Lower Bounding Ground State Energies of Local Hamiltonians

Tractable relaxations of the quantum marginal problem

Ilya Kull, Norbert Schuch, Ben Dive and Miguel Navascues

University of Vienna

European Research Council

Established by the European Commission

Local Hamiltonians and Marginal States

$H = \sum_{i \in I} h_{a_i}$ a_i local patches on a lattice Λ

$$E_0 = \min \langle \psi | H | \psi \rangle \quad = \quad \min \sum_{i \in I} \langle \psi | h_{a_i} | \psi \rangle =$$

$$\text{s.t.} ||\psi|| = 1 \qquad\qquad \text{s.t.} ||\psi|| = 1$$

$$= \min \sum_{i \in I} \operatorname{Tr}\left(h_{a_i} \rho_{a_i} \right)$$

s.t. $\{\rho_{a_i}\}_{i \in I}$ are all marginals of some $\psi \in \mathcal{H}_\Lambda$

$\operatorname{Tr}(\rho_{a_i}) = 1$

This is known as the quantum marginal problem.
(for electrons "N-representability")

Local Hamiltonians and Marginal States

$H = \sum_{i \in I} h_{a_i}$ $\qquad$ a_i local patches on a lattice Λ

$$E_0 = \min \langle \psi | H | \psi \rangle \quad = \quad \min \sum_{i \in I} \langle \psi | h_{a_i} | \psi \rangle =$$

$$\text{s.t.} ||\psi|| = 1 \qquad \qquad \text{s.t.} ||\psi|| = 1$$

$$= \min \sum_{i \in I} \mathrm{Tr}\left(h_{a_i} \rho_{a_i} \right)$$

$$\text{s.t.} \{\rho_{a_i}\}_{i \in I} \text{ are all marginals of some } \psi \in \mathcal{H}_\Lambda$$

$$\mathrm{Tr}(\rho_{a_i}) = 1$$

This is known as the quantum marginal problem.
(for electrons "N-representability")

Local Hamiltonians and Marginal States

$H = \sum_{i \in I} h_{a_i}$ $\qquad$ a_i local patches on a lattice Λ

$$E_0 = \min \langle \psi | H | \psi \rangle \quad = \quad \min \sum_{i \in I} \langle \psi | h_{a_i} | \psi \rangle =$$

$$\text{s.t.} ||\psi|| = 1 \qquad\qquad \text{s.t.} ||\psi|| = 1$$

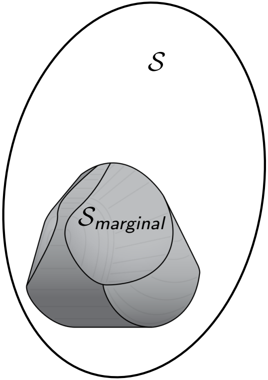
$$= \min \sum_{i \in I} \mathrm{Tr}\left(h_{a_i} \rho_{a_i} \right)$$

$$\text{s.t.} \{\rho_{a_i}\}_{i \in I} \text{ are all marginals of some } \psi \in \mathcal{H}_\Lambda$$

$$\mathrm{Tr}(\rho_{a_i}) = 1$$

This is known as the quantum marginal problem.
(for electrons "N-representability")

Convex Sets of Quantum States



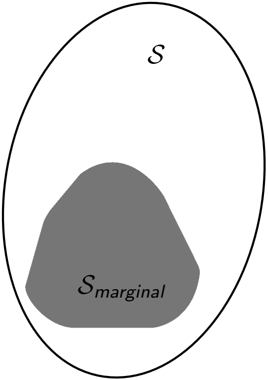
$$\{\rho_{a_i} \geq 0\}_{i \in I} \quad \longleftrightarrow \quad \vec{\boldsymbol{\rho}} \in \mathcal{S}$$

$$H = \sum_{i \in I} h_{a_i} \quad \longleftrightarrow \quad \vec{\boldsymbol{H}}$$

$$\sum_{i \in I} \mathrm{Tr}(h_{a_i} \rho_{a_i}) \quad \longleftrightarrow \quad \vec{\boldsymbol{H}} \cdot \vec{\boldsymbol{\rho}}$$

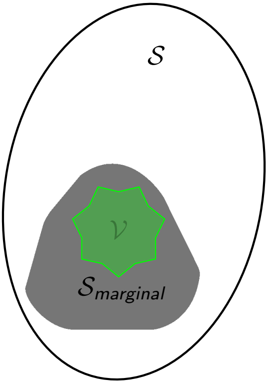
It's Hard...

- Local energy problem is QMA-complete
  [Aharonov et al. Comm Math Phys (2009)]
- **Variational Methods:**
  $E_{\mathcal{V}} = \min_{\vec{\rho} \in \mathcal{V}} \vec{H} \cdot \vec{\rho} \quad \Longrightarrow E_0 \leq E_{\mathcal{V}}$
- **Relaxation methods:**
  $E_{\mathcal{R}} = \min_{\vec{\rho} \in \mathcal{R}} \vec{H} \cdot \vec{\rho} \quad \Longrightarrow E_0 \geq E_{\mathcal{R}}$



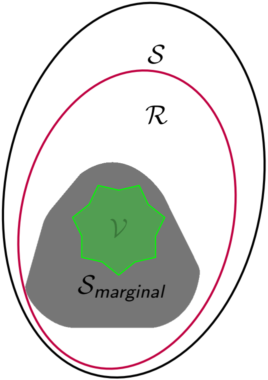
It's Hard...

