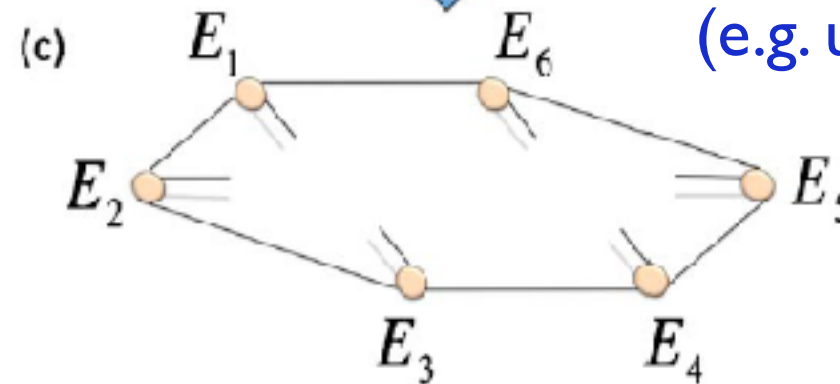
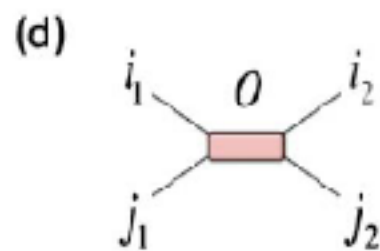
- ▶ **No** crossings anymore
- ▶ Fermionic signs taken into account **locally!**
- ▶ Only small modification to bosonic PEPS

# Fermionic (i)PEPS: expectation values



**environment**

compute environment approximately  
(e.g. using MPS)



Connect two-body operator

insert swap tensors

Contract this network!



# Summary: Fermionic TN

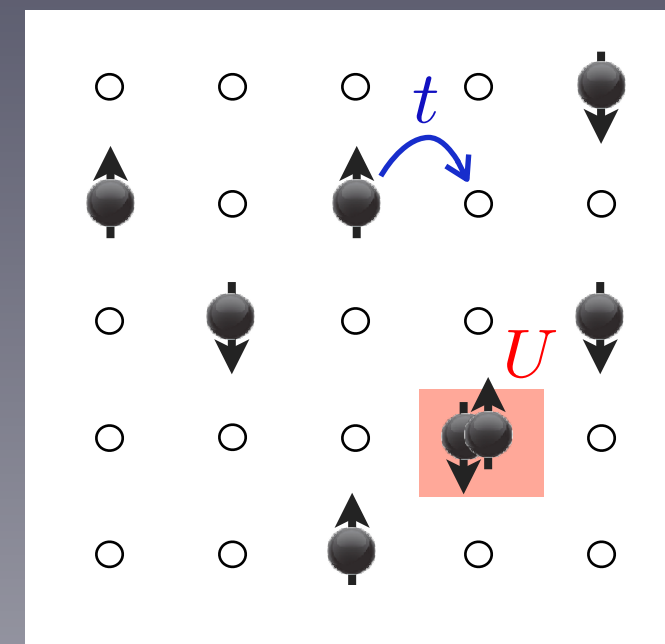
- ➔ Simulate fermionic systems with 2D tensor networks
  - ➔ Replace crossings by swap tensors & use parity preserving tensors
- ➔ Same leading computational cost in  $\mathcal{D}$



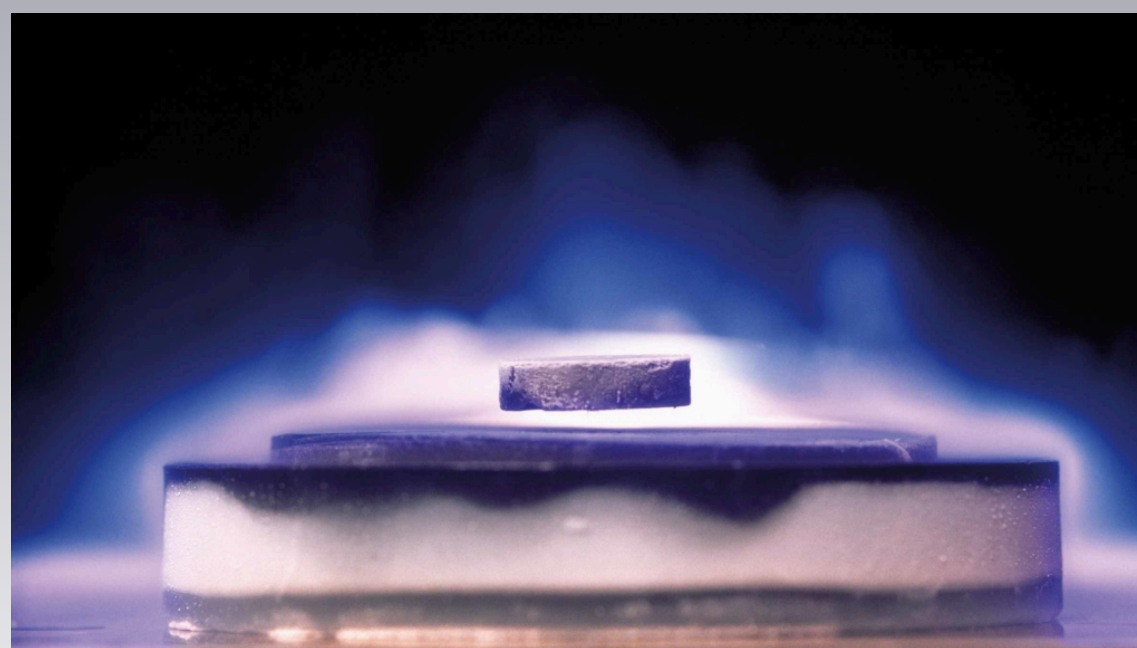
# The 2D Hubbard model

★ *The most basic model of strongly correlated electrons*

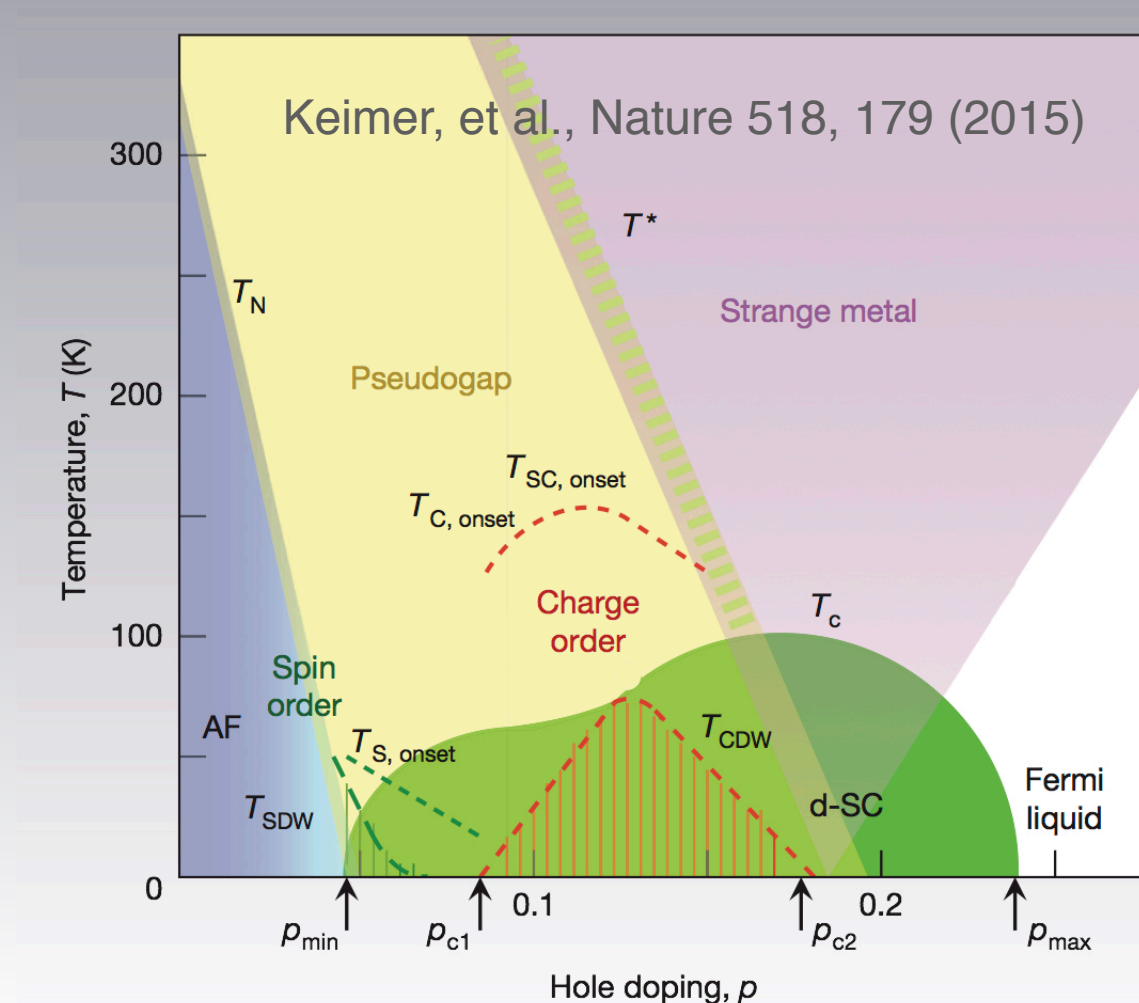
$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + h.c. + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$



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

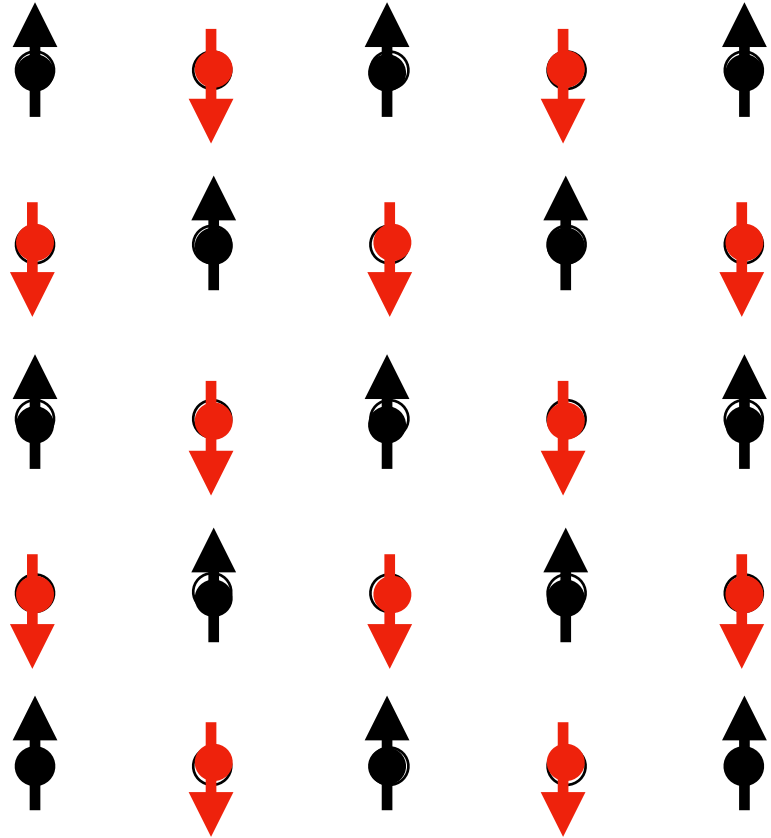


Physics World, Oct 2018



# Hubbard model: Main candidates for $U/t \sim 8$ , $\delta \sim 1/8$

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



$\delta = 0$ : Antiferromagnet

$\delta > 0$ : finite density of holes

**What do the holes do??**

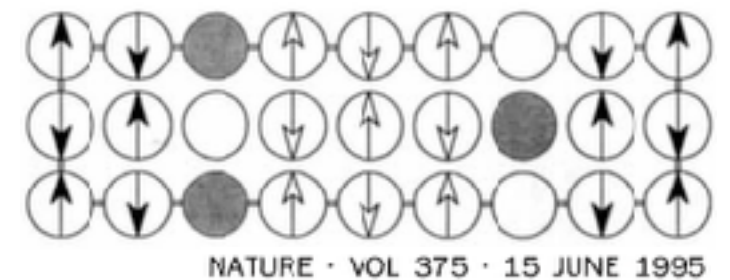
# Hubbard model: Main candidates for $U/t \sim 8$ , $\delta \sim 1/8$

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



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)  
Capone & Kotliar, PRB 74 (2006)  
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 ...

## Theory:

Zaanen & Gunnarsson, PRB 40 (1989)  
Poilblanc & Rice, PRB 39 (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 ...

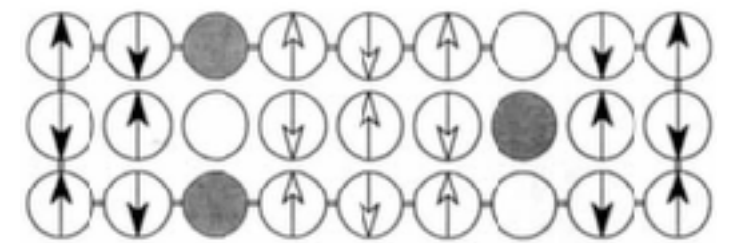
# Hubbard model: Main candidates for $U/t \sim 8$ , $\delta \sim 1/8$

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

**Uniform d-wave  
superconducting state**

VS

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



NATURE · VOL 375 · 15 JUNE 1995

Yokoyama & Shiba, IPS 157 (1988)

Gros, PR

Dagotto &

S. Sorella

Maier et al

Senechal

Capone &

Aichhorn

Lugas, et

Aimi & Im

Yokoyama

Yokoyama

Eichenbe

Macridin,

Hu, Becc

Gull, Parc

Misawa & Imada, PRB 90 (2014)

... and ma

Schulz, J. Phys. 50 (1989)

? Which is the true ground state ?

**Goal:** get conclusive answer  
for  $U/t=8$ ,  $\delta=1/8$  using  
**iPEPS, DMRG, AFQMC, DMET**

Zheng, Chung, PC, Ehlers, Qin, Noack, Shi,

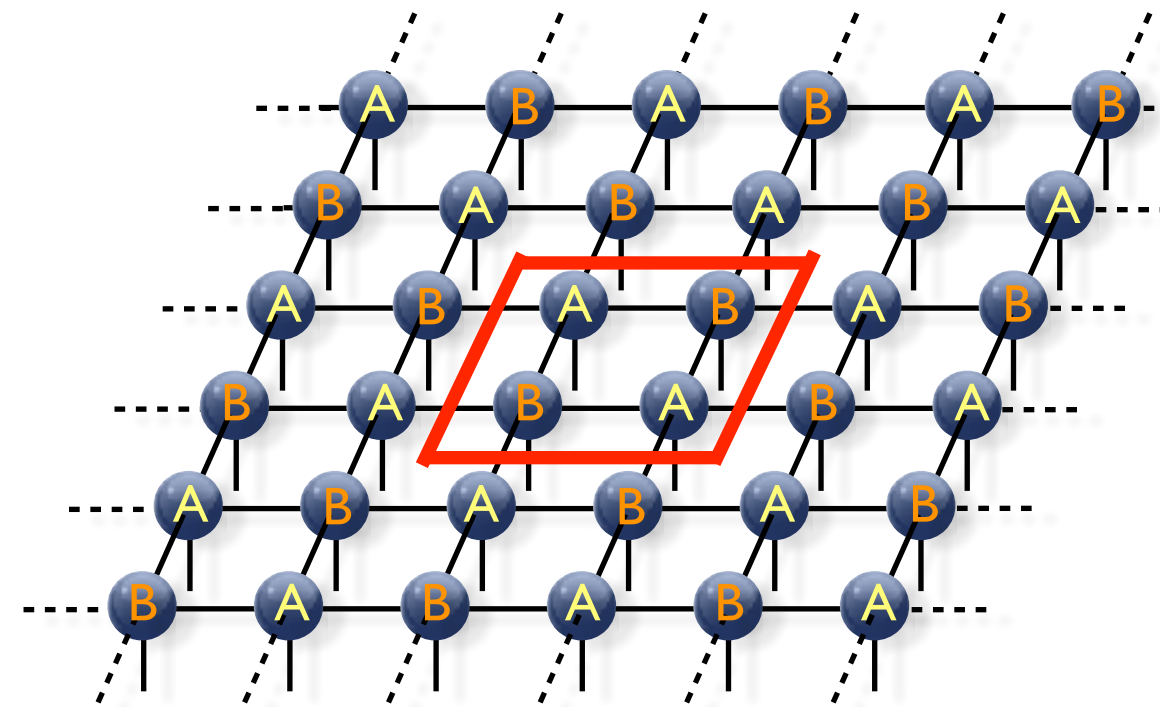
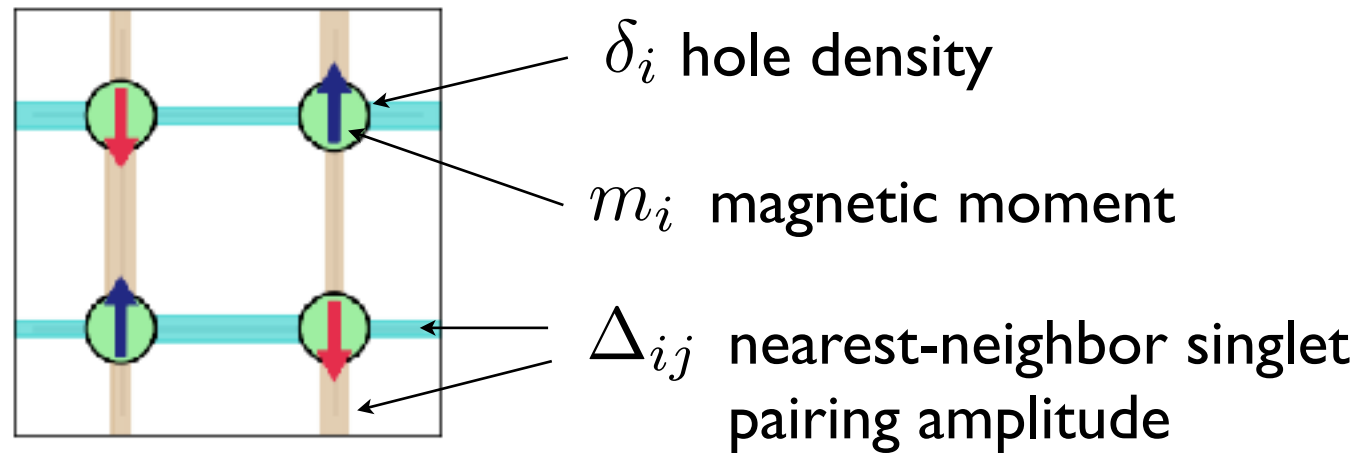
White, Zhang, Chan, Science 358, 1155 (2017)

