Fermionic tensor networks

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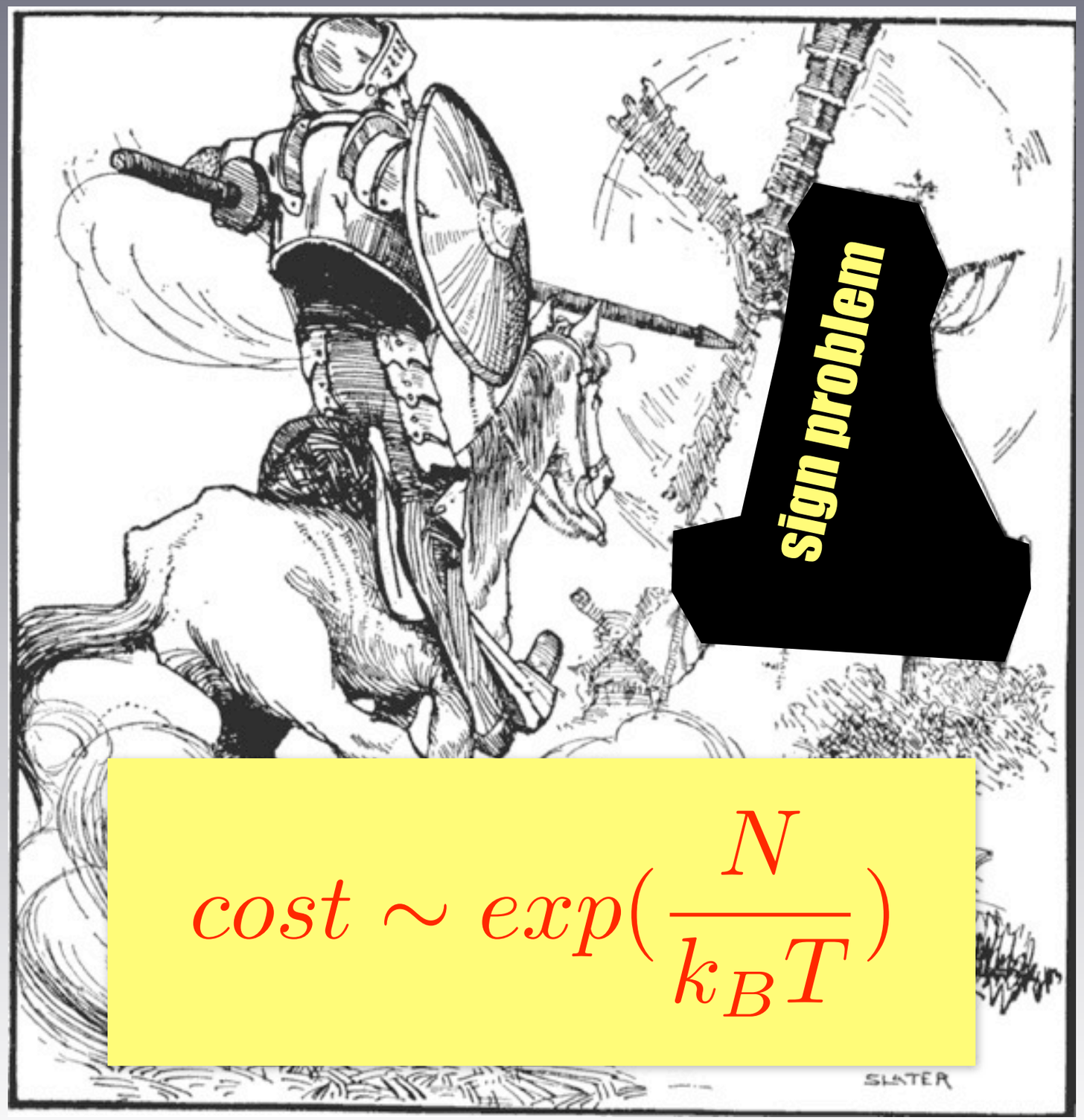
University of Vienna: Frank Verstraete

ETH/EPFL: Bela Bauer, Matthias Troyer, Frederic Mila

Acknowledgments: Luca Tagliacozzo, Robert Pfeifer

P. Corboz, G. Evenbly, F. Verstraete, G. Vidal, PRA 81, 010303(R) (2010)
P. Corboz, G. Vidal, Phys. Rev. B 80, 165129 (2009)
P. Corboz, R. Orus, B. Bauer, G. Vidal. PRB 81, 165104 (2010)
P. Corboz, J. Jordan, G. Vidal, arXiv:1008:3937

Attack the sign problem



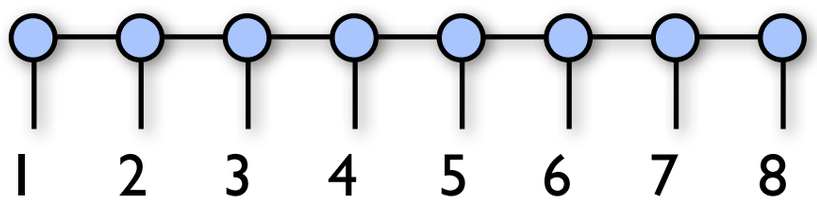
$$cost \sim exp(\frac{N}{k_B T})$$

Overview: tensor networks in 1D and 2D

1D

MPS

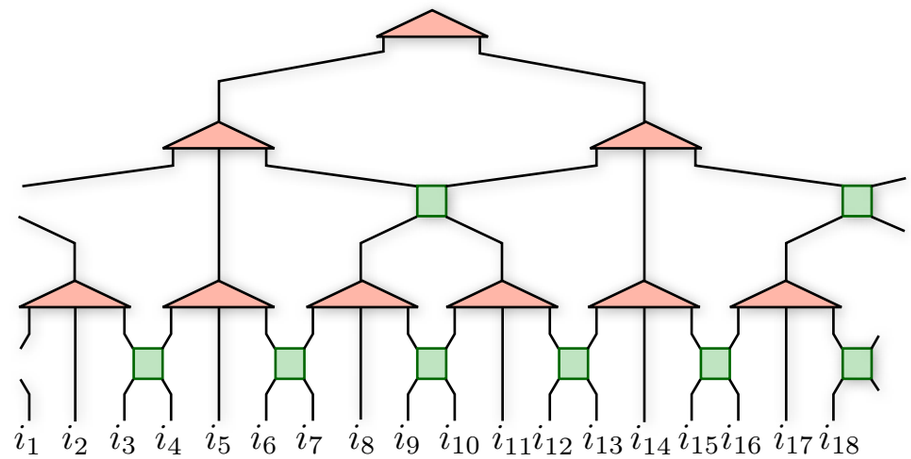
Matrix-product state



Related to the famous density-matrix renormalization group (DMRG) method

1D MERA

Multi-scale entanglement renormalization ansatz



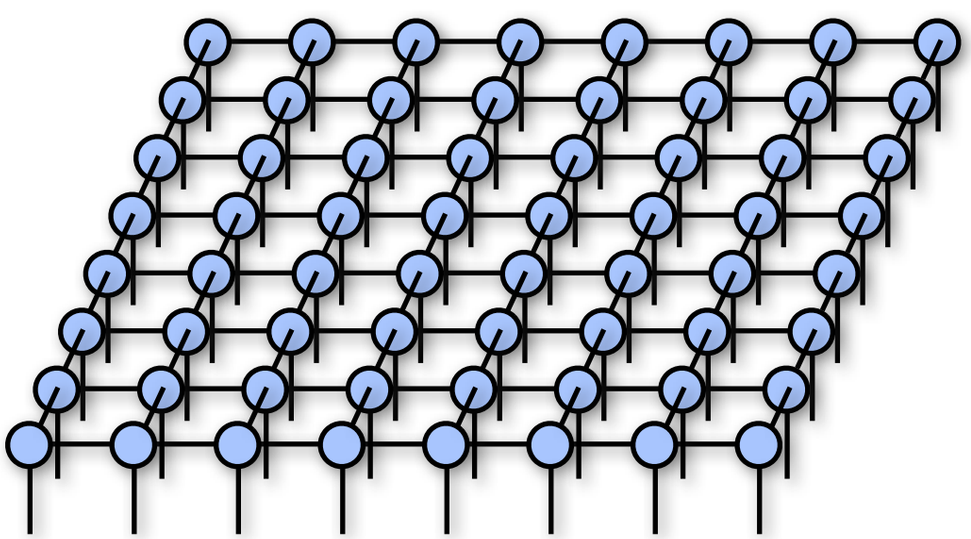
and more

- 1D tree tensor network
- ...

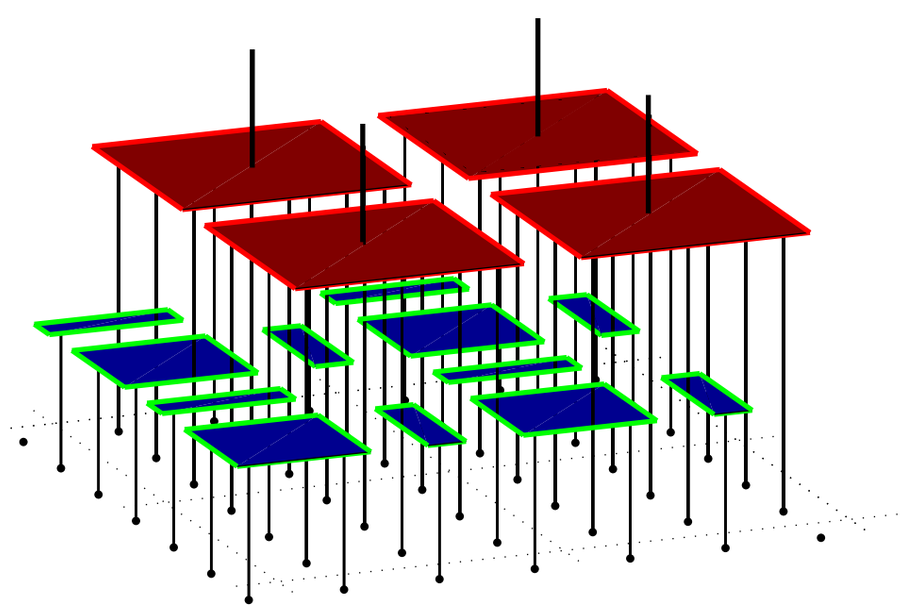
2D

(i)PEPS

(infinite) projected pair-entangled state



2D MERA



and more

- 2D tree tensor network
- String-bond states
- Entangled-plaquette states
- ...

Fermions in 2D & tensor networks

Simulate fermions in 2D?

Before April 2009: **NO!**

Since April 2009: **YES!**

P. Corboz, G. Evenbly, F. Verstraete, G. Vidal, arXiv:0904:4151

C. V. Kraus, N. Schuch, F. Verstraete, J. I. Cirac, arXiv:0904.4667

C. Pineda, T. Barthel, J. Eisert, arXiv:0905.0669

P. Corboz, G. Vidal, Phys. Rev. B 80, 165129 (2009)

T. Barthel, C. Pineda, J. Eisert, PRA 80, 042333 (2009)

Q.-Qian Shi, S.-Hao Li, J-Hui Zhao, H-Qiang Zhou, arXiv:0907.5520

P. Corboz, R. Orus, B.Bauer, G. Vidal, PRB 81, 165104 (2010)

S.-Hao Li, Q.-Qian Shi, H-Qiang Zhou, arXiv:1001:3343

I. Pizorn, F. Verstraete. arXiv:1003.2743

Z.-C. Gu, F. Verstraete, X.-G. Wen. arXiv:1004.2563

...

Outline

- Short introduction to tensor networks
  - Idea: efficient representation of quantum many-body states
  - Examples: Tree Tensor Network, MERA, MPS, PEPS
- Fermionic systems in 2D & tensor networks
  - Simple rules
  - Computational cost compared to bosonic systems
- Results (iPEPS) & comparison with other methods
  - Free and interacting spinless fermions
  - t-J model
- Summary: What's the **status**?

Tensor networks: Efficient representation of QMB states

$\{|\uparrow\rangle, |\downarrow\rangle\}$

6 site system $|\Psi\rangle = \sum \Psi_{i_1 i_2 i_3 i_4 i_5 i_6} |i_1 \otimes i_2 \otimes i_3 \otimes i_4 \otimes i_5 \otimes i_6\rangle$

$\tilde{\mathbb{V}}$ dimension χ

χ different states

Tensor/multidimensio

j_3

Big tensor $\Psi_{i_1 i_2}$

$C^{j_3}_{i_5 i_6}$

tensor network

$_4 i_5 i_6$

n!

