

Title: Simulation of quantum many-body systems with tensor network methods

Date: Oct 08, 2008 04:00 PM

URL: <http://pirsa.org/08100025>

Abstract: In this talk I will give an introduction to the simulation of quantum many-body systems using the so-called tensor networks. After a brief historical review, I will introduce the basics on tensor network representations of quantum states, and will explain some recent developments. In particular, in the last part of my talk I will focus on recent results obtained in the simulation of 2-dimensional quantum lattice systems of infinite size.



THE UNIVERSITY
OF QUEENSLAND
AUSTRALIA

Quantum many-body systems and tensor networks: simulation methods and applications

Román Orús

*School of Physical Sciences,
University of Queensland, Brisbane (Australia)*

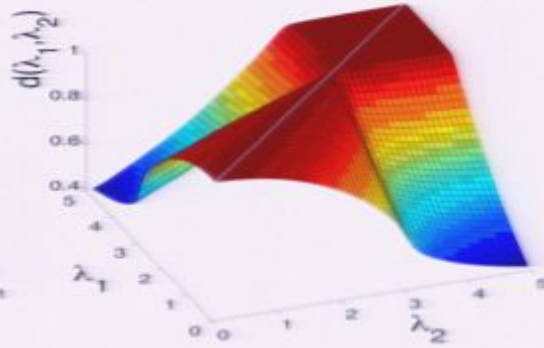
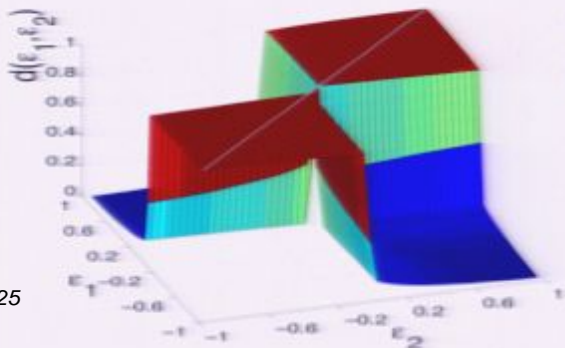
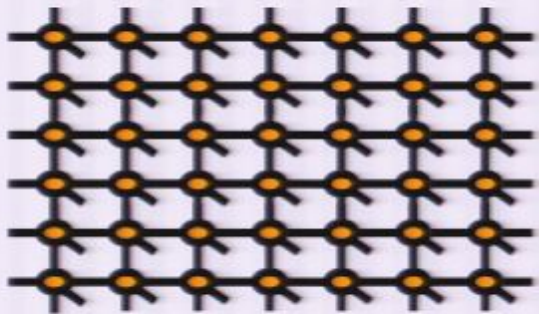


PERIMETER INSTITUTE
FOR THEORETICAL PHYSICS

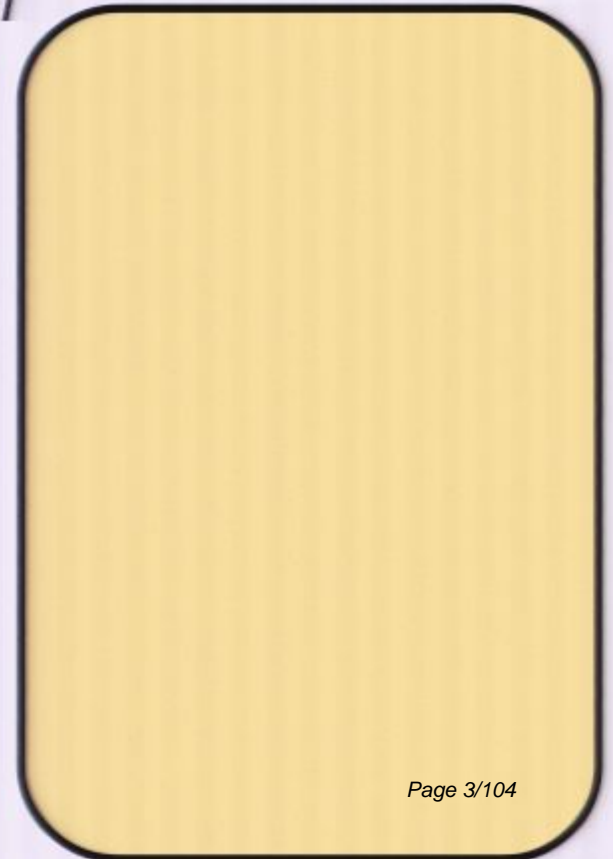
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Explain the background and basics of methods to *simulate quantum many-body systems with tensor networks*, together with some recent results and applications

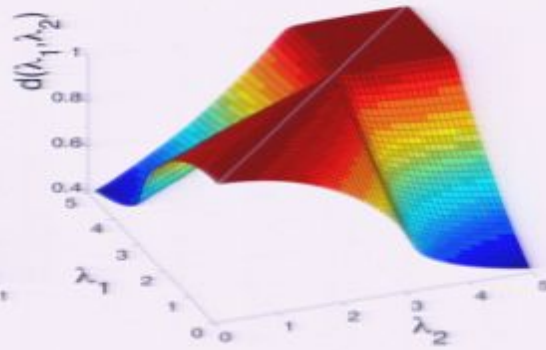
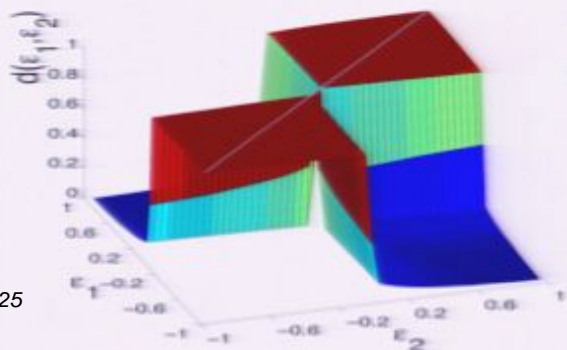
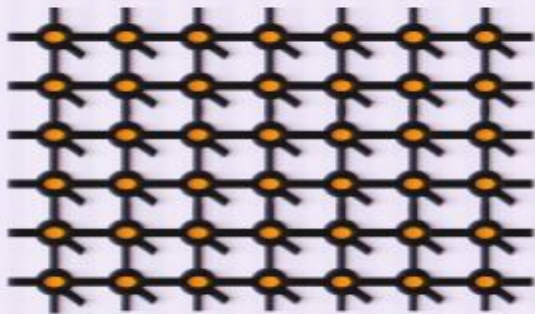


ROADMAP



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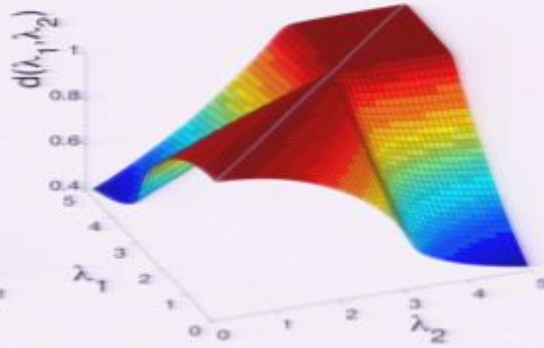
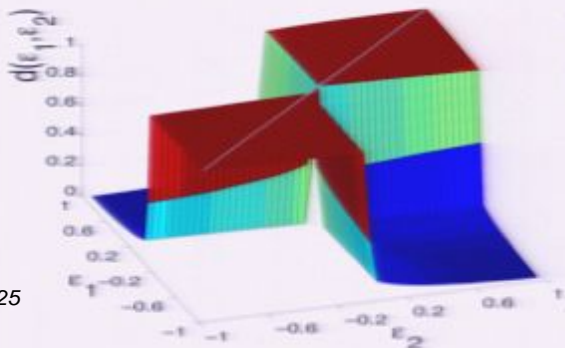
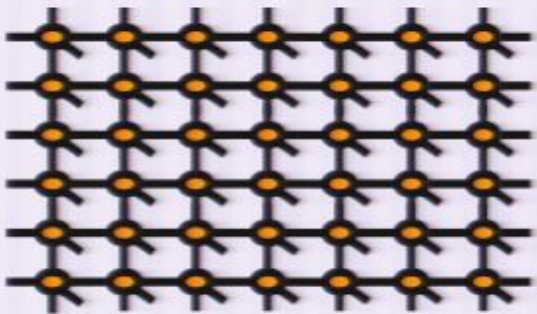


ROADMAP

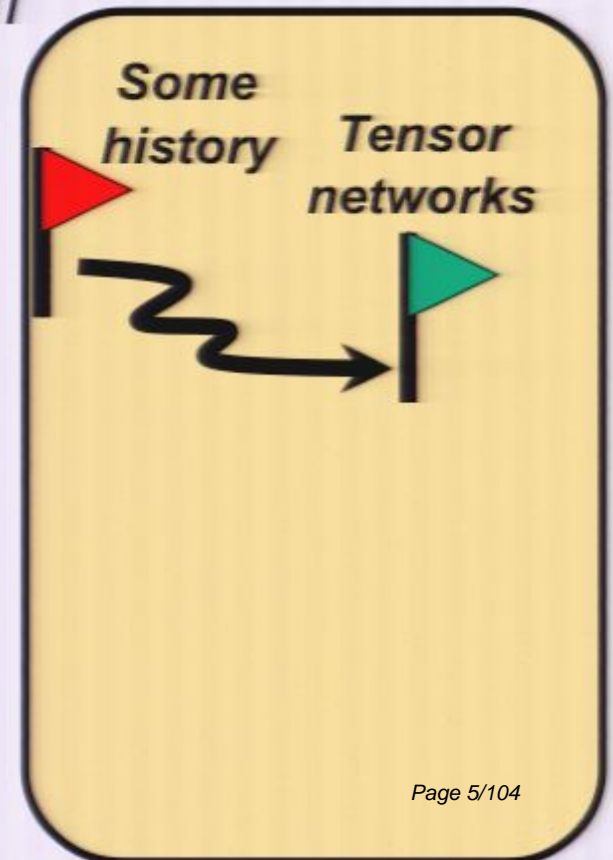
Some history

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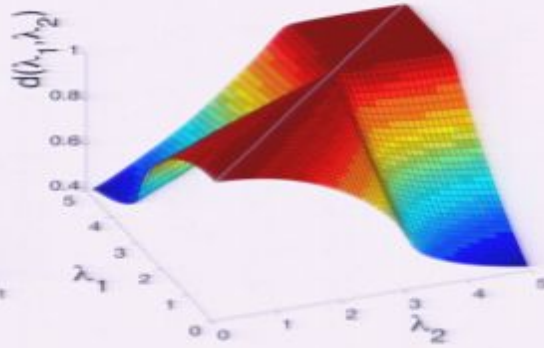
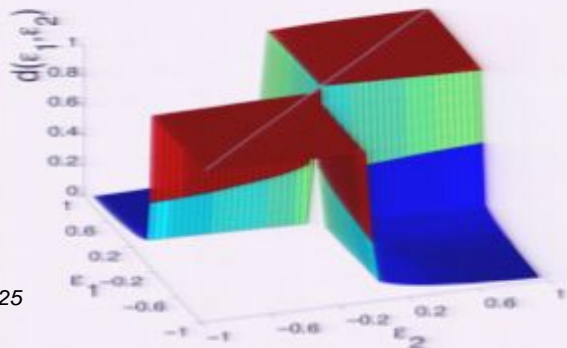
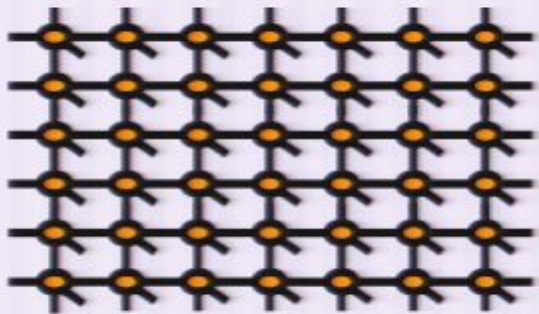


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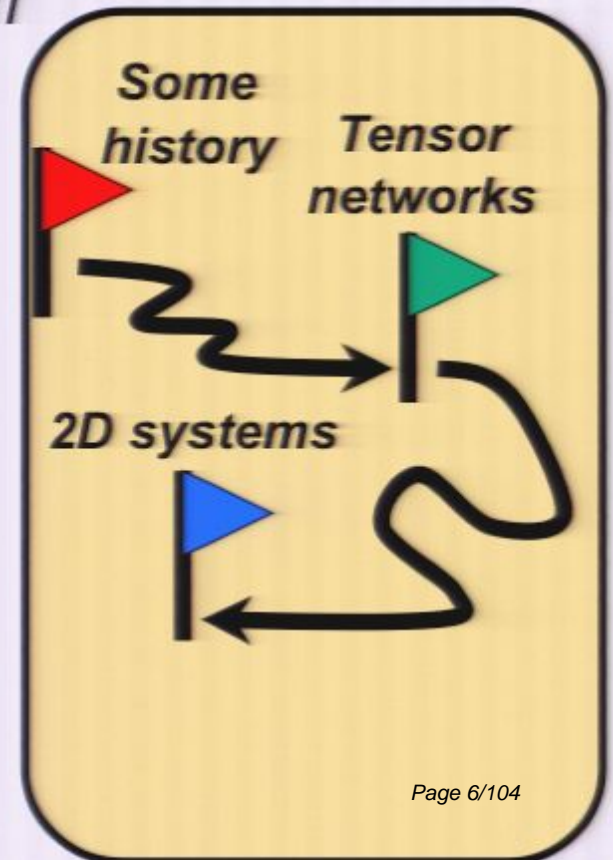


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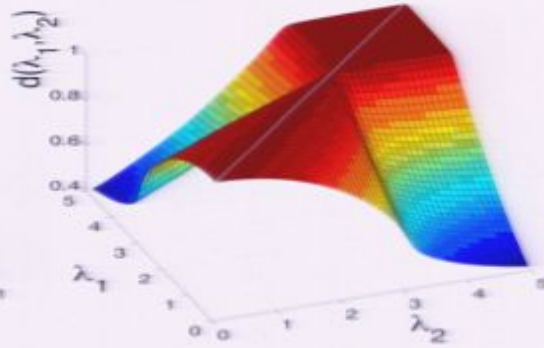
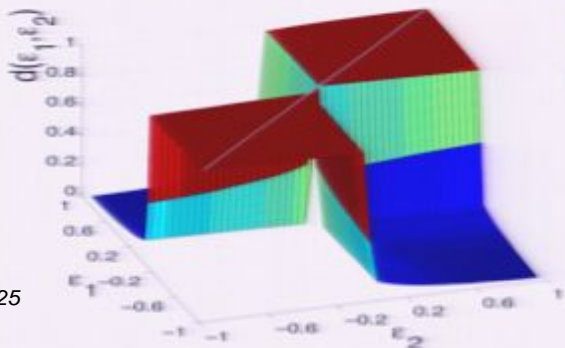
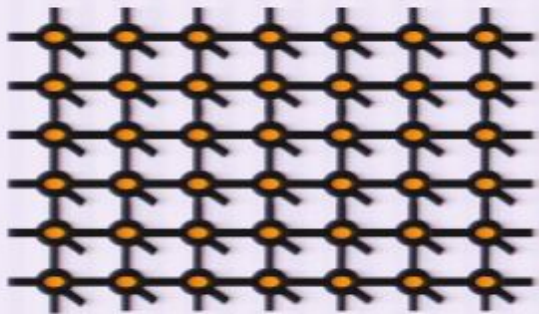


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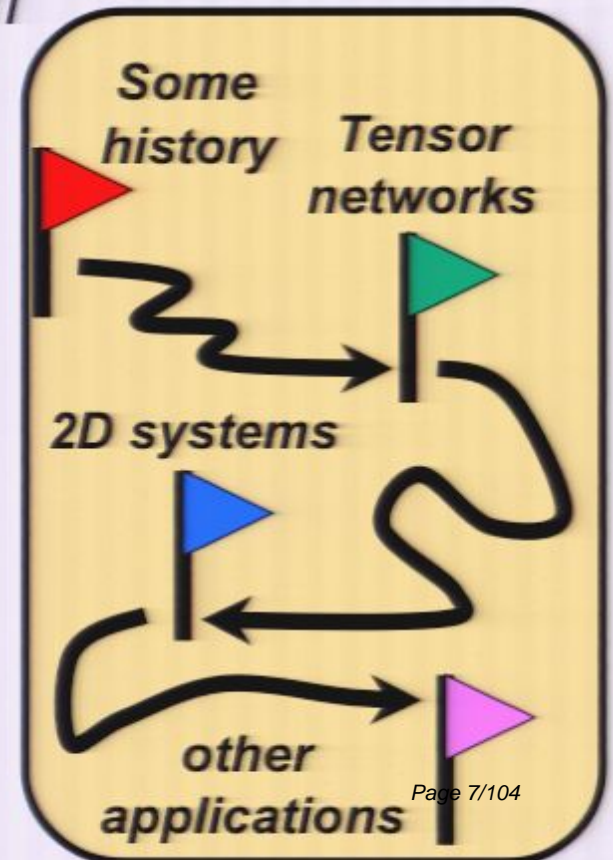


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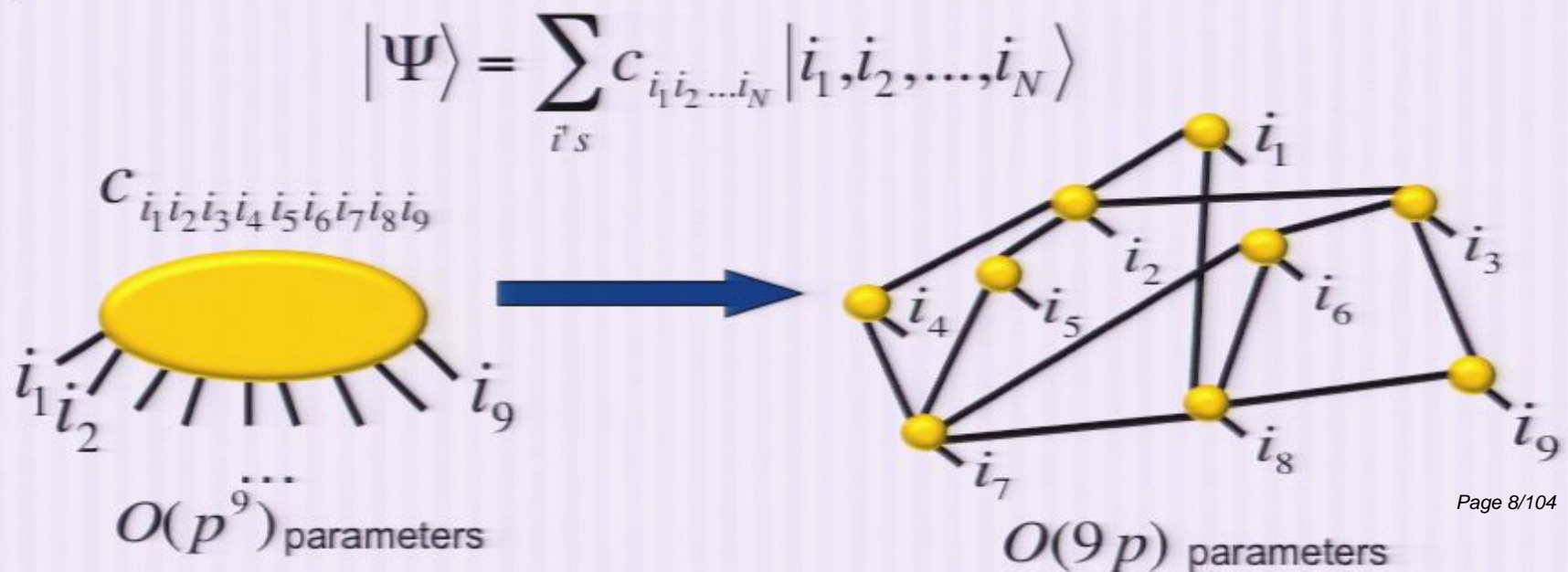


ROADMAP



Main idea

- **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



Outline

- 1.- Brief historical review
- 2.- What are Tensor Networks and why are they useful?
- 3.- Simulation results for 2-dim quantum systems
- 4.- Applications in the study of many-body entanglement

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→ **1.- Brief historical review**

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How it all began...



K. Wilson

Renormalization Group (RG), 1971
(Nobel Prize in 1982)

*Identification of the relevant degrees of freedom
of a physical system at long distances*

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Identification of the relevant degrees of freedom of a physical system at long distances



About 20 years later...