Zheng, Chan, PRB 90 (2014)

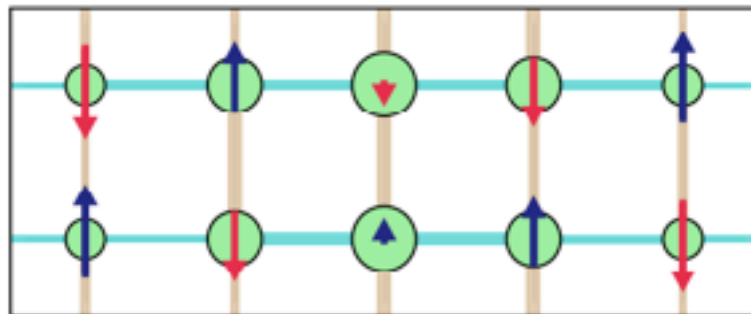
Ground state: **stripe state**

# iPEPS: main competing states ( $U/t=8, \delta=1/8$ )

## Uniform d-wave SC state (+ AF order)

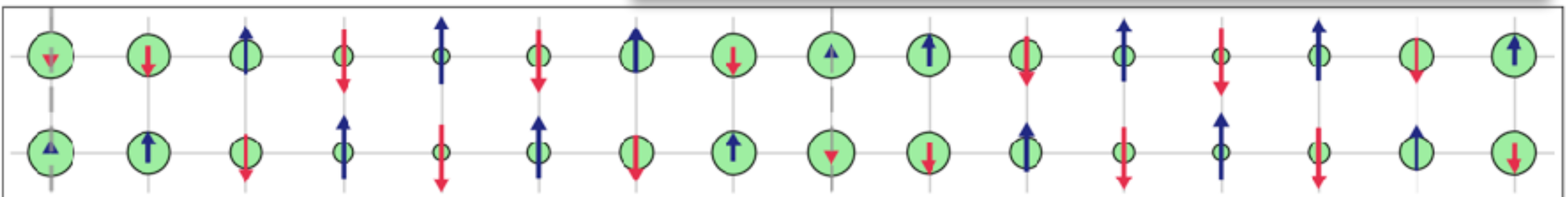


## Period $\lambda=5$ (W5 stripe)



- ★ Modulation in the charge, AF, and SC order
- ★ “Site-centered” stripe
- ★  $\pi$ -phase shift in the AF order

## Period $\lambda=8$ (W8 stripe)

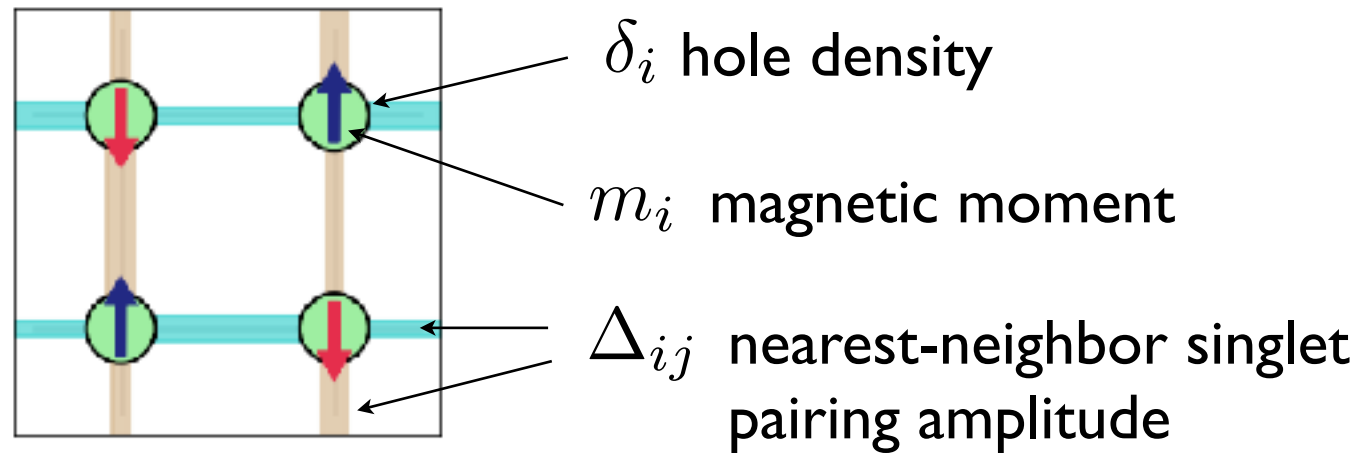


- ★ Superconductivity suppressed (1 hole per unit length)

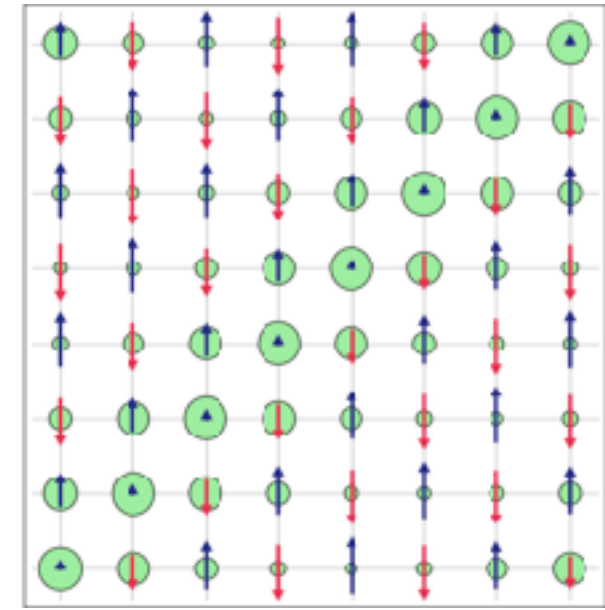


# iPEPS: main competing states ( $U/t=8, \delta=1/8$ )

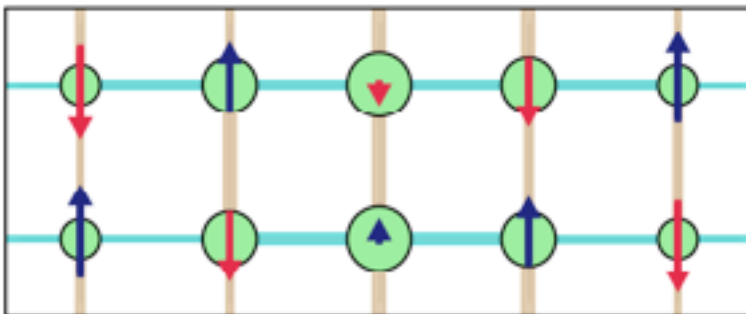
## Uniform d-wave SC state (+ AF order)



## Diagonal stripe (16x16 cell)

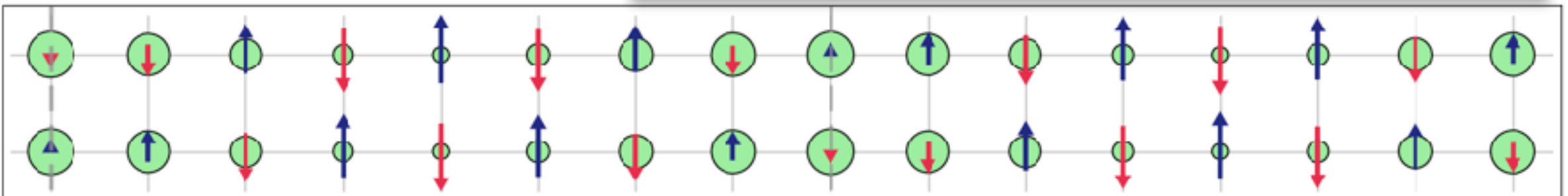


## Period $\lambda=5$ (W5 stripe)



- ★ Modulation in the charge, AF, and SC order
- ★ “Site-centered” stripe
- ★  $\pi$ -phase shift in the AF order

## Period $\lambda=8$ (W8 stripe)



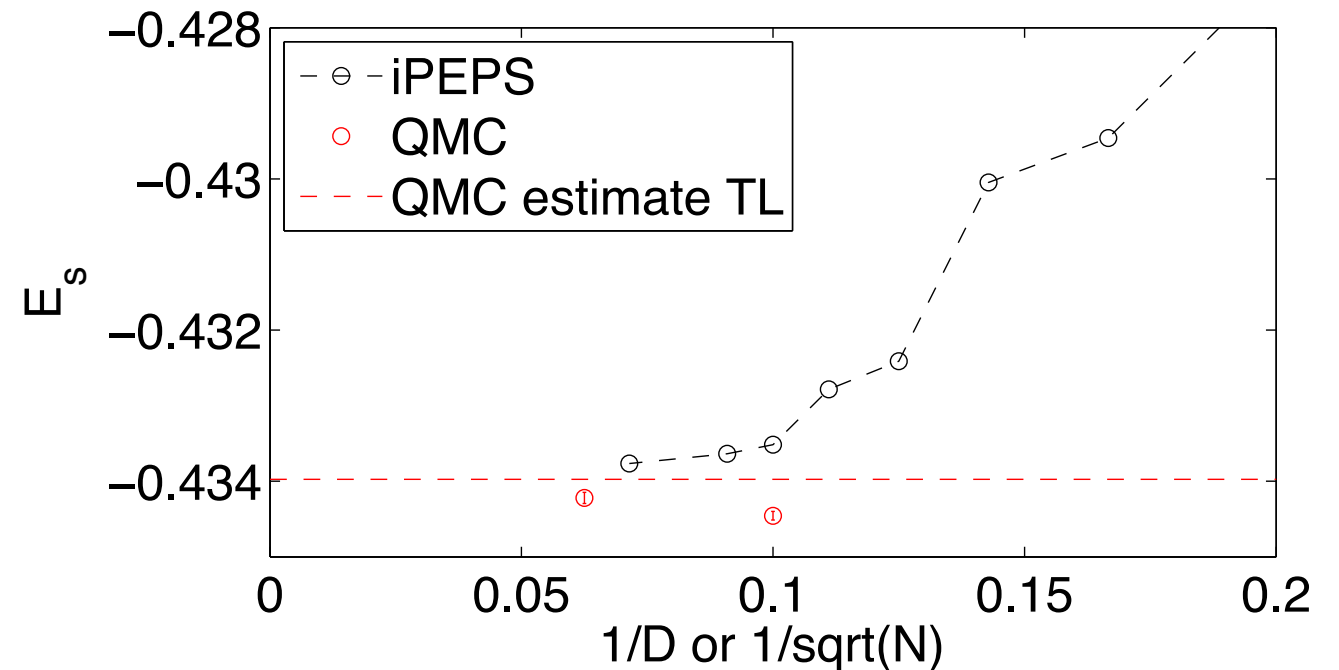
- ★ Superconductivity suppressed (1 hole per unit length)



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

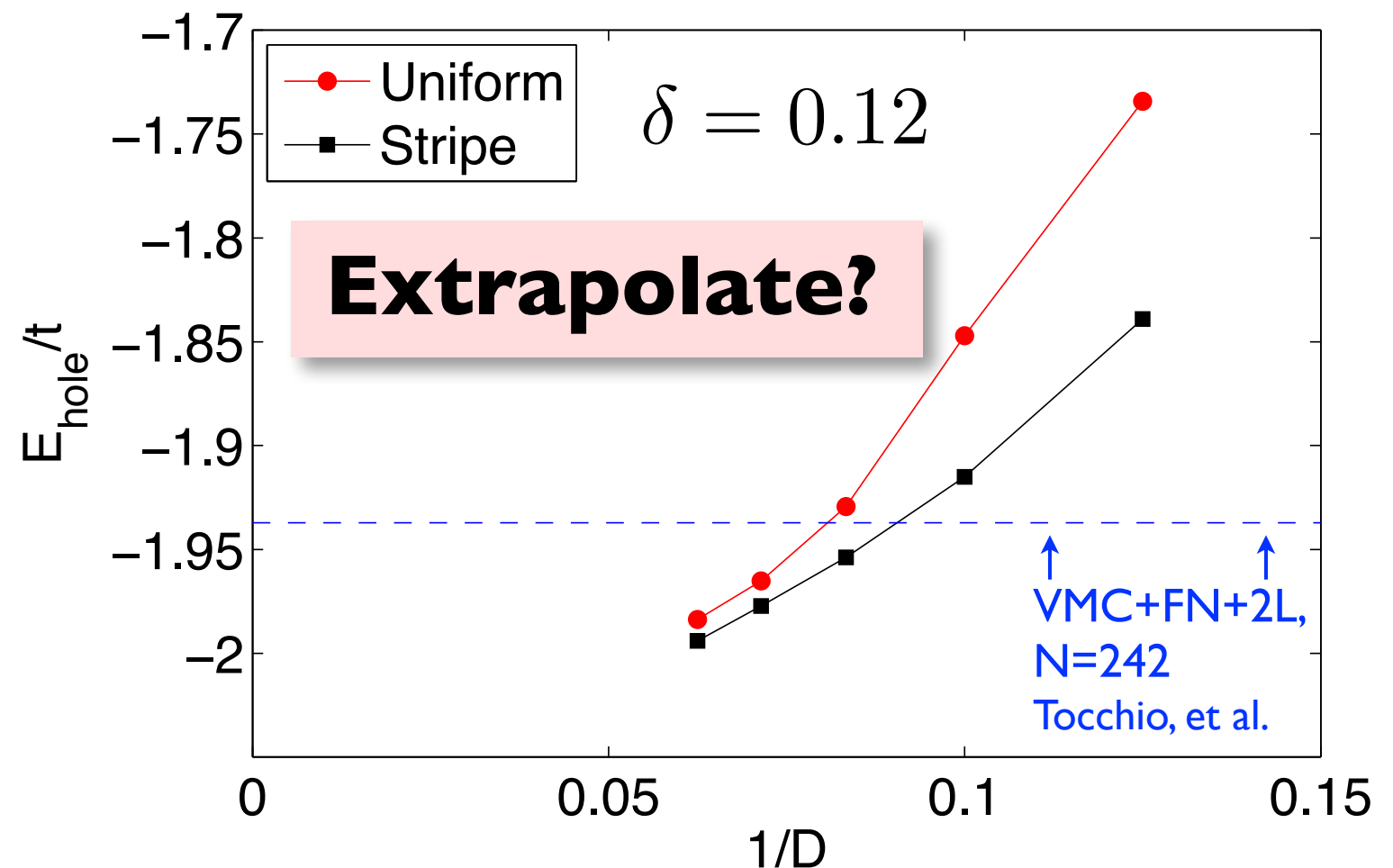
## Half-filled case ( $n=1$ ):

- ▶ Relative error in the TL:  $O(\mathbf{0.05\%})$   
( $D=14$  without extrapolation!)
- ▶ QMC estimate by S. Sorella (unpublished)



