Improved Approximation Algorithms for Bounded-Degree Local Hamiltonians

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Joint work with

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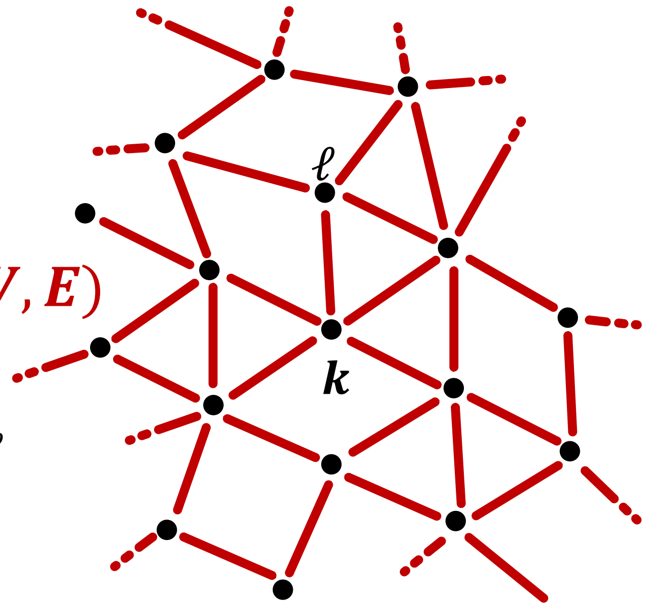
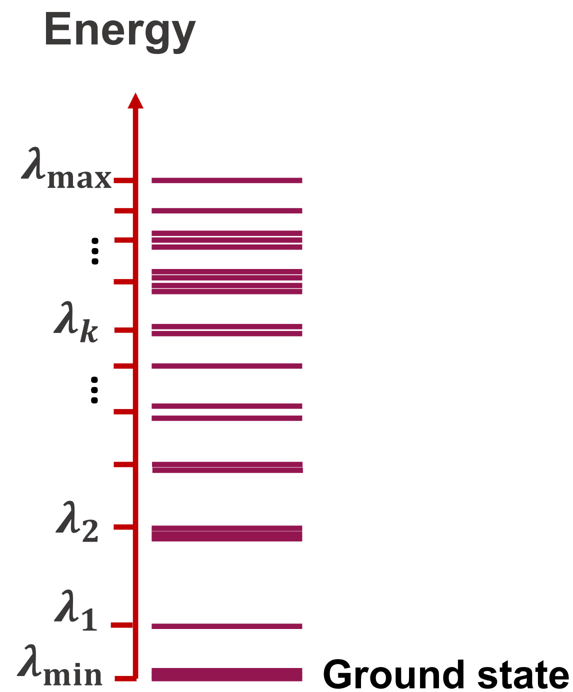
Problem Statement and Background

Bounded-degree Local Hamiltonians

Interaction graph $G = (V, E)$
$|V| = n$ **qubits**
$|E| = m$ **local term $h_{k\ell}$**





Local Hamiltonian $H = \sum_{\{k,\ell\}\in E} h_{k\ell}$

Degree-d interaction graph:
Each qubit is involved in $\leq d$ interactions

Ground state of H captures the low-temperature physics

Believed to generally require $\exp(n)$ resources to compute

1 Worst-Case Complexity and Rigorous Algorithms

2 Heuristic Quantum Algorithms

Worst-Case Complexity

- **Ground state energy** $= \lambda_{\min}(H) := \min_{\psi} \langle \psi | H | \psi \rangle$

- **QMA-hard to estimate** $\lambda_{\min}(\mathrm{H})$ **with** $\frac{1}{\mathrm{poly}(n)}$ **additive error**

[Kitaev'99, Kempe-Kitaev-Regev'04]

- **PCP Theorem: For some constant** $0 < \varepsilon < 1$,
remains NP-hard to estimate $\lambda_{\min}$ **within additive error** $\varepsilon \cdot m$

QMA-hard? qPCP conjecture

[Arora-Lund-Motwani-Sudan-Szegedy'98,
Arora-Safra'98, Dinur'07]

Worst-Case Complexity

What is the best approximation of $\lambda_{\min}(\mathrm{H})$ achievable with efficient algorithms?