S. R. White

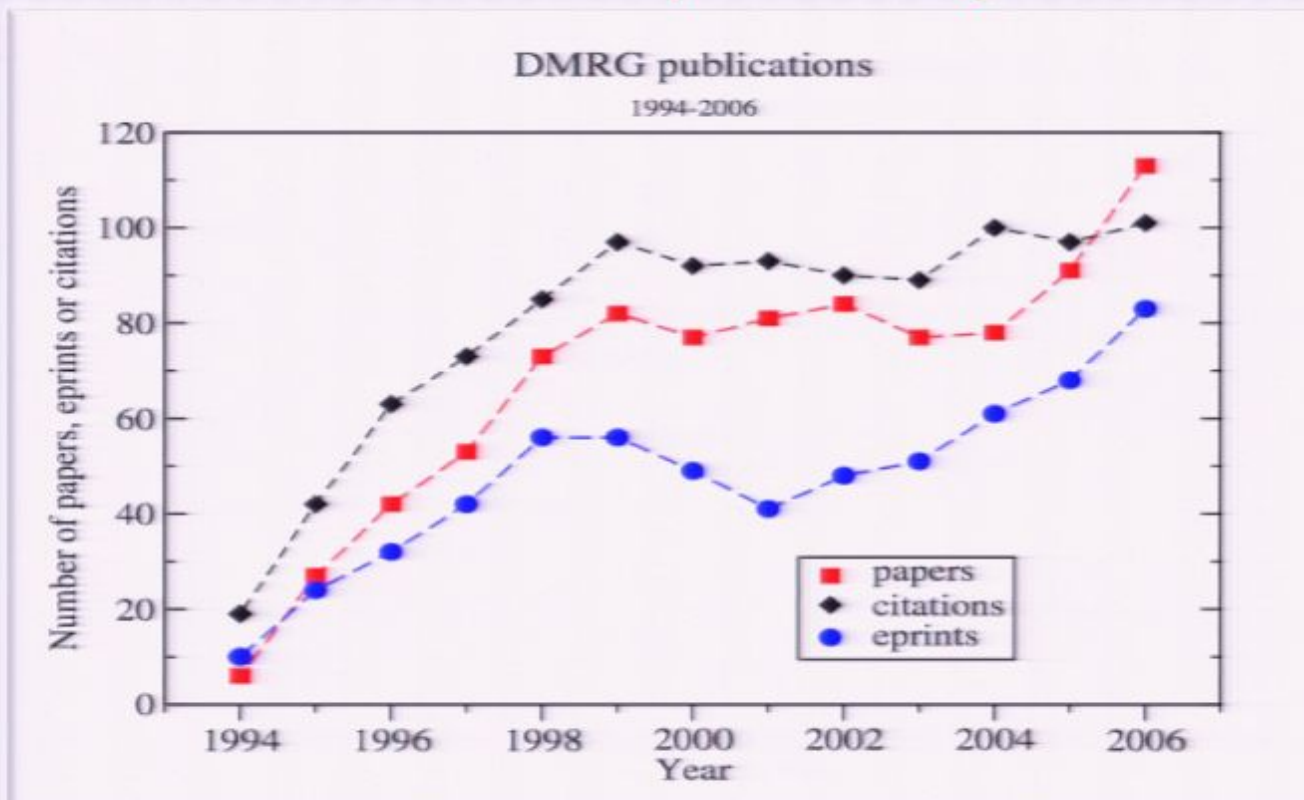
Density Matrix Renormalization Group (DMRG), 1992

Impact of DMRG


- DMRG is a numerical method to compute the low-energy properties of quantum systems, and has been the method of reference to simulate **1-dim quantum systems for the last 15 years.**

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Generalization to **Matrix Product States (MPS)**



- 1995 S. Ostlund,
S. Rommer



Connection between DMRG and Matrix Product States

Deep connection to quantum information theory

- 2003 G. Vidal

VOLUME 91, NUMBER 14

PHYSICAL REVIEW LETTERS

week ending
3 OCTOBER 2003

Efficient Classical Simulation of Slightly Entangled Quantum Computations

Guifré Vidal

Institute for Quantum Information, California Institute of Technology, Pasadena, California 91125, USA
(Received 25 February 2003; published 1 October 2003)

We present a classical protocol to efficiently simulate any pure-state quantum computation that involves only a restricted amount of entanglement. More generally, we show how to classically simulate pure-state quantum computations on n qubits by using computational resources that grow linearly in n and exponentially in the amount of entanglement in the quantum computer. Our results imply that a necessary condition for an exponential computational speedup (with respect to classical computations) is that the amount of entanglement increases with the size n of the computation, and provide an explicit lower bound on the required growth.

DOI: 10.1103/PhysRevLett.91.147902

PACS numbers: 03.67.Lx, 03.65.Ud, 03.67.Hk, 03.67.Mn

Classical simulation of quantum computations which involve a small amount of entanglement

Deep connection to quantum information theory

- 2003 G. Vidal →

Connection between MPS and
quantum computing

Deep connection to quantum information theory

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Time evolution of 1-dim systems with
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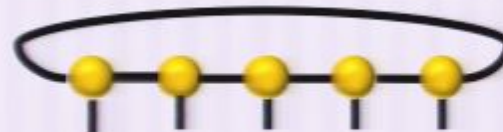
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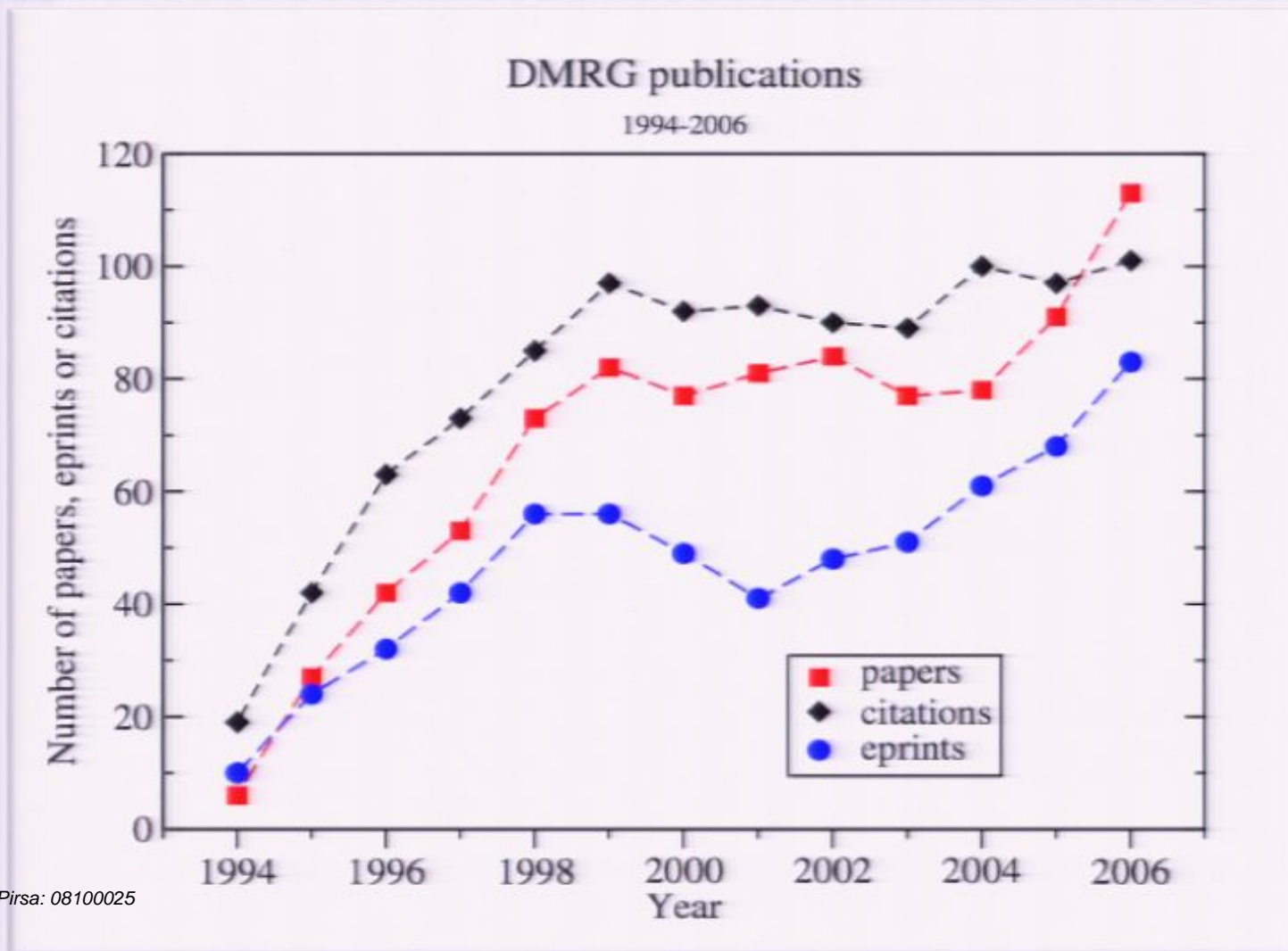


- 2004 F. Verstraete,
D. Porras,
J. I. Cirac →

Periodic boundary conditions



Deep connection to quantum information theory



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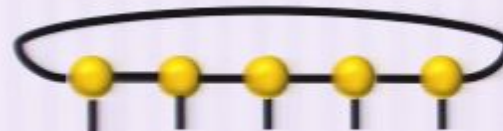
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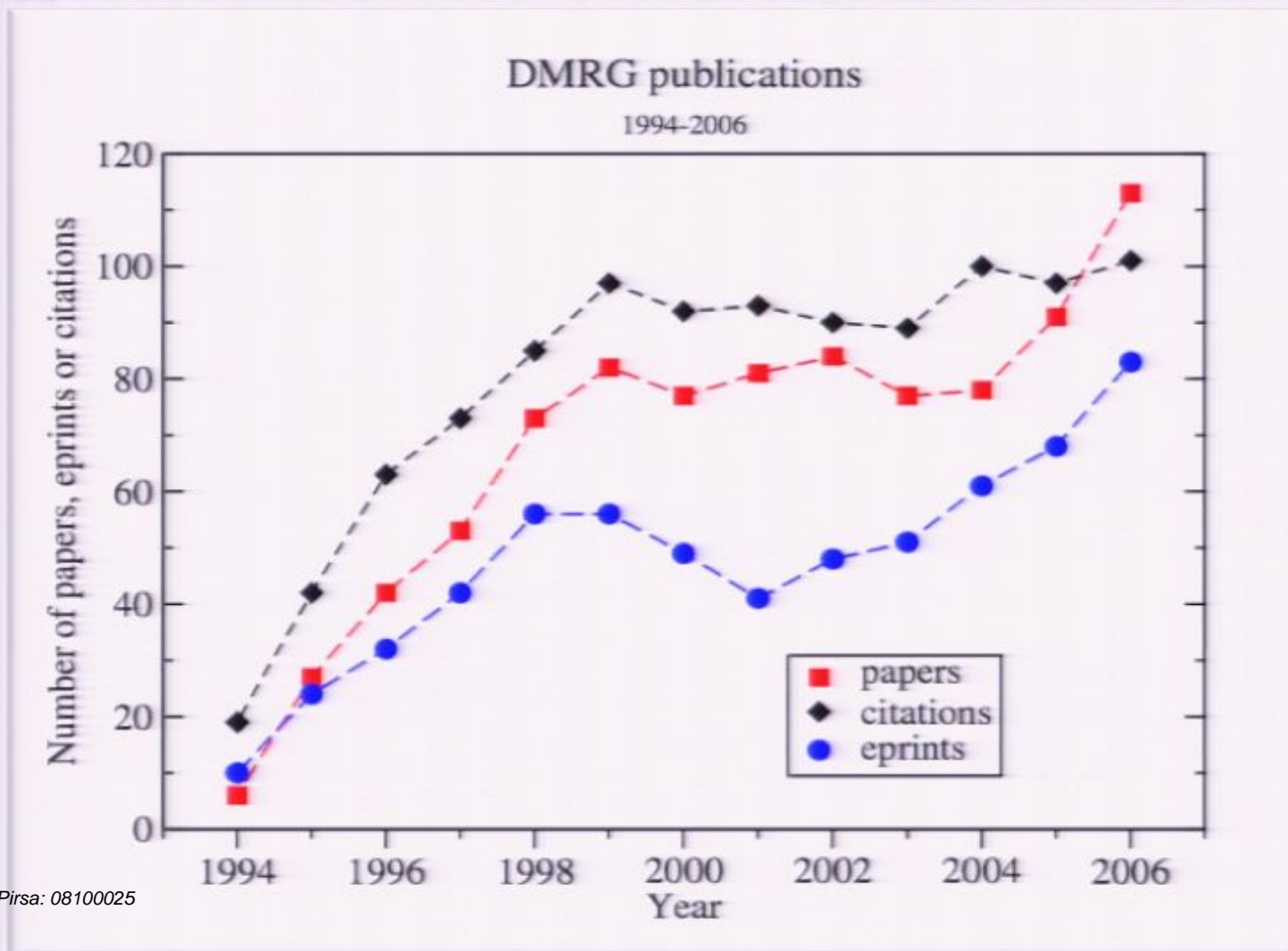


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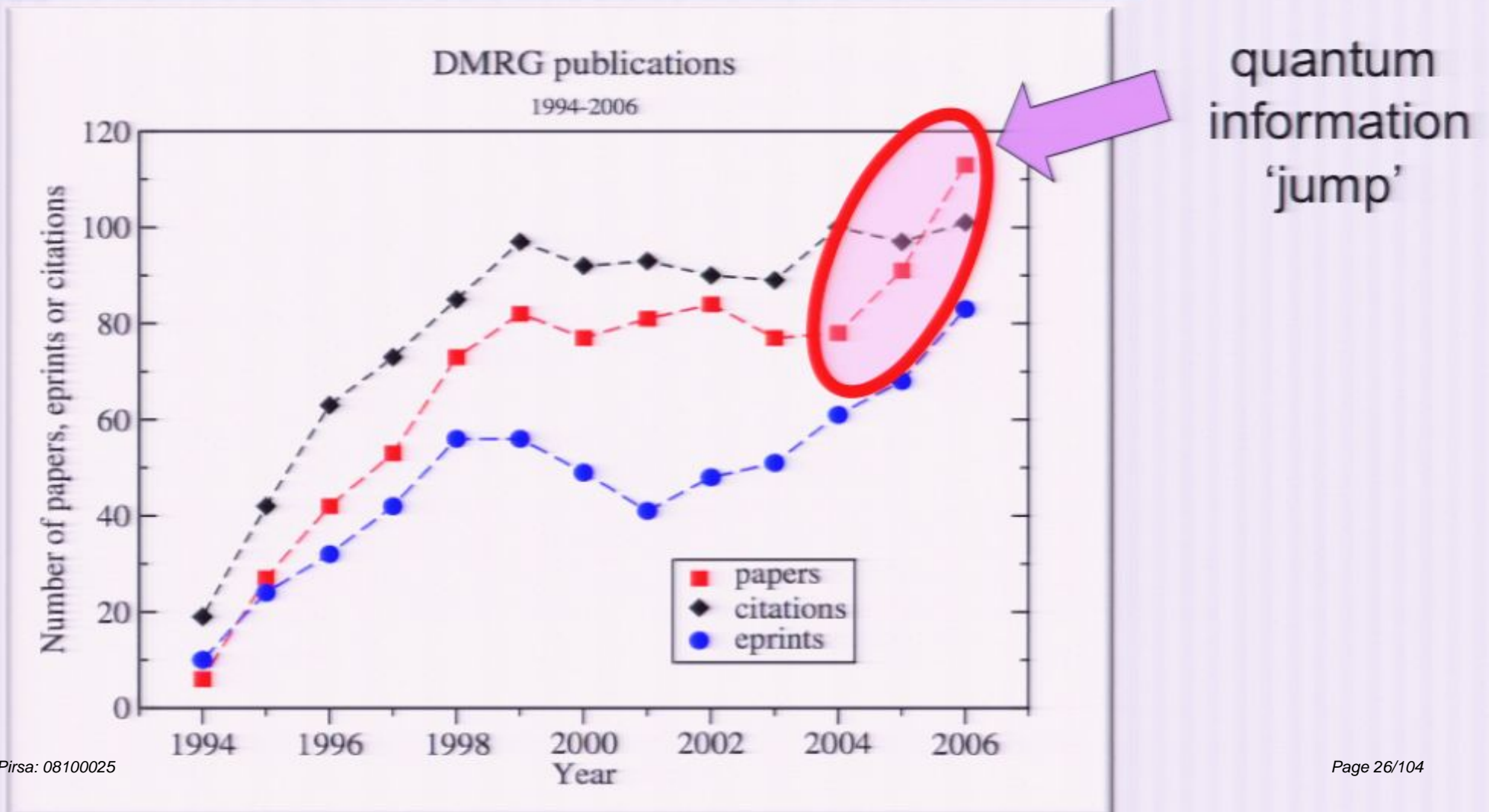
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
Deep connection to quantum information theory



Deep connection to quantum information theory



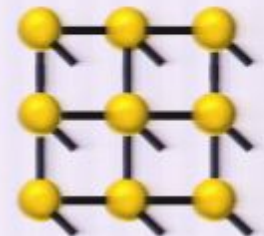
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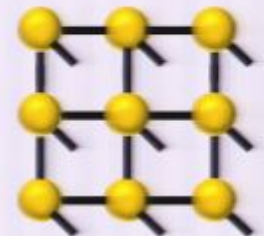
- 2004 F. Verstraete, J. I. Cirac → **Method of Projected Entangled Pair States (PEPS)** for d-dim systems



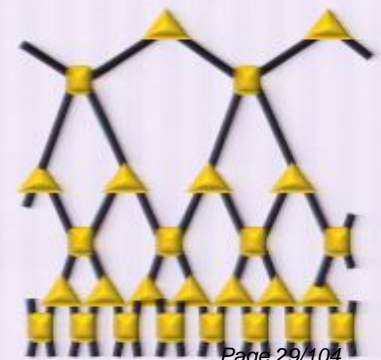
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- 2005 G. Vidal → **Multiscale Entanglement Renormalization Ansatz (MERA)**, for scale-invariant systems



Summary of history

- 1-dim

MPS



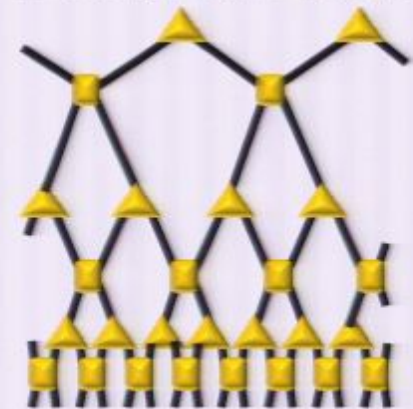
1992 & 2003

MPS PBC



2004

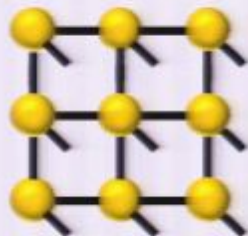
1-dim MERA



2005

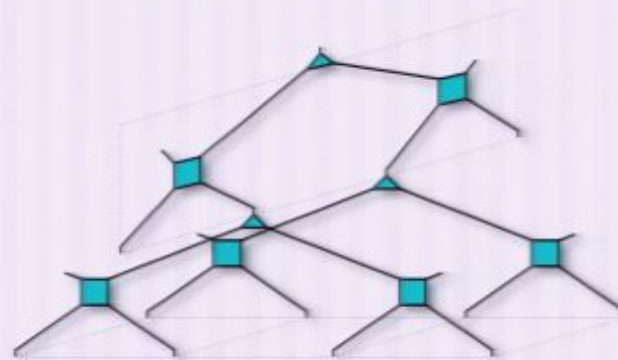
- d-dim

TPS / PEPS



2000 & 2004

d-dim MERA



2005

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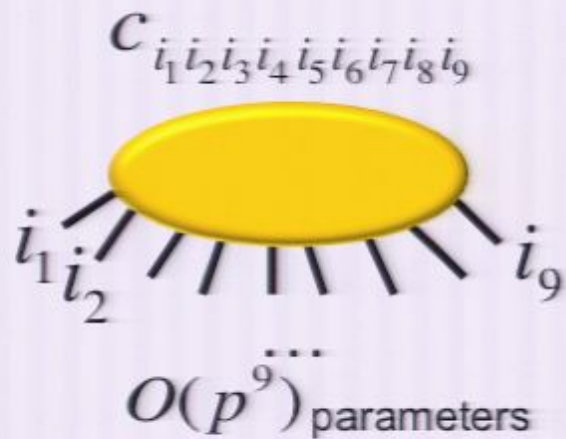
4.- Applications in the study of many-body entanglement

Tensor Networks (TN)

$$|\Psi\rangle = \sum_{i_s} c_{i_1 i_2 \dots i_N} |i_1, i_2, \dots, i_N\rangle \in (\mathbf{C}^p)^{\otimes N} \quad p^N \text{ complex parameters}$$

