Lower bounds on ground-state energies of local Hamiltonians through the renormalization group

arxiv:2212.03014

Ilya Kull, Norbert Schuch, Ben Dive and Miguel Navascues

University of Vienna, IQOQI Vienna

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Outline

$H = \sum_i h_i$, h_i act locally, $\dim \mathcal{H} = d^N$

$$\text{Find } \min_{\psi \in \mathcal{H}} \langle \psi | H | \psi \rangle$$

Intro:

- Locality $\Rightarrow$ **variational** vs. **relaxation** (aka **bootstrap**) approaches
- **Variational** principle + **renormalization group**
  $\Rightarrow$ tensor-networks methods (e.g. DMRG)
- ...still need good lower bounds,
  existing methods scale as $\exp(n)$

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Our method:

- **Relaxation** + **renormalization group** $\Rightarrow$ efficient* lower bounds

"Corner of Hilbert Space" — The Variational Approach

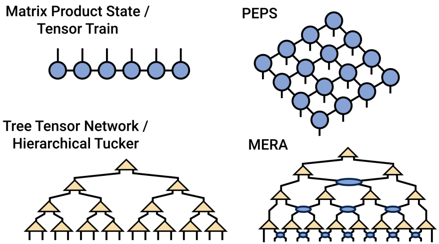
$H = \sum_i h_i$, h_i act locally, $\dim \mathcal{H} = d^N$

$$\min_{\psi \in \mathcal{C} \subset \mathcal{H}} \langle \psi | H | \psi \rangle \approx \min_{\psi \in \mathcal{H}} \langle \psi | H | \psi \rangle$$

"Corner of Hilbert Space" — The Variational Approach

$H = \sum_i h_i$, h_i act locally, $\dim \mathcal{H} = d^N$

$$\min_{\psi \in \mathcal{C} \subset \mathcal{H}} \langle \psi | H | \psi \rangle \geq \min_{\psi \in \mathcal{H}} \langle \psi | H | \psi \rangle \geq ?$$



[tensornetwork.org]
[Cirac and Verstraete, J.Phys.A (2009)]

Lower Bounds — Relaxation Methods

$H = \sum_i h_i$, h_i act locally, $\dim \mathcal{H} = d^N$

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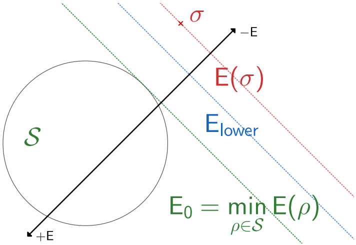

Applications

- Central to physics and chemistry:
  Certify variational solutions,
  benchmark methods
- Quantum information and foundations:
  detection, certification, falsification
- Quantum complexity theory
  MAX-k-SAT $\xrightarrow{\text{quantum}}$ k-local H min. energy

Lower Bounds Through Constraints Relaxation

$$\min_{\psi \in \mathcal{H}} \langle \psi | H | \psi \rangle$$

$$H = \sum_i h_i,\ h_i = h_{a_i} \otimes \mathbb{I}_{a_i^c}$$

Lower Bounds Through Constraints Relaxation

$$\min_{\psi \in \mathcal{H}} \langle \psi | H | \psi \rangle = \min_{\psi \in \mathcal{H}} \sum_i \langle \psi | h_i | \psi \rangle$$

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Lower Bounds Through Constraints Relaxation

$$\min_{\psi\in\mathcal{H}}\langle\psi|H|\psi\rangle = \min_{\psi\in\mathcal{H}}\sum_i \langle\psi|h_i|\psi\rangle$$
$$= \min_{\{\rho_i\}\leftarrow\psi}\sum_i \mathrm{Tr}(h_i\rho_i)$$

"$\{\rho_i\} \leftarrow \psi$" $\Leftrightarrow$ there exists a state $\psi \in \mathcal{H}$ such that ρ_i are its reduced states. Hard!!

$H = \sum_i h_i,\ h_i = h_{a_i} \otimes \mathbb{I}_{a_i^c}$
ρ_i local reduced state on $a_i \subset \Lambda$

Lower Bounds Through Constraints Relaxation

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$$\geq \min_{\{\rho_i\}\in\mathcal{S}_?}\sum_i \mathrm{Tr}(h_i\rho_i) \qquad \text{(Relaxation)}$$

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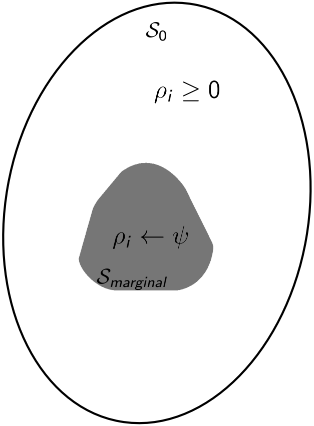
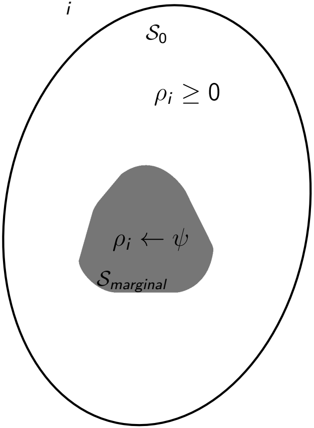
Convex Sets of Local States



