Title: Simulation of Fermionic and Frustrated Systems with 2D Tensor Networks

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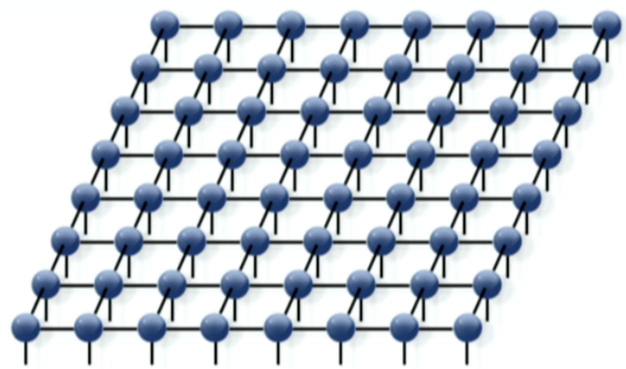
Abstract: The study of fermionic and frustrated systems in two dimensions is one of the biggest challenges in condensed matter physics. Among the most promising tools to simulate these systems are 2D tensor networks, including projected entangled-pair states (PEPS) and the 2D multi-scale entanglement renormalization ansatz (MERA), which have been generalized to fermionic systems recently.
In the first part of this talk I will present a simple formalism how to include fermionic statistics into 2D tensor networks. The second part covers recent simulation results showing that infinite PEPS (iPEPS) can compete with the best known variational methods. In particular, for the t-J model and the SU(4) Heisenberg model iPEPS yields better variational energies than obtained in previous variational- and fixed-node Monte Carlo studies. Future perspectives and open problems are discussed.

Simulation of fermionic and frustrated lattice models with 2D tensor networks

Philippe Corboz, ETH Zurich, Switzerland



Collaborators (part I&II)
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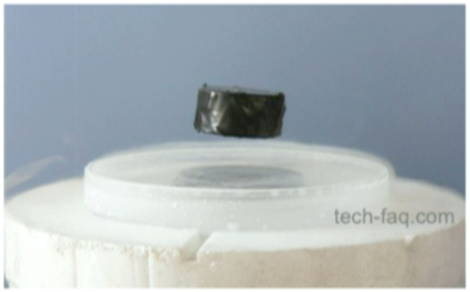
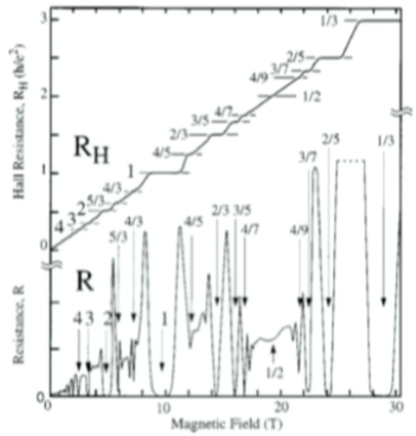
Andreas Läuchli (ITP, Innsbruck)
Karlo Penc (RISSPO, Budapest)

Motivation: Strongly correlated quantum many-body systems

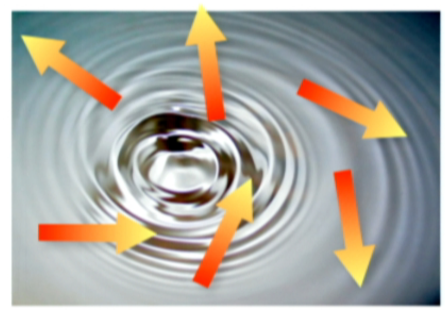
High-temperature superconductivity



Fractional QH Effect



Quantum magnetism / spin liquids



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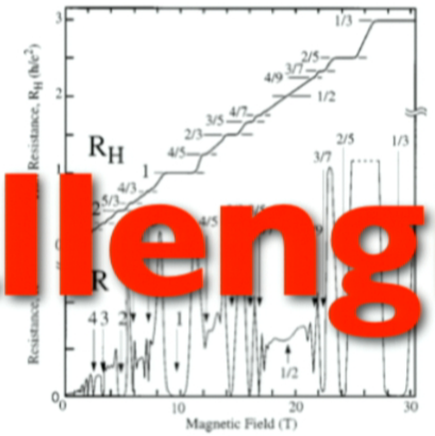


Quantum magnetism / spin liquids

Challenging!

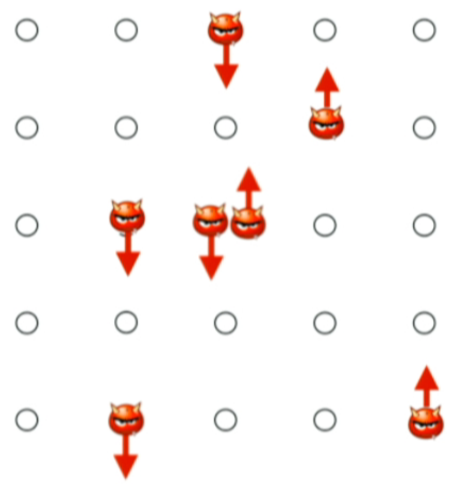
Quantum Monte Carlo

Main idea: Statistical sampling of the exponentially large configuration space

✓ **Very** powerful!

Strongly correlated fermionic systems

2D Hubbard model



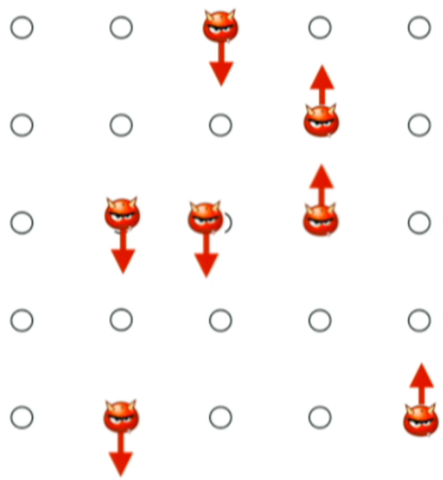
$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

Hopping between nearest-neighbor sites

On-site repulsion between electrons with opposite spin

Strongly correlated fermionic systems

2D Hubbard model



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Is it the relevant model of high-temperature superconductors?

Strongly correlated fermionic systems

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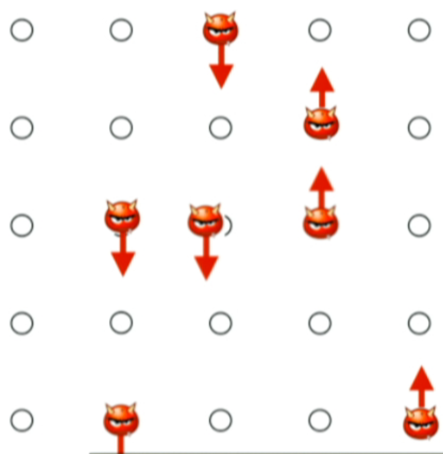

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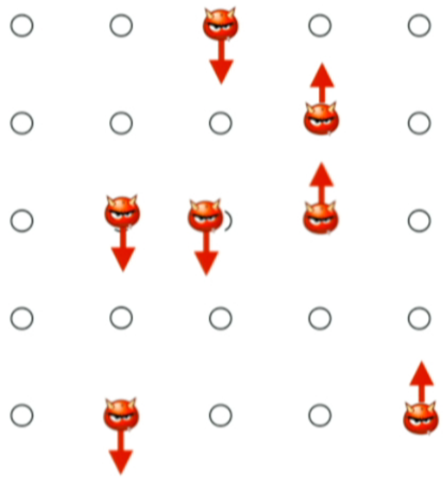
Methods to study strongly correlated fermions in 2D

- Exact diagonalization of small systems
- Density matrix renormalization group (small 2D systems / ladders)
- Variational approaches
- (Cluster) dynamical mean field theory
- Fixed-node Monte Carlo
- Diagrammatic Monte Carlo
- Gaussian Monte Carlo
- ... and more ...

Strongly correlated fermionic systems

2D Hubbard model



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Hopping between nearest-neighbor sites

On-site repulsion between electrons with opposite spin

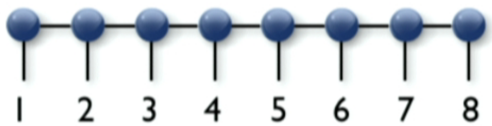
Is it the relevant model of high-temperature superconductors?

➡ **Still controversial!!**

Overview: tensor networks in 1D and 2D

1D

MPS
Matrix-product state



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

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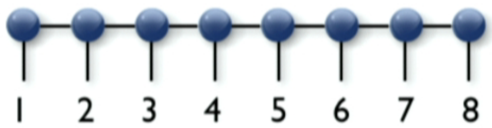
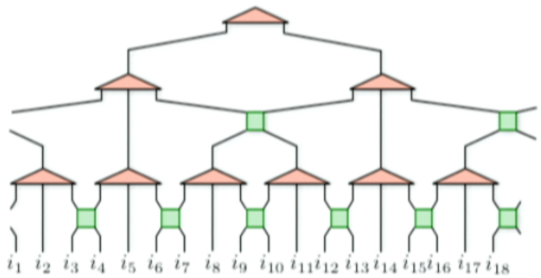


Related to the famous density-matrix renormalization group (DMRG) method

1D MERA
Multi-scale entanglement renormalization ansatz



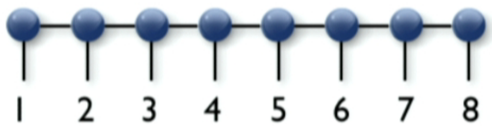
and more

- 1D tree tensor network
- ...

Overview: tensor networks in 1D and 2D

1D

MPS
Matrix-product state



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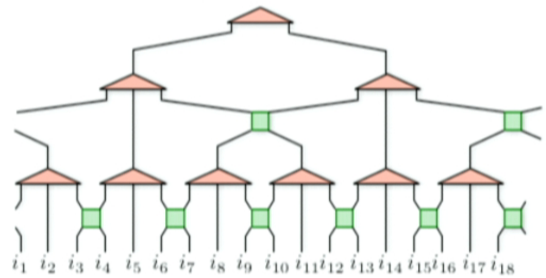
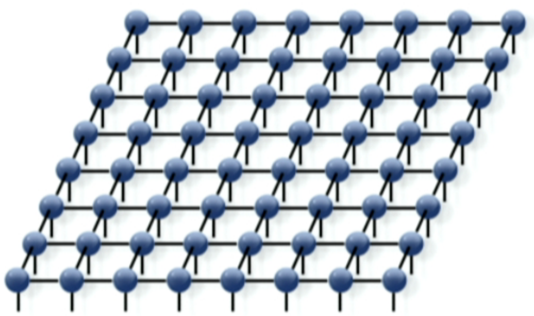
1D MERA
Multi-scale entanglement renormalization ansatz



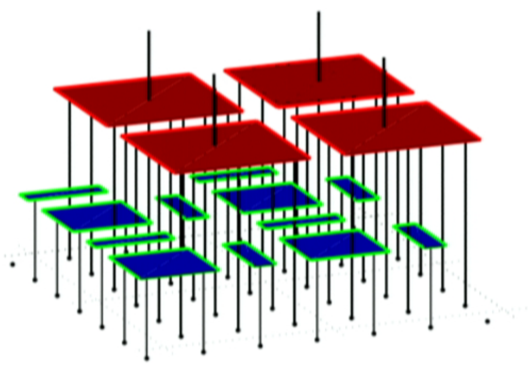
and more
- 1D tree tensor network
- ...

2D

(i)PEPS
(infinite) projected entangled-pair state



2D MERA



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

Fermions with 2D tensor networks

Simulate fermions in 2D?

Fermions with 2D tensor networks

Simulate fermions in 2D?

