How local is the information in a MPS/PEPS tensor-network ?

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arXiv: 1603.06049

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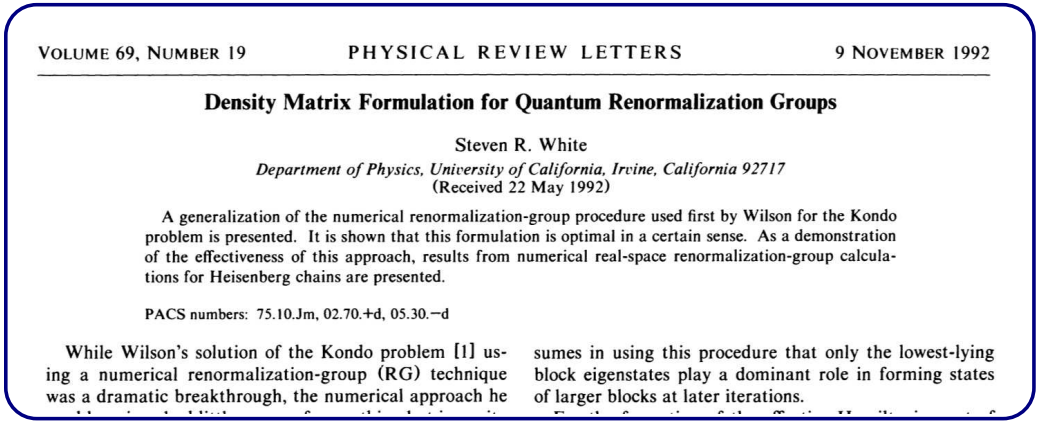
Hehuan Mountain

In 1992 Steven White introduced DMRG



VOLUME 69, NUMBER 19 PHYSICAL REVIEW LETTERS 9 NOVEMBER 1992

Density Matrix Formulation for Quantum Renormalization Groups

Steven R. White

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(Received 22 May 1992)

A generalization of the numerical renormalization-group procedure used first by Wilson for the Kondo problem is presented. It is shown that this formulation is optimal in a certain sense. As a demonstration of the effectiveness of this approach, results from numerical real-space renormalization-group calculations for Heisenberg chains are presented.

PACS numbers: 75.10.Jm, 02.70.+d, 05.30.−d

While Wilson's solution of the Kondo problem [1] using a numerical renormalization-group (RG) technique was a dramatic breakthrough, the numerical approach he

sumes in using this procedure that only the lowest-lying block eigenstates play a dominant role in forming states of larger blocks at later iterations.

DMRG = Density Matrix Renormalization Group

A variational algorithm to approximate the ground state of spin chains using a 1D tensor-network ansatz (MPS)

Example: ground energy of S=1 anti-ferromagnetic Heisenberg chain:

Monte-Carlo	**DMRG ('92)**	**DMRG ('93)**
-1.401 5(5)	-1.401 484(2)	-1.401 484 038 971(4)

Fast-forward 23 years...

PHYSICAL REVIEW X **5,** 041041 (2015)

Solutions of the Two-Dimensional Hubbard Model: Benchmarks and Results from a Wide Range of Numerical Algorithms

J. P. F. LeBlanc,[1] Andrey E. Antipov,[1] Federico Becca,[2] Ireneusz W. Bulik,[3] Garnet Kin-Lic Chan,[4] Chia-Min Chung,[5] Youjin Deng,[6] Michel Ferrero,[7] Thomas M. Henderson,[3,8] Carlos A. Jiménez-Hoyos,[3] E. Kozik,[9] Xuan-Wen Liu,[6] Andrew J. Millis,[10] N. V. Prokof'ev,[11,12] Mingpu Qin,[13] Gustavo E. Scuseria,[3,8] Hao Shi,[13] B. V. Svistunov,[11,12] Luca F. Tocchio,[2] I. S. Tupitsyn,[11] Steven R. White,[5] Shiwei Zhang,[13] Bo-Xiao Zheng,[4] Zhenyue Zhu,[5] and Emanuel Gull[1,*]