Convex Sets of Local States

XXZ chain:

$$H = \sum_i (\sigma_x^i \sigma_x^{i+1} + \sigma_y^i \sigma_y^{i+1} + \Delta \sigma_z^i \sigma_z^{i+1})$$



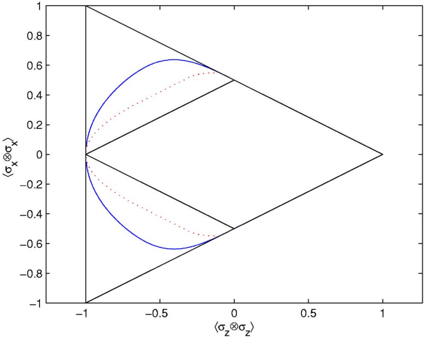
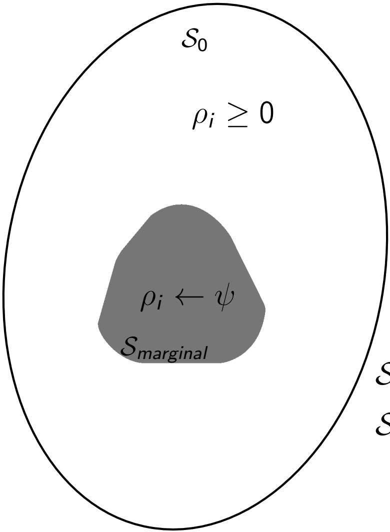


FIG. 1. (Color online) Convex sets of the possible reduced density operators of translational invariant states in the *XX-ZZ* plane: the big triangle represents all positive density operators, the inner parallellogram represents the separable states, the union of the separable cone and the convex hull of the full curved line is the complete convex set in the case of a 1D geometry, and the dashed lines represent extreme points in the 2D case of a square lattice. The singlet corresponds to the point with coordinates (−1,−1).

[Verstraete and Cirac, PRB (2006)]

Existing methods — Complete Hierarchies

$$\min_{\{\rho_i\} \leftarrow \psi} \sum_i \mathrm{Tr}(h_i \rho_i)$$



$$\mathcal{S}_0 = \{\rho_i \geq 0\}$$

$$\mathcal{S}_{\text{marginal}} = \{\{\rho_i\} \leftarrow \psi\}$$

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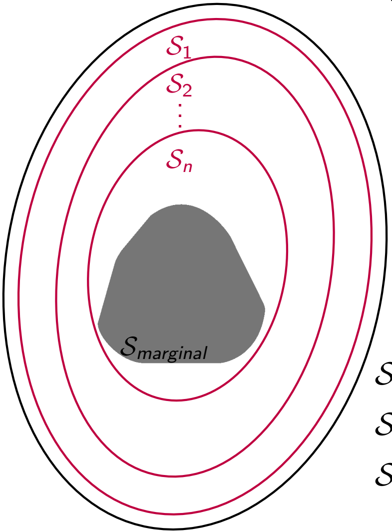


$$\mathcal{S}_0 = \{\rho_i \geq 0\}$$

$$\mathcal{S}_{\text{marginal}} = \{\{\rho_i\} \leftarrow \psi\} = \mathcal{S}_\infty$$

$$\mathcal{S}_0 \supset \mathcal{S}_1 \supset \mathcal{S}_2 \supset \ldots \supset \mathcal{S}_n \supset \ldots \supset \mathcal{S}_{\text{marginal}}$$

Existing methods — Complete Hierarchies

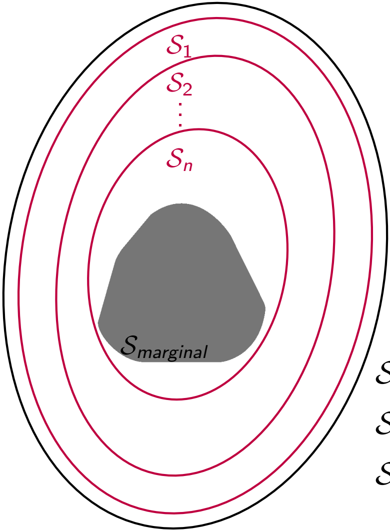
$$\min_{\{\rho_i\}\leftarrow\psi}\sum_i \mathrm{Tr}(h_i\rho_i) \geq \ldots \geq \min_{\{\rho_i\}\in\mathcal{S}_n}\sum_i \mathrm{Tr}(h_i\rho_i)$$

