Improved Approximation Algorithms for Bounded-Degree Local Hamiltonians

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Joint work with

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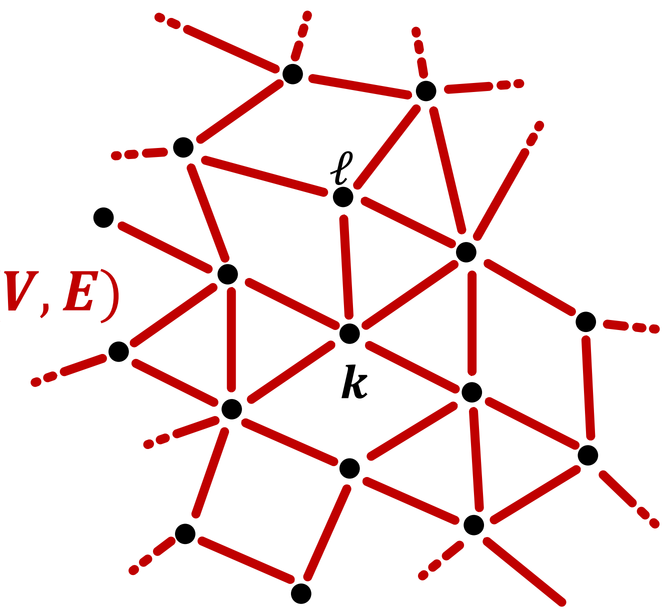
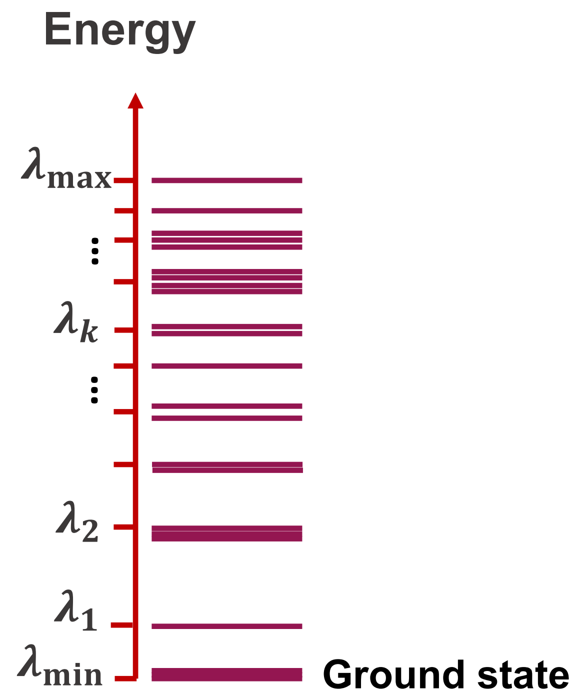
Problem Statement and Background

Interacting Quantum Systems

Interaction graph $G = (V, E)$
$|V| = n$ qubits
$|E| = m$ interactions





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

Degree-d interaction graph

Ground state of H captures the low-temperature physics

Believed to require $\exp(n)$ resources to compute in the worst case

1 Worst-Case Complexity and Rigorous Algorithms

2 Heuristic Quantum Algorithms

Worst-Case Complexity

- **Although ground state energy $= \lambda_{\min}(H)$, more convenient to consider estimating**

$$\lambda_{\max}(H) = \max_{\psi} \langle \psi | H | \psi \rangle$$

Equivalent because $\lambda_{\min}(H) = -\lambda_{\max}(-H)$

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

[Kitaev 1999, Kempe, Kitaev, Regev 2004]

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

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

QMA-hard? qPCP conjecture

Worst-Case Complexity

Approximation algorithms: compute estimate $\hat{\lambda} \leq \lambda_{\max}$ s.t.

$$r = \hat{\lambda}/\lambda_{\max}$$

is as large as possible.

What is the largest approximation ratio r achievable with efficient algorithms?

Known Algorithms e.g. for

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

  [Gharibian, Parekh 2019, Anshu, Gosset, Morenz Korol 2020]

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

  [Gharibian, Kempe 2012]

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

  [Bravyi, Gosset, König, Temme 2019]

- **Dense or Planar graphs**

  [Bansal, Bravyi, Terhal 2009, Gharibian, Kempe 2012, Brandão, Harrow 2014]

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
with high approximation ratio?**

Worst-Case Complexity

What is the structure of states with high approximation ratio?