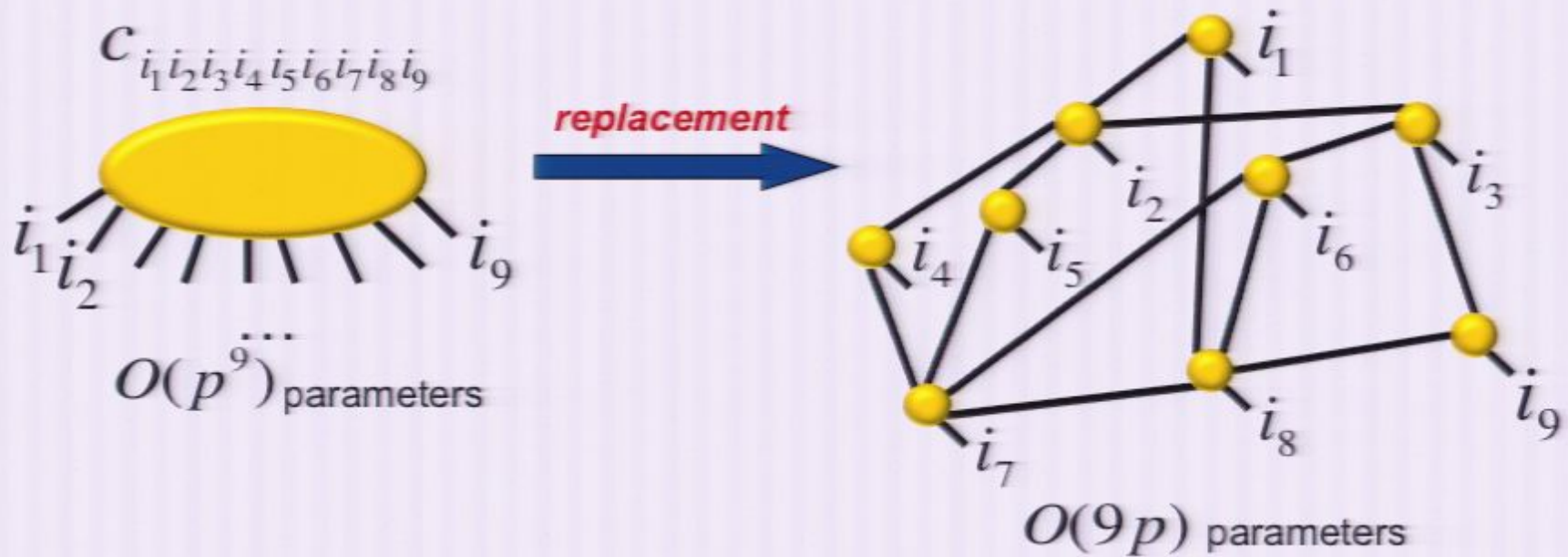
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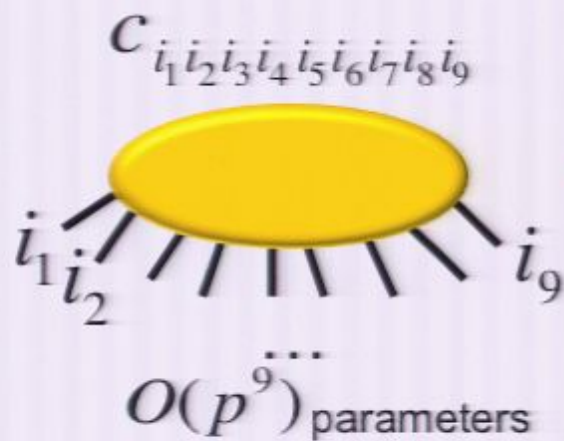
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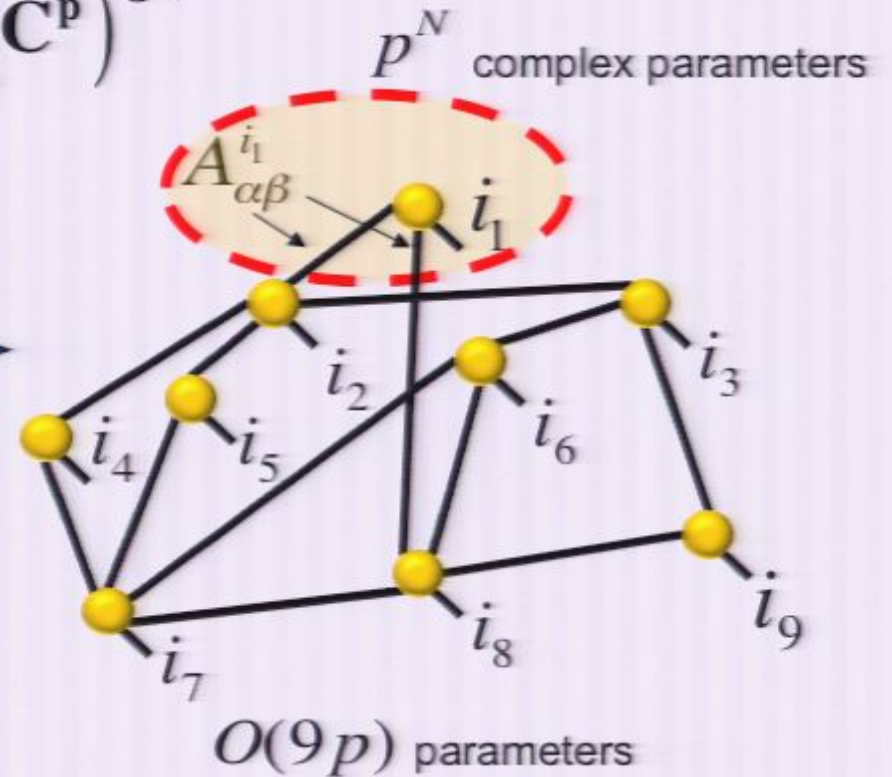


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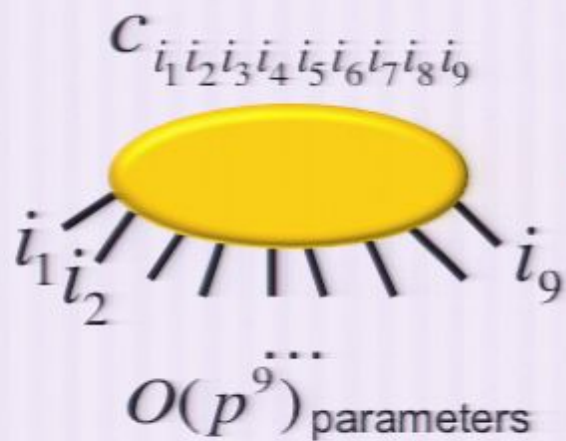


replacement 

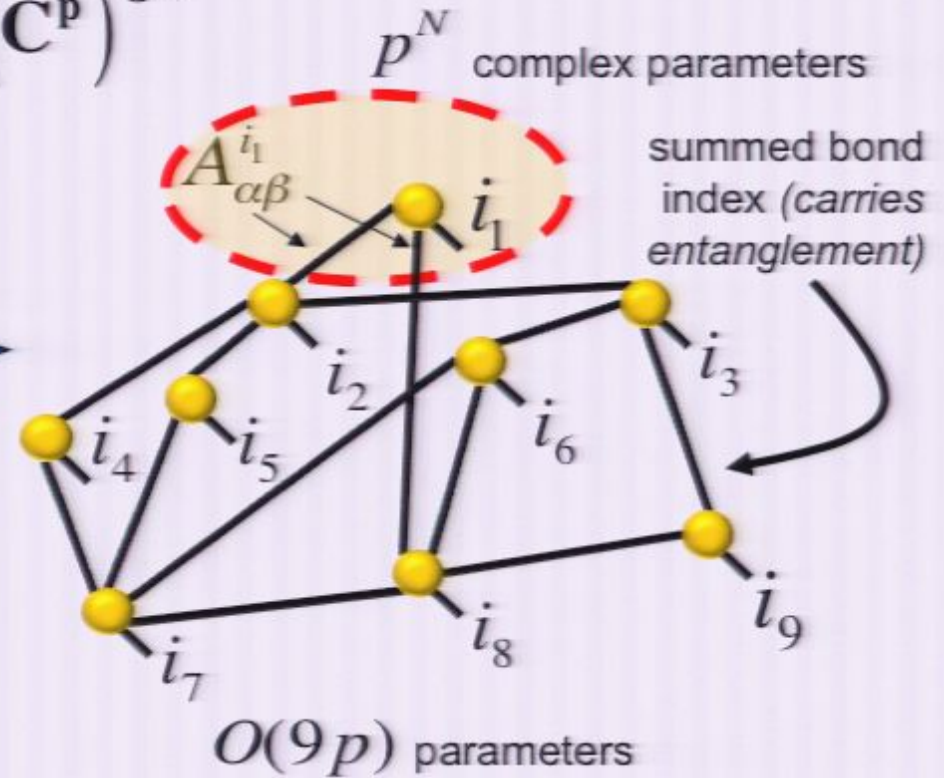


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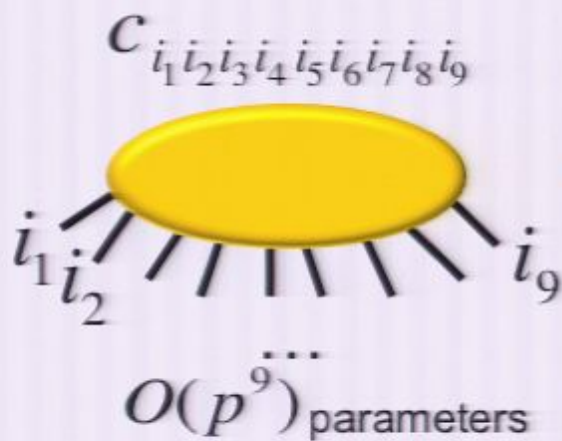


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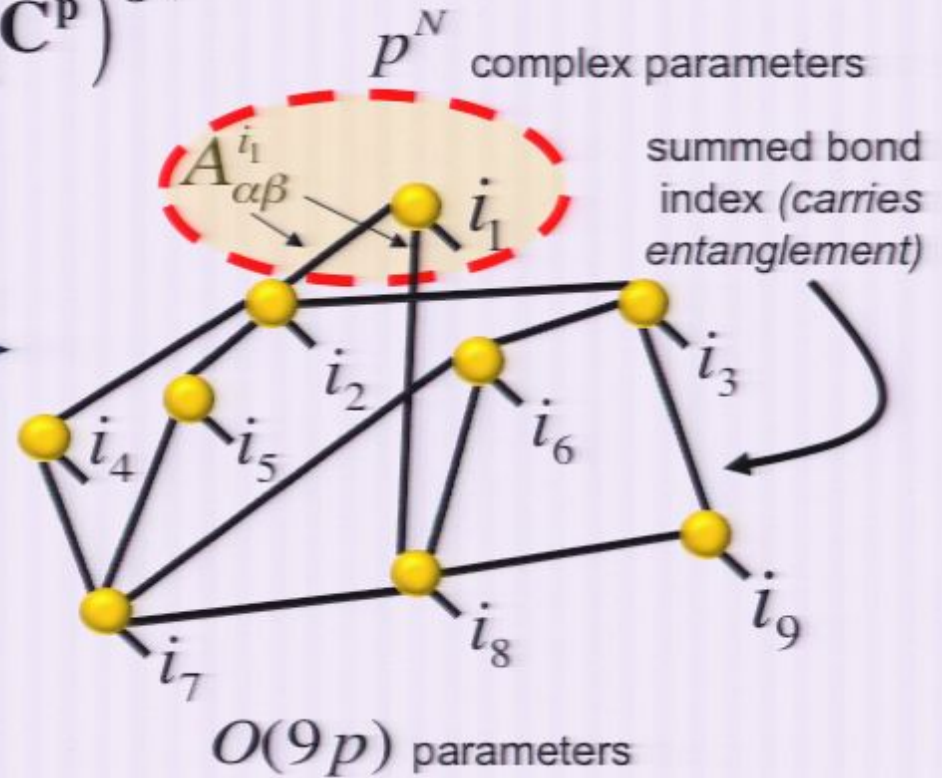


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replacement →



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)*

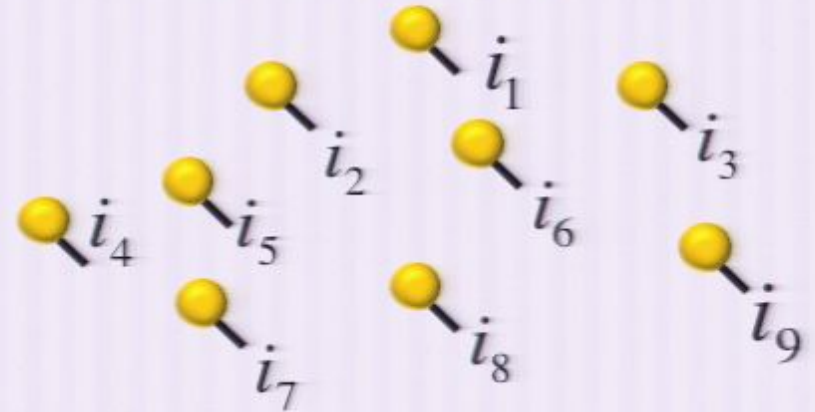
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Product state



*Efficiency OK
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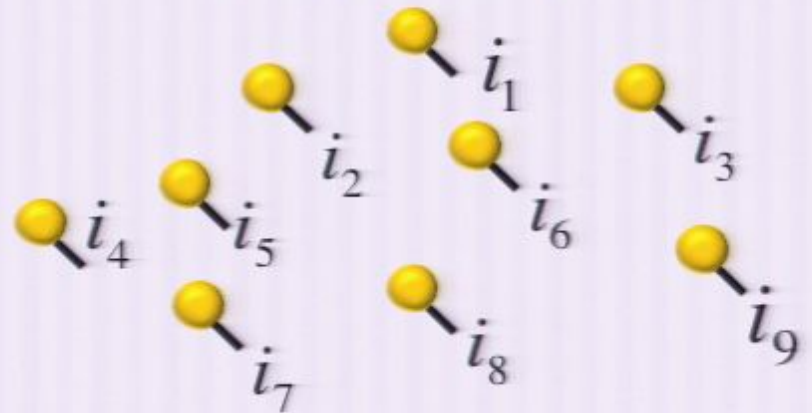
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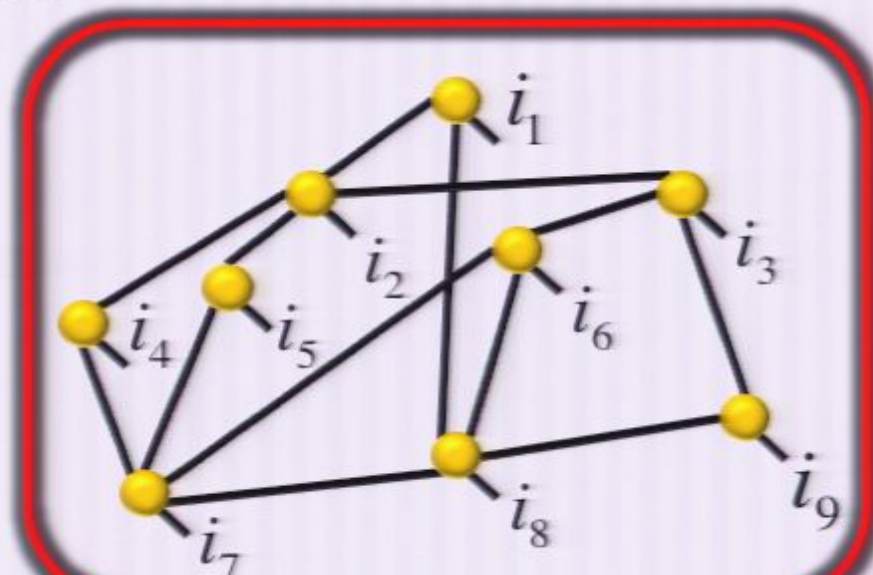
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Tensor network



Efficient and correlated

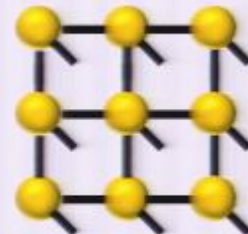
Examples of TN

Matrix Product States (MPS)



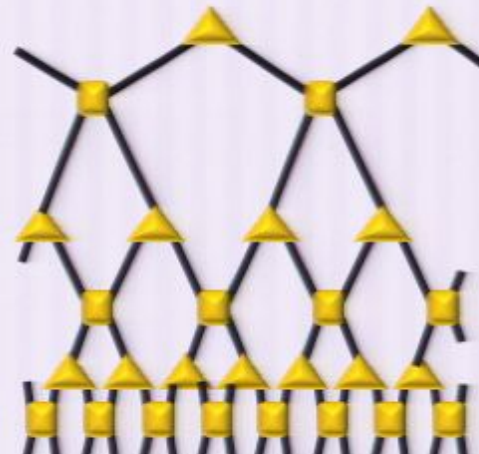
1-dim systems

Projected Entangled Pair States (PEPS)



*d-dim systems,
 $d > 1$*

Multiscale Entanglement Renormalization Ansatz (MERA)



Scale-invariant systems

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)

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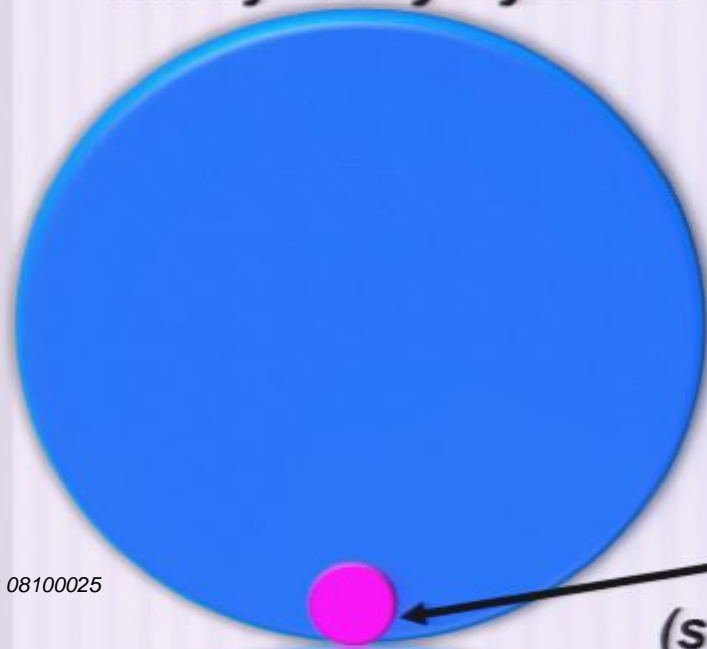
Hilbert space of a many-body system



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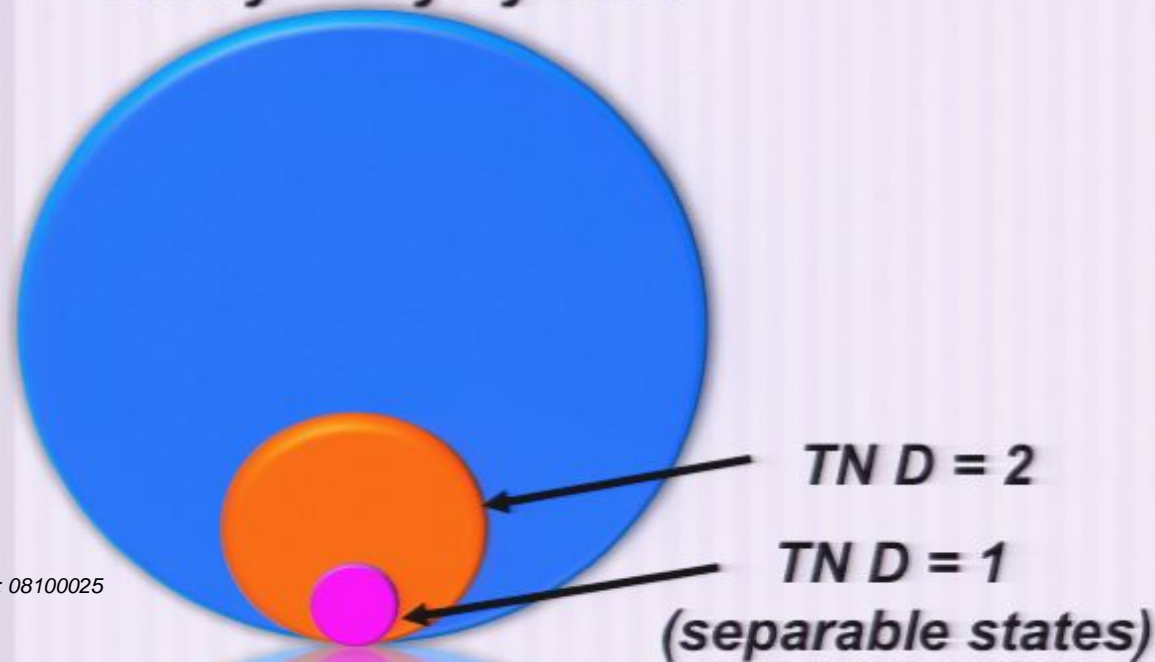


$TN D = 1$
(separable states)