Before April 2009: **NO!**

Since April 2009: **YES!**

Different formulations:

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

T. Barthel, C. Pineda, and J. Eisert, Phys. Rev. A 80, 042333 (2009)

C. V. Kraus, N. Schuch, F. Verstraete, J. I. Cirac, Phys. Rev. A 81, 052338 (2010)

Q.-Q. Shi, S.-H. Li, J.-H. Zhao, and H.-Q. Zhou, arXiv:0907.5520

P. Corboz, G. Evenbly, F. Verstraete, G. Vidal, Phys. Rev. A 81, 010303(R) (2010)

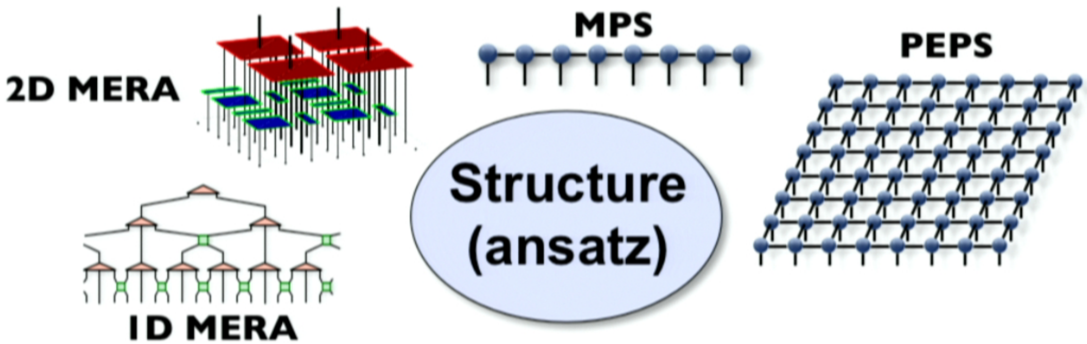
C. Pineda, T. Barthel, and J. Eisert, Phys. Rev. A 81, 050303(R) (2010)

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

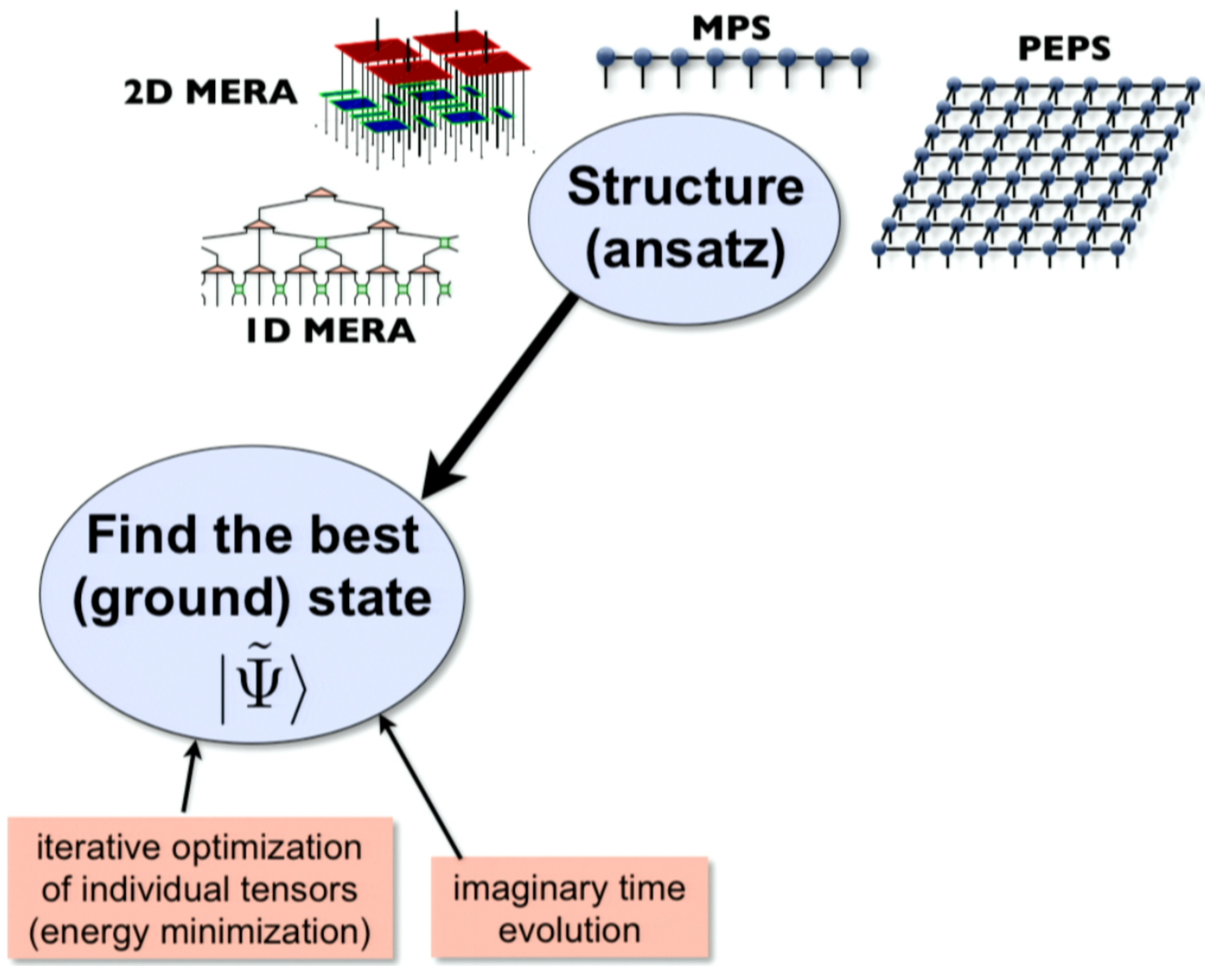
I. Pizorn, F. Verstraete, Phys. Rev. B 81, 245110 (2010)

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

Summary: Tensor network algorithms



Summary: Tensor network algorithms



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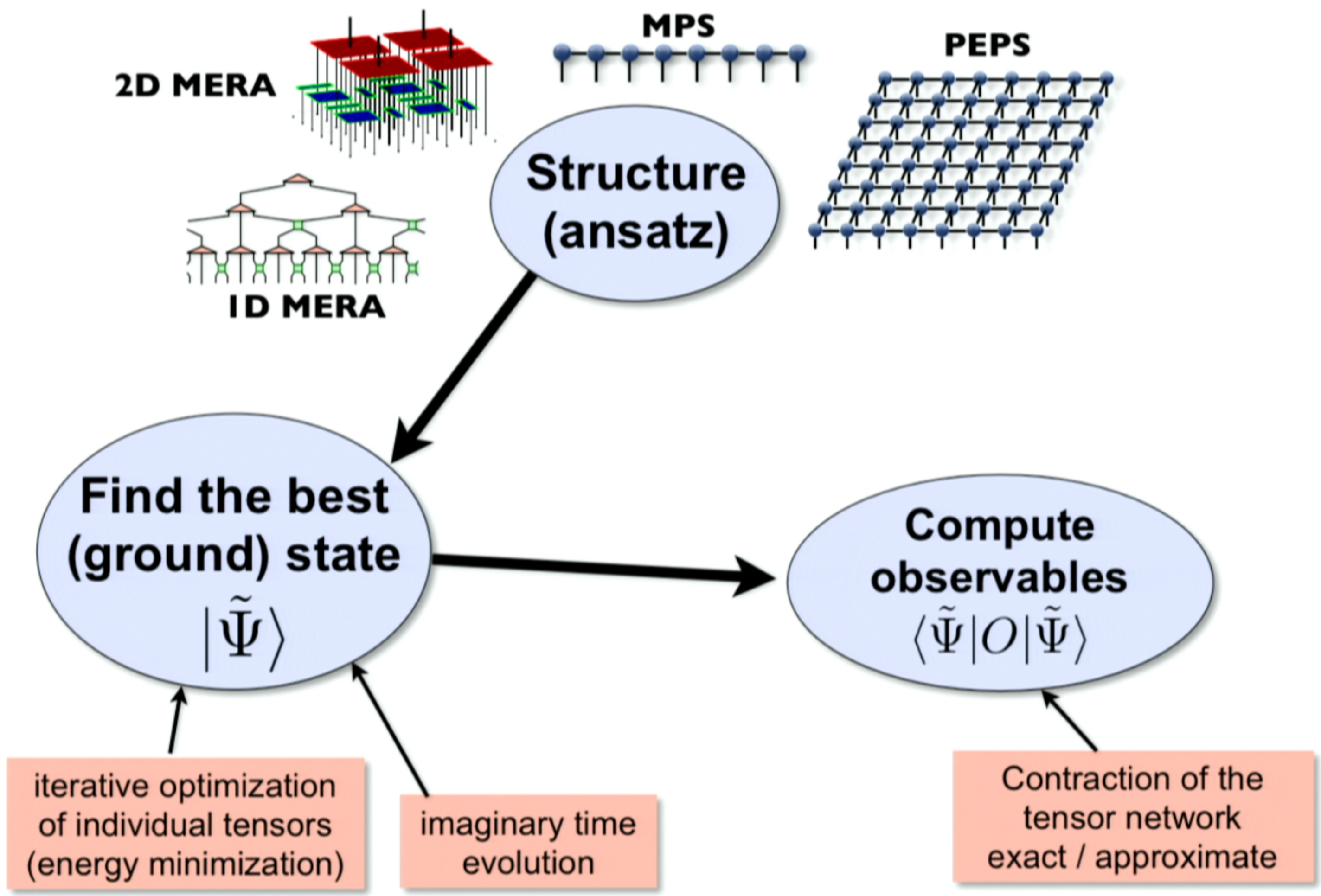

Outline

- Motivation
- **Part I:** Fermionic tensor networks
  - ✦ Formalism to take fermionic statistics in 2D tensor networks into account!
- **Part II:** Benchmark results (exactly solvable model)
  - ✦ Accuracy depends on the amount of entanglement in the system
- **Part III:** Recent studies with **iPEPS**
  - ✦ Infinite PEPS can compete with the best known variational methods
  - ✦ t-J model: **stripes**
  - ✦ SU(4) Heisenberg model: **new prediction for the ground state**
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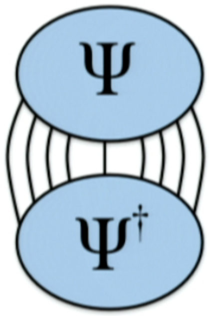
Crossings in 2D tensor networks

$\langle \Psi | \Psi \rangle$



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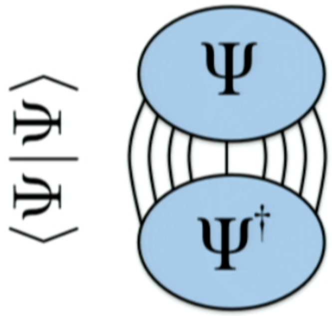
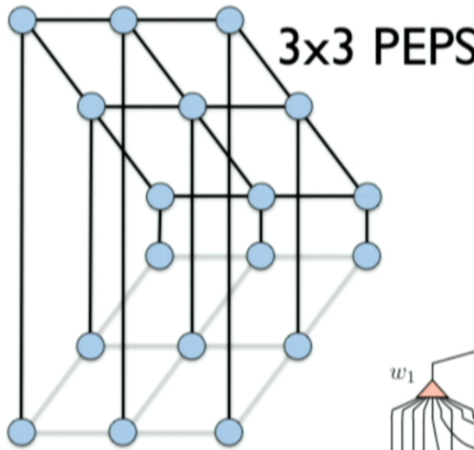
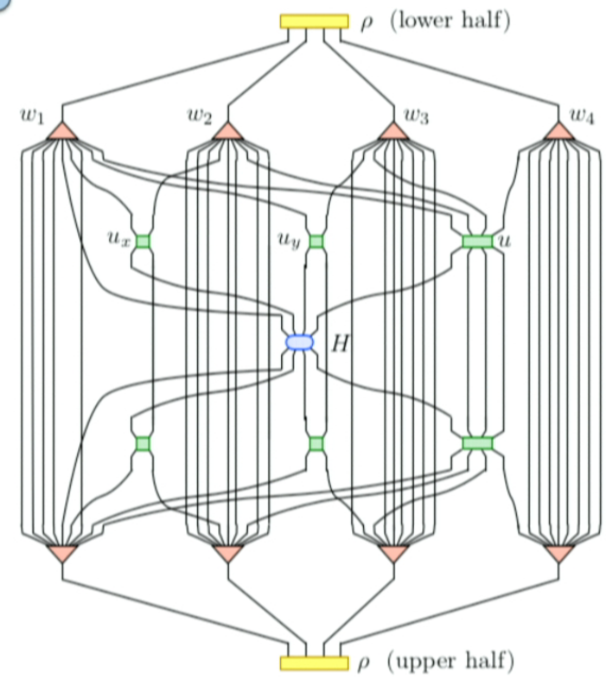
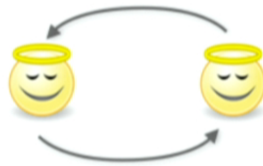




Example network of the 2D MERA

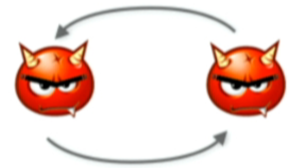


Bosons vs Fermions



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

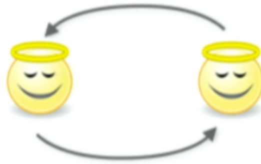
symmetric!



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

antisymmetric!