For high degree graphs,
product states provide good approximations

Monogamy of Entanglement
Mean-field Approximation

[Brandão, Harrow 2014]

For Hamiltonians on degree-d graph 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.

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

This work:
Extensive improvement over product states for bounded-degree graphs using shallow (low-depth) quantum circuits

1 Worst-Case Complexity and Rigorous Algorithms

2 Heuristic Quantum Algorithms

- Many heuristic classical or quantum algorithms for estimating ground state energy

- Ground states could be highly entangled
  Potential advantage in using quantum computers

- E.g. variationally optimize energy over output states of shallow (low-depth) quantum circuits

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

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

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

- Many heuristic classical or quantum algorithms for estimating ground state energy

- Ground states could be highly entangled
  Potential advantage in using quantum computers

- E.g. variationally optimize energy over output states of shallow (low-depth) quantum circuits
  - Can be implemented on small quantum computers
  - Some known limitations in efficacy

[McClean et al 2018]
[Bravyi, Kliesch, Koenig, Tang 2020]
[Farhi, Gamarnik, Gutmann 2020]
[Bravyi, Gosset, Movassagh 2021]

Rigorous bounds on the performance of shallow 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 shallow quantum circuits

How can we rigorously bound their performance?

Main Results

Result: Improving product state approx.

Define variance of a state $|v\rangle$ by

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

Given a degree-d Hamiltonian H and a product state $|v\rangle$, we can efficiently compute a depth-$(d+1)$ quantum circuit U such that the state $|\psi\rangle = U|v\rangle$ satisfies

$$\langle \psi|H|\psi\rangle \geq \langle v|H|v\rangle + \Omega\left(\frac{\mathrm{Var}_v(H)^2}{d^2\, m}\right)$$

- 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 an eigenstate of Hamiltonian (e.g. purely classical case)

Proof Idea of 1st Result

Choice of circuit U for state $|v\rangle = |v_1\rangle \otimes |v_2\rangle \otimes \cdots \otimes |v_n\rangle$

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

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

- **Generalizes level-1 QAOA** $\quad P_i = e^{i\beta\sum_{k\in V}X_k} Z_k e^{-i\beta\sum_{k\in V}X_k}$
- **Locally & slightly rotates $|v_i\rangle|v_j\rangle$ towards the ground space**

Example: Antiferromagnetic Heisenberg Interactions

[Anshu, Gosset, Morenz Korol 2020]

$$H = \sum_{\{i,j\}\in E} w_{ij}h_{ij}$$

$$h_{ij} = \frac{1}{4}\left(I - X_iX_j - Y_iY_j - Z_iZ_j\right) = \left|\Psi_{ij}\right\rangle\left\langle\Psi_{ij}\right|$$

$$\left|\Psi_{ij}\right\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle_i|1\rangle_j - |1\rangle_i|0\rangle_j\right)$$

$$e^{-i\theta_{ij}X_iY_j}|0\rangle_i|1\rangle_j = \cos\left(\theta_{ij}\right)|0\rangle_i|1\rangle_j - \sin\left(\theta_{ij}\right)|1\rangle_i|0\rangle_j$$

Bounding improvement in energy

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

$$|\psi\rangle = U(\boldsymbol{\theta})|v\rangle$$

$$\langle\psi|h_{ij}|\psi\rangle = \langle v|U(\boldsymbol{\theta})^\dagger h_{ij}\, U(\boldsymbol{\theta})|v\rangle$$

$$= \langle v|h_{ij}|v\rangle - i\,\theta_{ij}\ \langle v|[P_iP_j\,, h_{ij}]|v\rangle\ + \mathbf{Err}$$

$$\langle v_i|P_i|v_i\rangle = 0$$

Bounding improvement in energy

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$$\langle v_i|P_i|v_i\rangle = 0$$

$$\theta_{k\ell} = \theta_0 \cdot \mathrm{sign}\left(-i\langle v|[P_kP_\ell\,,h_{ij}]|v\rangle\right)$$

Bounding improvement in energy

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$$\langle v_i|P_i|v_i\rangle = 0$$

$$|\mathrm{Err}| \le O\left(\theta_0^2 d\right)$$

Bounding improvement in energy

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$$\langle v_i|P_i|v_i\rangle = 0$$

