Efficient Algorithm for Ground State of 1D Hamiltonians

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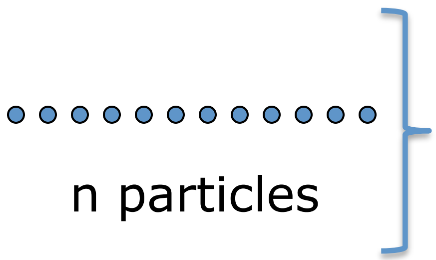
[Feynman ’81] Exponential description of quantum states poses challenge to classical simulation.



Classical: $O(n)$ parameters.

Quantum: $2^{O(n)}$ parameters.

Use a quantum computer.

What do we do until we have quantum computers?

Numerical techniques have been remarkably successful in practice for 1D systems:

- Good Ansatz for Ground state: MPS

- DMRG algorithm[White ’92] very successful for 1D

- Doesn’t always work. Artificial hard examples known.

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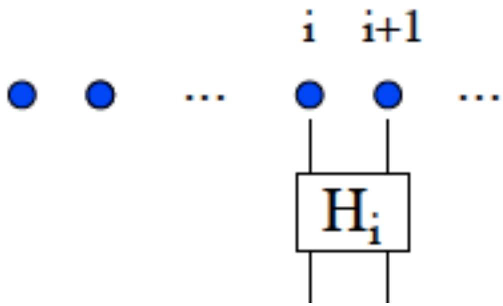
   Are 1D systems easy?
2. 2D systems?

1D Ground States



$$H = H_1 + \cdots + H_m$$

- Qudits

- Each H_i is $d^2 x d^2$, positive, norm ≤ 1

- Wish to compute ground state |GS>,
  state that minimizes energy E = <GS|H|GS>

- Given the H_i as input (to some precision), calculate a classical description of |GS> (to some precision). The classical description must allow efficient evaluation of local observables.

Matrix Product States (MPS)

$$|\psi\rangle = \sum_{i=1}^{B} |A_i\rangle \otimes |B_i\rangle$$

Bond dimension = Schmidt rank across cut

Quantum Complexity Theory Perspective

[Kitaev ’99]:
Introduction of QMA – quantum analogue of NP.
Finding ground states of general local Hamiltonians
is QMA complete.
Conjecture: no sub-exponential size classical witness
for QMA-complete problems.

[Aharonov, et. al. ’04][Oliveira, Terhal ’05]:
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[Aharonov, Gottesman, Irani, Kempe 07]
QMA-complete for 1D Hamiltonians

[Gottesman, Irani 09] Hard even for translation
invariant 1D Hamiltonians

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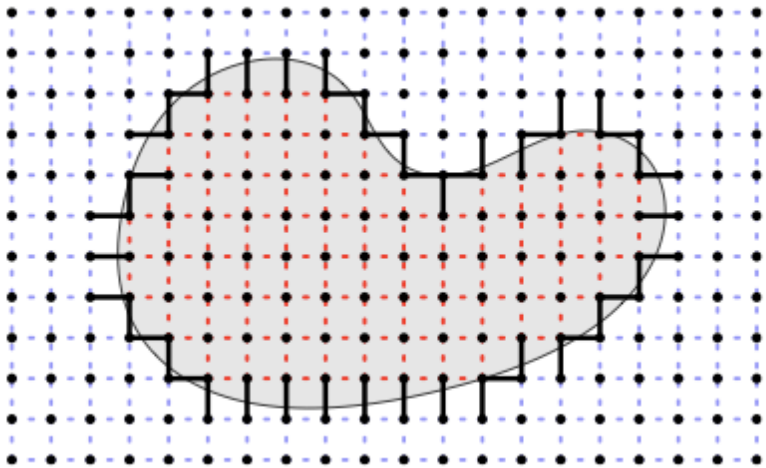
Area Law

For gapped local Hamiltonians $H = H_1 + \ldots + H_m$, entanglement entropy of the ground state scales like surface area, rather than volume.