## Doped case ( $n=0.88$ ):

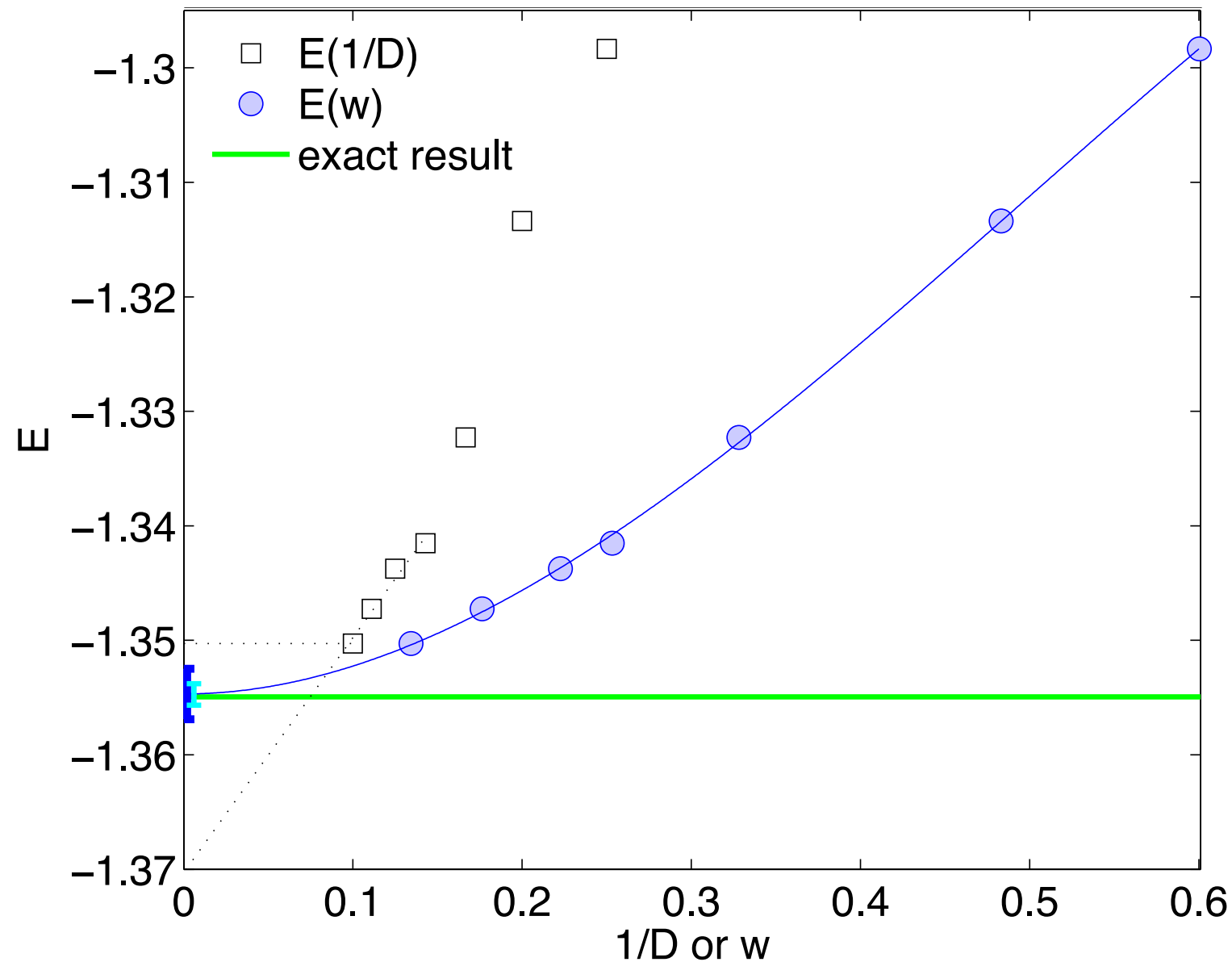
- ▶ Lower variational energy than best data from VMC+FN+2L  
[Tocchio, Becca, Sorella, unpublished]



# Improving energy extrapolations

PC, PRB 93 (2016)

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

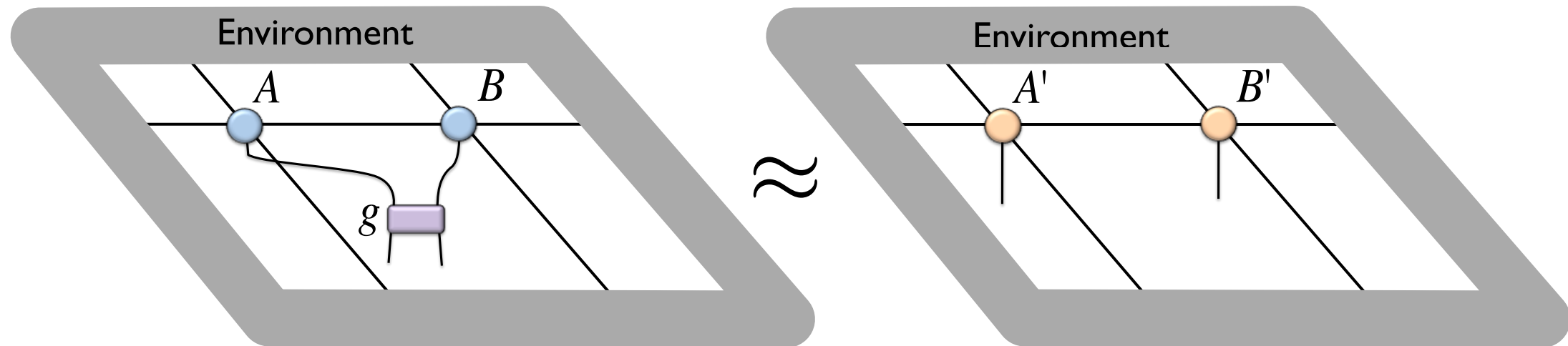


Bad estimate based  
on 1/D data!

Extrapolate in  
**truncation error**  
instead!

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

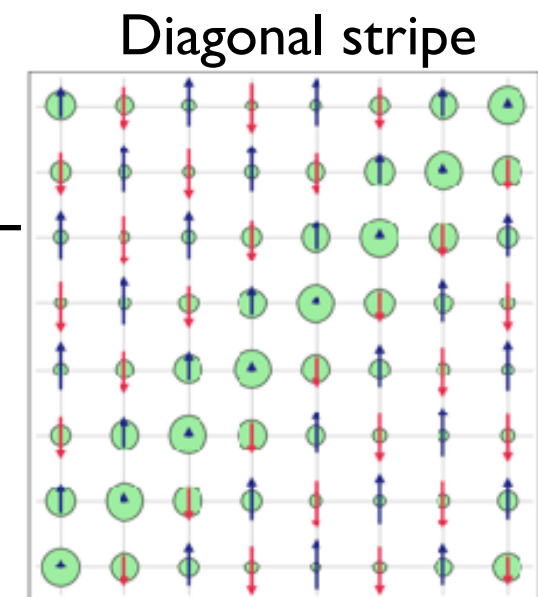
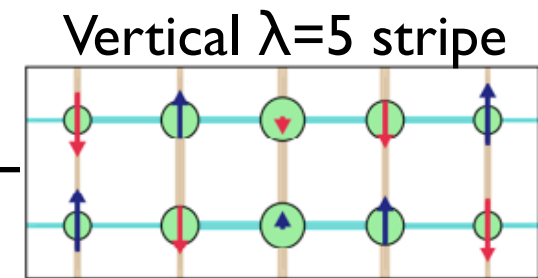
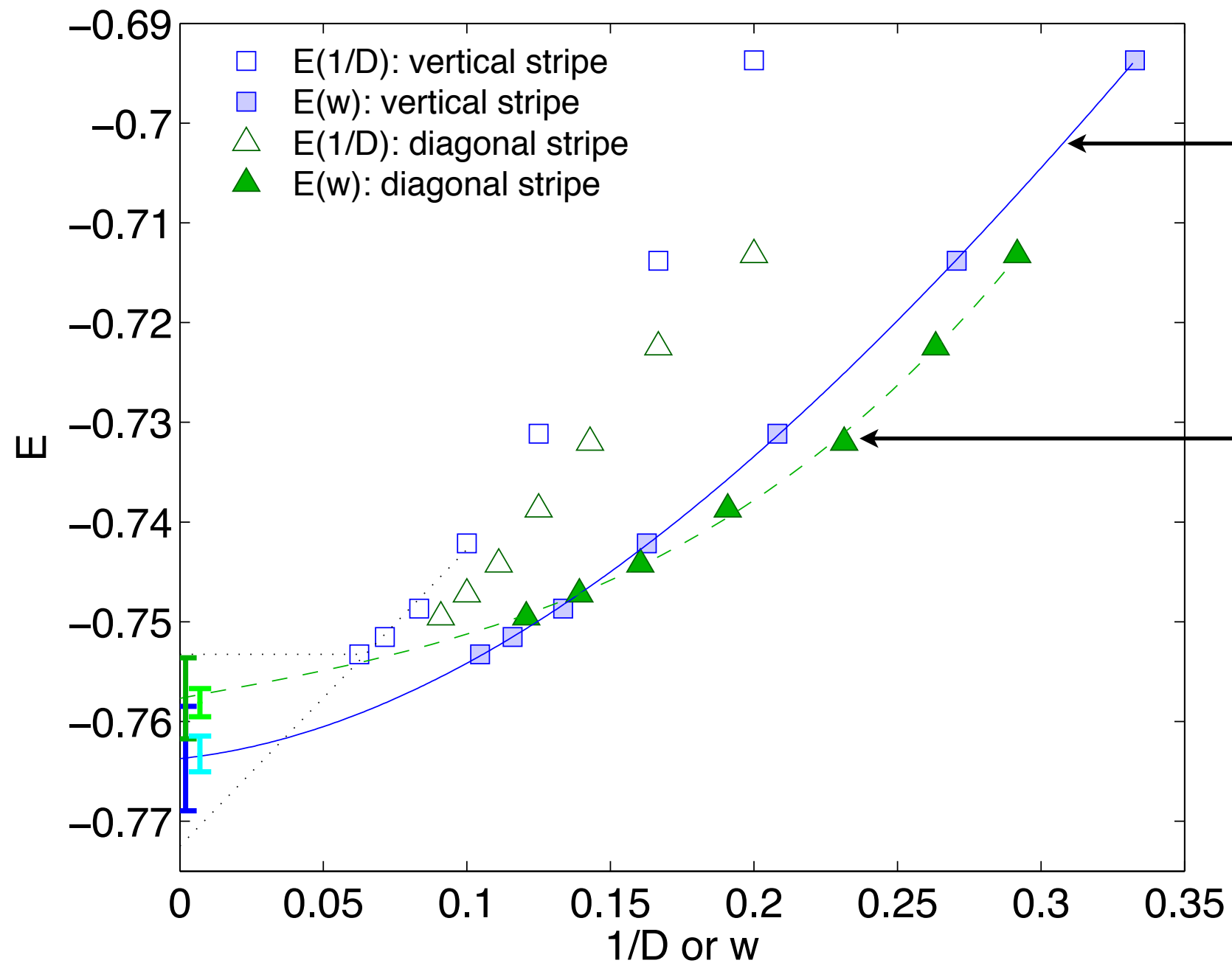
# Truncation error in the full update algorithm



$$|\tilde{\Psi}\rangle = g|\Psi\rangle \approx |\Psi'\rangle$$

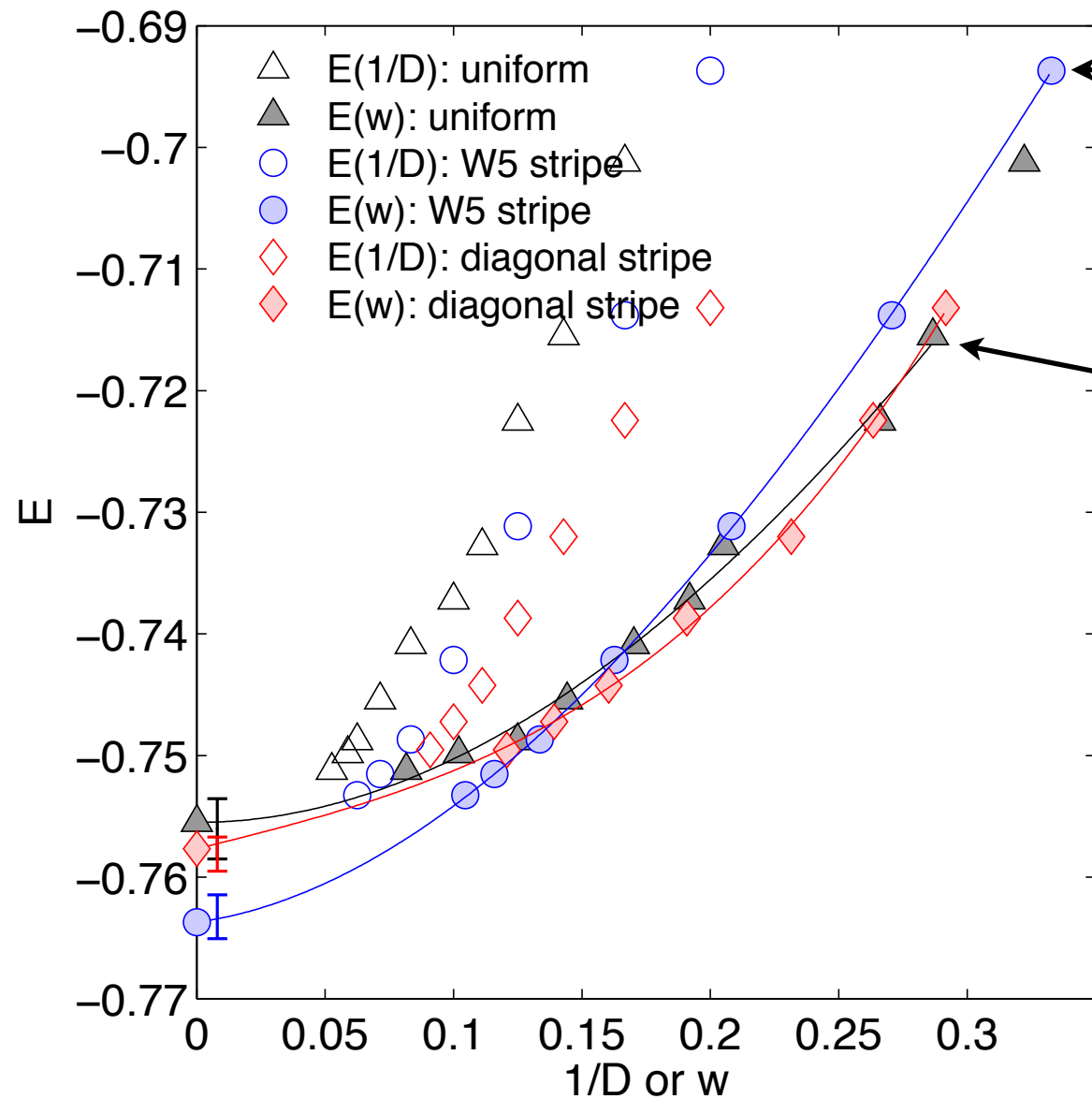
- Cost function:  $C = || |\tilde{\Psi}\rangle - |\Psi'\rangle ||$
- Truncation error:  $w(D) = C(D, \beta \rightarrow \infty) / \tau$

