Progress on Infinite TPS/PEPS Algorithms

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Numerical Approaches to

Quantum Many-Body Systems,

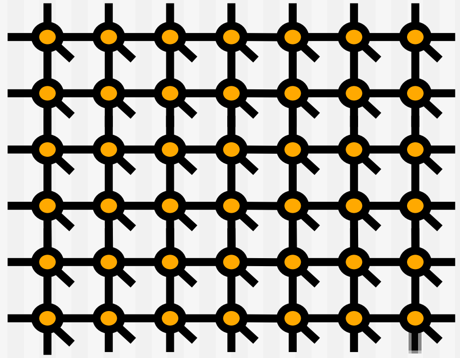
IPAM / UCLA January 28th 2009

Collaborators: G. Vidal, J. Jordan, A. Doherty,

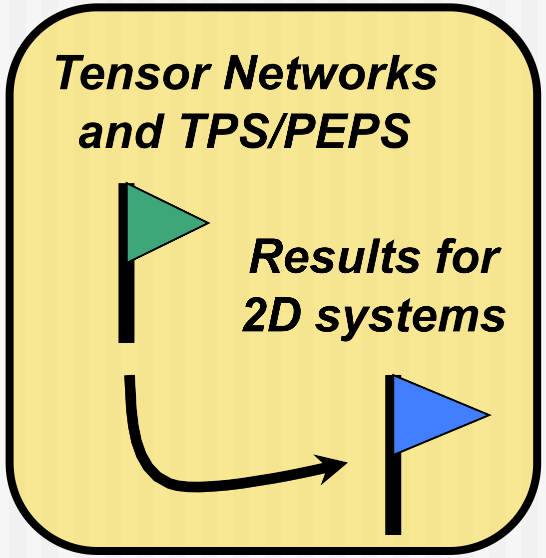
F. Verstraete, I. Cirac, H.-Q. Zhou

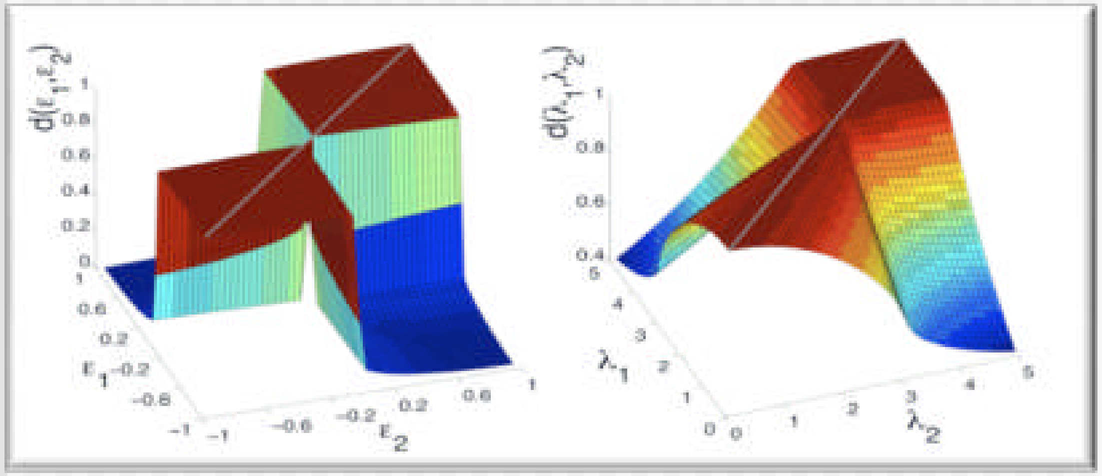
Goal of this talk:

Explain recent results in the simulation of infinite-size quantum many-body systems in 2 dimensions using methods based on Tensor Product States / Projected Entangled Pair States



ROADMAP

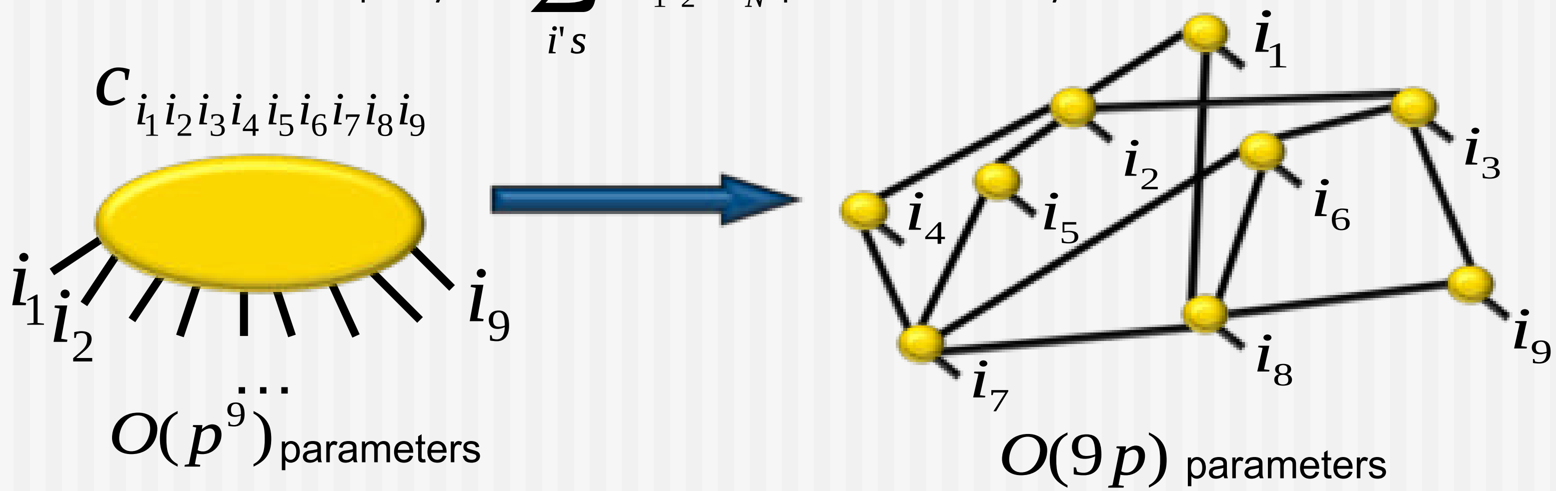




Main idea of Tensor Networks

- **Problem:** how to represent efficiently quantum states of a quantum lattice system
- **Solution:** divide the coefficient of the quantum state in a *Tensor Network that only depends on a small number of parameters*

$$|\Psi\rangle = \sum_{i's} c_{i_1 i_2 \ldots i_N} |i_1, i_2, \ldots, i_N\rangle$$



Outline

1.- Basics on Tensor Networks

* Tensor Networks
* Tensor Product States / Projected Entangled Pair States
* Tensor Network Algorithms

2.- Simulation results for 2-dim quantum systems

* Infinite-PEPS algorithm (iPEPS)
* 2-dim Quantum Ising
* Infinite-PEPS and the Fidelity approach to Quantum Phase Transitions
* 2-dim Quantum Compass model
* 2-dim Hard-Core Bose-Hubbard model

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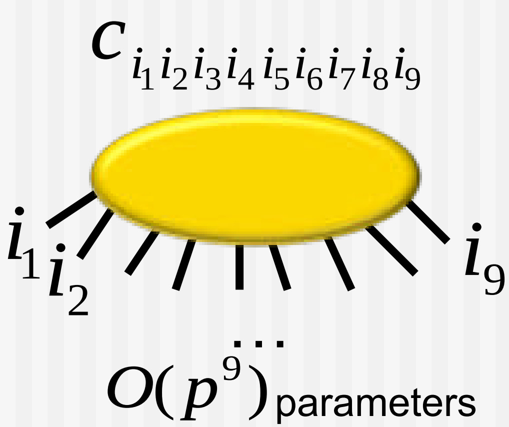
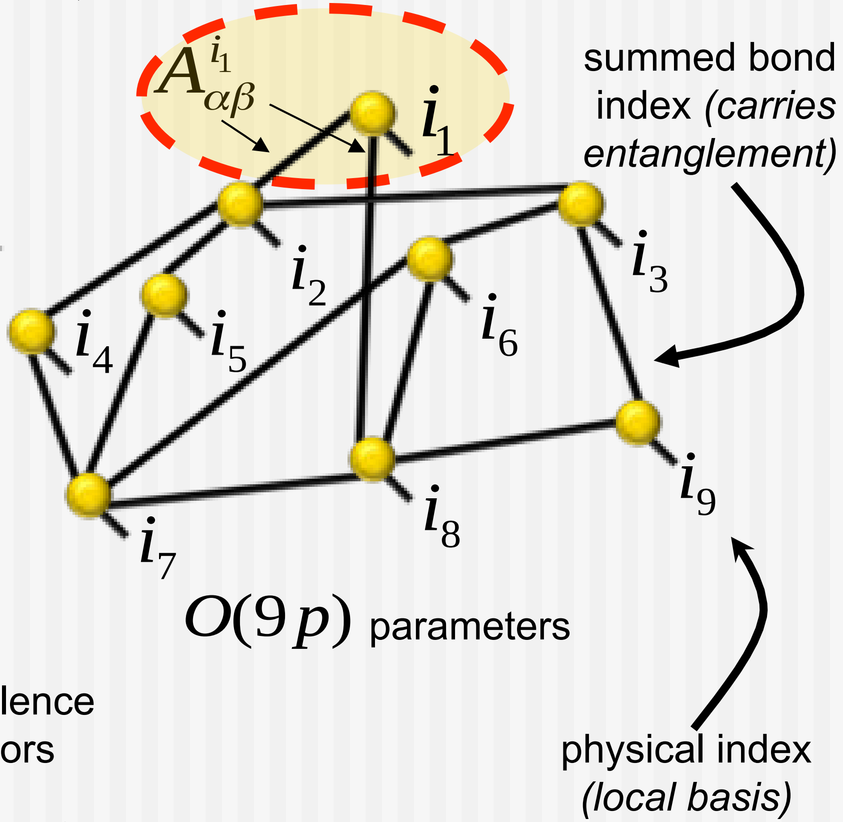
Tensor Networks (TN)

$$|\Psi\rangle = \sum_{i's} c_{i_1 i_2 \ldots i_N} |i_1, i_2, \ldots, i_N\rangle \in (\mathbf{C}^{\mathbf{p}})^{\otimes N}$$