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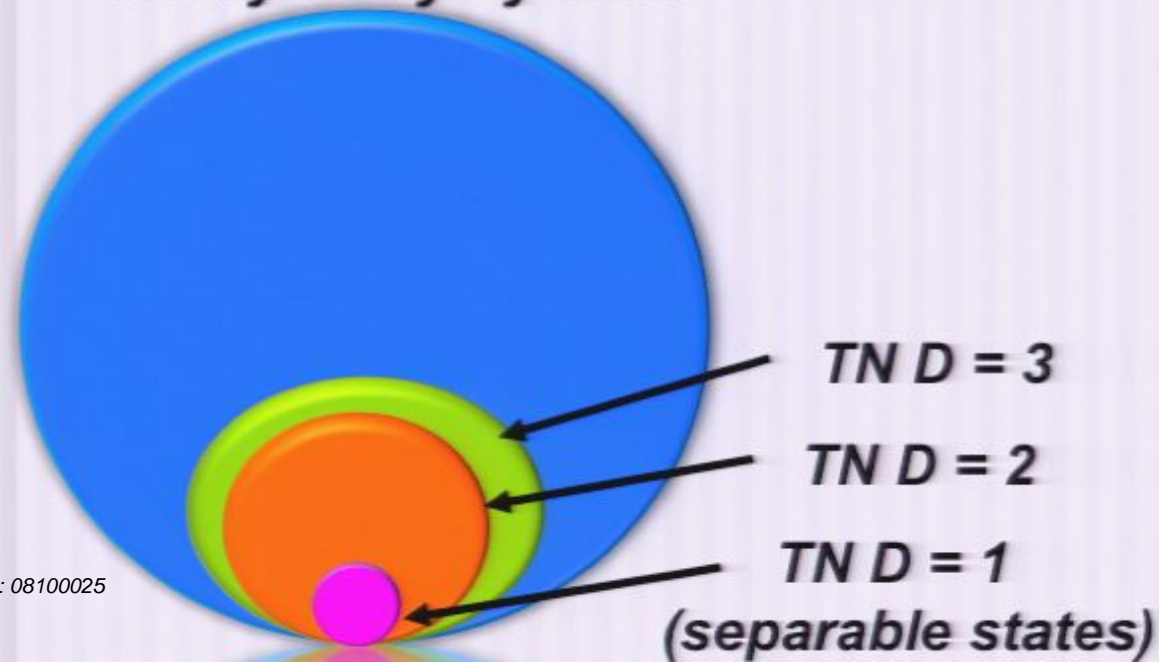
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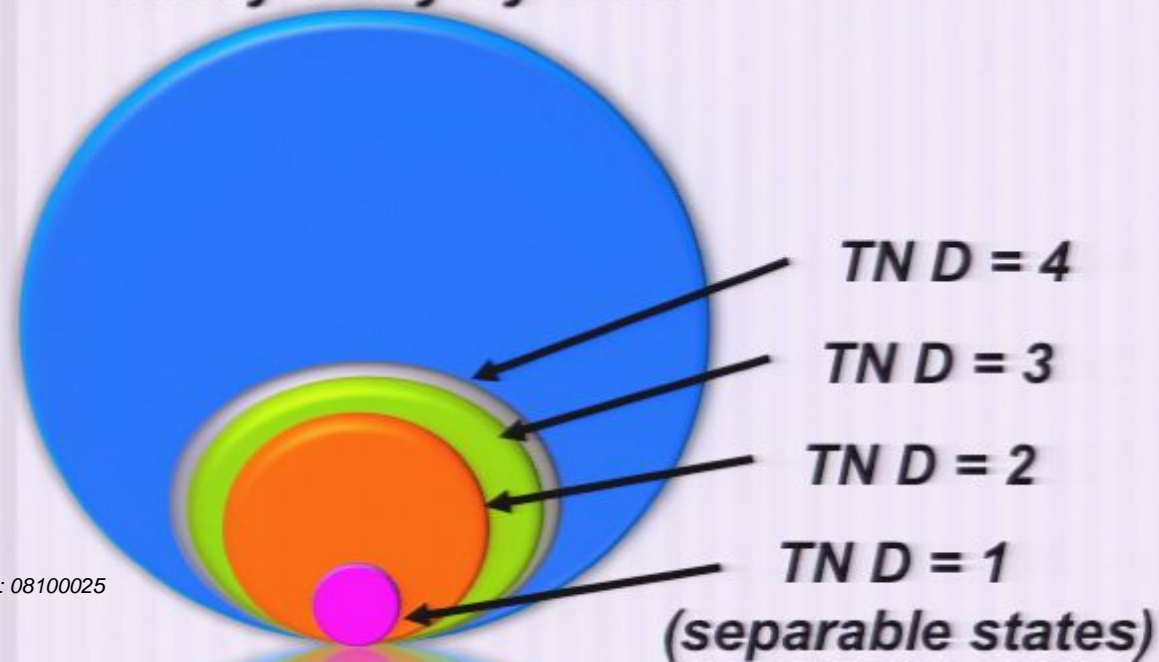
Hilbert space of a many-body system



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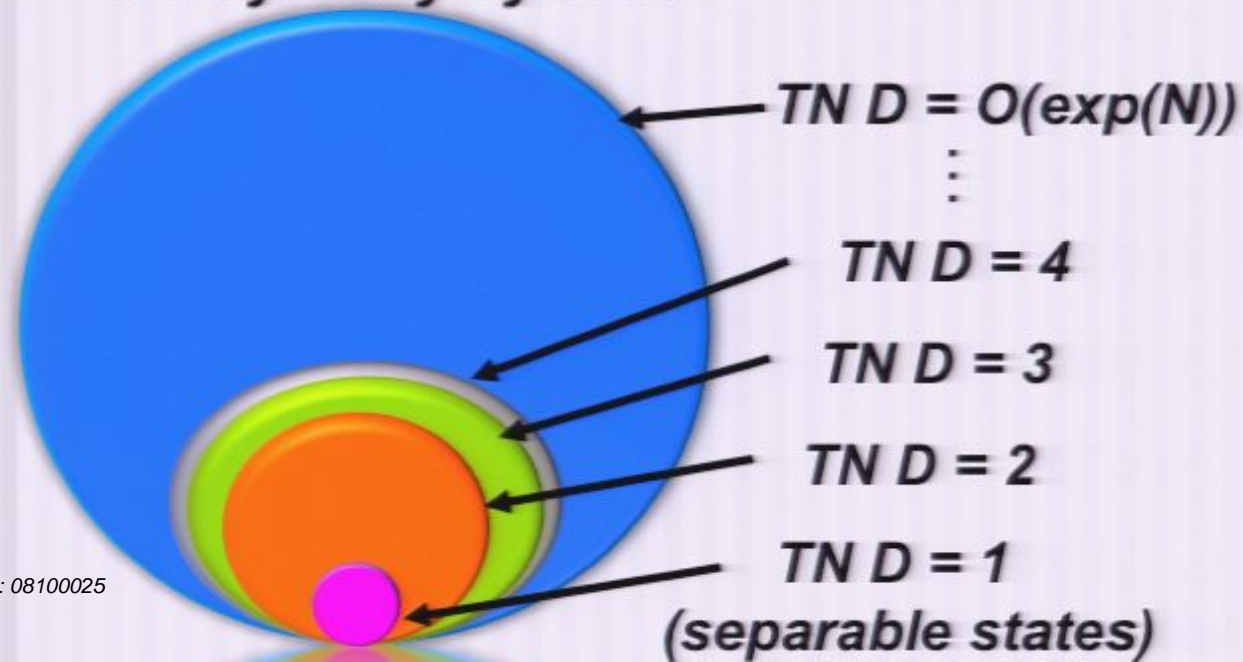
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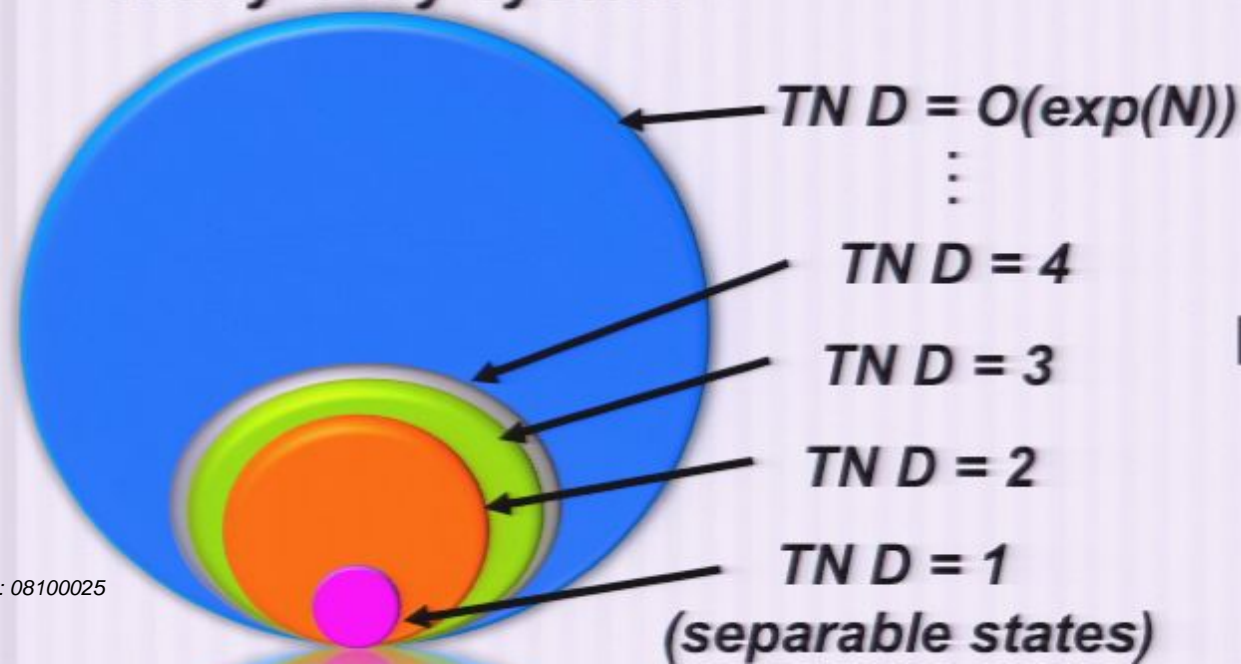
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Tensor Network Algorithms

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

Hilbert space of a many-body system



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?

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- Evaluation of ***expectation values*** $\langle \Psi | O | \Psi \rangle$ (order parameters, correlators...) - exact in 1-dim, approximate in d-dim $d > 1$ (NP-Hard) -

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dynamics

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ground states

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ground states

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

$$\min_{|\Psi\rangle \in PEPS} \langle \Psi | H | \Psi \rangle$$

ground states

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

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- Efficient **updating** after an operation, e.g.

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

dynamics *ground states*

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

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

ground states

- Allow to deal with **infinite lattices (thermodynamic limit)** for translationally invariant systems

Why Tensor Networks?

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ground states

- Allow to deal with **infinite lattices (thermodynamic limit)** for translationally invariant systems
- **Fastest simulation algorithms.** E.g., 1 month of quantum Monte Carlo in a supercomputer vs 1 day of TN in a desktop PC

Outline



1.- Brief historical review



2.- What are Tensor Networks and why are they useful?

3.- Simulation results for 2-dim quantum systems

4.- Applications in the study of many-body entanglement

Outline



1.- Brief historical review



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Infinite 2-dim quantum systems (iPEPS algorithm)

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

*J. Jordan, R. Orús, G. Vidal, F. Verstraete, J.I. Cirac,
cond-mat/0703788*



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INPUT: 2-dim lattice
Hamiltonian

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

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INPUT: 2-dim lattice Hamiltonian imaginary-time evolution

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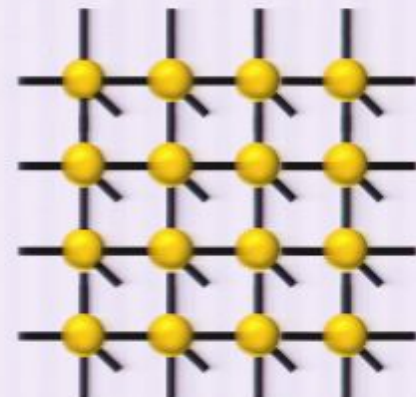
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imaginary-time
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iPEPS for the
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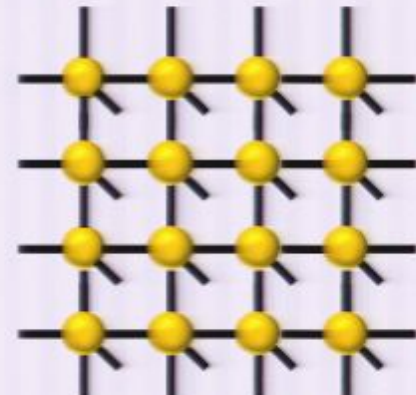
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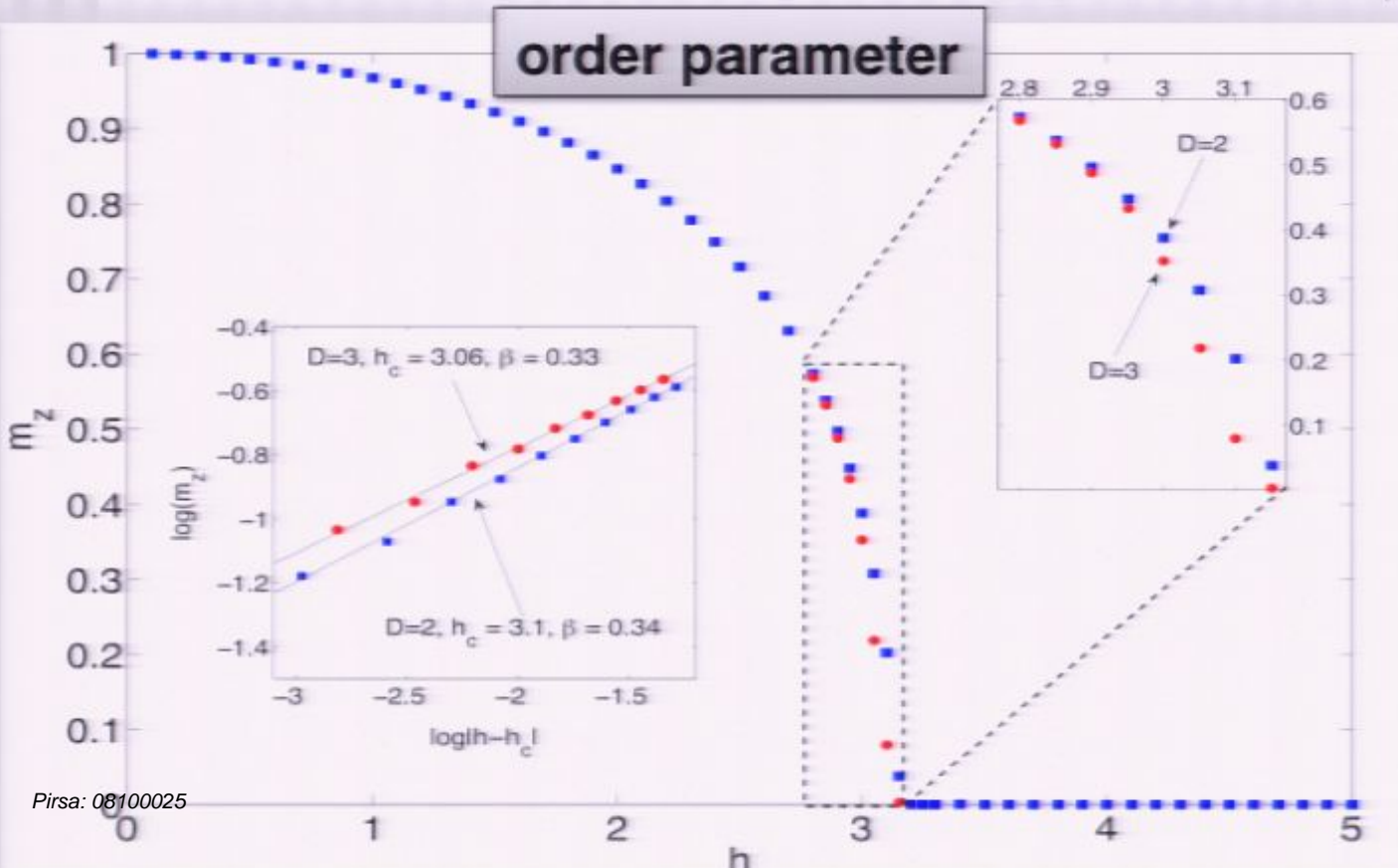
OUTPUT: expectation values