[13]*Department of Physics, College of William and Mary, Williamsburg, Virginia 23187, USA*

(Received 9 May 2015; revised manuscript received 30 October 2015; published 14 December 2015)

Numerical results for ground-state and excited-state properties (energies, double occupancies, and Matsubara-axis self-energies) of the single-orbital Hubbard model on a two-dimensional square lattice are presented, in order to provide an assessment of our ability to compute accurate results in the thermodynamic limit. Many methods are employed, including auxiliary-field quantum Monte Carlo, bare and bold-line diagrammatic Monte Carlo, method of dual fermions, density matrix embedding theory, density matrix renormalization group, dynamical cluster approximation, diffusion Monte Carlo within a fixed-node approximation, unrestricted coupled cluster theory, and multireference projected Hartree-Fock methods. Comparison of results obtained by different methods allows for the identification of uncertainties and systematic errors. The importance of extrapolation to converged thermodynamic-limit values is emphasized. Cases where agreement between different methods is obtained establish benchmark results that may be useful in the validation of new approaches and the improvement of existing methods.

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Why are 2D T.N. methods not as successful as 1D T.N. methods?

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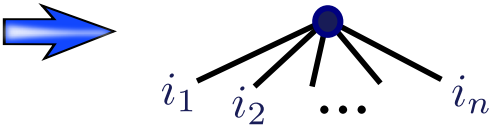
Why are 2D T.N. methods not as successful as 1D T.N. methods?

Can they be improved?

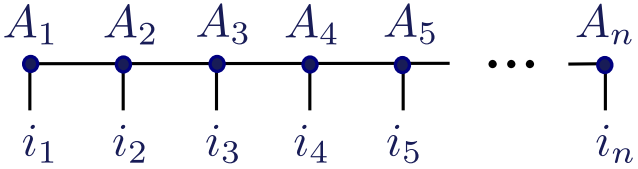
Tensor networks

$$|\psi\rangle = \sum_{i_1,\ldots,i_n} c_{i_1\ldots i_n} |i_1 \ldots i_n\rangle$$

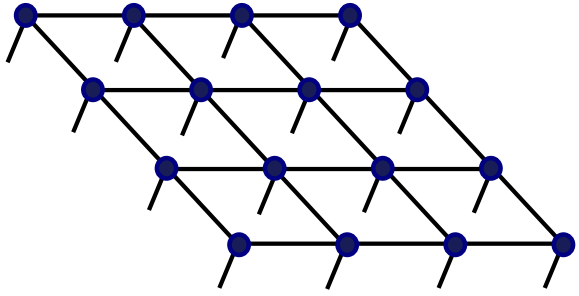


rank-n tensor

Matrix Product State (MPS)



Projected Entangled Pairs (PEPS)



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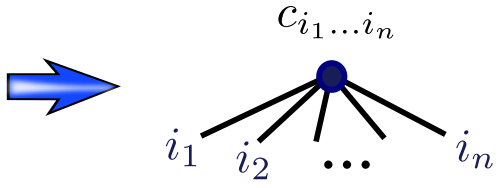

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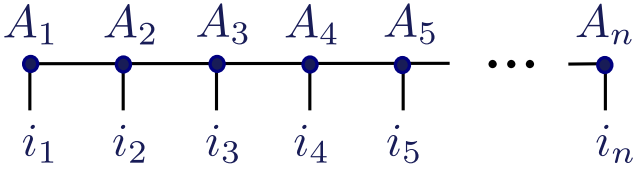