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

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$$= \langle v|h_{ij}|v\rangle - i\,\theta_{ij}\ \langle v|[P_iP_j\,, h_{ij}]|v\rangle\ + \mathbf{Err} \qquad \langle v_i|P_i|v_i\rangle = 0$$

$$\geq\ \langle v|h_{ij}|v\rangle + \theta_0|\langle v|[P_iP_j\,, h_{ij}]|v\rangle| - \Omega(\theta_0^2 d)$$

There are choices of $\{P_i\}$ such that for $\theta_0 \leq O(1/d)$,

$$\langle\psi|H|\psi\rangle \geq \langle v|H|v\rangle + \Omega\left(\frac{\mathrm{Var}_v(H)^2}{d^2\, m}\right)$$

Extensions 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,

$$\langle\psi|H|\psi\rangle \geq \langle v|H|v\rangle + \Omega\left(\frac{\mathrm{Var}_v(H)^2}{d\, m}\right)$$

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

$$\lambda_{\max} - \langle v|H|v\rangle \leq O\left(\frac{\mathrm{Var}_v(H)^2}{d^2\, m}\right)$$

Result: k-local Hamiltonians

Improvement for k-local Hamiltonians

Given a degree-d k-local Hamiltonian H and a product state $|v\rangle$, we can efficiently compute a shallow quantum circuit U such that the state $|\psi\rangle = U|v\rangle$ satisfies

$$\langle\psi|H|\psi\rangle \geq \langle v|H|v\rangle + \Omega\left(\frac{\mathrm{Var}_v(H)^2}{2^{O(k)} d^4\, m}\right)$$

Result: Improving entangled states

Let $|v\rangle = W|0^n\rangle$ where W is a quantum circuit of $\boxed{\text{depth } D.}$

We can **efficiently** compute a quantum circuit U

such that the state $|\psi\rangle = U|v\rangle$ satisfies

Lightcone ℓ

$$\langle\psi|H|\psi\rangle \geq \langle v|H|v\rangle + \Omega\left(\frac{\mathrm{Var}_v(H)^2}{\boxed{2^{O(D)}}d^2\, m}\right)$$

ℓ^{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

Generic Performance and Comparison with Local Classical Algorithms

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

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

There is an efficient randomized algorithm which computes a depth-$(d+1)$ quantum circuit U such that $|\psi\rangle = U|v\rangle$ satisfies

$$\mathbb{E}_v \langle \psi | H | \psi \rangle \geq \mathbb{E}_v \langle v | H | v \rangle + \Omega\left(\frac{\mathrm{quad}(H)^2}{d\, m} \right)$$

For triangle-free graphs, we have

$$\mathbb{E}_v \langle \psi | H | \psi \rangle \geq \mathbb{E}_v \langle v | H | v \rangle + \Omega\left(\frac{\mathrm{quad}(H)}{\sqrt{d}} \right)$$

Result: Local Classical Algorithm

For triangle free graphs, there is an efficient randomized algorithm that computes the product state $|v\rangle$ satisfying

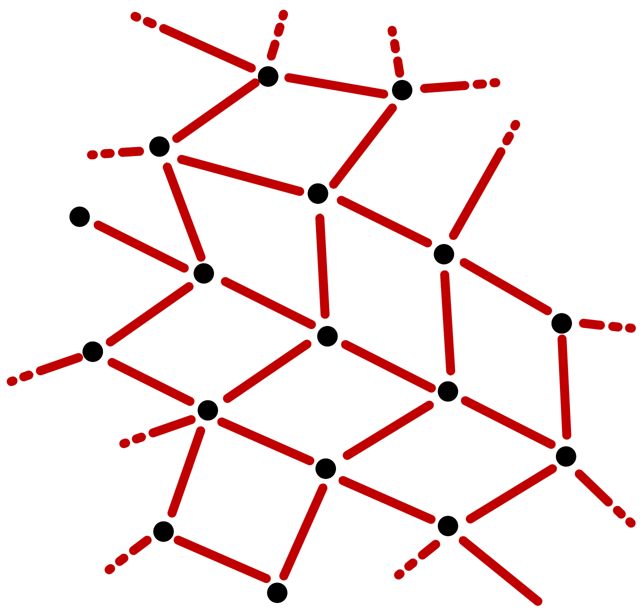
$$\mathbb{E}_v\langle v|H|v\rangle \geq \frac{1}{4}\mathrm{Tr}(H) + \Omega\left(\frac{\mathrm{quad}(H)}{\sqrt{d}}\right)$$