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

iPEPS: results

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

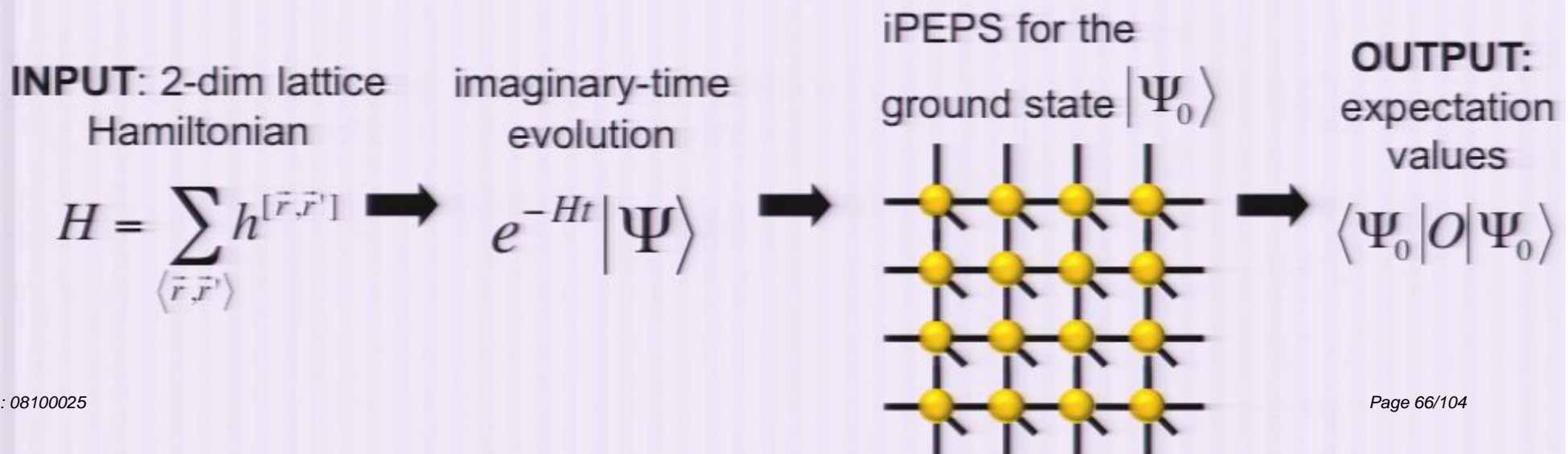
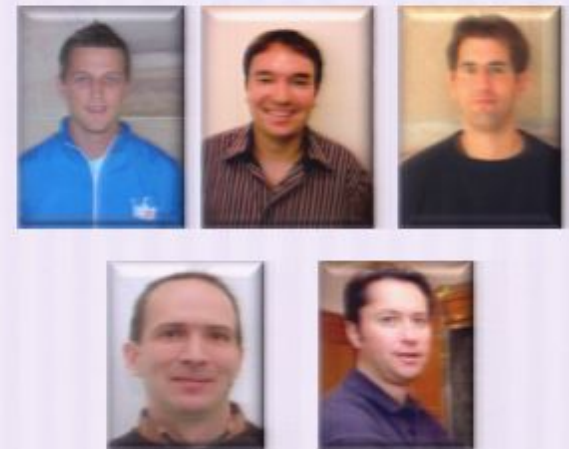
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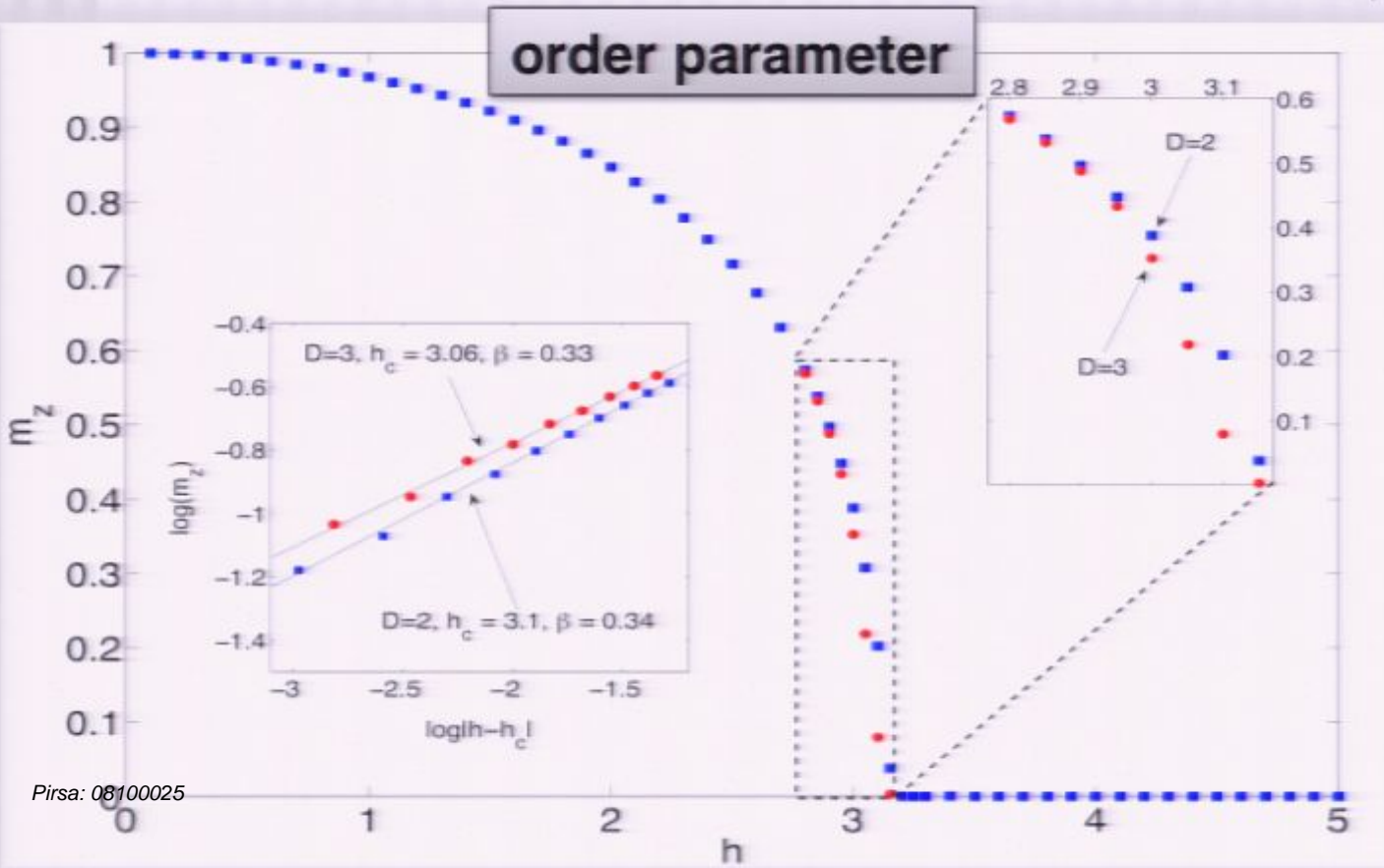
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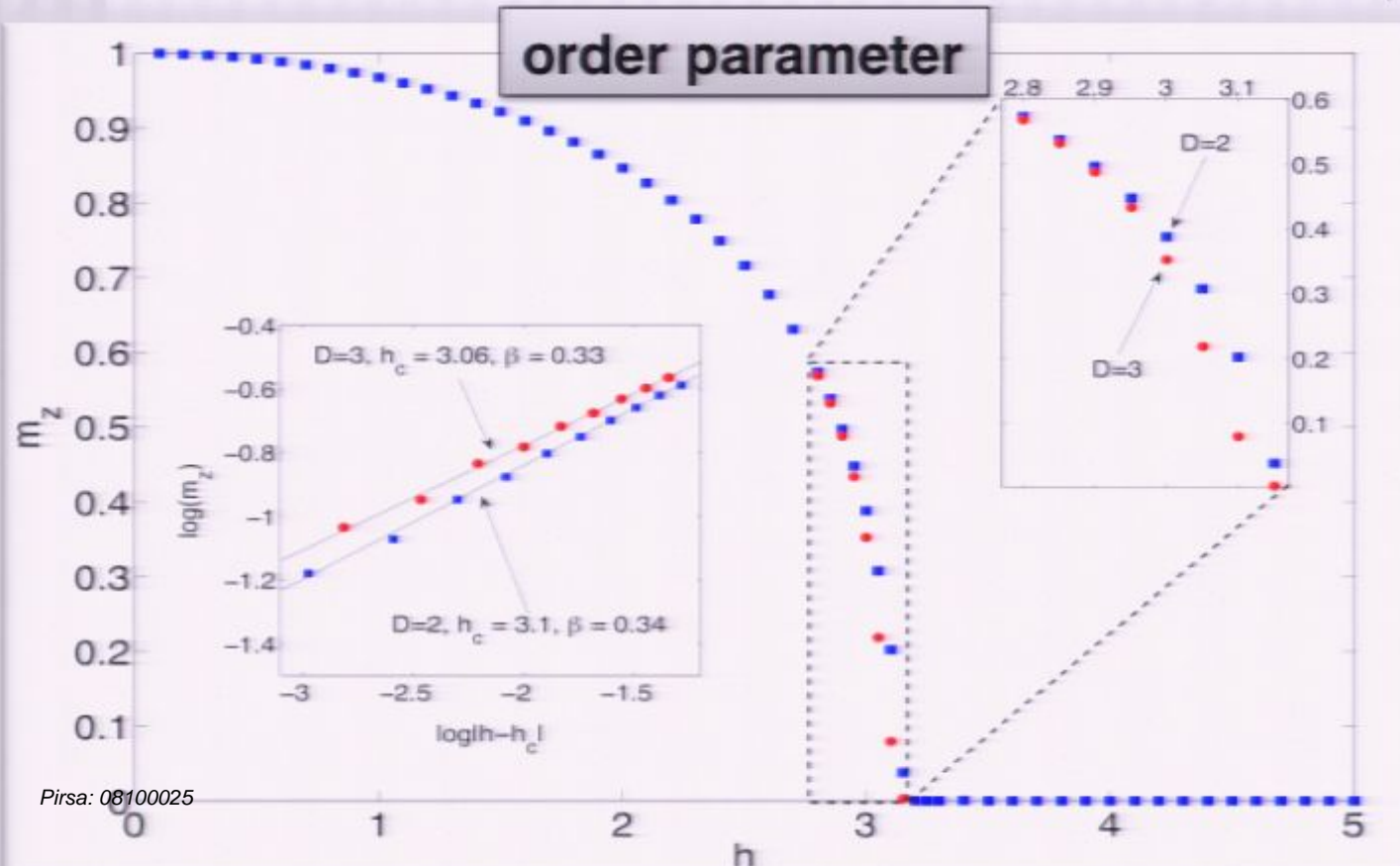
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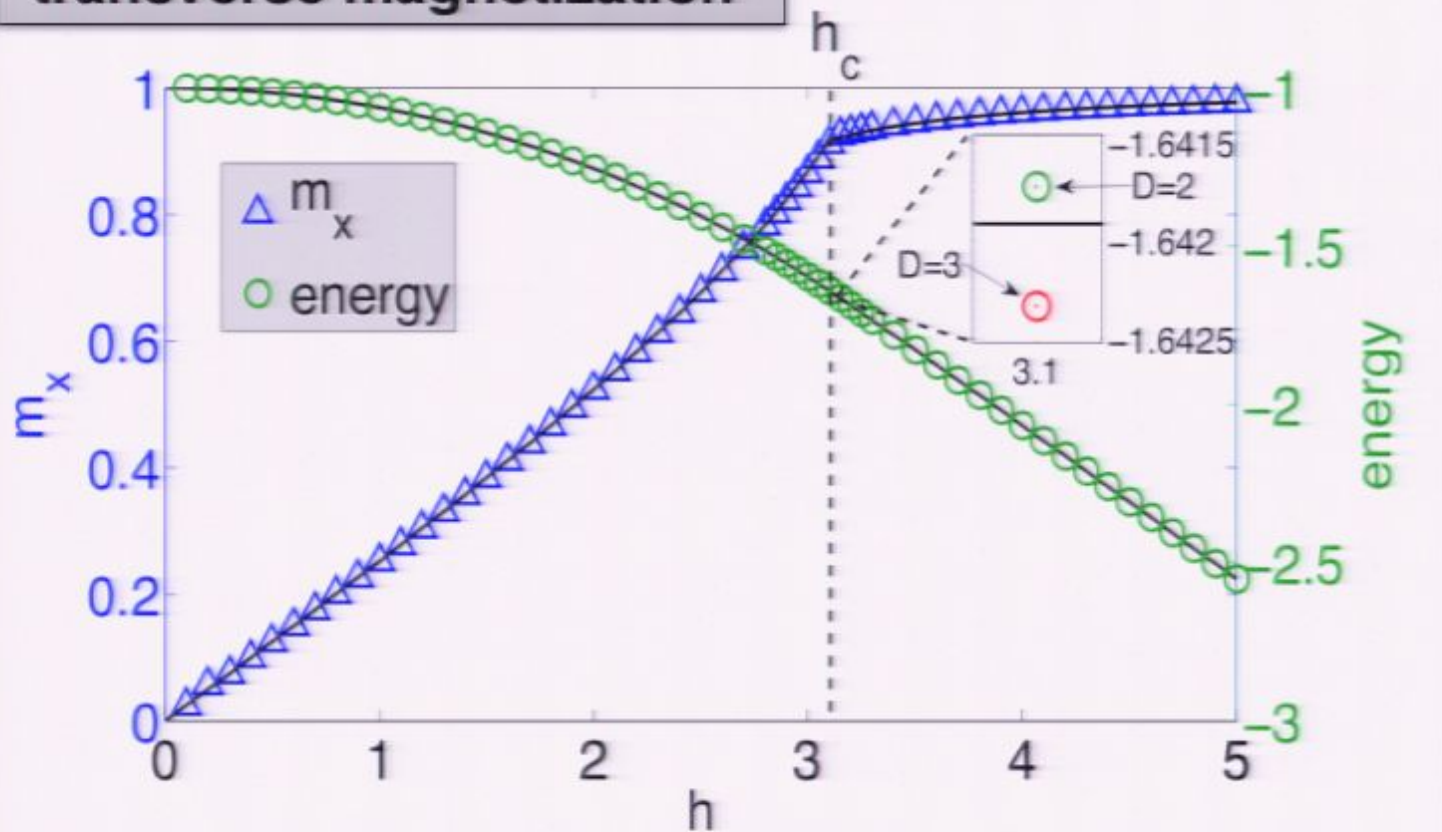
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The critical point and the critical exponents match those from the best Quantum Monte Carlo simulation with less than 1% of relative error

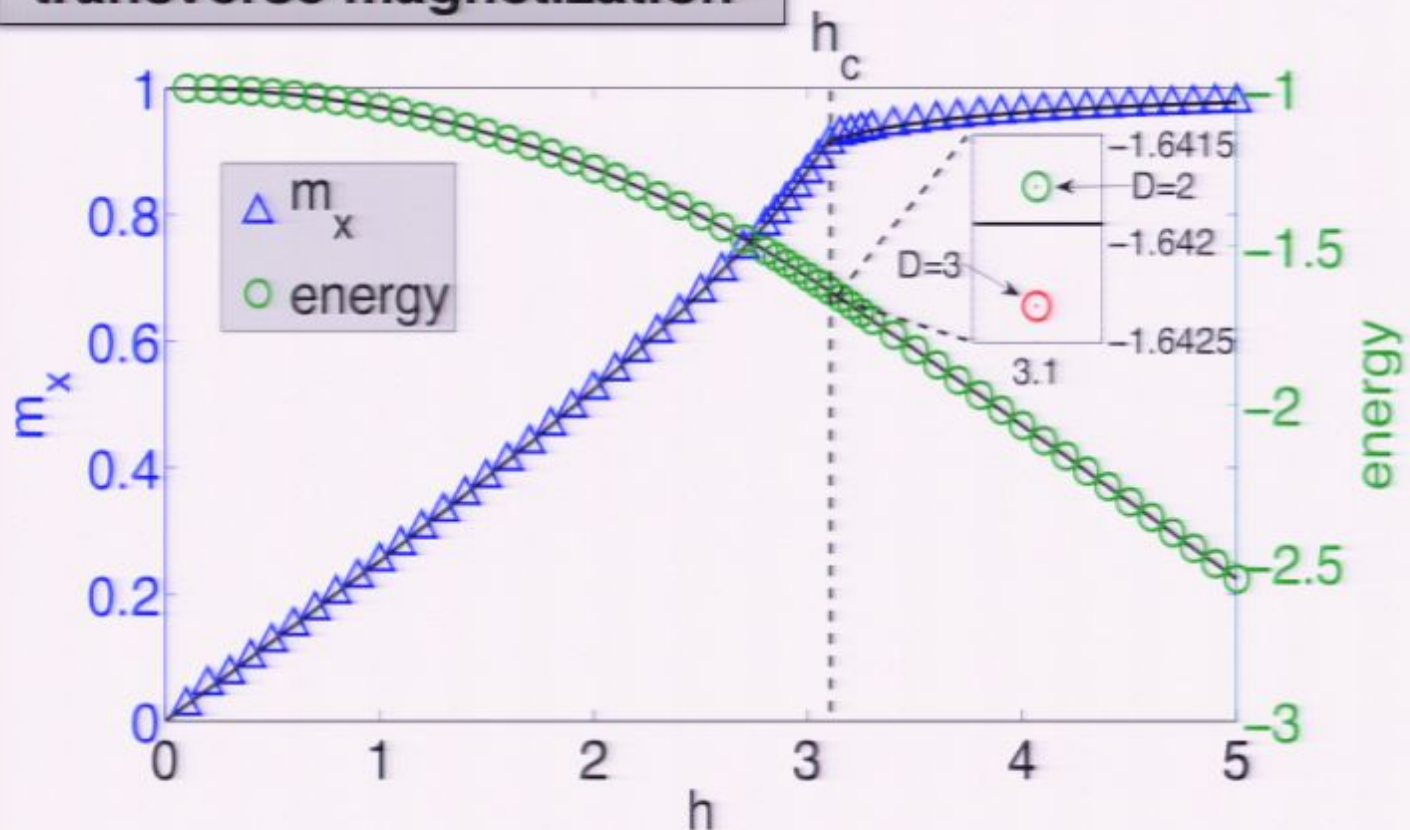
iPEPS: results

Ground state energy and transverse magnetization



iPEPS: results

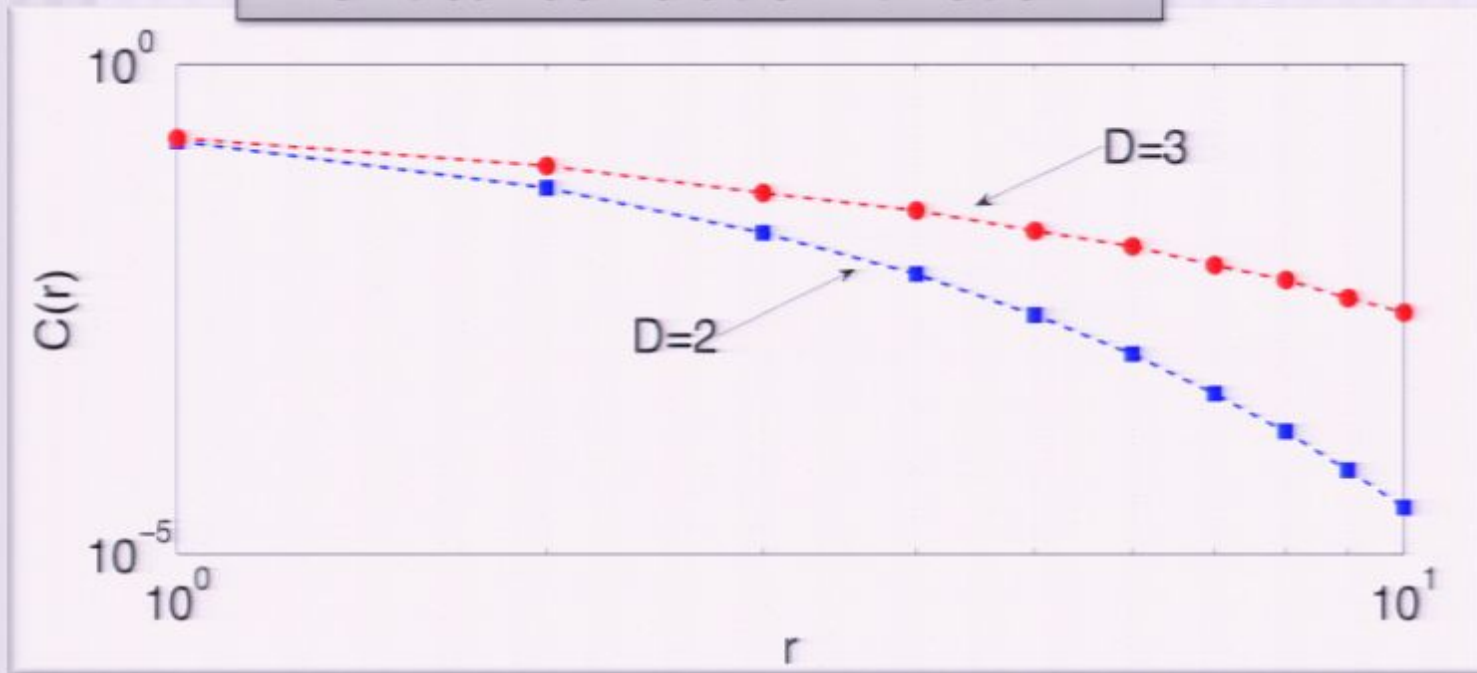
Ground state energy and transverse magnetization



Good agreement with simple perturbative series expansions calculation (black line)

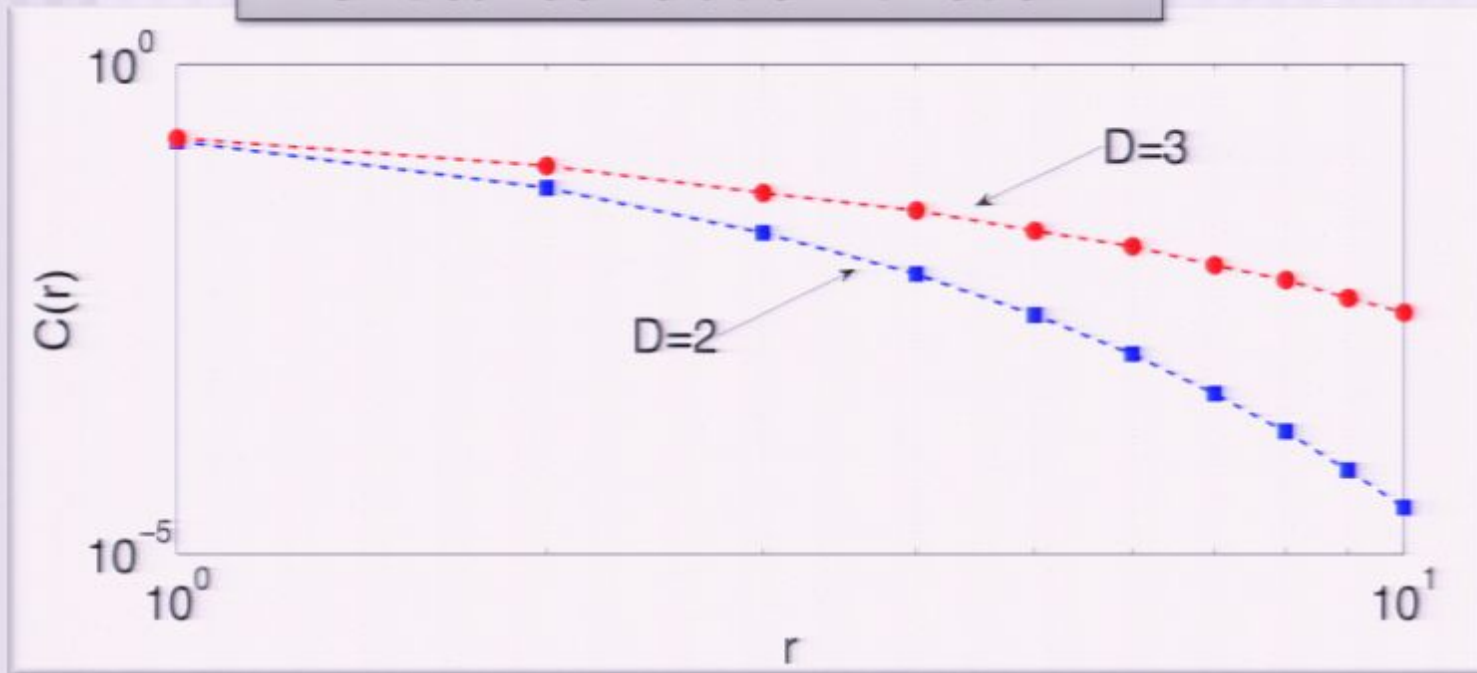
iPEPS: results

Critical correlation function



iPEPS: results

Critical correlation function

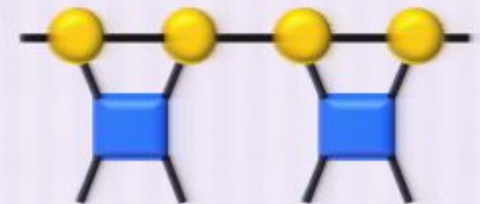


Easy to compute,
and non-trivial
even for small
values of D

Infinite 2-dim classical systems (iTEBD+ algorithm)

The iTEBD algorithm is a method that allows to compute the evolution of infinite 1-dim quantum systems as driven by local (e.g. two-body) *unitary* operations

G. Vidal, PRL 98, 070201 (2007)

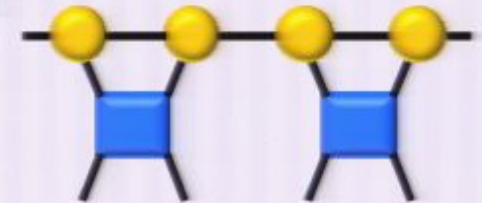


2-body gates

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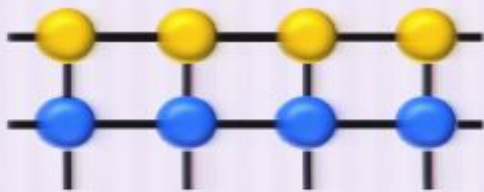
G. Vidal, PRL 98, 070201 (2007)



2-body gates

We have generalized iTEBD so that it can be used to **simulate infinite-size classical lattice systems in 2-dim**

R. Orús, G. Vidal, PRB ?, (2008)



Matrix Product Operators (MPO)