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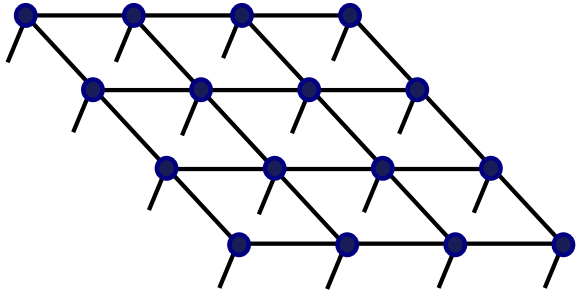
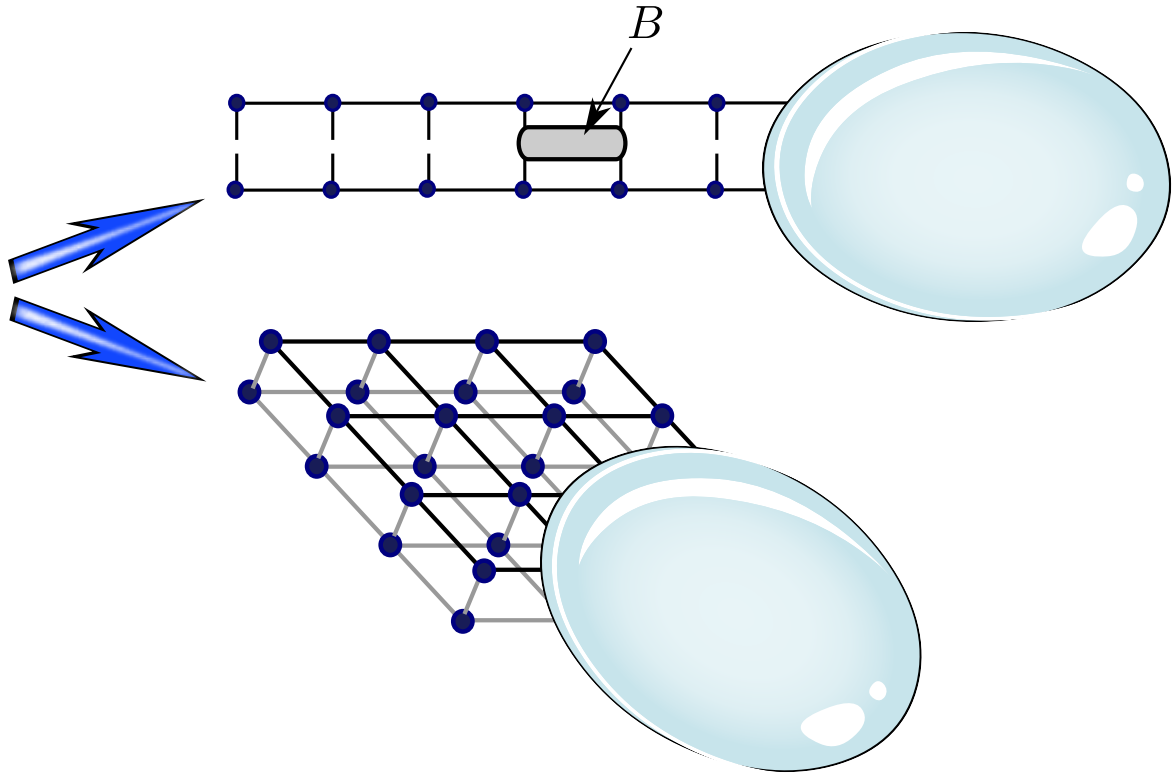


Advantages

- $2^{\mathcal{O}(n)} \rightarrow \mathcal{O}(n)$ parameters
- Network structure corresponds to entanglement structure
- Allows variational algorithms

