Title: Recent Developments in Computational Physics with Tensor Network States

Date: Oct 06, 2015 03:30 PM

URL: http://pirsa.org/15100075

Abstract: In this talk, I will present our latest results on the development of algorithms for computer simulations based on tensor network states (TNS). The major part of this talk is concerned with finite projected entangled pair states (PEPS) in 2D: I will discuss their algorithmic properties as well as their performance for typical benchmark Hamiltonians [1, 2]. A minor part of this talk deals with the question whether TNS methods can be useful for density functional theory (DFT).

[1] M. Lubasch, J. I. Cirac, and M.-C. Ba\~{n}uls, New J. Phys. \textbf{16}, 033014 (2014).

[2] M. Lubasch, J. I. Cirac, and M.-C. Ba\~{n}uls, Phys. Rev. B \textbf{90}, 064425 (2014).

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Perimeter Institute for Theoretical Physics
6th October 2015

Michael Lubasch

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Finite PEPS Algorithms

Motivation

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Motivation

Finite PEPS algorithms:

- represent one generalization of *DMRG algorithms*

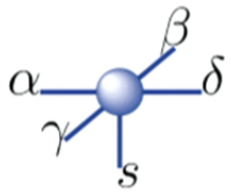
Finite PEPS Algorithms

Finite PEPS

Verstraete and Cirac, arXiv:cond-mat/0407066 (2004).

- here: *variational ansatz* for *N quantum spins* on *square lattice*
  - composed of *N tensors*
  - *one tensor* represents *one quantum spin*

$$A^{s}_{\alpha,\beta,\gamma,\delta} =$$



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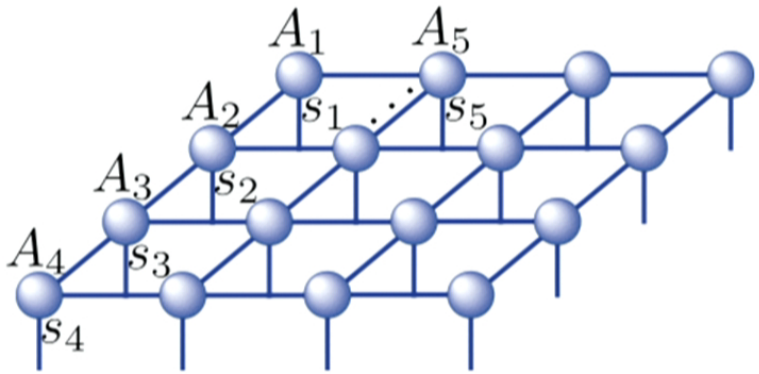

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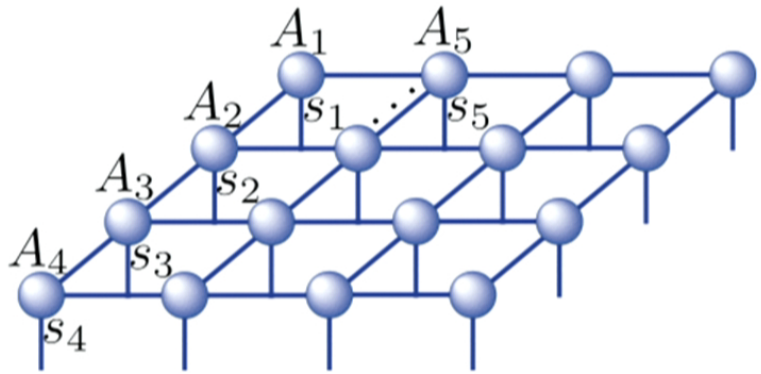


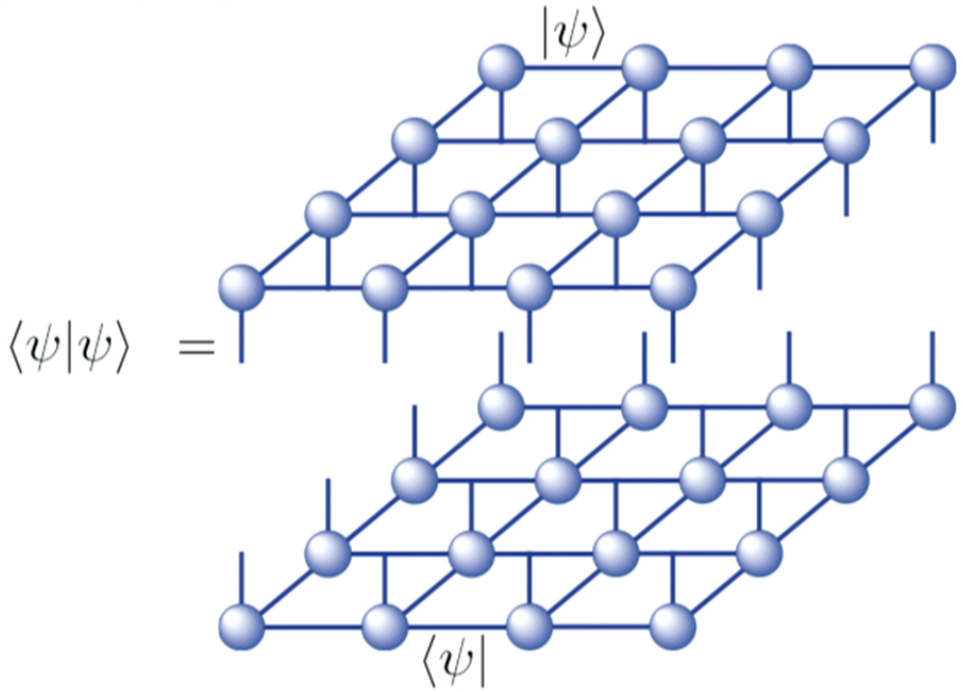
$$|\psi\rangle = \sum_{s_1,s_2,\ldots,s_N} \mathcal{F}(A_1^{s_1} A_2^{s_2} \ldots A_N^{s_N})|s_1 s_2 \ldots s_N\rangle$$

Finite PEPS Algorithms

Original Contraction

Verstraete and Cirac, arXiv:cond-mat/0407066 (2004).