~ex

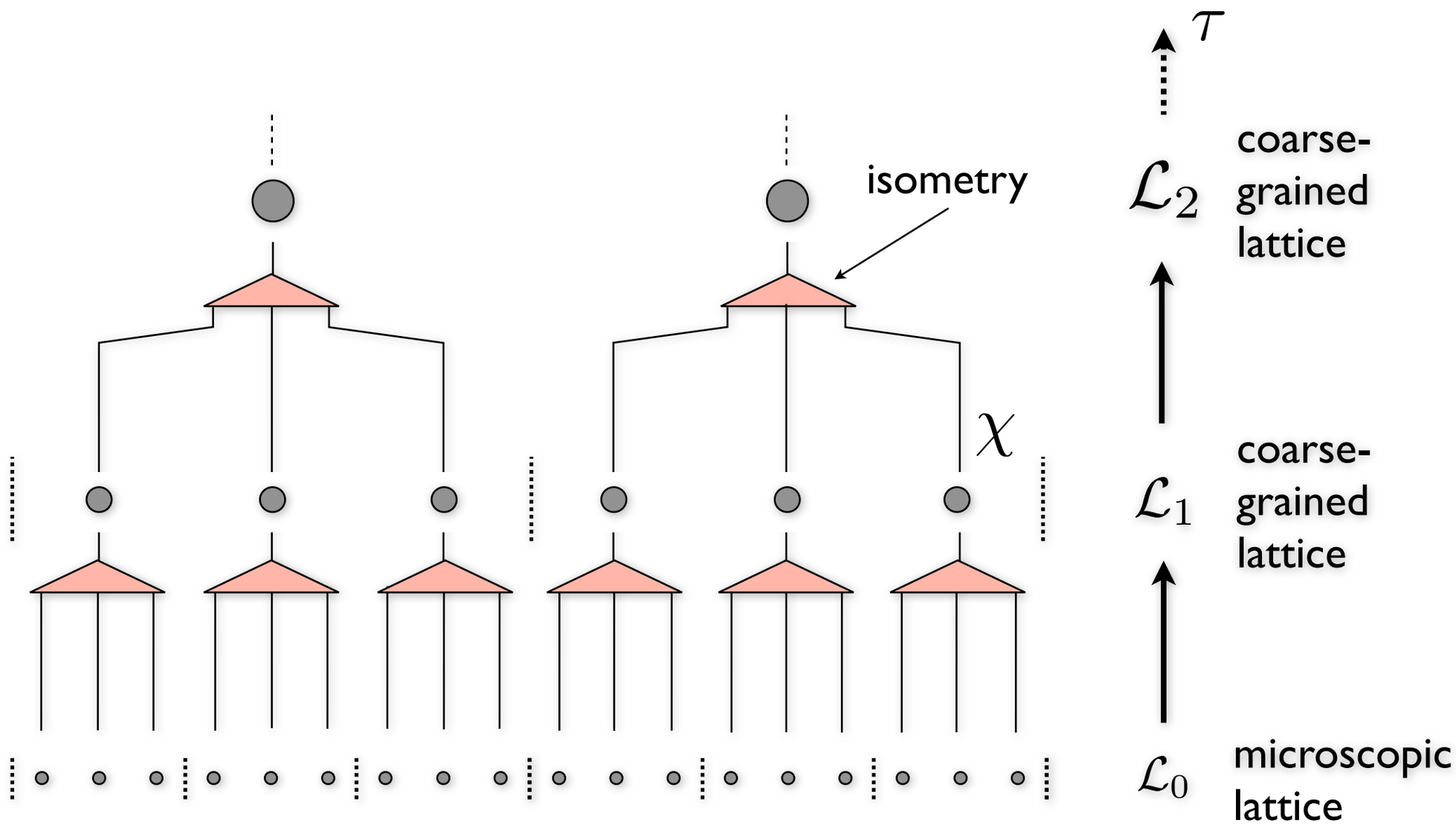
Why is this possible??

Entanglement entropy

General state	**Ground state** (local Hamiltonian)
$S(L) \sim L^D$ (volume)	$S(L) \sim L^{D-1}$ **(area law)**

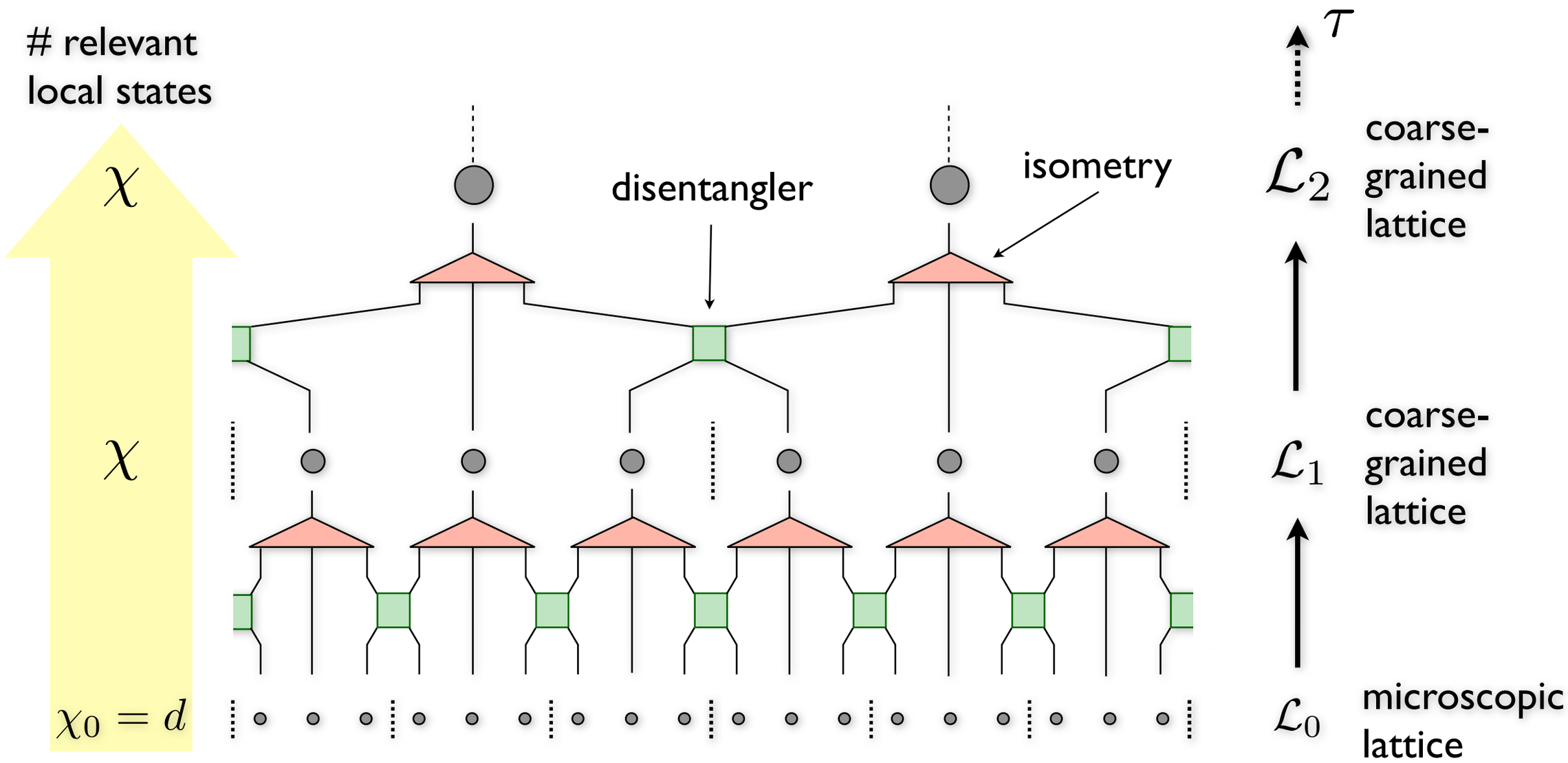
Note: Some (critical) ground states exhibit a **logarithmic correction** to the area law

Tree Tensor Network (1D)



The MERA (The **M**ulti-scale **E**ntanglement **R**enormalization **A**nsatz)

G. Vidal, PRL 99, 220405 (2007), PRL 101, 110501 (2008)



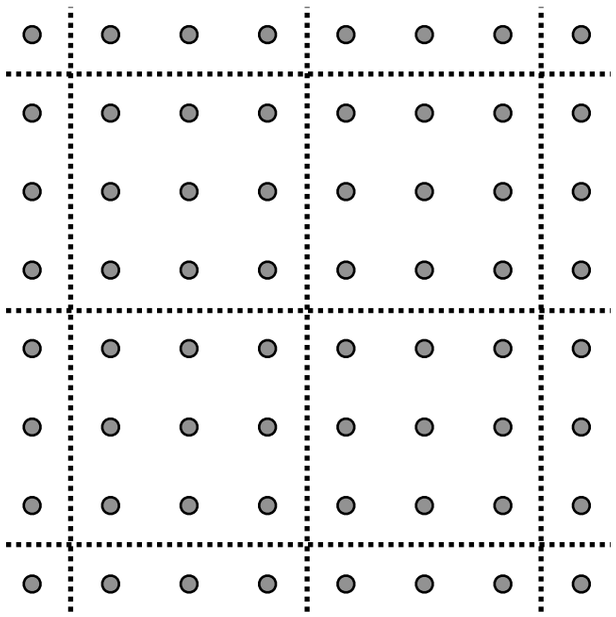
KEY: Disentanglers reduce the amount of short-range entanglement

➡ **Efficient ansatz** for critical and non-critical systems in 1D

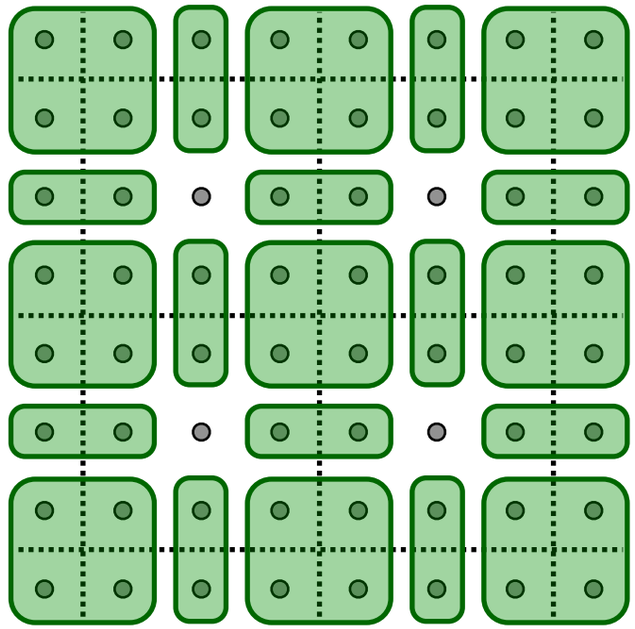
2D MERA (top view)

Evenbly, Vidal. PRL 102, 180406 (2009)