Contracting a tensor-network

$$\langle B \rangle = \langle \psi | B | \psi \rangle$$



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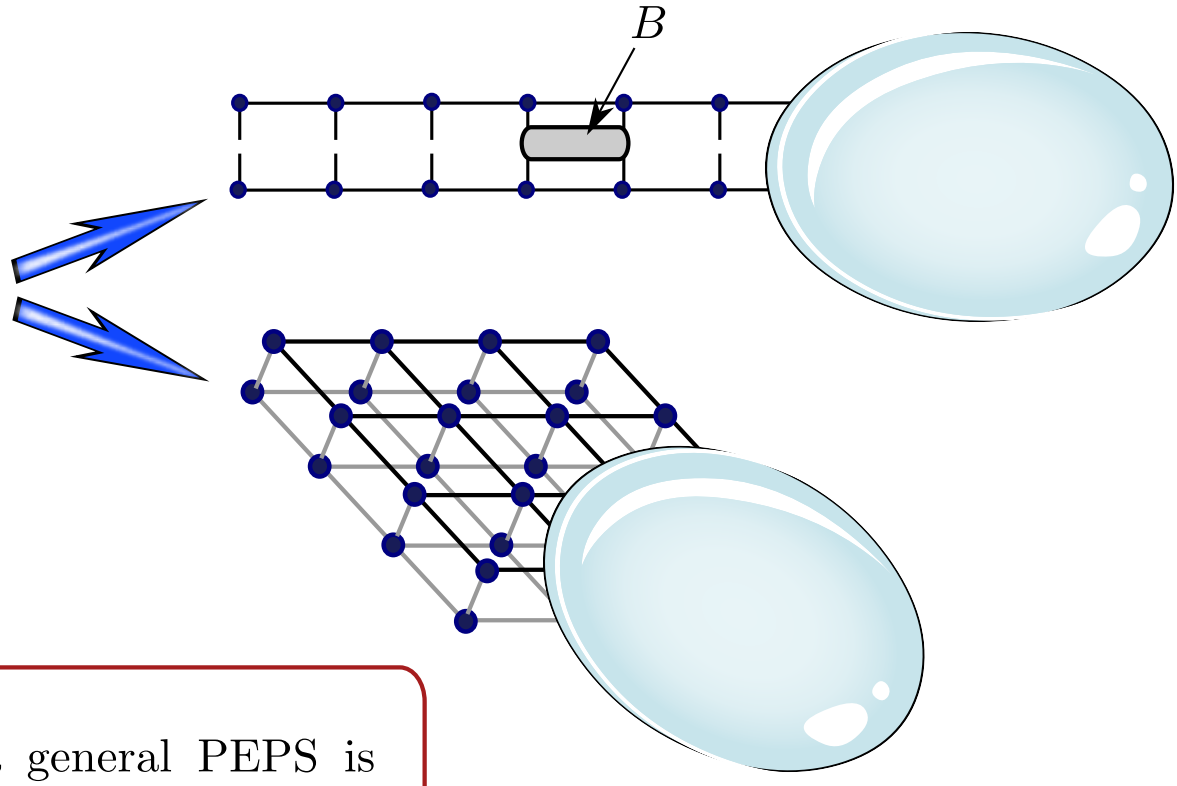

- Contracting a general PEPS is #P-hard (Schuch et. al. '07)
- One must use approximations (boundary MPS, CTM, TRG etc.)