# Example: vertical vs diagonal stripe, $U/t=8$ , $\delta=1/8$

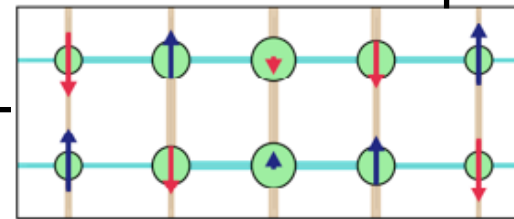


Vertical  $\lambda=5$  stripe is **lower** than diagonal stripe

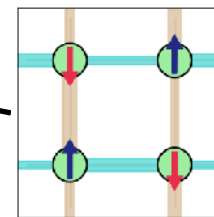
# iPEPS: extrapolated energies



Vertical  $\lambda=5$  stripe



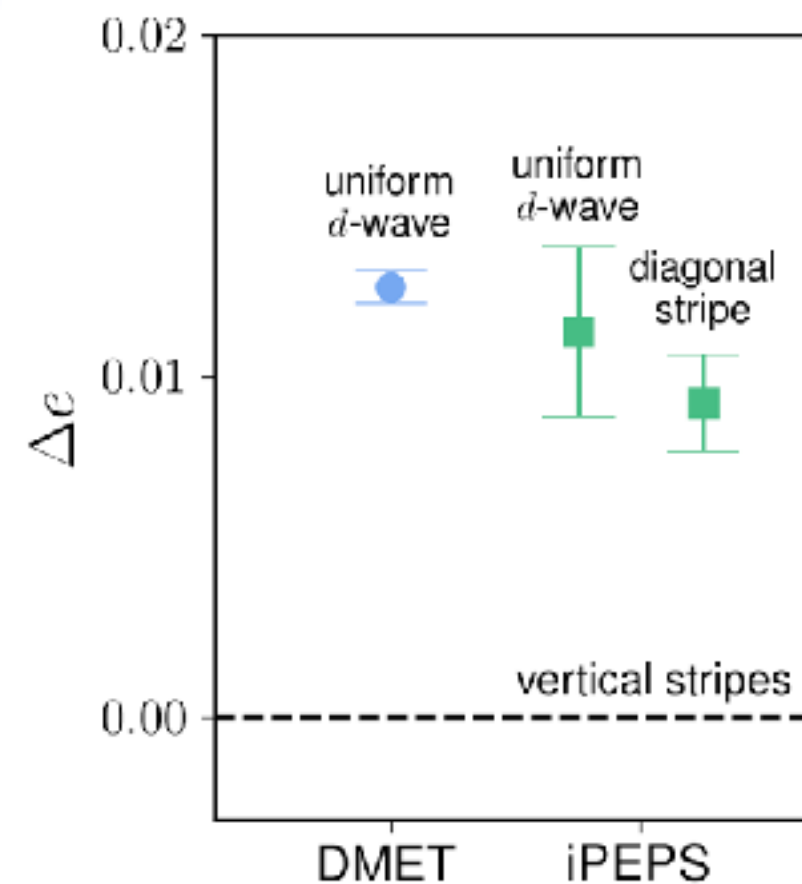
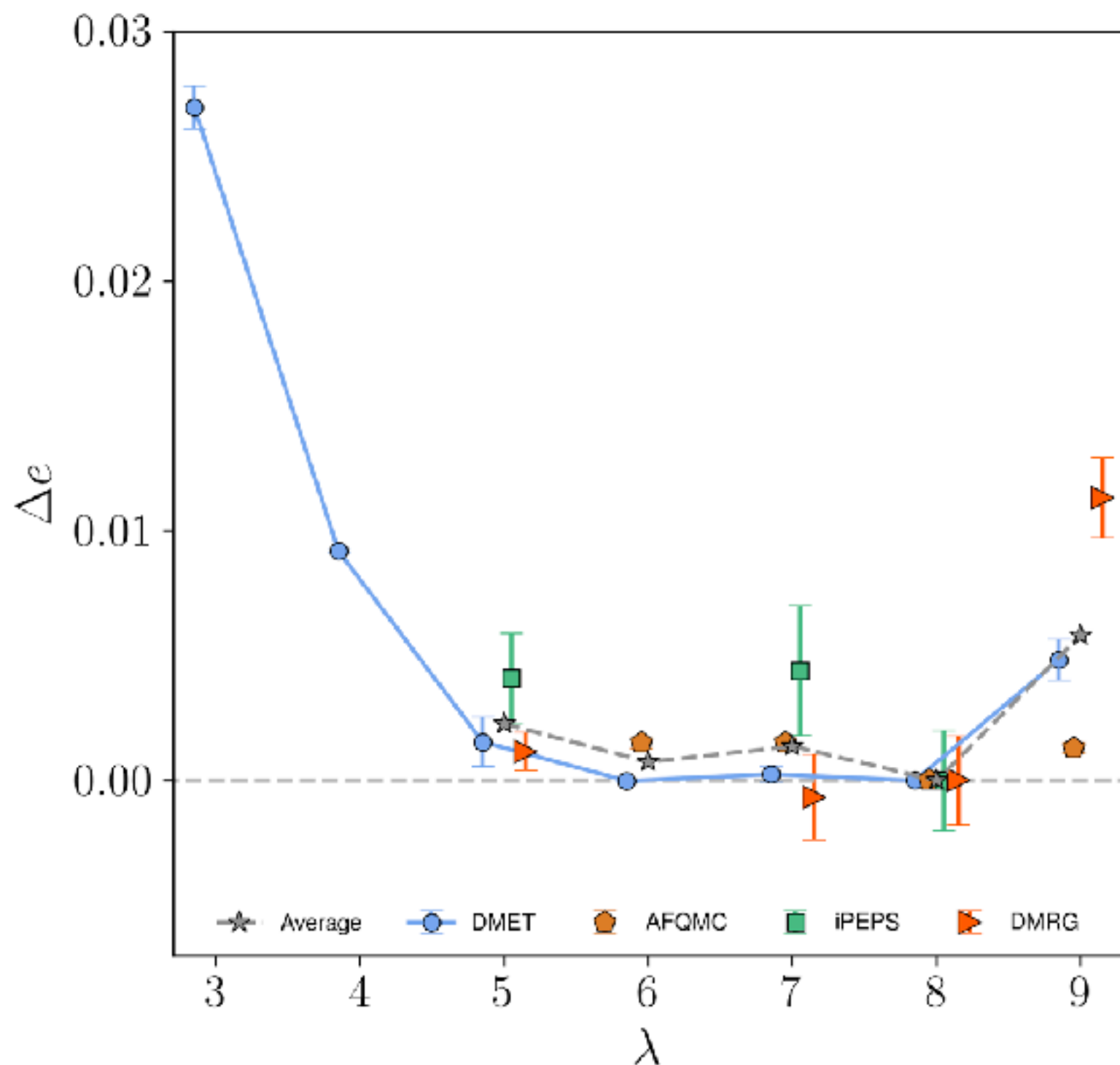
Uniform d-wave



**Stripe is lower than uniform state!**

**$\lambda=8$  stripe has lowest energy**

# Comparison with other methods



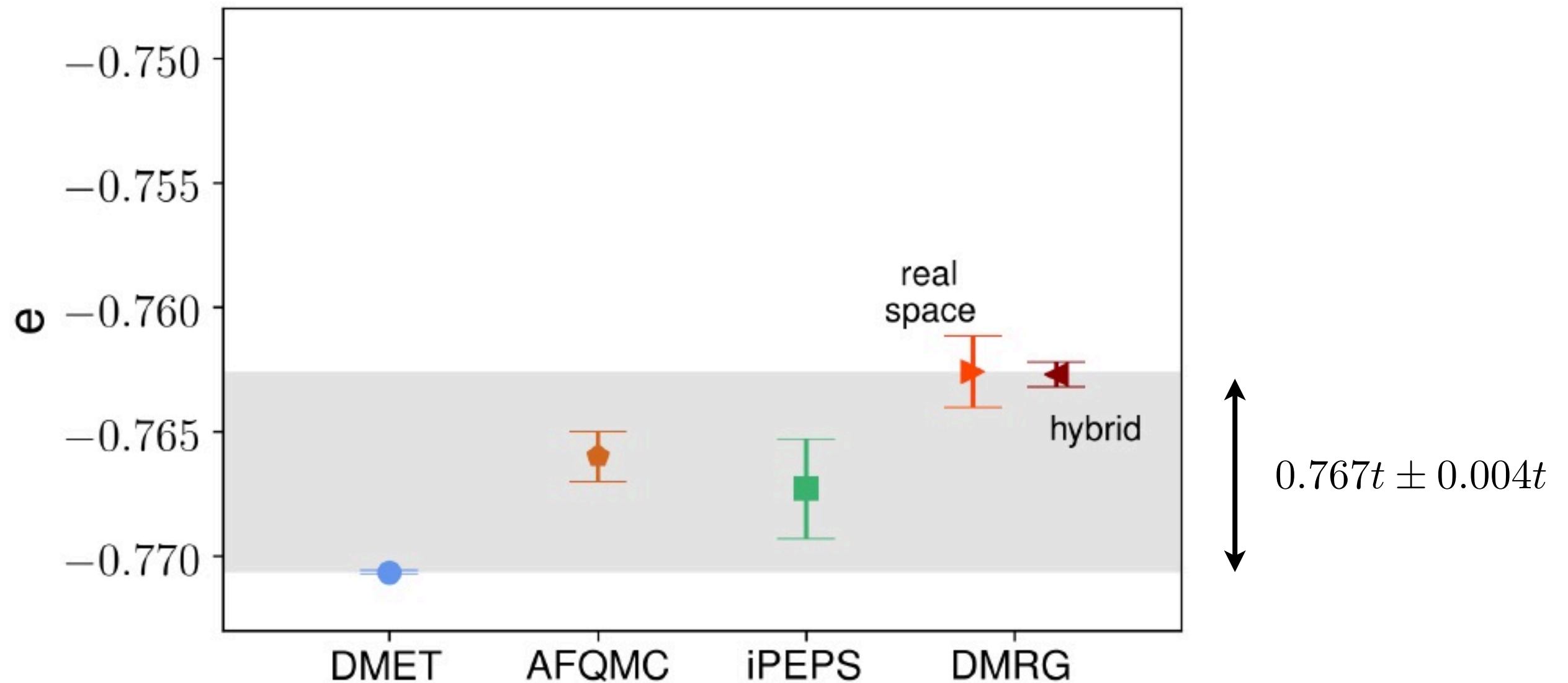
★ Uniform state: higher energy

★  $\lambda=5\dots 8$ : close in energy

★  $\lambda=8$  stripe: slightly lower

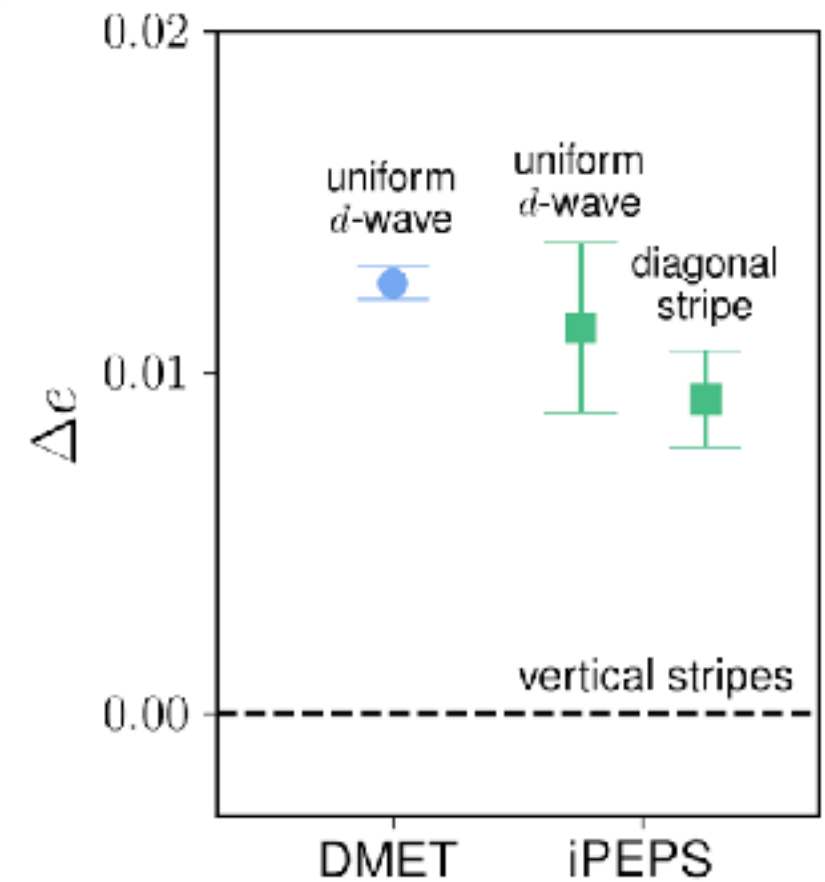
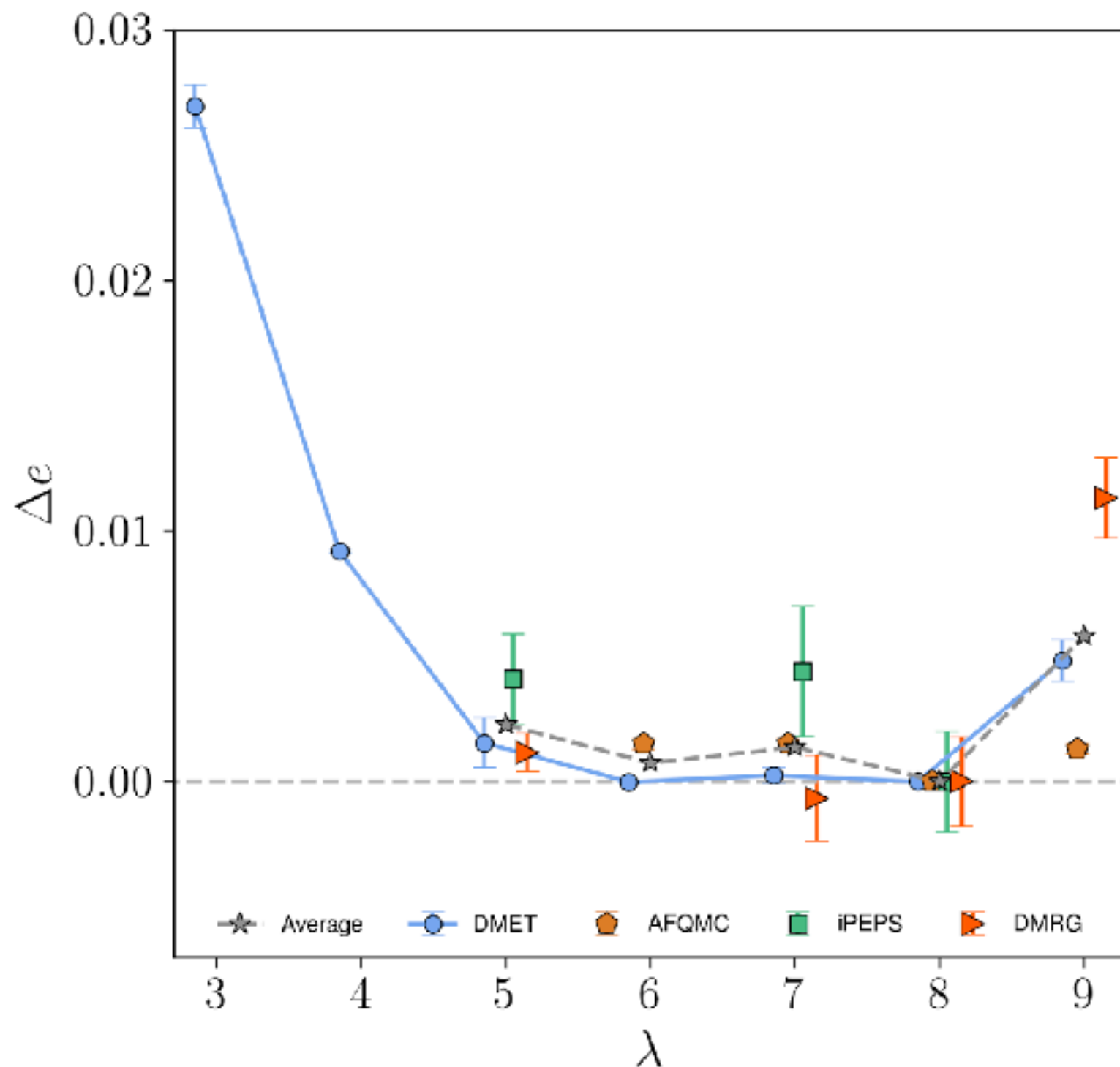
★ also compatible with fluctuating stripes

# Energy of $\lambda=8$ stripe



★ Close agreement between methods!

# Comparison with other methods



★ Uniform state: higher energy

★  $\lambda=5\dots 8$ : close in energy

★  $\lambda=8$  stripe: slightly lower

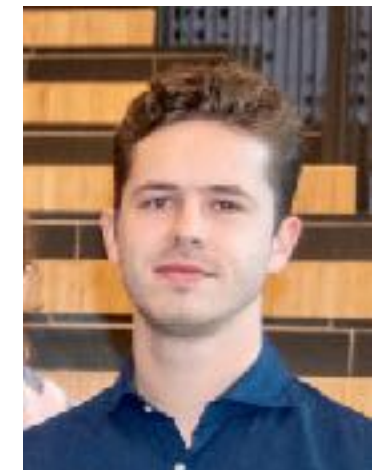
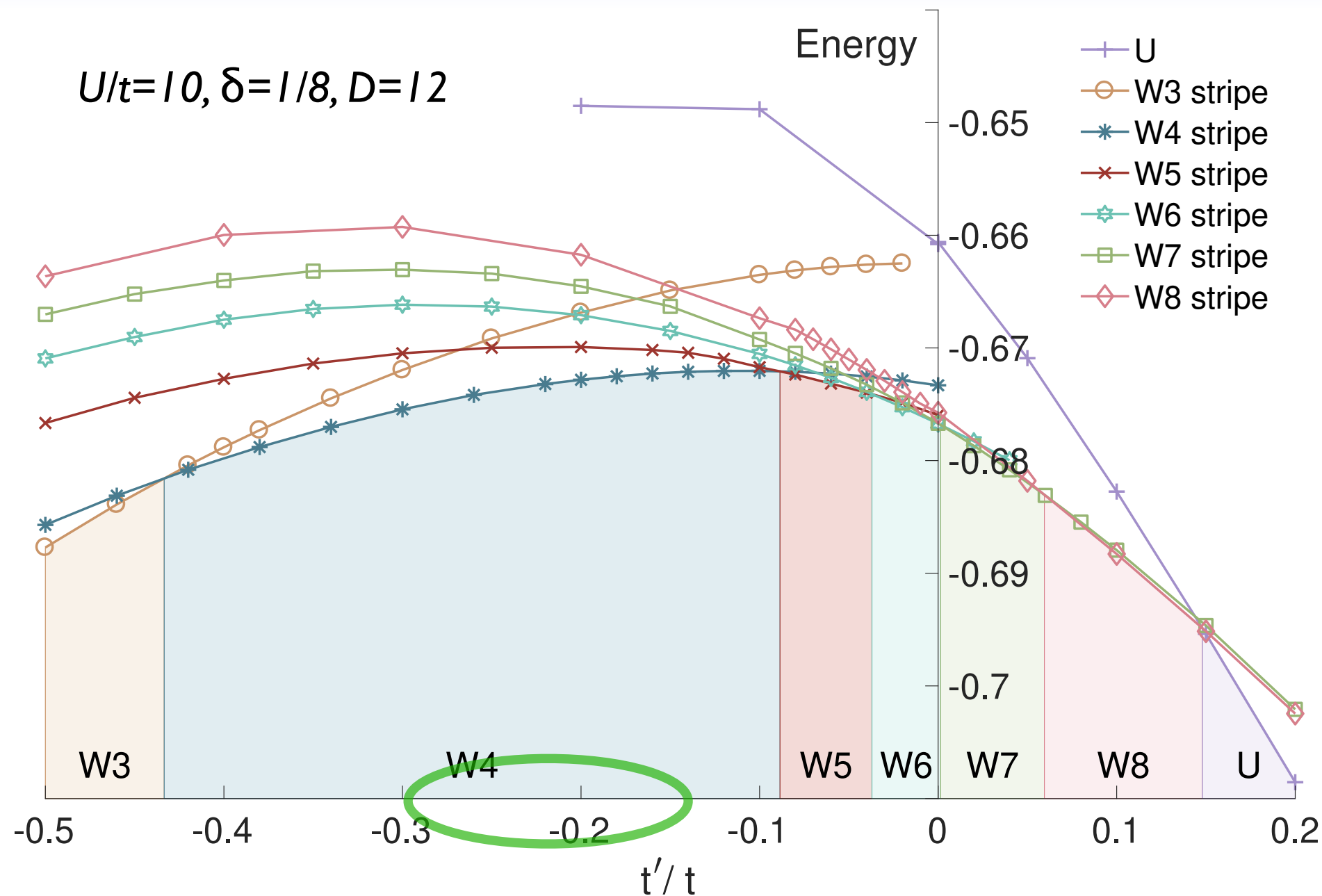
★ also compatible with fluctuating stripes

★ Experiments:  $\lambda \sim 4$ , but here higher in energy!

