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)

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

$\epsilon_0$ ground energy - the smallest eigenvalue of $H$

$|\Gamma\rangle$ ground state

How hard is it to find a $1/poly(n)$ approximation to $\epsilon_0$?
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

\[ H = \sum_{|X| \leq k} h_X \quad \|h_X\| \leq 1 \]

\[ H \text{ eigenvalues: } \epsilon_0 < \epsilon_1 < \epsilon_2 < \ldots \]

\[ \gamma := \epsilon_1 - \epsilon_0 \quad \text{Spectral gap} \]

Common belief:

When \( \gamma = \Omega(1) \), then \( |\Gamma\rangle \) becomes “more local”. May admit an efficient classical description
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The grand conjecture:
When \( \gamma = \Omega(1) \), the complexity of the LH problem becomes classical:

\[
\begin{align*}
\star & \quad \text{In 1D it is in P} \\
\star & \quad \text{In 2D and more it is inside NP}
\end{align*}
\]
Gapped systems

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\[ \checkmark \quad \star \quad \text{In 1D it is in P} \quad \text{Landau, Vazirani & Vidick '13} \]

\[ \star \quad \text{In 2D and more it is inside NP} \]
Efficient algorithms for 1D

Previous results:

★ Z. Landau, U. Vazirani & T. Vidick, 2013:
A randomized algorithm. Runs in $T = n^{2^\bigO{1/\gamma}}$

★ Y. Haung, 2014:
Deterministic algorithm. Runs in $T = 2^{2^\bigO{1/\gamma}} \cdot n^{\bigO{1/\gamma}}$

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

Our result:

A new randomized algorithm with $T = n^{\bigO{1/\gamma}}$ and:

★ A new framework - can be potentially improved

★ Much more programmer friendly; no eps-nets, better factors
\[ |\psi\rangle = \sum_{i_1,\ldots,i_n = 1}^d \Psi_{i_1,\ldots,i_n} |i_1\rangle \otimes \cdots \otimes |i_n\rangle \]

\[ \langle \phi | \psi \rangle \iff \begin{array}{c}
\langle \phi | \\
\cdots \\
\langle \phi |
\end{array} \]

\[ K = \sum_{i,j} K_{i_1\ldots i_n}^{j_1\ldots j_n} |i_1\rangle \langle j_1| \otimes \cdots \otimes |i_n\rangle \langle j_n| \]

\[ k |\psi\rangle \iff |\psi\rangle \begin{array}{c}
\cdots \\
K
\end{array} \]
\[ A_{ijklm} = \sum_{\alpha=1}^{D} B_{ijk,\alpha} \cdot C_{\alpha,lm} \]

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

The Schmidt rank between the two sides is bounded by D.

Tensor networks can describe the entanglement structure of a state.
Matrix Product States (MPS)

\[ \Psi_{i_1, \ldots, i_n} \]

\[ \mathbb{C}^d \quad \mathbb{C}^d \quad \mathbb{C}^d \quad \ldots \quad \mathbb{C}^d \]

\[ = \]

\[ D \quad D \quad \ldots \quad D \]

\[ A_{\alpha \beta}^i = \alpha \quad \beta \]

\[ D - \text{bond dimension} \]

\[ d^n \text{ parameters} \mapsto nD^2d \text{ parameters} \]

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 = \( O(nd^2 D^4) \)

Matrix Product Operators (MPO)

\[ K = \sum_{\alpha=1}^{D} A_\alpha \otimes B_\alpha \quad \Rightarrow \quad K = \]

\[ d \quad D \quad \cdots \]

\[ D_1 \quad D_2 \quad \cdots \]

\[ d \quad d \]

\[ D_1 \cdot D_2 \quad \cdots \]
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 \( \delta > 0 \),

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

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

\[ \| |\Gamma\rangle - |\Gamma_D\rangle \| \leq 1/\text{poly}(n). \]
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 $\beta = O(1)$ several times

\[ \begin{array}{c}
\cdots \\
|0\rangle^\otimes n \\
\vdots \\
\end{array} \]
Finding a MPS approximation for $|\Gamma\rangle$