2-to-1 gates



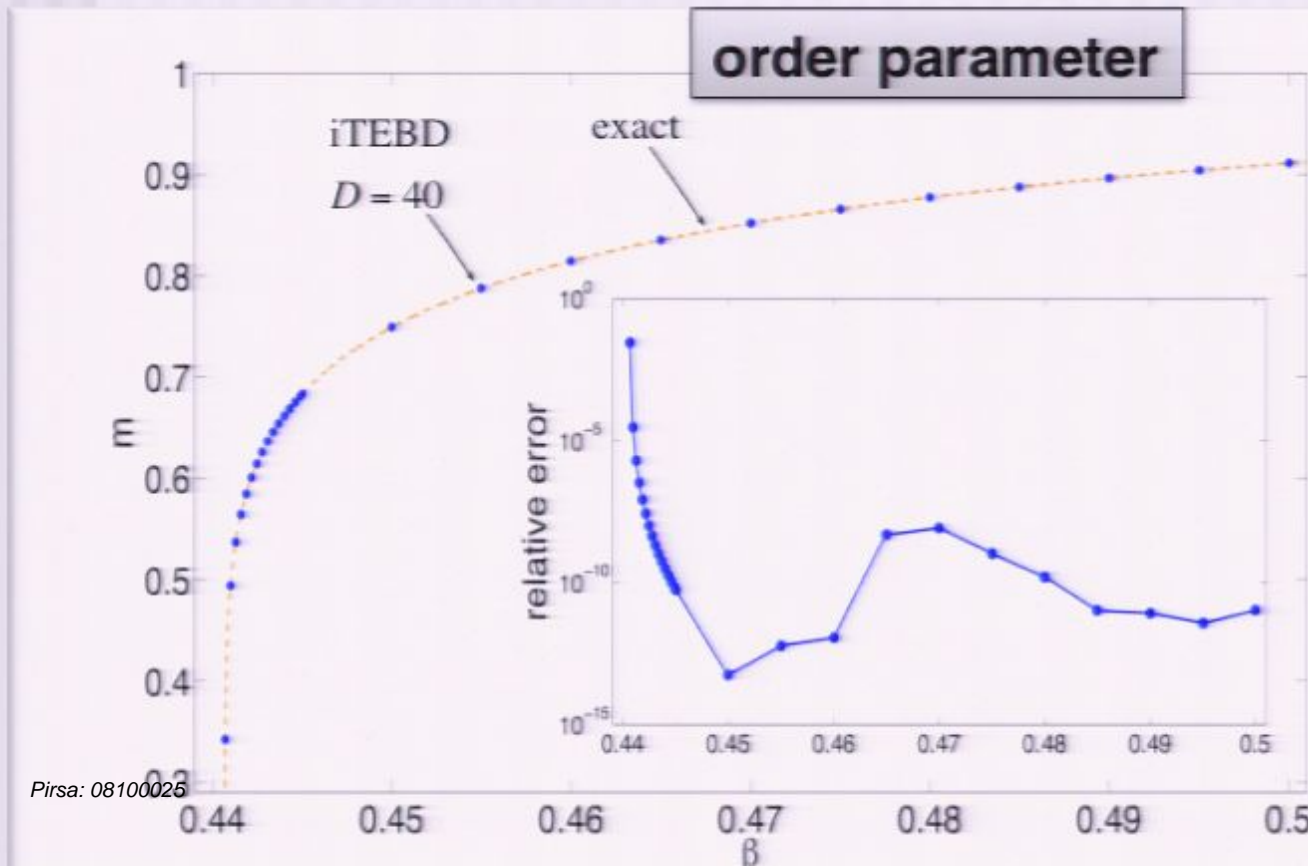
1-to-2 gates

iTEBD+: results

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

$$K(s, s') = -s s' \quad s, s' = \pm 1$$

$$Z(\beta) = \sum_{\{s\}} \exp(-\beta K(\{s\}))$$

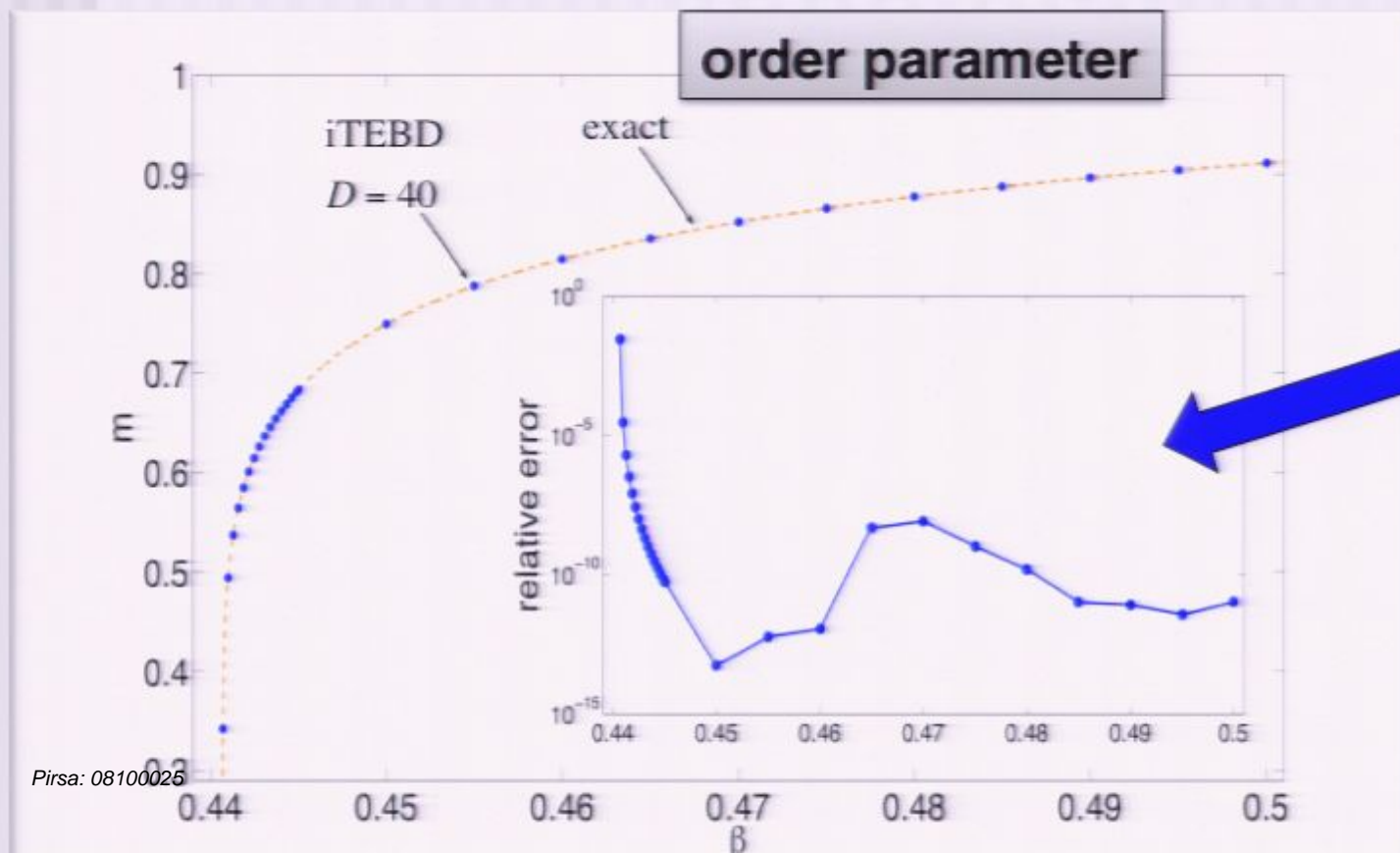


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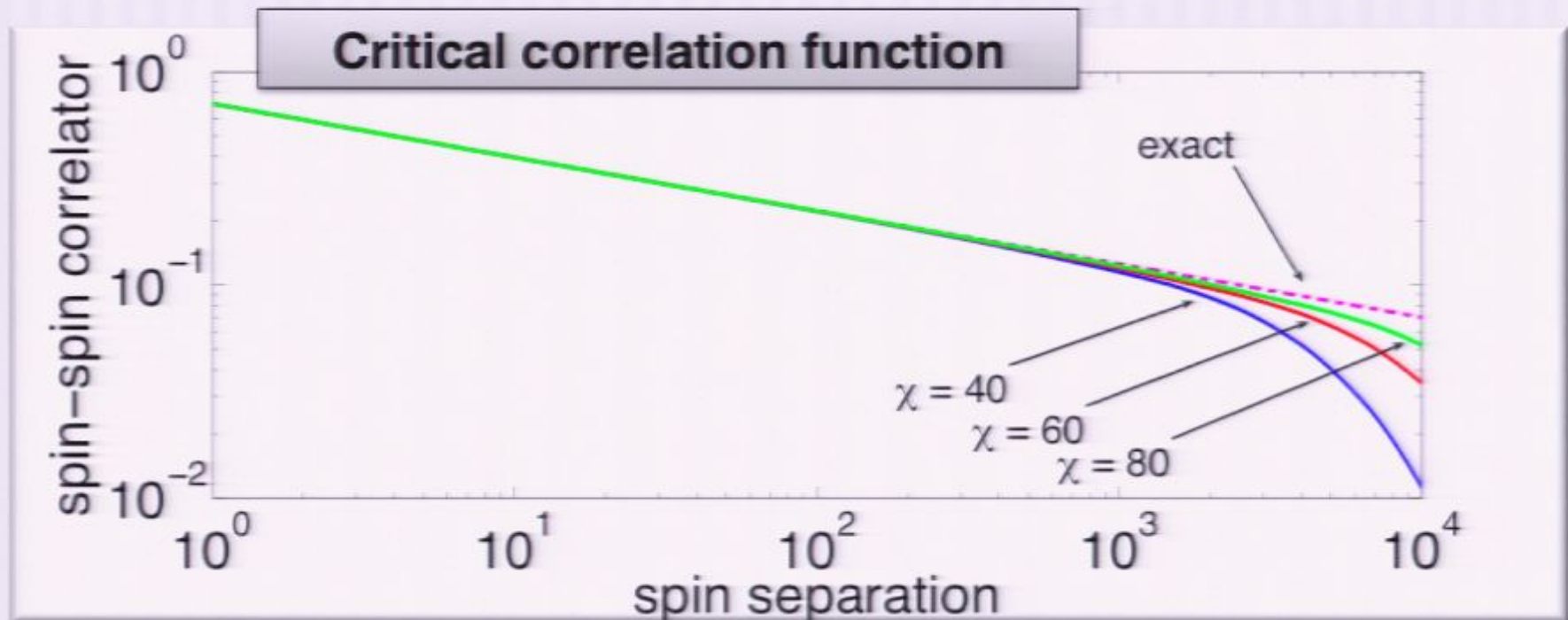
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Small relative error close to criticality, and the critical exponent matches the exact one with 0.2% of relative error

iTEBD+: results



Correct power-law decay up to several thousands of sites

Hard-core Bose-Hubbard model with iPEPS

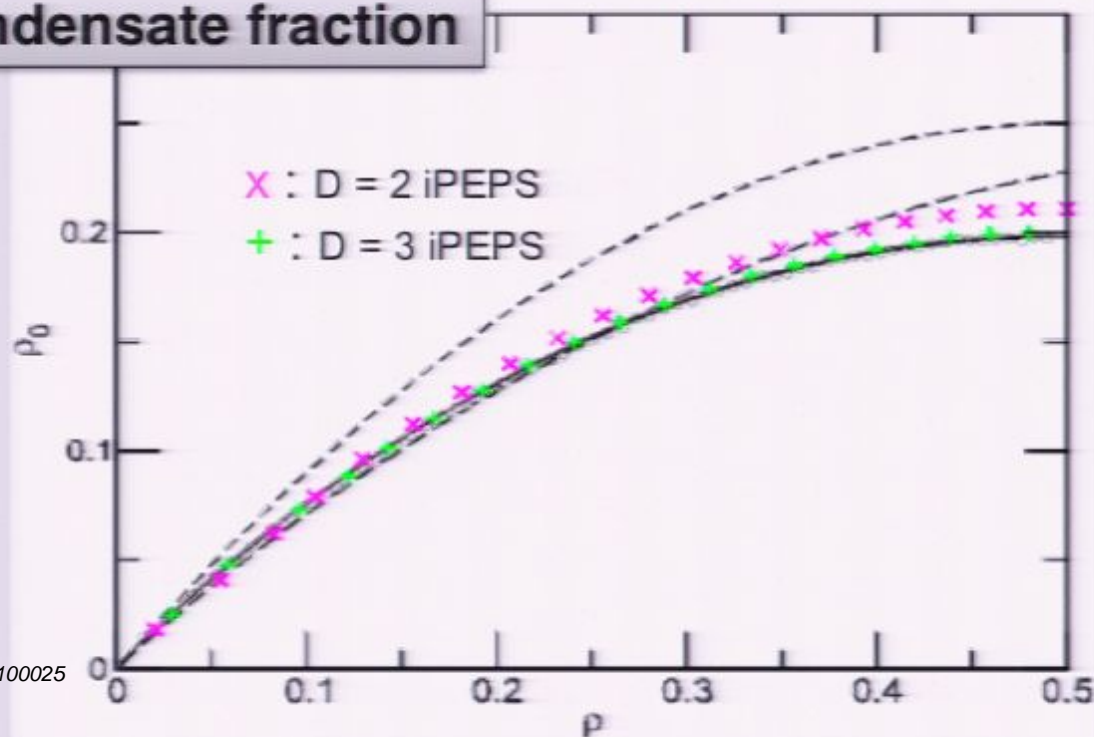
J. Jordan, R. Orús, G. Vidal, in preparation

$$H_{HC} = -J \sum_{\langle i,j \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) - \mu \sum_i n_i$$



Circles: sse, Solid: SW, dotted: MF, dashed: Hines

Condensate fraction



Hard-core Bose-Hubbard model with iPEPS

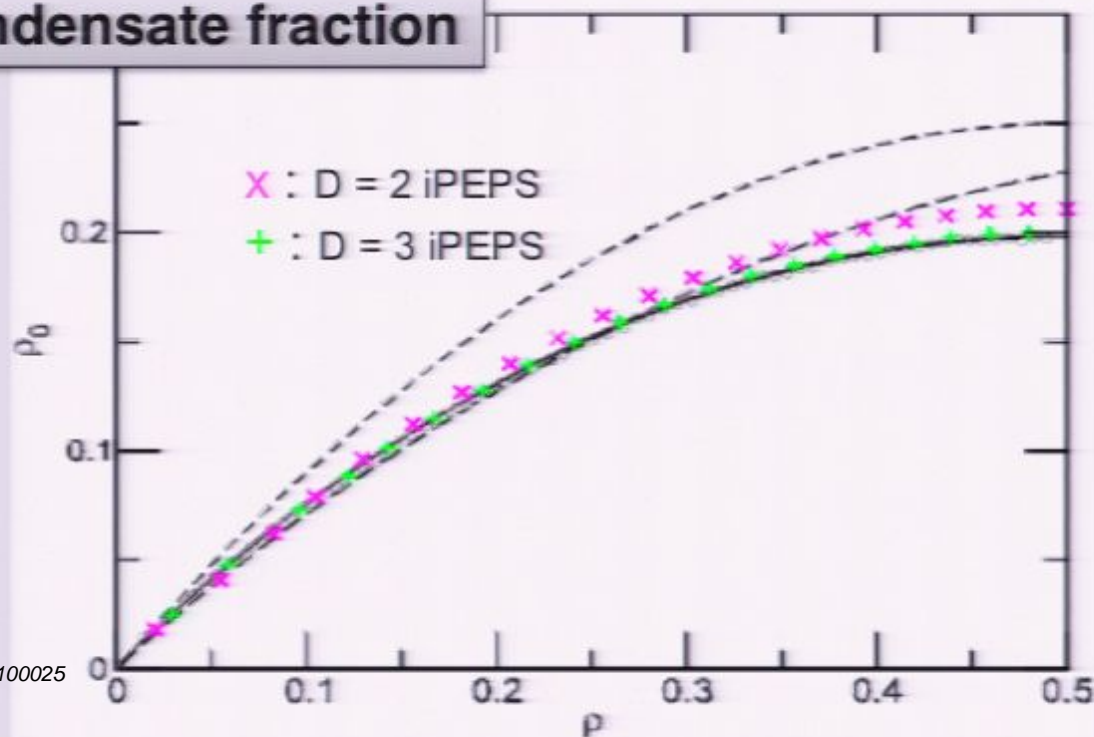
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Condensate fraction



Excellent agreement with other techniques, and possibility to compute new quantities (e.g. time evolution...)

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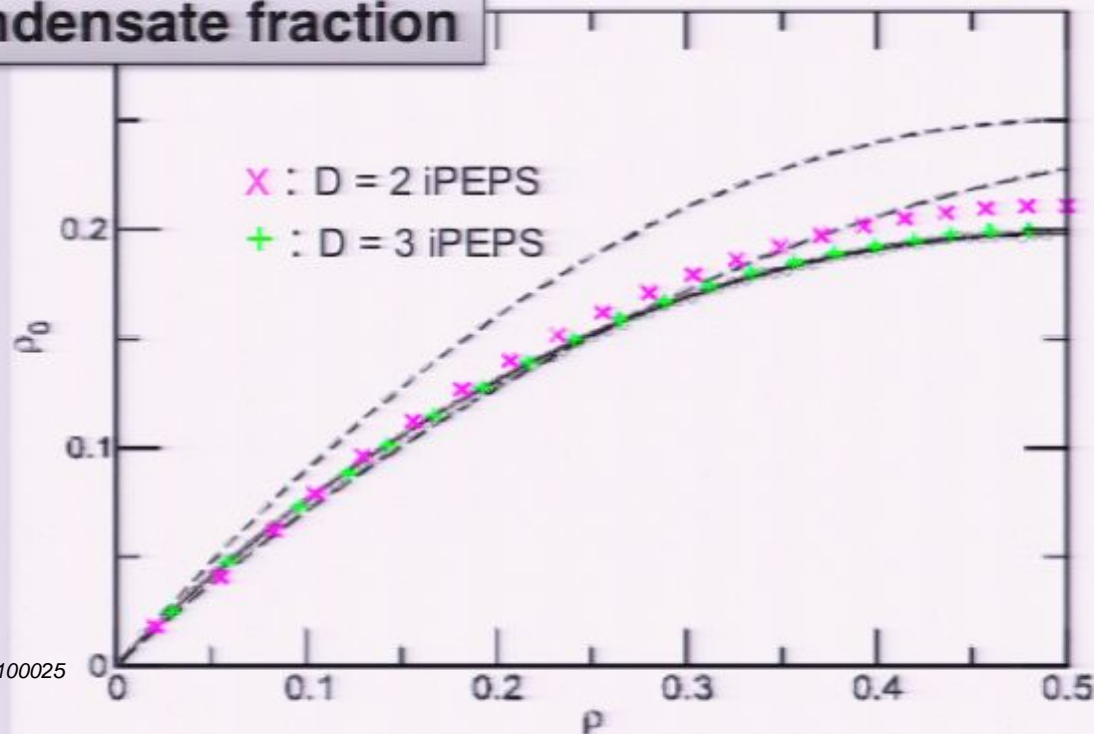
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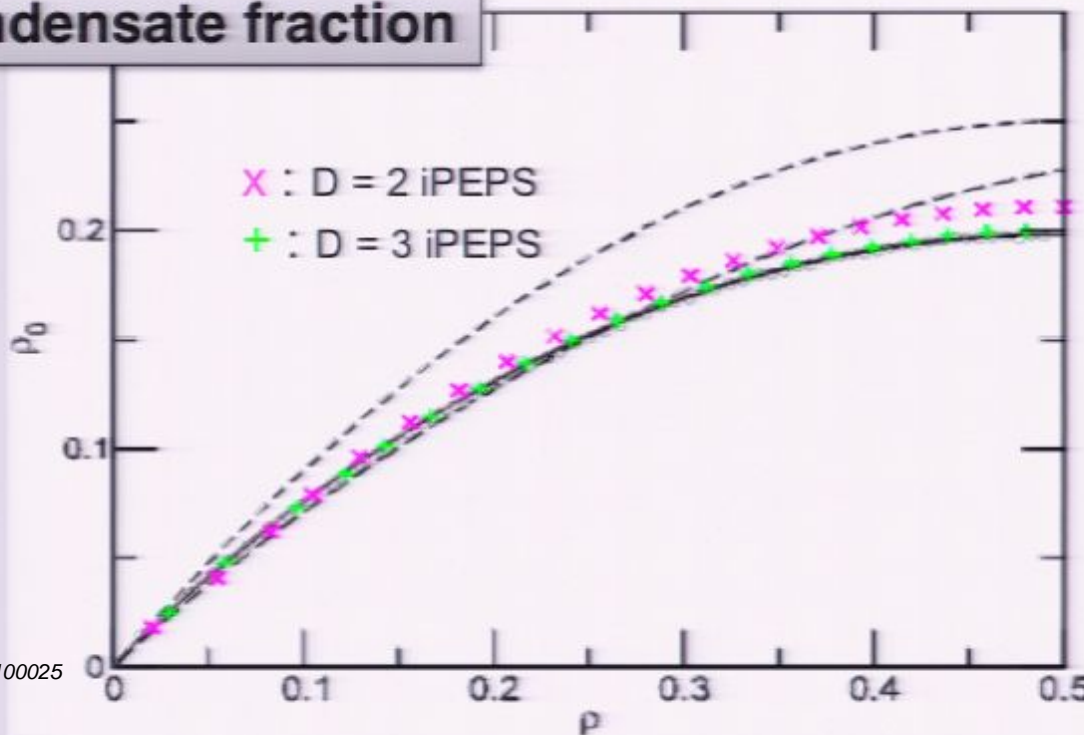
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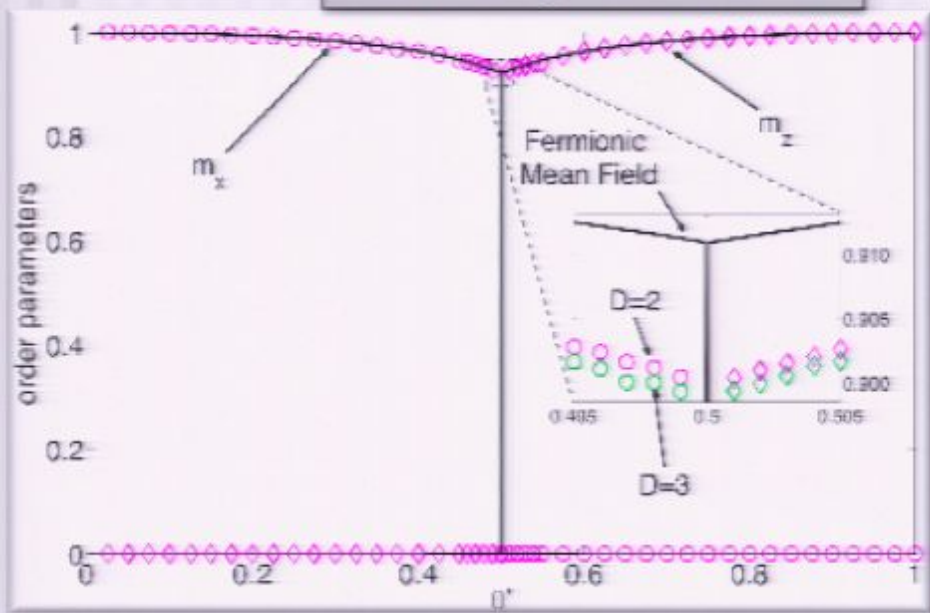
Anisotropic Quantum Orbital Compass Model with iPEPS