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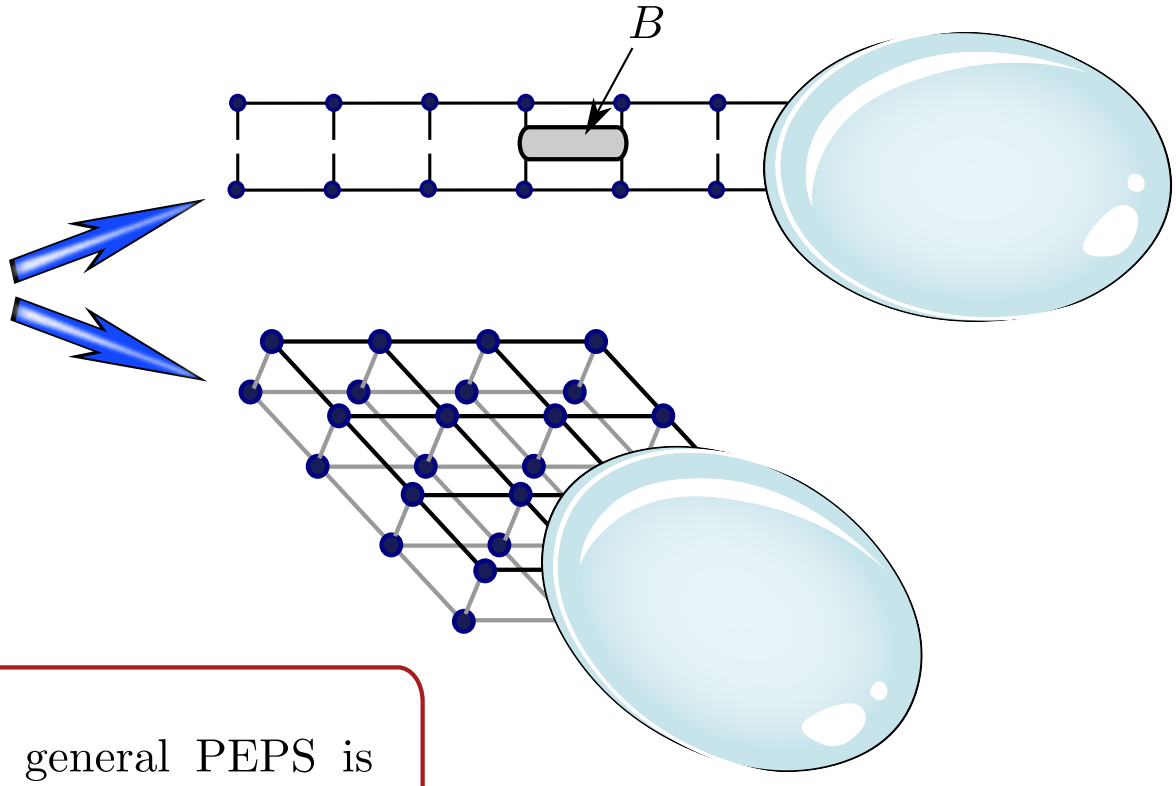


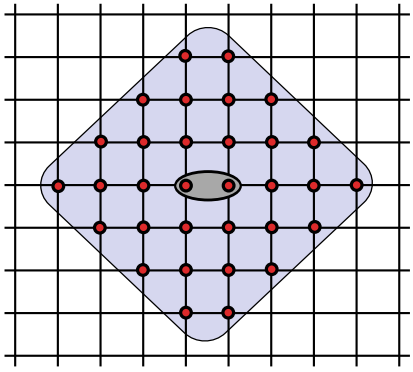
- Contracting a general PEPS is #P-hard (Schuch et. al. '07)
- One must use approximations (boundary MPS, CTM, TRG etc.)

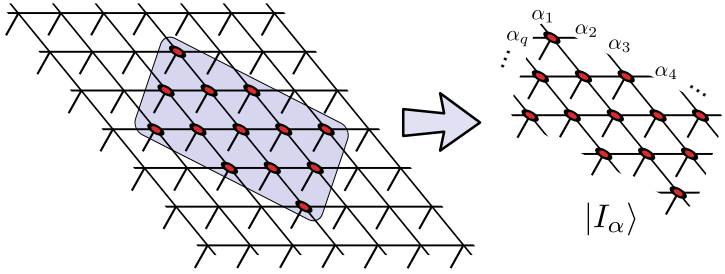
Can we approximate $\langle B \rangle$ using only a **local patch** of the T.N., assuming that $|\psi\rangle$ a ***ground state*** of a ***known*** local Hamiltonian H ?