- contraction of *norm*:



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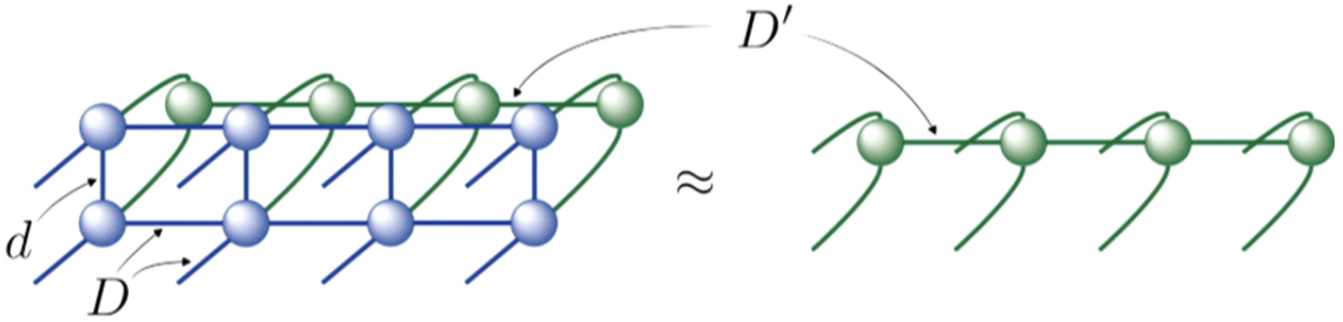
- contraction of *norm*:
  via *successive row-row approximations*



Cost: $\mathcal{O}(dD^6D'^2 + D^4D'^3)$

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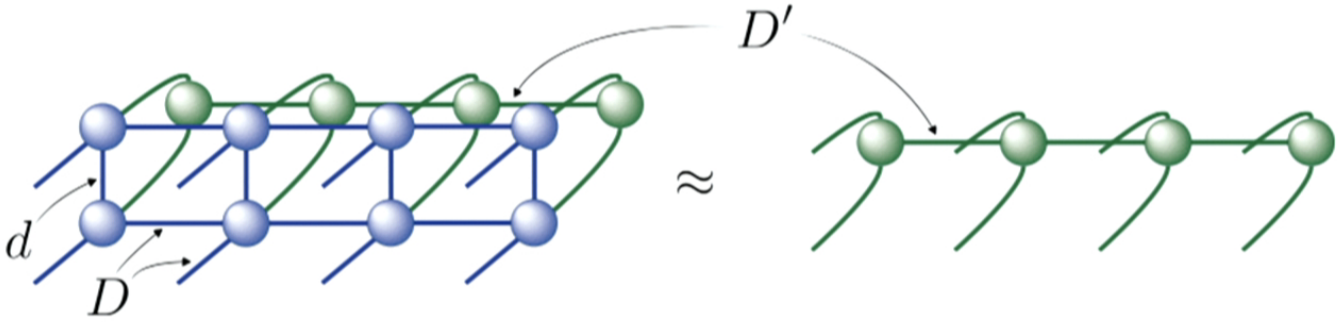

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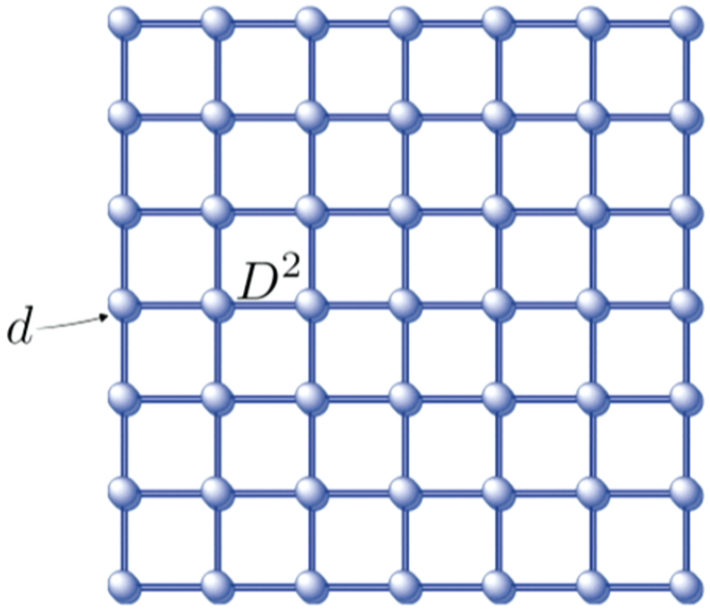

two-dimensional TN:
exact contraction is *hard*

Finite PEPS Algorithms

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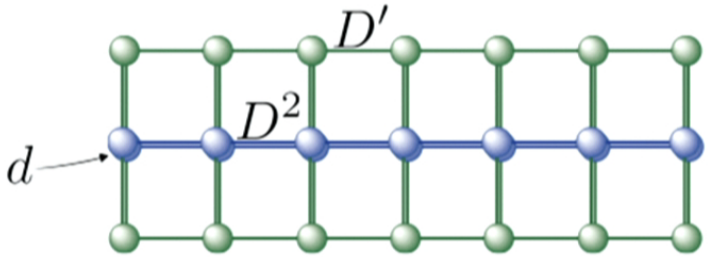

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exact contraction is *efficient*

approximate contraction via *successive row-row approximations*

Finite PEPS Algorithms

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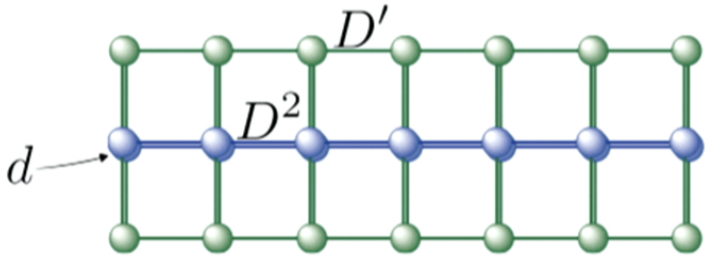