Gapped local Hamiltonians
spectral gap = $\varepsilon = E_1 - E_0$ = constant. $|H_i| \leq 1$

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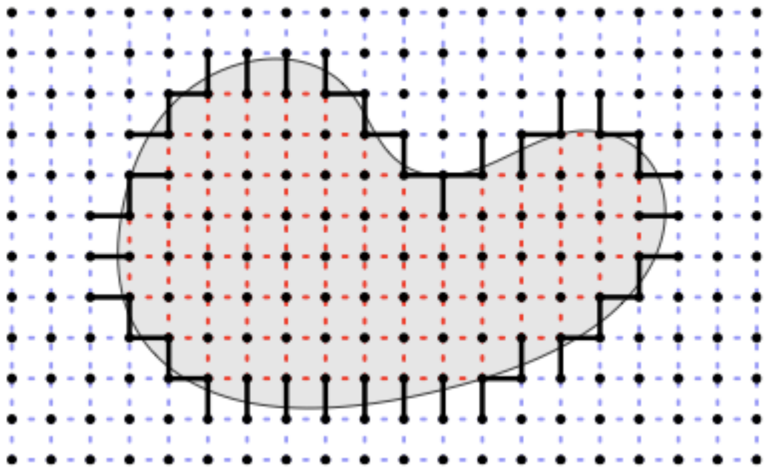
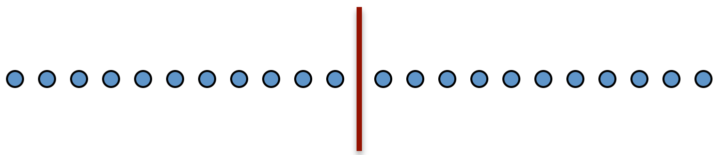


Related to Holographic Principle: Black hole entropy scales like surface area.

[Vidal, Latorre, Rico, Kitaev '02]

1D Area Law



[Hastings '07]: Rigorous proof for 1D systems:

$$S_{1D} = O(\exp(\log d/\varepsilon))$$

d = dimension of particle, ε = spectral gap.

- Implies 1D ground states in NP.

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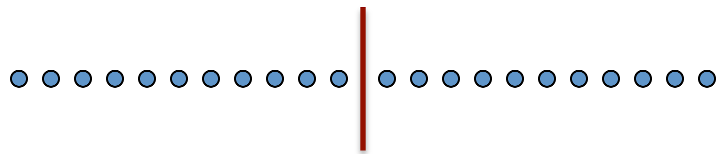

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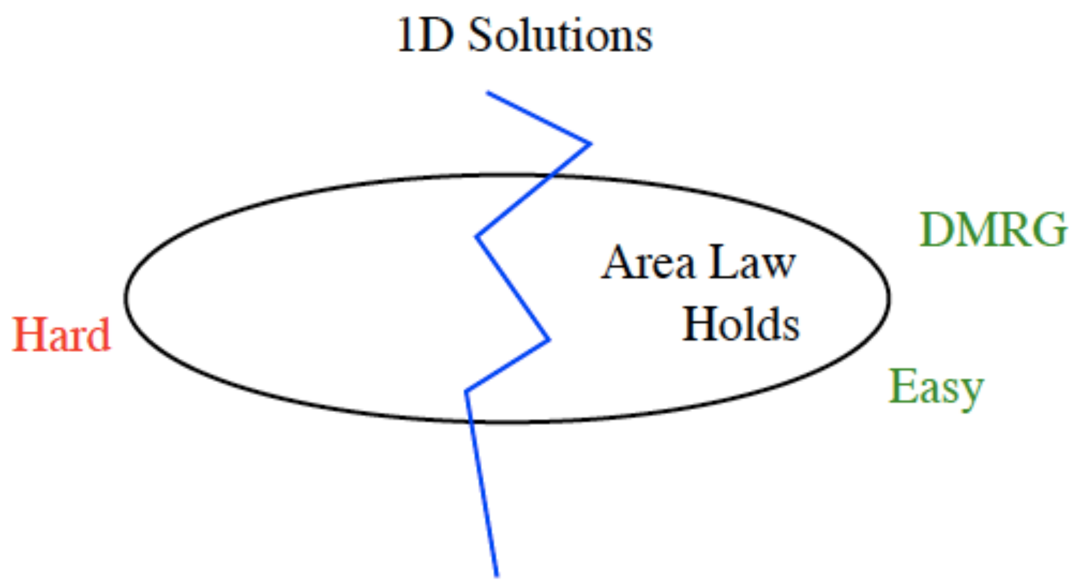