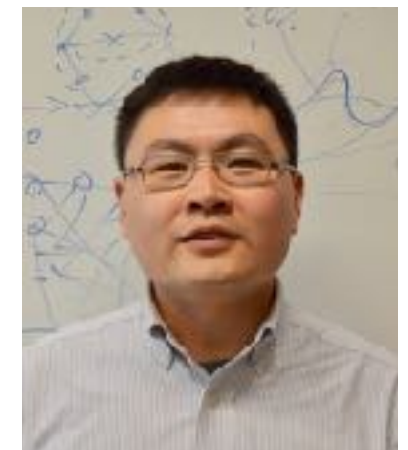


# Extended 2D Hubbard model (+ next-nearest neighbor hopping)

Ponsioen, Chung,  
PC, PRB 100 (2019)



Boris Ponsioen



Sangwoo Chung

- ★ Period-4 stripes are stabilized by including a realistic  $t'/t \sim -0.15 \dots -0.3$  [see also: Ido, Ohgoe & Imada, PRB **97** (2018), Jiang & Devereaux, Science 365 (2019)]
- ★ Competition is weaker in this region than for  $t'/t=0$
- ★ Superconductivity is suppressed in the period-4 stripe

## Summary: 2D Hubbard model, $\delta=1/8$ , $U/t=8$ ( $U/t=10$ )

- Doped 2D Hubbard model exhibits many competing low energy states
- Stripe has lower energy than uniform d-wave state ( $\delta=1/8$ )
- $\lambda=8$  stripe lowest energy ( $U/t=8$ ), with  $\lambda=5-7$  stripes very close in energy
- Realistic  $t'/t = -0.2\dots-0.3$ : period 4 stripe (with suppressed SC)

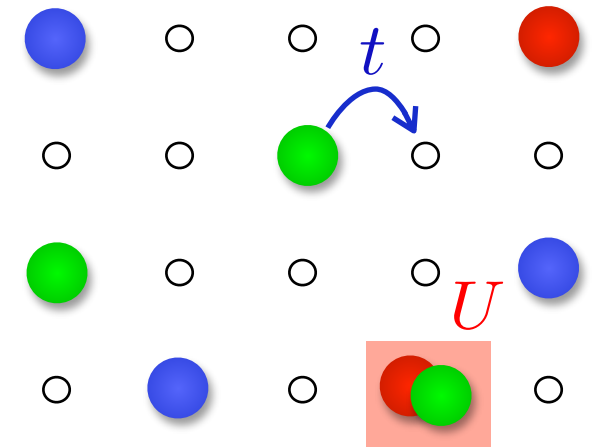
- ★ Next step: more realistic models of the cuprates (multi-band models)
- ★ Systematic study will help to get a better understanding of the various competing phases in the cuprates!

# SU(N) Hubbard models

- ▶ Generalization to N species (“colors”) of fermions

$$\hat{H} = -t \sum_{\langle i,j \rangle, \alpha} \hat{c}_{i\alpha}^\dagger \hat{c}_{j\alpha} + H.c. + U \sum_{i, \alpha < \beta} \hat{n}_{i\alpha} \hat{n}_{i\beta}$$

$\uparrow$   
 sum over all colors: ● ● ● ...



- ▶ Realizable in quantum simulators using alkaline-earth atoms in optical lattices

Nuclear spin

$$^{87}\text{Sr}: I = 9/2 \rightarrow N_{max} = 2I + 1 = 10$$

Cazalilla, Ho & Ueda, NJP 11(2009)  
 Gorshkov, et al, Nat. Phys. 6, 289 (2010).  
 Taie, Yamazaki, Sugawa & Takahashi, Nat. Phys. 8 (2012).  
 Scazza, et al., Nat. Phys. 10, 779 (2014).  
 Zhang, et al, Science 345 (2014).  
 Cazalilla & Rey, Rep. Prog. Phys. 77 (2014).  
 Hofrichter, et al, PRX 6 (2016).  
 Ozawa, Taie, Takasu & Takahashi, PRL 121 (2018).

⋮

⋮

⋮

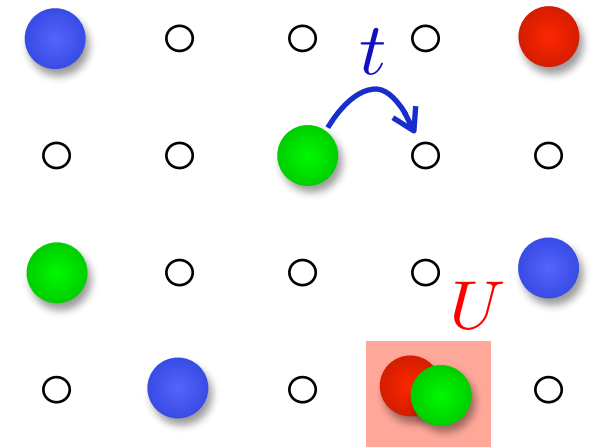
$$\begin{aligned}
 |I_z = 3/2\rangle & \leftrightarrow |\text{red}\rangle \\
 |I_z = 1/2\rangle & \leftrightarrow |\text{green}\rangle \\
 |I_z = -1/2\rangle & \leftrightarrow |\text{blue}\rangle \\
 |I_z = -3/2\rangle & \leftrightarrow |\text{yellow}\rangle \\
 \vdots & \\
 \vdots &
 \end{aligned}$$

# SU(N) Hubbard models

- ▶ Generalization to N species (“colors”) of fermions

$$\hat{H} = -t \sum_{\langle i,j \rangle, \alpha} \hat{c}_{i\alpha}^\dagger \hat{c}_{j\alpha} + H.c. + U \sum_{i, \alpha < \beta} \hat{n}_{i\alpha} \hat{n}_{i\beta}$$

$\uparrow$   
 sum over all colors:    ...



- ▶ Strong coupling limit ( $U \gg t$ ), integer filling: *SU(N) Heisenberg model*

$$H = \sum_{\langle i,j \rangle} P_{ij}$$

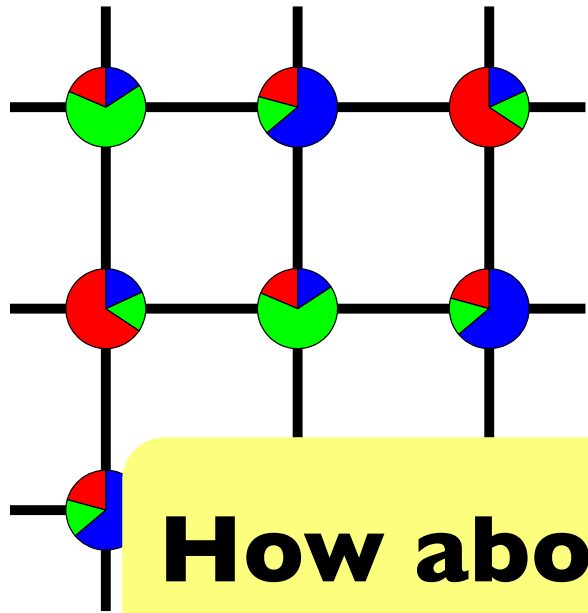
$\leftarrow$  permutation operator

The diagram illustrates the permutation operator  $P_{ij}$ . On the left, a red fermion is at site 'i' and a green fermion is at site 'j'. An arrow labeled  $P_{ij}$  points to the right, where the green fermion is now at site 'i' and the red fermion is at site 'j', representing the exchange of the two fermions.

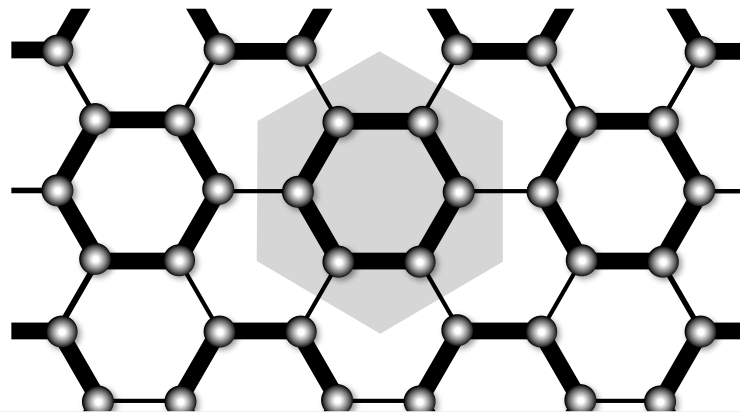
- ▶ **In general very challenging to study!**

# SU(N) Heisenberg models

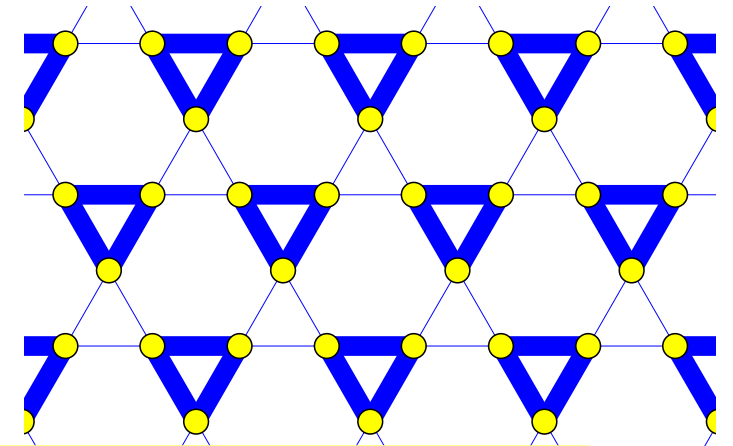
SU(3) square/triangular:  
*3-sublattice Néel order*  
Bauer, PC, et al., PRB 85 (2012)



SU(3) honeycomb: *Plaquette state*  
Zhao, Xu, Chen, Wei, Qin, Zhang, Xiang,  
PRB 85 (2012);  
PC, Läuchli, Penc, Mila, PRB 87 (2013)

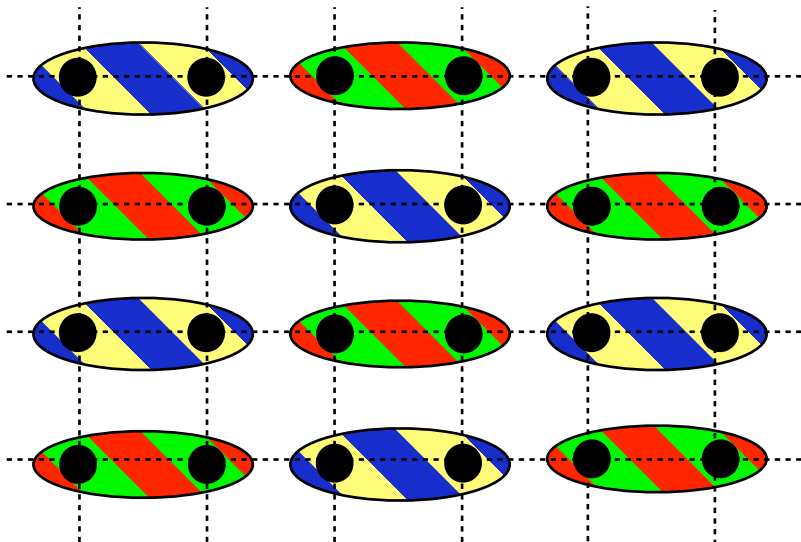


SU(3) kagome:  
*Simplex solid state*  
PC, Penc, Mila, Läuchli, PRB 86 (2012)

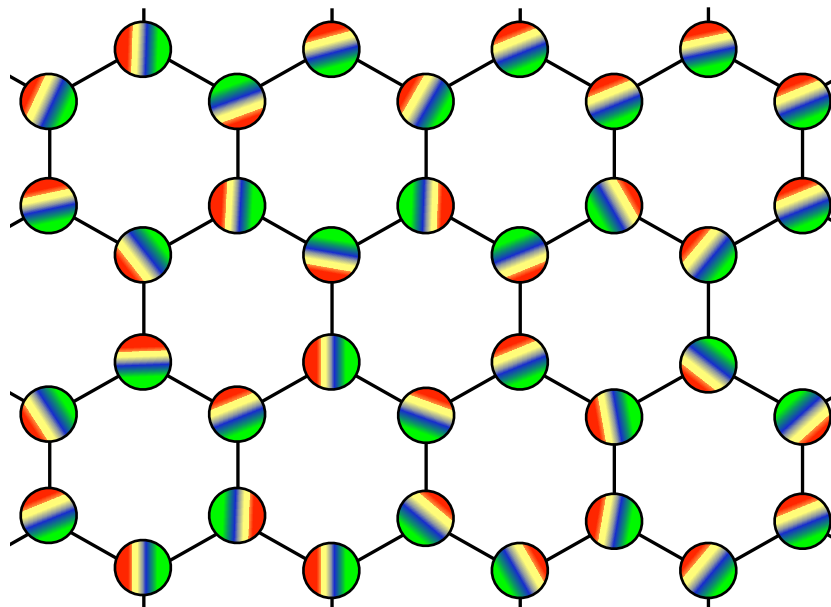


**How about SU(N) Hubbard models with iPEPS?**

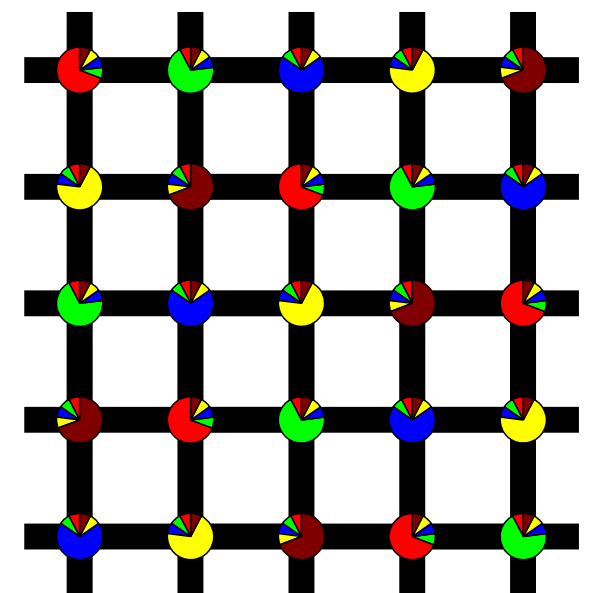
SU(4) square:  
*Dimer-Néel order*  
PC, Läuchli, Penc, Troyer,  
Mila, PRL 107 (2011)



SU(4) honeycomb:  
*spin-orbital (4-color) liquid*  
PC, Lajkó, Läuchli, Penc, Mila, PRX 2 ('12)