Expectaion value from a local patch

Main Problem

Given a g.s. $|\psi\rangle$ of a known local Hamiltonian H in the form of a PEPS and a local observable B, approximate $\langle\psi|B|\psi\rangle$ using only a local patch L of the PEPS around B.





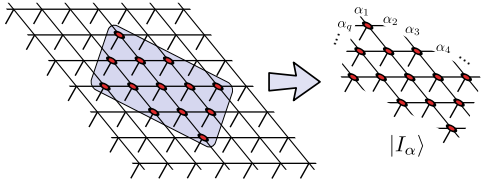
External states

Internal states

$$|\psi\rangle = \sum_{\alpha} |O_\alpha\rangle \otimes |I_\alpha\rangle$$

$$V_L := \mathrm{Span}\Big\{|I_\alpha\rangle\Big\}$$

The basic algorithm



$$|\psi\rangle = \sum_\alpha |O_\alpha\rangle \otimes |I_\alpha\rangle \qquad V_L := \mathrm{Span}\Big\{|I_\alpha\rangle\Big\}$$

Define: $\rho_L \stackrel{\text{def}}{=} \mathrm{Tr}_{L^c} |\psi\rangle\langle\psi|$ and $P_L \stackrel{\text{def}}{=}$ projector onto V_L

Then: $\rho_L = P_L \rho_L P_L$

Therefore: $\langle\psi|B|\psi\rangle = \mathrm{Tr}(\rho_L B) = \mathrm{Tr}(P_L \rho_L P_L B) = \mathrm{Tr}(\rho_L \cdot P_L B P_L)$

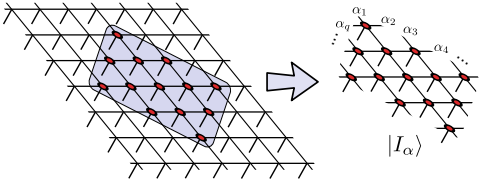
The basic method: Find b_{min}, b_{max}, the minimal/maximal eigenvalues of $P_L B P_L$. Then $\langle\psi|B|\psi\rangle \in [b_{min}, b_{max}]$

Lemma

If $|\psi\rangle$ has an exponential decay of correlations with correlation length ξ, and L is a patch of radius ℓ, then for every eigenvalue b_i of $P_L B P_L$,

$$|b_i - \langle\psi|B|\psi\rangle| \leq \frac{e^{-\ell/\xi}}{\min_{V_L} \langle x|\rho_L|x\rangle}$$

The basic algorithm



$$|\psi\rangle = \sum_\alpha |O_\alpha\rangle \otimes |I_\alpha\rangle \qquad V_L := \mathrm{Span}\Big\{|I_\alpha\rangle\Big\}$$

Define: ρ_L

Then: ρ_L

Therefore:

The basic lues

- In 1D we expect: $\min_{V_L} \langle x|\rho_L|x\rangle = \mathcal{O}(1)$
- In 2D we expect: $\min_{V_L} \langle x|\rho_L|x\rangle = \mathcal{O}\left(e^{-\mathcal{O}(\ell)}\right)$
- In 3D we expect: $\min_{V_L} \langle x|\rho_L|x\rangle = \mathcal{O}\left(e^{-\mathcal{O}(\ell^2)}\right)$

Can we do better?

Lemma

If $|\psi\rangle$ has an exponential decay of correlations with correlation length ξ, and L is a patch of radius ℓ, then for every eigenvalue b_i of $P_L B P_L$,

$$|b_i - \langle\psi|B|\psi\rangle| \leq \frac{e^{-\ell/\xi}}{\min_{V_L} \langle x|\rho_L|x\rangle}$$

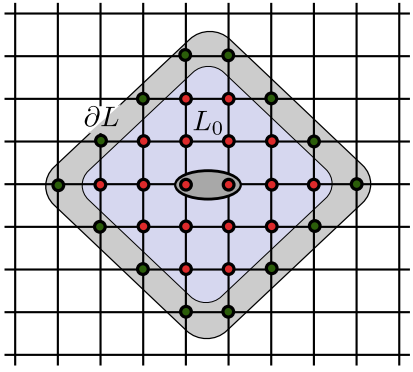
Commutator Gauge Optimization (CGO)