- Local energy problem is QMA-complete
  [Aharonov et al. Comm Math Phys (2009)]
- **Variational Methods:**
  $$E_{\mathcal{V}} = \min_{\vec{\boldsymbol{\rho}} \in \mathcal{V}} \vec{\boldsymbol{H}} \cdot \vec{\boldsymbol{\rho}} \quad \Longrightarrow \quad E_0 \leq E_{\mathcal{V}}$$
- **Relaxation methods:**
  $$E_{\mathcal{R}} = \min_{\vec{\rho} \in \mathcal{R}} \vec{\boldsymbol{H}} \cdot \vec{\rho} \quad \Longrightarrow \quad E_0 \geq E_{\mathcal{R}}$$



It's Hard...

- Local energy problem is QMA-complete
  [Aharonov et al. Comm Math Phys (2009)]
- **Variational Methods:**
  $E_{\mathcal{V}} = \min_{\vec{\rho} \in \mathcal{V}} \vec{\boldsymbol{H}} \cdot \vec{\boldsymbol{\rho}} \quad \Longrightarrow E_0 \leq E_{\mathcal{V}}$
- **Relaxation methods:**
  $E_{\mathcal{R}} = \min_{\vec{\rho} \in \mathcal{R}} \vec{\boldsymbol{H}} \cdot \vec{\boldsymbol{\rho}} \quad \Longrightarrow E_0 \geq E_{\mathcal{R}}$



In this Talk

- Our relaxation method
  - expand exact constraint into a hierarchy of constraints
  - coarse-grain and compress the variables
  - use tensor networks for coarse-graining maps
- Results for 1D translation-invariant models

How to relax?

$$E_0 = \min \langle \psi | H | \psi \rangle = \min \sum_{i \in I} \mathrm{Tr}\left(h_{a_i} \rho_{a_i}\right) \geq \min \sum_{i \in I} \mathrm{Tr}\left(h_{a_i} \rho_{a_i}\right)$$

$$\text{s.t.} ||\psi|| = 1 \qquad \text{s.t.} \{\rho_{a_i}\}_{i \in I} \in \mathcal{S}_{marginal} \qquad \text{s.t.} \ldots ???$$

How to relax?

$$E_0 = \min \langle \psi | H | \psi \rangle = \quad \min \sum_{i \in I} \mathrm{Tr}\left(h_{a_i} \rho_{a_i} \right) \qquad \geq \min \sum_{i \in I} \mathrm{Tr}\left(h_{a_i} \rho_{a_i} \right)$$

$$\text{s.t.} ||\psi|| = 1 \qquad \text{s.t.} \{\rho_{a_i}\}_{i \in I} \in \mathcal{S}_{marginal} \qquad \text{s.t.} \ldots ???$$

Which constraints NOT to relax?

- Nearest neighbors in $1D$: $H = \sum_i h_{i,i+1}$
- $\{\rho_{i,i+1}\}_i$ marginals of $\psi \in \mathcal{H}_\Lambda \Longrightarrow \{\rho_{i,i+1}\}_i$ **mutually compatible**

$$\mathrm{Tr}_1(\rho_{1,2}) = \rho_2 = \mathrm{Tr}_{1,3,4,\ldots,N}(|\psi\rangle\langle\psi|) = \mathrm{Tr}_3(\rho_{2,3})$$

- Keep the conditions $\mathrm{Tr}_i(\rho_{i,i+1}) = \mathrm{Tr}_{i+2}(\rho_{i+1,i+2})$

Which constraints NOT to relax?

- Nearest neighbors in $1D$: $H = \sum_i h_{i,i+1}$
- $\{\rho_{i,i+1}\}_i$ marginals of $\psi \in \mathcal{H}_\Lambda \Rightarrow \{\rho_{i,i+1}\}_i$ **mutually compatible**

$$\mathrm{Tr}_1(\rho_{1,2}) = \rho_2 = \mathrm{Tr}_{1,3,4,\ldots,N}(|\psi\rangle\langle\psi|) = \mathrm{Tr}_3(\rho_{2,3})$$

- Keep the conditions $\mathrm{Tr}_i(\rho_{i,i+1}) = \mathrm{Tr}_{i+2}(\rho_{i+1,i+2})$

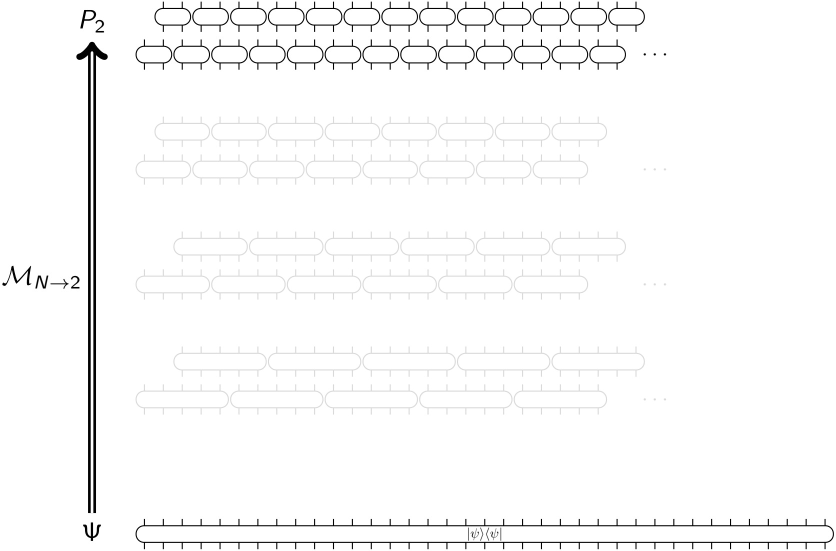
Which constraints NOT to relax?