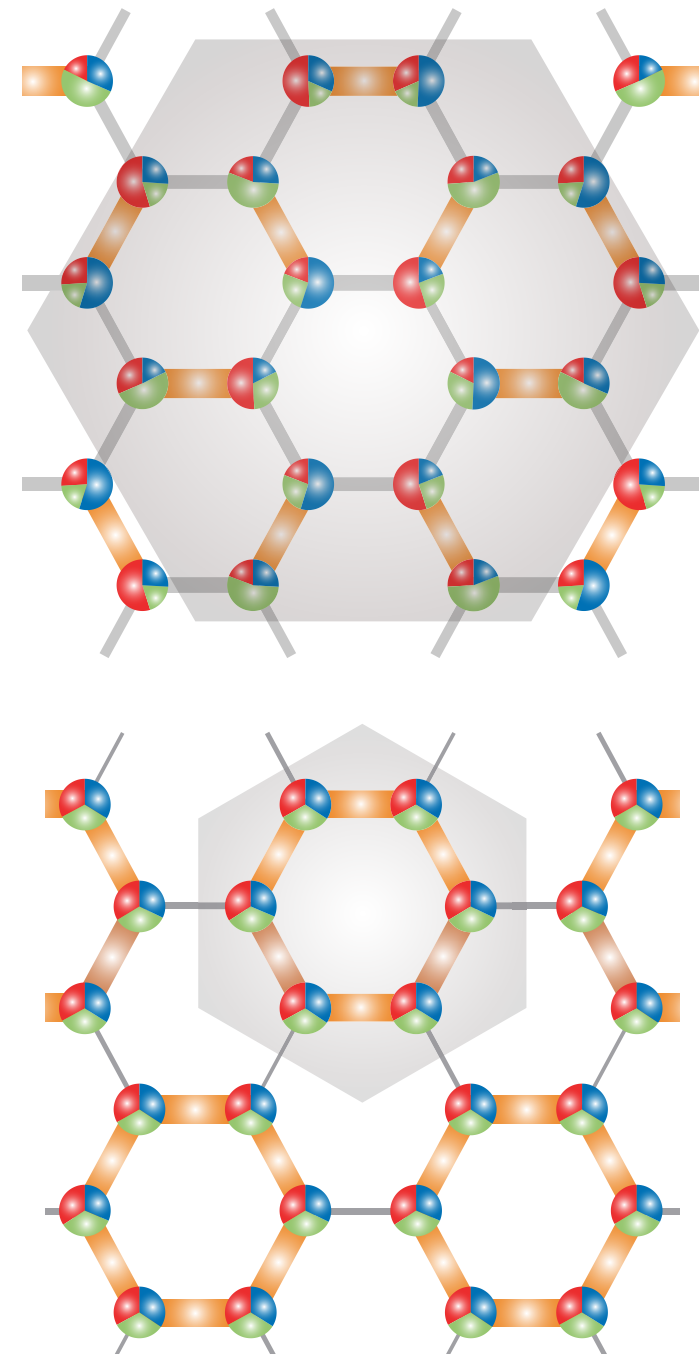
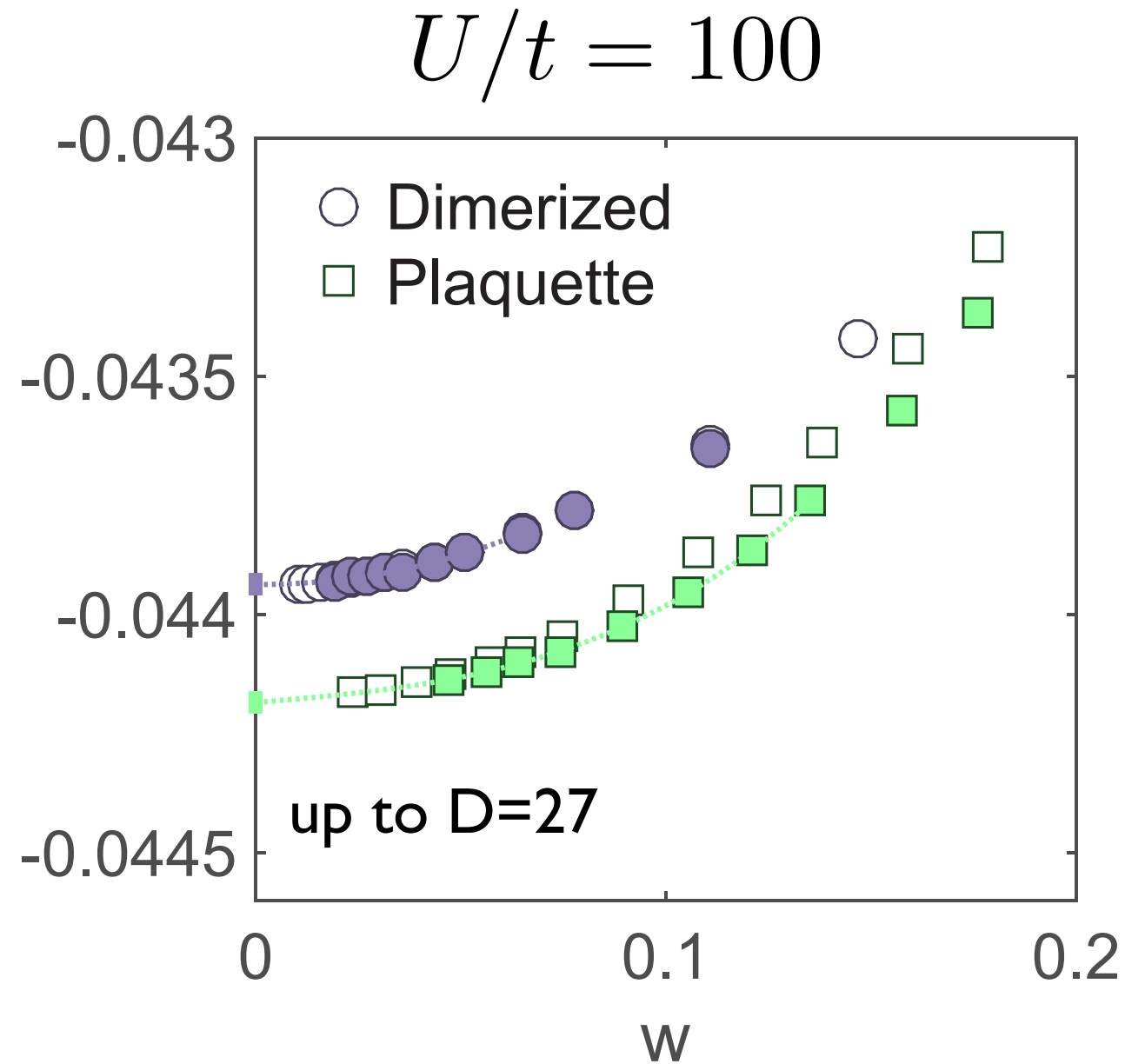


SU(5) square:  
*color order*  
PC, Mila, unpublished



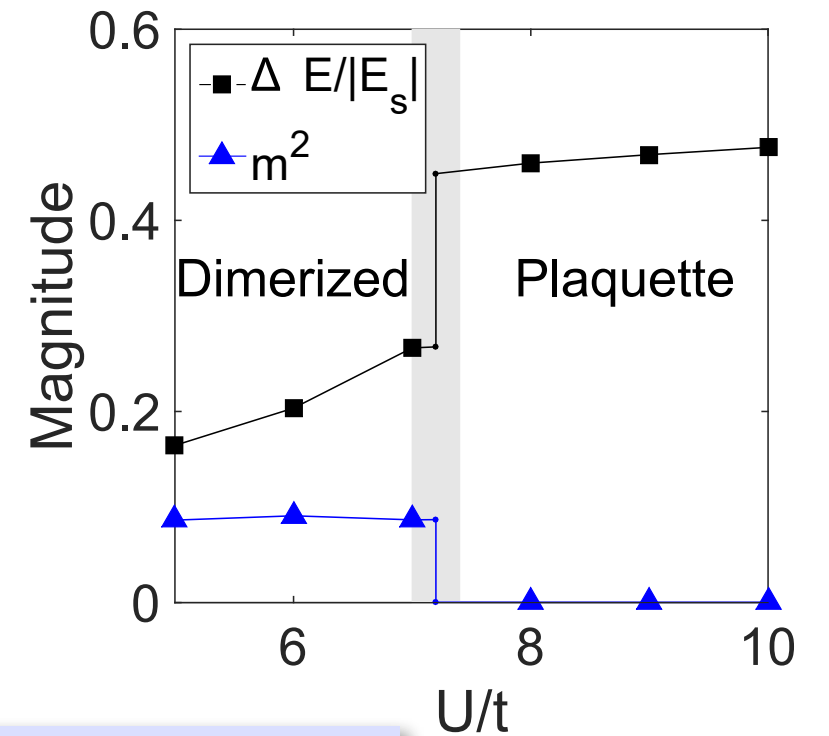
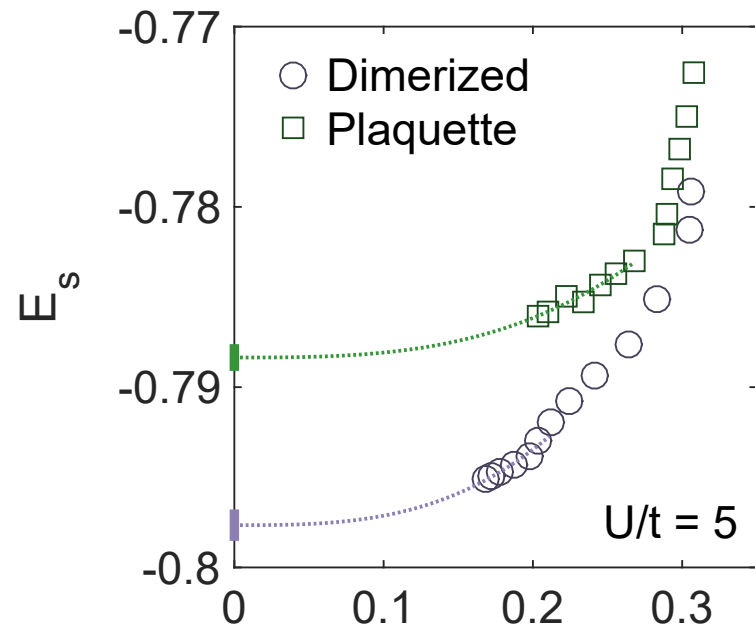
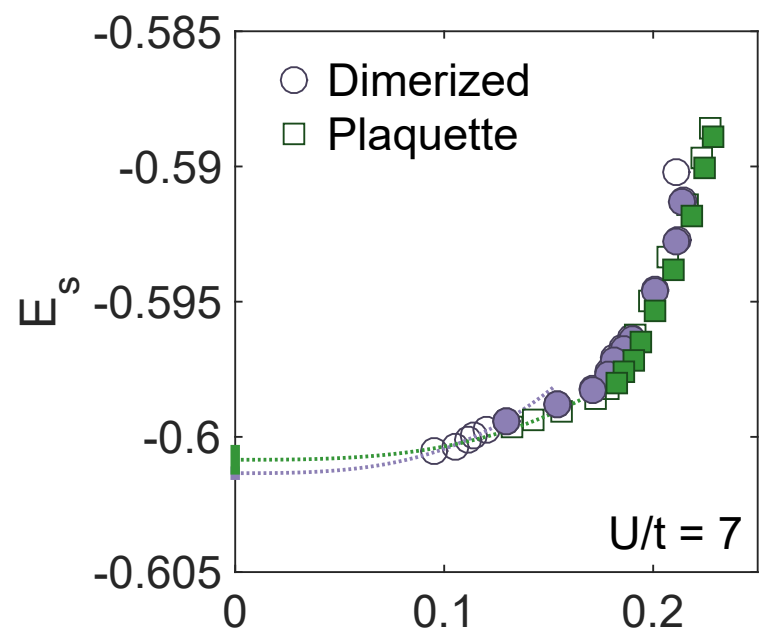
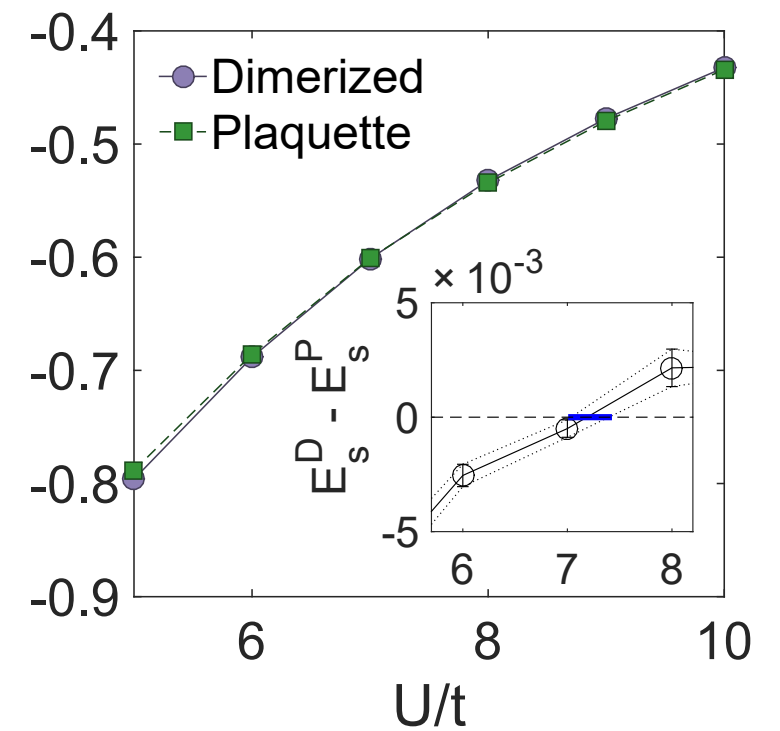
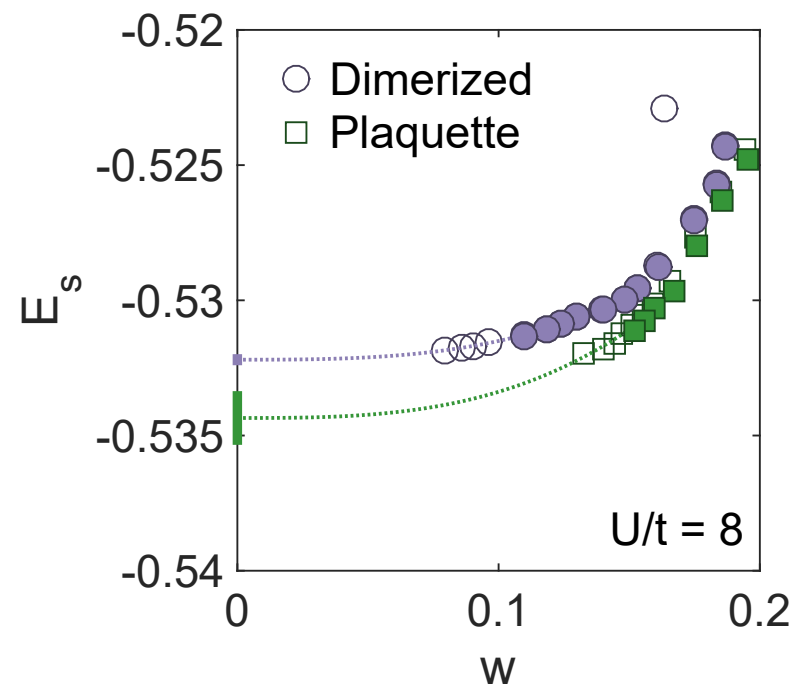
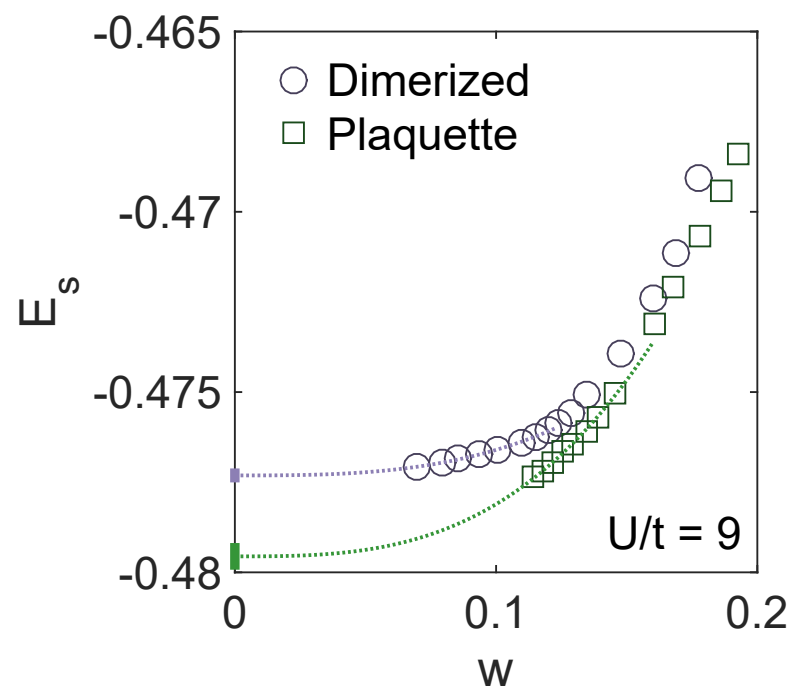
# SU(3) honeycomb Hubbard model ( $n=1/3$ )

S. S. Chung, PC, PRB 100, 035134 (2019)



Consistent with Heisenberg case!