Main idea: Optimize over all local operators K for which $\langle B \rangle = \langle K \rangle$

Construction: For any A supported on L_0, define

$$K_A \stackrel{\text{def}}{=} B + [H, A] = B + [H_L, A]$$

$$\langle\psi|[H, A]|\psi\rangle = 0 \quad \Longrightarrow \quad \langle\psi|B|\psi\rangle = \langle\psi|K_A|\psi\rangle$$



Algorithm:

- Fix a set of random operators A_i supported on L_0
- $$b_{max} = \min_{A_i} \lambda_{max}\left[P_L(B + [H_L, A_i])P_L\right]$$
- $$b_{min} = \max_{A_i} \lambda_{min}\left[P_L(B + [H_L, A_i])P_L\right]$$

This can be easily written as an SDP problem

The dual problem

If for every A, we have $\mathrm{Tr}_L(\rho_L[A, H_L]) = 0$, then

$$0 = \mathrm{Tr}_L(A[H_L, \rho_L]) = \mathrm{Tr}_{L_0} A \, \mathrm{Tr}_{\partial L}[H_L, \rho_L] \quad \Longrightarrow \quad \boxed{\mathrm{Tr}_{\partial L}[H_L, \rho_L] = 0}$$

The dual problem:

find $\quad b_{max} = \max_{\rho_L} \mathrm{Tr}(\rho_L B) \;\; , \;\; b_{min} = \min_{\rho_L} \mathrm{Tr}(\rho_L B)$

subject to:

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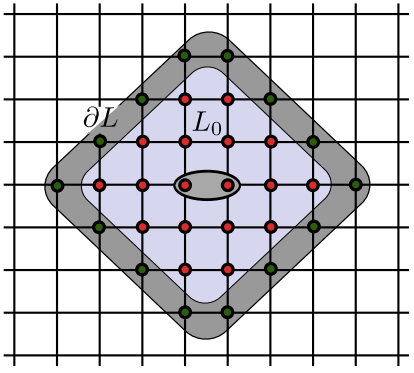

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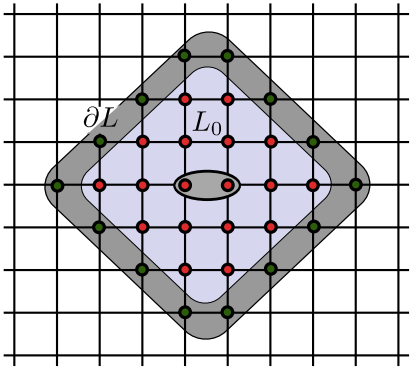

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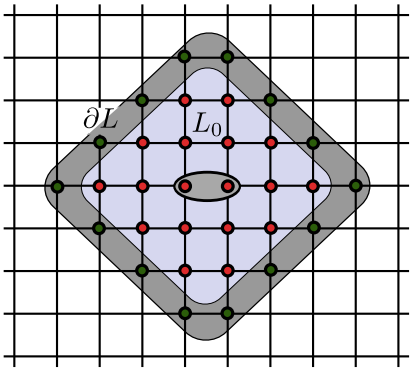

