A new efficient algorithm for finding the ground states of 1D gapped local Hamiltonians

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Joint work with
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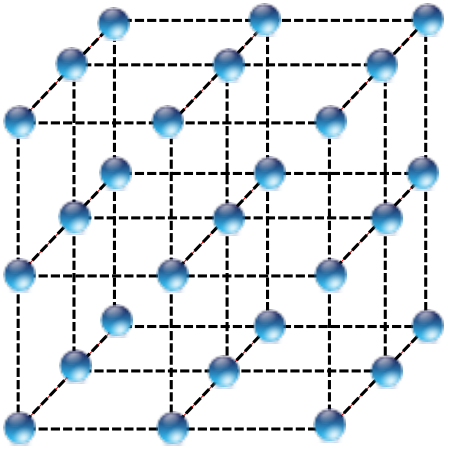
How hard is it to approximate the ground energy ?

The k-local Hamiltonian problem (Kitaev '98)

$$H = \sum_{|X| \leq k} h_X \qquad \|h_X\| \leq 1$$



ϵ_0 ground energy - the smallest eigenvalue of H

$|\Gamma\rangle$ ground state

How hard is it to find a $1/\mathrm{poly}(n)$ approximation to ϵ_0?
To other local observables?

The "quantum Cook-Levin" theorem, Kitaev' 98:

When $k = 5$ and $d = 2$, it is QMA hard

Some landmark results

The problem remains QMA hard when:

- Regev & Kempe '03: $k = 3$ and $d = 2$
- Regev & Kempe & Kitaev '04: $k = 2$ and $d = 2$
- Oliveira & Terhal '05 $k = 2$ and $d = 2$ on a 2D lattice
- Aharonov et. al. '07 $k = 2$, $d = 12$ in 1D lattice
- Hallgren et. al. '13 $k = 2$, $d = 8$ in 1D lattice

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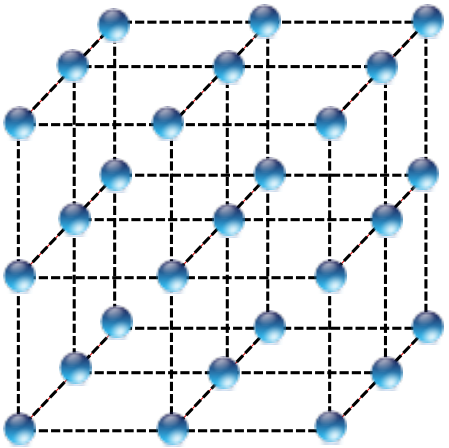
However, for physicists most 1D problems are easy (DMRG)
How can that be?

Gapped systems

$$H = \sum_{|X| \leq k} h_X \qquad \|h_X\| \leq 1$$

H eigenvalues : $\epsilon_0 < \epsilon_1 < \epsilon_2 < \ldots$

$\gamma := \epsilon_1 - \epsilon_0$ Spectral gap



Common belief:

When $\gamma = \Omega(1)$, then $|\Gamma\rangle$ becomes "more local". May admit an efficient classical description

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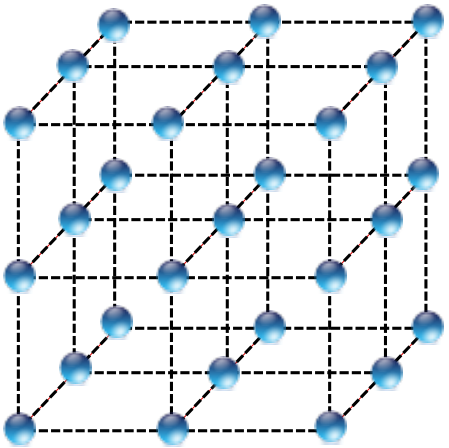

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When $\gamma = \Omega(1)$, the complexity of the LH problem becomes classical:

- ☆ In 1D it is in P
- ☆ In 2D and more it is inside NP

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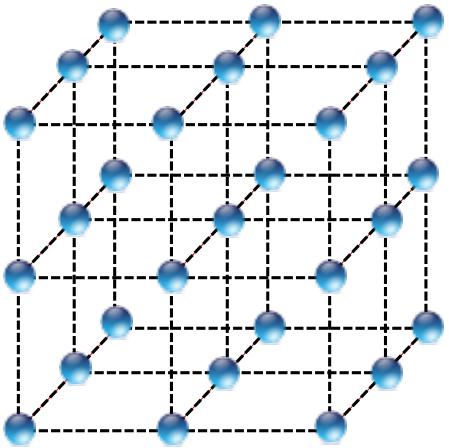

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- ✓ ☆ In 1D it is in P — Landau, Vazirani & Vidick '13
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Efficient algorithms for 1D

Previous results:

- Z. Landau, U. Vazirani & T. Vidick, 2013:
  A randomized algorithm. Runs in $T = n^{2^{O\left(1/\gamma\right)}}$

- Y. Haung, 2014:
  Deterministic algorithm. Runs in $T = 2^{2^{O\left(1/\gamma\right)}} \cdot n^{O\left(1/\gamma\right)}$

- C. T. Chubb & S. Flammia:
  Extends Huang's algorithm for degenerate ground states

Our result:

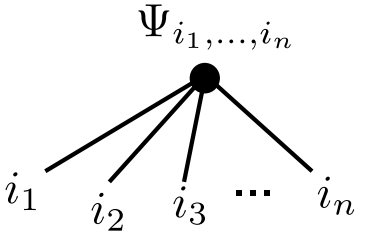
A new randomized algorithm with $T = n^{O\left(1/\gamma\right)}$ and:

- A new framework - can be potentially improved

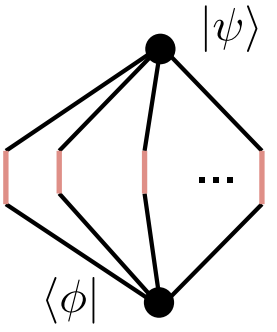
- **Much** more programmer friendly; no eps-nets, better factors

MPS & tensor networks Theory

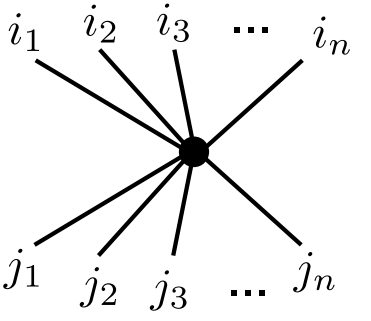
$$|\psi\rangle = \sum_{i_1,\ldots,i_n=1}^{d} \Psi_{i_1,\ldots,i_n} |i_1\rangle \otimes \cdots \otimes |i_n\rangle$$



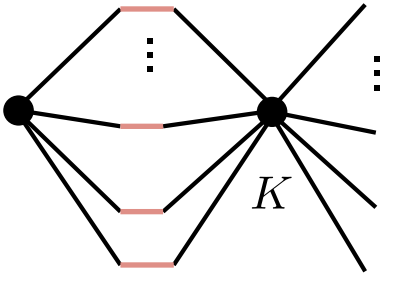
$\langle\phi|\psi\rangle \quad \Leftrightarrow$



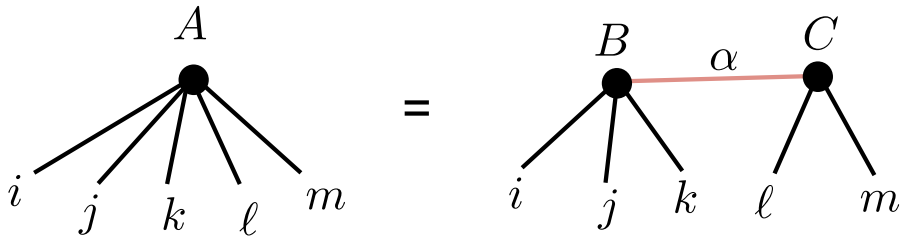
$$K = \sum_{\underline{i},\underline{j}} K^{j_1\ldots j_n}_{i_1\ldots i_n} |j_1\rangle\langle i_1| \otimes \cdots \otimes |j_n\rangle\langle i_n|$$