# Lowering $U/t$ ...

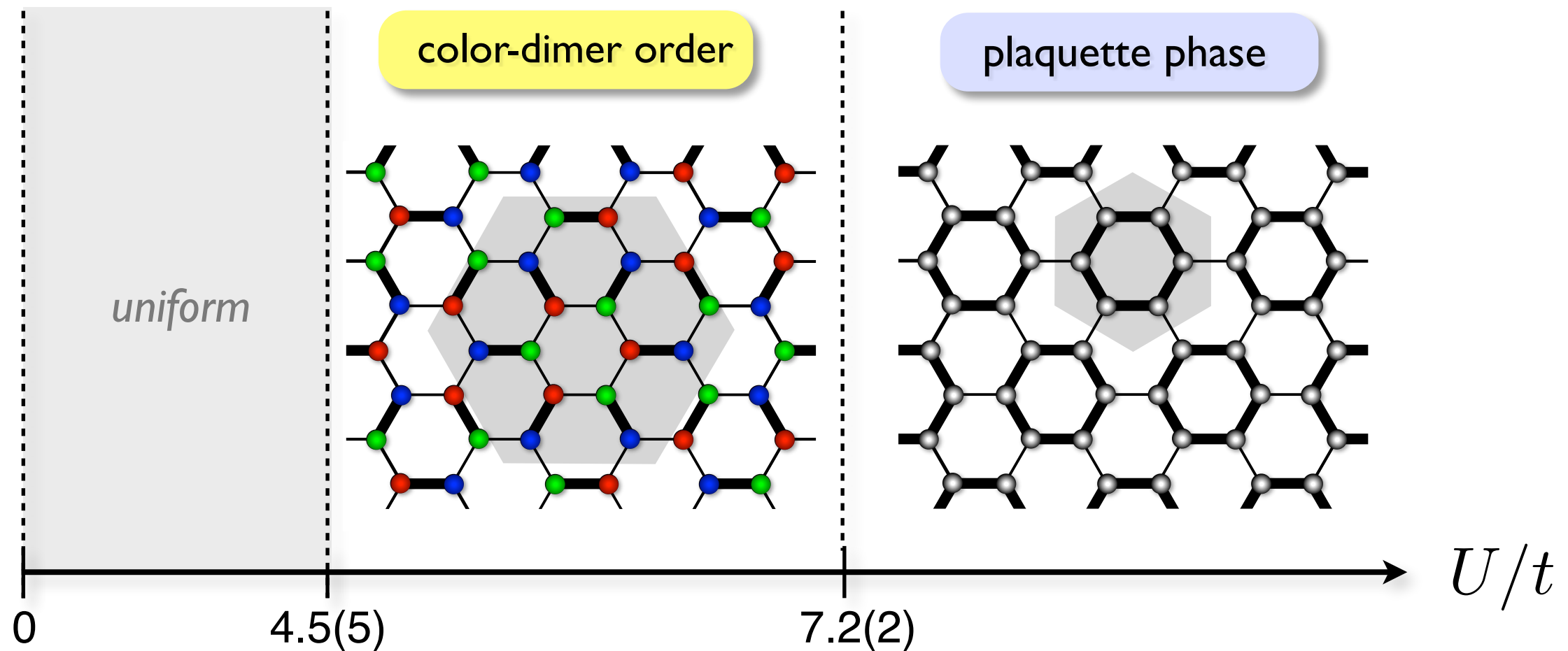


Transition between the two states:  $U/t = 7.2(2)$



# SU(3) honeycomb Hubbard model ( $n=1/3$ ): summary

S. S. Chung, PC, PRB 100, 035134 (2019)



*SU(N) Hubbard models: rich physics!*  
*Challenging, but within reach of iPEPS simulations*



# Finite temperature simulations with iPEPS

► Methodological developments:

Li et al. PRL 106 (2011); Czarnik et al. PRB 86 (2012); Czarnik & Dziarmaga PRB 90 (2014); Czarnik & Dziarmaga PRB 92 (2015); Czarnik et al. PRB 94 (2016); Dai et al PRB 95 (2017); Kshetrimayum, Rizzi, Eisert, Orus, PRL 122 (2019), P. Czarnik, J. Dziarmaga, PC, PRB 99 (2019), ...

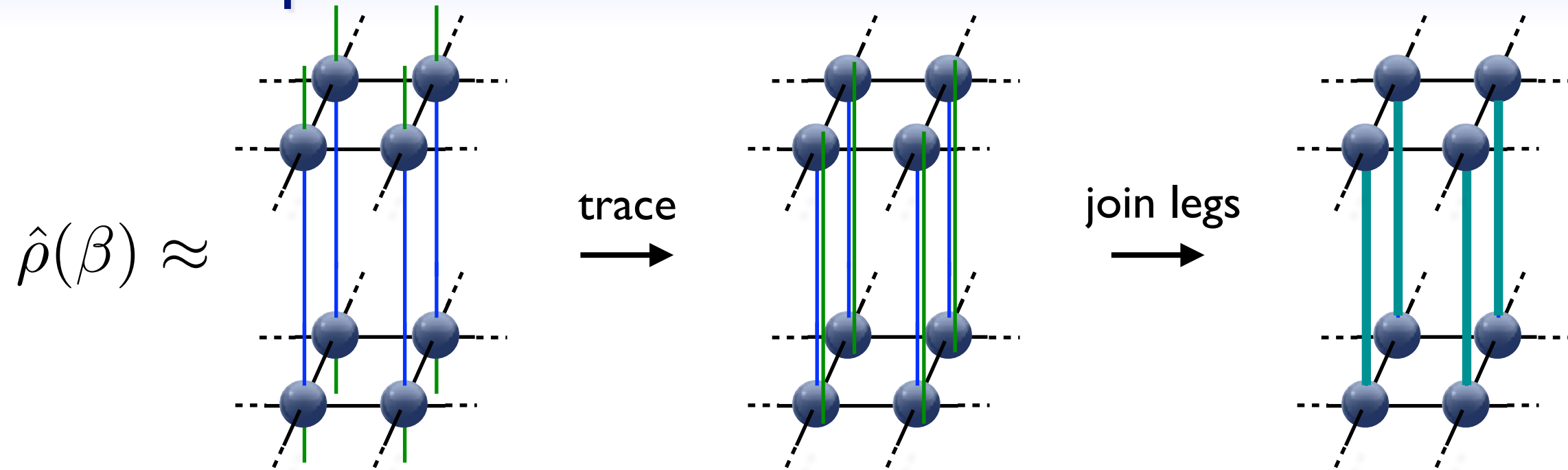
► Wave-function:  $|\Psi\rangle \approx$

► Density-operator:  $\hat{\rho} = e^{-\beta \hat{H}} \approx$

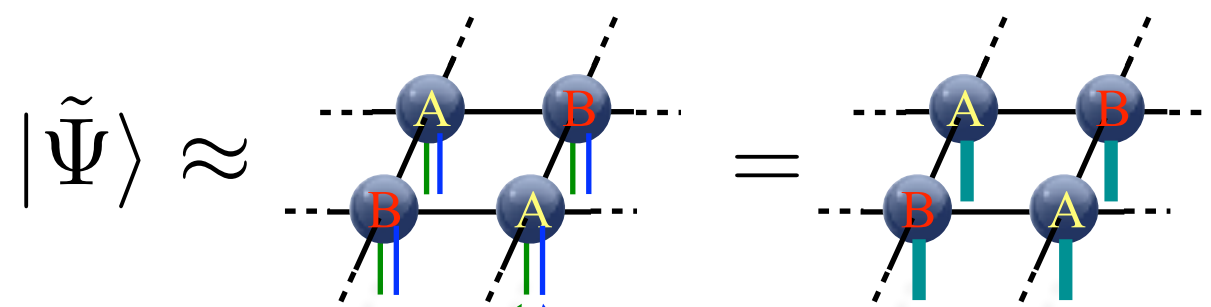
► Symmetric form:  $e^{-\beta \hat{H} / 2} \approx$   $\hat{\rho}(\beta) \approx$

$$\hat{\rho}(\beta) = \hat{\rho}^\dagger(\beta) \quad \text{by construction}$$

# Finite temperature simulations with iPEPS



same structure as  $\langle \tilde{\Psi} | \tilde{\Psi} \rangle$   
for wave functions



$$\hat{\rho}(\beta) = \text{Tr}_a |\tilde{\Psi}\rangle \langle \tilde{\Psi}|$$

**Recycle algorithms for wave functions!  
(CTM + imaginary time evolution)**

# Imaginary time evolution

- Start at infinite temperature:  $\hat{\rho}(\beta = 0) = \mathbb{I}$

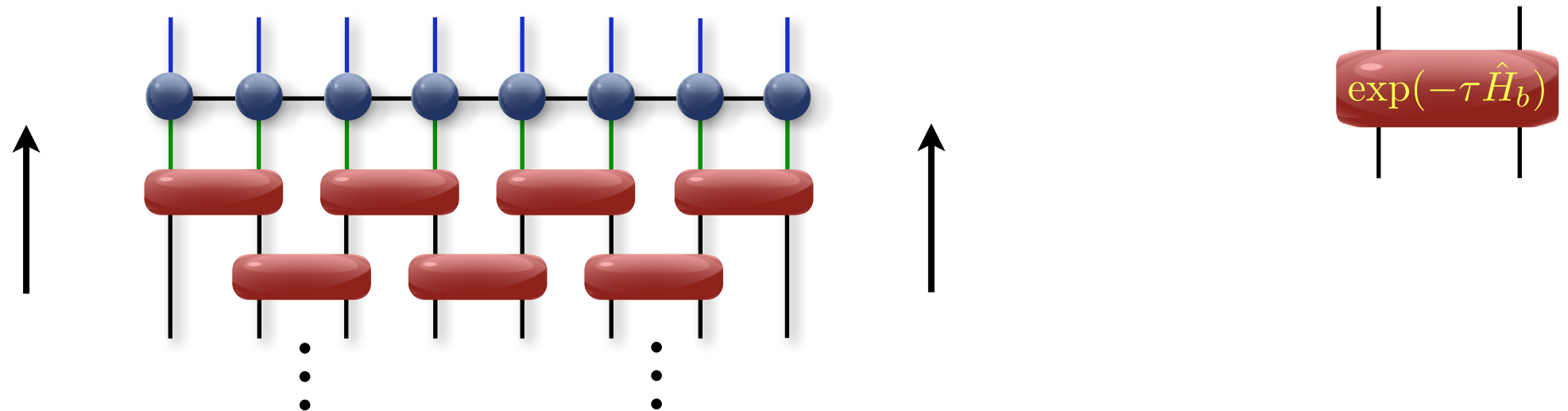
- Initial state:  **exact!**

- Evolve in imaginary time:  $\hat{\rho}(\beta) = e^{-\beta\hat{H}/2}\hat{\rho}(0)e^{-\beta\hat{H}/2}$

*Trotter-Suzuki decomposition:*  $\exp(-\beta\hat{H}) = \exp(-\beta \sum_b \hat{H}_b) = \left( \exp(-\tau \sum_b \hat{H}_b) \right)^n \approx \left( \prod_b \exp(-\tau \hat{H}_b) \right)^n$

$\tau = \beta/n$

- ID:

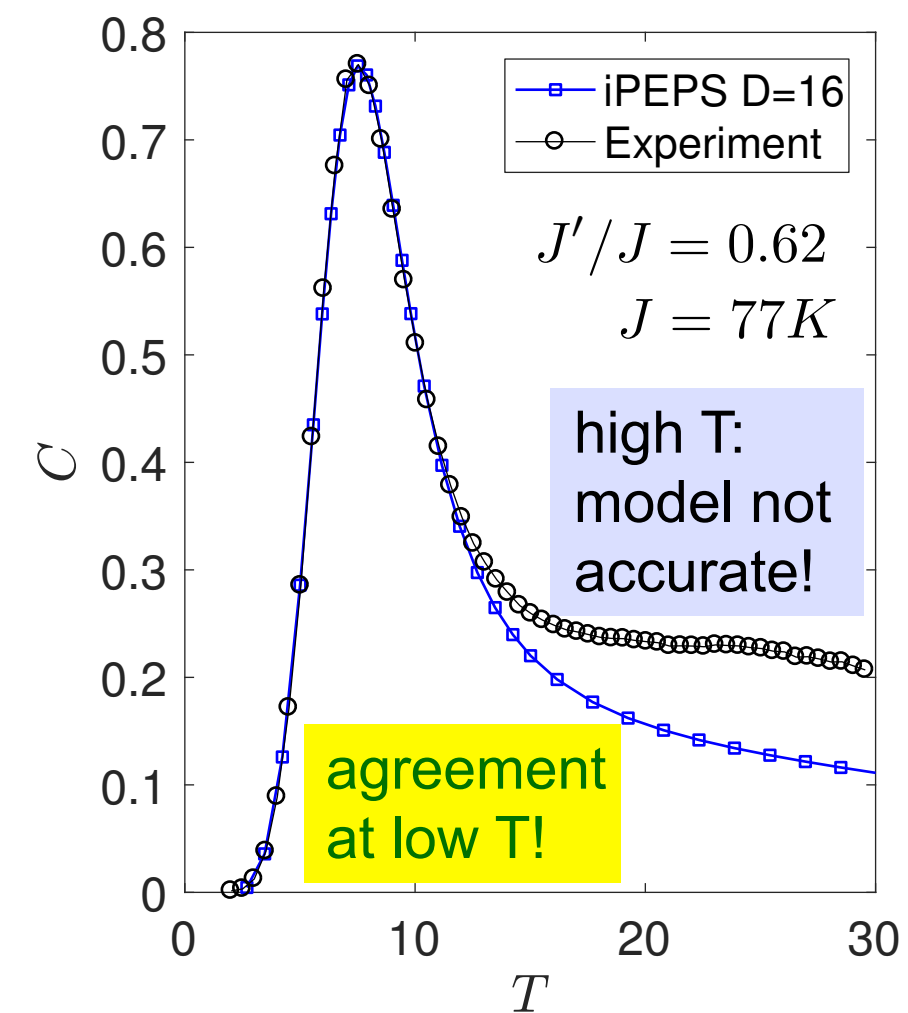
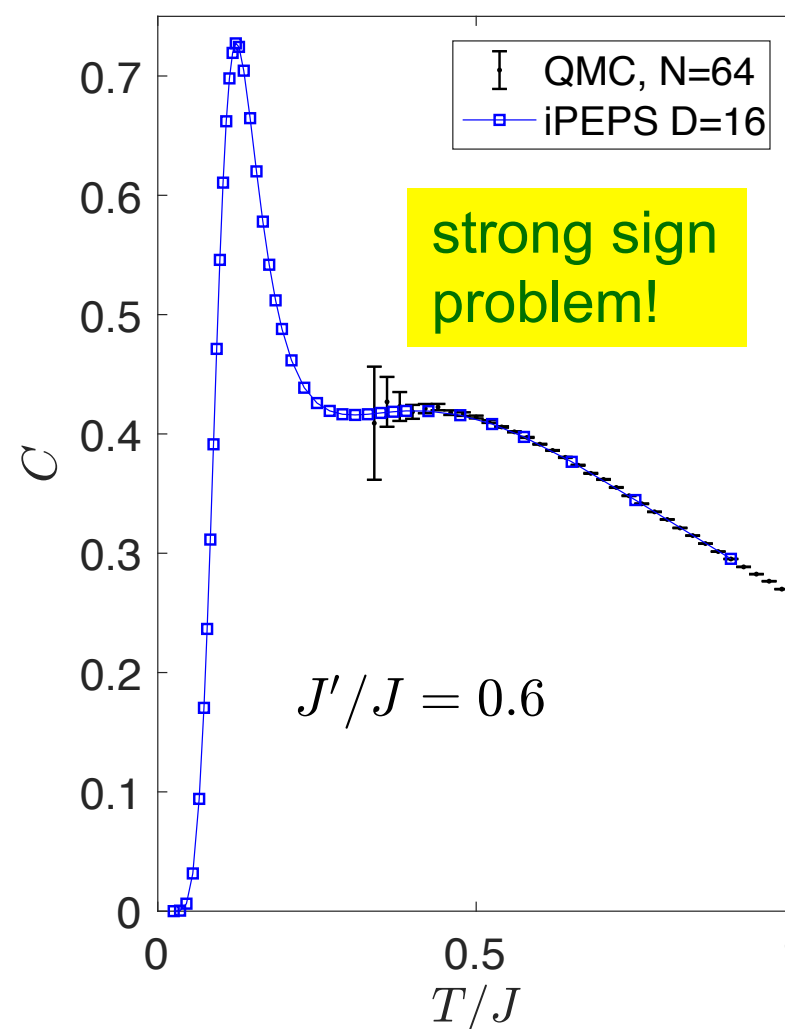
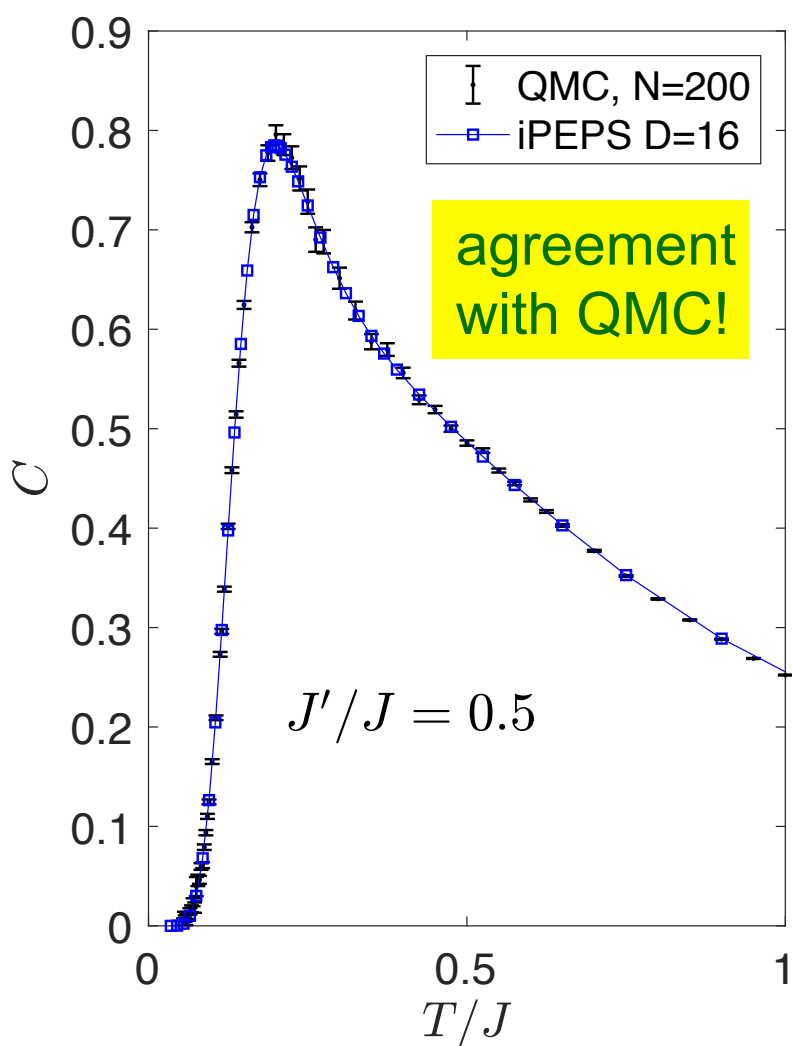
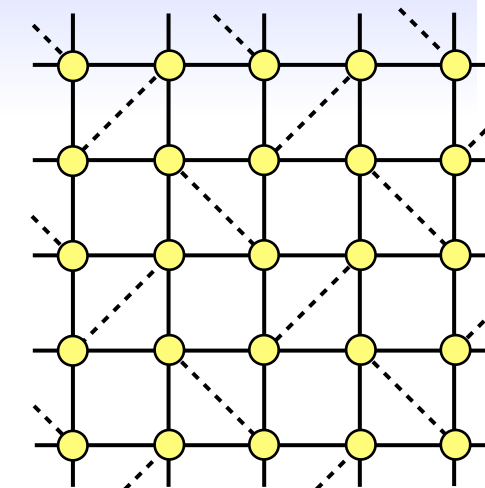