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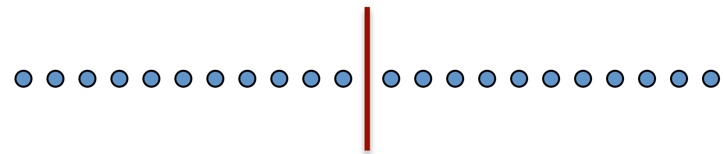

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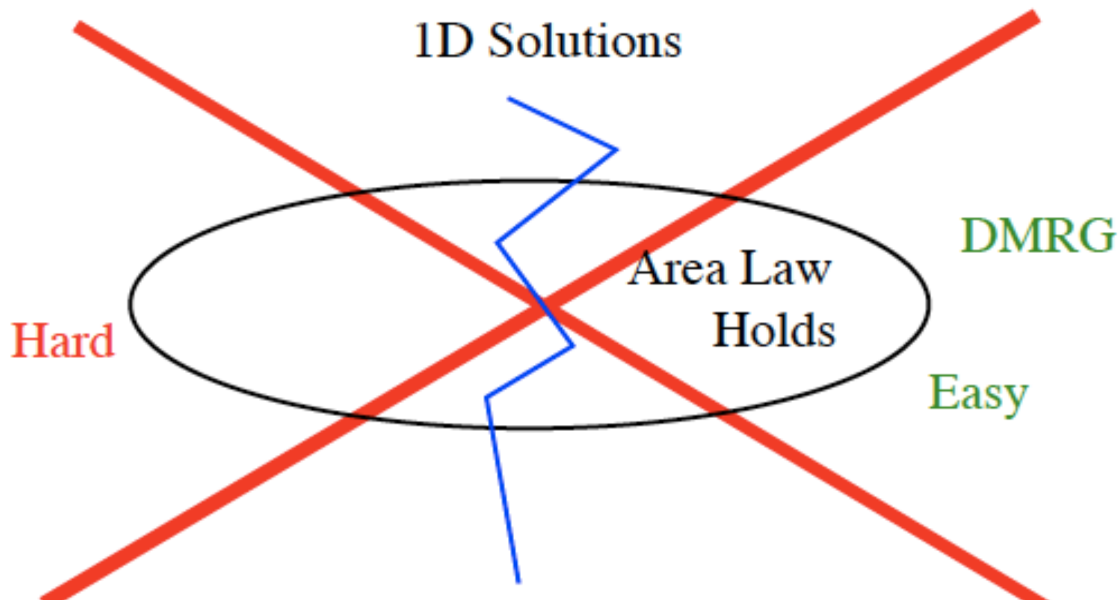

[Schuch, Cirac, Verstraete '08] Hard even when GS has poly size MPS.

←→ satisfies area law up to log correction

[Arad, Kitaev, Landau, Vazirani ’12] Exponential improvement in parameters of the 1D area law:

$$S_{1D} = O(\log^3 d/\varepsilon)$$

- Implies sublinear bond dimension MPS approximation.
- Sub-exponential time classical algorithm for finding MPS approximation to ground state.

Today: Algorithm that on input H_1, …, H_n outputs an MPS that has 1-η fidelity with |GS>.

Running time: $n^{c(d,\varepsilon)}\mathrm{poly}(\eta^{-1})$, where $c(d,\varepsilon) = 2^{O\left(\frac{\log^3 d}{\varepsilon}\right)}$

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How to reconcile these +ve results with the -ve results from Quantum Complexity Theory?

$$H = H_1 + \cdots + H_m$$

spectral gap = $\varepsilon = E_1 - E_0$

$$|H_i| \leq 1$$

- Gapped Hamiltonians: $\varepsilon = E_1 - E_0$ = constant
- QMA-complete instances: 1/poly(m) gap

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[Schuch, Cirac, Verstraete '08]