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Finite PEPS Algorithms

Cluster Contraction

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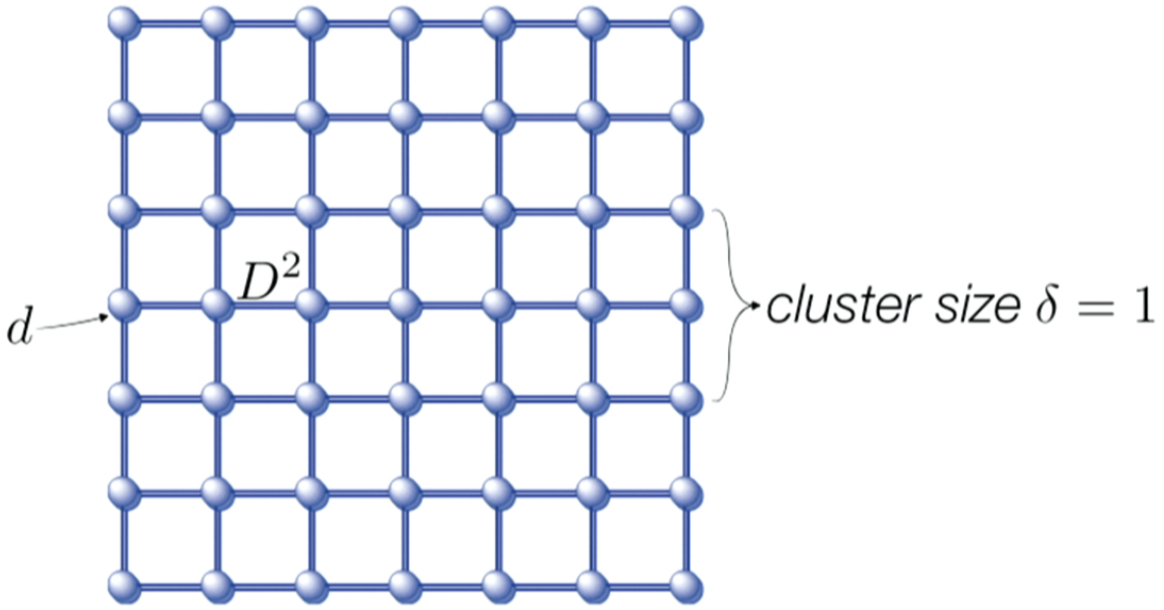

rough approximate contraction outside *cluster*

Finite PEPS Algorithms

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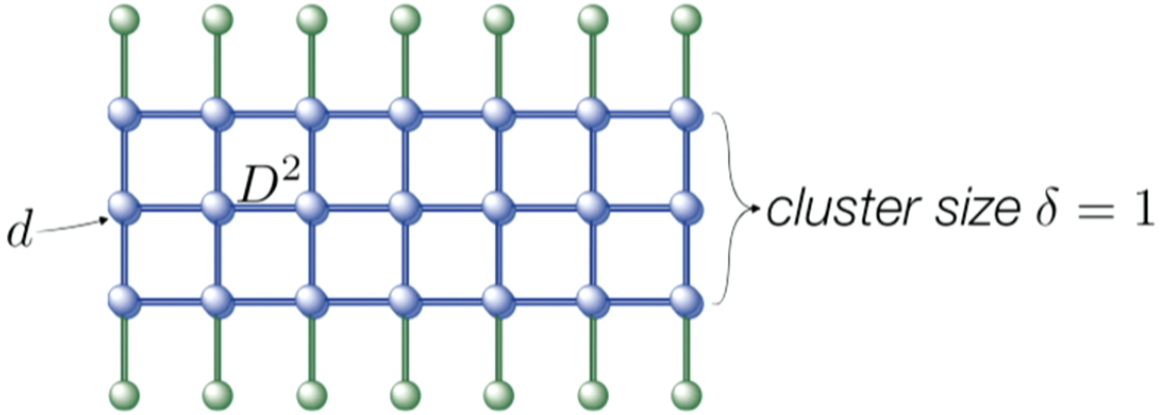

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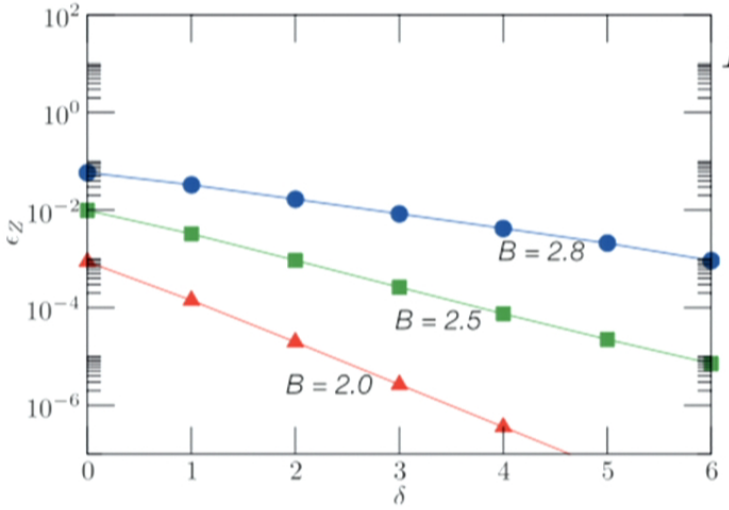
Finite PEPS Algorithms

Cluster Precision

Lubasch, Cirac, and Bañuls, PRB 90, 064425 (2014).