- Evolve up to target  $\beta/2$  using e.g. simple / full update

# Finite temperature simulations example

## ► Application to the Shastry-Sutherland model ( $\text{SrCu}_2(\text{BO}_3)_2$ )

Wietek, PC, Wessel, Normand, Mila, and Honecker, PRR I (2019)

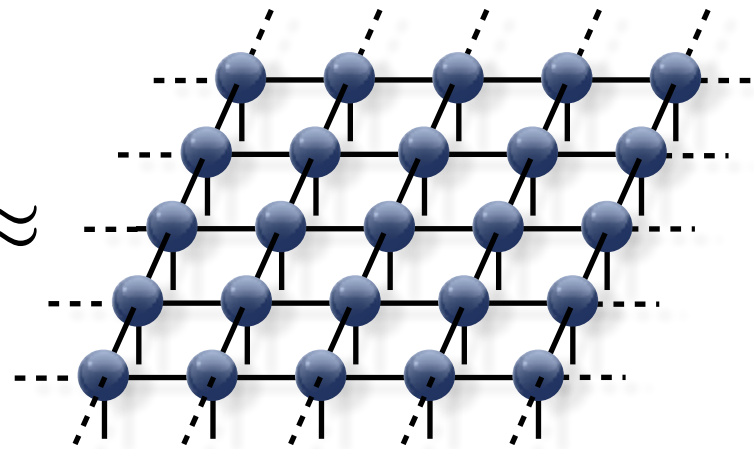


Miyahara and Ueda, arxiv:cond-mat/0004260

# iPEPS excitation ansatz

► Ground state:

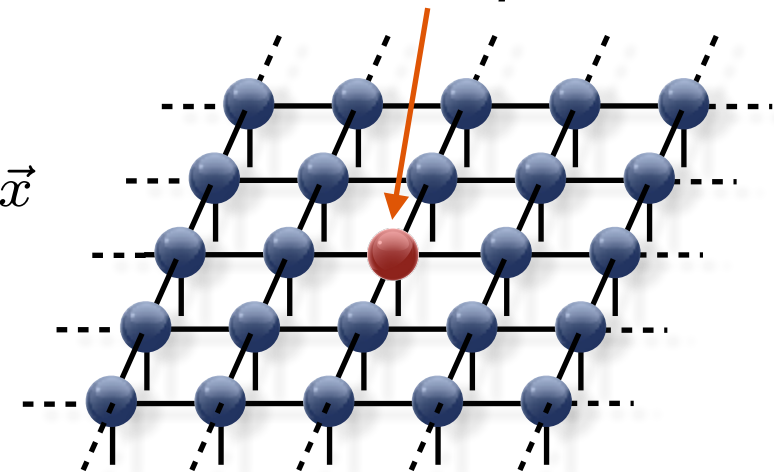
$$|\Psi\rangle \approx$$



► Excitation on top of ground state with momentum  $k$

$$|\Phi_{\vec{k}}(B)\rangle \approx \sum_{\vec{x}} e^{i\vec{k}\vec{x}}$$

*Tensor B at position  $\vec{x}$*

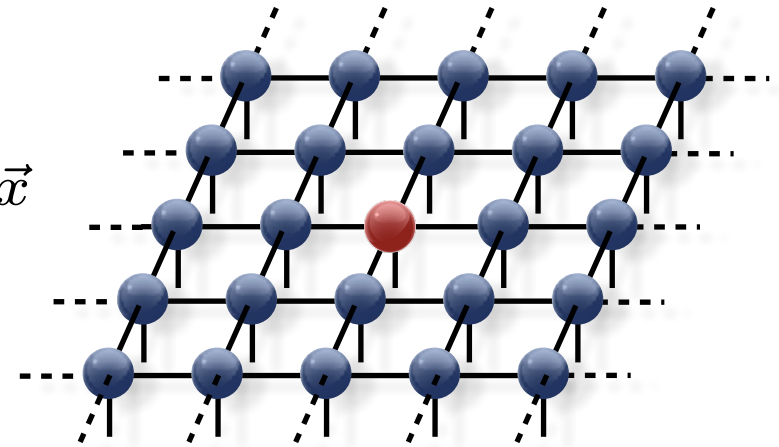


- Haegeman, Pirvu, Weir, Cirac, Osborne, Verschelde, and Verstraete, PRB 85, 100408(R) (2012).  
Haegeman, Michalakis, Nachtergaele, Osborne, Schuch, and Verstraete, PRL 111, 080401 (2013).  
Haegeman, Osborne, and Verstraete, PRB 88, 075133 (2013).  
Zauner, Draxler, Vanderstraeten, Degroote, Haegeman, Rams, Stojevic, Schuch, and Verstraete, New J. Phys. 17, 053002 (2015).  
Vanderstraeten, Marien, Verstraete, and Haegeman, PRB 92, 201111 (2015)  
Vanderstraeten, Haegeman, and Verstraete, PRB 99, 165121 (2019)  
Ponsioen and PC, ArXiv:2001.02645 (2020)

# iPEPS excitation ansatz: the challenge

- ▶ Excitation on top of ground state with momentum  $k$

$$|\Phi_{\vec{k}}(B)\rangle \approx \sum_{\vec{x}} e^{i\vec{k}\vec{x}}$$



Ansatz consists of an infinite sum!

- ▶ Minimizing:  $\langle \Phi_{\vec{k}}(B) | \hat{H} | \Phi_{\vec{k}}(B) \rangle$

Triple infinite sum!

Translational invariance  
→ Double infinite sum

- ▶ Use systematic summation:

**Channel environments**

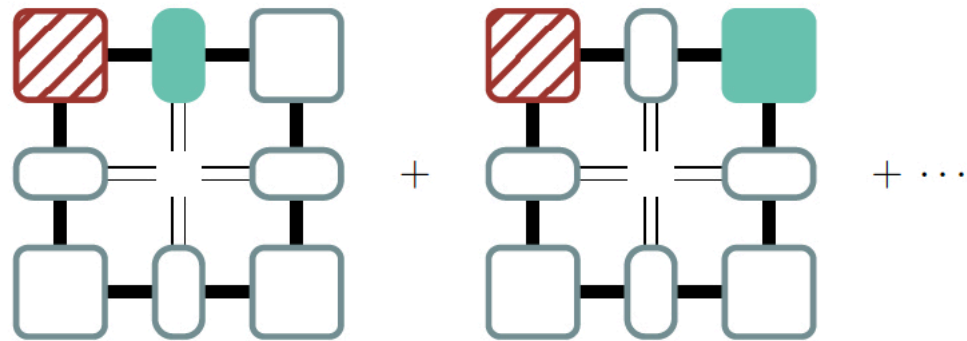
Vanderstraeten, Marien, Verstraete, and Haegeman, PRB 92 (2015)  
Vanderstraeten, Haegeman, and Verstraete, PRB 99(2019)

**CTM approach**

Ponsioen and PC, ArXiv:2001.02645 (2020)

# Systematic summation using CTM

$$\langle \Phi_{\vec{k}}(B) | \hat{H} | \Phi_{\vec{k}}(B) \rangle$$



Norm



Energy

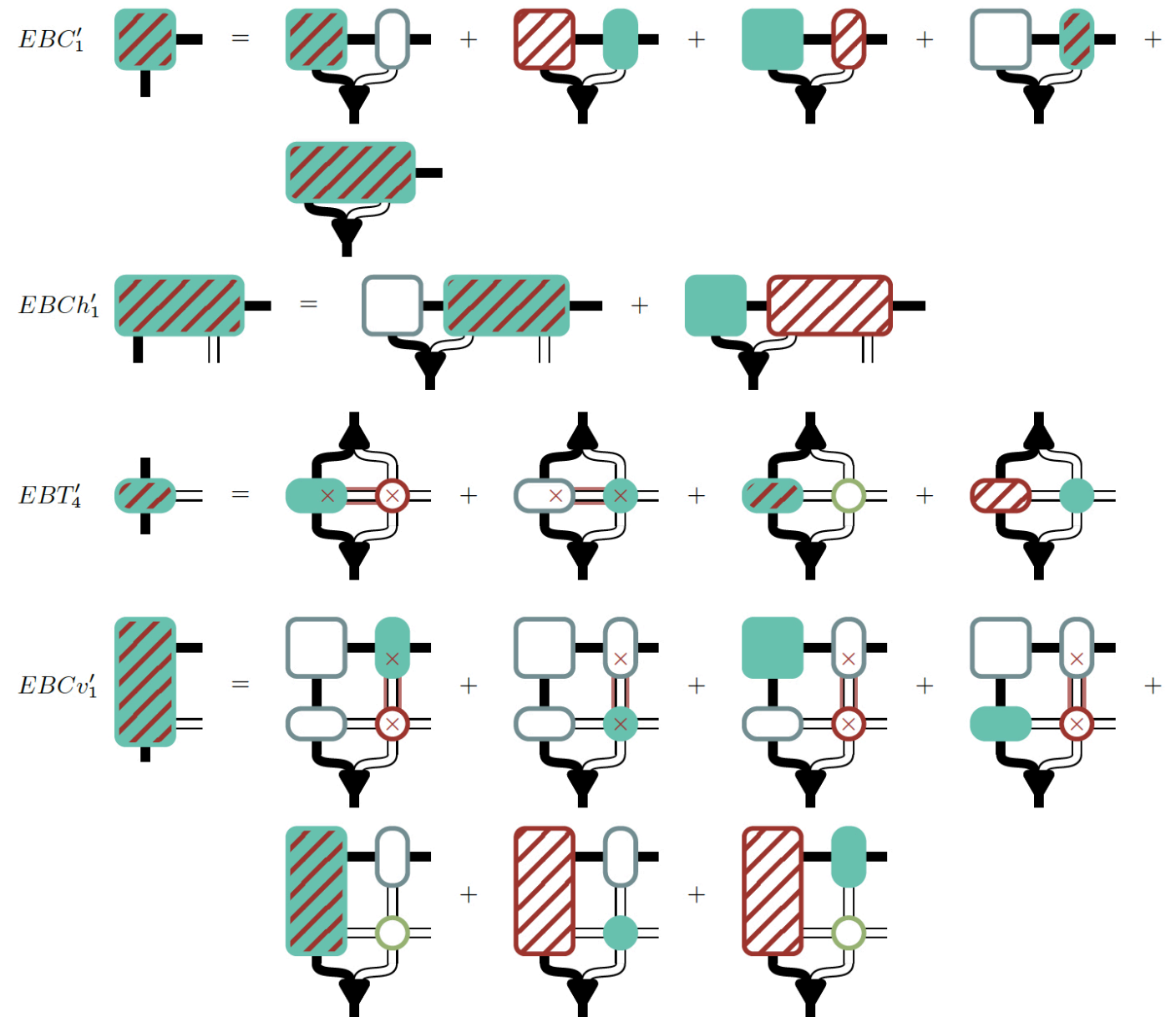


Excitation



Energy + excitation

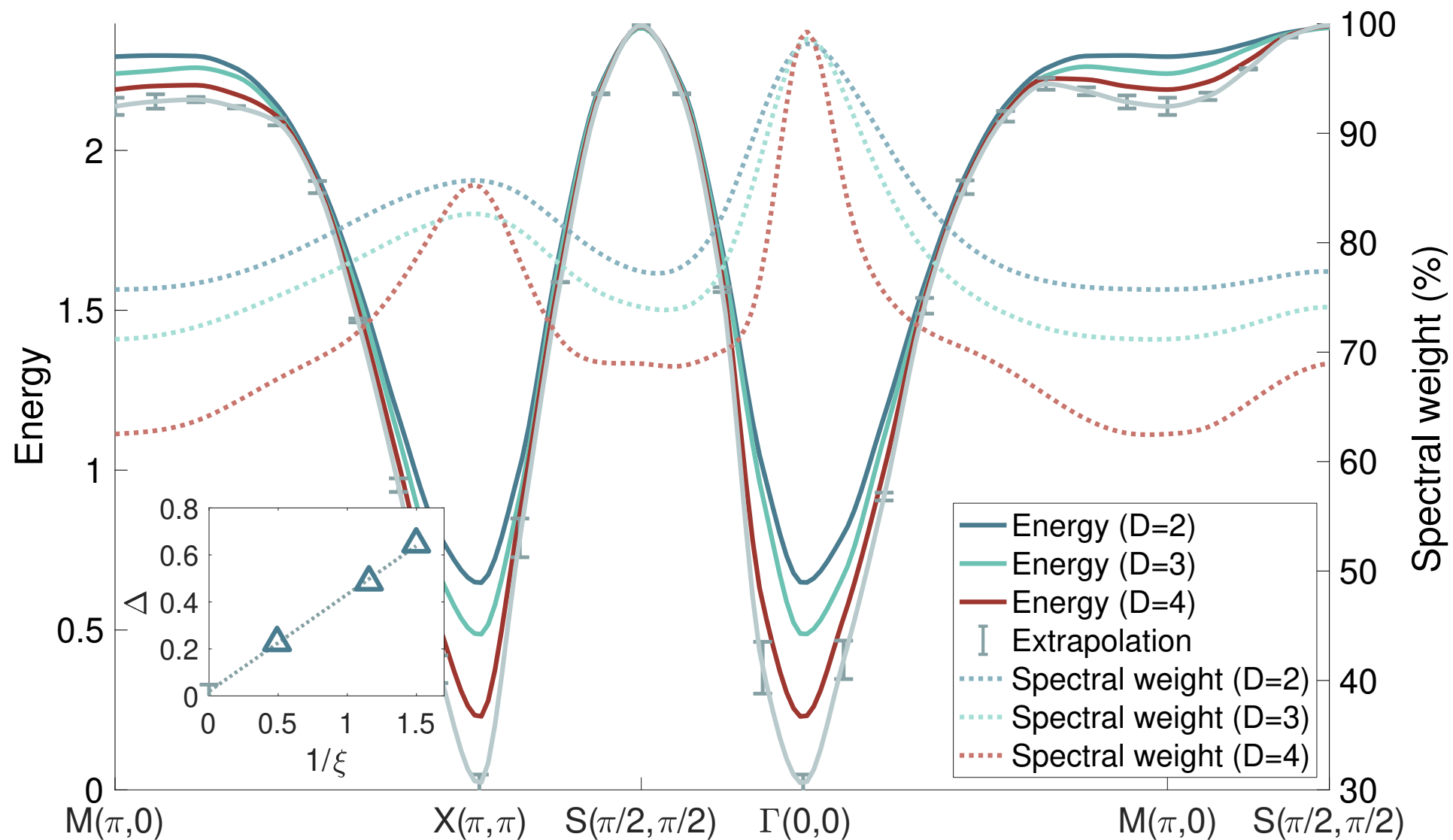
## Left move examples:



... it's just bookkeeping



# Benchmark: Heisenberg model



Ponsioen, PC, ArXiv:2001.02645

similar results in:

Vanderstraeten, Haegeman, Verstraete, PRB 99, 165121 (2019)

# Summary

- ✓ **1D** tensor networks: State-of-the-art (MPS, DMRG)
- ✓ **2D** tensor networks: A lot of progress in recent years!
  - ★ iPEPS has become a powerful tool to study challenging problems: Frustrated spin systems, fermionic systems,  $SU(N)$  systems, ...
  - ★ New approaches for finite temperature, excitations, time evolution, open systems, critical phenomena, classification of topologically ordered systems, ...
- ✓ Still big room for improvement & many possible extensions!

Thank you for your attention!