p^N complex parameters



replacement



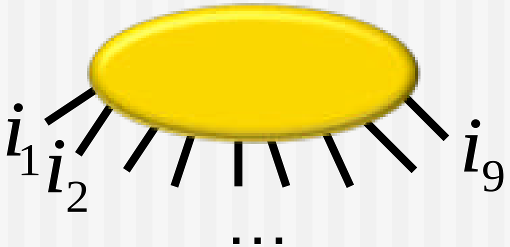
range of the bond indices

maximum valence of the tensors

In general, $O(NpD^V)$ parameters

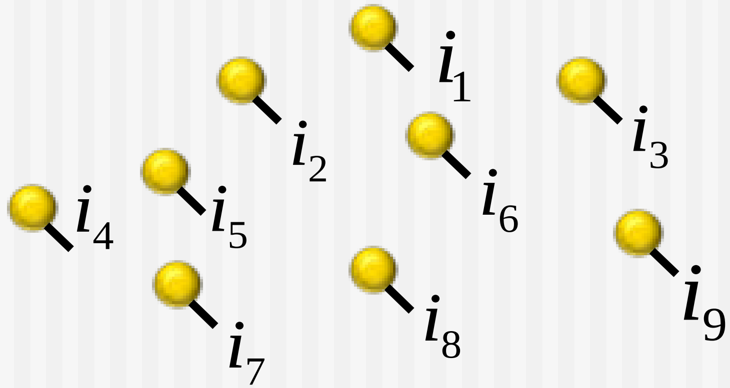
Justification

Generic state



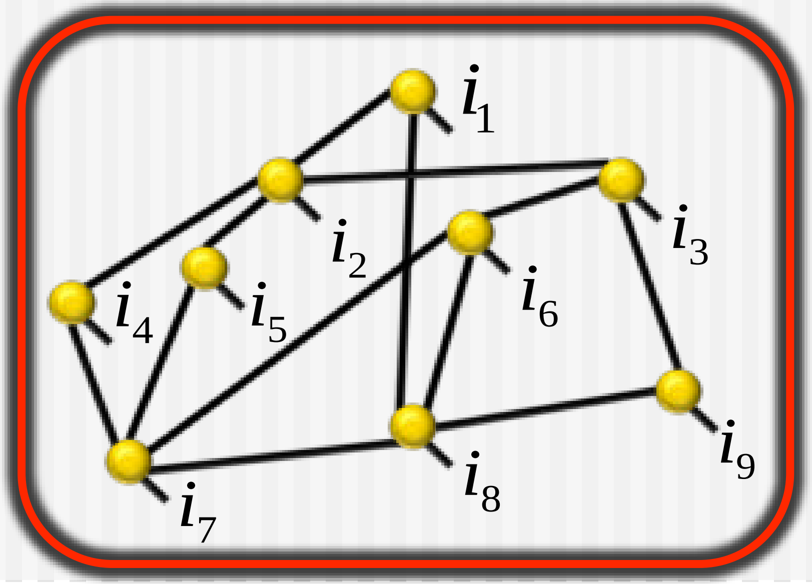
Correlations OK
but not efficient
(exact)

Product state



Efficiency OK
but not correlated
(mean field)

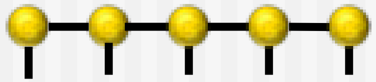
Tensor network



Efficient and correlated

Some types of TN

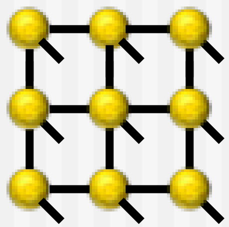
Matrix Product States (MPS)



1-dim systems

Density Matrix Renormalization Group (White, Schollwoeck, McCulloch…)
Power Wave Function Renormalization Group (Nishino, Okunishi…)
Time Evolving Block Decimation (Vidal…)

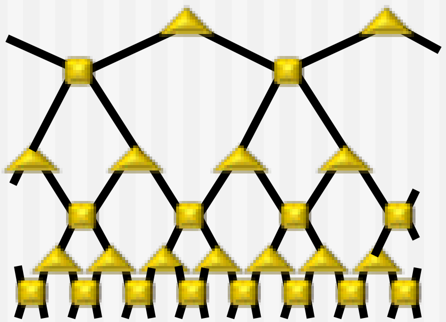
Tensor Product States (TPS), Projected Entangled Pair States (PEPS)



d-dim systems, d > 1

Tensor Product Variational Approach (Nishino, Okunishi, Hieida, Maeshima, Akutsu...)
PEPS algorithm (Verstraete, Cirac, Murg, Schuch…)
Infinite-PEPS algorithm (Jordan, Orus, Vidal, Verstraete, Cirac…)

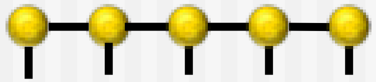
Multiscale Entanglement Renormalization Ansatz (MERA)



Scale-invariant systems

Entanglement Renormalization (Vidal, Evenbly, Pfeipfer…)

Some types of TN

Matrix Product States (MPS)  *1-dim systems*

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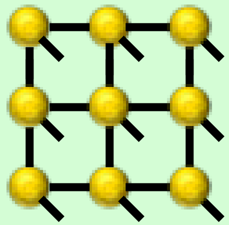

d-dim systems, $d > 1$

Tensor Product Variational Approach (Nishino, Okunishi, Hieida, Maeshima, Akutsu...)
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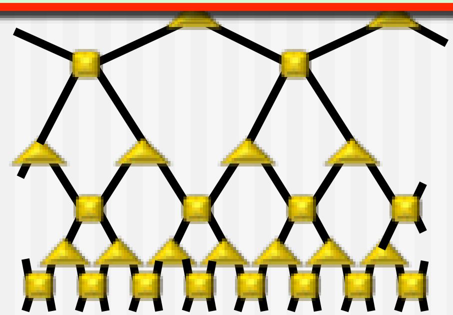


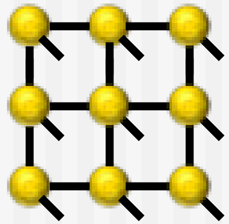
Scale-invariant systems

Entanglement Renormalization (Vidal, Evenbly, Pfeipfer…)

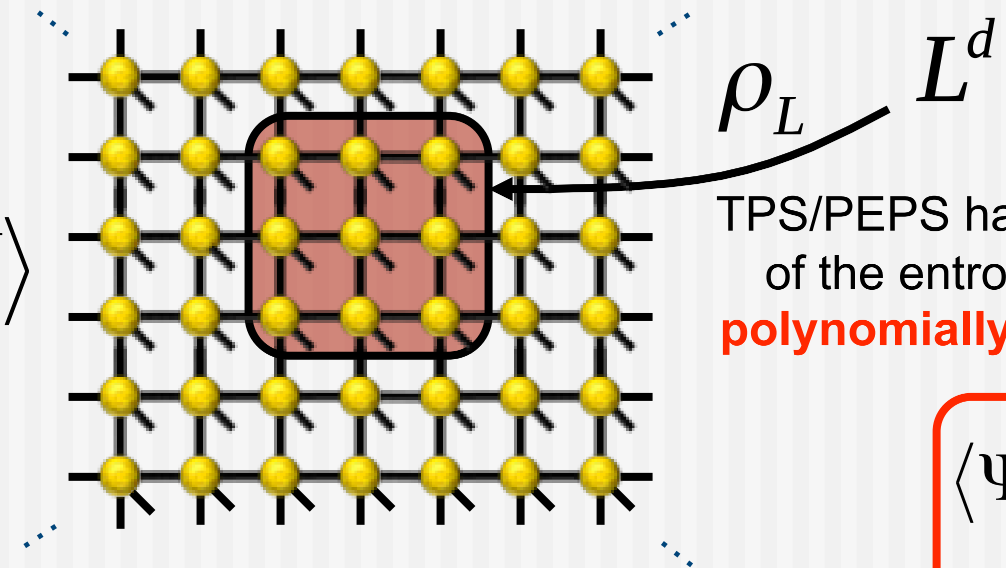
Tensor Product States, Projected Entangled Pair States

Tensor Product States (TPS), or Projected Entangled Pair States (PEPS) mimic the structure of entanglement in d-dim lattices

(see also talks by F. Verstraete and N. Schuch)



$|\Psi\rangle$



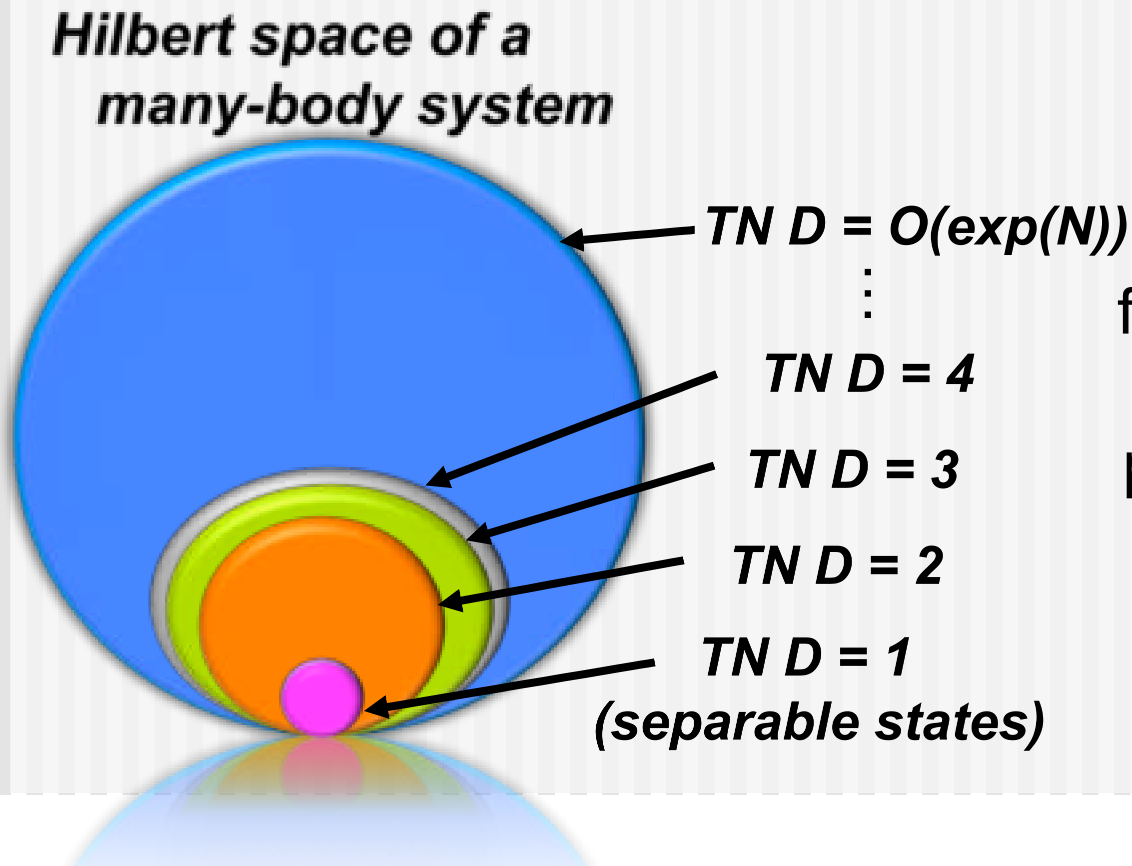
$$S(\rho_L) \leq \log(D)\, L^{d-1}$$

TPS/PEPS handle a **'boundary law' scaling** of the entropy of entanglement, and also **polynomially decaying** two-point correlators