Similar to [Hastings '19, Harrow, Montanaro '17, Barak et al '15]

Result: Local Classical Algorithm

Local Classical Algorithm

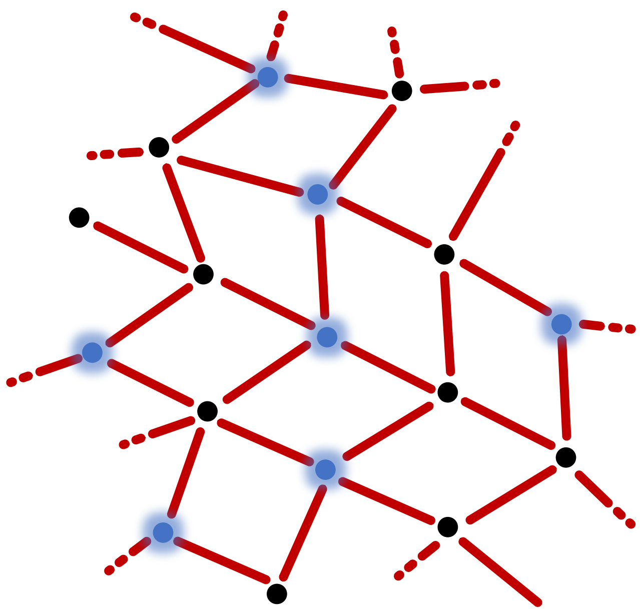
- **Assign i.i.d states to all vertices uniformly at random**



Result: Local Classical Algorithm

Local Classical Algorithm

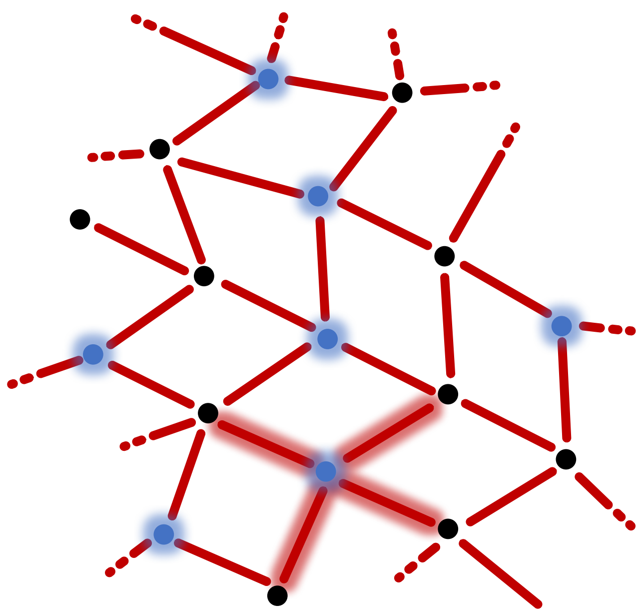
- **Assign i.i.d states to all vertices uniformly at random**
- **Randomly divide vertices into two sets {●}, {●}**



Result: Local Classical Algorithm

Local Classical Algorithm

- **Assign i.i.d states to all vertices uniformly at random**
- **Randomly divide vertices into two sets {●}, {●}**
- Update state of {●} **based on neighbors in {●} to maximize energy**



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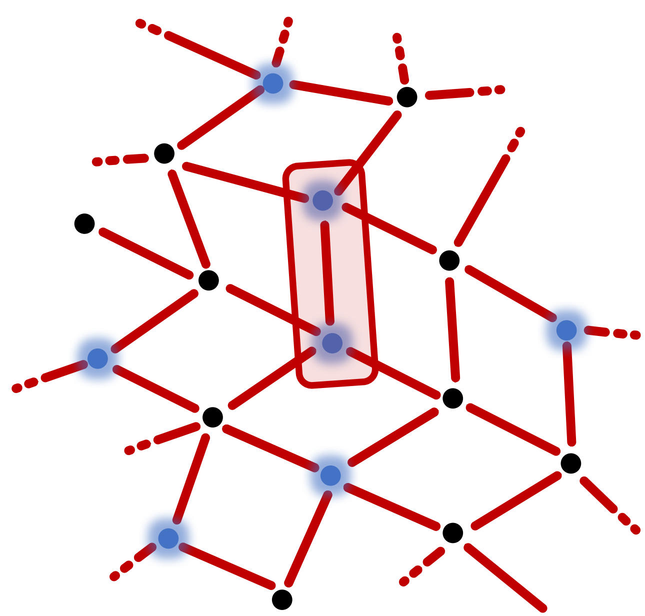