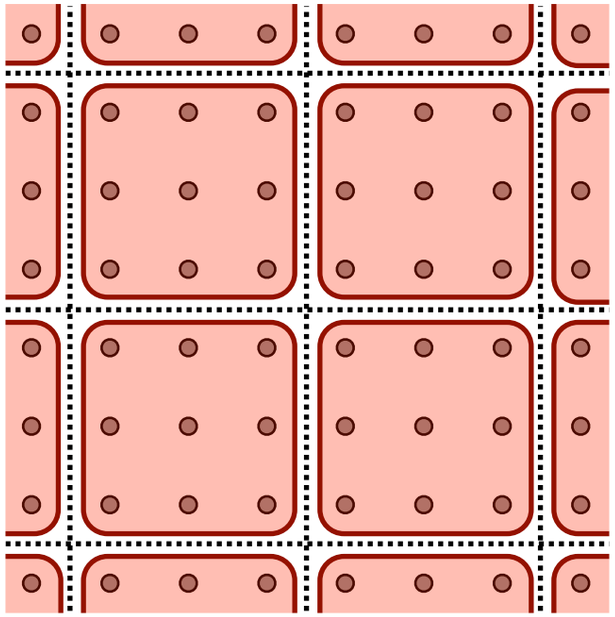
Original lattice



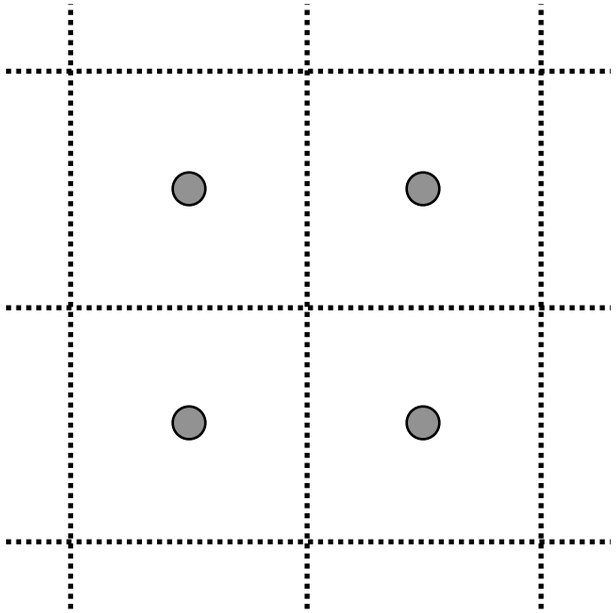
Apply disentanglers



Apply isometries



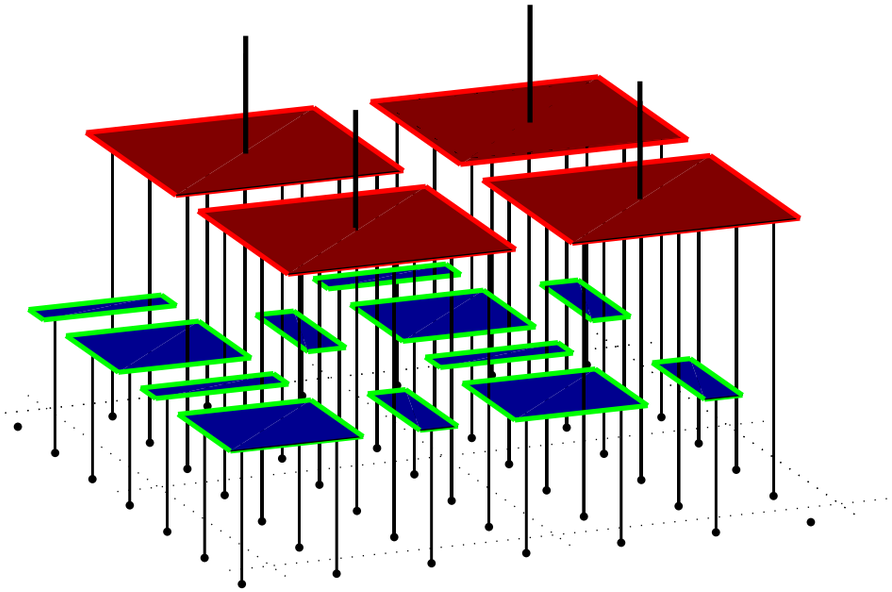
Coarse-grained lattice



✓ Accounts for area-law in 2D systems

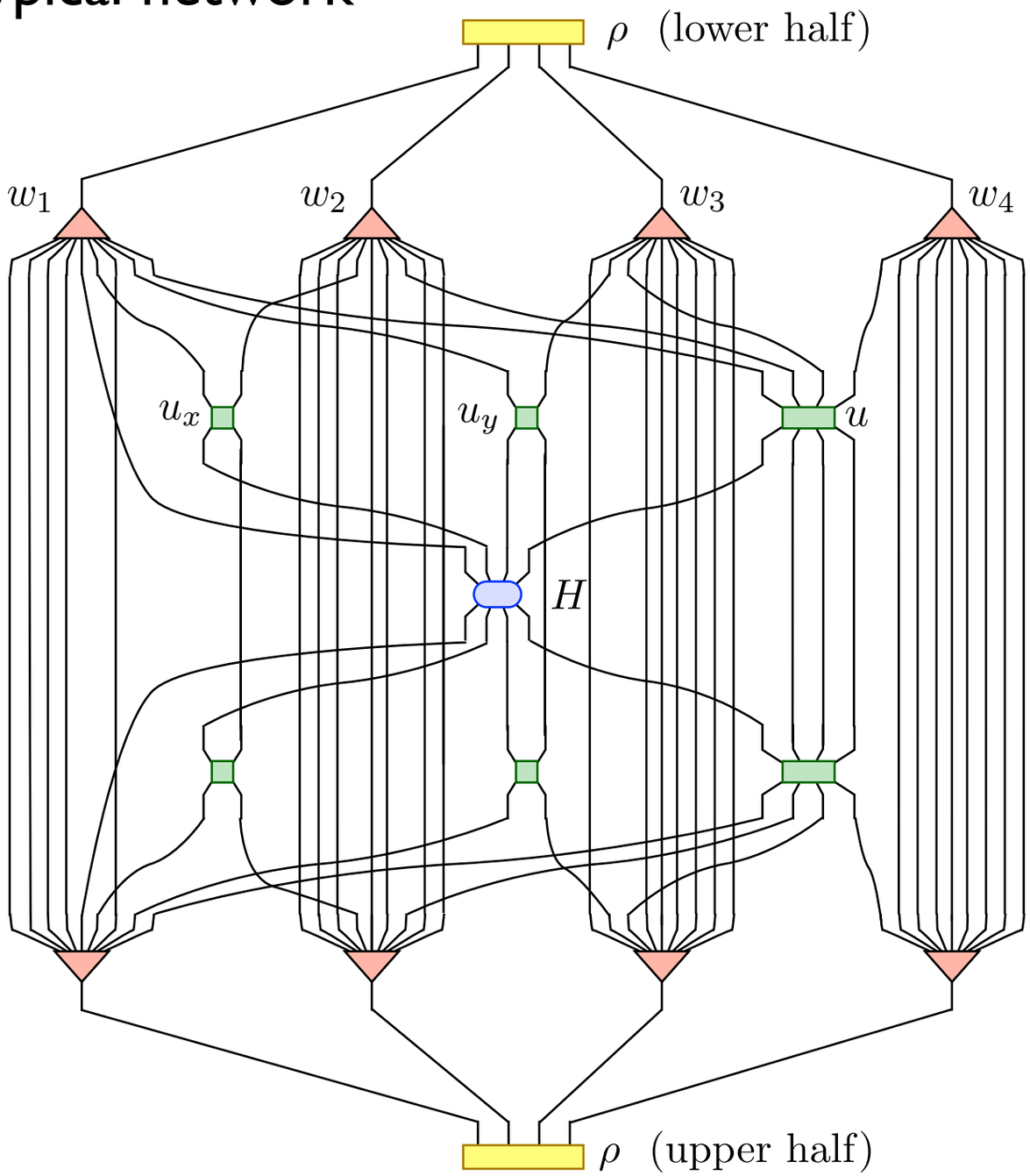
$$S(L) \sim L$$

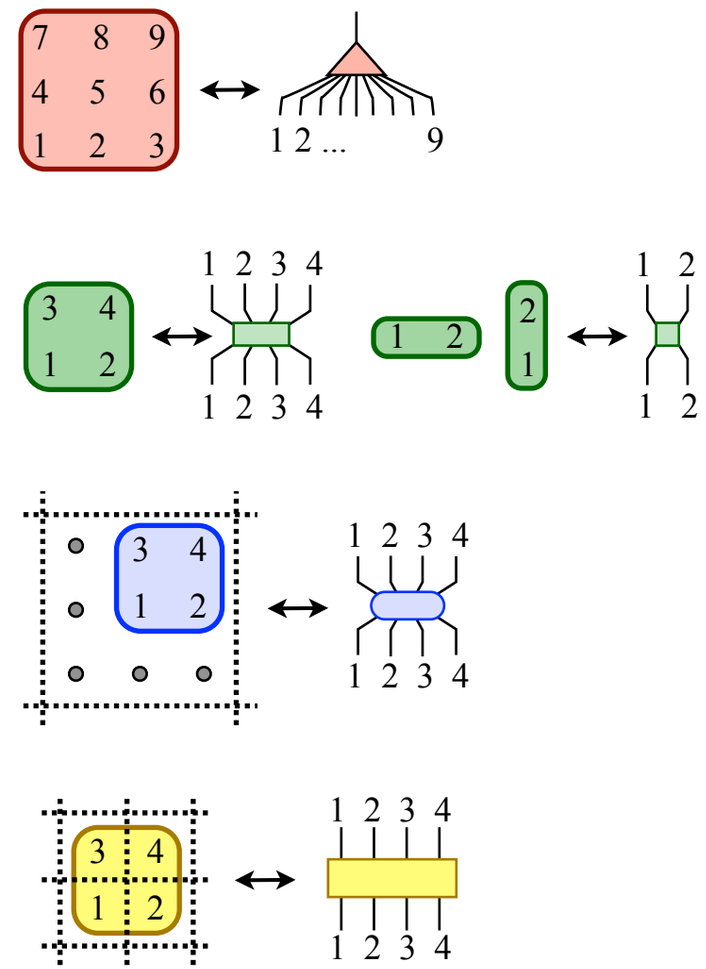
$$\chi_\tau = const$$



2D MERA represented as a 1D MERA

Typical network





Crossing lines play an important role for fermions!

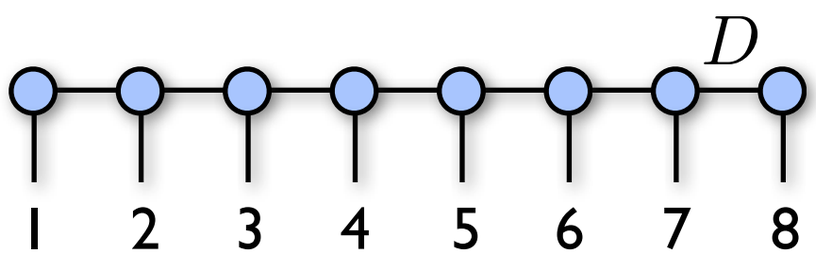
MPS & PEPS

1D

MPS

Matrix-product state

(Related to 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)

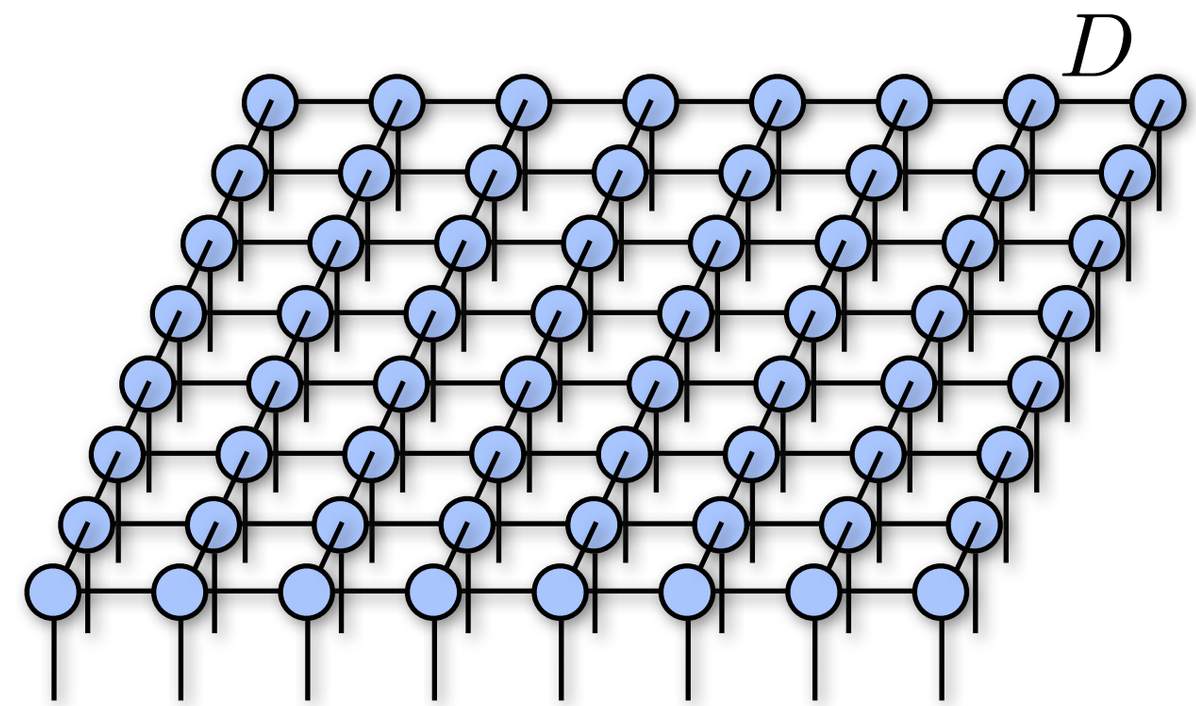
✓ Reproduces area-law in 1D

$$S(L) = const$$

2D

(i)PEPS

(infinite) projected pair-entangled state

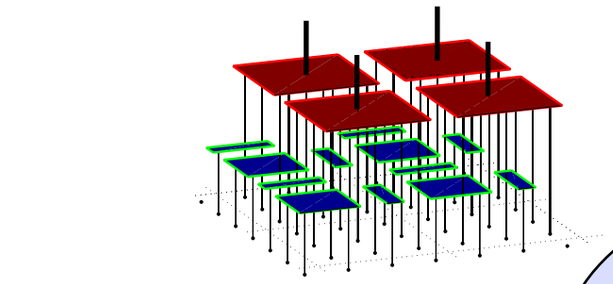


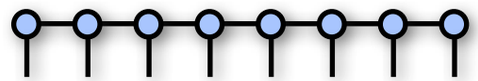
F. Verstraete, J. I. Cirac, cond-mat/0407066

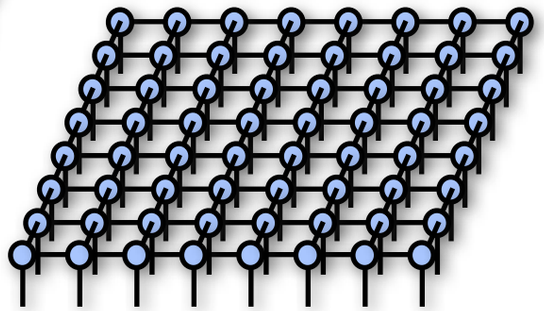
✓ Reproduces area-law in 2D

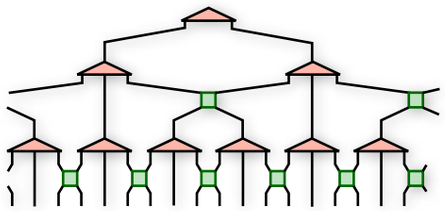
$$S(L) \sim L$$

Summary: Tensor network algorithms









Structure (ansatz)

Find the best (ground) state

$$|\tilde{\Psi}\rangle$$

Compute observables

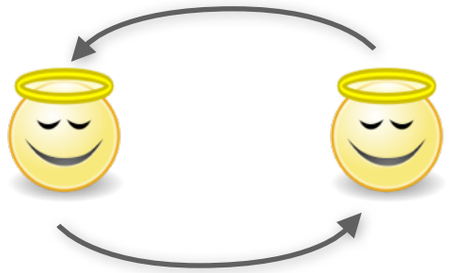
$$\langle\tilde{\Psi}|O|\tilde{\Psi}\rangle$$

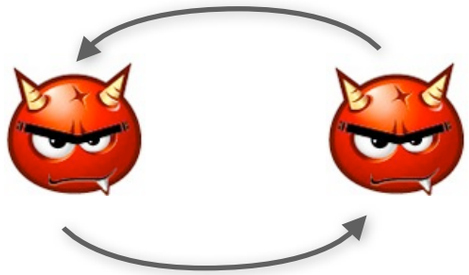
iterative optimization of individual tensors (energy minimization)

imaginary time evolution

Contraction of the tensor network exact / approximate

Bosons vs Fermions





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

$$2) = -\Psi_F(x_2, x_1)$$

symmetri

tisymmetric!