$$\langle \Psi | O_{\vec{r}} O_{\vec{r}\,'} | \Psi \rangle \approx \frac{1}{|\vec{r} - \vec{r}\,'|^{\eta}}$$

Tensor Network Algorithms

Observation: many relevant quantum states in Nature seem to be well represented by TN (e.g. ground states of some Hamiltonians with local interactions)



Idea: use TN with fixed and increasing D to compute the properties of quantum many-body systems, e.g. ground states, dynamics…

Why Tensor Networks?

- Efficient ***description*** of the system
- Evaluation of ***expectation values*** $\langle \Psi | O | \Psi \rangle$ (order parameters, correlators…) - exact in 1-dim, approximate in d-dim d > 1 (#P-Hard) -
- Efficient ***updating*** after an operation, e.g.

$$e^{-iHt}|\Psi\rangle \qquad e^{-Ht}|\Psi\rangle$$

dynamics ***ground states***

- Efficient ***optimization of cost functions***, e.g.

$$\min_{|\Psi\rangle \in PEPS} \langle \Psi | H | \Psi \rangle \qquad \min_{|\Psi\rangle \in PEPS} \left\| |\Psi\rangle - |\Psi'\rangle \right\|^2$$

ground states

- Allow to deal with ***infinite lattices (thermodynanic limit)*** for translationally invariant systems
- ***Fast simulation algorithms***
- ***No sign problem!*** *But* ***limited by the amount of entanglement***

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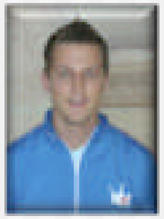
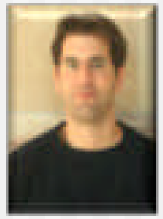
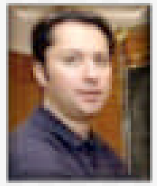
Infinite 2-dim quantum systems (iPEPS algorithm)

We developed an algorithm that uses infinite PEPS (or TPS) to evaluate the ground state properties of ***infinite-size quantum lattice systems in 2-dim***







J. Jordan, R. Orús, G. Vidal, F. Verstraete, I. Cirac, PRL 101, 250602 (2008)

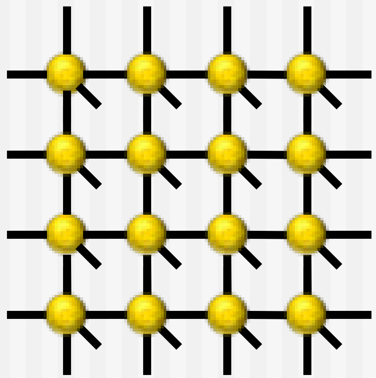
INPUT: 2-dim lattice Hamiltonian

$$H = \sum_{\langle \vec{r}, \vec{r}' \rangle} h^{[\vec{r}, \vec{r}']}$$

imaginary-time evolution

$$e^{-Ht} |\Psi\rangle$$

iPEPS for the ground state $|\Psi_0\rangle$



OUTPUT: expectation values

$$\langle \Psi_0 | O | \Psi_0 \rangle$$

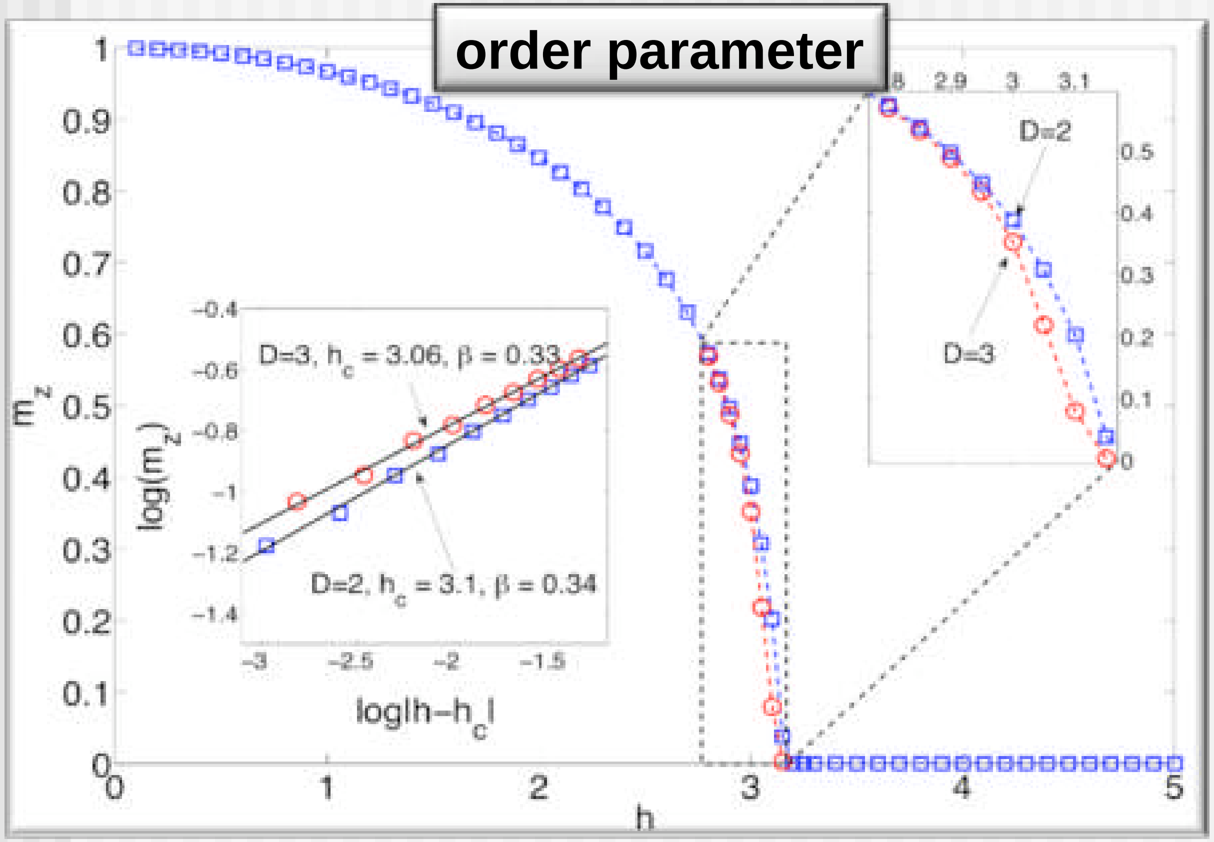
Trick: reduction to a 1-dim transfer matrix problem (dimensional reduction)

R. Orús, G. Vidal, PRB 78, 155117 (2008)

iPEPS Ising: results

Benchmark: 2D quantum Ising model on the infinite square lattice

$$H = -\sum_{\langle \vec{r},\vec{r}'\rangle} \sigma_z^{\vec{r}} \sigma_z^{\vec{r}'} + h \sum_{\vec{r}} \sigma_x^{\vec{r}}$$

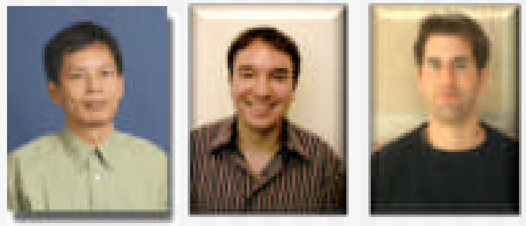


The critical point and the critical exponents match those from the best Quantum Monte Carlo simulation with less than 1% of relative error

iPEPS and the Fidelity Approach to Quantum Phase Transitions

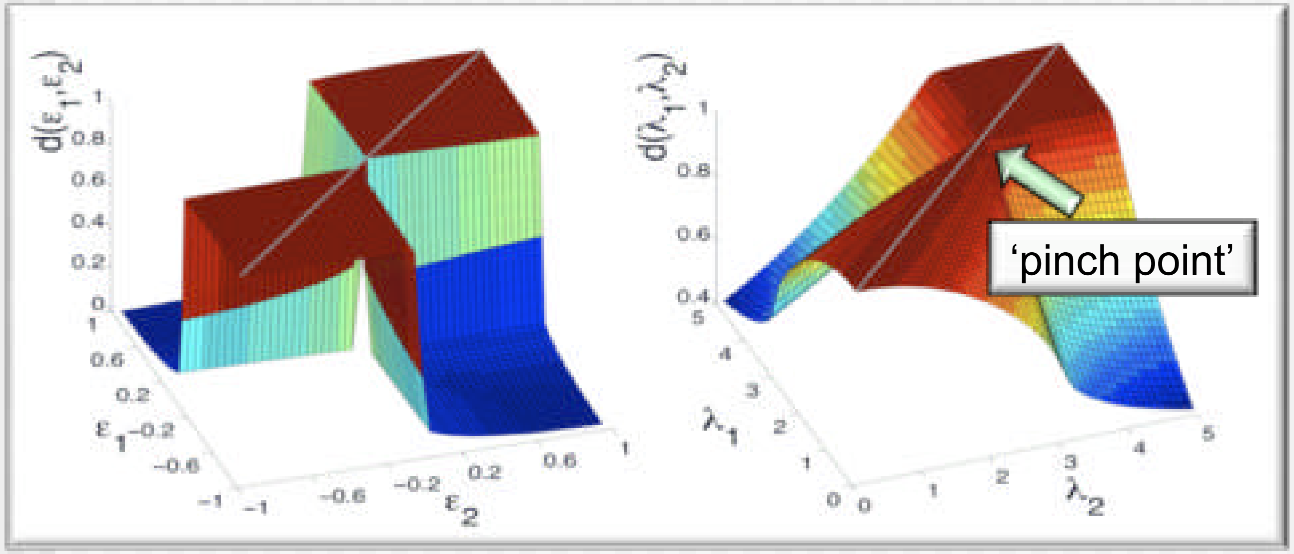
Fidelity between different ground states