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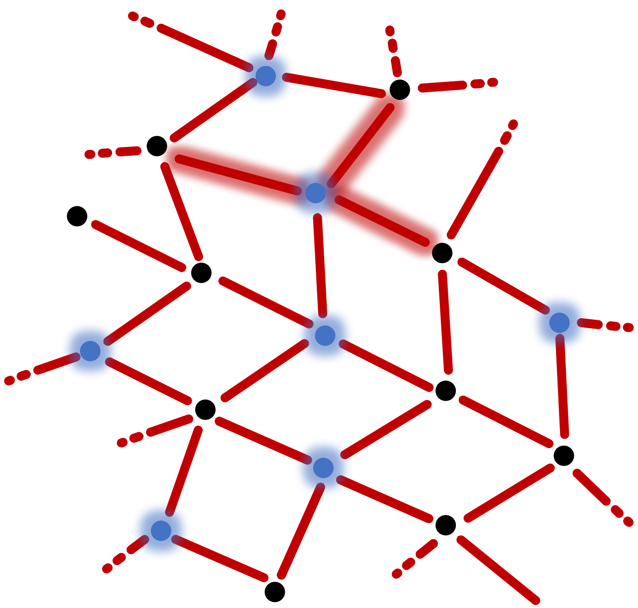

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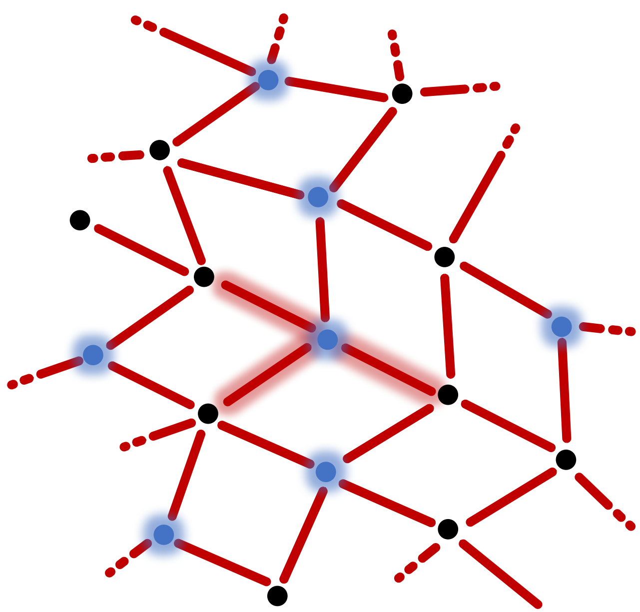


Classical local algorithms may achieve the **same scaling** with product states.

But their output can be **further improved** by our shallow circuit

We also saw

For **locally optimal states**,

$$\langle \psi | H | \psi \rangle \geq \langle v | H | v \rangle + \Omega\left(\frac{\mathrm{Var}_v(H)^2}{d\, m}\right)$$

Better energy improvement can be achieved with structured initial states.