$$\vdots$$

$$\geq \min_{\{\rho_i\}\in\mathcal{S}_2}\sum_i \mathrm{Tr}(h_i\rho_i)$$

$$\geq \min_{\{\rho_i\}\in\mathcal{S}_1}\sum_i \mathrm{Tr}(h_i\rho_i)$$

$$\geq \min_{\{\rho_i\}\in\mathcal{S}_0}\sum_i \mathrm{Tr}(h_i\rho_i)$$



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History and Related Methods

- **Anderson bounds:**
  [Anderson, Limits on the Energy of the Antiferromagnetic Ground State, Phys. Rev. 83, (1951)]
- **Quantum chemistry: (RDMT)**
  [Mazziotti and Rice, Reduced-Density-Matrix Mechanics, Wiley & Sons (2007)]
  [Klyachko, Quantum marginal problem and N-representability, J. Phys: Conf. Ser. 36, (2006)]
- **Quantum information / foundations: (NPA hierarchy)**
  Bounding the set of quantum correlations
  [Navascués, Pironio & Acín, Phys. Rev. Lett. 98, (2007)
- **Optimization, complexity theory:**
  Lasserre/Parrilo/SOS hierarchy [Lasserre, Global optimization with polynomials and the problem of moments, SIAM J. Optim. 11, (2001)]
- **Bootstrap methods:**
  Conformal bootstrap Poland, Rychkov & Vichi, Rev. Mod. Phys. 91, (2019), Random matrix models Lin, J. High Energ. Phys. 90 (2020) , 3D classical Ising model [Cho et. al. arxiv:2206.12538], Gap in 1D quantum Ising model [Nancarrow & Xin, arXiv:2211.03819] ...

Example: The LTI Hierarchy

Setting:
$H = \sum_i \tau_i(h)$, translation-invariant, nearest-neighbor interactions

$$E_{\mathsf{TI}} := \min_{\rho^{(2)},\psi_{\mathsf{TI}}} \mathrm{Tr}\left(h\rho^{(2)}\right)$$
$$\text{s.t. } \rho^{(2)} \leftarrow \psi_{\mathsf{TI}}$$

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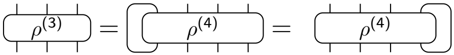
$$\rho^{(m-1)} \leftarrow \rho^{(m)}$$
$$\Updownarrow$$
$$\rho^{(m-1)} = \mathrm{Tr}_{\mathrm{L}}(\rho^{(m)}) = \mathrm{Tr}_{\mathrm{R}}(\rho^{(m)})$$



Example: The LTI Hierarchy

Setting:
$H = \sum_i \tau_i(h)$, translation-invariant, nearest-neighbor interactions

$$E_{\mathsf{TI}} \geq E_{\mathsf{LTI}}(n) = \min_{\{\rho^{(m)}\}, \cancel{\psi_{\mathsf{TI}}}} \mathrm{Tr}\left(h\rho^{(2)}\right)$$

$$\text{s.t. } \rho^{(2)} \leftarrow \rho^{(3)} \leftarrow \ldots \leftarrow \rho^{(n-1)} \leftarrow \rho^{(n)} \cancel{\leftarrow} \cancel{\psi_{\mathsf{TI}}}$$

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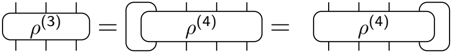
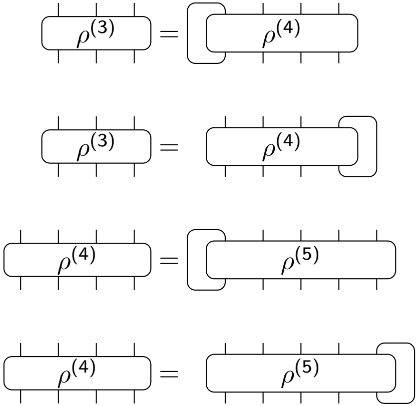
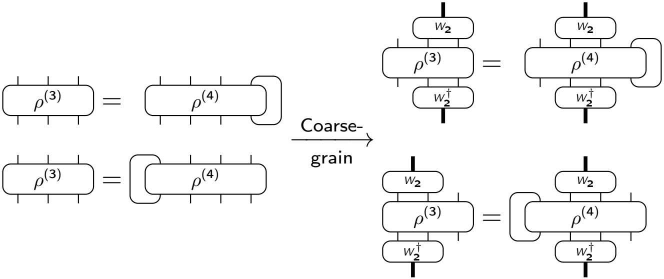


Renormalization of the LTI Constraints

We relax the constraints $\rho^{(3)} \leftarrow \rho^{(4)} \leftarrow \rho^{(5)}$