Bosons vs Fermions



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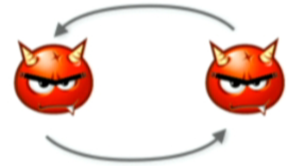

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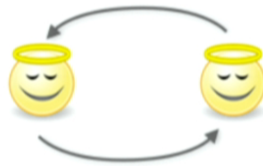
Bosons vs Fermions



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

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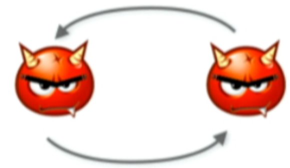
$$\hat{b}_i \hat{b}_j = \hat{b}_j \hat{b}_i$$

operators commute



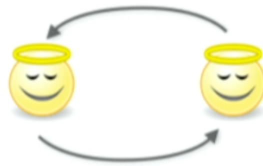
$$\Psi_F(x_1, x_2) = -\Psi_F(x_2, x_1)$$

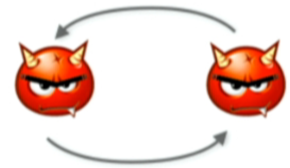
antisymmetric!

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

operators *anti*commute

Bosons vs Fermions



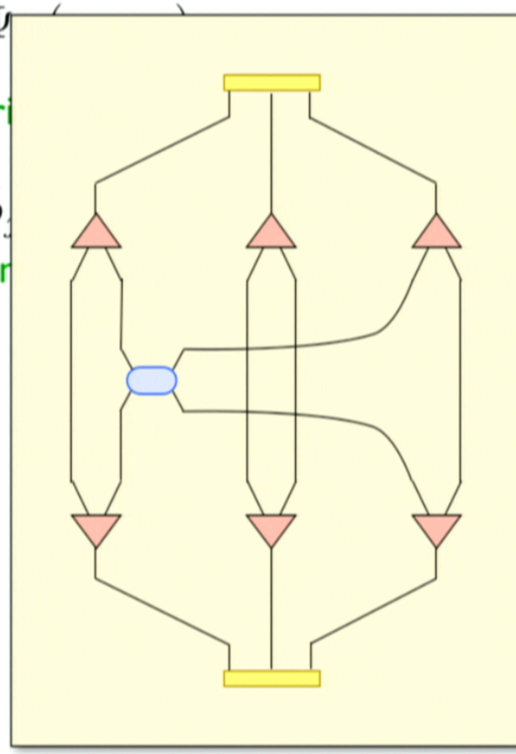


$\Psi_B(x_1, x_2) = \Psi$ … $_2) = -\Psi_F(x_2, x_1)$

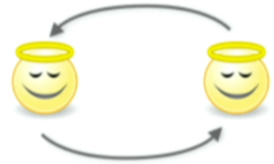
symmetri … tisymmetric!

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

operators co … ors *anti*commute



Bosons vs Fermions



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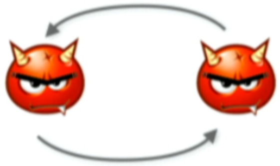


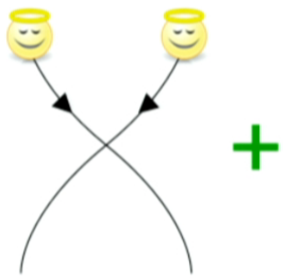
$$\Psi_F(x_1, x_2) = -\Psi_F(x_2, x_1)$$

antisymmetric!

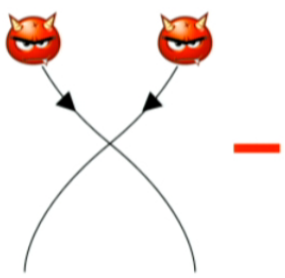
$$\hat{c}_i \hat{c}_j = -\hat{c}_j \hat{c}_i$$

operators *anti*commute

Crossings in a tensor network



ignore crossings

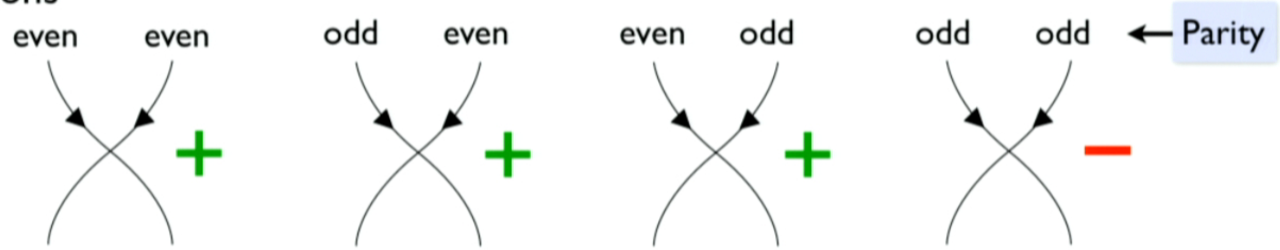


take care!

The swap tensor

Fermions

RULE:



The swap tensor

Fermions

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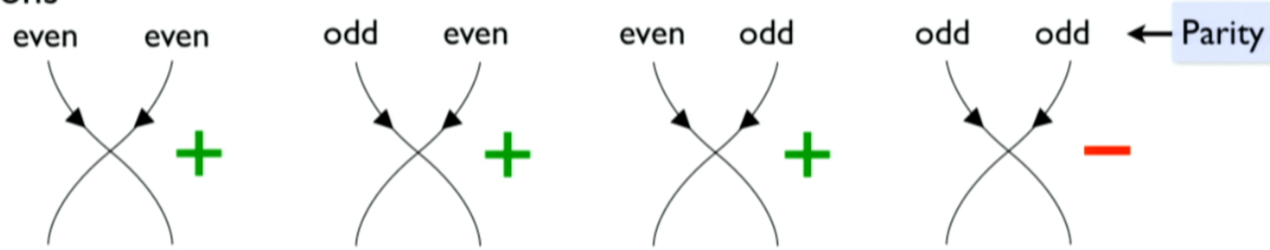
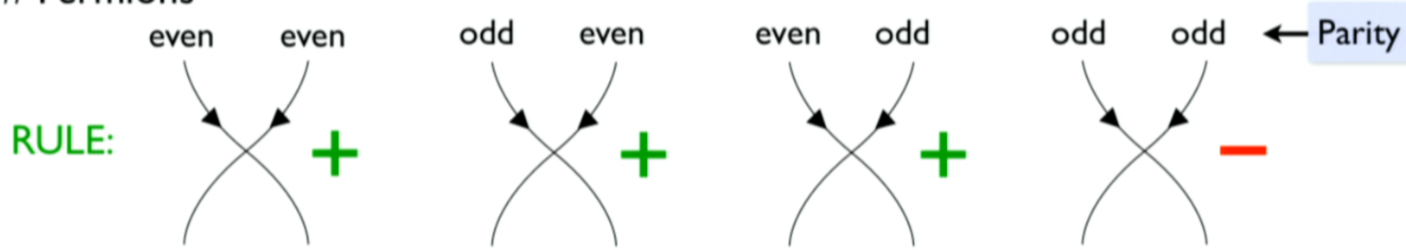


Parity P of a state: $\begin{cases} P=+1 & \text{(even parity), even number of particles} \\ P=-1 & \text{(odd parity), odd number of particles} \end{cases}$

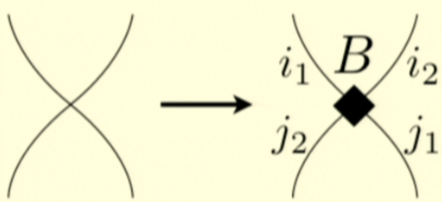
The swap tensor

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**



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

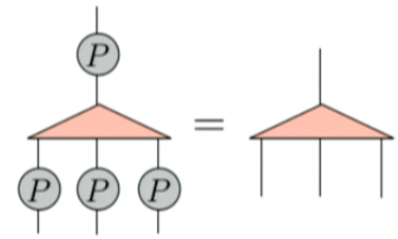
$$S(P(i_1), P(i_2)) = \begin{cases} -1 & \text{if } P(i_1) = P(i_2) = -1 \\ +1 & \text{otherwise} \end{cases}$$

Parity symmetry

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

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

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



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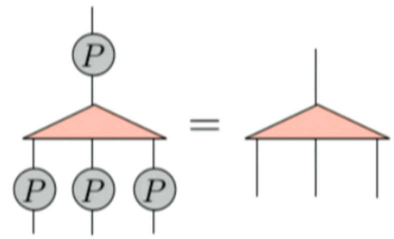


- Decomposing local Hilbert spaces into even and odd parity sectors

$$\mathbb{V} = \mathbb{V}^{(+)} \oplus \mathbb{V}^{(-)}$$

even odd

- Label state by a composite index

parity sector

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

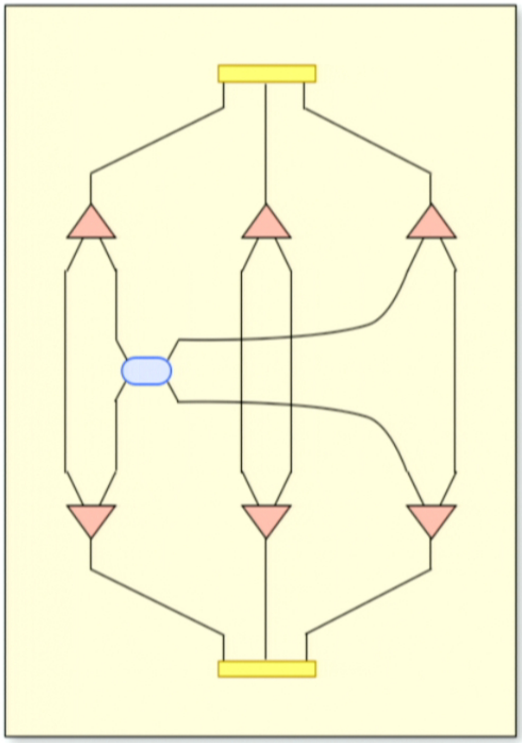
enumerate states in parity sector p

➡ tensor with a block structure (similar to a block diagonal matrix)

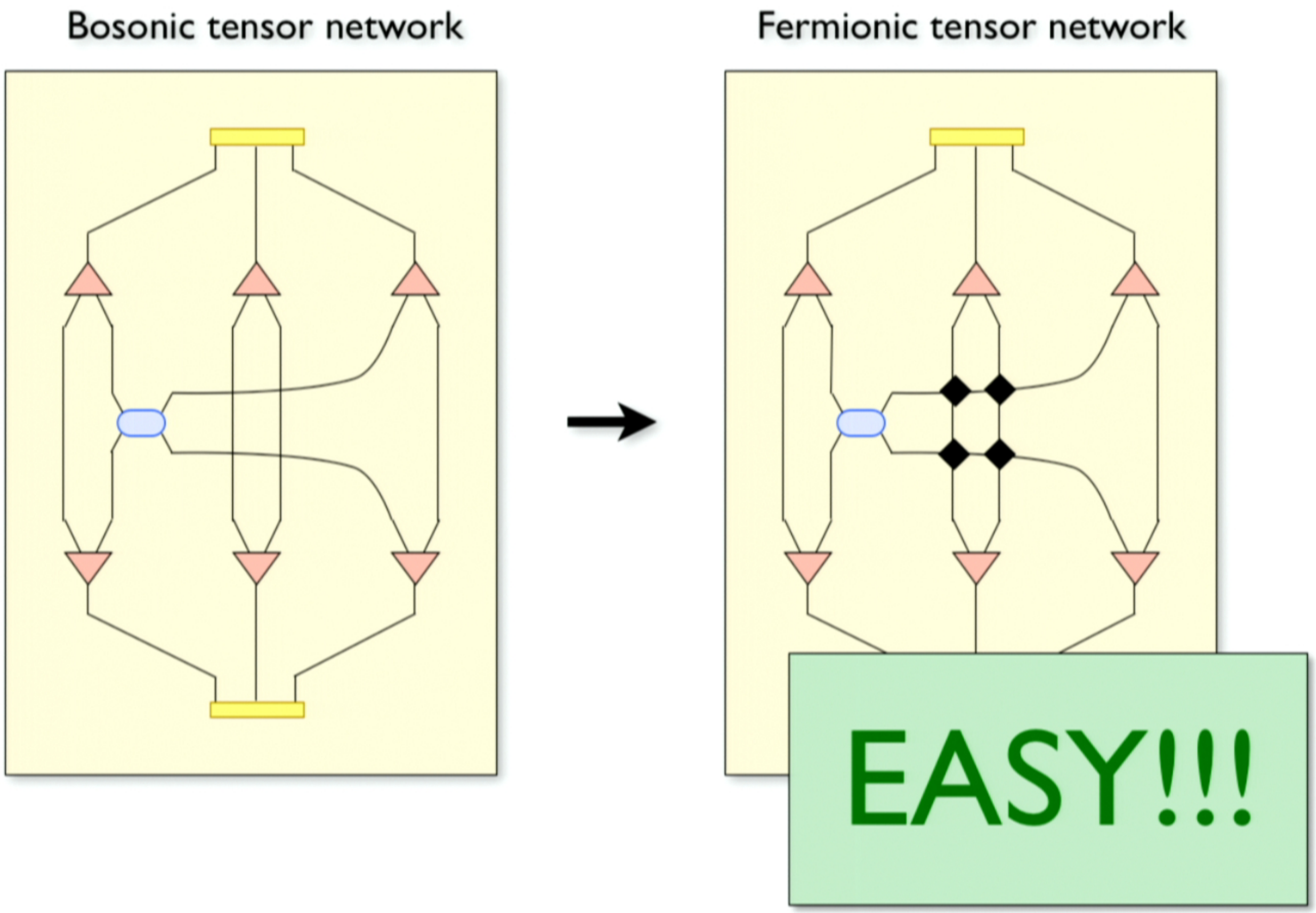
➡ Easy identification of the parity of a state!