$k|\psi\rangle \quad \Leftrightarrow \quad |\psi\rangle$



$$A_{ijk\ell m} = \sum_{\alpha=1}^{D} B_{ijk,\alpha} \cdot C_{\alpha,\ell m}$$

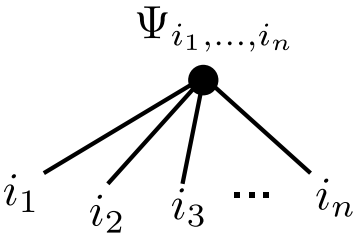


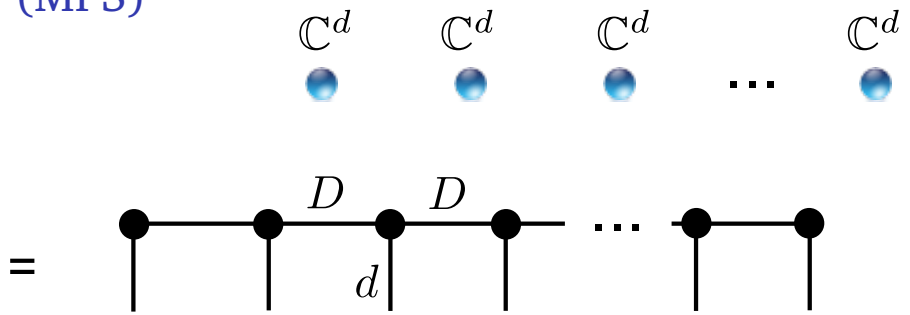
$$|A\rangle = \sum_{\alpha=1}^{D} |B_\alpha\rangle \otimes |C_\alpha\rangle$$

The Schmidt rank between the two sides is bounded by D

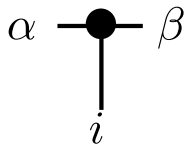
Tensor networks can describe the entanglement structure of a state

Matrix Proiduct States (MPS)





$A^i_{\alpha\beta}$ =



D – **bond dimension**

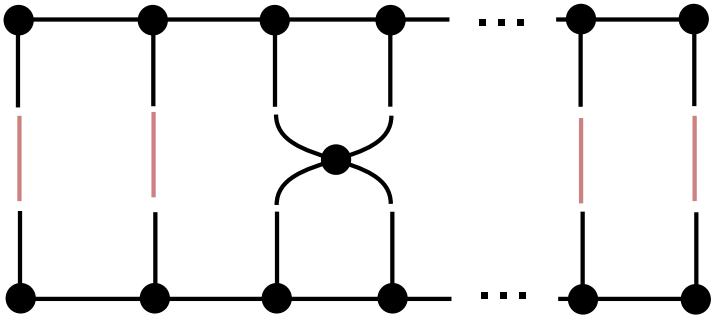
d^n parameters $\mapsto nD^2d$ parameters

Proposition

An ordered array of qudits of has an MPS representation with bond dimension D iff the Schmidt rank at every cut in the line $\leq D$.