PEPS Ground States of 21x21 *Quantum Ising Model*



$$\hat{H} = -\sum_{\langle l,m \rangle} \sigma_l^Z \sigma_m^Z - B \sum_l \sigma_l^X$$

$$\epsilon_Z(\delta) := |\langle \sigma^Z \rangle_\delta - \langle \sigma^Z \rangle| / |\langle \sigma^Z \rangle|$$

Finite PEPS Algorithms

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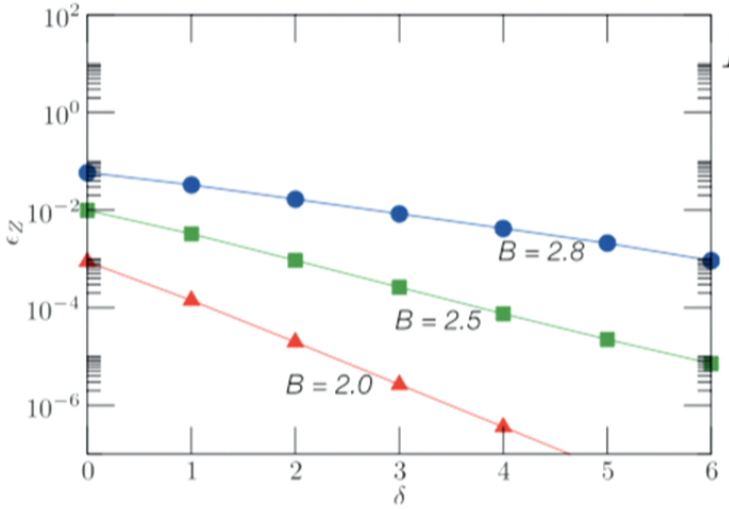

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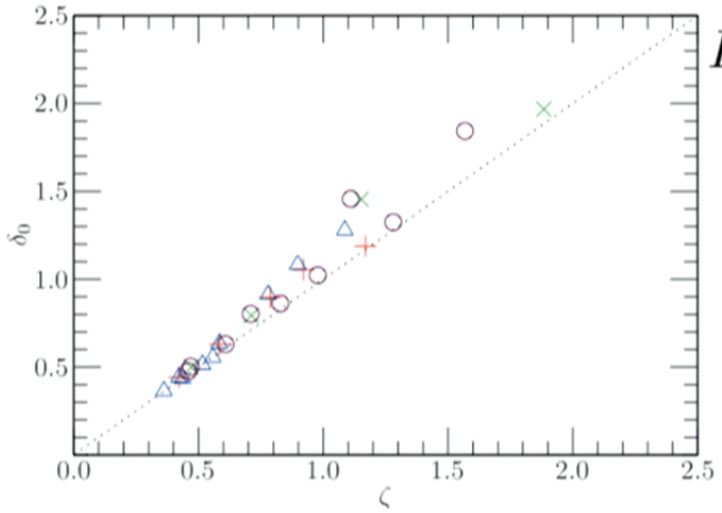

$$\hat{H} = -\sum_{\langle l,m \rangle} \sigma_l^Z \sigma_m^Z - B \sum_l \sigma_l^X$$

$$\epsilon_Z(\delta) \propto \exp(-\delta/\delta_0)$$

$$G_Z(x) \propto \exp(-x/\zeta)$$

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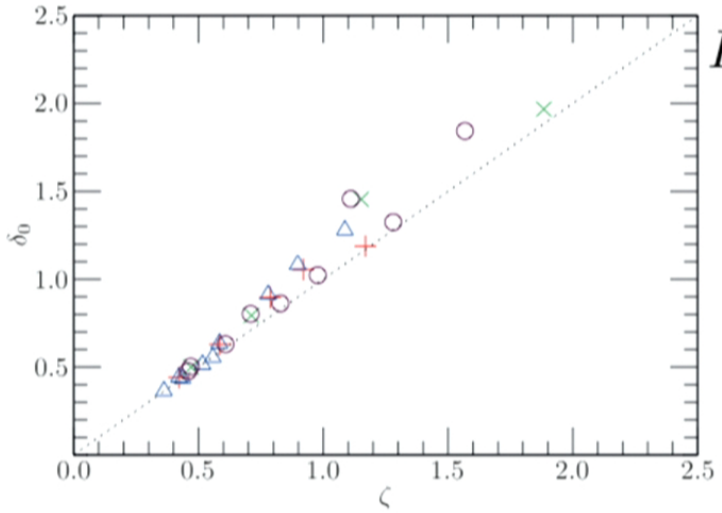

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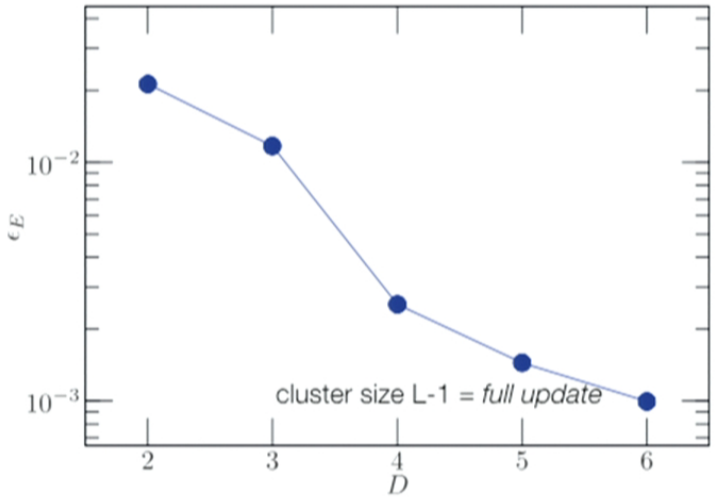
$$\left.\begin{aligned} \epsilon_Z(\delta) &\propto \exp(-\delta/\delta_0) \\ G_Z(x) &\propto \exp(-x/\zeta) \end{aligned}\right\} \rightarrow \delta_0 \approx \zeta$$

Finite PEPS Algorithms

Finite PEPS Performance

Lubasch, Cirac, and Bañuls, PRB 90, 064425 (2014).