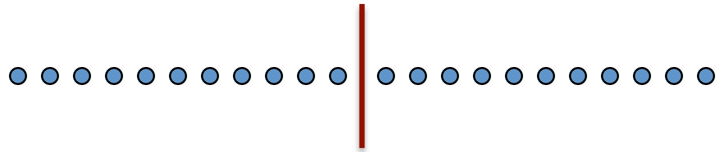
Gapped 1D Hamiltonian

Succinct description of ground state

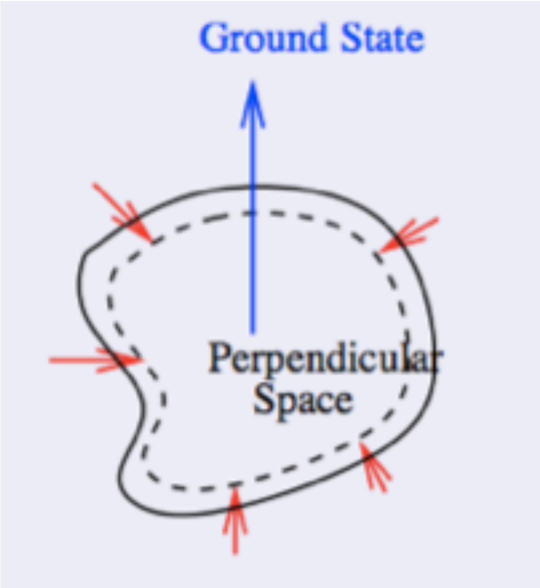
AGSP

1D algorithm

AGSP: Approximate Ground State Projector



An AGSP is an operator K that is not "too complex" and approximately projects onto the ground state:



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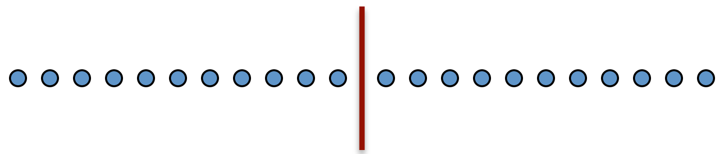
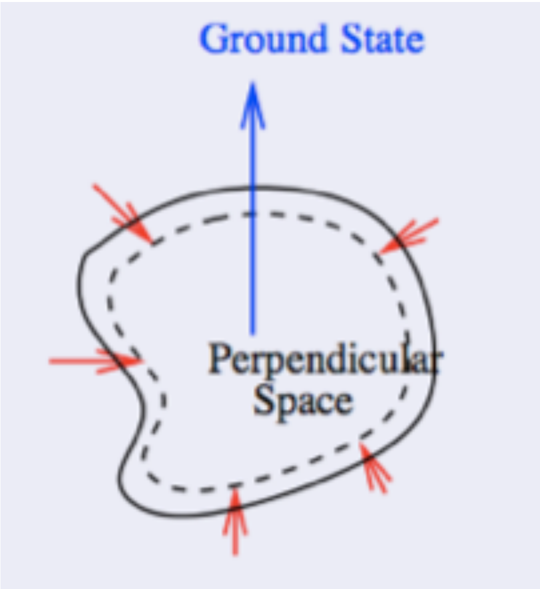
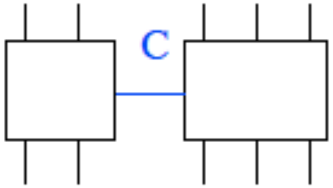