Local observables can be evaluated efficiently

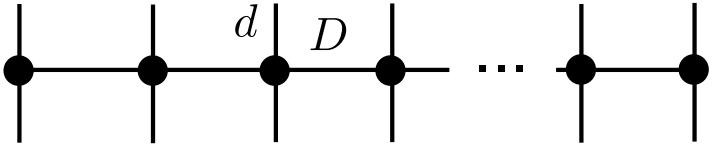
$\langle\psi|A|\psi\rangle$

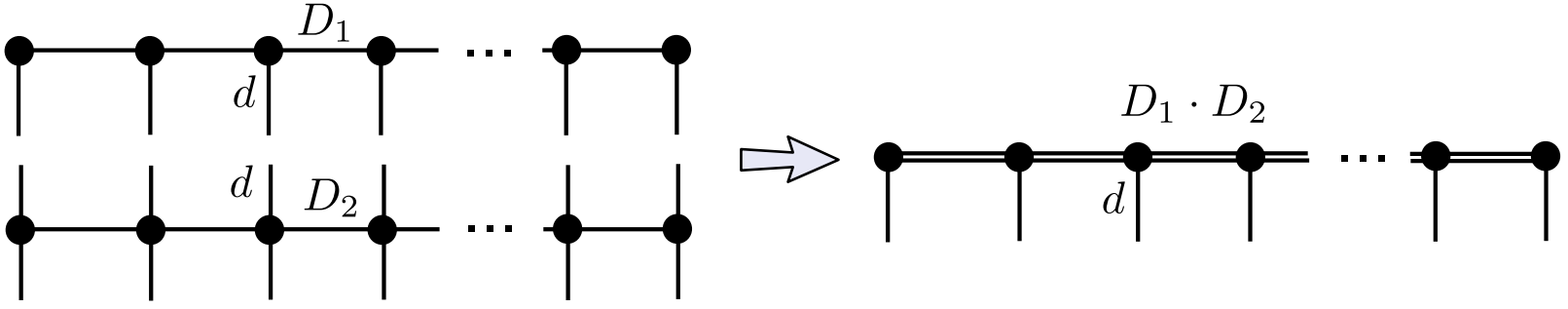


Contraction time $= \mathrm{O}\left(nd^2D^4\right)$

Matrix Product Operators (MPO)

$$K = \sum_{\alpha=1}^{D} A_\alpha \otimes B_\alpha \qquad \Rightarrow \qquad K =$$

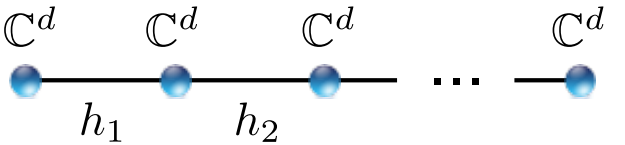




The 1D area law

Theorem (AKLV '13)

$H = \sum_{i=1}^{n-1} h_i \quad \|h_i\| \leq 1$



Spectral gap $\gamma = \epsilon_1 - \epsilon_0 > 0$

Consider the Schmidt decomposition of the g.s. $|\Gamma\rangle$ across the $(i, i+1)$ cut:

$$|\Gamma\rangle = \sum_{\alpha} \lambda_\alpha |L_\alpha\rangle \otimes |R_\alpha\rangle$$

Then for any $\delta > 0$,

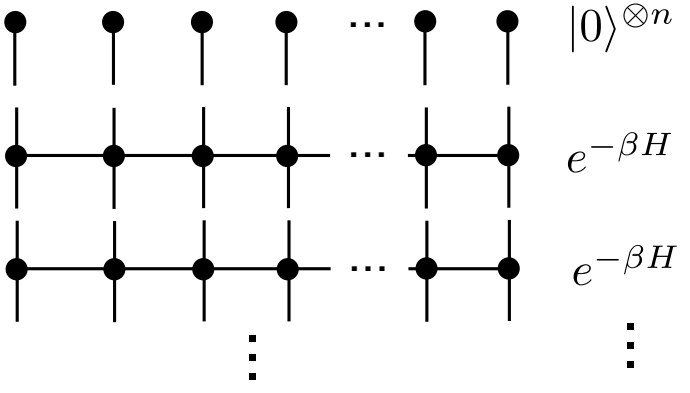
$$\sum_{\alpha \geq k_0} \lambda_\alpha^2 \leq \delta \quad \text{for } k_0 := e^{\tilde{\mathrm{O}}\left(\gamma^{-1/4} \cdot \log^{3/4}(\delta^{-1}) \cdot \log d\right)}$$

Corollary: For any polynomial $\mathrm{poly}(n)$, there is an MPS $|\Gamma_D\rangle$ with bond dimension $D = e^{\tilde{\mathrm{O}}\left(\gamma^{-1/4} \cdot \log^{3/4} n \cdot \log d\right)}$ such that $\||\Gamma\rangle - |\Gamma_D\rangle\| \leq 1/\mathrm{poly}(n)$.

Finding a MPS approximation for $|\Gamma\rangle$

A naive approach:

1. Start with a product state $|0\rangle^{\otimes n}$
2. Apply $e^{-\beta H}$ for some $\beta = \mathrm{O}(1)$ several times