PEPS Ground States of 14x14 *Heisenberg Model*



$$\hat{H} = \sum_{\langle l,m \rangle} \vec{S}_l \cdot \vec{S}_m$$

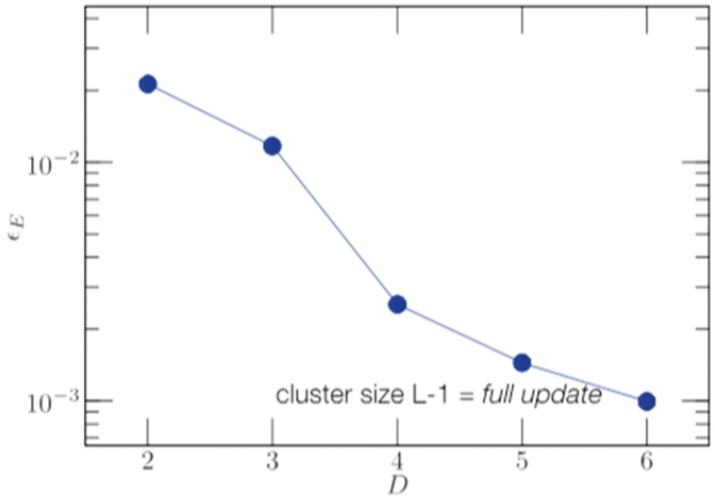
$$\epsilon_E(D) := |E(D) - E_{\text{exact}}|/|E_{\text{exact}}|$$

Finite PEPS Algorithms

Finite PEPS Performance

Lubasch, Cirac, and Bañuls, PRB 90, 064425 (2014).

PEPS Ground States of 14x14 *Heisenberg Model*



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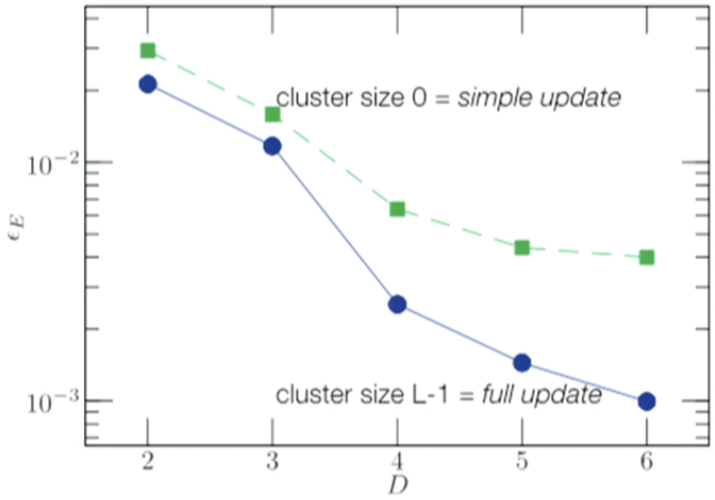

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Finite PEPS Algorithms

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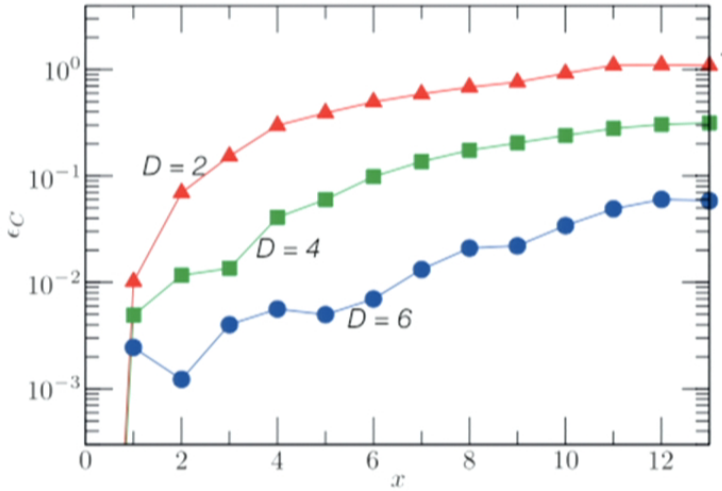
PEPS Ground States of 14x14 *Heisenberg Model*

filled symbols:
full update



$$\hat{H} = \sum_{\langle l,m \rangle} \vec{S}_l \cdot \vec{S}_m$$

$$C(x) := |\langle \vec{S}_l \cdot \vec{S}_{l+x} \rangle|$$

$$\epsilon_C(x) := |C(x) - C_{\text{exact}}(x)|/|C_{\text{exact}}(x)|$$

An Application of Finite PEPS

Adiabatic Preparation of Heisenberg AFM

Motivation

Simulation of *t-J model*:

- might explain *high-temperature superconductivity in cuprates*
- is *hard for classical computers*

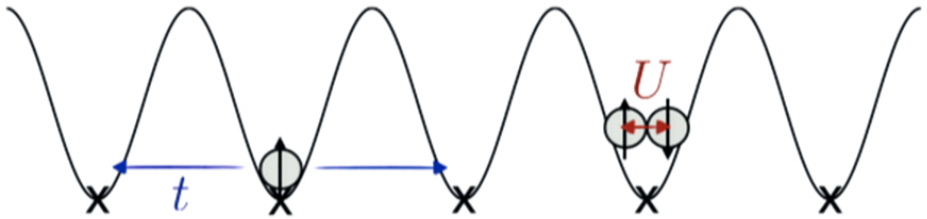
Adiabatic Preparation of Heisenberg AFM

Experimental Status

Schneider *et al.*, Science 322, 1520 (2008).

Jördens *et al.*, Nature 455, 204 (2008).