Example

Bosonic tensor network



Example



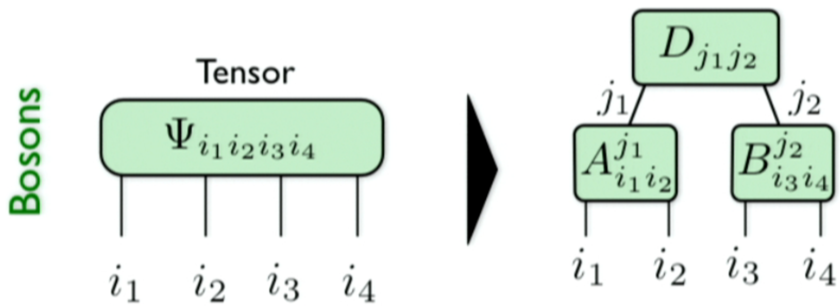
Fermionic "operator networks"

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

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

Fermionic "operator networks"

State of 4 site system $|\Psi\rangle = \sum_{i_1 i_2 i_3 i_4} \Psi_{i_1 i_2 i_3 i_4} |i_1 i_2 i_3 i_4\rangle$, with $i_4 \in \{|0\rangle, |1\rangle\}$

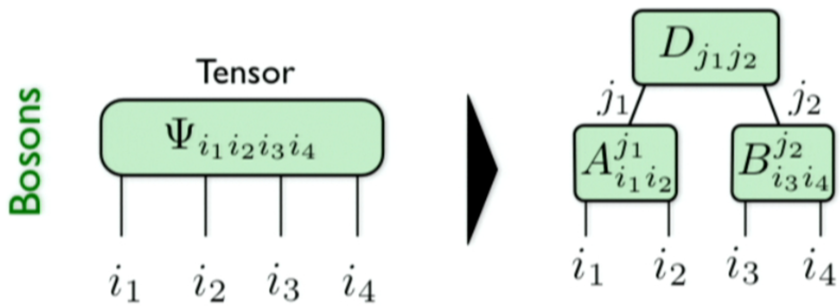


bosonic tensor network

Contract

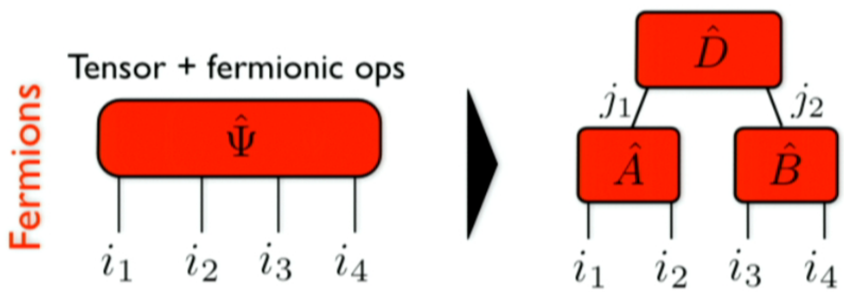
Fermionic "operator networks"

State of 4 site system $|\Psi\rangle = \sum_{i_1 i_2 i_3 i_4} \Psi_{i_1 i_2 i_3 i_4} |i_1 i_2 i_3 i_4\rangle$ where $i_4 \in \{|0\rangle, |1\rangle\}$



bosonic tensor network

Contract



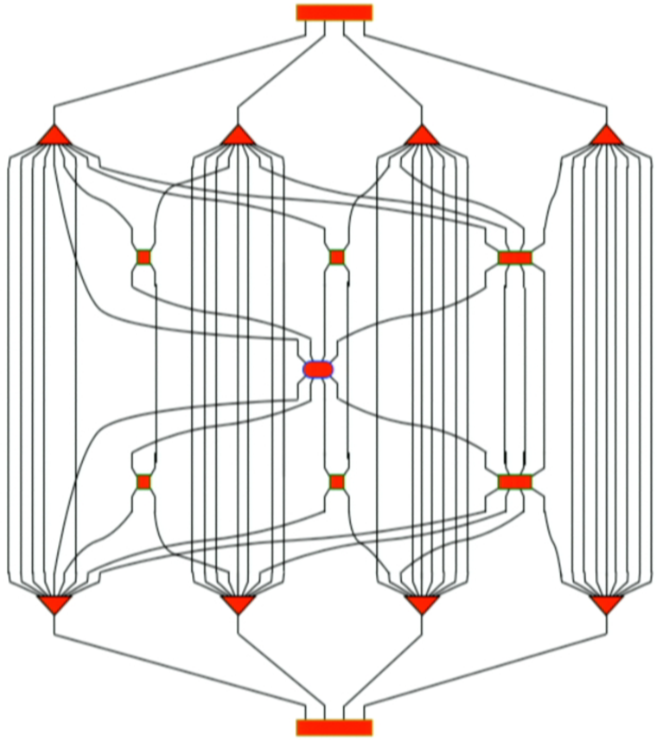
fermionic operator network

Contract + operator calculus

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

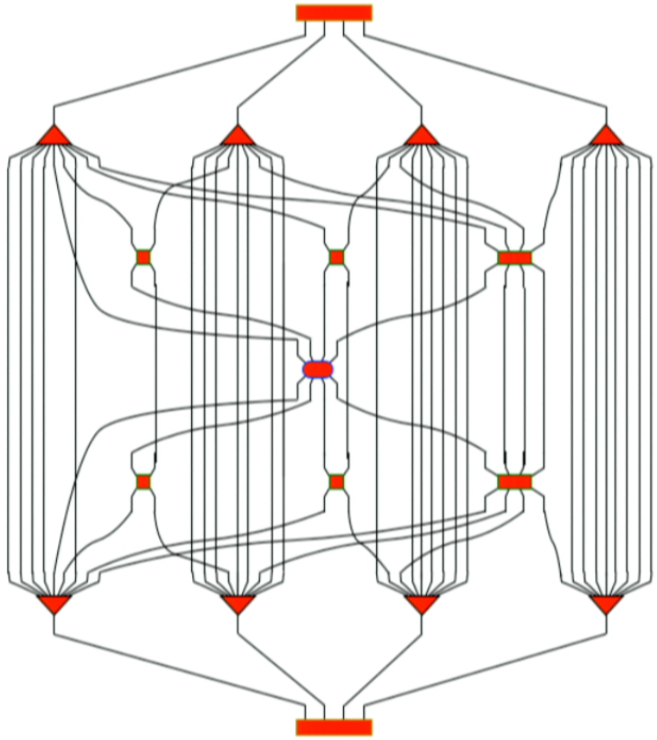
Fermionic "operator network"

Use anticommutation rules to evaluate fermionic operator network:



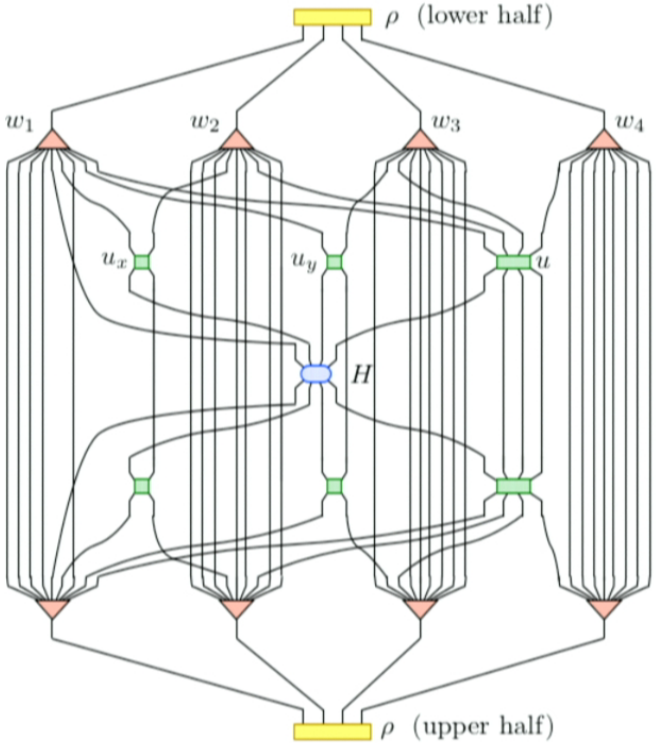
Fermionic "operator network"

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??**

The "jump" move

The "jump" move

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

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

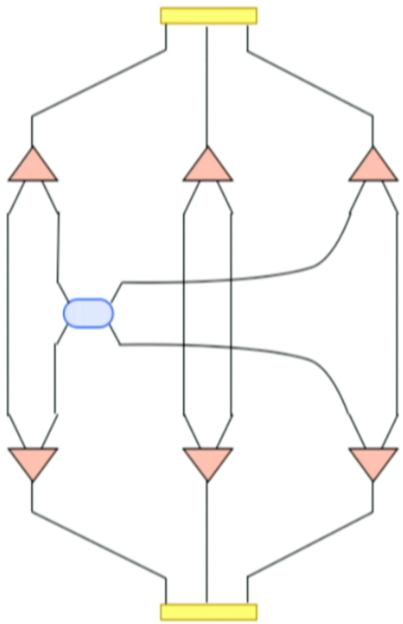
The "jump" move

- 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



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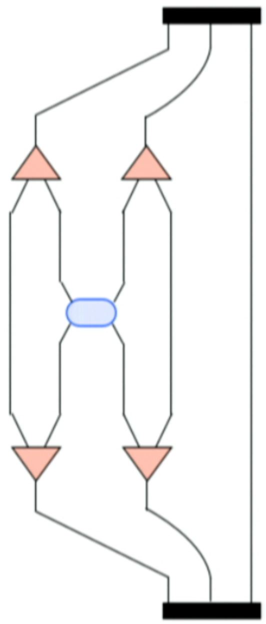
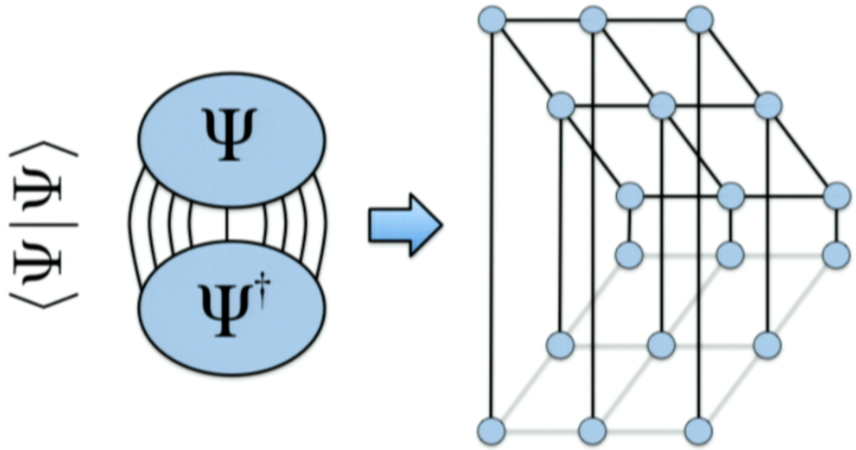
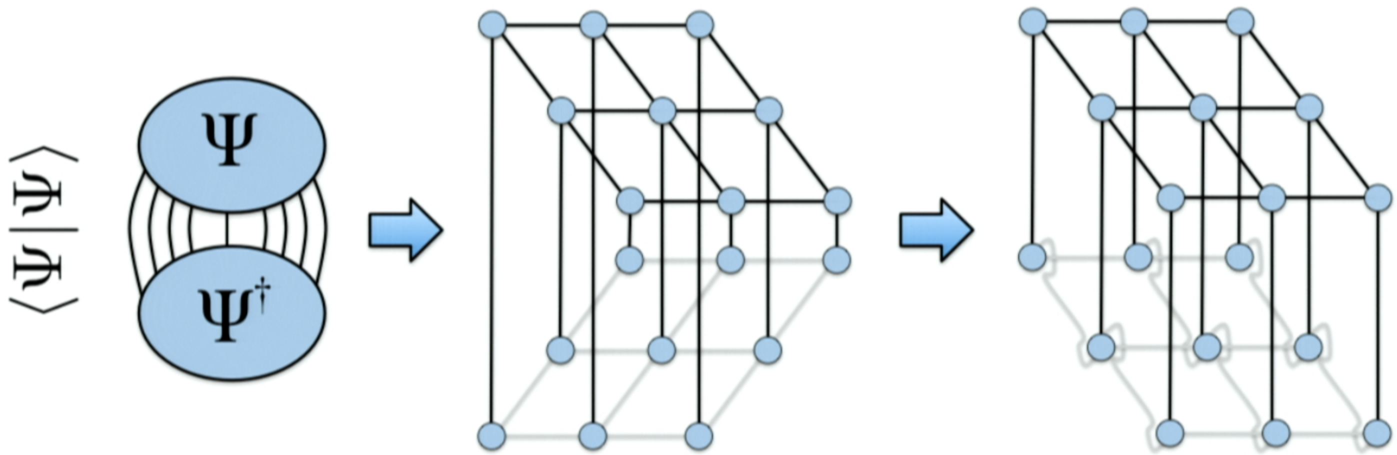


now
contract as usual!