Coarse-Graining and Compression Step



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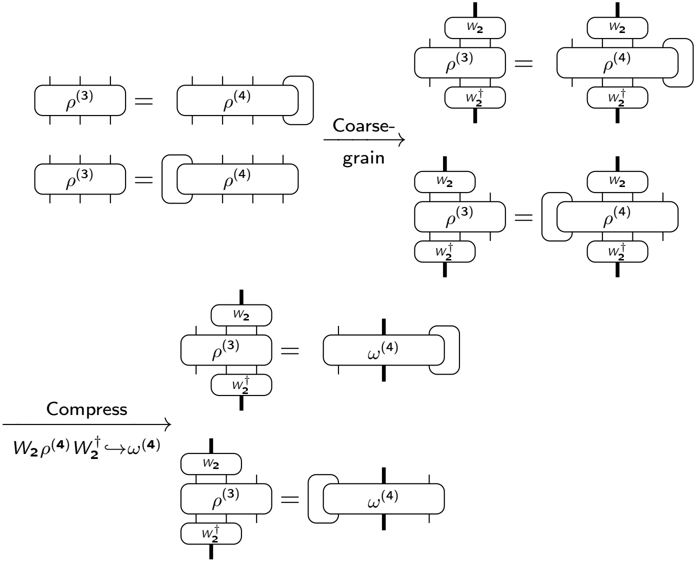
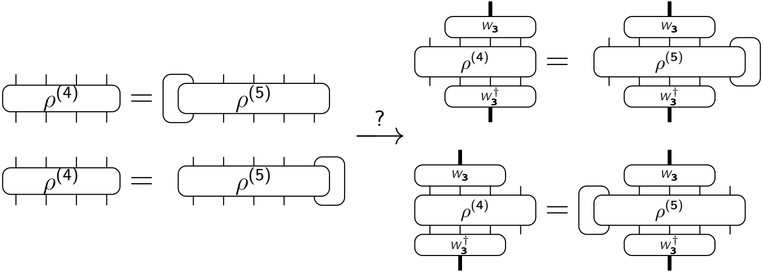
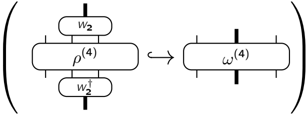


Iterative Coarse-Graining

We want:



But $\rho^{(4)}$ is no longer available



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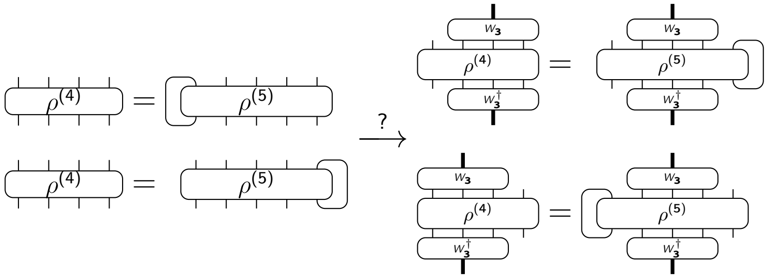

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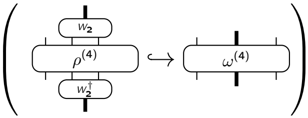

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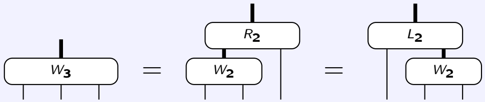

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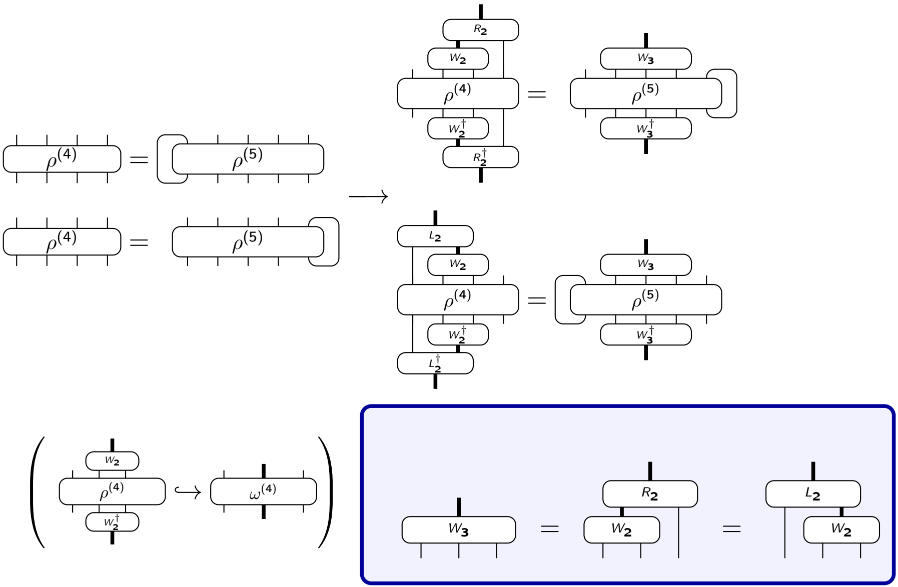

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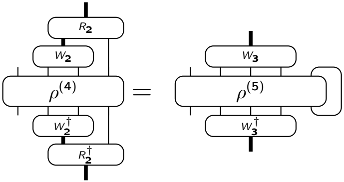
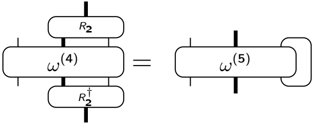
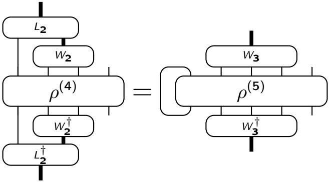
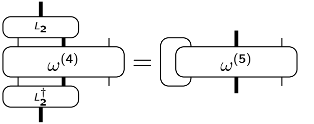
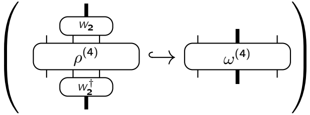