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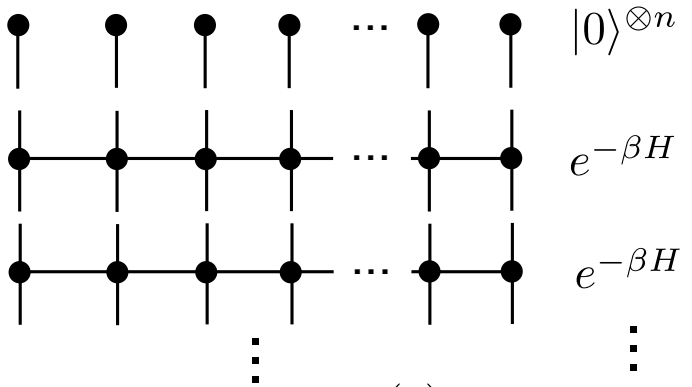

Problem: $|\langle 0^{\otimes n}|\Gamma\rangle| \leq d^{-\Omega(n)}$

$\Rightarrow$ we will need to apply $e^{-\beta H}$ for $\Omega(n)$ times resulting in an MPS with an exponential bond dimension

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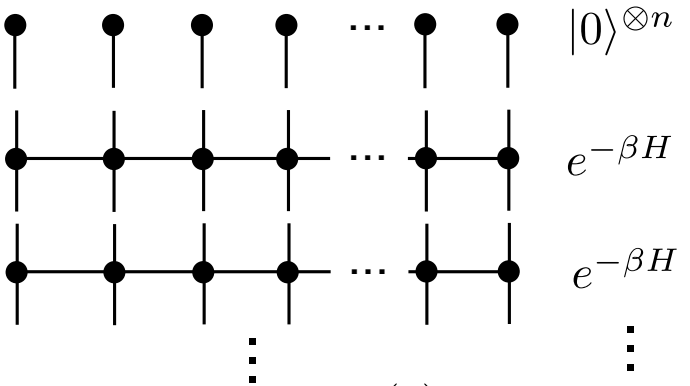

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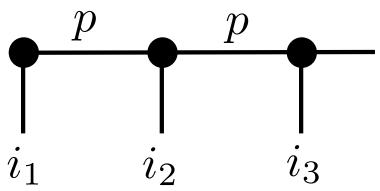
However: For $\rho_1 := \mathrm{Tr}_{[2,n]}\, |\Gamma\rangle\langle\Gamma|$ we know $\exists |\alpha\rangle$ such that $\langle\alpha|\rho_1|\alpha\rangle = \mathrm{O}(1)$

Can we gradually approximate $\rho_{[1,k]}$ for k=1,2,3,... ?

Definition: a viable set



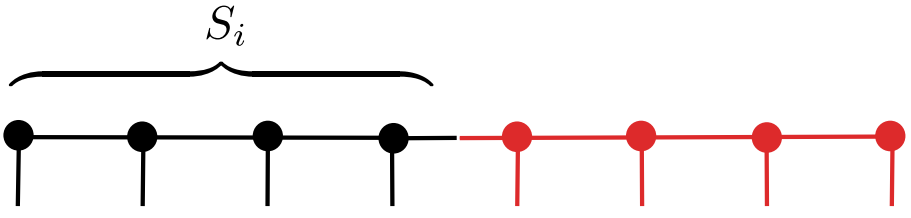
$\alpha = 1, \ldots, s$ $\quad\Leftrightarrow\quad$ $\{|\phi_\alpha\rangle\}_{\alpha=1}^{s}$

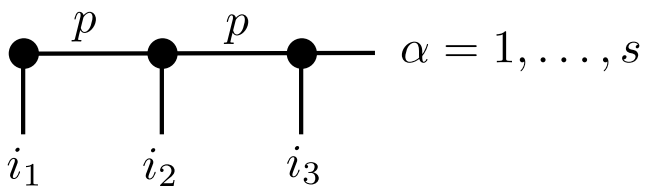
A subspace $S_i \subseteq \mathcal{H}_{[1,i]}$ is a (i, s, p, η)-viable set for $|\Gamma\rangle$ if:

- S_i is an s-dimensional subspace spanned by $|\phi_\alpha\rangle$ as above
- $\exists |\psi\rangle$ such that $|\langle\psi|\Gamma\rangle|^2 \geq \eta$ and $\mathrm{Tr}_{[i+1,n]}\, |\psi\rangle\langle\psi|$ supported in S_i
- Bond dimension of the partial MPS is at most p

Graphically, $\mathrm{Tr}_{[i+1,n]}\, |\psi\rangle\langle\psi|$ is supported in S_i iff:

$|\psi\rangle \quad =$





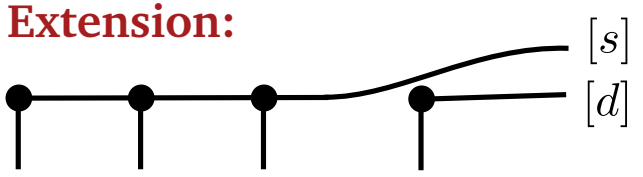
At every step we construct a (i, s, p, η)-viable set S_i for $|\Gamma\rangle$ with:

- $s = \Theta\big(\log n\big)$
- $p = \tilde{\mathrm{O}}\big(n\big)$
- $\eta = \frac{1}{2} \qquad \Rightarrow \qquad |\langle\psi|\Gamma\rangle|^2 \geq \frac{1}{2}$

Constructing S_1 is easy - just take the entire local Hilbert space

$S_{i-1} \to S_i$

1. Extension:



$S_i^{(1)}$ is a $(i, sd, p, \frac{1}{2})$-V.S.

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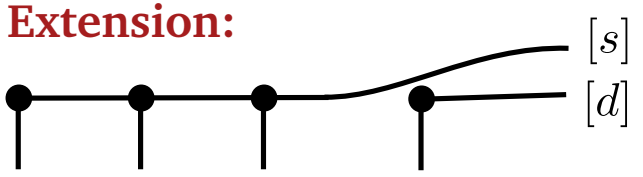
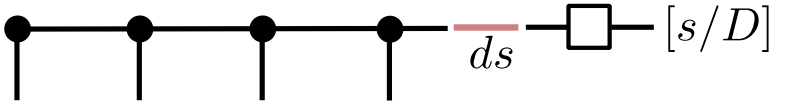


$S_i^{(1)}$ is a $(i, sd, p, \frac{1}{2})$-V.S.

2. Size reduction: project to a random s/D subspace



$S_i^{(2)}$ is a $(i, s/D, p, \frac{1}{8dD})$-V.S.

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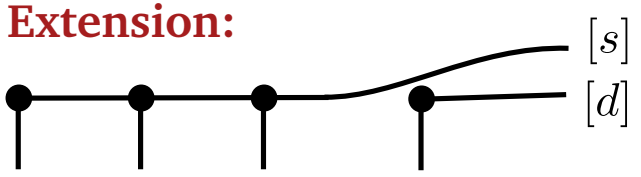

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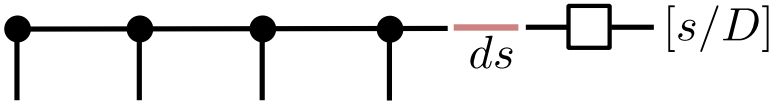
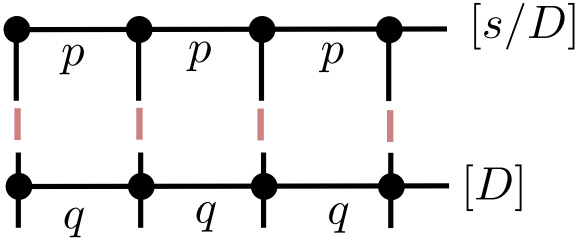


$S_i^{(2)}$ is a $(i, s/D, p, \frac{1}{8dD})$-V.S.

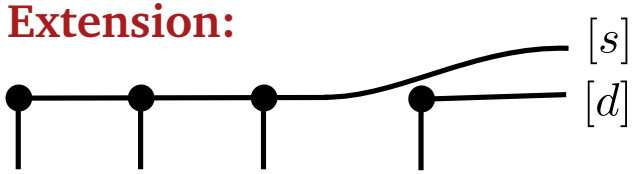
3. Amplification: Apply an AGSP K



$S_i^{(3)}$ is a $(i, s, pq, \frac{3}{4})$-V.S.