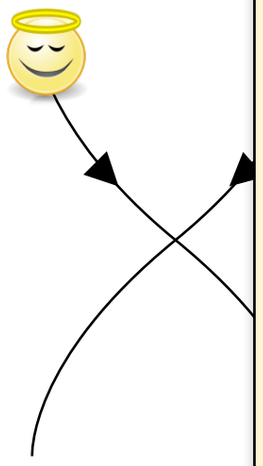
$$\hat{b}_i\hat{b}_j = \hat{b}$$

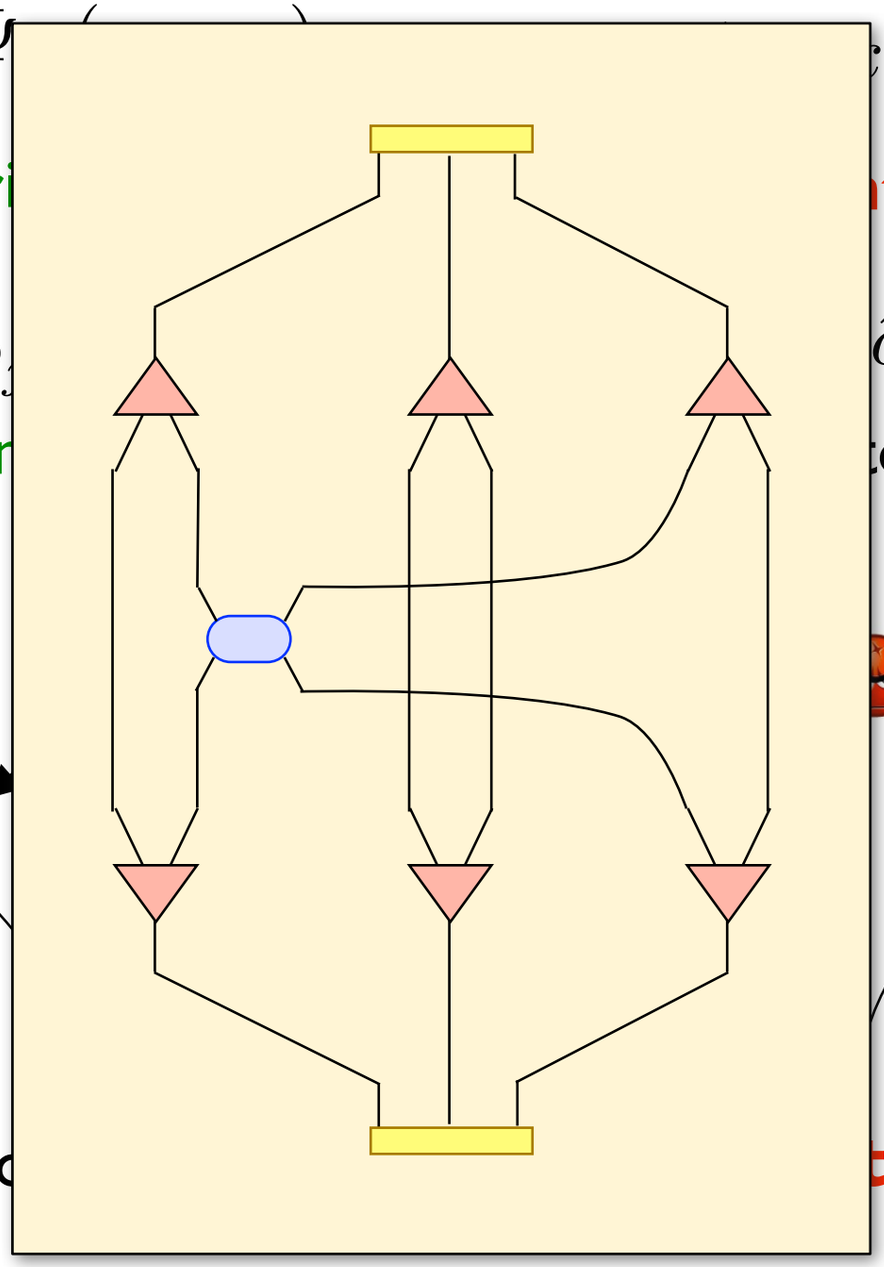
$$\hat{c}_j = -\hat{c}_j\hat{c}_i$$

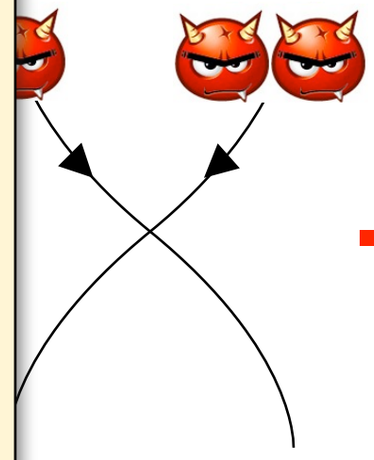
operators cor

tors *anti*commute

Crossings in a tensor network







$$- - = +$$

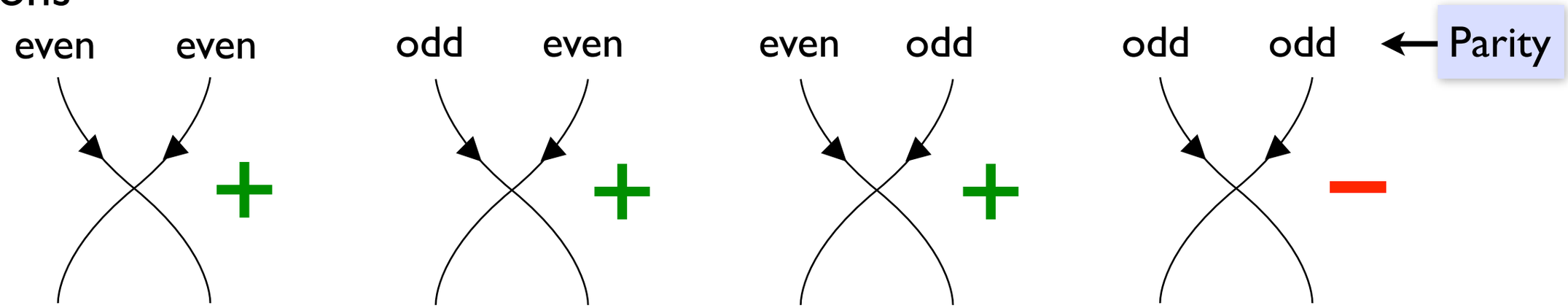
ignore cro

take care!

The swap tensor

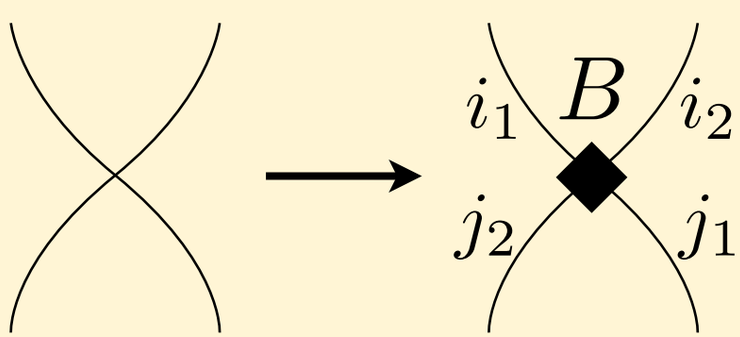
Fermions

RULE:



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**



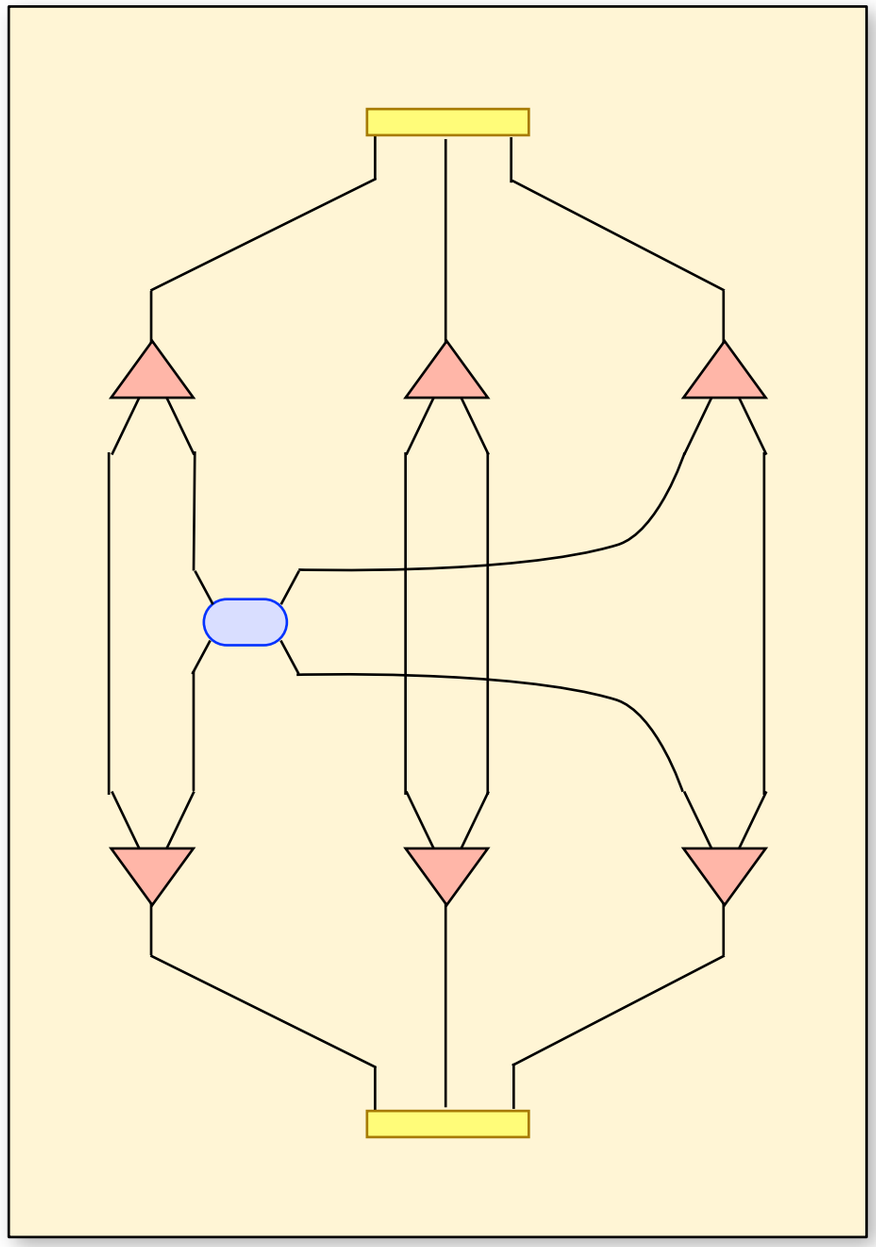
$$B^{i_1 i_2}_{j_2 j_1} = \delta_{i_1,j_1}\delta_{i_2,j_2} S(P(i_1), P(i_2))$$

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

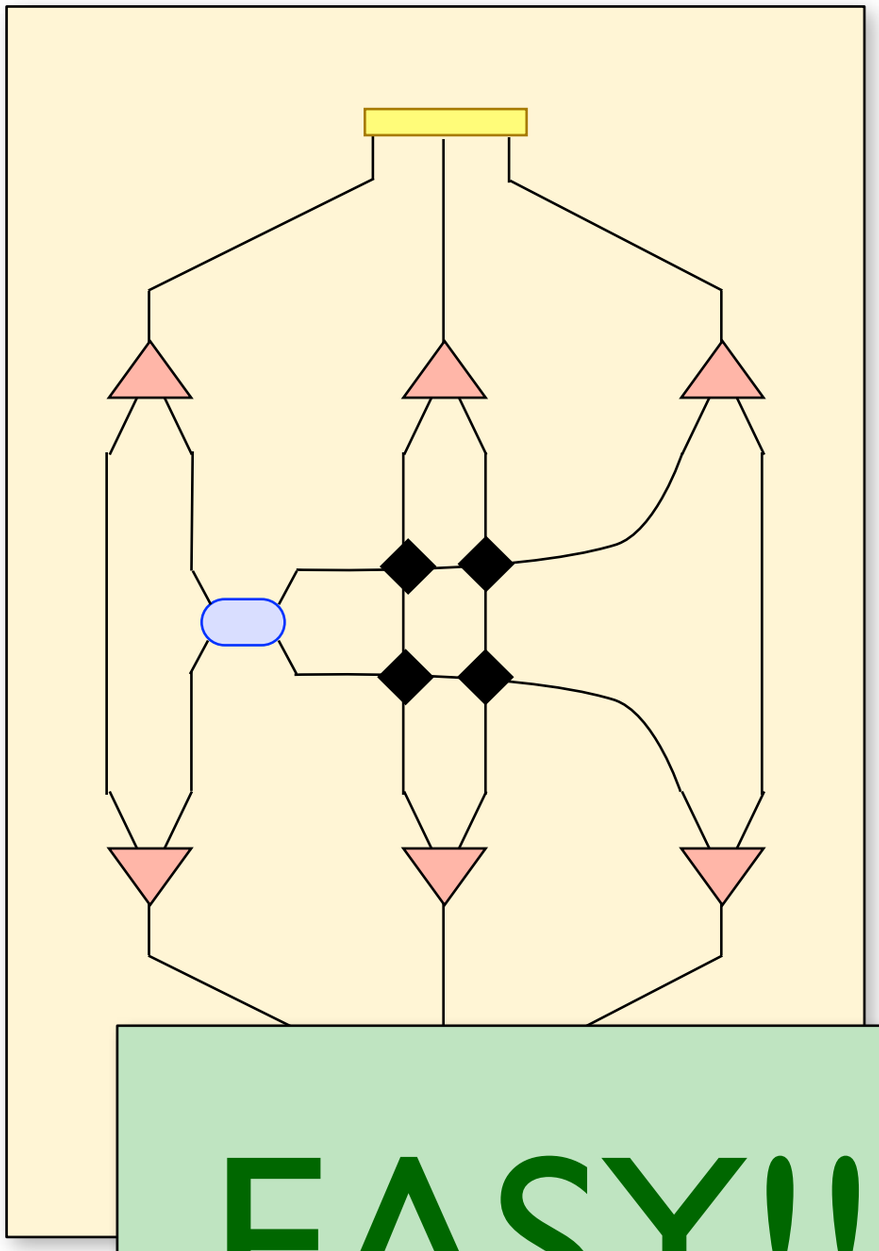
Use **parity** preserving tensors: $T_{i_1 i_2 \ldots i_M} = 0$ if $P(i_1)P(i_2)\ldots P(i_M) \neq 1$

Example

Bosonic tensor network



Fermionic tensor network



EASY!!!