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![Diagram](image)

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

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

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

\[ p \quad \bullet \quad \bullet \quad p \quad \alpha = 1, \ldots, s \]

\[ \Rightarrow \quad \{ |\phi_\alpha\rangle \}_{\alpha=1}^{s} \]

A subspace \( S_i \subseteq \mathcal{H}_{[1,i]} \) is a \((i, s, p, \eta)\)-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 \( \text{Tr}_{[i+1,n]} |\psi\rangle\langle\psi| \) supported in \( S_i \)
- Bond dimension of the partial MPS is at most \( p \)

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

\[ |\psi\rangle = \underbrace{\bullet \quad \bullet \quad \bullet \quad \bullet}_{S_i} \overbrace{\bullet \quad \bullet \quad \bullet \quad \bullet}^{p} \]
At every step we construct a \((i, s, p, \eta)\)-viable set \(S_i\) for \(|\Gamma\rangle\) with:

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

**Constructing** \(S_1\) is easy - just take the entire local Hilbert space
$S_{i-1} \rightarrow S_i$

1. Extension:

\[ \begin{array}{c}
\text{[s]} \\
\text{[d]}
\end{array} \]

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

1. **Extension:**

```
[ s ]
[ d ]
```

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

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

```
[ s/D ]
```

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

1. **Extension:**

   $S_i^{(1)}$ 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.

3. **Amplification:** Apply an AGSP $K$

   $S_i^{(3)}$ is a $(i, s, pq, \frac{3}{4})$-V.S.
\[ S_{i-1} \rightarrow S_i \]

1. **Extension:**

\[ \begin{array}{c}
\bullet \\
\bullet \\
\bullet \\
\bullet \\
\bullet \\
\bullet \\
\bullet \\
\end{array} \]

\[
\begin{bmatrix}
\mathbf{s} \\
\mathbf{d}
\end{bmatrix}
\]

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

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

\[ ds \]

\[ \begin{array}{c}
\bullet \\
\bullet \\
\bullet \\
\bullet \\
\bullet \\
\bullet \\
\bullet \\
\bullet \\
\end{array} \]

\[
\begin{bmatrix}
s/D
\end{bmatrix}
\]

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

3. **Amplification:** Apply an AGSP K

\[ p \quad p \quad p \]

\[ \begin{array}{c}
\bullet \\
\bullet \\
\bullet \\
\bullet \\
\end{array} \]

\[
\begin{bmatrix}
s/D
\end{bmatrix}
\]

\[ q \quad q \quad q \]

\[ \begin{array}{c}
\bullet \\
\bullet \\
\bullet \\
\bullet \\
\end{array} \]

\[
\begin{bmatrix}
D
\end{bmatrix}
\]

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

4. **Truncation:** Truncate the high Schmidt coefficients

\[ \begin{array}{c}
p \\
p \\
p
\end{array} \]

\[ \begin{array}{c}
\bullet \\
\bullet \\
\bullet \\
\bullet \\
\end{array} \]

\[ \begin{bmatrix}
s
\end{bmatrix}
\]

\( S_i = S_i^{(4)} \) is a \((i, s, p, \frac{1}{2})\)-V.S.
AGSP - Approximate Ground State Projectors

\[ K = \]

\[ q \quad q \quad q \quad D \quad q \quad q \quad q \quad q \]

Definition:
An operator \( K \) is a \((i, q, D, \Delta)\) 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 \((i, q, D, \Delta)\)-AGSP for \(|\Gamma\rangle\) such that:
\[
q = n \tilde{O}\left( \frac{\log^5 d}{\gamma} \right), \quad D = e \tilde{O}\left( \frac{\log^3 d}{\gamma} \right), \quad 8dD \cdot \Delta \leq \frac{3}{4}
\]
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: $|\phi\rangle := \frac{1}{\|K|\psi\|}K|\psi\rangle$

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

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:

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

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

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

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

\[ H_L \rightarrow H_L^t, \quad H_R \rightarrow H_R^t \]

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

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

The cluster expansion for \( e^{-\beta H} \)

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!