- realization of *fermionic Hubbard model* in optical lattice:



$$\hat{H} = -t \sum_{\langle l,m \rangle,\sigma} (c^{\dagger}_{l,\sigma} c_{m,\sigma} + c^{\dagger}_{m,\sigma} c_{l,\sigma}) + U \sum_{l} \hat{n}_{l,\uparrow} \hat{n}_{l,\downarrow}$$

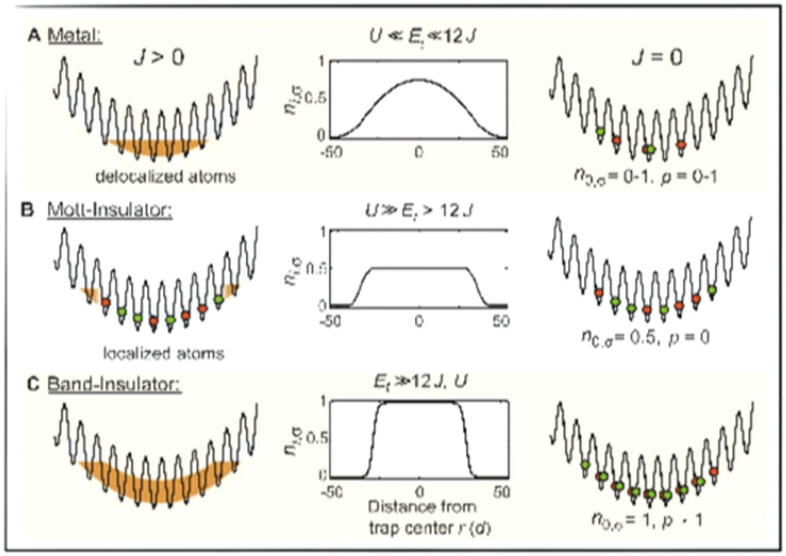
Adiabatic Preparation of Heisenberg AFM

Experimental Status

Schneider *et al.*, Science 322, 1520 (2008).

- realization of *various phases*:

$$\hat{H} + V_{\mathrm{t}} \sum_{l} (l - l_0)^2 \hat{n}_l$$



- difficulty: *temperatures too high* for magnetic order

Adiabatic Preparation of Heisenberg AFM

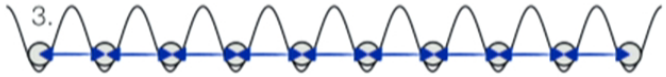
Adiabatic Protocol

Lubasch, Murg, Schneider, Cirac, and Bañuls, PRL 107, 165301 (2011).

initial state:
band insulator

intermediate state:
decoupled singlets

final state:
desired AFM



Tensor Networks and Density Functional Theory?

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Approximating the Universal Functional

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Motivation

- *density functional theory (DFT)* can deal with *realistic materials*

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- however, typically, *systematically improving a final DFT result* is *difficult*

Approximating the Universal Functional

Motivation

- *density functional theory (DFT)* can deal with *realistic materials*
- however, typically, *systematically improving a final DFT result* is *difficult*
- within *tensor network states (TNS)* a *systematic improvement* is *straightforward*

↓

Can we merge the good properties of DFT and TNS?

Approximating the Universal Functional

Setting

- space: *one-dimensional*, *discretized* and *finite*

$$l \in \{1, 2, \ldots, L\}$$

lattice site ↔ l ; L ↔ lattice length

Approximating the Universal Functional

Setting

- space: *one-dimensional*, *discretized* and *finite*

$$l \in \{1, 2, \ldots, L\}$$

lattice site ↔ l; L → lattice length

- density: *finite-dimensional* vector

$$\vec{n} := (n_1, n_2, \ldots, n_L)^{\mathrm{t}}$$

- Hubbard model with *local on-site interaction*:

$$\hat{H} = -t \sum_{l,\sigma} (c^\dagger_{l,\sigma} c_{l+1,\sigma} + c^\dagger_{l+1,\sigma} c_{l,\sigma}) + U \sum_l \hat{n}_{l,\uparrow} \hat{n}_{l,\downarrow} + \sum_l v_l \hat{n}_l$$

- Soft-Coulomb model with *non-local long-range interaction*:

$$\hat{H} = -t \sum_{l,\sigma} (c^\dagger_{l,\sigma} c_{l+1,\sigma} + c^\dagger_{l+1,\sigma} c_{l,\sigma}) + U \sum_{l \leq m} \frac{\hat{n}_l \hat{n}_m}{\sqrt{(l-m)^2 + 1}} + \sum_l v_l \hat{n}_l$$

Approximating the Universal Functional

Universal Functional and our Ansatz

- *universal functional* from energy minimization:

general Hamiltonian:

$$\hat{H} = \hat{H}_0 + \sum_l v_l \hat{n}_l$$

$$\begin{aligned}
E &= \min_{|\psi\rangle} \langle\psi|\hat{H}|\psi\rangle \\
&= \min_{\vec{n}} \left(\min_{|\psi_{\vec{n}}\rangle} \langle\psi_{\vec{n}}|\hat{H}|\psi_{\vec{n}}\rangle \right) \\
&= \min_{\vec{n}} \left(\min_{|\psi_{\vec{n}}\rangle} \langle\psi_{\vec{n}}|\hat{H}_0 + \sum_l v_l \hat{n}_l |\psi_{\vec{n}}\rangle \right) \\
&= \min_{\vec{n}} \left(\min_{|\psi_{\vec{n}}\rangle} \langle\psi_{\vec{n}}|\hat{H}_0|\psi_{\vec{n}}\rangle + \sum_l v_l n_l \right) \\
&=: \min_{\vec{n}} \left(F(\vec{n}) + \sum_l v_l n_l \right)
\end{aligned}$$

Approximating the Universal Functional

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\end{aligned}
$$

general Hamiltonian:

$$\hat{H} = \hat{H}_0 + \sum_l v_l \hat{n}_l$$

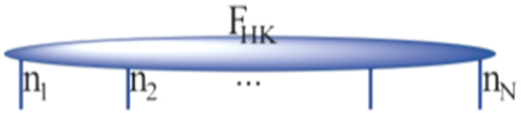
- *approximate* exact functional by our ansatz:

exact functional $F(\vec{n}) \approx G(\vec{n})$ our ansatz

Approximating the Universal Functional

MPS Approximation

- we construct the *exact functional*:



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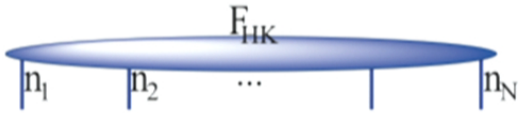
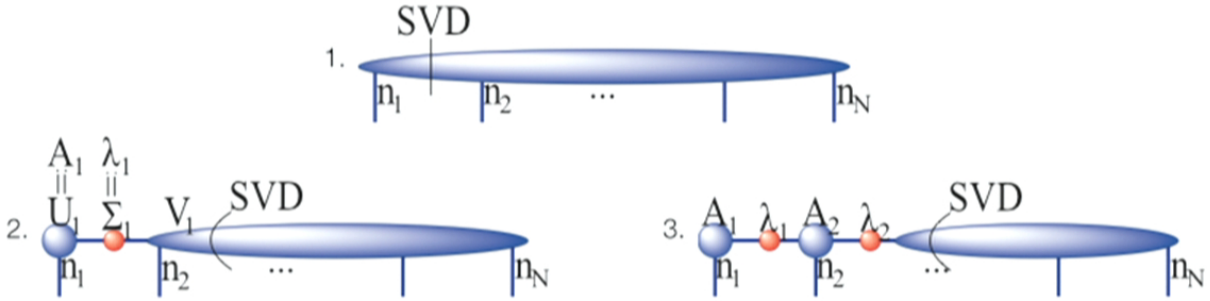


- we find its optimal *MPS approximation*:



Approximating the Universal Functional

Our Ansatz

$$G_X(\vec{n}) = \sum_{x=0}^{X} \sum_{l=1}^{L-x} g_{x,l}(n_l, n_{l+x})$$

$$= \sum_{l=1}^{L} g_{x=0,l}(n_l) + \sum_{l=1}^{L-1} g_{x=1,l}(n_l, n_{l+1}) + \sum_{l=1}^{L-2} g_{x=2,l}(n_l, n_{l+2}) +$$

$$\sum_{l=1}^{L-3} g_{x=3,l}(n_l, n_{l+3}) + \sum_{l=1}^{L-4} g_{x=4,l}(n_l, n_{l+4}) + \dots$$

Approximating the Universal Functional

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$$\sum_{l=1}^{L-3} g_{x=3,l}(n_l, n_{l+3}) + \sum_{l=1}^{L-4} g_{x=4,l}(n_l, n_{l+4}) + \dots$$

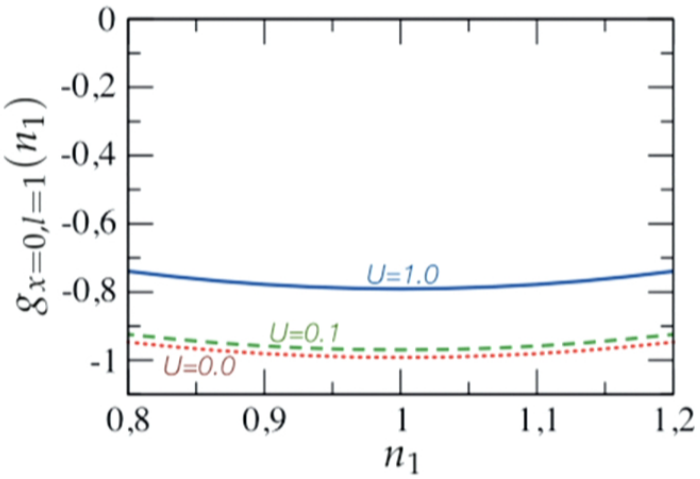
- *non-locality* can be increased *systematically*

Approximating the Universal Functional

Our Ansatz: General Tensors

L=4=N

- our *local terms*:

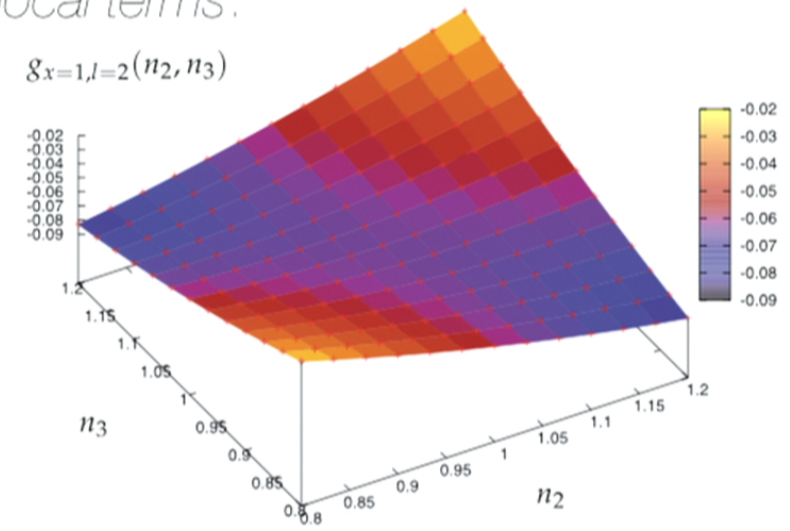


Approximating the Universal Functional

Our Ansatz: General Tensors

$L=4=N$

- our *non-local terms*:



$$g_{x>0,l}(n_l, n_{l+x}) \propto (n_l - 1)(n_{l+x} - 1)$$

(Taylor expansion around uniform density)