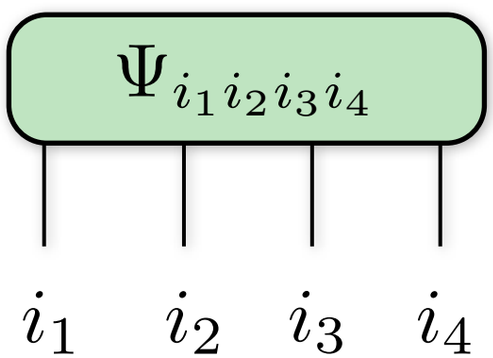
Fermionic "operator networks"

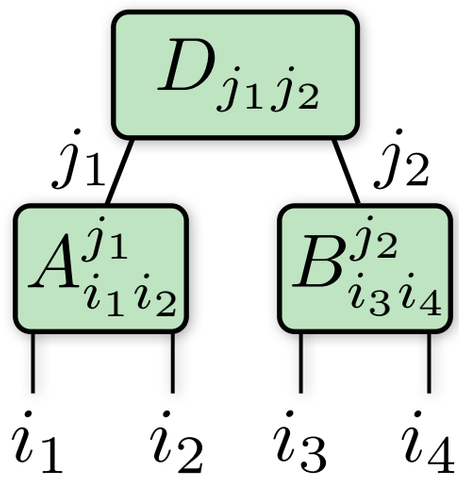
State of 4 site system $|\Psi\rangle = \sum_{i_1 i_2 i_3 i_4} \Psi_{i_1 i_2 i_3 i_4} |i_1 i_2 i_3 i_4\rangle$

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

Bosons

Tensor



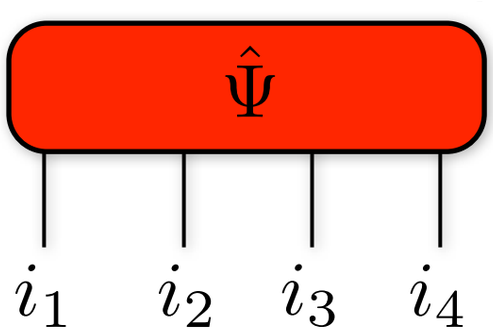


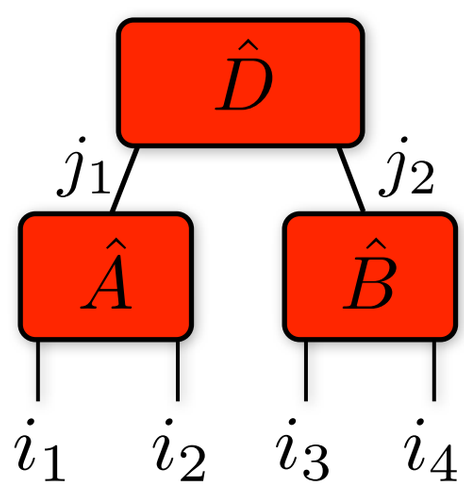
bosonic tensor network

Contract

Fermions

Tensor + fermionic ops





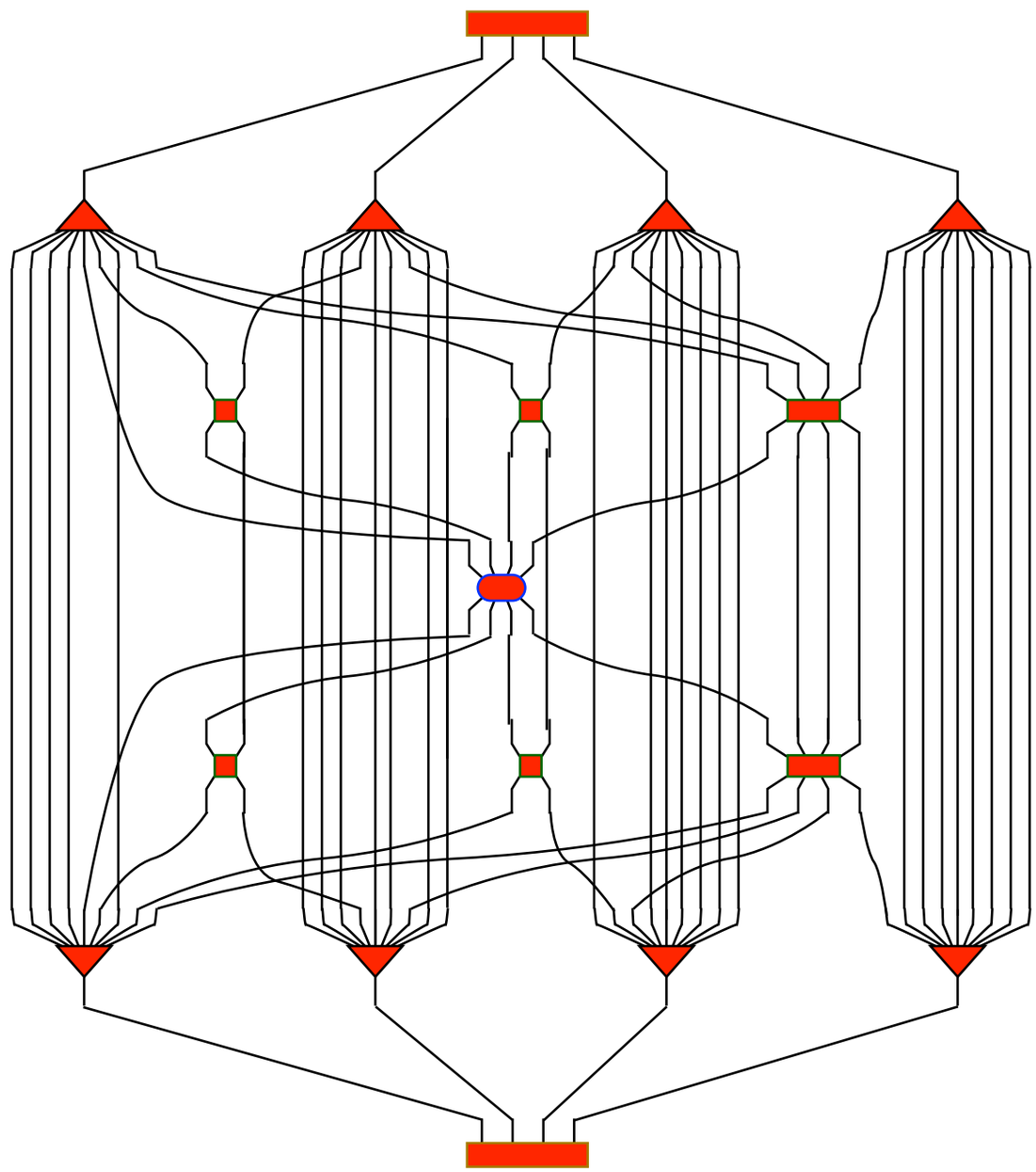
fermionic operator network

Contract + operator calculus

$$\hat{A} = A^{j_1}_{i_1 i_2} |i_1 i_2\rangle\langle j_1| = A^{j_1}_{i_1 i_2} \hat{c}_1^{\dagger i_1} \hat{c}_2^{\dagger i_2} |0\rangle\langle 0| \hat{c}_{1'}^{j_1}$$

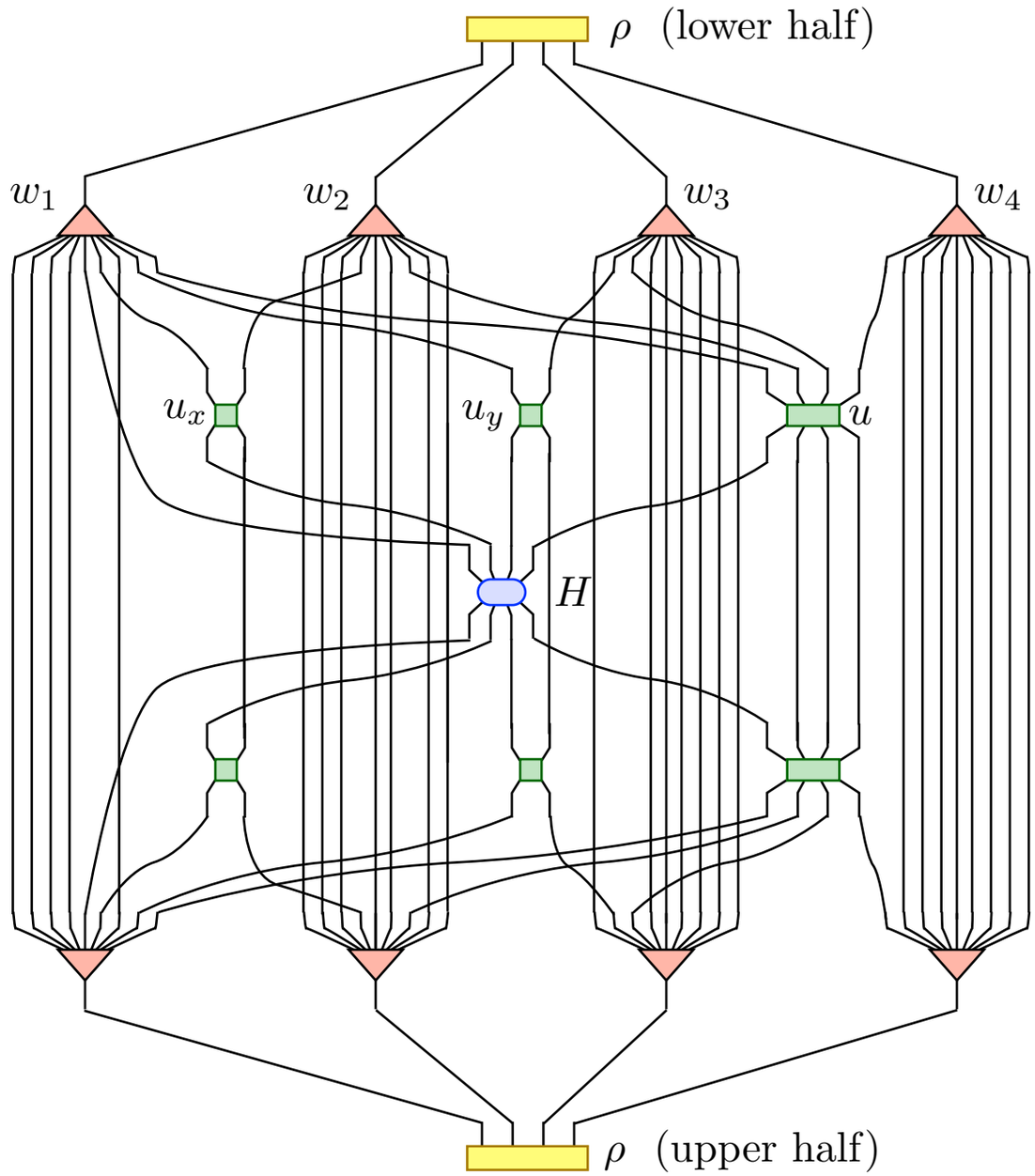
Fermionic "operator network"

Use anticommutation rules to evaluate fermionic operator network:



Easy solution:
Map it to a tensor network by replacing crossings by swap tensors

Cost of fermionic tensor networks??



First thought:

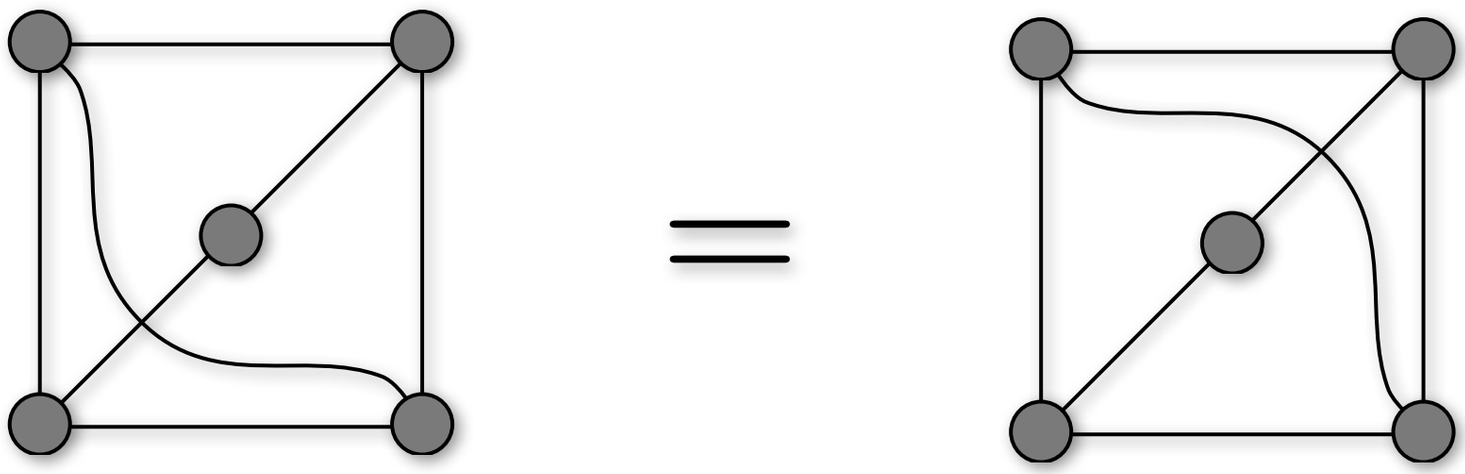
Many crossings → many more tensors

→ **larger computational cost??**

NO!

Same computational cost

The "jump" move

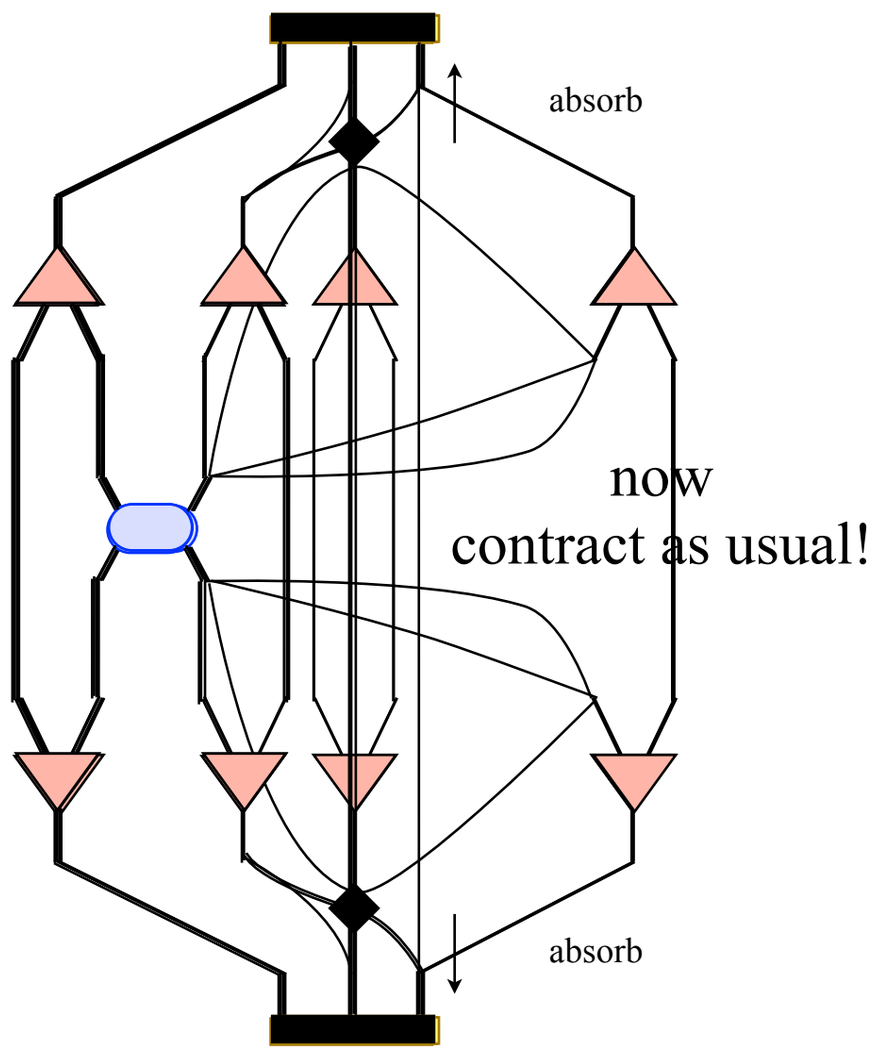


- Jumps over tensors leave the tensor network **invariant**
- Follows form parity preserving tensors

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

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

Example of the "jump" move



Message:

- Taking fermionic statistics into account is **easy!**
  - Replace crossings by swap tensors & use parity preserving tensors
- Computational cost does not depend a priori on the particle statistics, but on the amount of entanglement in the system!