H-Q. Zhou, R. Orús, G. Vidal, PRL 100, 080602 (2008)



$$H(g) \Longleftrightarrow d(g_1, g_2) = \lim_{N\to\infty} -\frac{1}{N}\log\left|\langle\Psi_0(g_1)|\Psi_0(g_2)\rangle\right|$$

$$H = -\sum_{\langle\vec{r},\vec{r}'\rangle}\sigma_z^{\vec{r}}\sigma_z^{\vec{r}'} + \varepsilon\sum_{\vec{r}}\sigma_z^{\vec{r}} \qquad H = -\sum_{\langle\vec{r},\vec{r}'\rangle}\sigma_z^{\vec{r}}\sigma_z^{\vec{r}'} + \lambda\sum_{\vec{r}}\sigma_x^{\vec{r}}$$

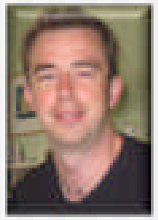


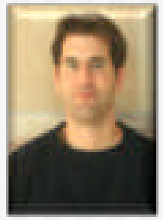
1st order QPT **2nd order QPT**

Easy to compute with TN, and shows the phase diagram without relying on any local order parameter

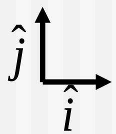
Anisotropic Quantum Orbital Compass Model with iPEPS

A. Doherty, R. Orús, G. Vidal, arXiv:0809.4068 (PRL)

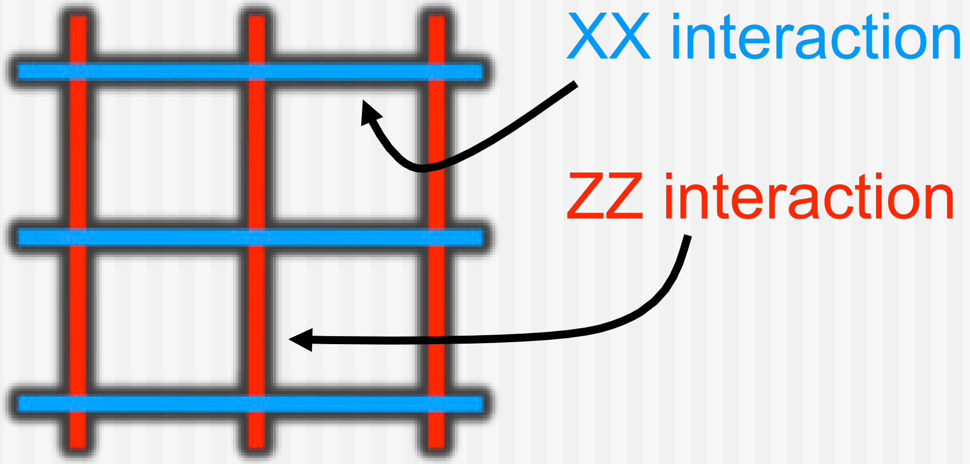




$$H = -J_x \sum_{\vec{r}} \sigma_x^{\vec{r}} \sigma_x^{\vec{r}+\hat{i}} - J_z \sum_{\vec{r}} \sigma_z^{\vec{r}} \sigma_z^{\vec{r}+\hat{j}}$$



spins ½ at the nodes of a square lattice



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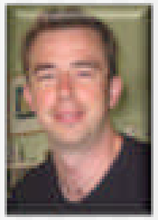
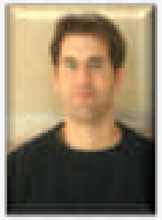
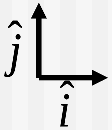




$$H = -J_x \sum_{\vec{r}} \sigma_x^{\vec{r}} \sigma_x^{\vec{r}+\hat{i}} - J_z \sum_{\vec{r}} \sigma_z^{\vec{r}} \sigma_z^{\vec{r}+\hat{j}}$$



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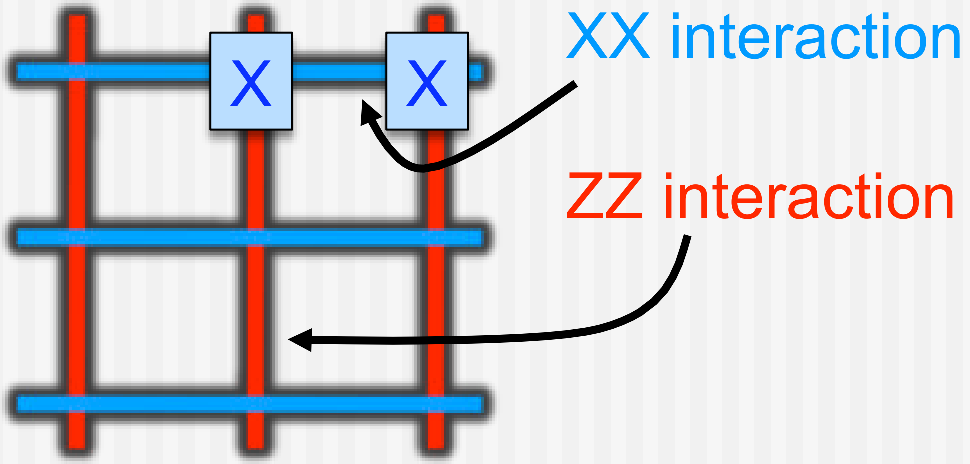

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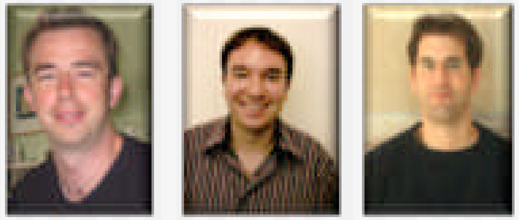

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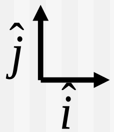

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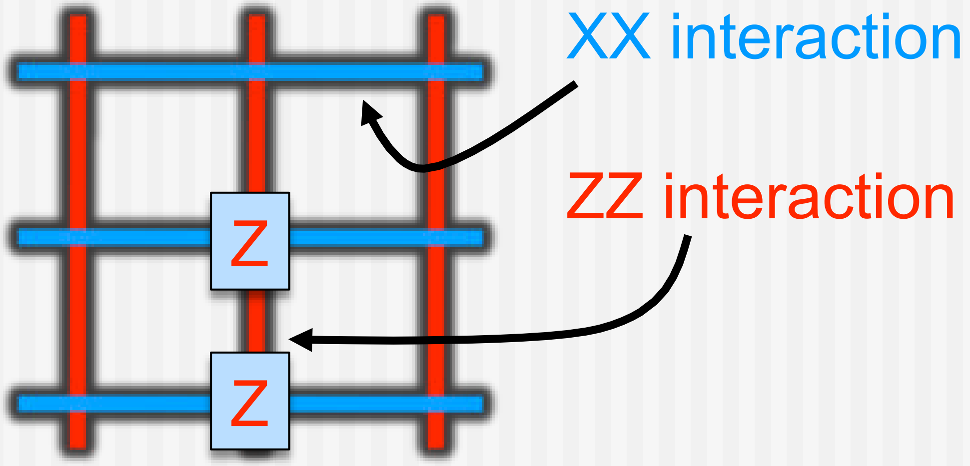

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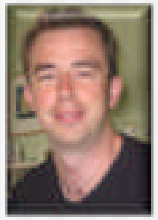

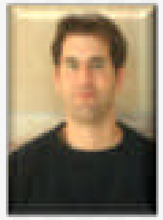

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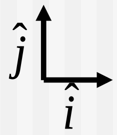
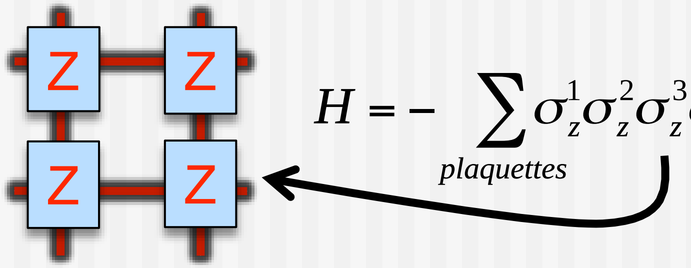


spins ½ at the nodes of a square lattice

Dual to…

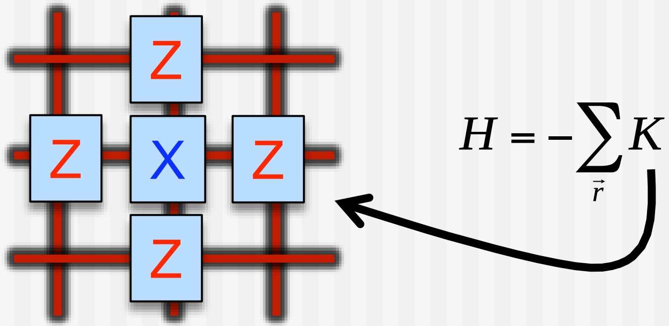


$$H = -\sum_{plaquettes} \sigma_z^1 \sigma_z^2 \sigma_z^3 \sigma_z^4 - h \sum_{\vec{r}} \sigma_x^{\vec{r}}$$

p+ip superconducting array model (e.g. Sr_2RuO_4)

Xu, Moore, PRL 93, 047003 (2004)