- Nearest neighbors in $1D$: $H = \sum_i h_{i,i+1}$
- $\{\rho_{i,i+1}\}_i$ marginals of $\psi \in \mathcal{H}_\Lambda \Rightarrow \{\rho_{i,i+1}\}_i$ **mutually compatible**

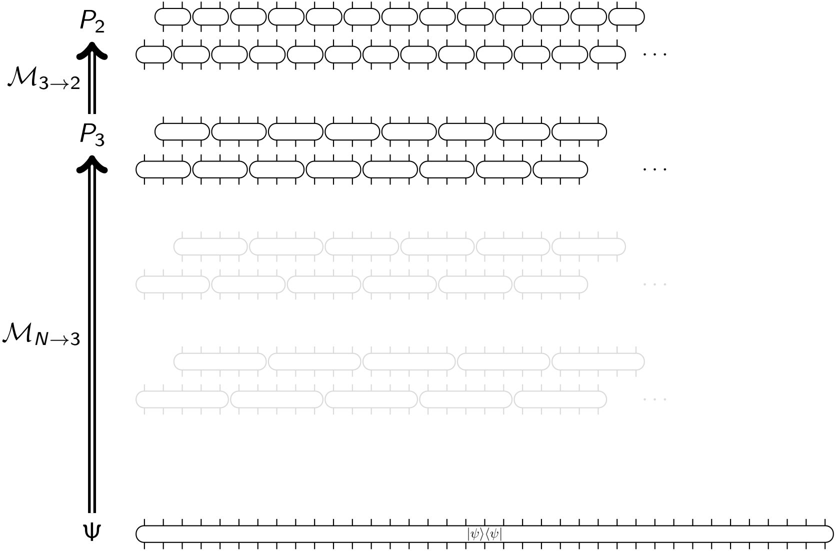
$$\mathrm{Tr}_1(\rho_{1,2}) = \rho_2 = \mathrm{Tr}_{1,3,4,\ldots,N}(|\psi\rangle\langle\psi|) = \mathrm{Tr}_3(\rho_{2,3})$$

- Keep the conditions $\mathrm{Tr}_i(\rho_{i,i+1}) = \mathrm{Tr}_{i+2}(\rho_{i+1,i+2})$

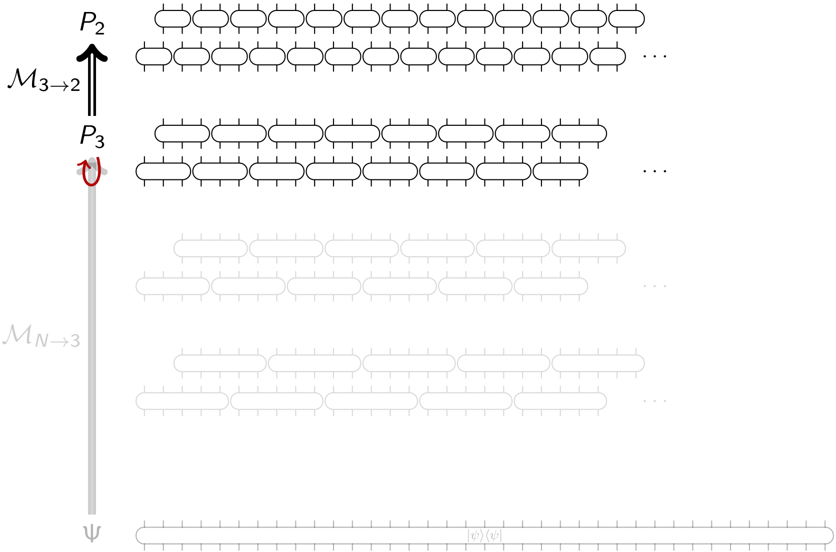
Ingredient 1: a hierarchy of constraints



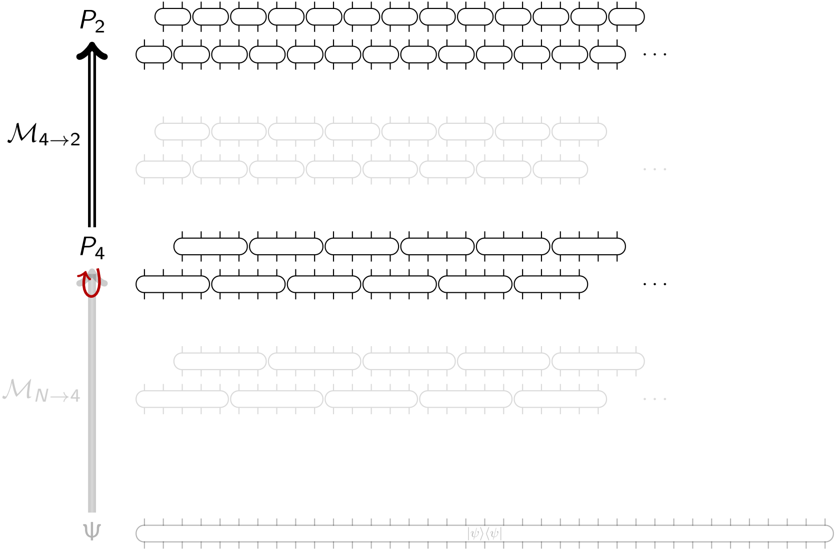
Ingredient 1: a hierarchy of constraints