$S_{i-1} \to S_i$

1. Extension:



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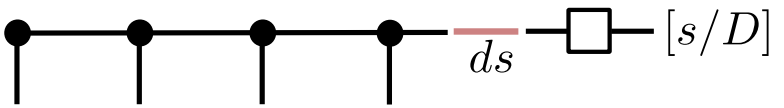

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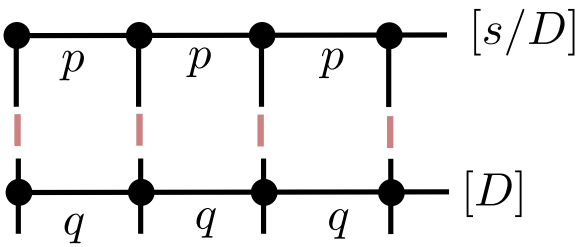
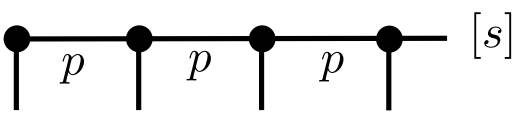


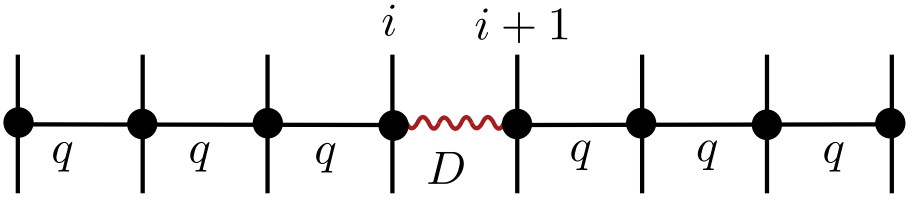
$S_i^{(3)}$ is a $(i, s, pq, \frac{3}{4})$-V.S.

4. Truncation: Truncate the high Schmidt coefficients



$S_i = S_i^{(4)}$ is a $(i, s, p, \frac{1}{2})$-V.S.

AGSP - Approximate Ground State Projectors

$K =$ 

Definition:

An operator K is a (i, q, D, Δ) AGSP for $|\Gamma\rangle$ if:

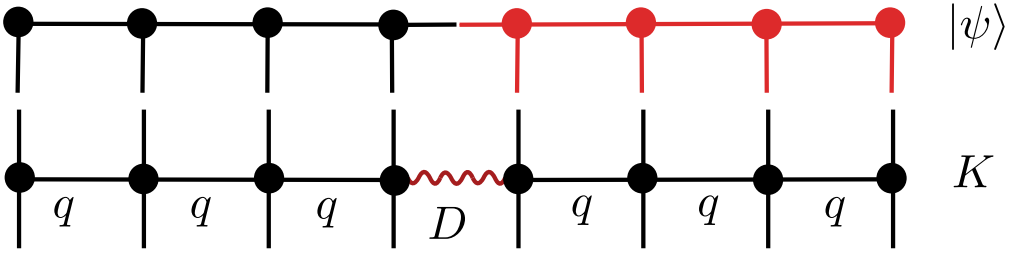
- Given as MPO with bond D between $i, i+1$ and q elsewhere
- $K|\Gamma\rangle = |\Gamma\rangle$ and $\|K|\Gamma^{\perp}\rangle\|^2 \leq \Delta \cdot \||\Gamma^{\perp}\rangle\|^2$

Theorem:

There is an efficiently constructable (i, q, D, Δ)-AGSP for $|\Gamma\rangle$ such that:

$$q = n^{\tilde{\mathrm{O}}\left(\frac{\log^5 d}{\gamma}\right)}, \qquad D = e^{\tilde{\mathrm{O}}\left(\frac{\log^3 d}{\gamma}\right)}, \qquad 8dD \cdot \Delta \leq \frac{3}{4}$$

Amplification



Let $|\psi\rangle$ be a witness for $|\Gamma\rangle$ with $|\langle\psi|\Gamma\rangle|^2 = \eta$

$$|\psi\rangle = \sqrt{\eta}|\Gamma\rangle + \sqrt{1-\eta}|\Gamma^\perp\rangle$$

A new witness for the amplified set: $|\phi\rangle := \frac{1}{\|K|\psi\rangle\|} K|\psi\rangle$

New overlap: $$|\langle\phi|\Gamma\rangle|^2 = \frac{\eta}{\eta + \Delta(1-\eta)} \geq 1 - \frac{\Delta}{\eta}$$