Nussinov, Fradkin, PRB 71, 195120 (2005)



$$H = -\sum_{\vec{r}} K^{\vec{r}} - h \sum_{\vec{r}} \sigma_x^{\vec{r}}$$

Cluster state Hamiltonian in a magnetic field

Doherty, Bartlett, arXiv:0802.4314

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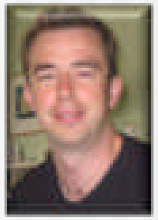
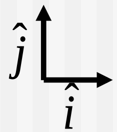


$$H = -J_x \sum_{\vec{r}} \sigma_x^{\vec{r}} \sigma_x^{\vec{r}+\hat{i}} - J_z \sum_{\vec{r}} \sigma_z^{\vec{r}} \sigma_z^{\vec{r}+\hat{j}}$$



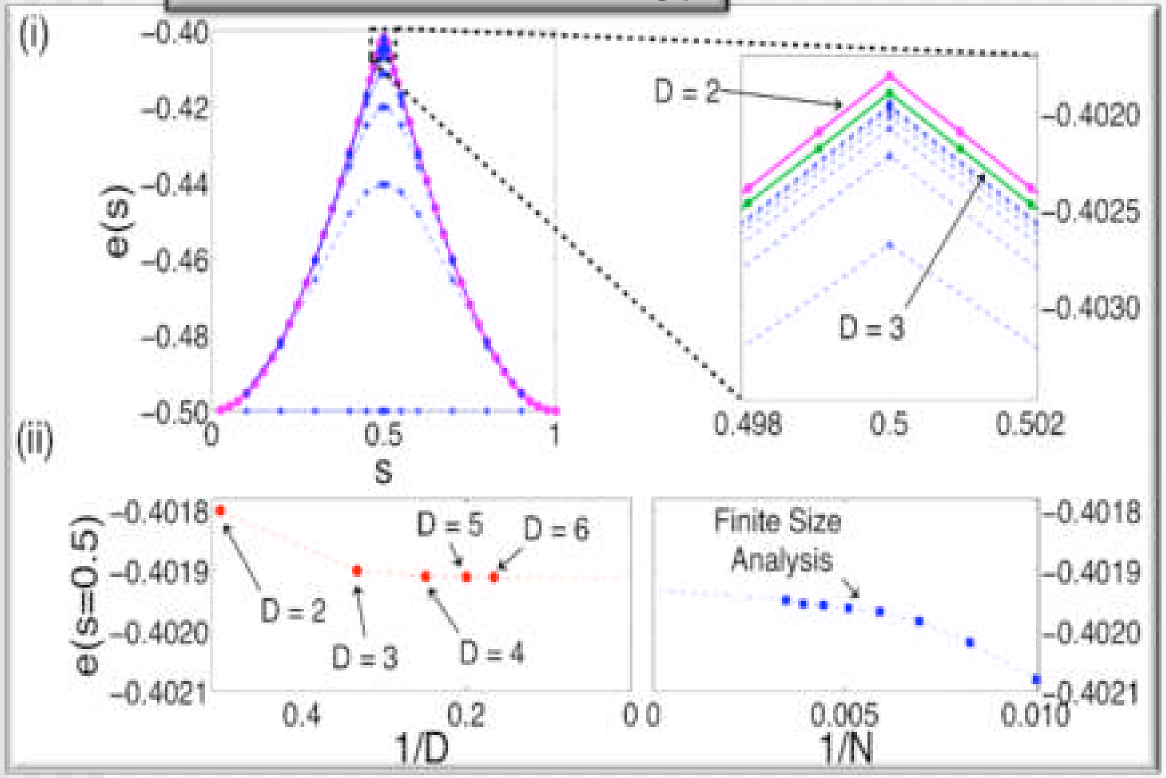
spins ½ at the nodes of a square lattice

Question: what is the ORDER of the phase transition?

Our answer: 1st order

Anisotropic Quantum Orbital Compass Model with iPEPS

Ground state energy



$$J_x = \cos(s\pi/2)$$

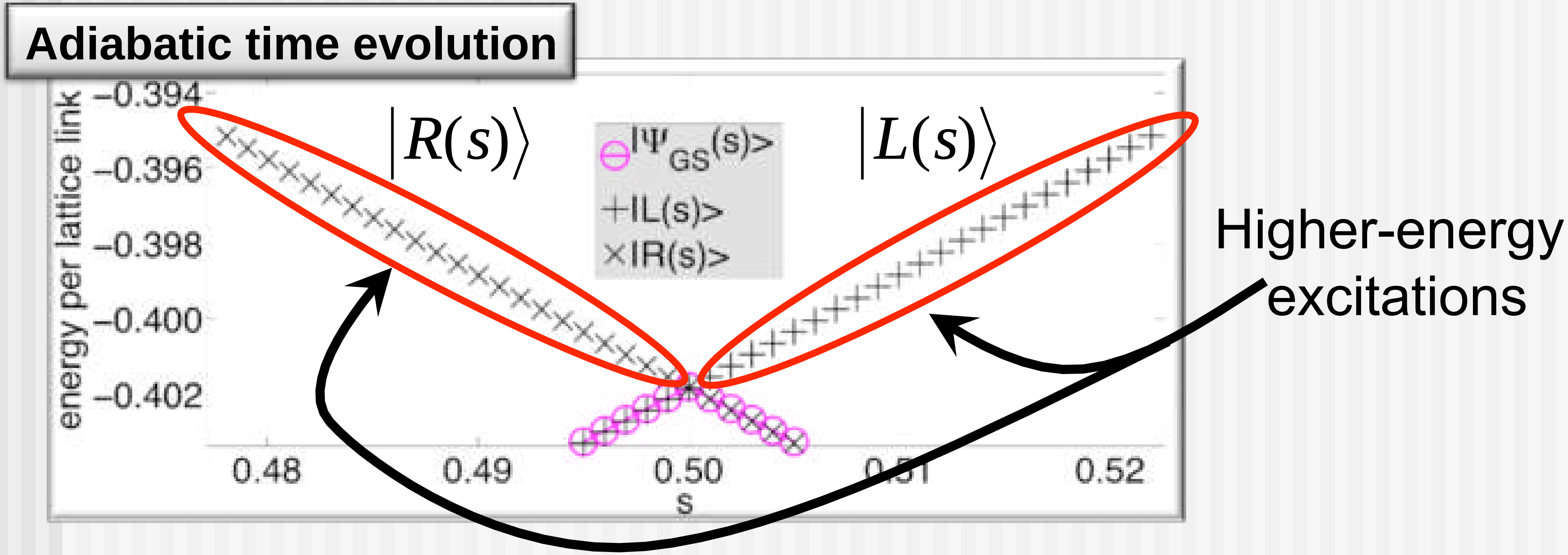
$$J_z = \sin(s\pi/2)$$

$$s \in [0,1]$$

Compatible with Monte Carlo results up to 16 x 16 sites

(*Dorier, Beca Mila, PRB 72, 024448 (2005)*)

Anisotropic Quantum Orbital Compass Model with iPEPS

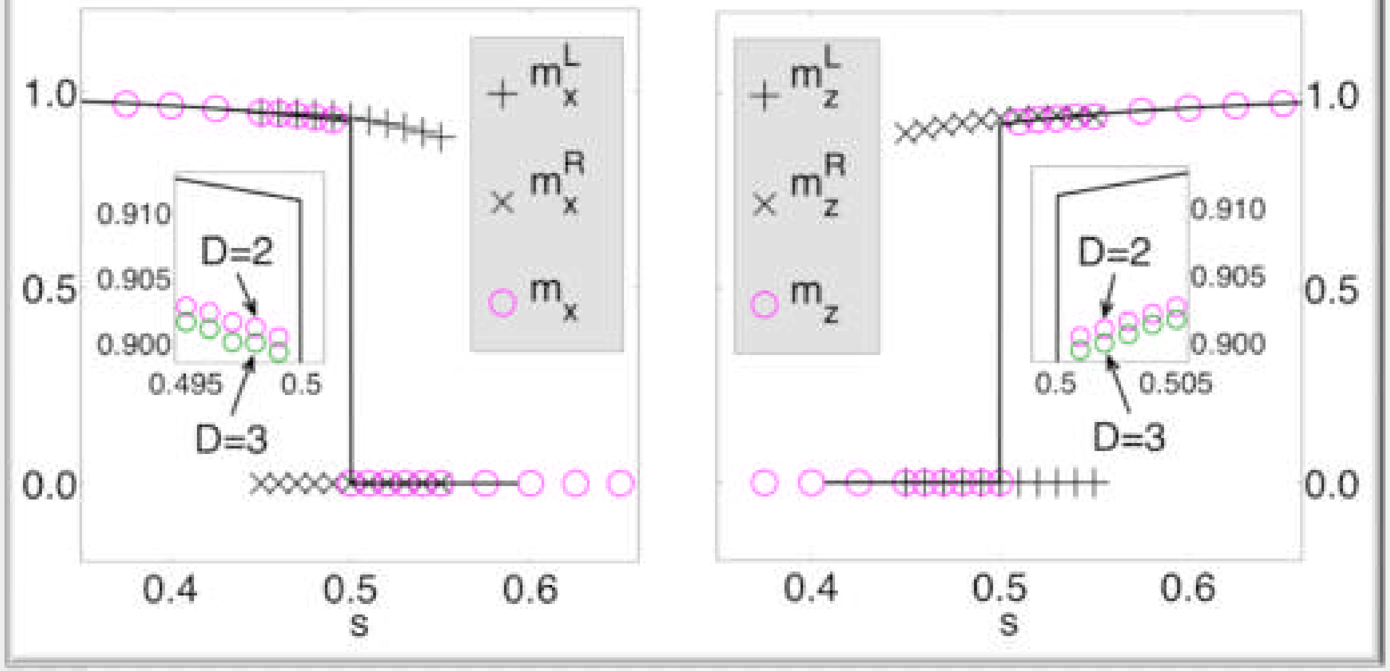


$$|\Psi_{GS}(s)\rangle \approx \begin{cases} |L(s)\rangle & \text{if } s < 1/2 \\ |R(s)\rangle & \text{if } s > 1/2 \end{cases}$$

Two possible ground states at s=1/2: $|L(1/2)\rangle$ and $|R(1/2)\rangle$

Anisotropic Quantum Orbital Compass Model with iPEPS

Discontinuity of local order parameters



1.5% Better than fermionization + mean field (black line)