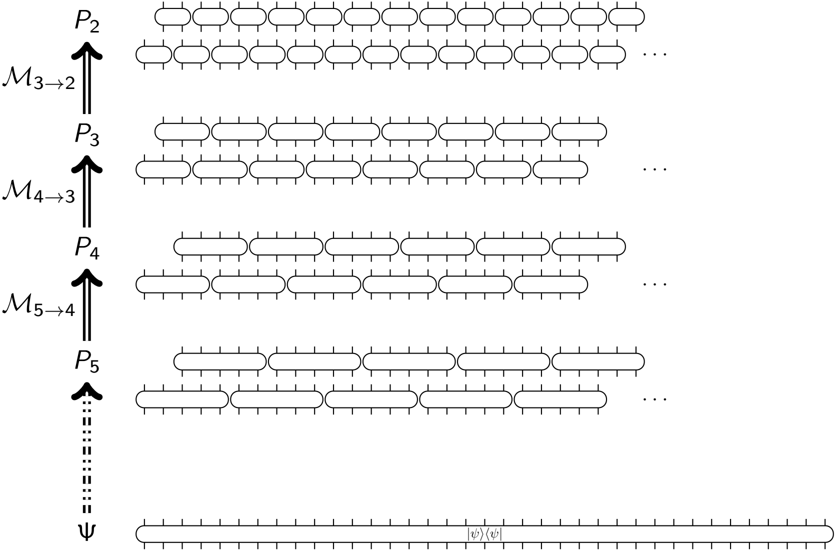
Ingredient 1: a hierarchy of constraints



Ingredient 1: a hierarchy of constraints



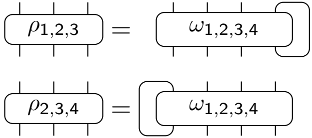
Ingredient 1: a hierarchy of constraints



Ingredient 2: relaxation via coarse-graining and compression

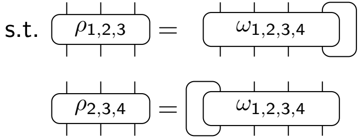
$\min \mathcal{F}(\rho_{1,2,3}, \rho_{2,3,4})$

s.t.

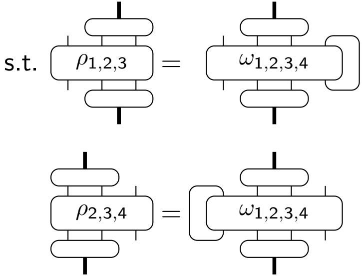


Ingredient 2: relaxation via coarse-graining and compression

$\min \mathcal{F}(\rho_{1,2,3}, \rho_{2,3,4})$



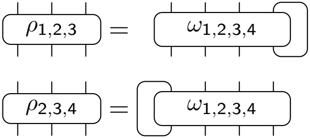
$\geq \min \mathcal{F}(\rho_{1,2,3}, \rho_{2,3,4})$



Ingredient 2: relaxation via coarse-graining and compression

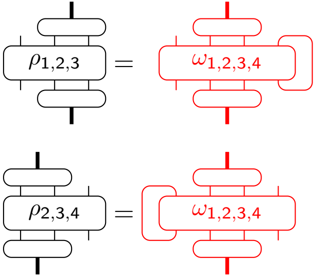
$\min \mathcal{F}(\rho_{1,2,3}, \rho_{2,3,4})$

s.t.

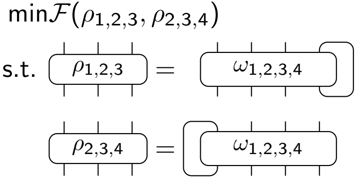


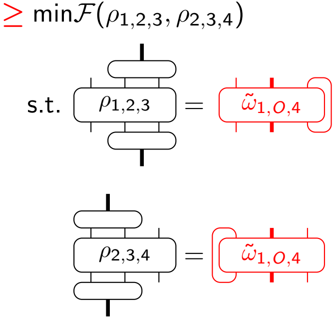
$\geq \min \mathcal{F}(\rho_{1,2,3}, \rho_{2,3,4})$

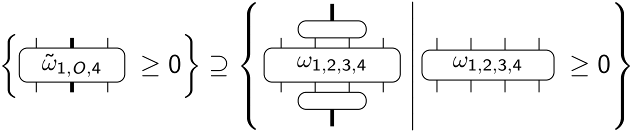
s.t.



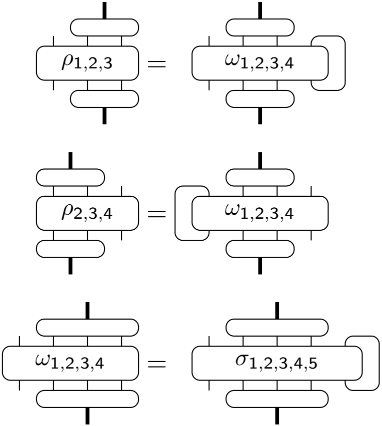
Ingredient 2: relaxation via coarse-graining and compression





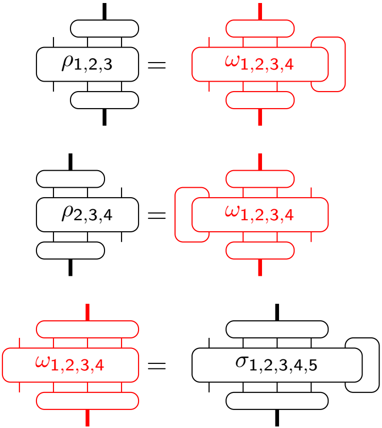


The last ingredient: composable coarse-graining maps



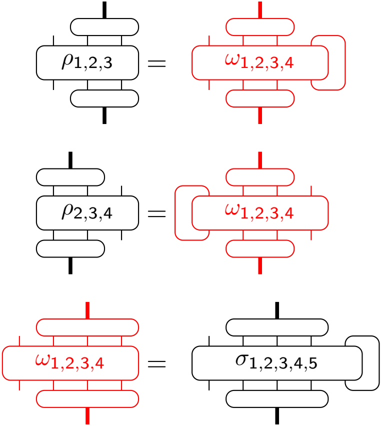
But which tensor to use??