Known rigorous algorithms e.g. for

- **Heisenberg-like interactions:** $h_{ij} = I - X_i X_j - Y_i Y_j - Z_i Z_j$

  [Gharibian-Parekh'19, Anshu-Gosset-Morenz Korol'20]

- **Positive semidefinite:** $h_{ij} \geq 0$

  [Gharibian-Kempe'12]

- **Traceless:** $\mathrm{Tr}[h_{ij}] = 0$

  [Bravyi-Gosset-König-Temme'19]

- **Dense or planar graphs**

  [Bansal-Bravyi-Terhal'09, Gharibian-Kempe'12, Brandão-Harrow'14]

Worst-Case Complexity

Most of these algorithms compute a quantum state $|v\rangle$ that

$$|v\rangle = |v_1\rangle \otimes |v_2\rangle \otimes \cdots \otimes |v_n\rangle$$

or

$|v\rangle =$ tensor product of few-qubit states

But ground states may be highly entangled,

What is the structure of states
which provide good approximations?

Worst-Case Complexity

What is the structure of states which provide good approximations?

For high degree graphs, product states provide good approximations

Monogamy of entanglement
Mean-field approximation

[Brandão, Harrow 2014]

For Hamiltonians on degree-d graphs with n qubits and m interactions, there exists $|v\rangle = |v_1\rangle \otimes |v_2\rangle \otimes \cdots \otimes |v_n\rangle$ s.t.

$$\langle v|H|v\rangle \leq \lambda_{\min}(H) + O\left(\frac{m}{d^{1/3}}\right)$$

Are there improved approximation algorithms for $\lambda_{\min}(H)$ using entangled states?

What is the structure of states which provide good approximations?

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This work:
Extensive improvement over product states for bounded-degree interactions via low-depth quantum circuits

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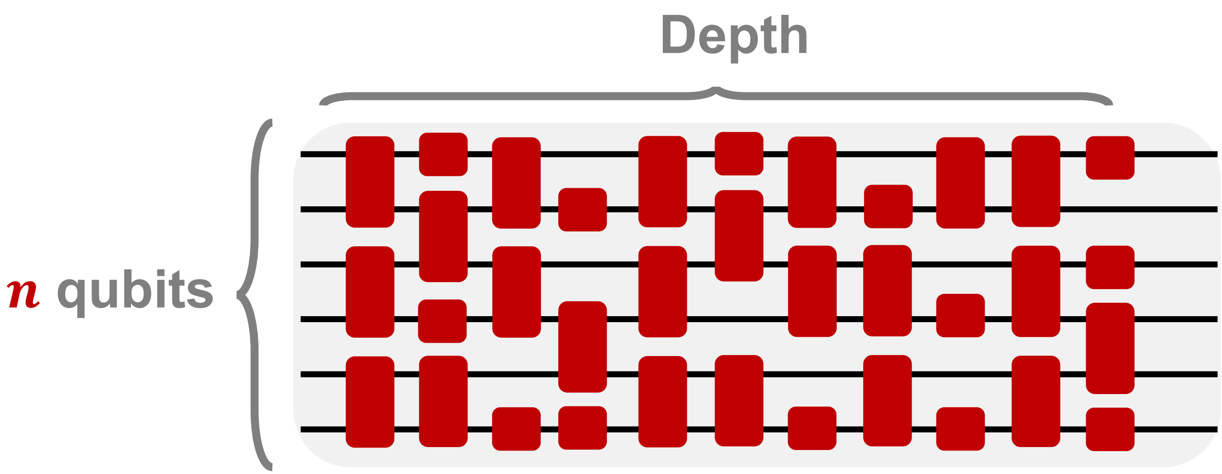
Ground states may be highly entangled

So potential advantage in using quantum computers

Some near-term quantum computers can be modeled with low-depth quantum circuits model



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Many heuristic algorithms use low-depth quantum circuits

E.g. variational algorithms:

$$|\psi(\theta)\rangle = U(\theta)|0^n\rangle$$

$\langle\psi(\theta)|H|\psi(\theta)\rangle$
Measure with quantum computer

$\min_\theta \langle\psi(\theta)|H|\psi(\theta)\rangle$
Optimize with classical computer

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Many heuristic algorithms use low-depth quantum circuits

Rigorous bounds on the performance of low-depth quantum circuits for estimating ground energy?

Recap

Many known rigorous algorithms output product states.