Approximating the Universal Functional

Our Ansatz: Cubic Splines

- we express our ansatz in terms of *cubic splines*

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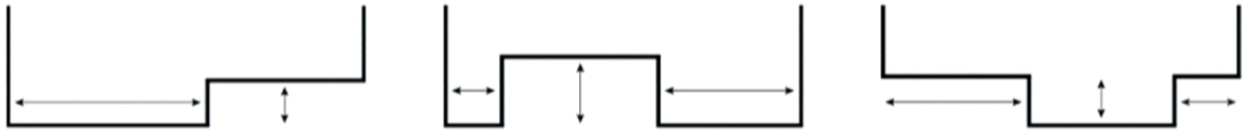
- we express our ansatz in terms of *cubic splines*
- *large systems*: exact functional is not feasible
- physically motivated *training sets*:

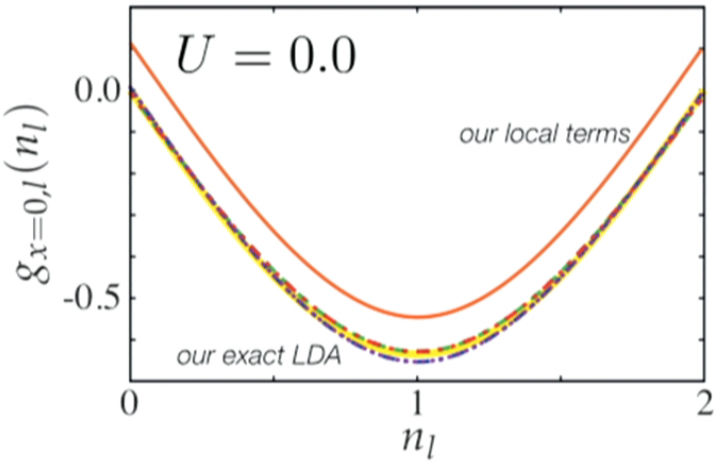


- *target sets* shall be different from *training sets*

Approximating the Universal Functional

Our Ansatz: Cubic Splines

- we can reproduce *our exact LDA*:



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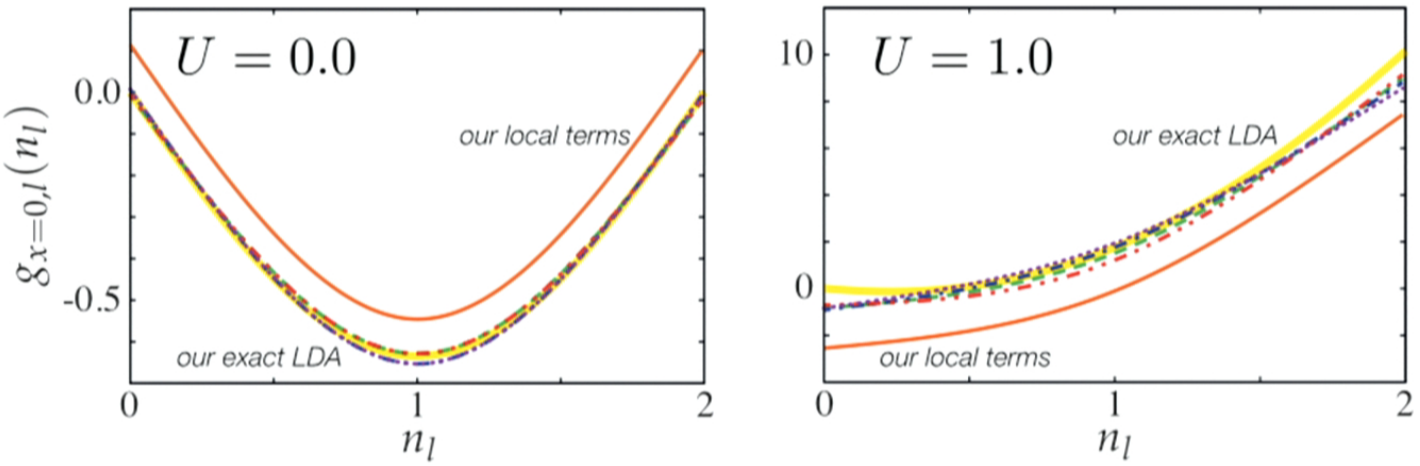
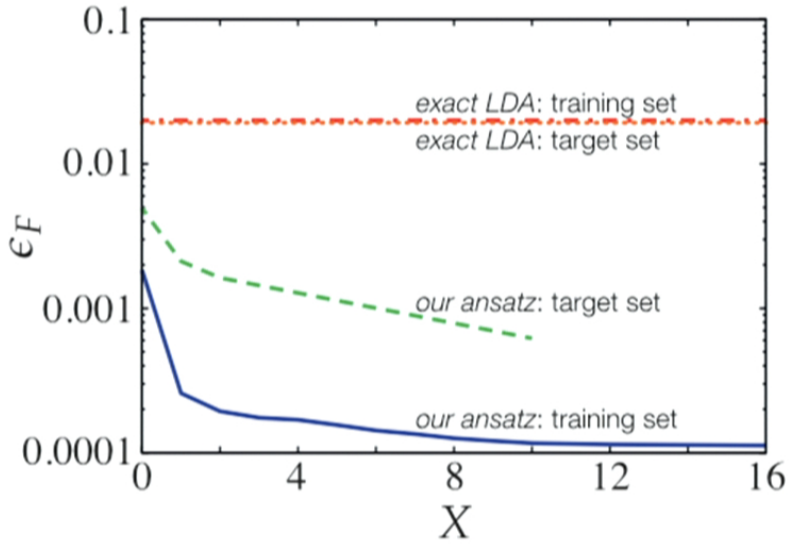


Approximating the Universal Functional

Performance of our Ansatz

Non-interacting Fermions



ϵ_F : *mean relative approximation error*

Recent Developments with Tensor Networks

Conclusions

- Finite PEPS Algorithms
  - Motivation
  - Finite PEPS
  - PEPS Contraction
  - Finite PEPS Performance

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- Tensor Networks and Density Functional Theory?

work in progress together with: Fuks, Appel, Rubio, Bañuls, and Cirac.