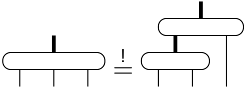
The last ingredient: composable coarse-graining maps



But which tensor to use??

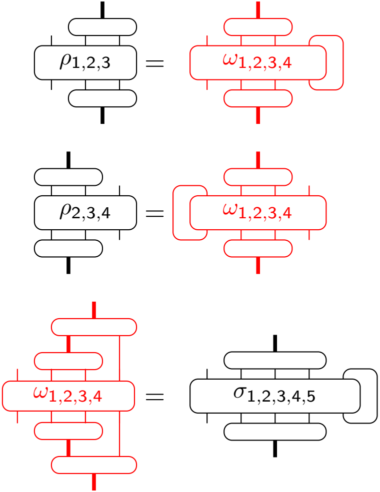
The last ingredient: composable coarse-graining maps

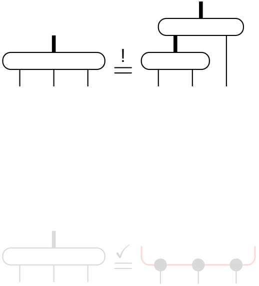




But which tensor to use??

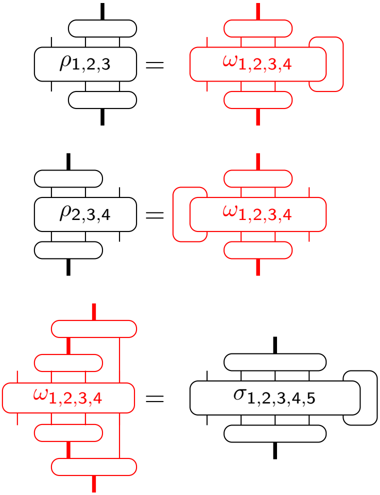
The last ingredient: composable coarse-graining maps

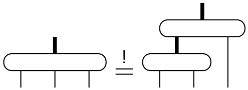


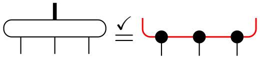


But which tensor to use??

The last ingredient: composable coarse-graining maps

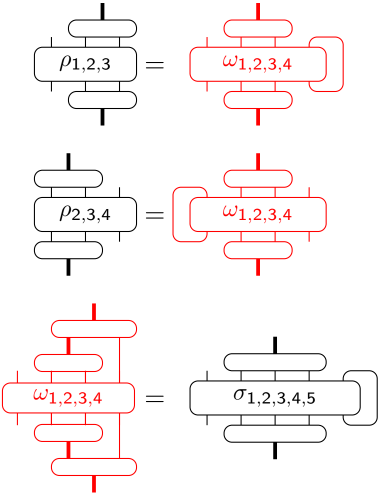


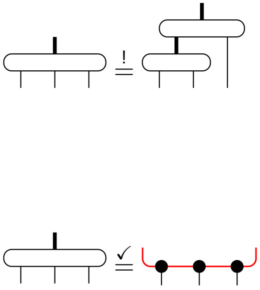




But which tensor to use??

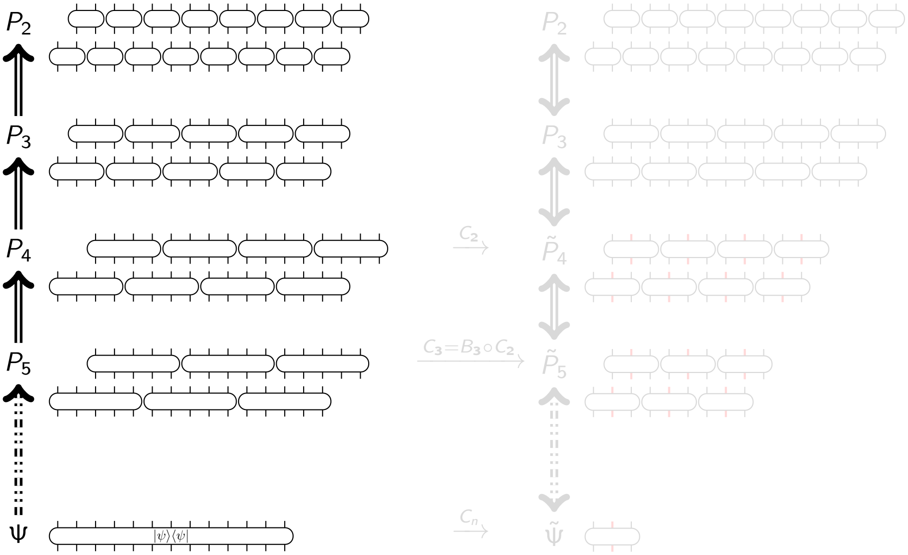
The last ingredient: composable coarse-graining maps