Chen, Fang, Hu, Yao, PRB 75, 144401 (2007)

Coexistence of ground states with different local properties at s=1/2 implies first order transition

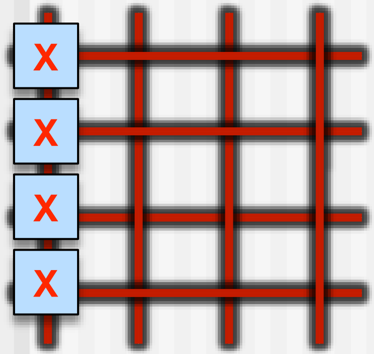
Anisotropic Quantum Orbital Compass Model with iPEPS

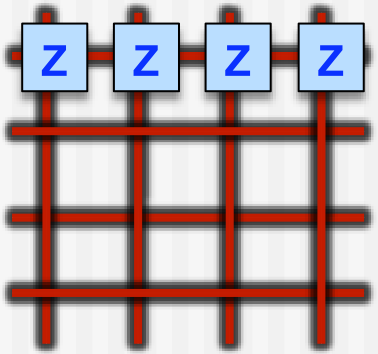
column operators

$$P_i = \prod_j \sigma_x^{[j,i]}$$

row operators

$$Q_j = \prod_i \sigma_z^{[j,i]}$$





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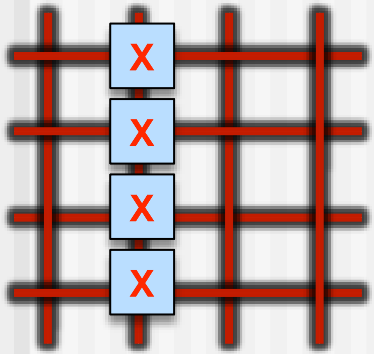

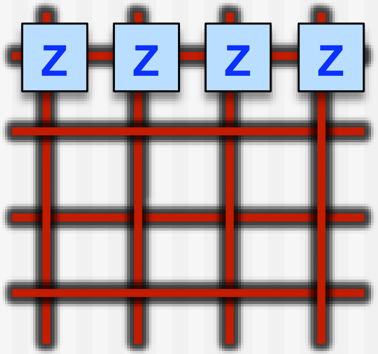

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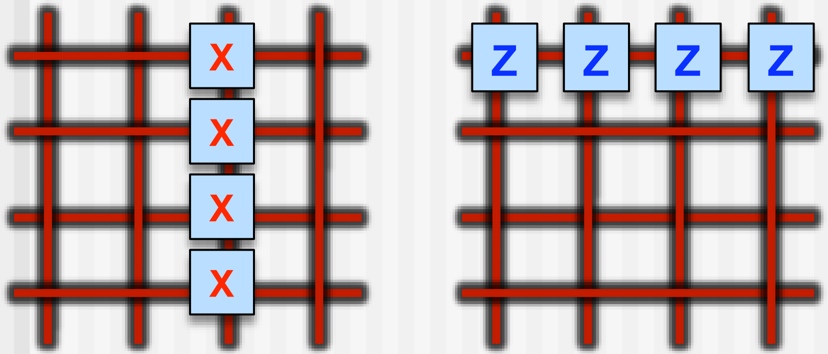

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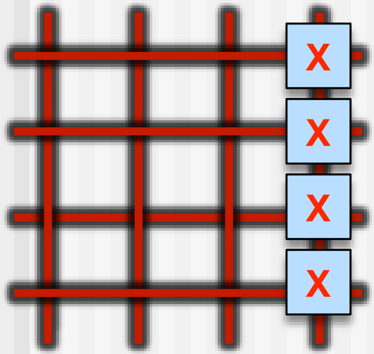

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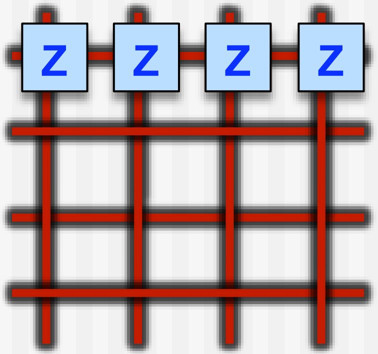

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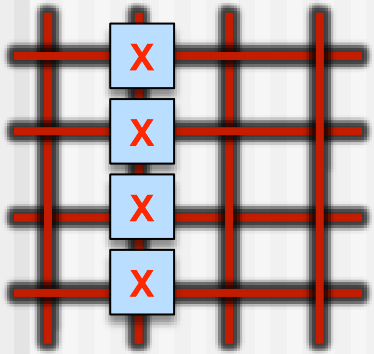

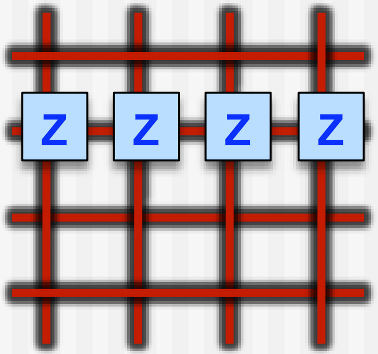

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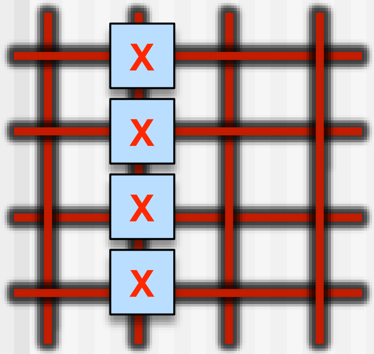

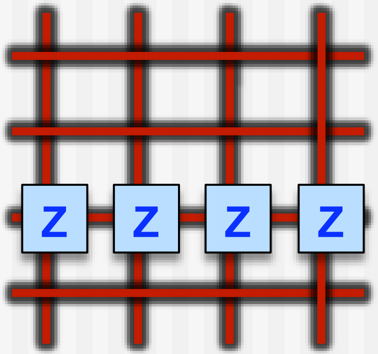

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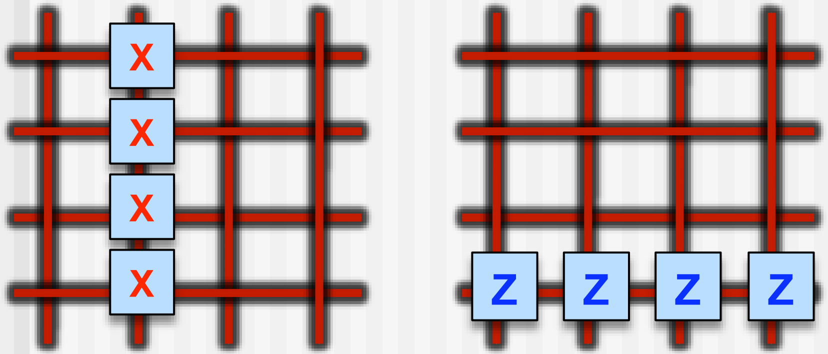

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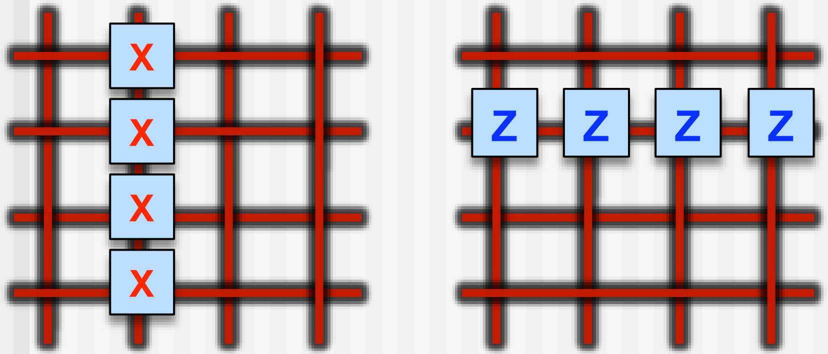

$$[H, P_i] = 0, \quad [H, Q_j] = 0, \quad [P_i, Q_j] \neq 0 \quad \forall i, j$$

(incompatible symmetries)

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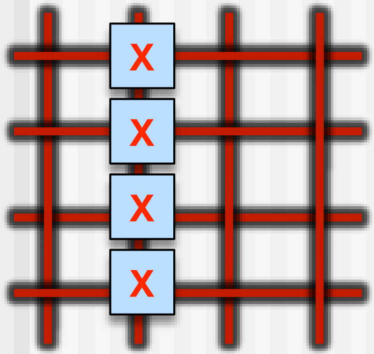

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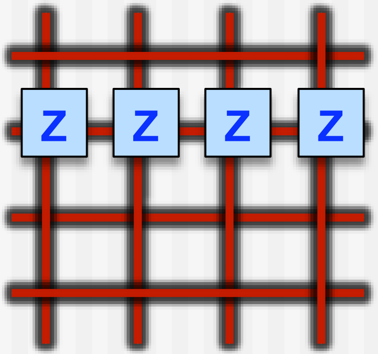

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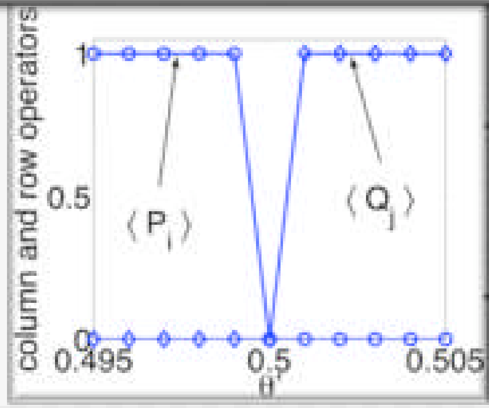
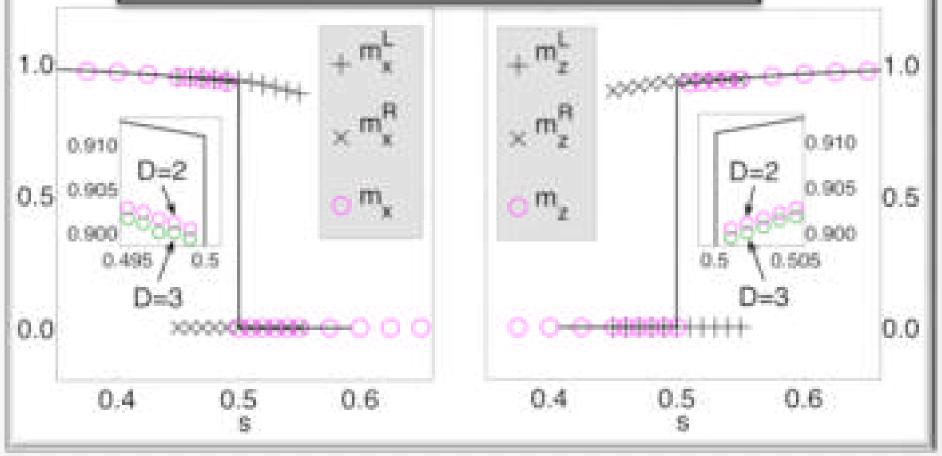
Different symmetry broken on each phase