How can we improve them by applying quantum circuits?

Many near-term algorithms use low-depth quantum circuits

How can we rigorously bound their performance?

Main Results

Result: Improving product state approx.

Given a product state $|v\rangle = |v_1\rangle \otimes |v_2\rangle \otimes \cdots \otimes |v_n\rangle$

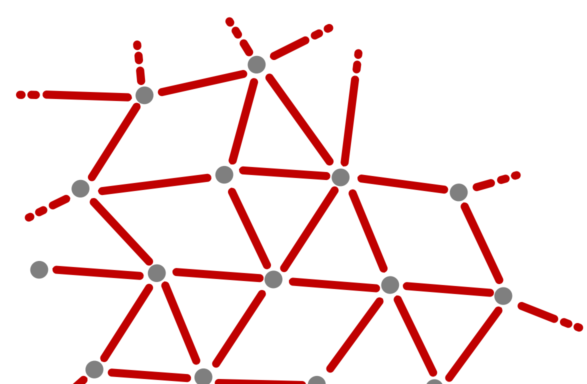
With variance

$$\mathrm{Var}_v(H) = \langle v|H^2|v\rangle - \langle v|H|v\rangle^2$$

There is a constant-depth quantum circuit U s.t. $|\psi\rangle = U|v\rangle$ satisfies

$$\langle\psi|H|\psi\rangle \le \langle v|H|v\rangle - \mathrm{constant} \cdot \frac{\mathrm{Var}_v(H)^2}{d^2\, m}$$

n qubits
m local terms h_{ij}
d neighbors



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- **An improvement of** $\Omega(m)$ **in estimated energy when**

$$\mathrm{Var}_v(H) = \Omega(m) \text{ and } d = O(1)$$

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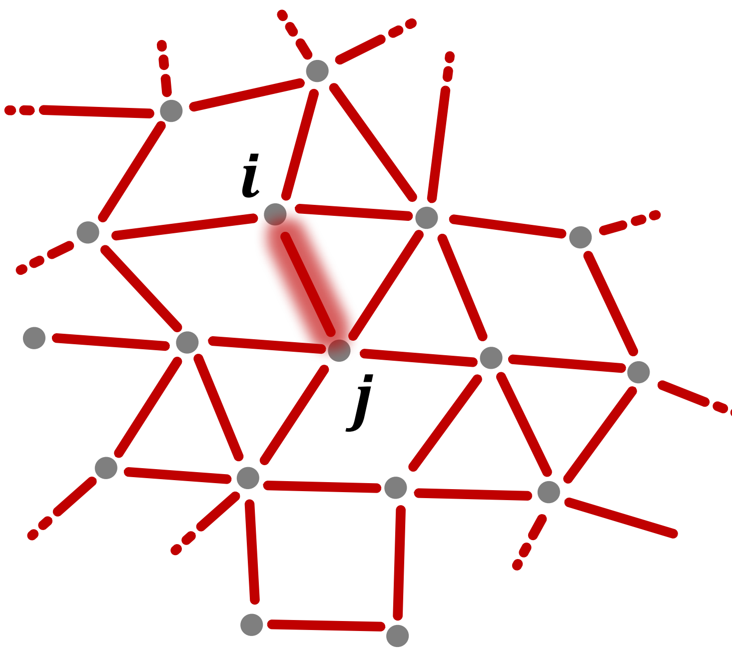
- **An improvement of** $\Omega(m)$ **in estimated energy when** $\mathrm{Var}_v(H) = \Omega(m)$ **and** $d = O(1)$
- **No improvement when** $|v\rangle$ **is eigenstate of Hamiltonian (e.g. purely classical case)**

Proof Idea of 1st Result

Circuit U for state $|v\rangle = |v_1\rangle \otimes |v_2\rangle \otimes \cdots \otimes |v_n\rangle$

$$U(\theta) = \Pi_{\{i,j\}\in E}\, e^{i\theta_{ij}P_iP_j} = e^{i\sum_{\{i,j\}\in E}\theta_{ij}P_iP_j}$$

$$\|P_i\| \leq 1, \qquad \langle v_i|P_i|v_i\rangle = 0 \qquad \forall i \in V$$



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- **Generalizes level-1 QAOA** $\quad P_i = e^{i\beta\sum_{i\in V}X_i}Z_i e^{-i\beta\sum_{i\in V}X_i}$
- **The circuit can be efficiently found. It has depth $= d+1$**