Fermionic (i)PEPS



Fermionic (i)PEPS



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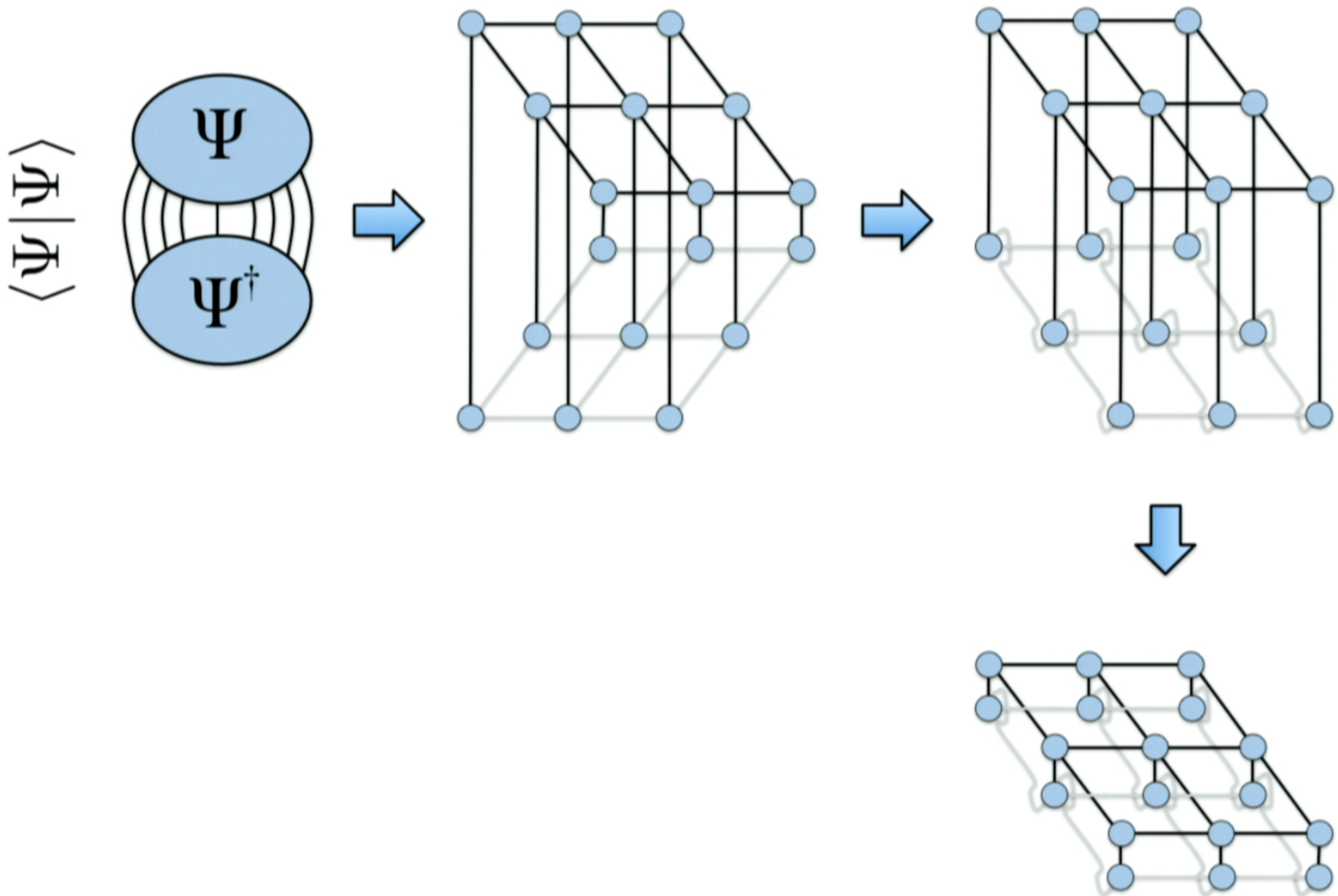

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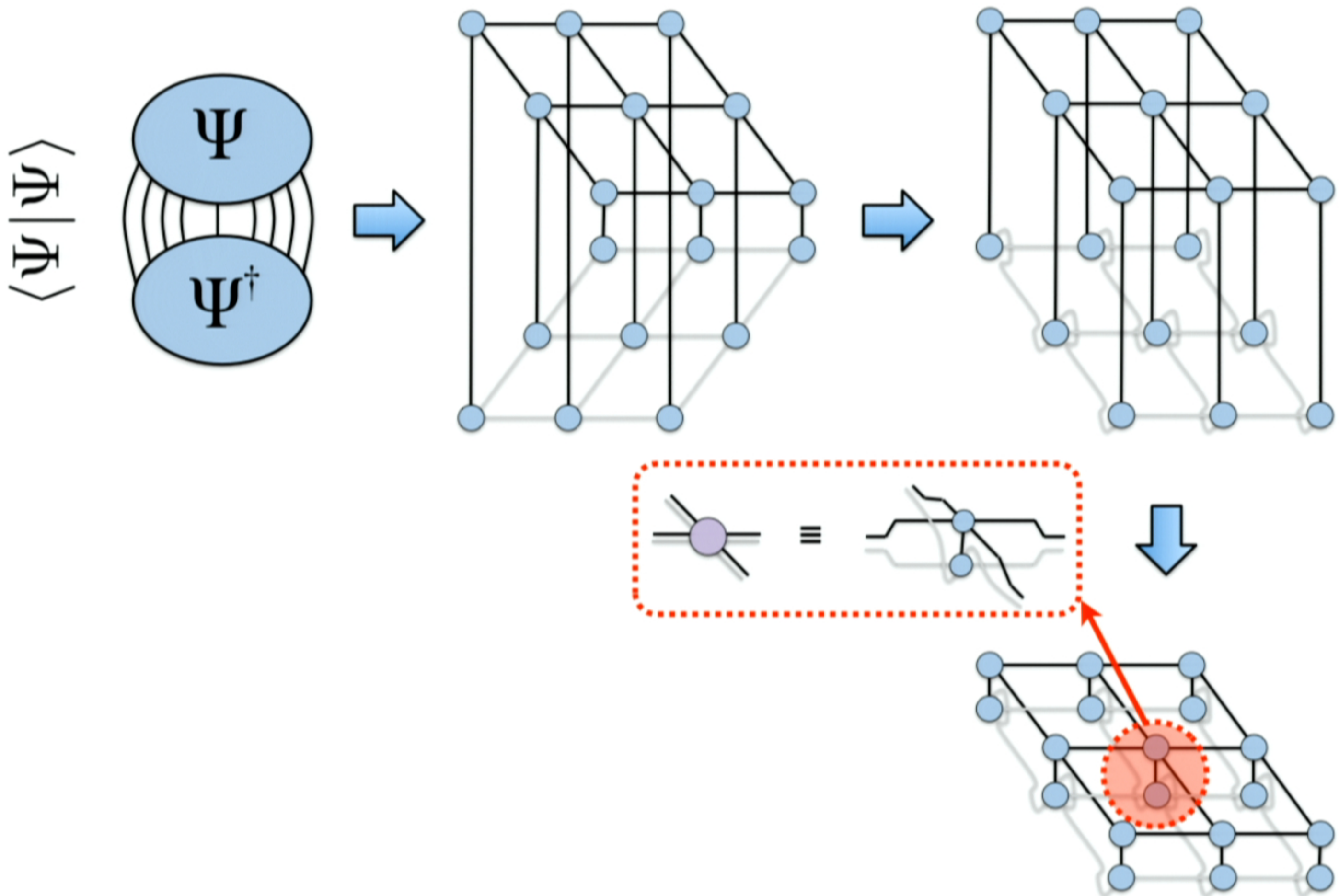
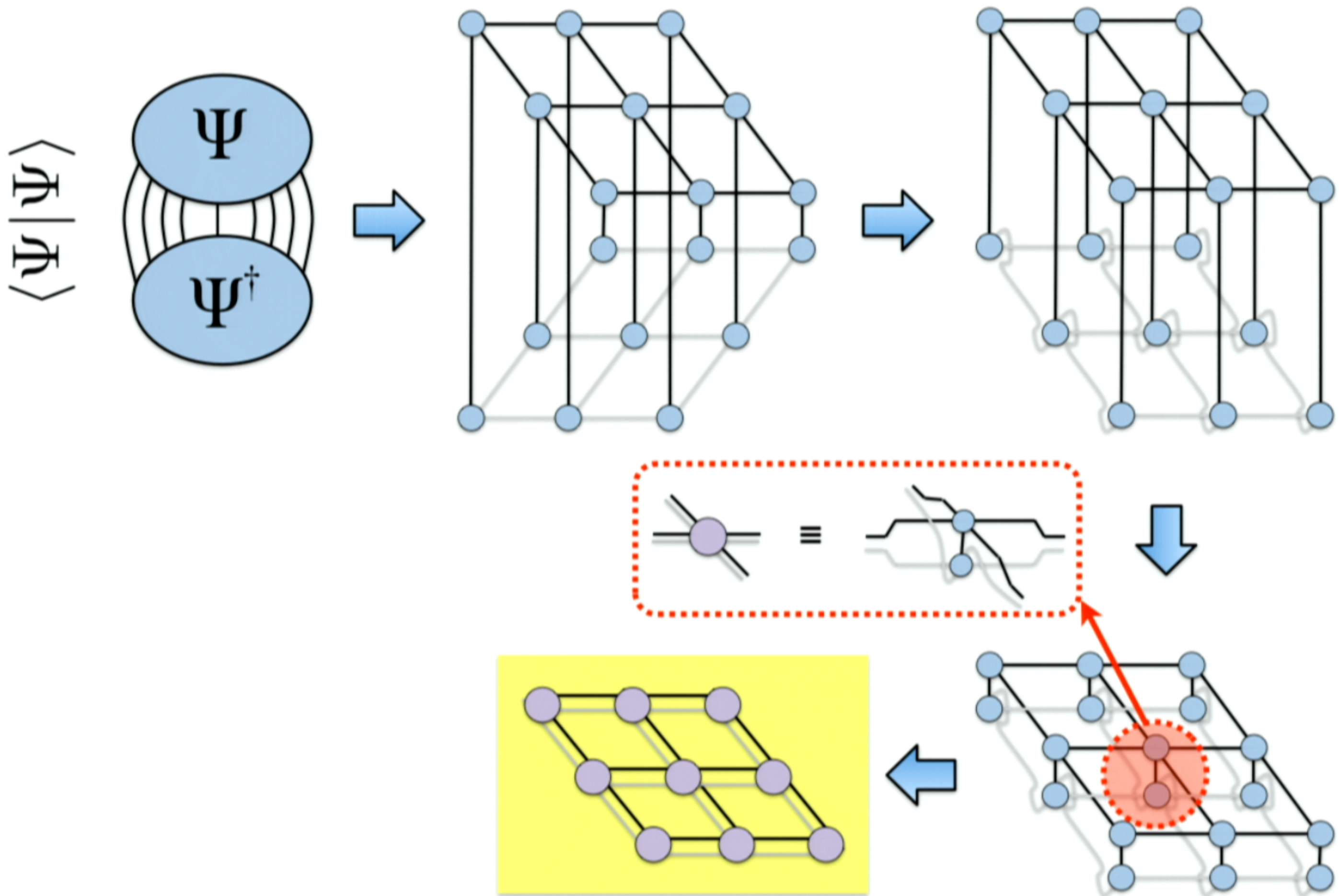
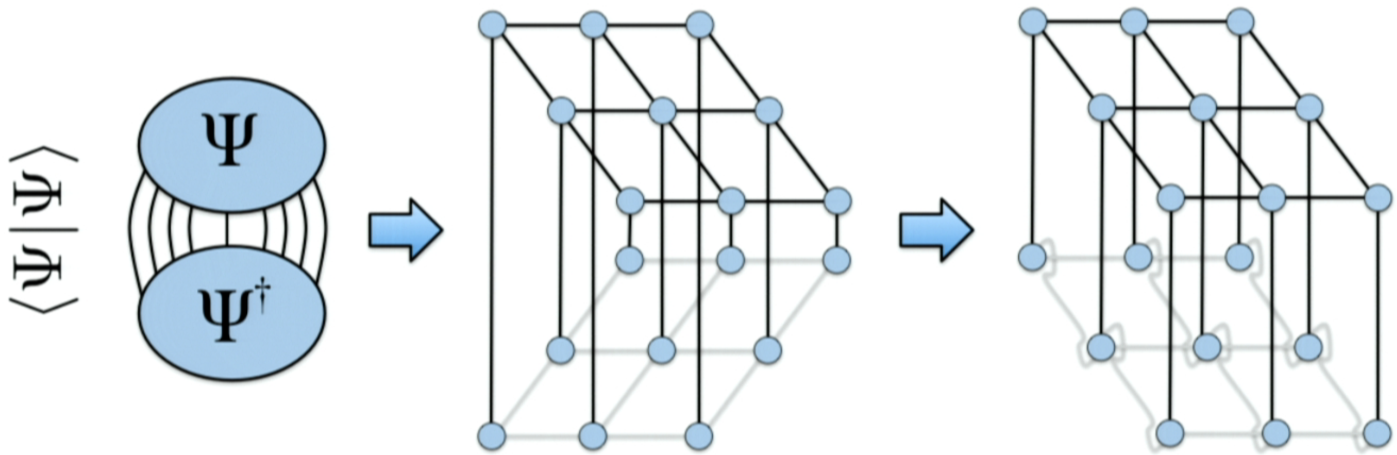