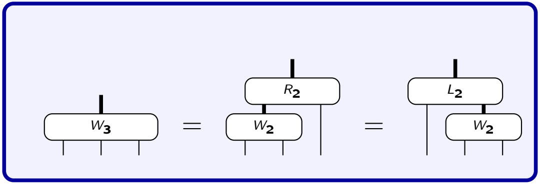


$$\xrightarrow[W_3\,\rho^{(\mathbf{5})}\,W_3^\dagger \hookrightarrow \omega^{(\mathbf{5})}]{W_2\,\rho^{(\mathbf{4})}\,W_2^\dagger \hookrightarrow \omega^{(\mathbf{4})}}$$

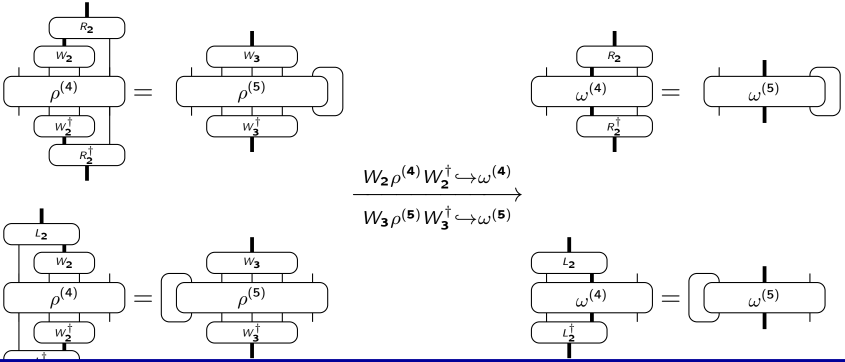




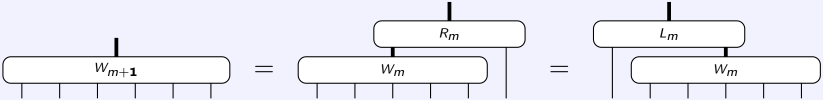




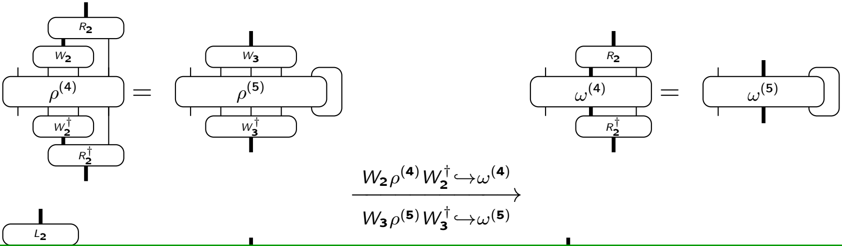
Iterative Coarse-Graining



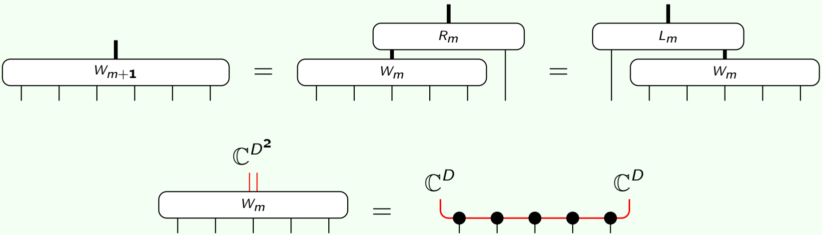
We need for all $m = 1, \ldots, n-2$



Iterative Coarse-Graining



The solution: Matrix Product States



Recap

$$E_{\mathsf{TI}} \geq E_{\mathsf{LTI}}(n) = \min_{\{\rho^{(m)}\}} \mathrm{Tr}\left(h\rho^{(2)}\right)$$

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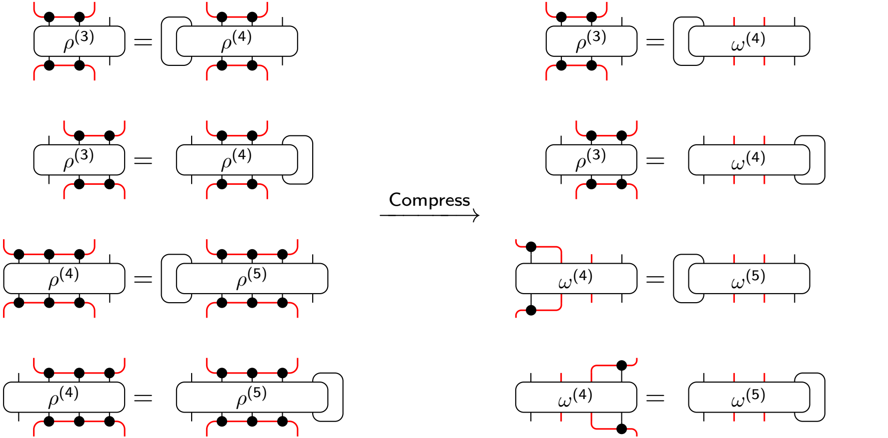
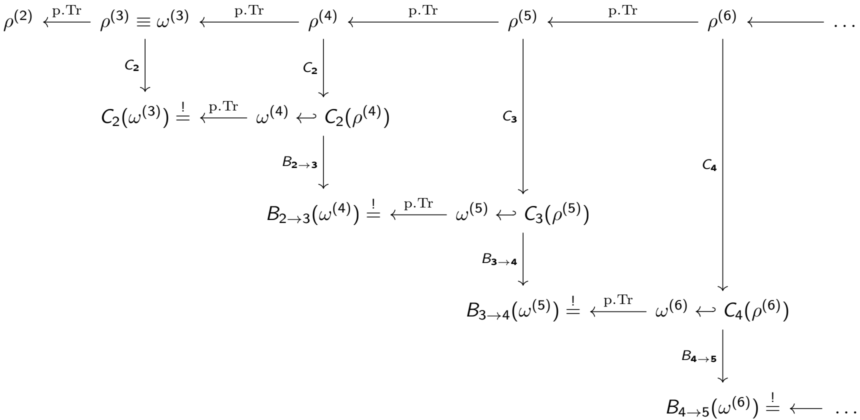