Computational cost

- Leading cost: $\mathcal{O}(D^k)$

MPS: $k = 3$

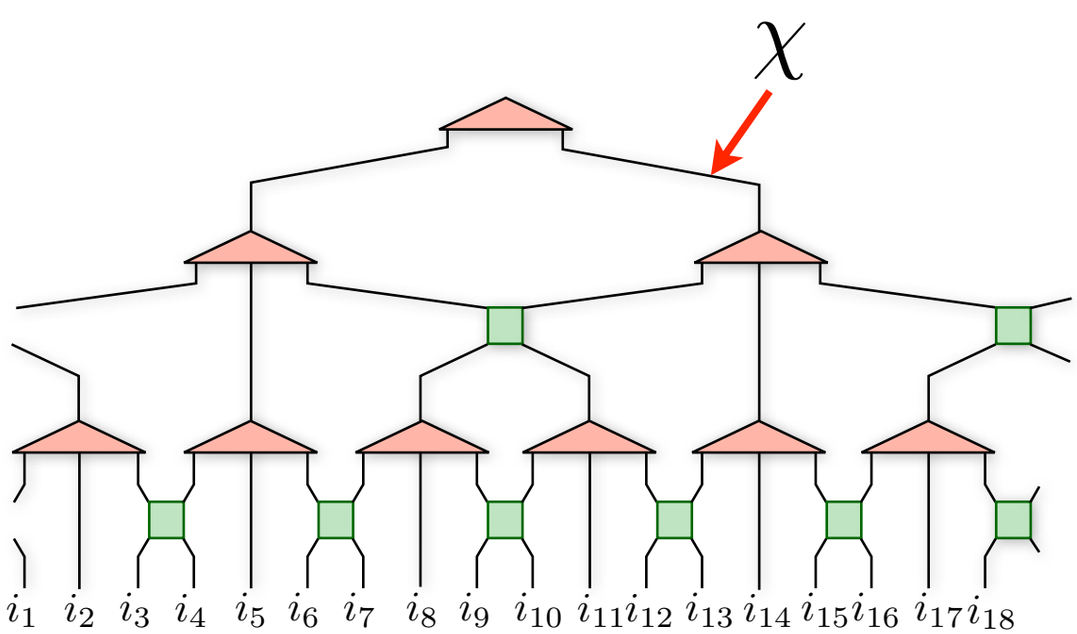
PEPS: $k \approx 10 \ldots 12$

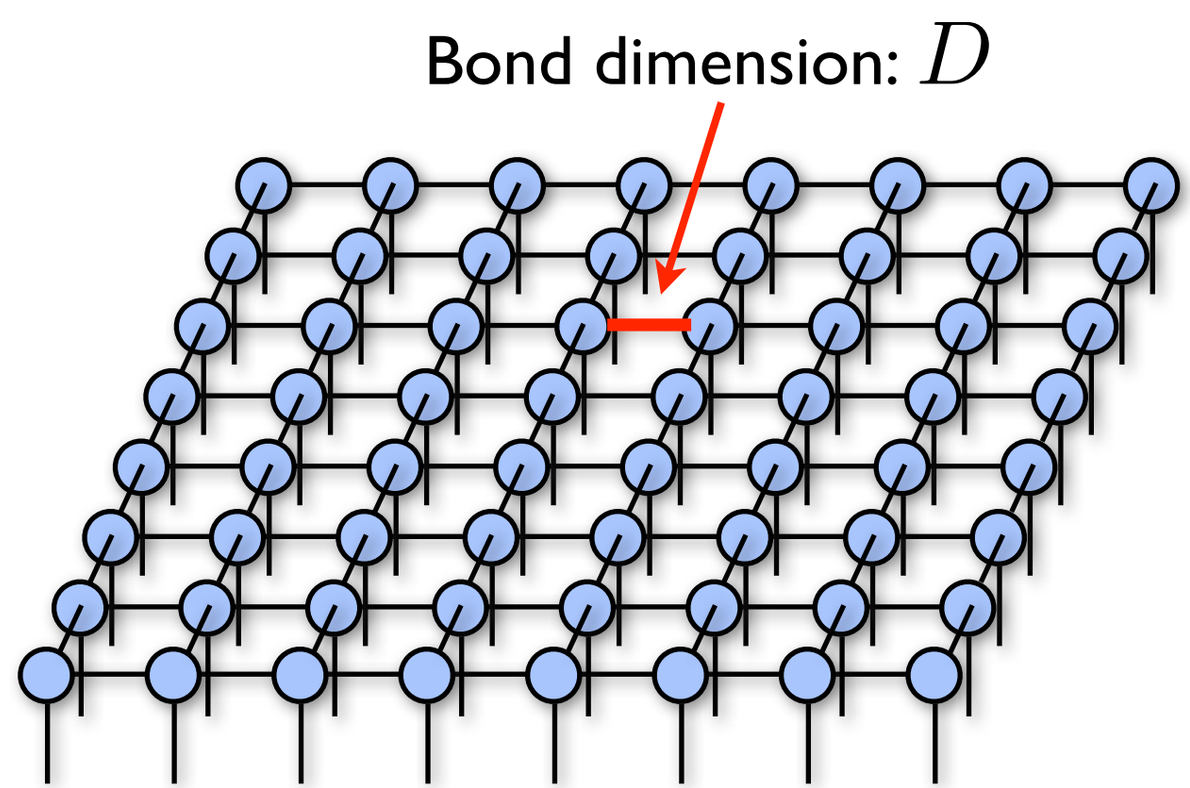
2D MERA: $k = 16$

polynomial scaling but large exponent!

- How large does D have to be?

It depends on the amount of entanglement in the system!





Classification by entanglement

Entanglement

low

high

gapped systems

band insulators,
valence-bond crystals,
s-wave superconductors,
...

gapless systems

Heisenberg model,
p-wave superconductors,
Dirac Fermions,
...

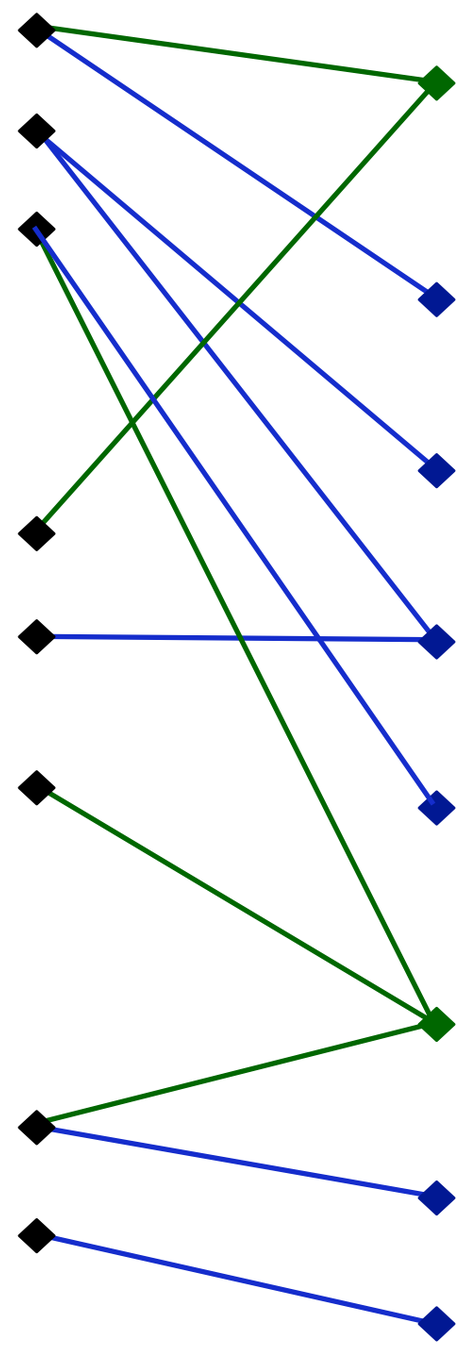
systems with "1D fermi surface"

free Fermions, Fermi-liquid type phases, bose-metals?

$$S(L) \sim L \log L$$

Overview: Results / benchmarks

- Free spinless fermions
  - Finite systems (MERA, TTN)
  - Finite systems (PEPS)
  - Infinite systems (iPEPS)
- Interacting spinless fermions
  - Finite systems (MERA, TTN)
  - Finite systems (PEPS)
  - Phase diagram of t-V model (iPEPS)
- t-J model
  - Benchmark (iPEPS)
  - Phase diagram (iPEPS)



Corboz, Evenbly, Verstraete, Vidal, PRA 81, 010303(R) (2010), Corboz, Vidal, PRB 80, 165129 (2009)

Pineda, Barthel, Eisert, arXiv:0905.0669

Kraus, Schuch, Verstraete, Cirac, arXiv:0904.4667

Pizorn, Verstraete. arXiv:1003.2743

Z.-C. Gu, F. Verstraete, X.-G. Wen. arXiv: 1004.2563

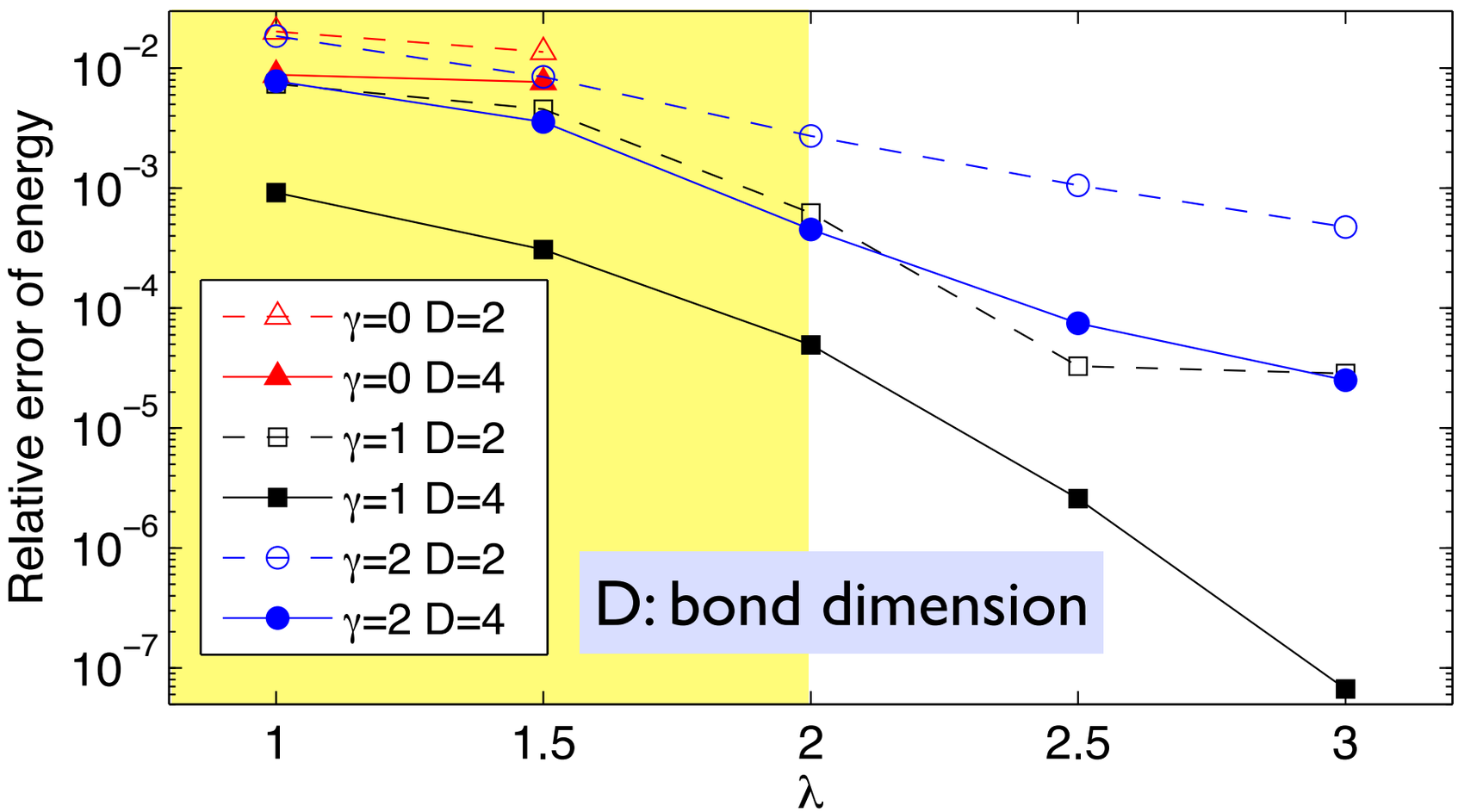
Corboz, Orus, Bauer, Vidal, PRB 81, 165104 (2010)