Fermionic (i)PEPS

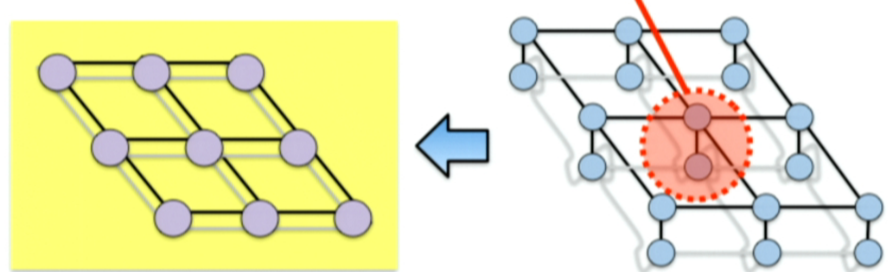


Fermionic (i)PEPS



- Fermionic character taken into account **locally!**

- **No** crossings left!

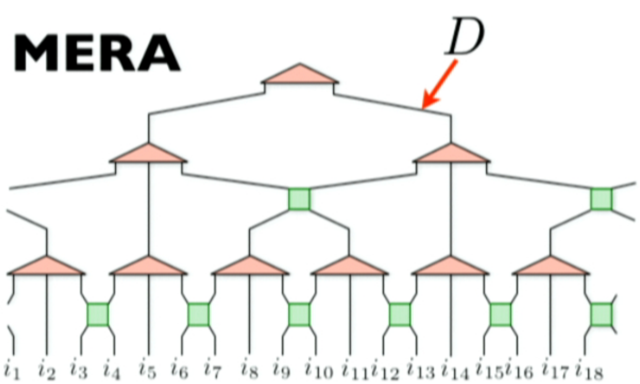


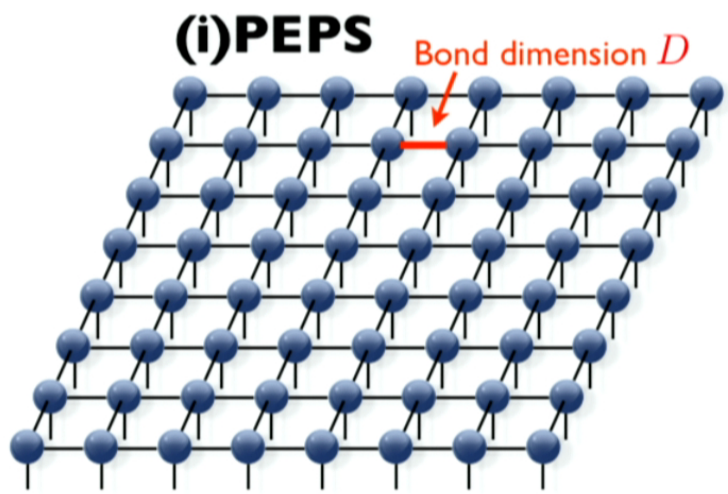
Summary Part I:

➡ Simulate fermionic systems with 2D tensor networks

Computational cost

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





Computational cost

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

MPS: $k = 3$

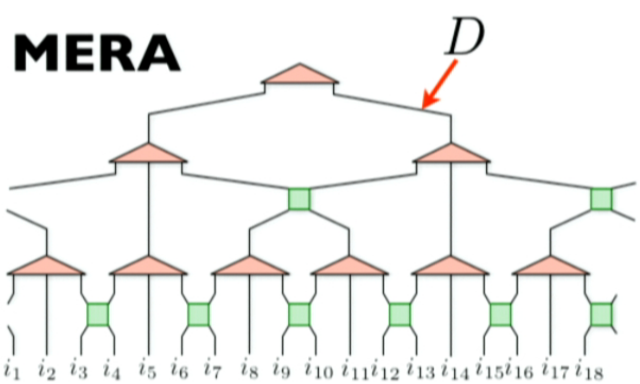
PEPS: $k \approx 10 \ldots 12$

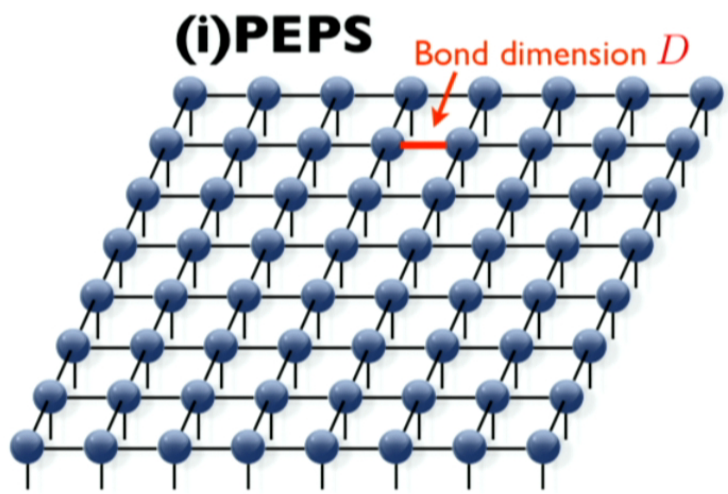
2D MERA: $k = 16$

polynomial scaling but large exponent!

- How large does D have to be?

▶ It depends on the amount of entanglement in the system!





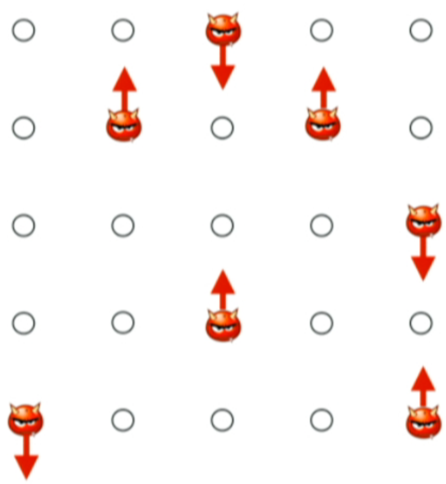
t-J model

$$H_{\text{t-J}} = -t \sum_{\langle ij \rangle \sigma} \tilde{c}^{\dagger}_{i\sigma} \tilde{c}_{j\sigma} + H.c. + J \sum_{\langle ij \rangle} (S_i S_j - \frac{1}{4} n_i n_j)$$

Nearest-neighbor hopping

Antiferro interaction

constraint: only one electron per site!



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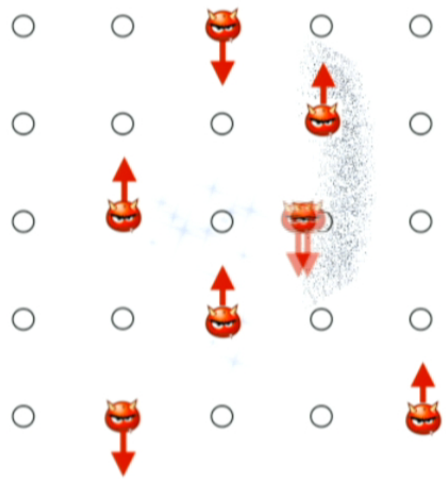


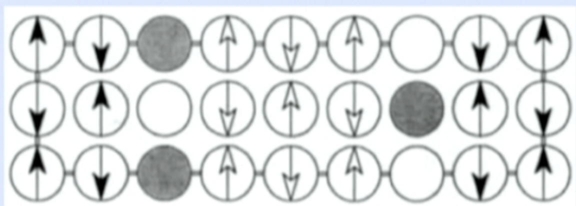
NATURE · VOL 375 · 15 JUNE 1995

Evidence for stripe correlations of spins and holes in copper oxide superconductors

J. M. Tranquada*, B. J. Sternlieb†, J. D. Axe*, Y. Nakamura† & S. Uchida†

* Physics Department, Brookhaven National Laboratory, Upton, New York 11973, USA
† Superconductivity Research Course, The University of Tokyo, Yayoi 2-11-16, Bunkyo-ku, Tokyo 113, Japan

ONE of the long-standing mysteries associated with the high-temperature copper oxide superconductors concerns the anomalous suppr... ertain relate... Here we ex... mical two-d... the crysta... O_4 by neutr... mmen-surabi... n and charg... s are separated by periodically spaced domain walls to which the holes segregate[5–9]. An ordered stripe phase of this type has recently been observed in hole-doped La_2NiO_4 (refs 10–12). We present evidence from neutron diffraction that in the copper oxide material $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$, with $x = 0.12$, a static analogue of the dynamical stripe phase is present, and is associated with an anomalous suppression of superconductivity[13,14]. Our results thus provide an explanation of the '$\frac{1}{8}$' conundrum, and also support the suggestion[15] that spatial modulations of spin and charge density are related to superconductivity in the copper oxides.



$- \frac{1}{4} n_i n_j)$

nteraction

constraint: only one electron per site!

Does it reproduce "striped" states observed in some cuprates?

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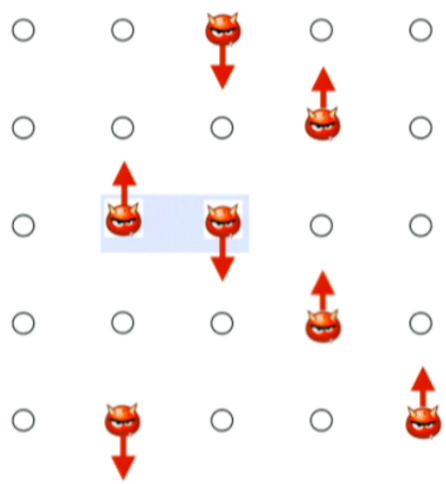


? Does it reproduce "striped" states observed in some cuprates? ?