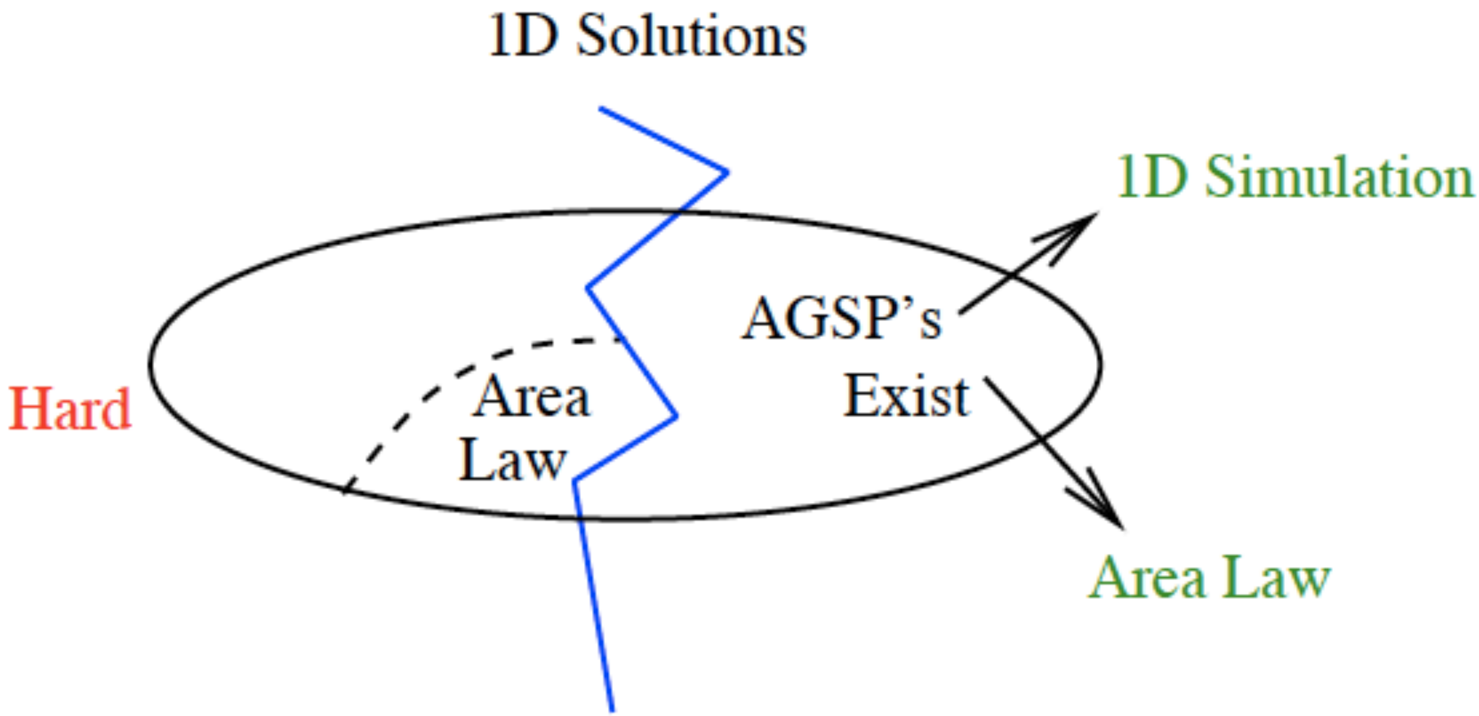


An AGSP is an operator K that is not "too complex" and approximately projects onto the ground state:

- K|GS> = |GS>
- Shrinks orthogonal space by Δ < 1
- Has low entanglement rank.

An operator on $\mathcal{H}_1 \otimes \mathcal{H}_2$ of the form $\sum_1^C A_i \otimes B_i$ will be said to have entanglement rank C.

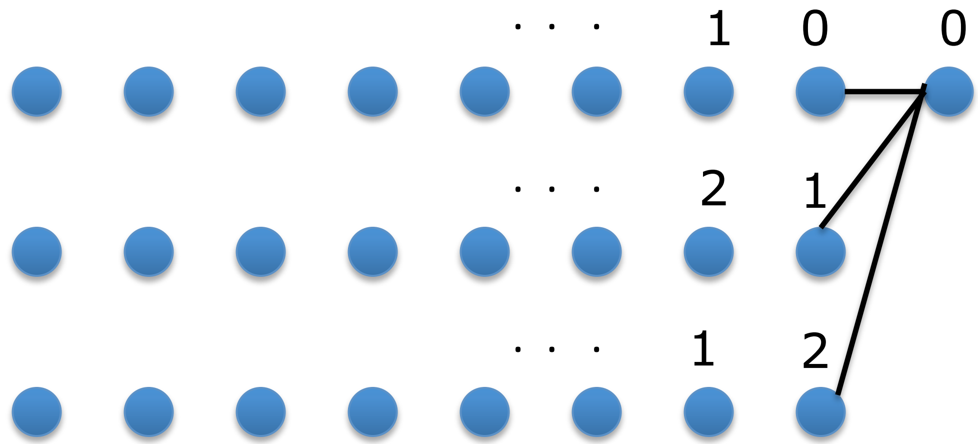



1D Solutions
1D Simulation
AGSP's
Exist
Hard
Area
Law
Area Law

Gap ➔ AGSP

1D Problems

Classical



Decoupling: Once you fix x_i can decouple left and right subproblems.