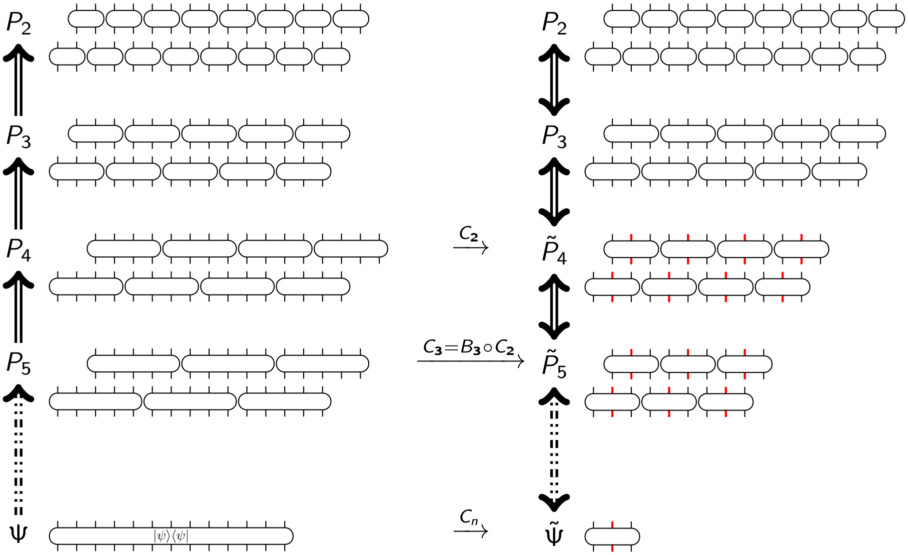


But which tensor to use??

Method overview



Method overview



Application: The 1D Translation-Invariant Local Energy Problem

The translation-invariant problem

$$H = \sum_{i=-\infty}^{\infty} h_{i,i+1} \ , \quad h_{i,i+1} \equiv h \quad \forall i$$

$$e_{TI} := \min \mathrm{Tr}\left(h\rho_{\{1,2\}}\right) \quad \text{s.t.} \rho_{\{1,2\}} \in \mathcal{S}^{TI}_{marginal}$$

$\overset{\text{Relax}}{\Longrightarrow}$

$$e^{n}_{LTI} := \min \mathrm{Tr}\left(h\rho_{\{1,2\}}\right)$$
$$\text{s.t.} \mathrm{Tr}\rho_{\{1,2\}} = 1 \ ,$$
$$\rho_{\{1,2\}} = \mathrm{Tr}_{\{3,4,\ldots n\}}\sigma_{\{1,2,\ldots n\}} \ ,$$
$$\sigma \geq 0 \ ,$$
$$\mathrm{Tr}_{\{1\}}\sigma = \mathrm{Tr}_{\{n\}}\sigma$$

Models:

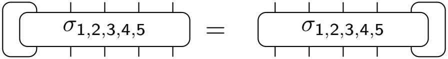
- $H_{TFI}(h_z) = -\sum_i X_i X_{i+1} - h_z \sum_i Z_i$ (Transverse field Ising)
- $H^{S}_{XXZ}(\Delta) = \sum_i X_i X_{i+1} + Y_i Y_{i+1} + \Delta Z_i Z_{i+1}$ (XXZ $S = 1/2$ and $S = 1$)

The translation-invariant problem

$$H = \sum_{i=-\infty}^{\infty} h_{i,i+1} \ , \quad h_{i,i+1} \equiv h \quad \forall i$$

$$e_{TI} := \min \mathrm{Tr}\left(h\rho_{\{1,2\}}\right) \quad \text{s.t.}\ \rho_{\{1,2\}} \in \mathcal{S}^{TI}_{marginal} \quad \overset{\text{Relax}}{\Longrightarrow} \quad e^{n}_{LTI} := \min \mathrm{Tr}\left(h\rho_{\{1,2\}}\right)$$

$$\begin{aligned} \text{s.t.}\ & \mathrm{Tr}\rho_{\{1,2\}} = 1 \ , \\ & \rho_{\{1,2\}} = \mathrm{Tr}_{\{3,4,\dots n\}}\sigma_{\{1,2,\dots n\}} \ , \\ & \sigma \geq 0 \ , \\ & \mathrm{Tr}_{\{1\}}\sigma = \mathrm{Tr}_{\{n\}}\sigma \end{aligned}$$



Models:

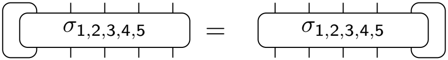
- $H_{TFI}(h_z) = -\sum_i X_i X_{i+1} - h_z \sum_i Z_i$ (Transverse field Ising)
- $H^{S}_{XXZ}(\Delta) = \sum_i X_i X_{i+1} + Y_i Y_{i+1} + \Delta Z_i Z_{i+1}$ (XXZ $S = 1/2$ and $S = 1$)

The translation-invariant problem

$$H = \sum_{i=-\infty}^{\infty} h_{i,i+1} \ , \quad h_{i,i+1} \equiv h \quad \forall i$$

$$e_{TI} := \min \mathrm{Tr}\left(h\rho_{\{1,2\}}\right) \quad \text{s.t.}\ \rho_{\{1,2\}} \in \mathcal{S}^{TI}_{marginal} \quad \overset{\text{Relax}}{\Longrightarrow} \quad e^{n}_{LTI} := \min \mathrm{Tr}\left(h\rho_{\{1,2\}}\right)$$

$$\text{s.t.}\ \mathrm{Tr}\rho_{\{1,2\}} = 1 \ ,$$
$$\rho_{\{1,2\}} = \mathrm{Tr}_{\{3,4,\ldots n\}}\sigma_{\{1,2,\ldots n\}} \ ,$$
$$\sigma \geq 0 \ ,$$
$$\mathrm{Tr}_{\{1\}}\sigma = \mathrm{Tr}_{\{n\}}\sigma$$