The "triangle of renormalization"



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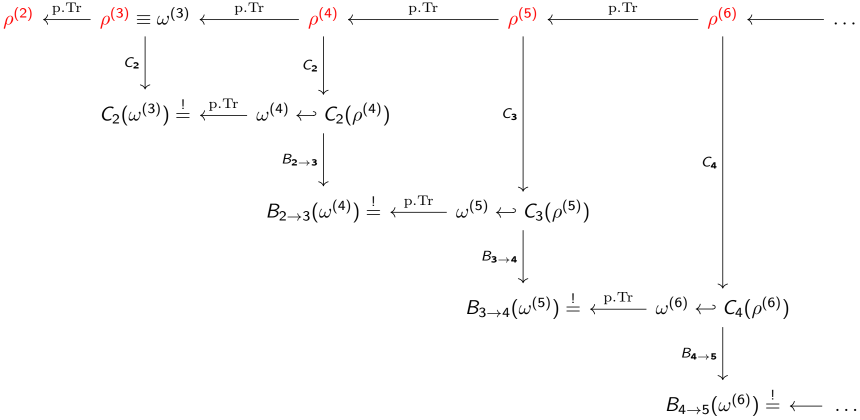

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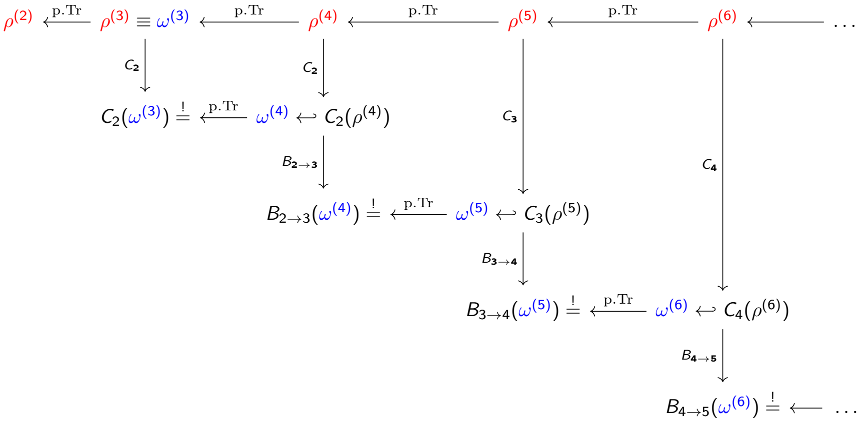
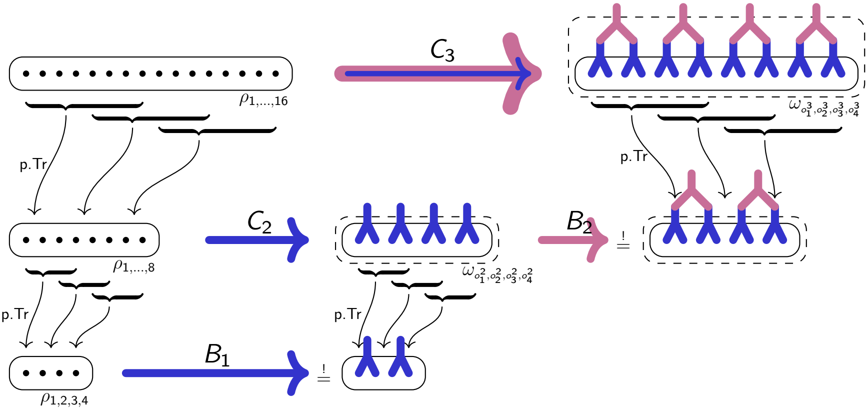