A. Doherty, R. Orús, G. Vidal, arXiv:0809.4068

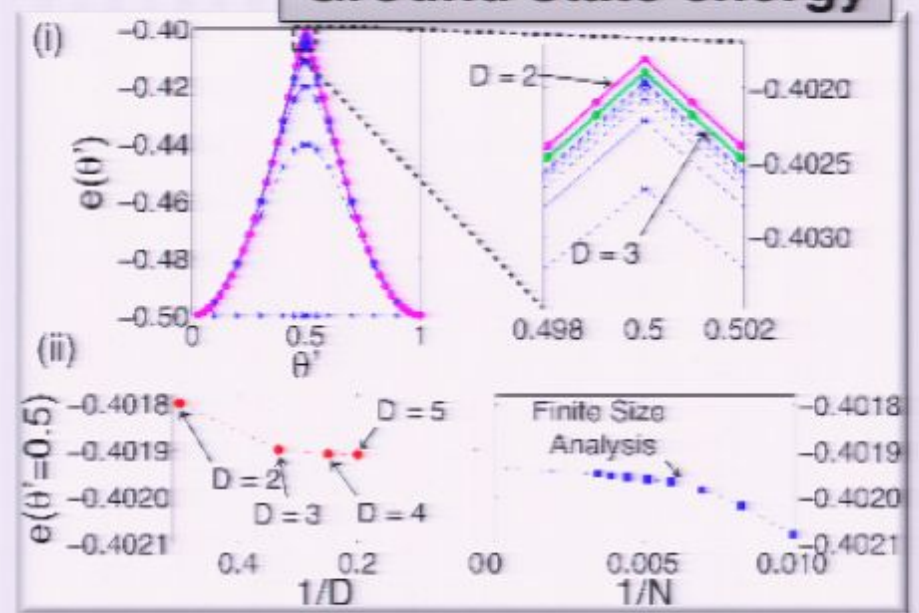


$$H = -\sin(\theta) \sum_{\vec{r}} \sigma_z^{\vec{r}} \sigma_z^{\vec{r}+\hat{i}} - \cos(\theta) \sum_{\vec{r}} \sigma_x^{\vec{r}} \sigma_x^{\vec{r}+\hat{j}}$$

Order parameters



Ground state energy

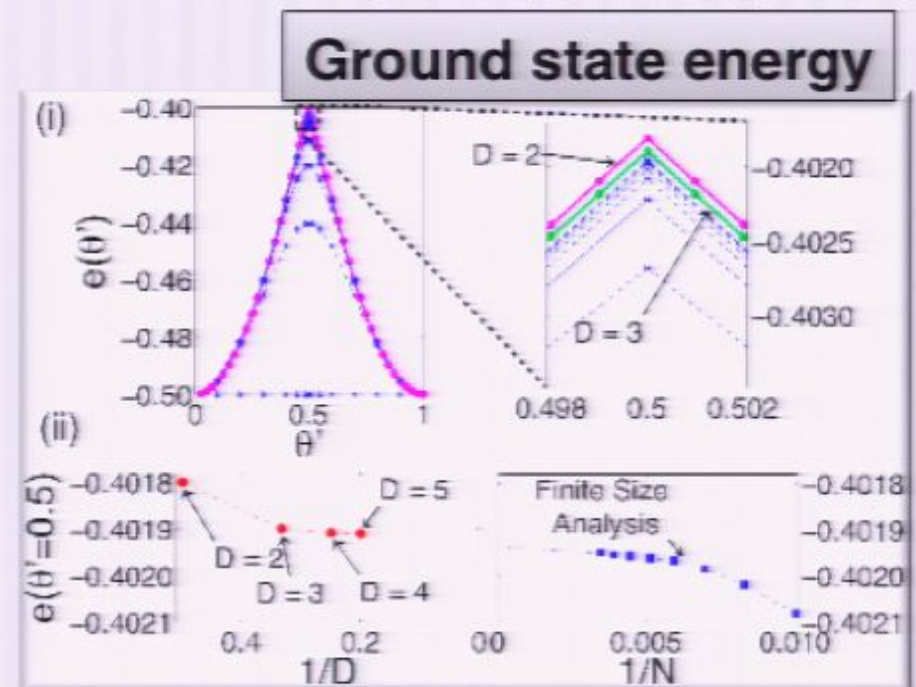
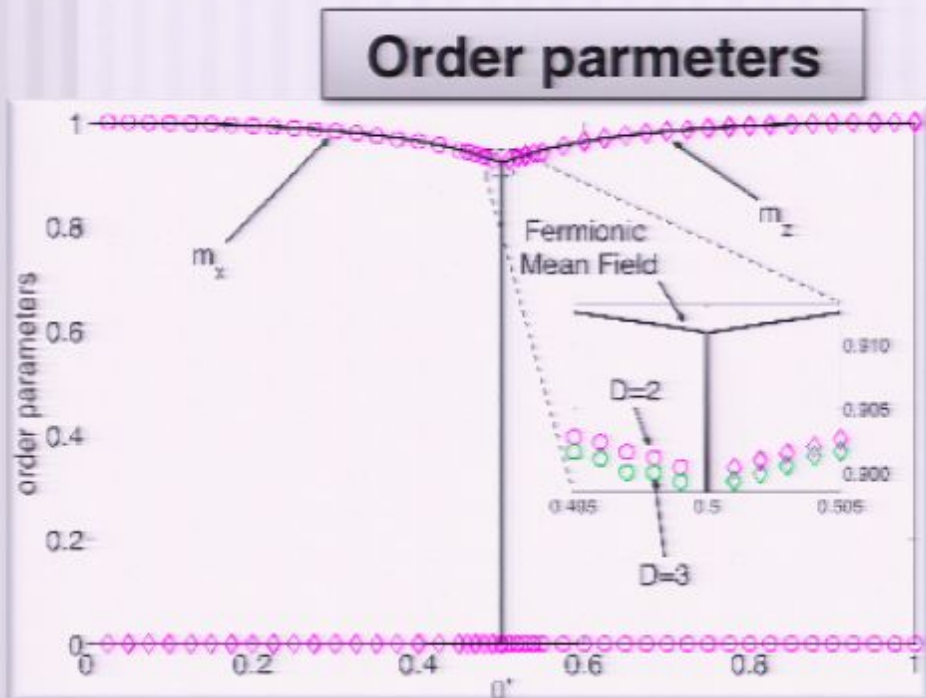


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Pirsa: 08100025 **Improves upon previous results, and conclusively determines a 1st order phase transition** Page 83/104

iPEPS and the Fidelity Approach to quantum phase transitions

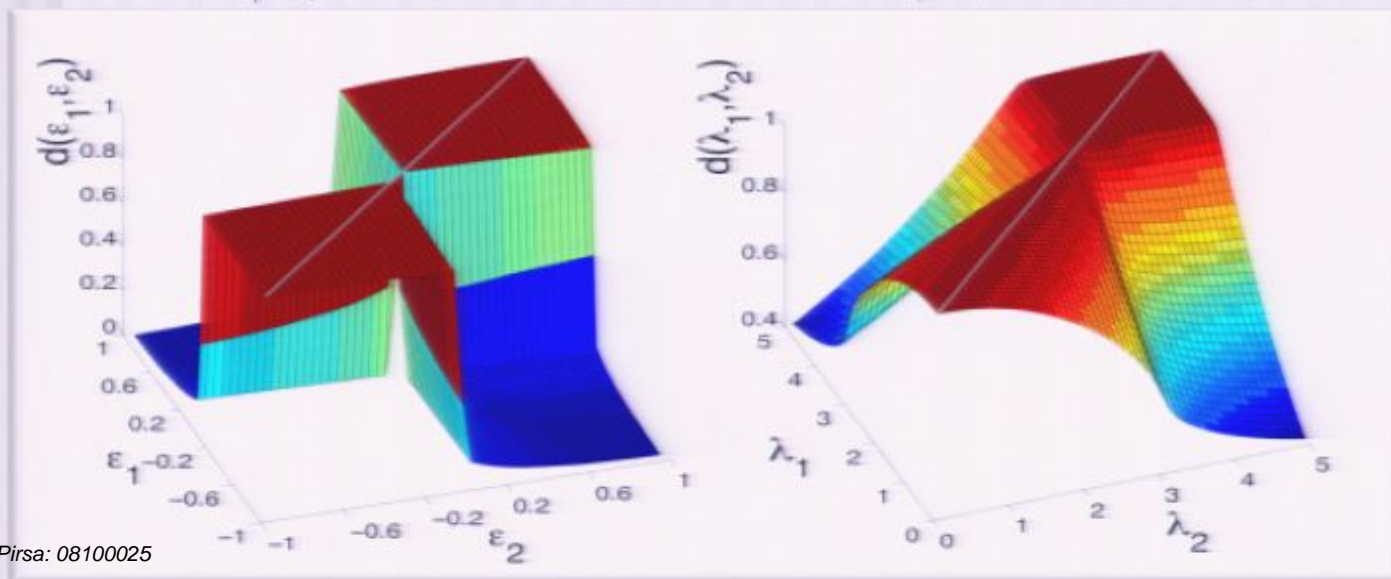
Fidelity between different ground states

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

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

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1st order QPT

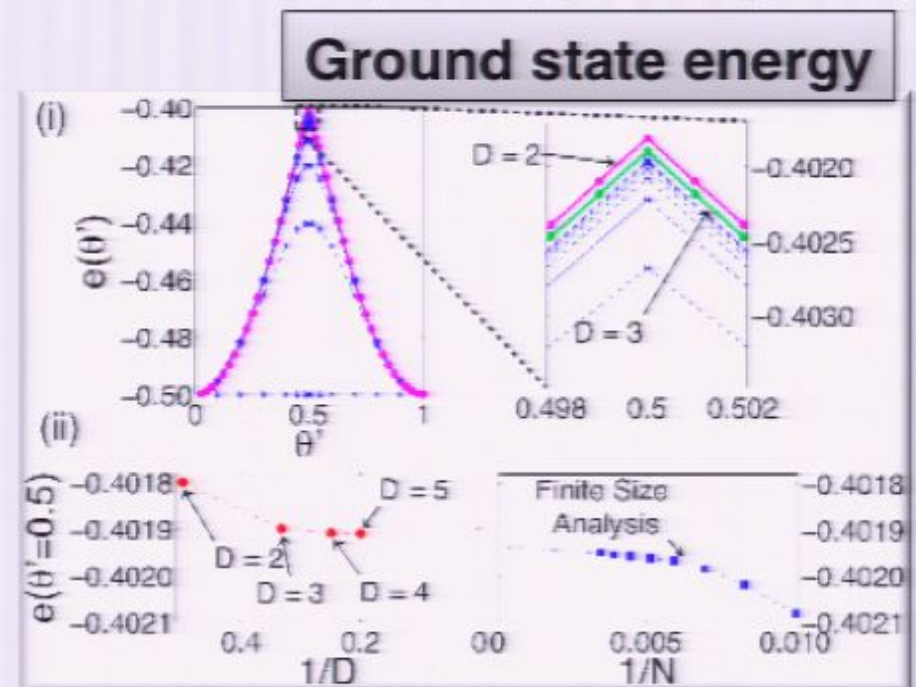
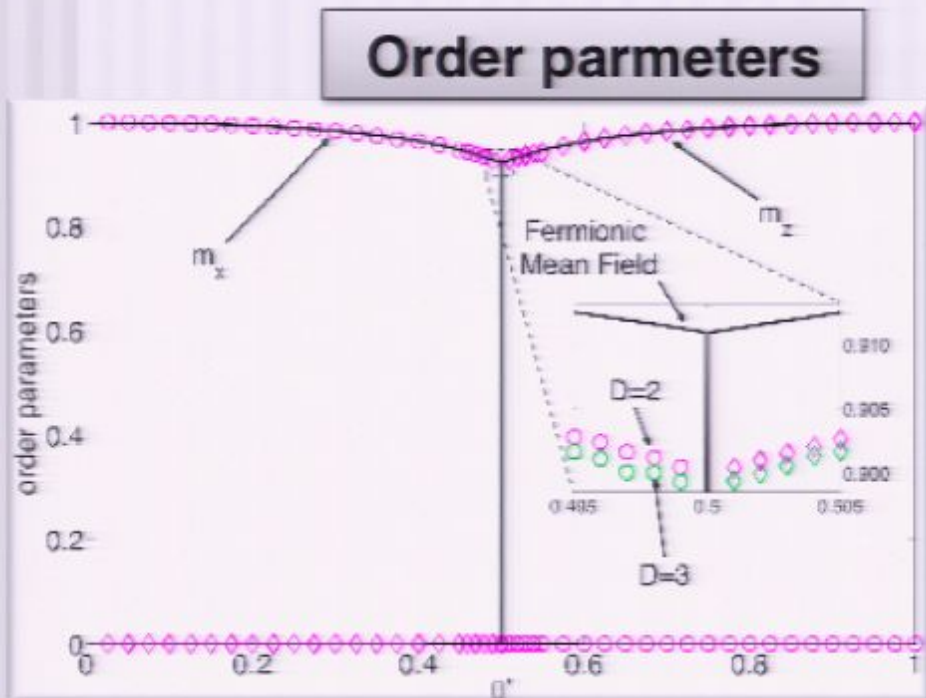
2nd order QPT

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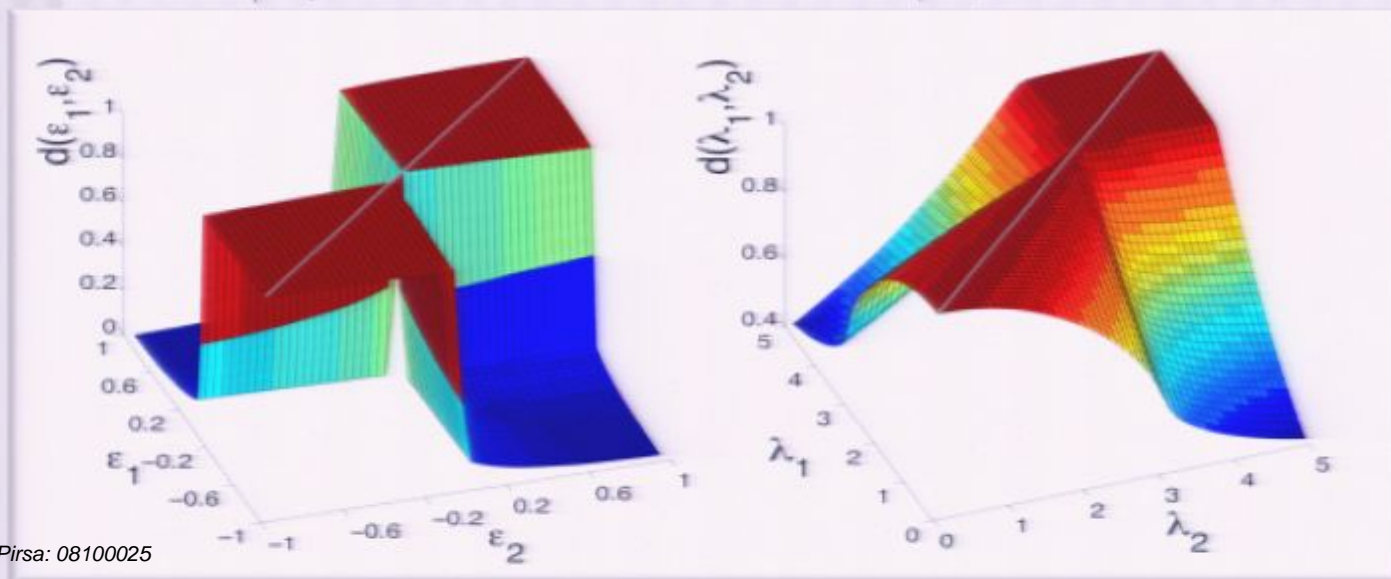
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1st order QPT

2nd order QPT

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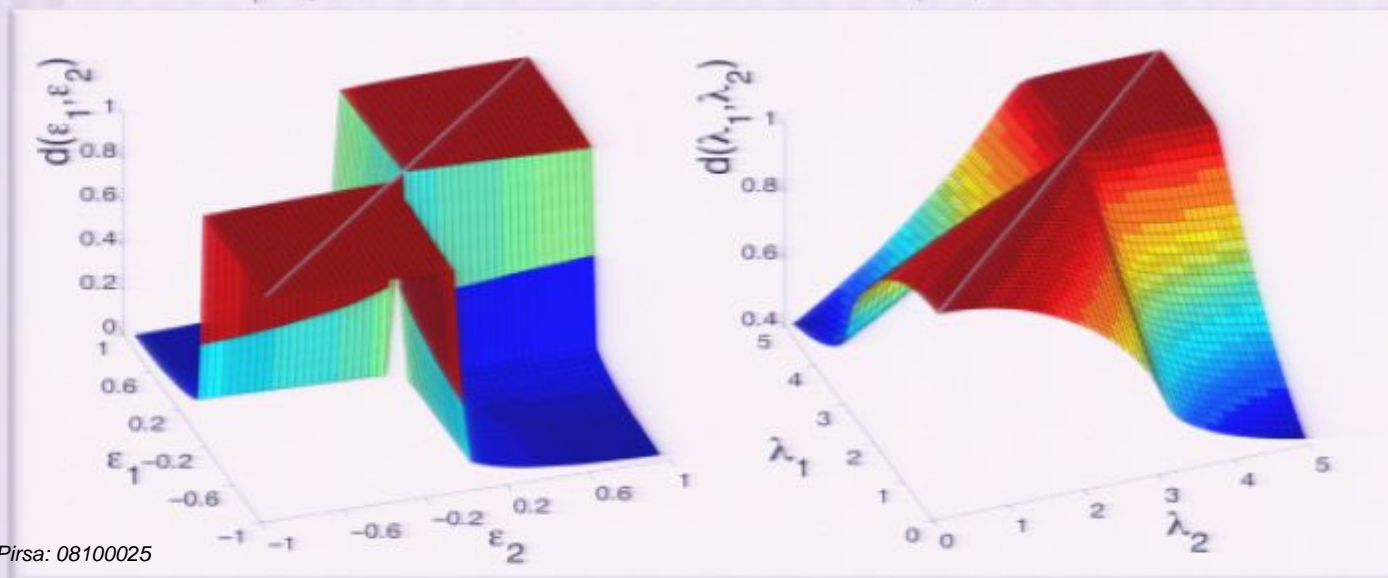
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Easy to compute with TN, and shows the phase diagram without relying on any local order parameter

2-dim quantum lattice systems with symmetries



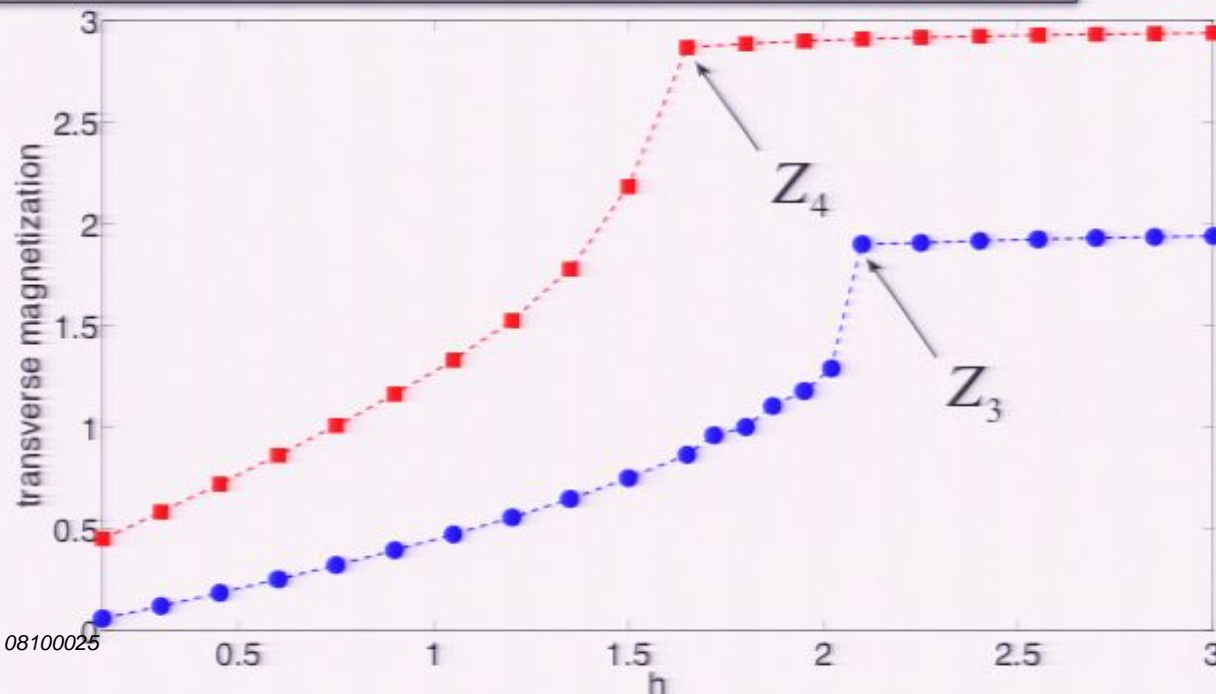
R. Orús, G. Vidal, ..., work in progress

Implementation of the symmetries directly at the level of the PEPS/iPEPS



...