Non-local symmetry operators

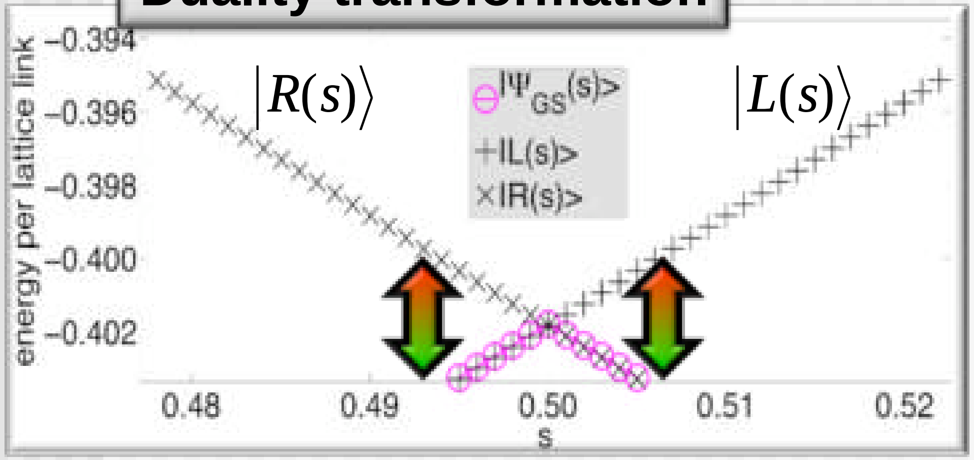


Local order parameters

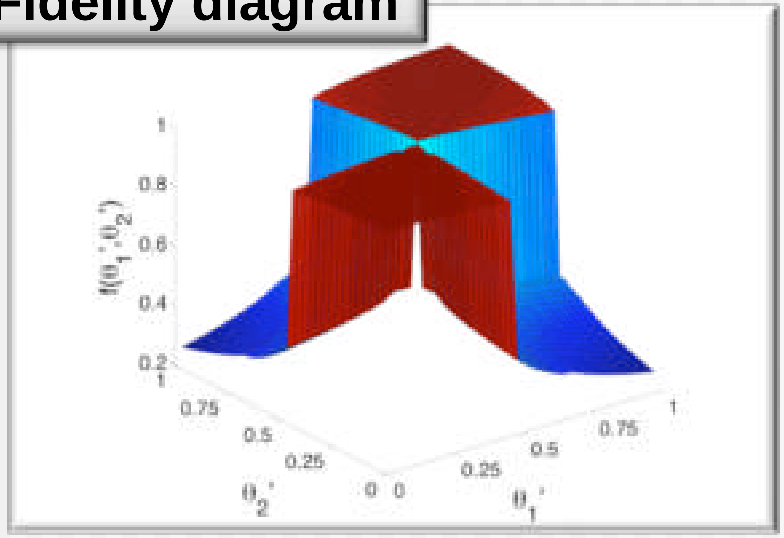


Anisotropic Quantum Orbital Compass Model with iPEPS

Duality transformation



Fidelity diagram



Transformation:

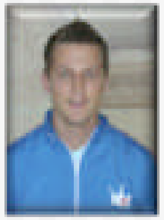
$\pi/2$ rotation of the lattice and all the spins around the Y-axis (**non-local** transformation)

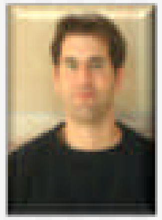
$$|L(s)\rangle = W(\pi/2)w(\pi/2)|R(s)\rangle$$

Typical of a first order transition

Hard-core Bose-Hubbard model with iPEPS

J. Jordan, R. Orús, G. Vidal, arXiv:0901.0420

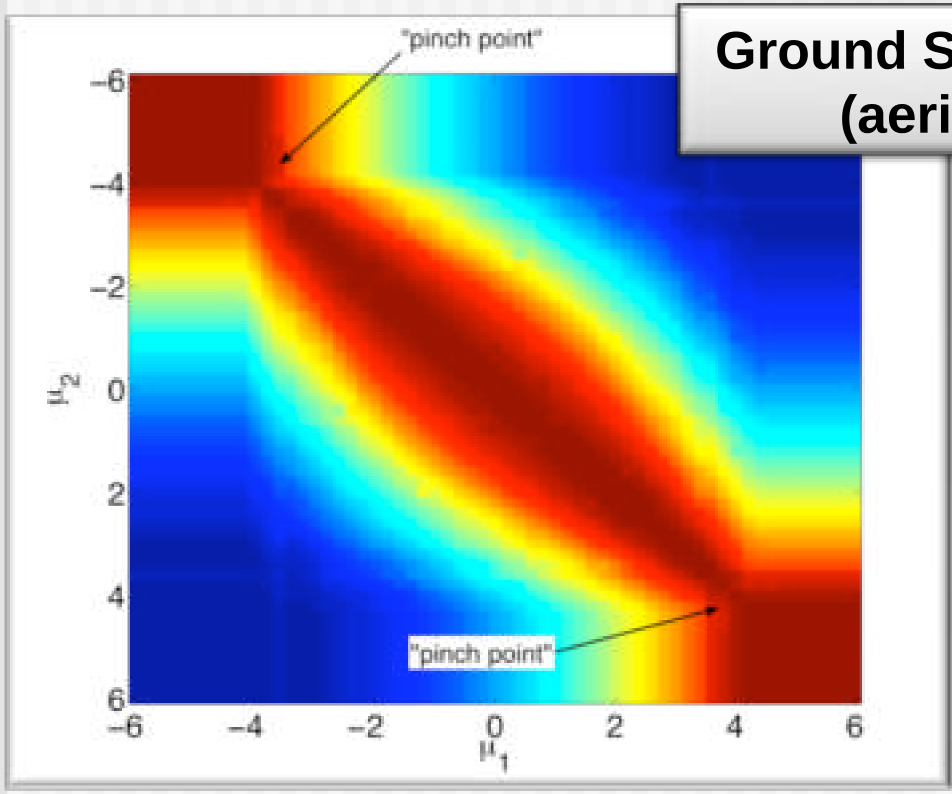




$$H_{HC} = -J\sum_{<i,j>}\left(a_i^{\dagger}a_j + a_j^{\dagger}a_i\right) - \mu\sum_i n_i$$

0 or 1 bosons per site
(hard-core limit)
Infinite square lattice

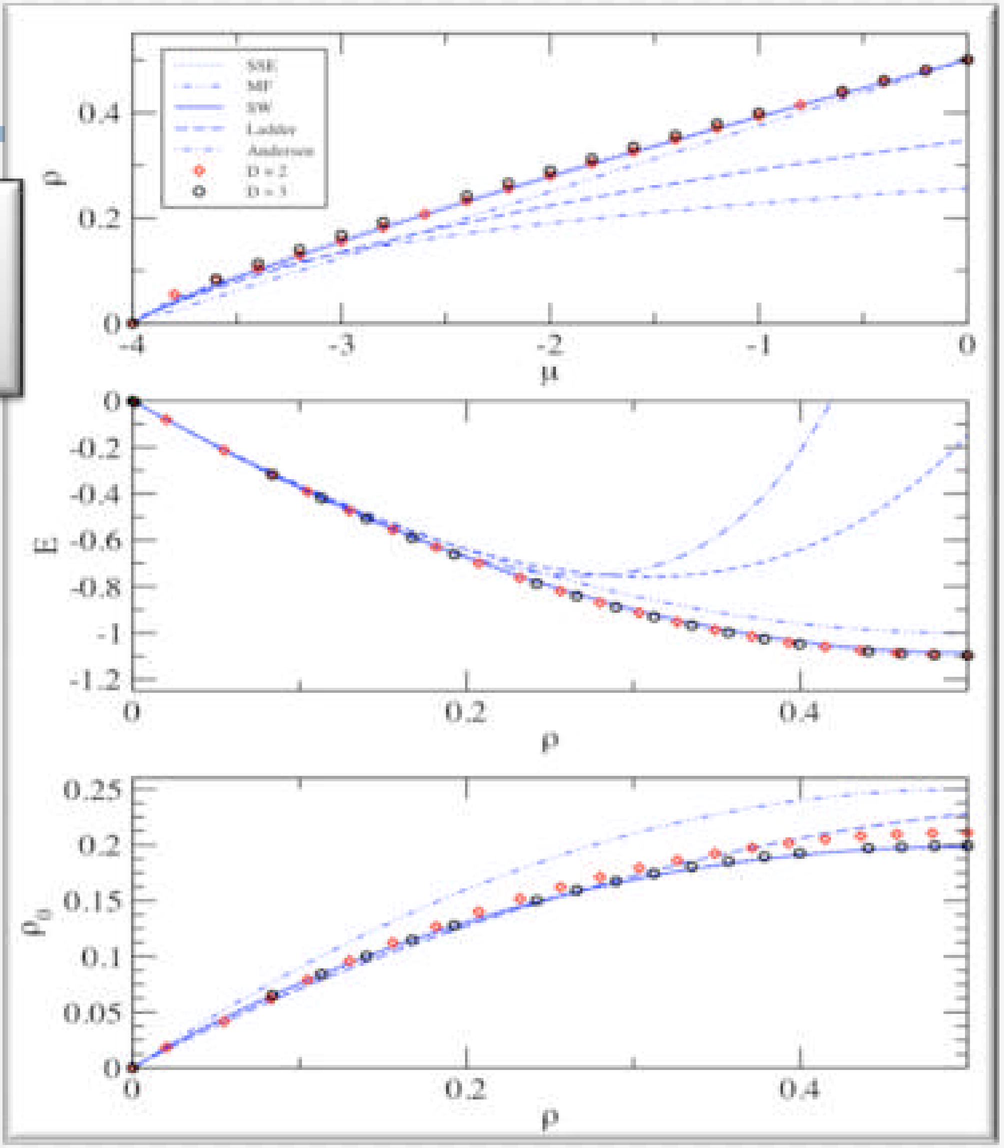
Ground State Fidelity (aerial view)