Coarse-graining using tree tensor networks



Benchmarking Results

Translation-invariant spin chains

	Model Name	Hamiltonian	Gap?
(**a**)	Critical Ising	$H_{\mathsf{TFI}}(1)$	Critical
(**b**)	S = 1/2 Heisenberg	$H^{1/2}_{\mathsf{XXZ}}(1)$	Critical
(**c**)	$S = 1/2$ symmetry broken XXZ	$H^{1/2}_{\mathsf{XXZ}}(2)$	Gapped
(**d**)	$S = 1/2$ XX model	$H^{1/2}_{\mathsf{XXZ}}(0)$	Critical
(**e**)	S = 1 Heisenberg	$H^{1}_{\mathsf{XXZ}}(1)$	Gapped
(**f**)	$S = 1/2$ J_1-J_2 Heisenberg	$H_{\mathsf{J_1\text{-}J_2}}(4.15, 1)$	Critical

$$H_{\mathsf{TFI}}(h_z) = -\sum_i X_i X_{i+1} - h_z \sum_i Z_i$$ Transverse field Ising model

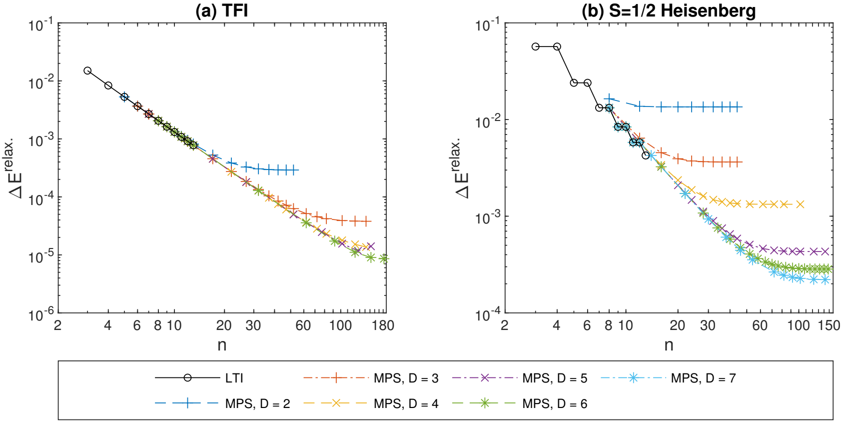
$$H^S_{\mathsf{XXZ}}(\Delta) = \sum_i X_i X_{i+1} + Y_i Y_{i+1} + \Delta Z_i Z_{i+1}$$ XXZ spin S

$$H_{\mathsf{J_1\text{-}J_2}}(J_1, J_2) = \sum_i J_1 \vec{S}_i \cdot \vec{S}_{i+1} + J_2 \vec{S}_i \cdot \vec{S}_{i+2}$$ J_1-J_2 Heisenberg spin 1/2

Results: TFI & S=1/2 Heisenberg model

(**a**) Critical TFI: $H_{\mathrm{TFI}}(1)$

(**b**) Isotropic antiferromagnetic S $= 1/2$ Heisenberg: $H^{1/2}_{\mathrm{XXZ}}(1)$



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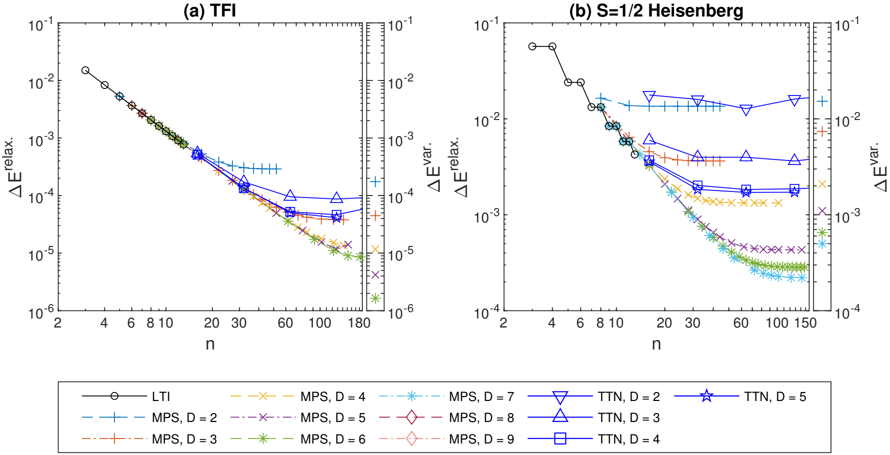
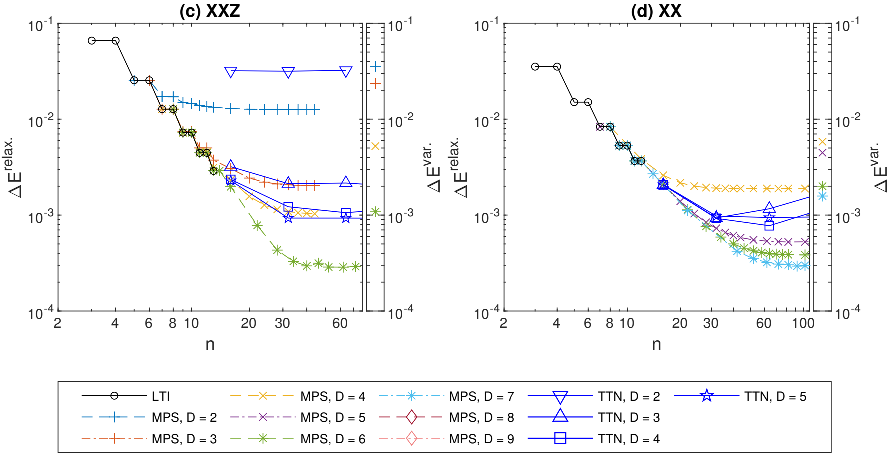