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$$\|P_i\| \leq 1, \qquad \langle v_i|P_i|v_i\rangle = 0 \qquad \forall i \in V$$

- **Slightly rotates** each $|v_i\rangle|v_j\rangle$ towards the ground space:

For some $\theta_0 \leq O(1/d)$:

$$\langle v|U(\theta_0)^\dagger\, h_{ij}\, U(\theta_0)|v\rangle$$

$$\leq \langle v|h_{ij}|v\rangle - \theta_0 \cdot \left|\langle v|[P_iP_j, h_{ij}]|v\rangle\right| + O(\theta_0^2 d)$$

Improved Bound and Tightness

Result: locally optimal states & tightness

Improved bound:

A product state $|v\rangle$ is locally optimal if for any single-qubit operator Q,

$$\frac{d}{d\phi}\langle v|e^{-i\phi Q}He^{i\phi Q}|v\rangle = 0 \quad \text{at} \quad \phi = 0$$

For locally optimal states,

$$\langle\psi|H|\psi\rangle \leq \langle v|H|v\rangle - \text{constant} \cdot \frac{\mathrm{Var}_v(H)^2}{d\,m}$$

Result: locally optimal states & tightness

Tightness:

For simple Hamiltonians e.g. $h_{ij} = Z_i + Z_j$ and

$$|v\rangle = (\cos(\theta)\,|0\rangle - \sin(\theta)|1\rangle)^{\otimes n}$$

We have

$$\langle v|H|v\rangle - \lambda_{\min} \leq \text{constant} \cdot \frac{\mathrm{Var}_v(H)^2}{d^2\, m}$$

Generic Performance

Result: Improvement for random states

Write H in terms of Pauli operators $\sigma_1, \sigma_2, \sigma_3$, and $\sigma_0 = I$:

$$H = \sum_{\{i,j\}\in E} \sum_{x,y} f_{xy}^{ij}\, \sigma_x^i \otimes \sigma_y^j$$

Define

$$\mathbf{quad}(H) = \sum_{\{i,j\}\in E} \sum_{x>0,y>0} \left(f_{xy}^{ij}\right)^2$$

Improvement for random product states

$$\mathbb{E}_v\langle\psi|H|\psi\rangle \leq \mathbb{E}_v\langle v|H|v\rangle - \mathbf{constant} \cdot \frac{\mathbf{quad}(H)^2}{d\, m}$$

For triangle-free graphs, we have

$$\mathbb{E}_v\langle\psi|H|\psi\rangle \leq \mathbb{E}_v\langle v|H|v\rangle - \mathbf{constant} \cdot \frac{\mathbf{quad}(H)}{\sqrt{d}}$$

Extensions of our Bounds

Result: k-local Hamiltonians

Given a degree-d k-local Hamiltonian H

and a product state $|v\rangle$,

there is a low-depth quantum circuit U s.t. $|\psi\rangle = U|v\rangle$ satisfies

$$\langle\psi|H|\psi\rangle \leq \langle v|H|v\rangle - \text{constant} \cdot \frac{\text{Var}_v(H)^2}{2^{O(k)} d^4\, m}$$

Result: Improving entangled states

Let $|v\rangle = W|0^n\rangle$ where W is a quantum circuit of depth D.
We can **efficiently** compute a quantum circuit U
such that the state $|\psi\rangle = U|v\rangle$ satisfies

$$\langle\psi|H|\psi\rangle \leq \langle v|H|v\rangle - \text{constant} \cdot \frac{\mathrm{Var}_v(H)^2}{2^{O(D)} d^2\, m}$$

$2^{O(D)} \rightarrow \ell^{10}$

- The circuit U is not constant-depth anymore
- The bound extends to when $|\psi\rangle$ is the **unique ground state** of some ℓ-local **gapped** Hamiltonian

Open Questions

Open questions

- Can output of SDP relaxations be directly rounded to entangled states?

  [Parekh-Thompson'20, Anshu-Gosset-Morenz Korol'20]

- Can similar strategies derive limitations on energy of low-depth circuits?

  NLTS [Freedman-Hastings'14, Eldar-Harrow'15, Anshu-Nirkhe'21]

- Rigorous results on performance of variational algorithms?

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