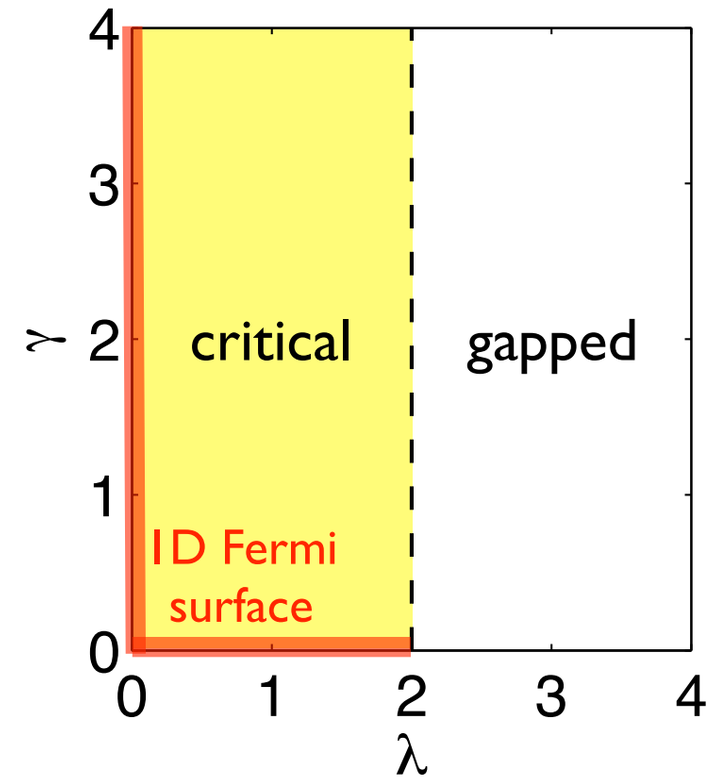
Shi, Li, Zhao, Zhou, arXiv:0907.5520

Li, Shi, Zhou, arXiv:1001:3343

Non-interacting spinless fermions: infinite systems (iPEPS)

$$H_{\text{free}} = \sum_{\langle rs \rangle} [c_r^\dagger c_s + c_s^\dagger c_r - \gamma(c_r^\dagger c_s^\dagger + c_s c_r)] - 2\lambda \sum_r c_r^\dagger c_r$$





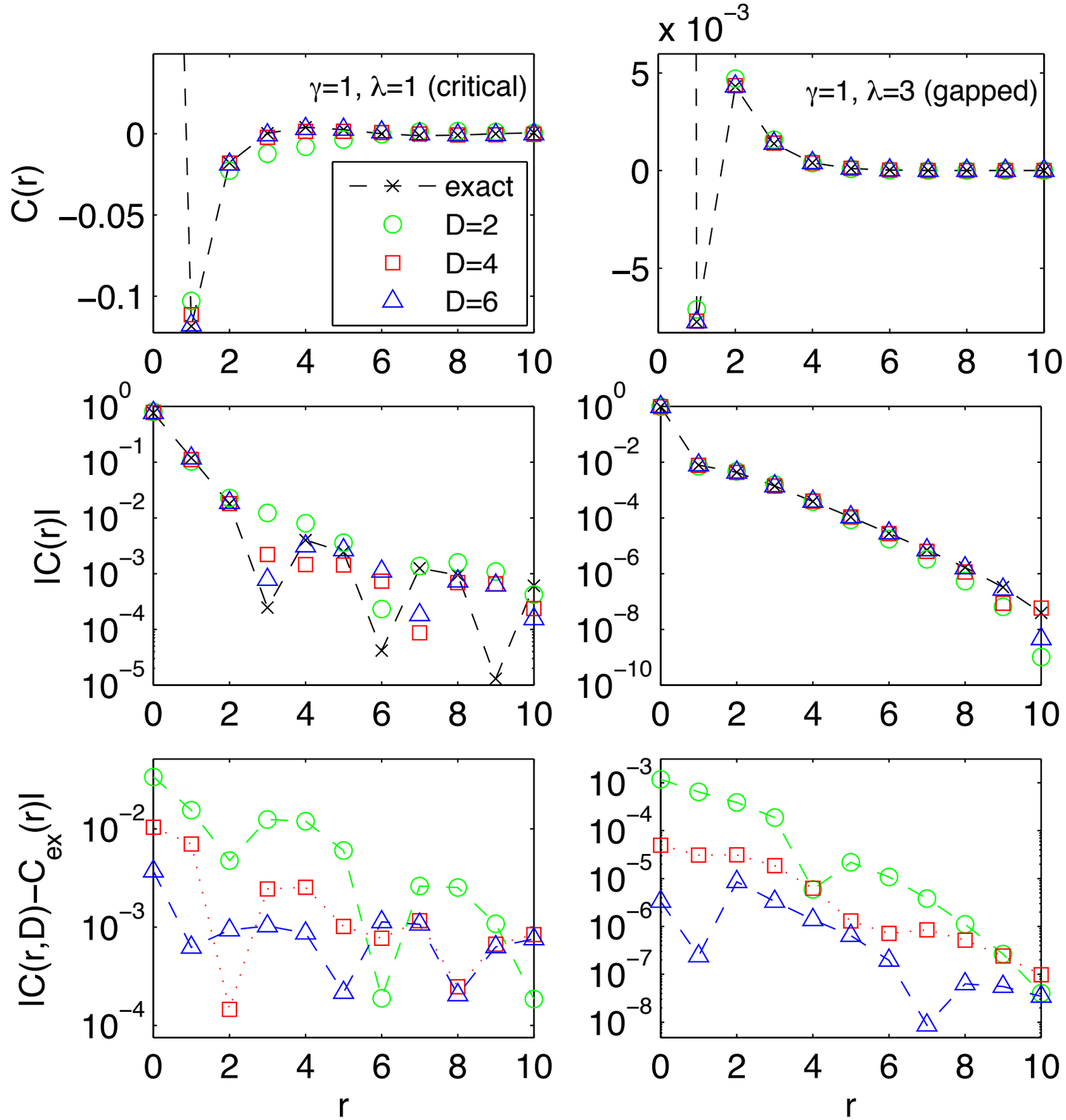
Li et al.,
PRB 74, 073103 (2006)

fast convergence with D in gapped phases

slow convergence in phase with 1D Fermi surface

Correlators

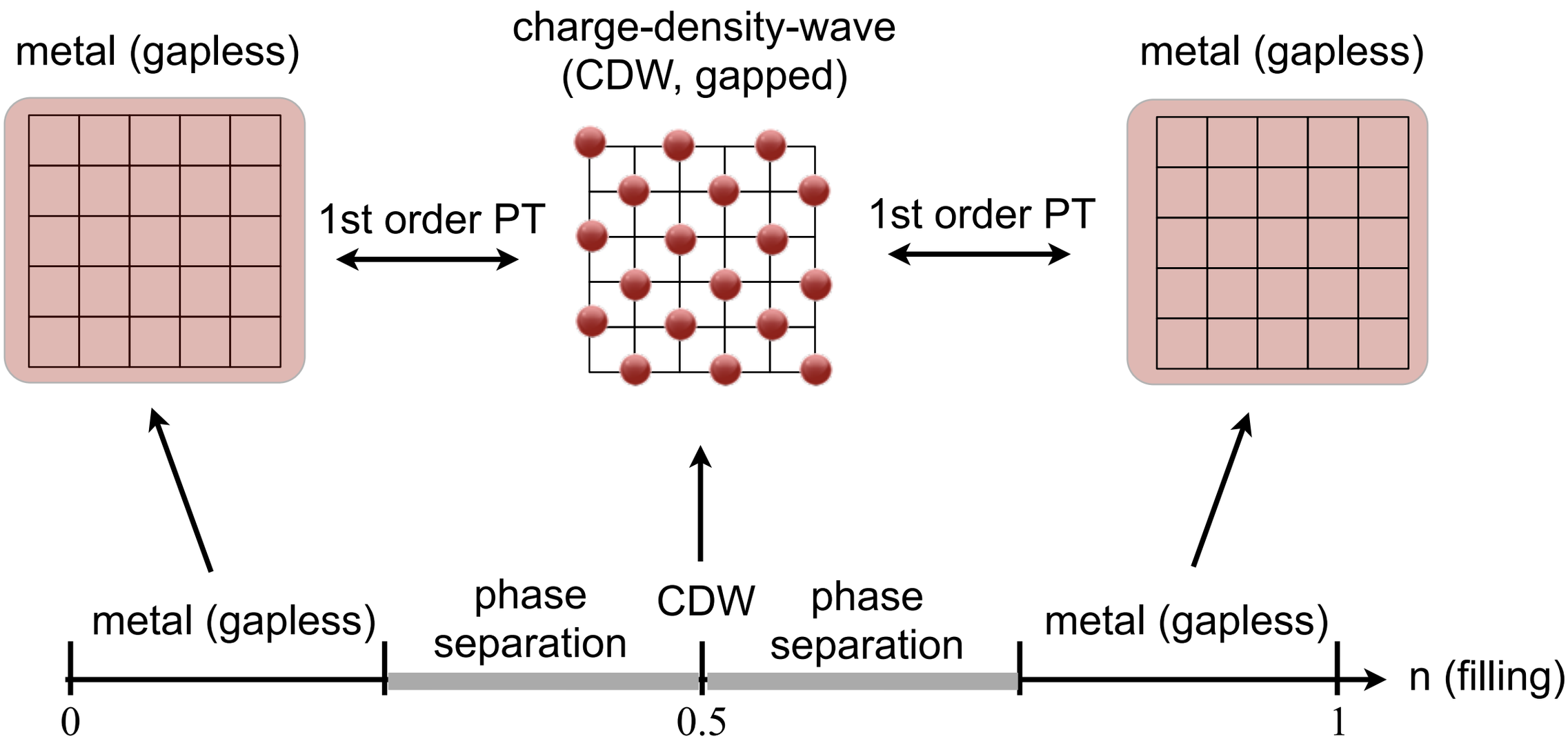
$$C(\vec{r}) = \langle c^\dagger_{\vec{r}_0} c_{\vec{r}_0+\vec{r}} \rangle$$



Phase diagram of interacting spinless fermions (iPEPS)

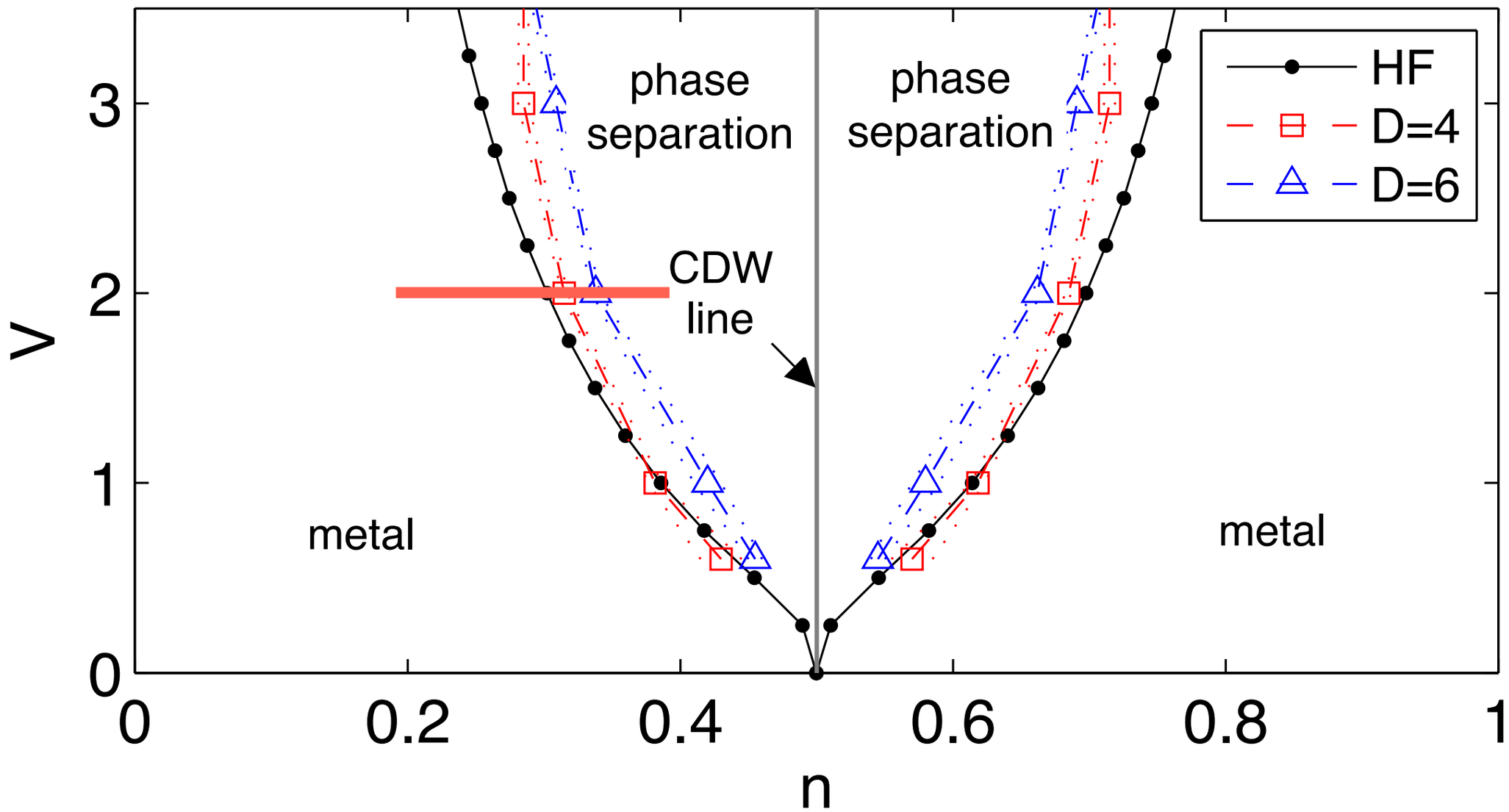
$$\hat{H} = -t \sum_{\langle i,j \rangle} \left[\hat{c}_i^\dagger \hat{c}_j + H.c. \right] - \mu \sum_i \hat{c}_i^\dagger \hat{c}_i + V \sum_{\langle i,j \rangle} \hat{c}_i^\dagger \hat{c}_i \hat{c}_j^\dagger \hat{c}_j$$

Restricted Hartree-Fock (HF) results: Woul&Langmann. J. Stat Phys. 139, 1033 (2010)



iPEPS vs Hartree-Fock

Woul, Langmann. J. Stat Phys. 139, 1033 (2010)
Corboz, Orus, Bauer, Vidal. PRB 81, 165104 (2010)