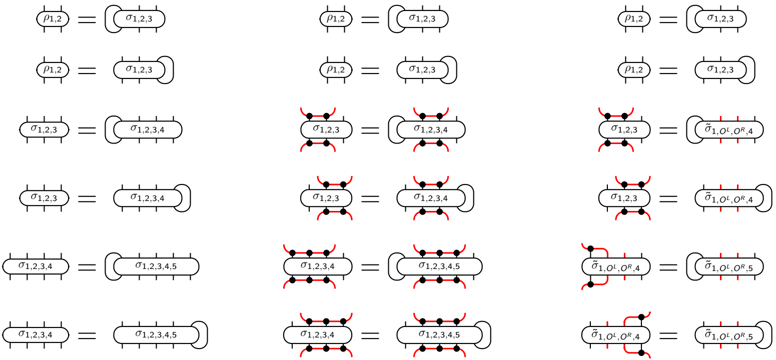


Models:

- $H_{TFI}(h_z) = -\sum_i X_i X_{i+1} - h_z \sum_i Z_i$ (Transverse field Ising)
- $H^{S}_{XXZ}(\Delta) = \sum_i X_i X_{i+1} + Y_i Y_{i+1} + \Delta Z_i Z_{i+1}$ (XXZ $S = 1/2$ and $S = 1$)

Translation invariant relaxation scheme

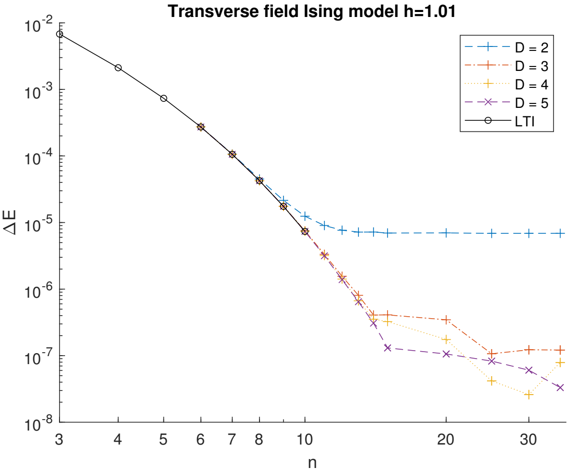
Exact 5-body Loc.T.I. problem	Relxation due to applied C.G. maps	Compressed relaxation



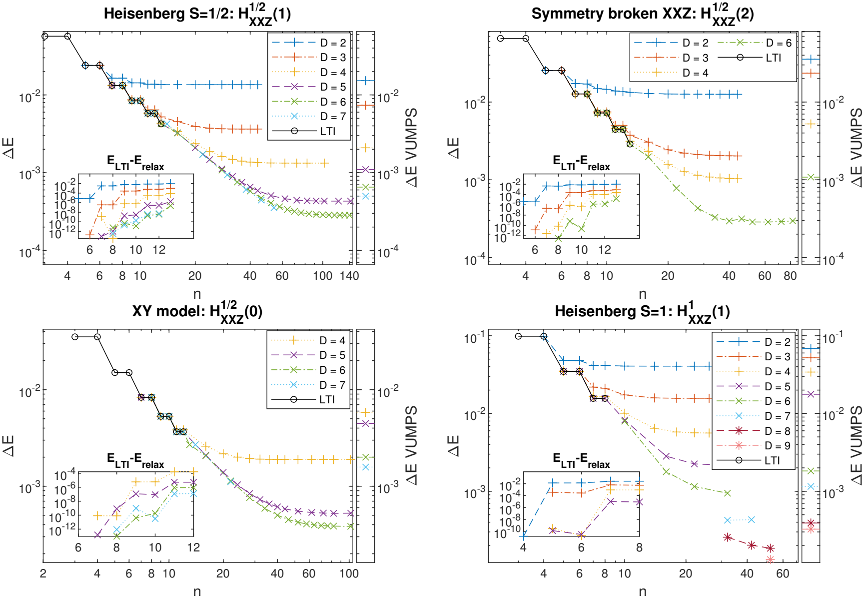
The MPS tensor is the VUMPS solution for the same Hamiltonian [Zauner-Stauber et al. PRB (2018)].