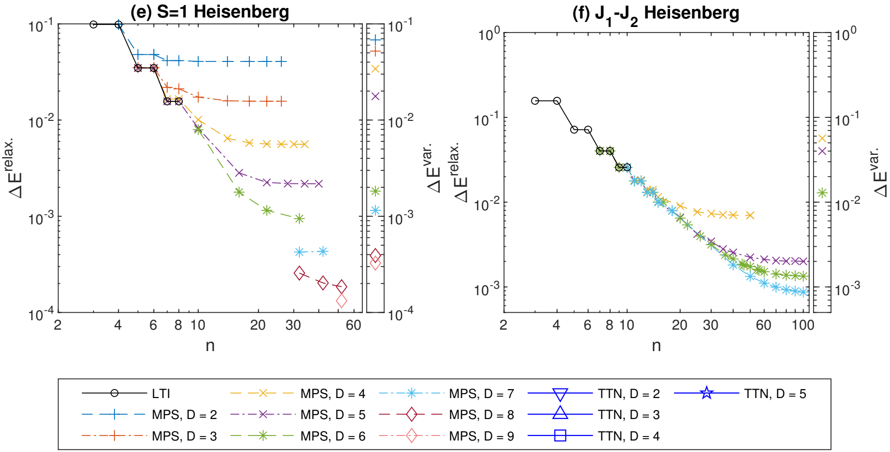
Results: XXZ & XX

(**c**) $S = 1/2$ symmetry broken XXZ: $H^{1/2}_{\mathrm{XXZ}}(2)$
(**d**) $S = 1/2$ XX model: $H^{1/2}_{\mathrm{XXZ}}(0)$

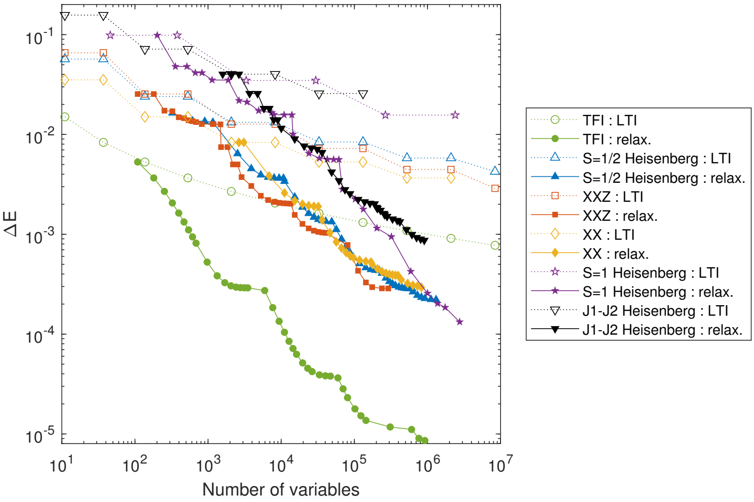


Results: S=1 Heisenberg & J_1-J_2

(**e**) Isotropic antiferromagnetic S $= 1$ Heisenberg: $H^1_{\mathrm{XXZ}}(1)$
(**f**) Critical $S = 1/2$ J_1-J_2 Heisenberg: $H_{\mathrm{J_1\text{-}J_2}}(4.15, 1)$

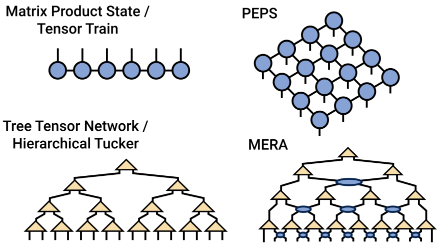


Results: Memory scaling vs. precision

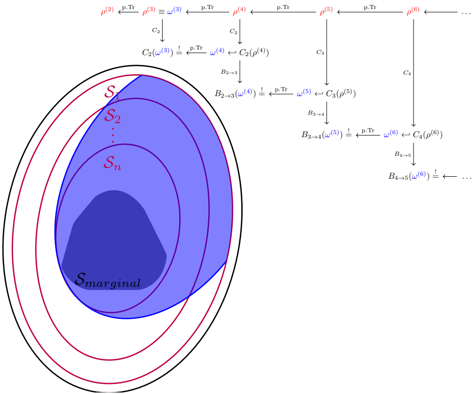


Conclusion

$$\min_{\psi \in \mathcal{C} \subset \mathcal{H}} \langle \psi | H | \psi \rangle \geq \min_{\psi \in \mathcal{H}} \langle \psi | H | \psi \rangle \geq E_{\text{relax.}}(\{C_i\})$$



[tensornetwork.org]
[Cirac and Verstraete, J.Phys.A (2009)]



Results: Relaxation precision vs. VUMPS precision