Z_q Quantum Potts Model, 10x10 lattice



Geometric Entanglement in 1-dim Valence Bond Solids

R. Orús, arXiv:0808.0938



Spin-1 AKLT chain

$$H = \sum_{r=1}^{N-1} \left(\vec{S}^{[r]} \vec{S}^{[r+1]} + \frac{1}{3} (\vec{S}^{[r]} \vec{S}^{[r+1]})^2 \right) + \pi^{[0,1]} + \pi^{[N,N+1]}$$

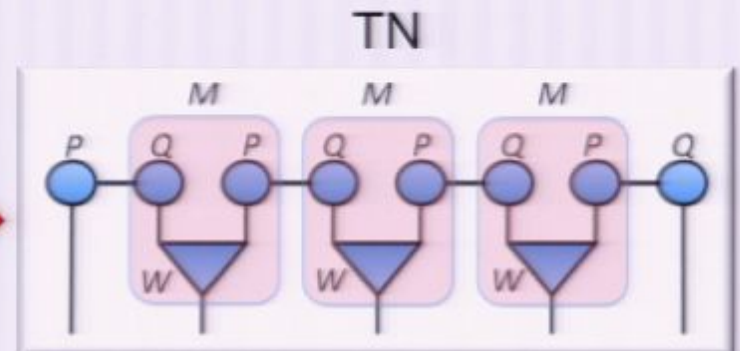
Gapped 1-dim Heisenberg-like system (Haldane conjecture)

Ground state is a Valence Bond Solid

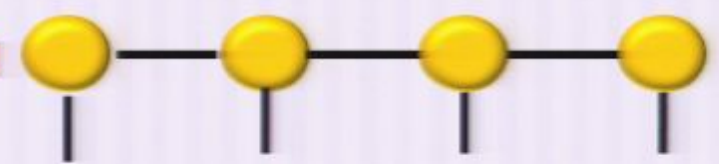
$$|\Psi\rangle = \left(\otimes_{r=1}^N W^{[r,r']} \right) |\Psi^-\rangle^{[0,1]} |\Psi^-\rangle^{[1,2]} \dots |\Psi^-\rangle^{[N,N+1]}$$

Isometries

Spin 1/2 - singlets



MPS



$$\epsilon(L) = \log 2 - \log \left(1 + \left(-\frac{1}{3} \right)^L \right)$$

Exponentially fast saturation in L

Closing the loop...

Quantum Information + Condensed Matter Physics

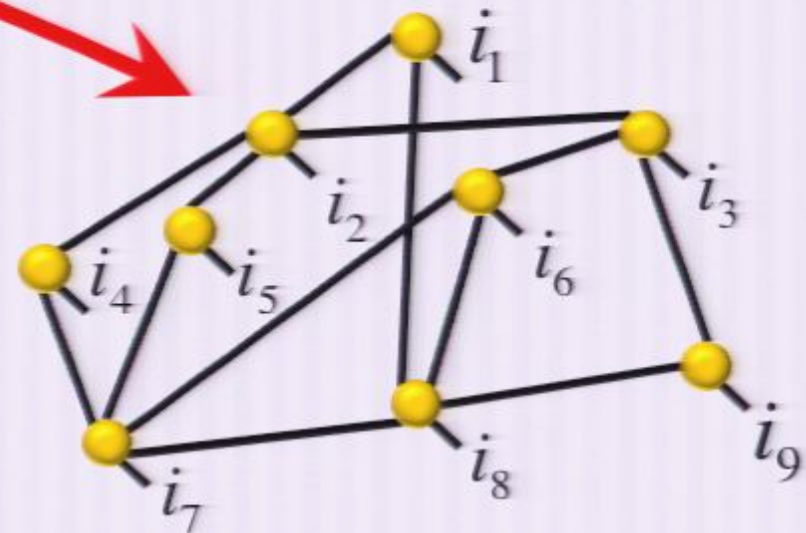
Entanglement in
many-body systems



Ruth Bloch: *Entanglement*
(bronze, 71 cm, 1995)



Tensor Networks



Outline



1.- Brief historical review



2.- What are Tensor Networks and why are they useful?



3.- Simulation results for 2-dim quantum systems

4.- Applications in the study of many-body entanglement

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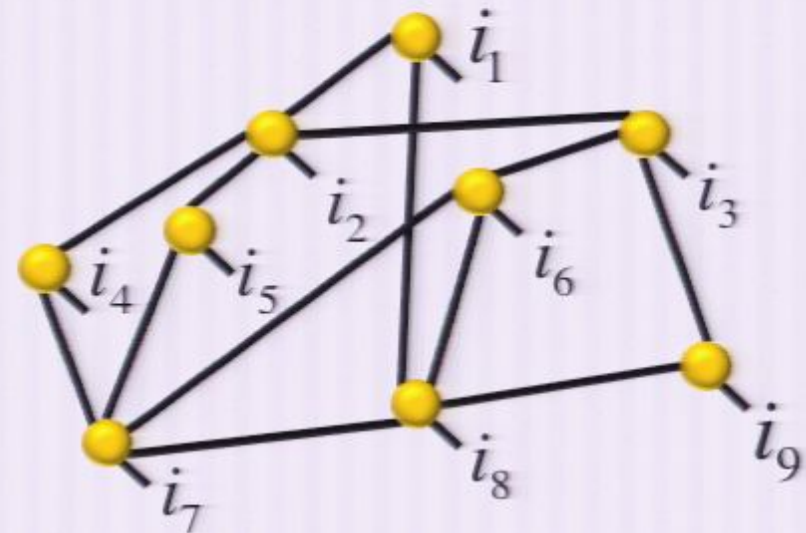
Quantum Information + Condensed Matter Physics

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Tensor Networks



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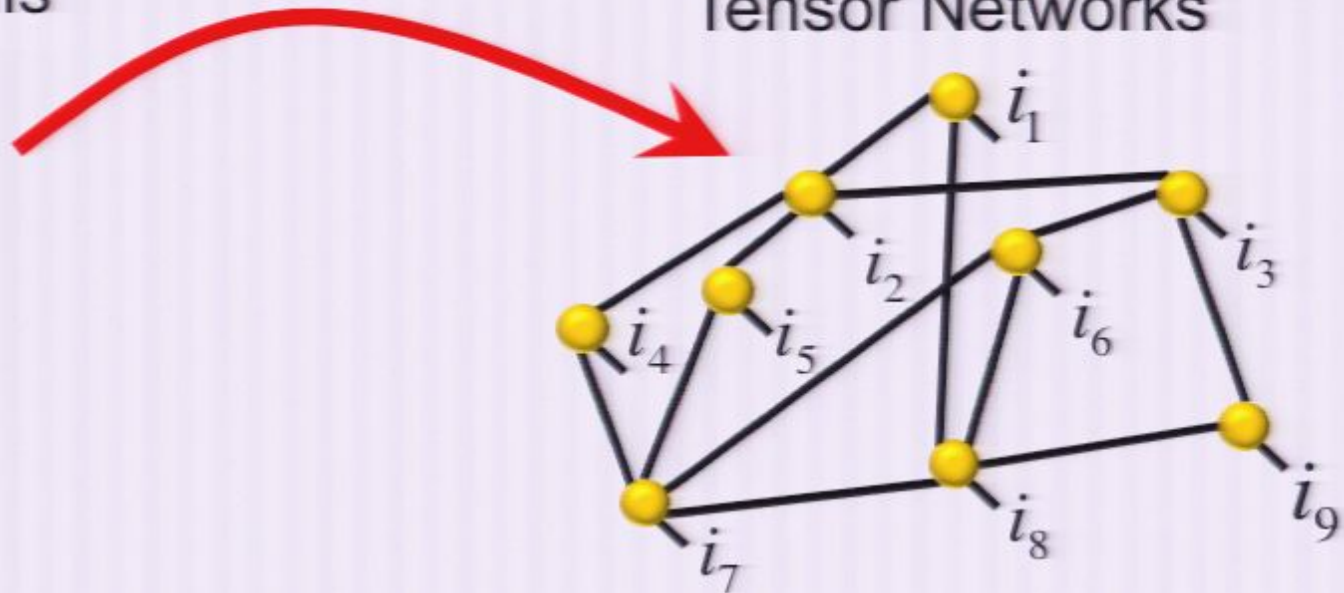
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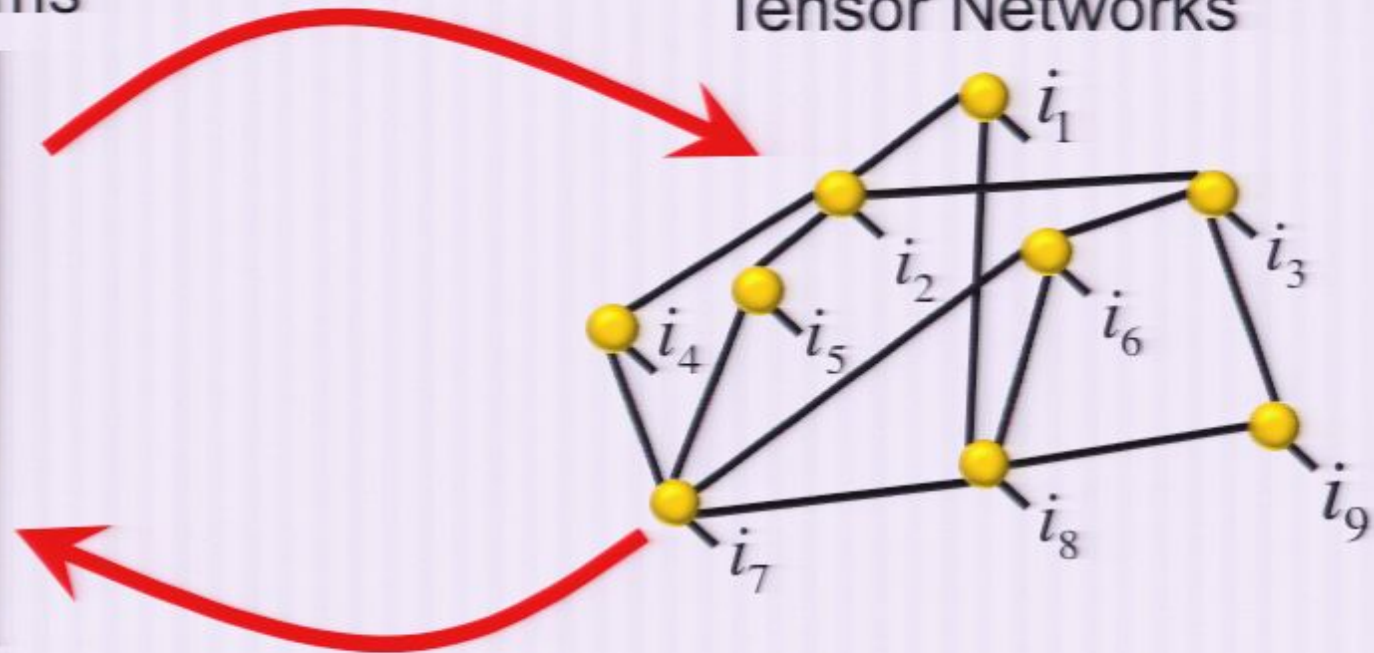
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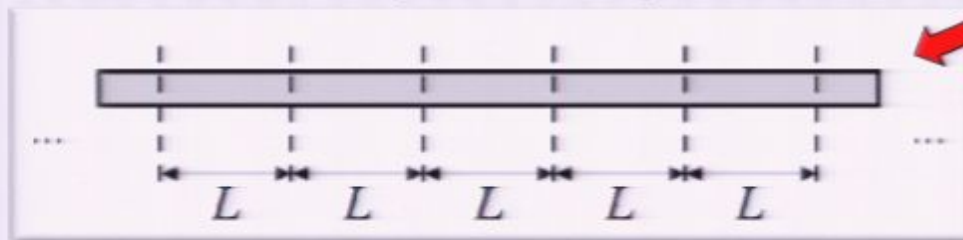


Geometric Entanglement and Conformal Field Theory

R. Orús, PRL 100, 130502 (2008)



1-dim quantum system



Divide into N blocks of length L

Global Geometric Entanglement
per block:

$$\varepsilon = \lim_{N \rightarrow \infty} -\frac{1}{N} \log \left| \langle \Phi_{\max} | \Psi \rangle \right|^2$$

Separable state of the blocks

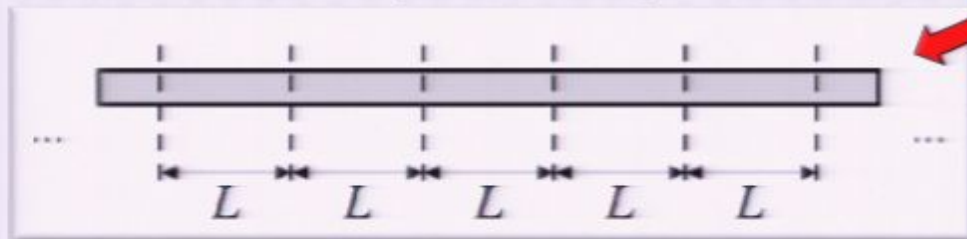
(Wei, Goldbart, Botero, Reznik)

Geometric Entanglement and Conformal Field Theory



R. Orús, PRL 100, 130502 (2008)

1-dim quantum system



Divide into N blocks of length L

central charge of the underlying 1+1-dim Conformal Field Theory

Global Geometric Entanglement per block:

$$\varepsilon = \lim_{N \rightarrow \infty} -\frac{1}{N} \log \left| \langle \Phi_{\max} | \Psi \rangle \right|^2$$

Separable state of the blocks

(Wei, Goldbart, Botero, Reznik)

$$\varepsilon = \frac{c}{12} \log \left(\frac{\xi}{\eta} \right)$$

Close to criticality

$$\varepsilon < \frac{c}{6} \log \left(\frac{L}{\eta} \right)$$

At criticality

Trick: use MPS



Geometric Entanglement in 1-dim Valence Bond Solids

R. Orús, arXiv:0808.0938



Spin-1 AKLT chain

$$H = \sum_{r=1}^{N-1} \left(\vec{S}^{[r]} \vec{S}^{[r+1]} + \frac{1}{3} (\vec{S}^{[r]} \vec{S}^{[r+1]})^2 \right) + \pi^{[0,1]} + \pi^{[N,N+1]}$$

Gapped 1-dim Heisenberg-like system (Haldane conjecture)

Ground state is a Valence Bond Solid

$$|\Psi\rangle = \left(\otimes_{r=1}^N W^{[r,r']} \right) |\Psi^-\rangle^{[0,1]} |\Psi^-\rangle^{[1,2]} \dots |\Psi^-\rangle^{[N,N+1]}$$

↑
Isometries

↑
Spin 1/2 - singlets

Geometric Entanglement in 1-dim Valence Bond Solids



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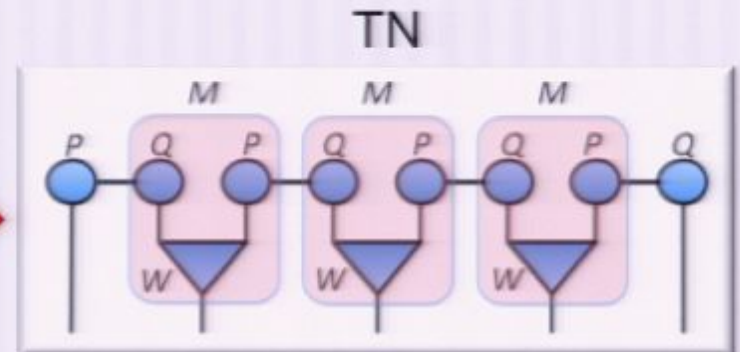
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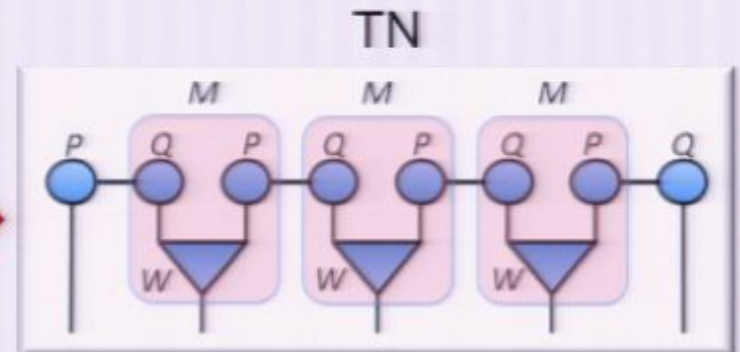
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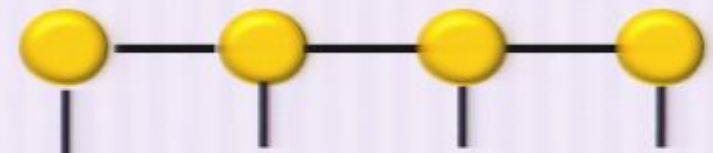
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Isometries

Spin 1/2 - singlets



MPS



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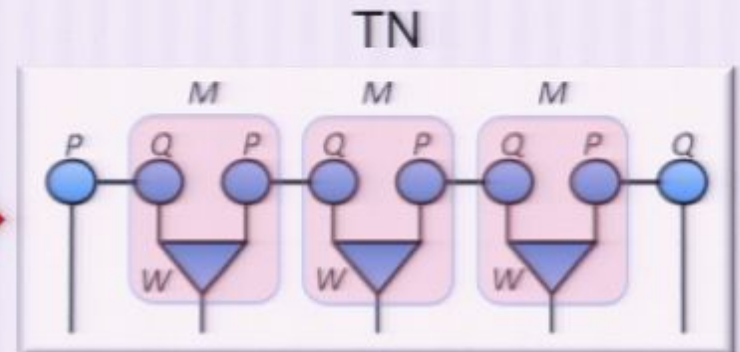
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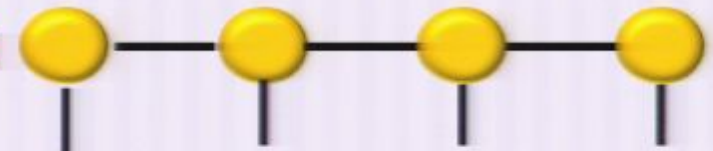
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Isometries

Spin 1/2 - singlets



MPS



$$\epsilon(L) = \log 2 - \log \left(1 + \left(-\frac{1}{3} \right)^L \right)$$

Exponentially fast saturation in L

More work in progress...



SU(N) AKLT chain

Finite-size effects

Topological order

Mean-field theory

Symmetries

2-dim Bose-Hubbard model

2-dim fermionic lattice systems

Thank you!

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Quantum many-body systems networks: simulation methods

Román Orús
School of Physical Science
University of Queensland, Brisbane

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Matlab2

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