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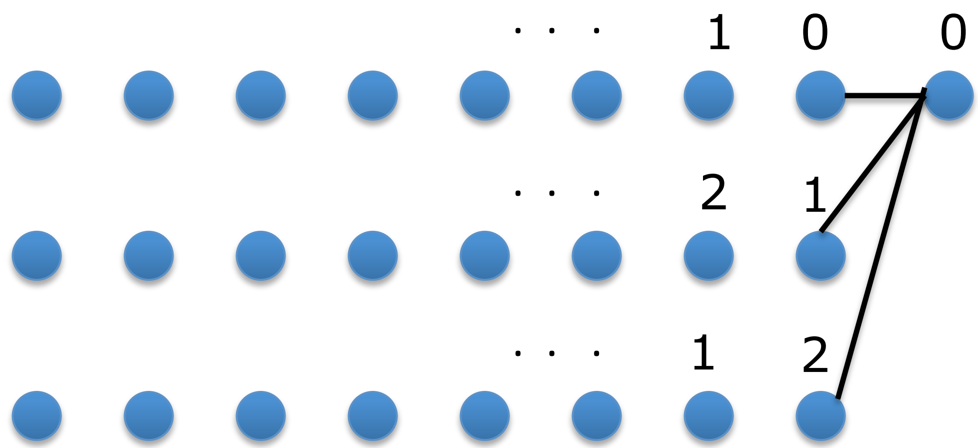

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Quantum: Fixing i-th qubit does not decouple.

Problem: Entanglement. Schmidt rank could grow with n.

1D Problems

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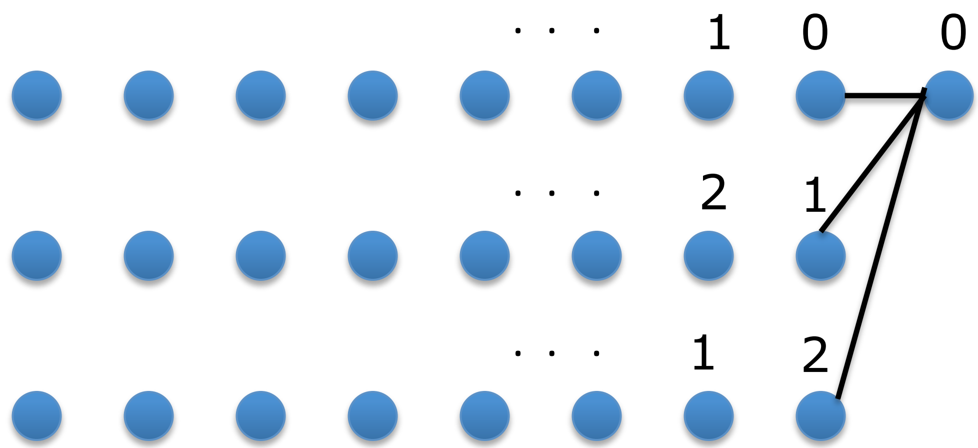

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Quantum: Boundary contraction. Density matrix on qubit + bond

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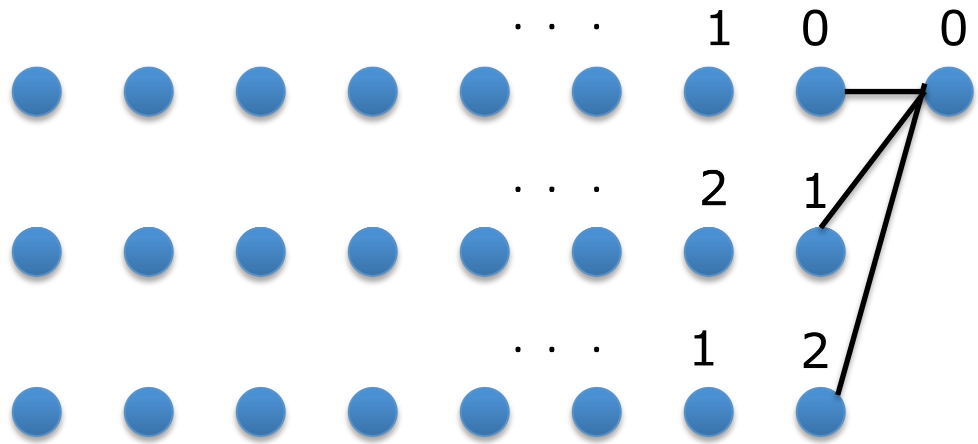