Clear quantum phase transition between superfluid and Mott-insulating phases

Hard-core Bose-Hubbard model with iPEPS

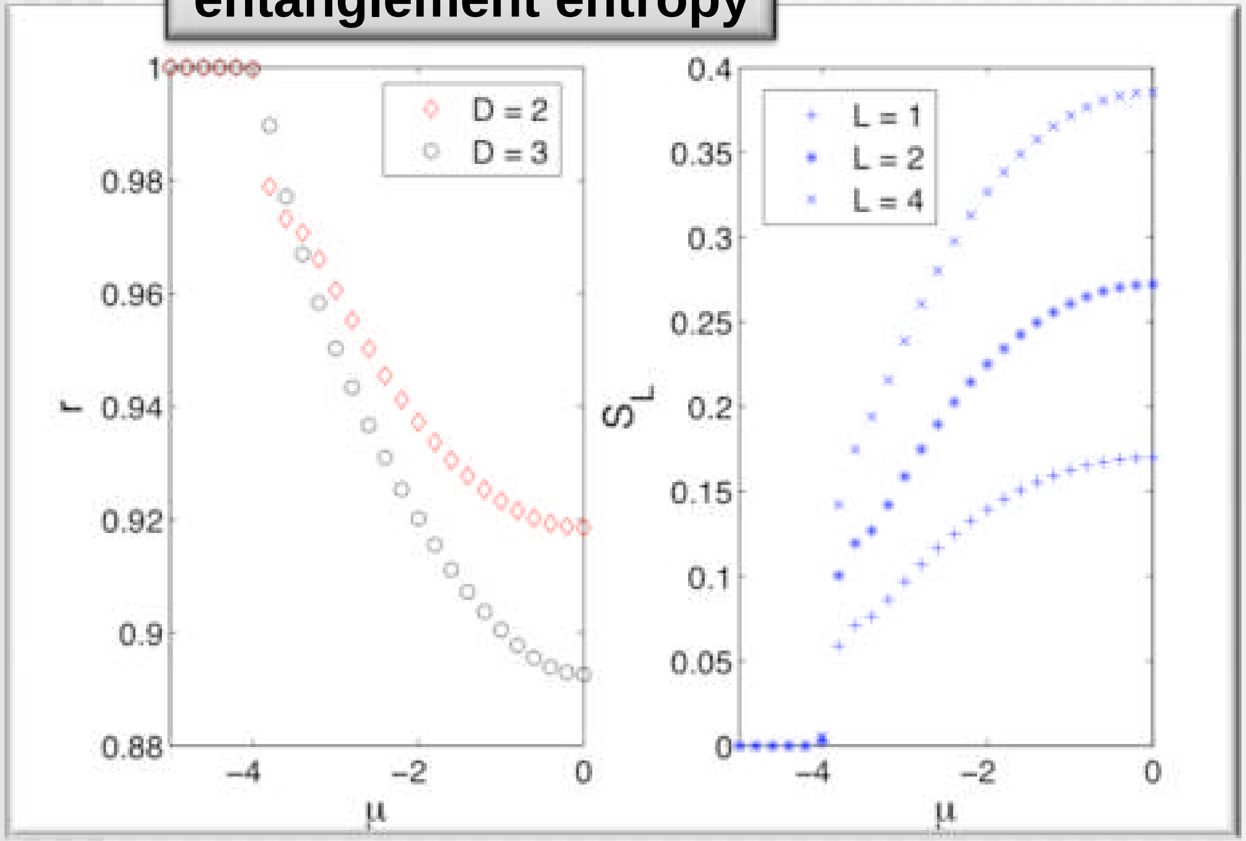
Particle density, energy, and condensate fraction



Good agreement with other techniques

Hard-core Bose-Hubbard model with iPEPS

Bloch vector, and entanglement entropy



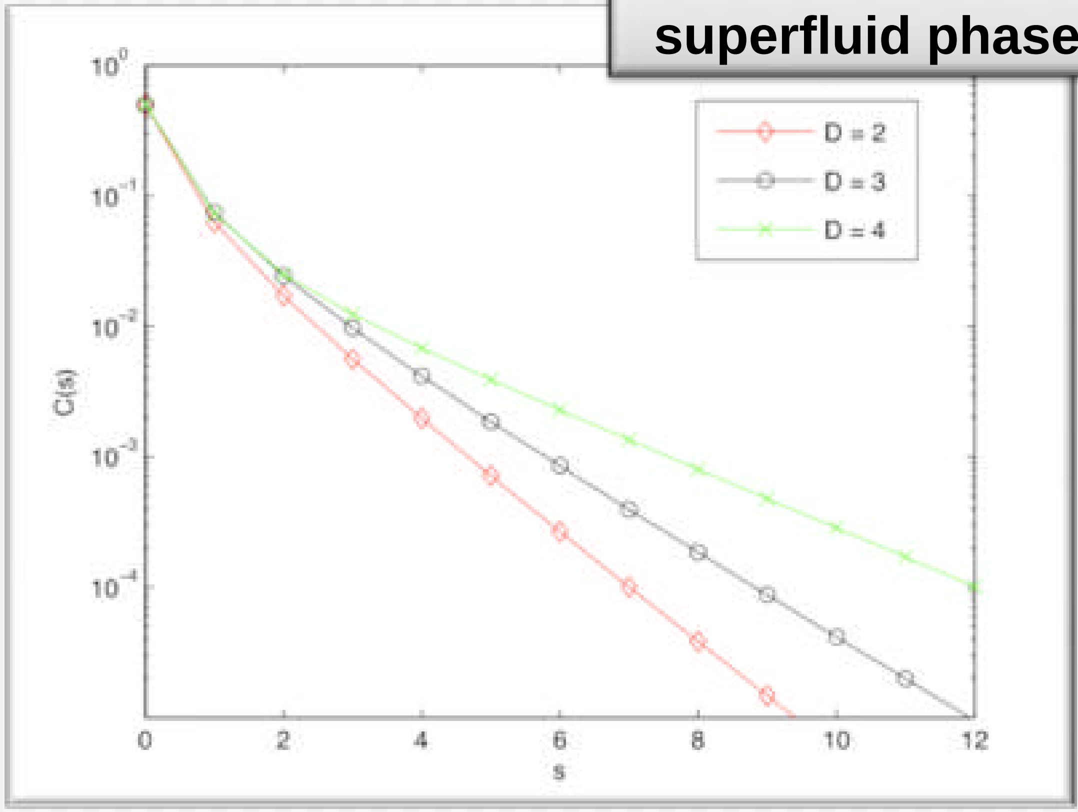
$$\rho_1 = \frac{I + \vec{r} \cdot \vec{\sigma}}{2}$$

$$S_L = -\mathrm{tr}\left(\rho_L \log \rho_L\right)$$

More entanglement deep into the superfluid region

Hard-core Bose-Hubbard model with iPEPS

Correlator in the superfluid phase



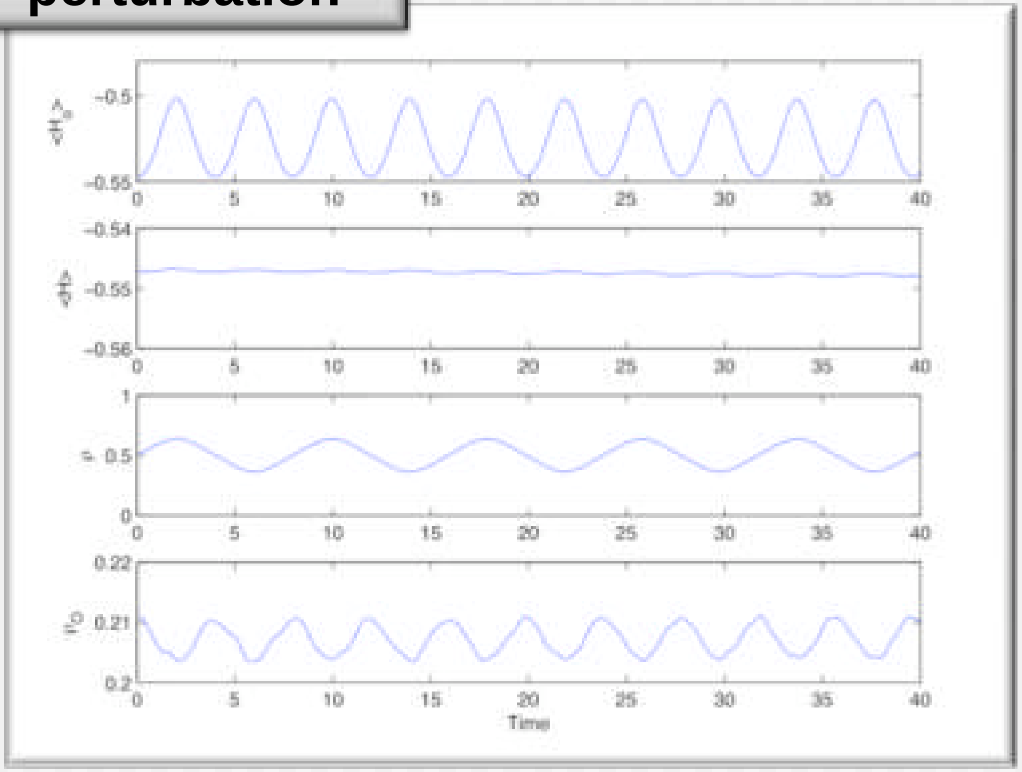
Easy to compute, and shows exponential decay

(slow convergence of non-local properties with D, higher D needed!)

Hard-core Bose-Hubbard model with iPEPS

Time evolution under sudden perturbation

$$H = H_{HC} - i\gamma \sum_k \left(a_k - a_k^+ \right)$$



Non-trivial time evolution of observable quantities

Thank you!