Results

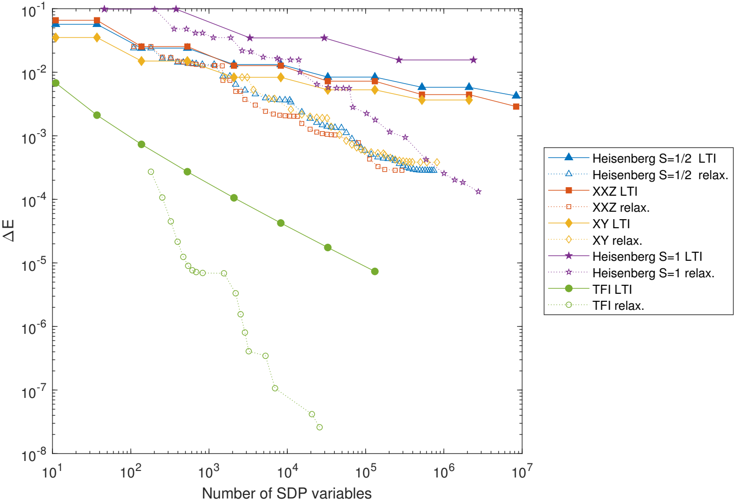
Results: transverse field Ising model



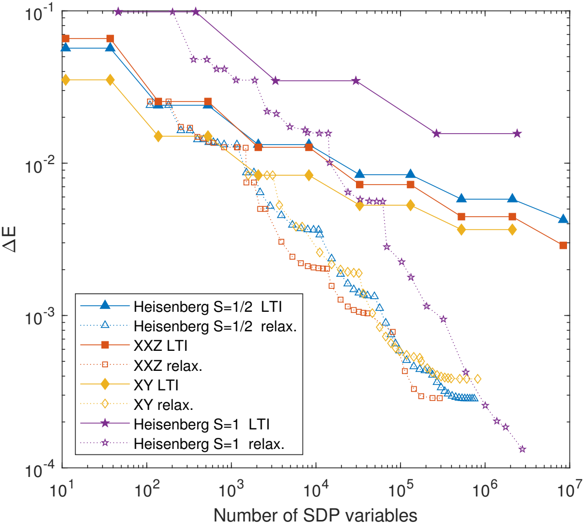
Results: XXZ models for S=1/2 and S=1 systems



Results: memory scaling vs. precision



Results: Memory scaling vs. precision



Discussion

Why does this work?

- we enforce the constraints only in subspaces spanned by MPS tensors
- keep constraints relevant to the given Hamiltonian
- optimal variational MPS $\not\Leftrightarrow$ optimal coarse-graining for relaxation

Not in this talk

- Works also for finite systems
- One can optimize over the coarse-graining maps
- Issues with SDP solvers: memory scaling is not everything
- Ideas beyond 1D and beyond lattice spin systems

Thanks!

Not in this talk

- Works also for finite systems
- One can optimize over the coarse-graining maps
- Issues with SDP solvers: memory scaling is not everything
- Ideas beyond 1D and beyond lattice spin systems

Thanks!

Not in this talk

- Works also for finite systems
- One can optimize over the coarse-graining maps
- Issues with SDP solvers: memory scaling is not everything
- Ideas beyond 1D and beyond lattice spin systems

Thanks!

Not in this talk

- Works also for finite systems
- One can optimize over the coarse-graining maps
- Issues with SDP solvers: memory scaling is not everything
- Ideas beyond 1D and beyond lattice spin systems

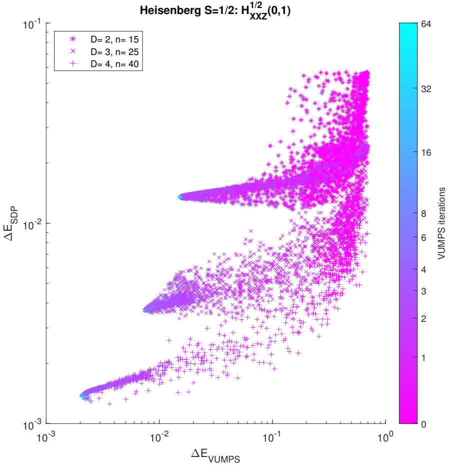
Thanks!

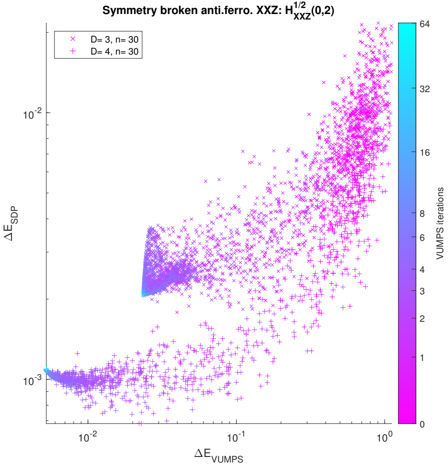
Not in this talk

- Works also for finite systems
- One can optimize over the coarse-graining maps
- Issues with SDP solvers: memory scaling is not everything
- Ideas beyond 1D and beyond lattice spin systems

Thanks!

Results: Relaxation precision vs. VUMPS precision





Near phase boundary

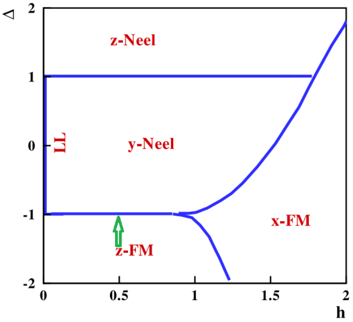
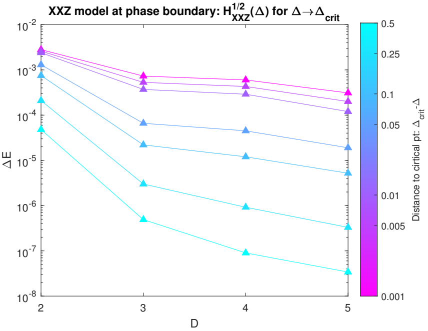


Fig. 1 Ground state magnetic phase diagram of the 1D spin-1/2 XXZ model in a transverse magnetic field. The z-Neel and y-Neel phases represent the staggered magnetization along z and y axis respectively. In the z-FM and x-FM regions, the long-range magnetization exist along the z and x axis, respectively (Color figure online)



Moradmard et al. J Supercond Nov Magn 27, (2014).