Quantum: Boundary contraction. Density matrix on qubit + bond

[Hastings '07] Bond dimension is poly(n).
To discretize, need an ε-net of size exp(n).

[Arad, Kitaev, Landau, Vazirani '12] Sublinear $2^{O\left(\log^{2/3} n\right)}$ bond dimension ➔ subexponential time algorithm

Two Ideas

1. For any given cut, and constant δ, there is a δ-approximation to |GS> with constant bond dimension B_δ across that cut (and poly(n) across other cuts).

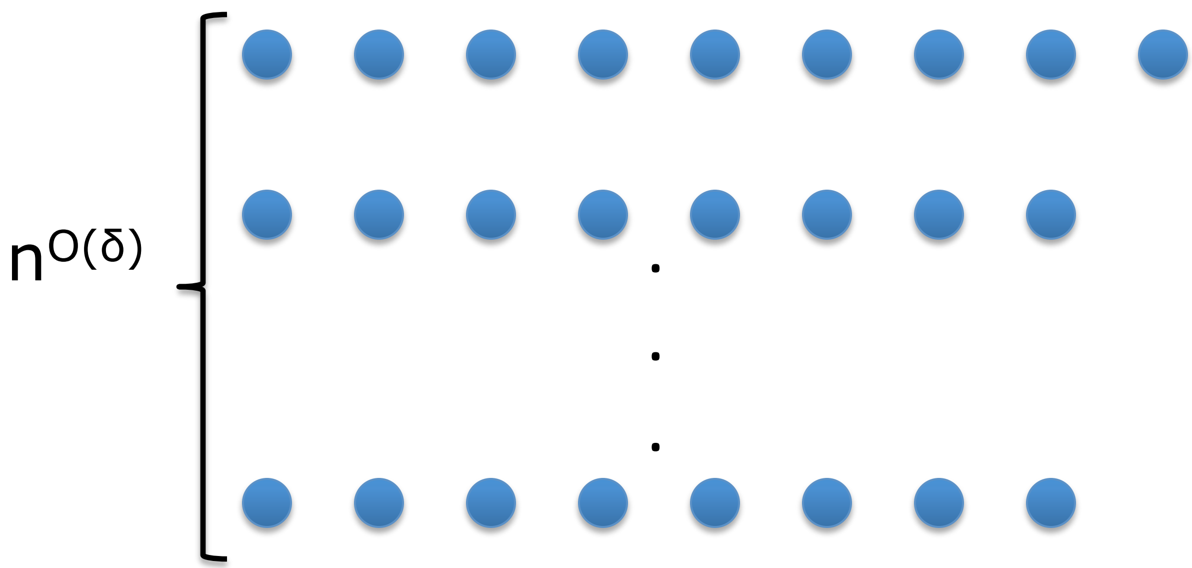
Pros:
Can use a $n^{O(\delta)}$-net for the boundary contractions across this cut to perform the extension step.

Cons:
Need to repeat this process across n cuts, and the error will blow up.

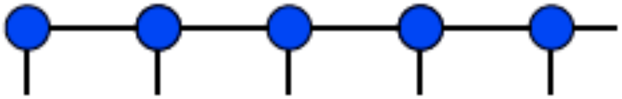
Two Ideas

1. For any given cut, and constant δ, there is a δ-approximation to |GS> with constant bond dimension B_δ across that cut (and poly(n) across other cuts).

2. Use an AGSP to reduce the error to 1/poly(n).



Upon Closer Examination



1. After the i-th iteration, the algorithm constructs an approximation to the left-half of |GS>.

   Can measure bond to decompose into a mixture of pure states on the first i qudits.