In the amplification step we start with $\eta = \frac{1}{8dD}$ $\Rightarrow$ we need $8dD\Delta \leq \frac{3}{4}$

Constructing a good AGSP

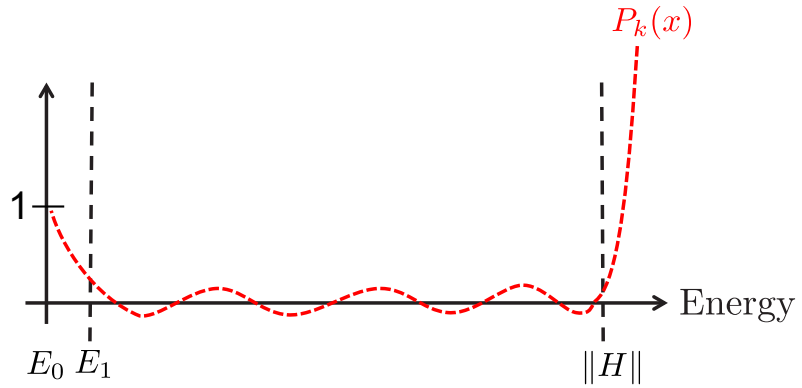
We need $K|\Gamma\rangle = |\Gamma\rangle, \quad \|K|\Gamma^\perp\rangle\|^2 \leq \Delta \||\Gamma^\perp\rangle\|^2$

Take $K = P_k(H)$ such that: $P_k(\epsilon_0) = 1$ and $|P_k(x)|^2 \leq \Delta$ for $\epsilon_1 \leq x \leq \|H\|$.

Rescaled Chebyshev polynomial:

$$\Delta = 4e^{-4k\sqrt{\gamma/(\|H\|-\epsilon_0)}}$$

$$D = d^{\mathrm{O}\left(\sqrt{k}\right)}$$



To have $D \cdot \Delta \ll 1$ we must truncate the norm of H

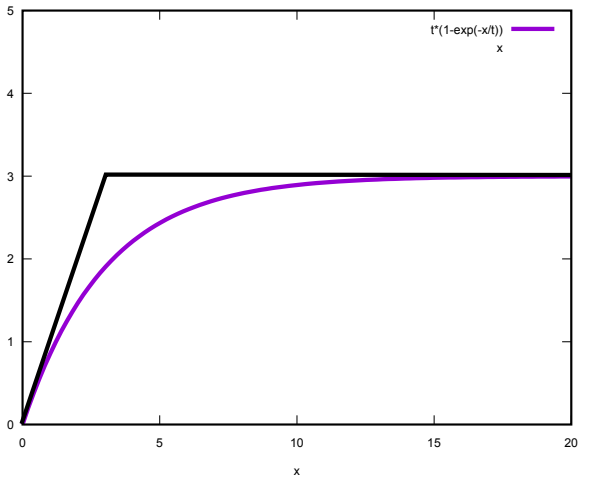
Soft truncation

$$H = H_L + h_{i-\ell} + \ldots + h_i + \ldots + h_{i+\ell} + H_R$$

$$H_L \to H_L^t, \qquad H_R \to H_R^t$$

In the Area-law proof: $H_L^t := H_L P_{\leq t} + t P_{>t}$

Soft truncation: $H_L^t := t(\mathbb{I} - e^{-H_L/t})$



The cluster expansion for $\mathbf{e^{-\beta H}}$

Kliesch et al '14 + Molnar et al '15:
There exists a good MPO approximation for $e^{-H_L/t}$

$\Rightarrow$ good MPO approximations for $H_t := H_L^t + h_{i-\ell} + \ldots + h_i + \ldots + h_{i+\ell} + H_R^t$

$\Rightarrow$ good MPO approximations for $K_i = P_k(H_t)$

Summary & open problems

- ★ A new algorithm for finding the g.s. of 1D systems, based on **good AGSPs**
- ★ More natural, and more friendly to program

- ? Can we improve the running time to linear?
  - ★ Need better AGSPs
  - ★ Better truncation scheme
- ? Can we de-randomize it?
- ? Run in parallel?
- ? Handle degeneracy?
- ? Can it teach us something new about the structure of gapped g.s. ?

Thank you !