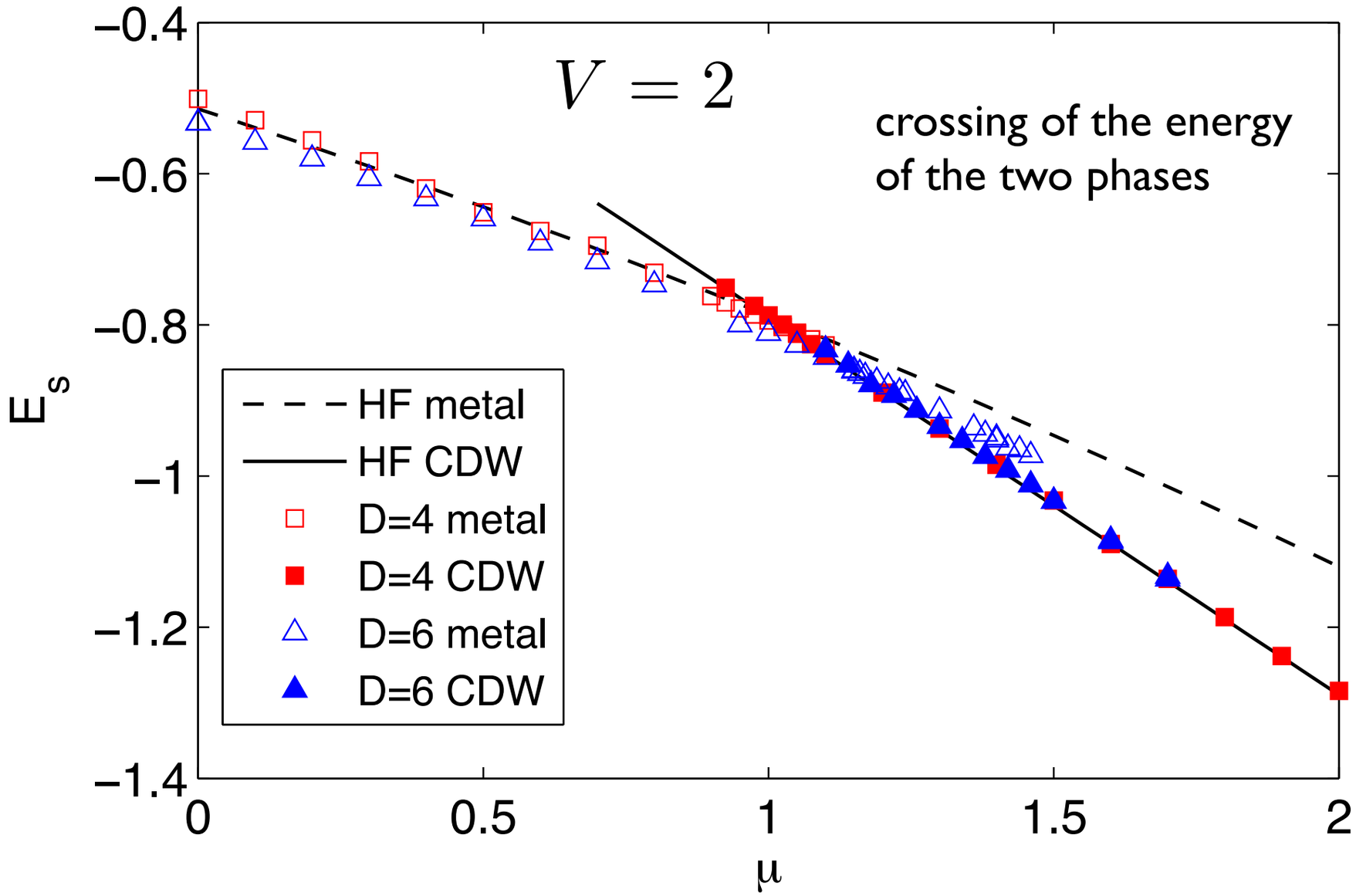


qualitative agreement

Phase boundary moves away from HF result with increasing D

iPEPS vs Hartree-Fock

Woul, Langmann. J. Stat Phys. 139, 1033 (2010)
Corboz, Orus, Bauer, Vidal. PRB 81, 165104 (2010)



D=4 result ~ HF result

D=6: lower (better) energies in the metal phase

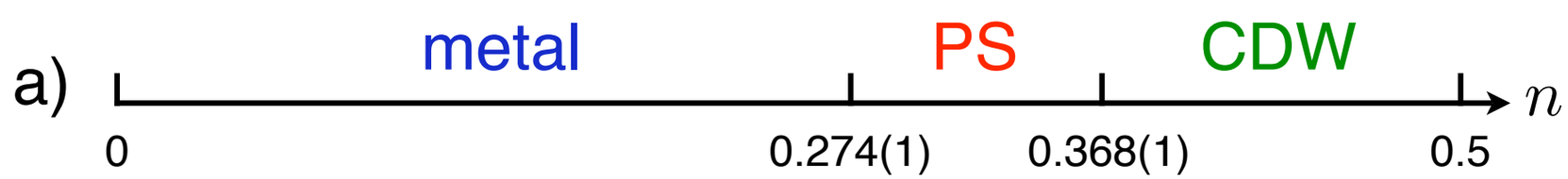
Adding a next-nearest neighbor hopping

Corboz, Jordan, Vidal, arXiv:1008:3937

$$\hat{H} = -t \sum_{\langle i,j \rangle} \left[\hat{c}_i^\dagger \hat{c}_j + H.c. \right] - \mu \sum_i \hat{c}_i^\dagger \hat{c}_i + V \sum_{\langle i,j \rangle} \hat{c}_i^\dagger \hat{c}_i \hat{c}_j^\dagger \hat{c}_j - t' \sum_{\langle\langle i,j \rangle\rangle} \left[\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + H.c. \right]$$

Hartree-Fock phase diagram: Woul, Langmann. J. Stat Phys. 139, 1033 (2010)

$V = 2 \qquad t' = -0.4$

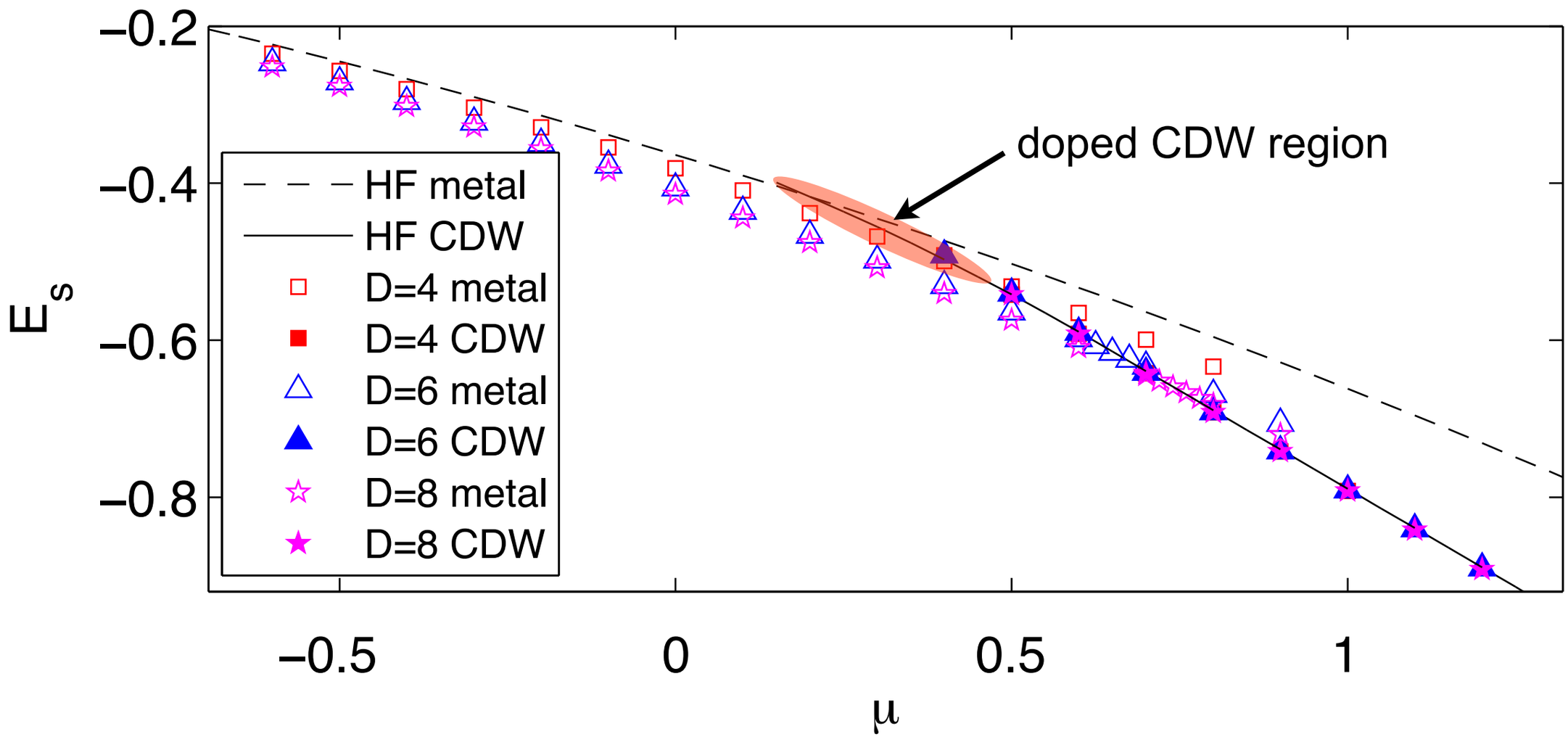


Is there a stable doped CDW phase beyond Hartree-Fock?

NO... (at least not for these parameters)

Adding a next-nearest neighbor hopping

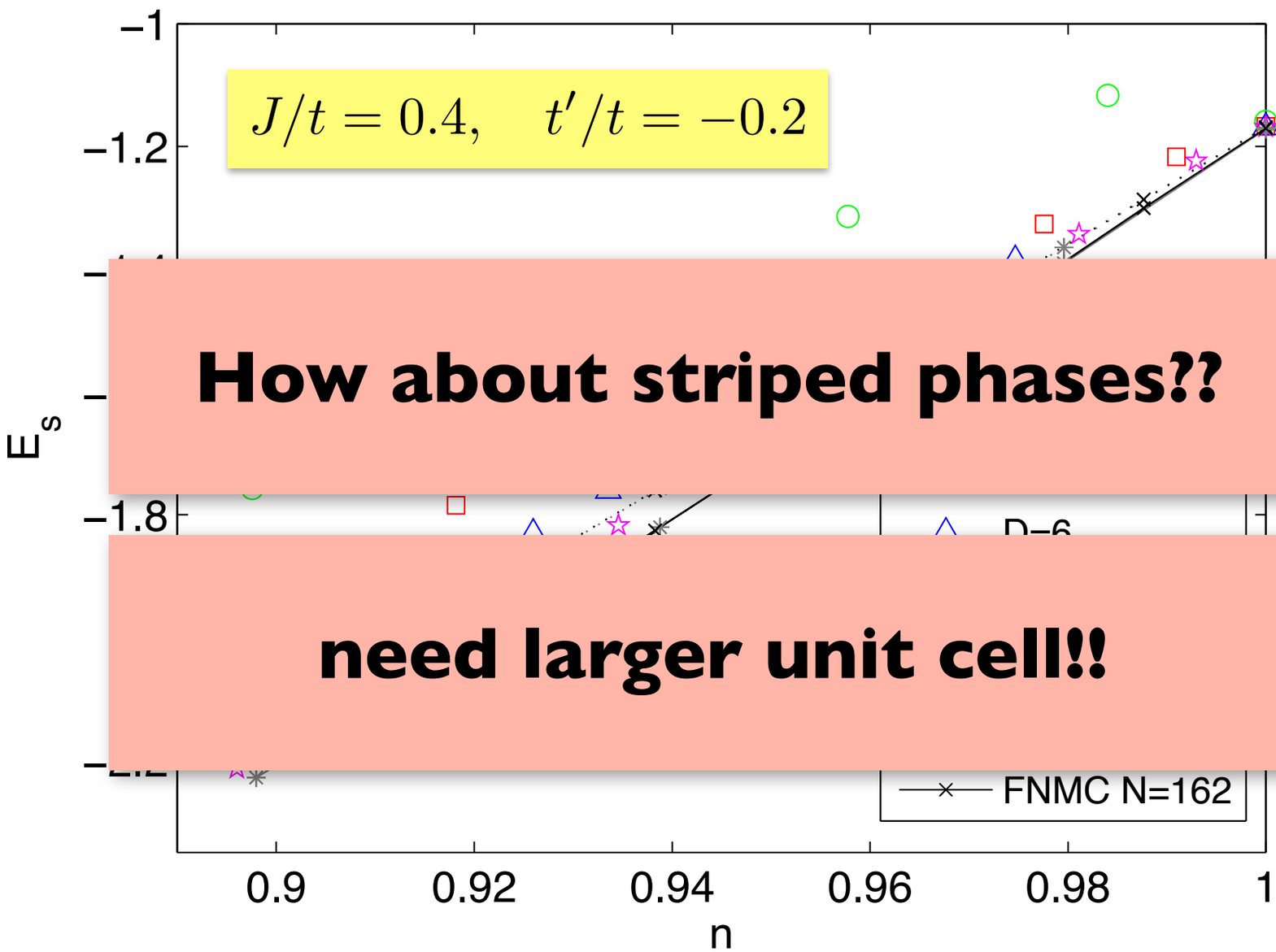
Corboz, Jordan, Vidal, arXiv:1008:3937



t-t'-J model

$$H_{\text{t-J}} = -t \sum_{\langle ij \rangle \sigma} \tilde{c}^{\dagger}_{i\sigma} \tilde{c}_{j\sigma} - t' \sum_{\langle\langle ij \rangle\rangle \sigma} \tilde{c}^{\dagger}_{i\sigma} \tilde{c}_{j\sigma} + J \sum_{\langle ij \rangle} (S_i S_j - \frac{1}{4} n_i n_j) - \mu \sum_i n_i$$

- Comparison with: L. Spanu, M. Lugas, F. Becca, S. Sorella. PRB 77, 024510 (2008).
  - **variational Monte Carlo** (VMC) (Gutzwiller projected ansatz wf)
  - state-of-the-art **fixed node Monte Carlo** (FNMC)



How about striped phases??

need larger unit cell!!

D=8 results in between VMC and FNMC

Corboz, Jordan, Vidal, arXiv:1008:3937

Summary: **status**

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- ✓ Variational ansatz with no (little) bias & controllable accuracy. Accuracy depends on the amount of entanglement in the system
- ✓ Accurate results for gapped systems
- ✓ Competitive compared to other variational wave functions
- ✓ Systematic improvement upon mean-field solution

- For which bond dimension is it converged?
- Limited accuracy for gapless systems
- no L log L scaling
- High computational cost

- Combine with Monte Carlo sampling (Schuch et al, Sandvik&Vidal, Wang et al.)
- Exploit symmetries of a model (Singh et al, Bauer et al.)
- Improve optimization/contraction schemes