2. How do we apply an AGSP to a state on i qudits?

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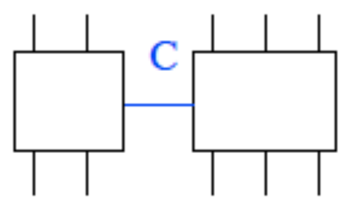

To get 1/poly(n) approximation, need C=poly(n).

Major Problem

- What we wanted: A poly(n) cardinality set of left-states on first i qudits, such that one of them of cardinality poly(n), such that one of them is (close to) the left-half of |GS>.

- What we obtained: a set of poly(n) states on first i qudits such that their span contains the left-half of (approx. to) |GS>.

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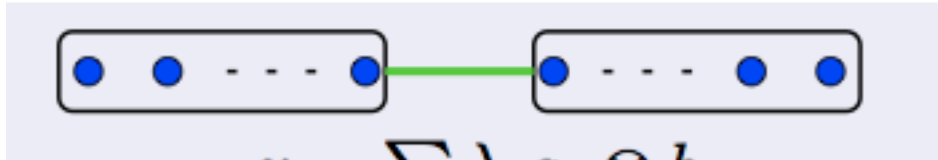
Idea: For a given boundary contraction on i+1-st qudit, finding a left-state which lies in the span of these poly(n) states on first i qudits, and with close to the specified boundary contraction can be expressed as a poly-sized convex program.

Convex Programming Framework for 1D Algorithm



$$v = \sum \lambda_i a_i \otimes b_i$$

min Tr[Hρ]

Tr[ρ]=1

ρ≥0

- But SDP is over an exponential dimensional space.
- Create a polynomial dimensional envelope that is guaranteed to contain a close approximation to ground state.

Viable Set

A set S of pure states on i-qudits is (i, s, b, δ) viable if:

- There is a δ-approx to |GS> whose left Schmidt vectors are in the span of S.
- Each element of S has an MPS representation with bond dimension ≤ B.
- |S| = s

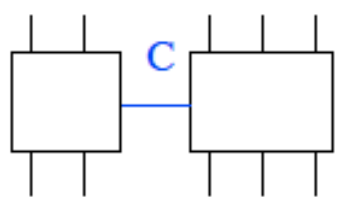
i →i+1: Four steps

Extension: Append a qudit. s → sd

Cardinality Reduction:
Fix a δ/n-net over the space of boundary contractions of constant dimension B_δ at i+1-st boundary.

$$\begin{aligned} \min \quad & \sum_{j=1}^{i-1} \mathrm{tr}(H_j \sigma) \\ \text{such that} \quad & \| \mathrm{tr}_{[1,\dots,i-1]}(\sigma) - X \|_1 \le \frac{c_\varepsilon}{2n}, \\ & \mathrm{tr}(\sigma)| = 1, \quad \sigma \ge 0. \end{aligned}$$

Error reduction: Apply AGSP to each element of S.



Bond Trimming: Truncate MPS representations.

Analysis

		i	s	B	δ
Start		$i-1$	$p(n)p_1(n)$	$p(n)p_2(n)$	c_ε/n
Extension:	$\rightarrow$	i	$dp(n)p_1(n)$	$p(n)p_2(n)$	c_ε/n
Size Trimming:	$\rightarrow$	i	$p_1(n)$	$p'(n)p_2(n)$	$1/12$
Bond Trimming:	$\rightarrow$	i	$p_1(n)$	$p_2(n)$	$1/2$
Error reduction:	$\rightarrow$	i	$p(n)p_1(n)$	$p(n)p_2(n)$	c_ε/n

Uniform AGSP

Assume frustration-free.

I – H/n stabilizes |GS> and |H|perp>| ≤ 1 – ε/n

So $(I - H/n)^n$ shrinks |perp> by constant factor

$$\frac{1}{n^n}(I - H_1)(I - H_2)\cdots(I - H_n)$$

$$= \frac{1}{n^n}\sum_{i_1\cdots i_n} H_{i_1}\cdots H_{i_n}$$

K = Sample poly(n) terms.

By matrix Chernoff bounds good approximation.

Conclusions

- A more local algorithm?
- AGSP
- 2D systems?
- Dependence on ε