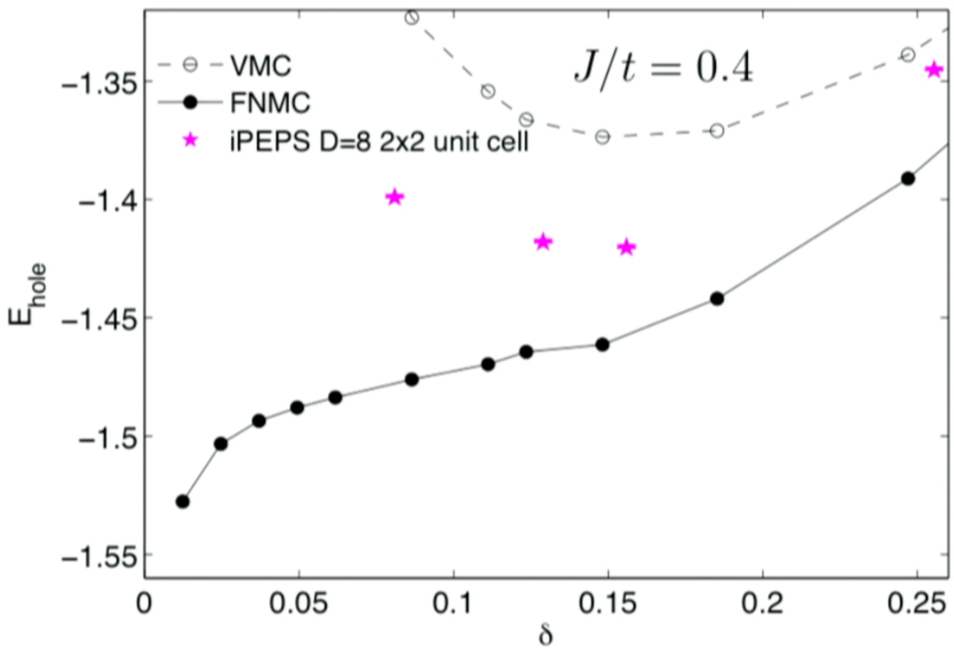
DMRG (wide ladders): **YES!**

Variational Monte Carlo
Fixed-node Monte Carlo **NO!**

t-J model: iPEPS results

Corboz, White, Vidal, Troyer, arXiv:1104.5463

- Comparison with: M. Lugas, L. Spanu, F. Becca, S. Sorella. PRB 74, 165122 (2006)
  - variational Monte Carlo (VMC) (Gutzwiller projected wavefunctions)
  - state-of-the-art fixed node Monte Carlo (FNMC)



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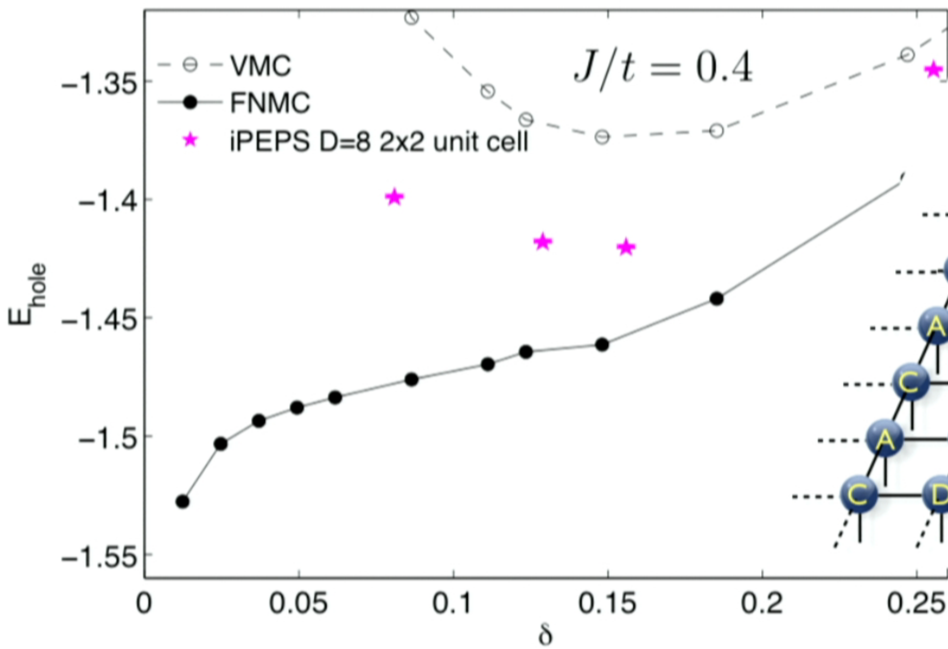
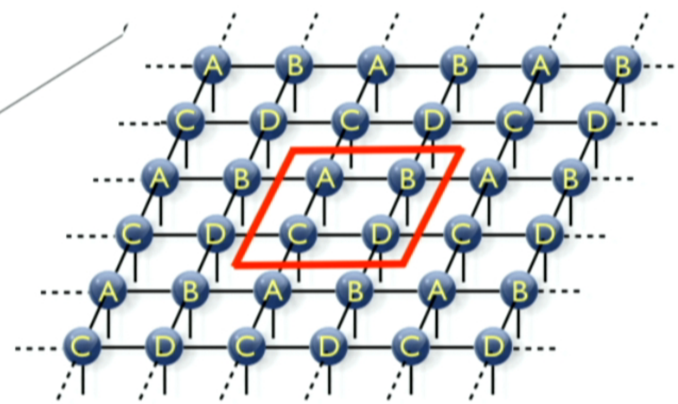


iPEPS with 2x2 unit cell



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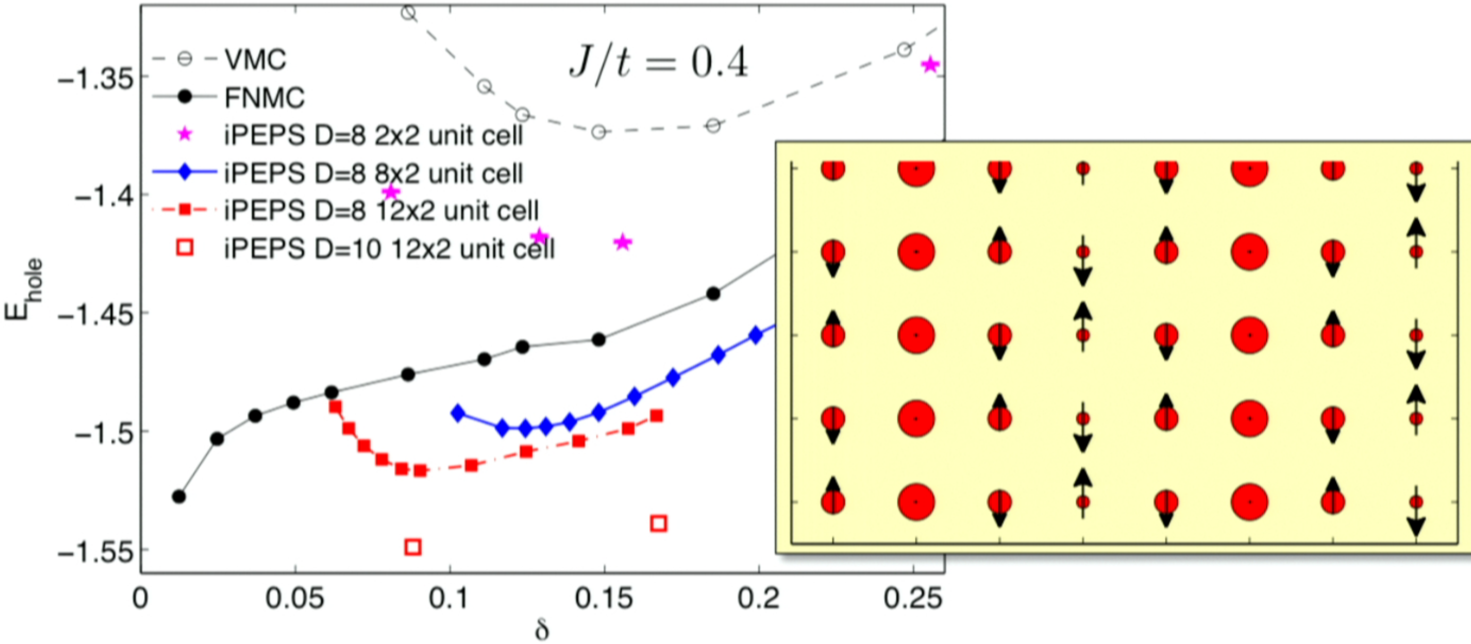

iPEPS: lower (better) variational energy: **stripes!**

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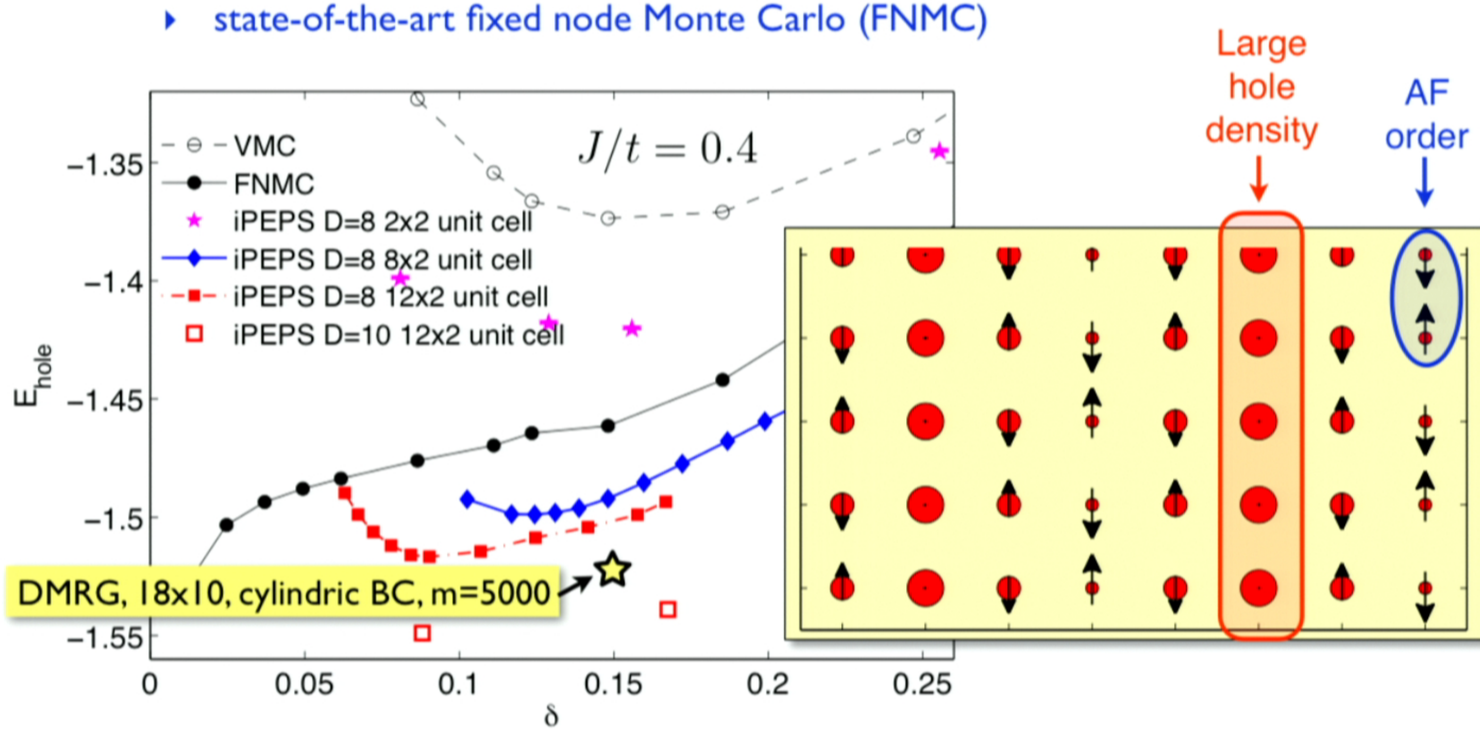

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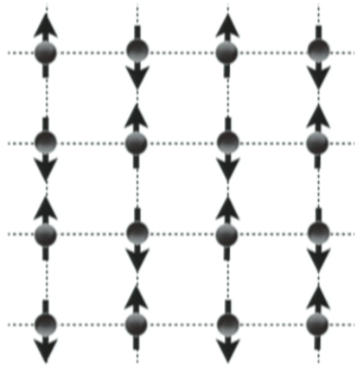
SU(N) Heisenberg models (square lattice)

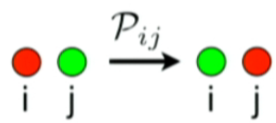
- N=2: $H = \sum_{\langle i,j \rangle} S_i S_j$

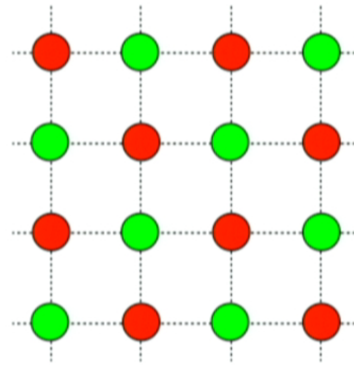
  local basis states: $|\uparrow\rangle, |\downarrow\rangle$



Néel order

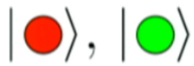
SU(N) Heisenberg models (square lattice)





Néel order

- N=2: $H = \sum_{\langle i,j \rangle} P_{ij}$

  local basis states: 

- N=3 

Ground state??