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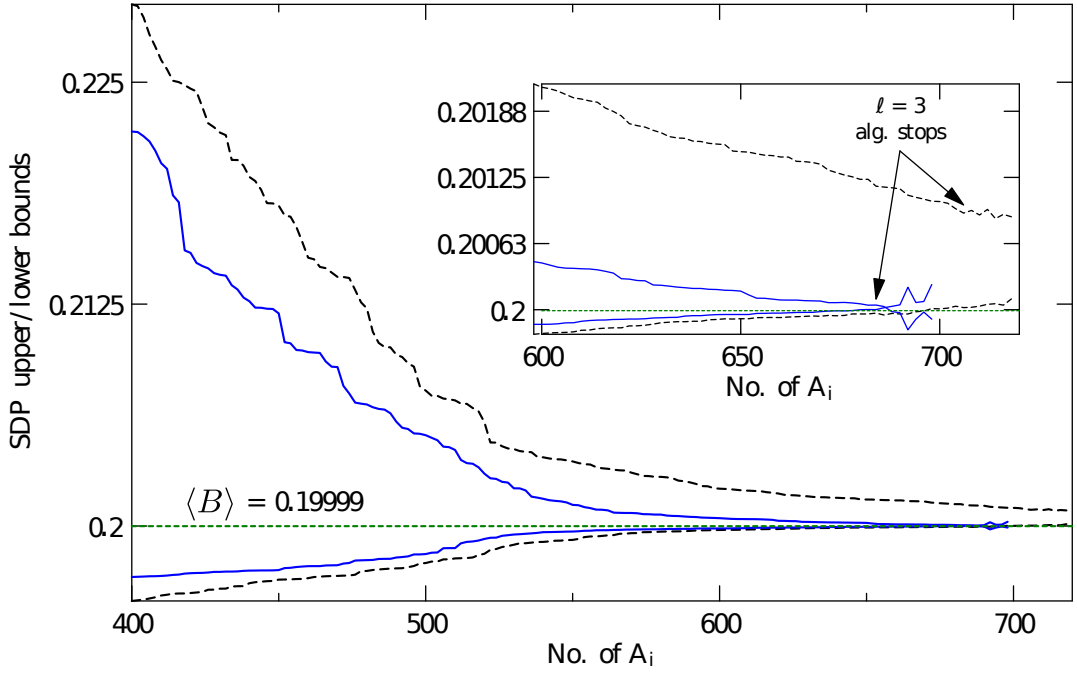
When there's an area-law, no. of variables $= \exp(\mathcal{O}(|\partial L|))$ while no. of equations $= \exp(\mathcal{O}(|L|))$ - CGO gives non-trivial results.

Numerical Results

We tested CGO and the basic method for several 1D chains

Example: XY model with random magnetic field (spectral gap=0.06)

Obs	exact $\langle B \rangle$	basic $\ell = 3$	CGO $\ell = 3$	basic $\ell = 4$	CGO $\ell = 4$
$P_x P_x$	0.19999	$[0.01222, 0.71539]$ (0.36)	$[0.19997, 0.20091]$ (0.0005)	$[0.02336, 0.66029]$ (0.32)	$[0.19999, 0.20007]$ (4×10^{-5})
$P_z P_z$	0.89168	$[0.20769, 0.98444]$ (0.39)	$[0.88757, 0.89180]$ (0.002)	$[0.19351, 0.97041]$ (0.39)	$[0.89144, 0.89168]$ (0.0001)
Random	0.27118	$[0.02703, 0.42696]$ (0.2)	$[0.27025, 0.27116]$ (0.0005)	$[0.03769, 0.49442]$ (0.23)	$[0.27109, 0.27116]$ (4×10^{-5})



Summary

- Efficient contraction of a 2D tensor-network is the main obstacle for good 2D tensor-based algorithms.
- If we assume that the T.N. is a good approximation to the ground state then local patches can be used to approximate a local expectation value
- Non-trivial local constraints for global eigenstates of H:

$$\mathrm{Tr}_{\partial L}[H_L, \rho_L] = 0$$

- Can we turn it into a practical algorithm?
- Can it be used as a criteria to test the proximity of the T.N. to the true ground state (other than just the energy)
- Can it be used to prove rigorous results about the complexity of the LH problem?
- Can it be used elsewhere: MC simulations, MBL, ...

Thank you !