- N=4 

nature physics

ARTICLES

PUBLISHED ONLINE: 28 FEBRUARY 2010 | DOI: 10.1038/NPHYS1535

Two-orbital *SU*(*N*) magnetism with ultracold alkaline-earth atoms

A. V. Gorshkov[1★], M. Hermele[2], V. Gurarie[2], C. Xu[1], P. S. Julienne[3], J. Ye[4], P. Zoller[5,6], E. Demler[1,7], M. D. Lukin[1,7] and A. M. Rey[4]

Nuclear spin

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

- N=3
- N=4

Ground state??

SU(2): Comparison with Quantum Monte Carlo

Energy:	QMC (extrap.):	-0.669437(5)J	A. Sandvik, PRB56, 11678 (1997)
	iPEPS (D=10):	-0.66939J	rel. error < 10^{-4}

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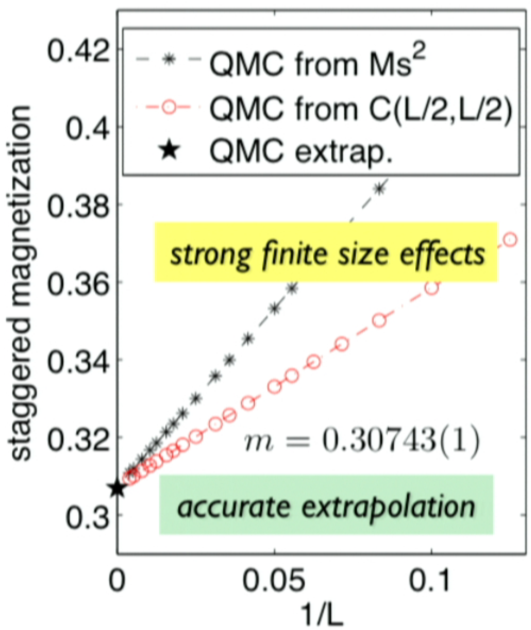
QMC study: Sandvik & Evertz, PRB82, 024407 (2010): system sizes up to 256x256



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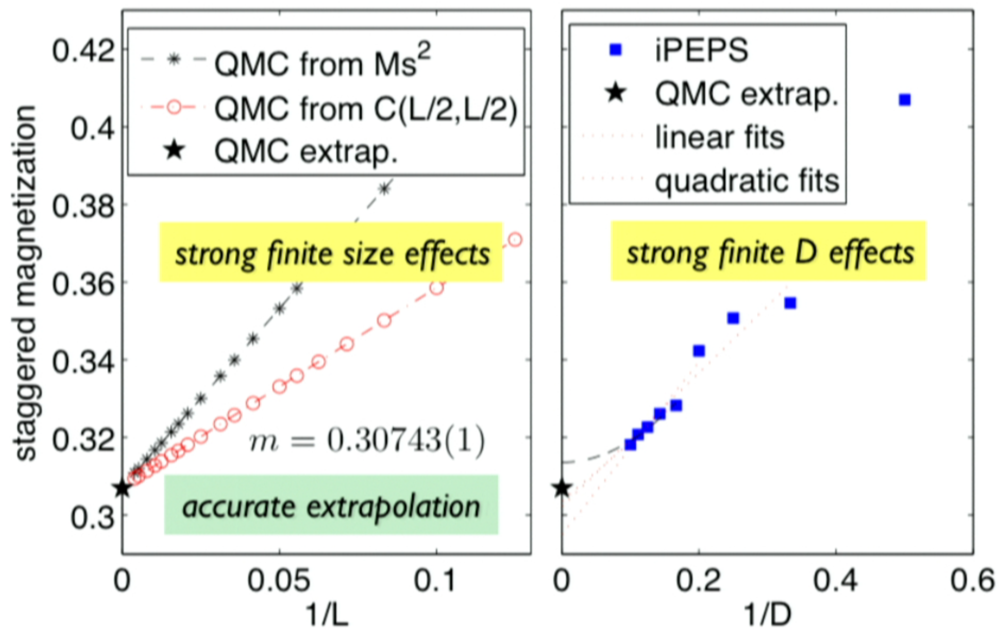
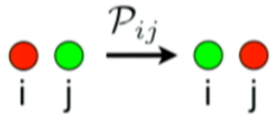
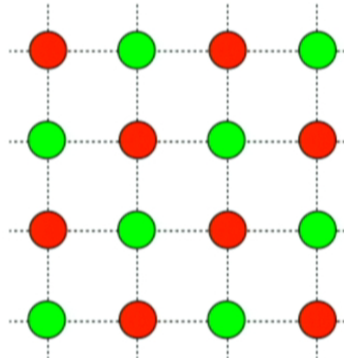


SU(N) Heisenberg models (square lattice)



- N=2: $H = \sum_{\langle i,j \rangle} P_{ij}$

local basis states: 



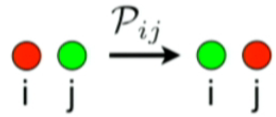
Néel order

- N=3 

- N=4 

Cannot use QMC because of the **sign problem**!!!

SU(N) Heisenberg models (square lattice)



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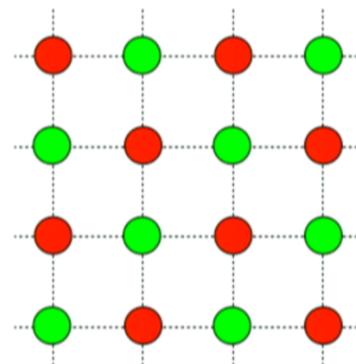

Néel order

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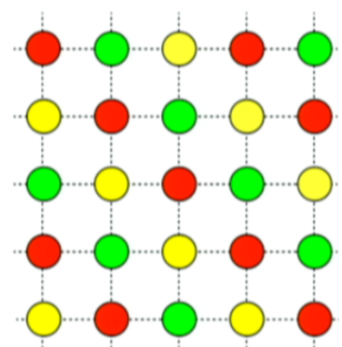


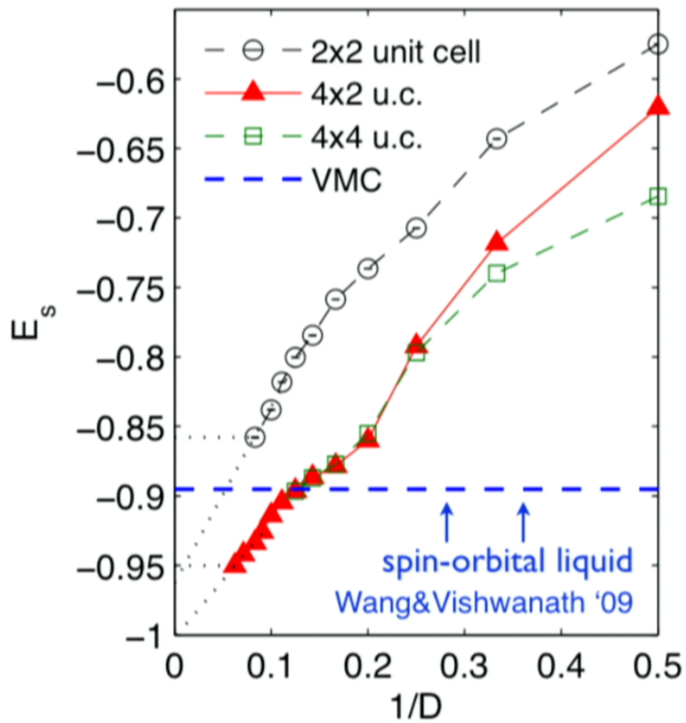
3 sub-lattice
Néel order

- N=4 

ED & flavor-wave theory (Toth et al.)
iPEPS & DMRG (Bauer et al.)

SU(4) Heisenberg model: iPEPS results

Corboz, Läuchli, Mila, Penc, Troyer, arXiv:1108.2857



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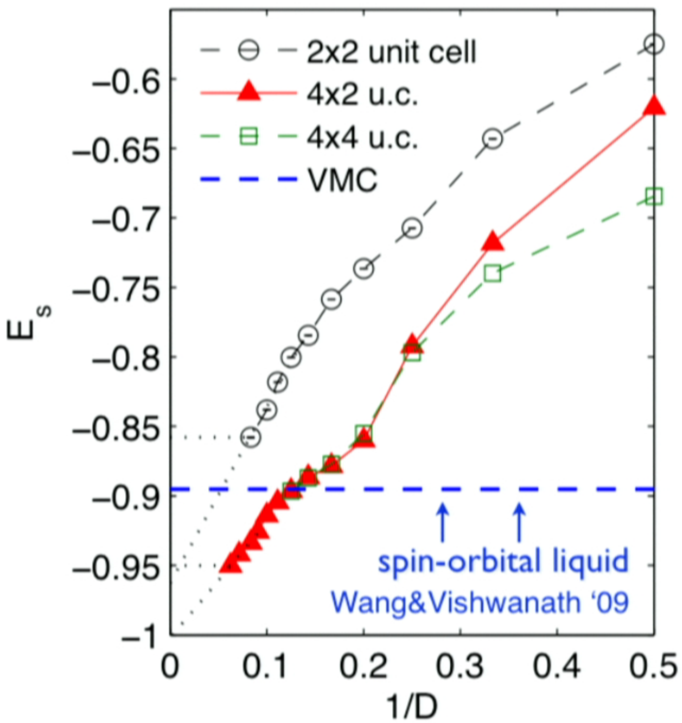
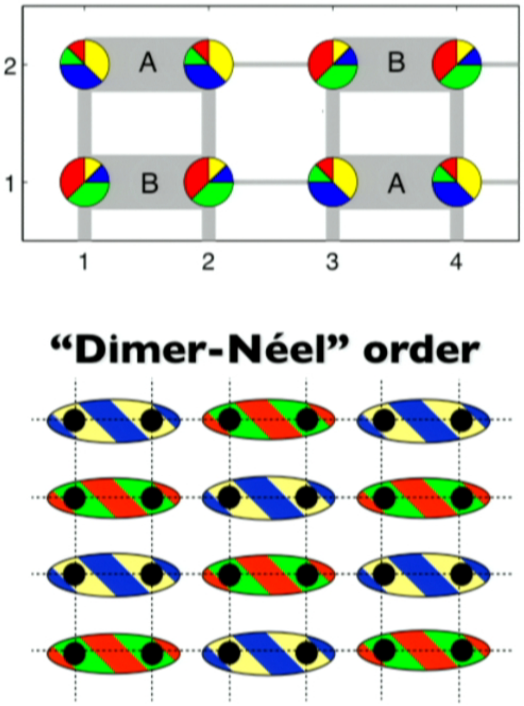
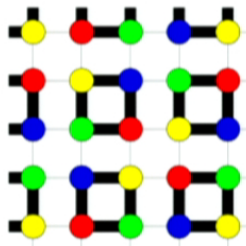




SU(4): Study as a function of bond dimension

infinite
ground
state
degeneracy



plaquette state

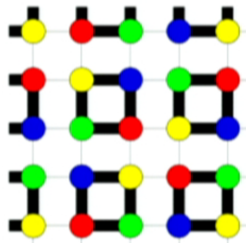
→ D

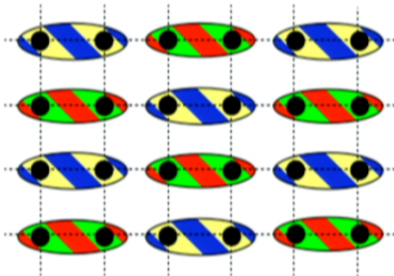
D=1
product state
(mean-field)

D=2
add quantum fluctuations
on top of product state
same solution as
linear flavor-wave theory

SU(4): Study as a function of bond dimension

infinite ground state degeneracy





studying extrapolations of the data for D=5-16 suggests that state is stable

D

D=1
product state (mean-field)

D=2
add quantum fluctuations on top of product state same solution as linear flavor-wave theory

D=5

D=16
largest D tested in this study

increase **quantum fluctuations** / increase **entanglement** D

Summary: tensor networks in 2D

- Variational ansatz with no (little) bias & controllable accuracy for bosonic/spin *and* fermionic systems

Recent progress with iPEPS: competitive method!

✓ t-J model: *striped state* with *better variational energy* than variational and fixed-node Monte Carlo

✓ SU(4) Heisenberg: *New type of ground state (Dimer-Néel ordered)*

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- High computational cost

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Ways to improve the efficiency:

- 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 (Pizorn et al., Vidal et al.)