Open Questions

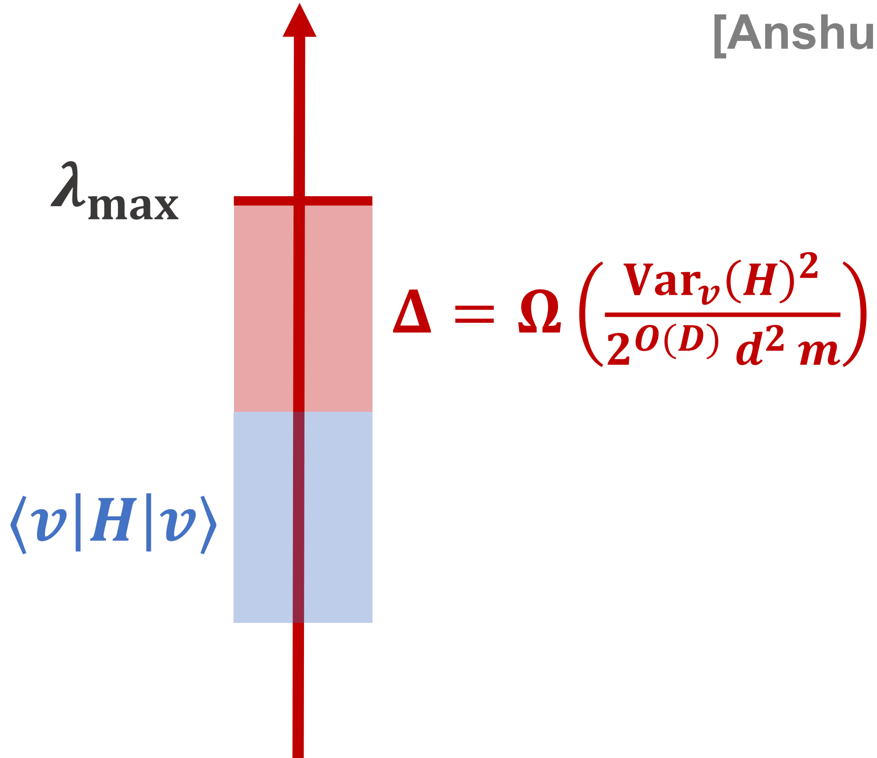
Open questions

- **Limitations on energy of states generated with low-depth circuits**

$$\langle v|H|v\rangle \leq \lambda_{\max} - \Omega\left(\frac{\mathrm{Var}_v(H)^2}{2^{O(D)}\, d^2\, m}\right)$$

Examples of Hamiltonians with almost NLTS property?

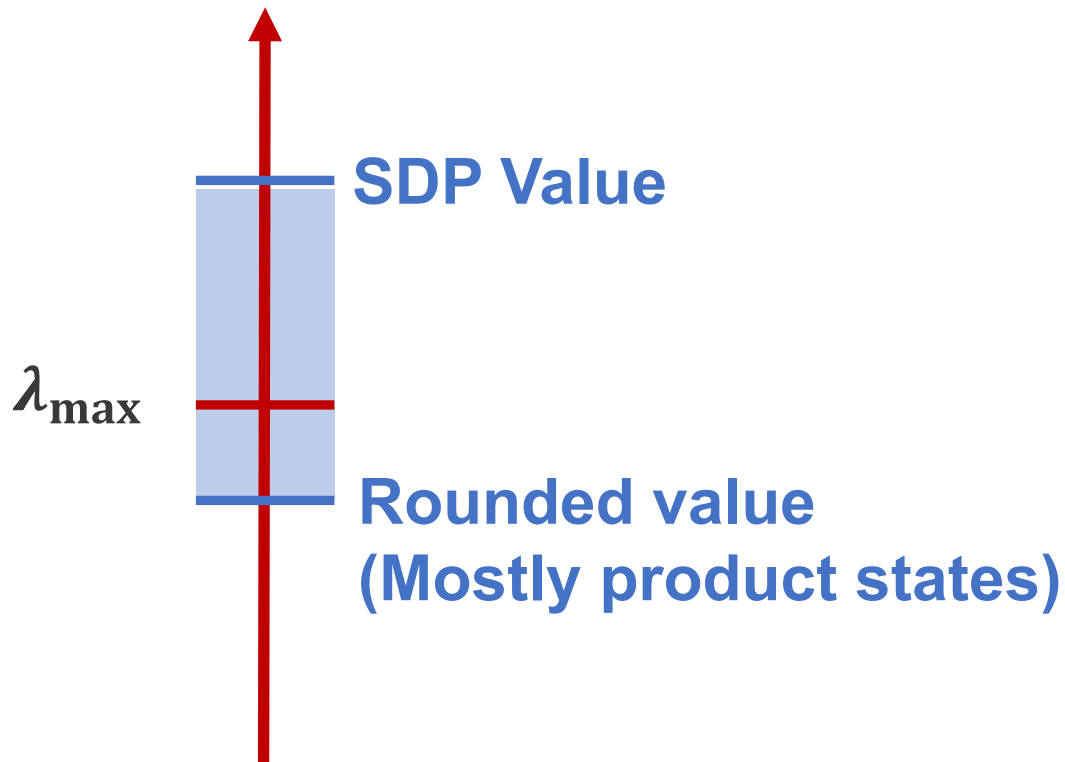
[Anshu, Nirkhe 2021]



Open questions

- **Rounding to entangled states in SDP relaxations?**

  [Parekh, Thompson 2020, Anshu, Gosset, Morenz Korol 2020]



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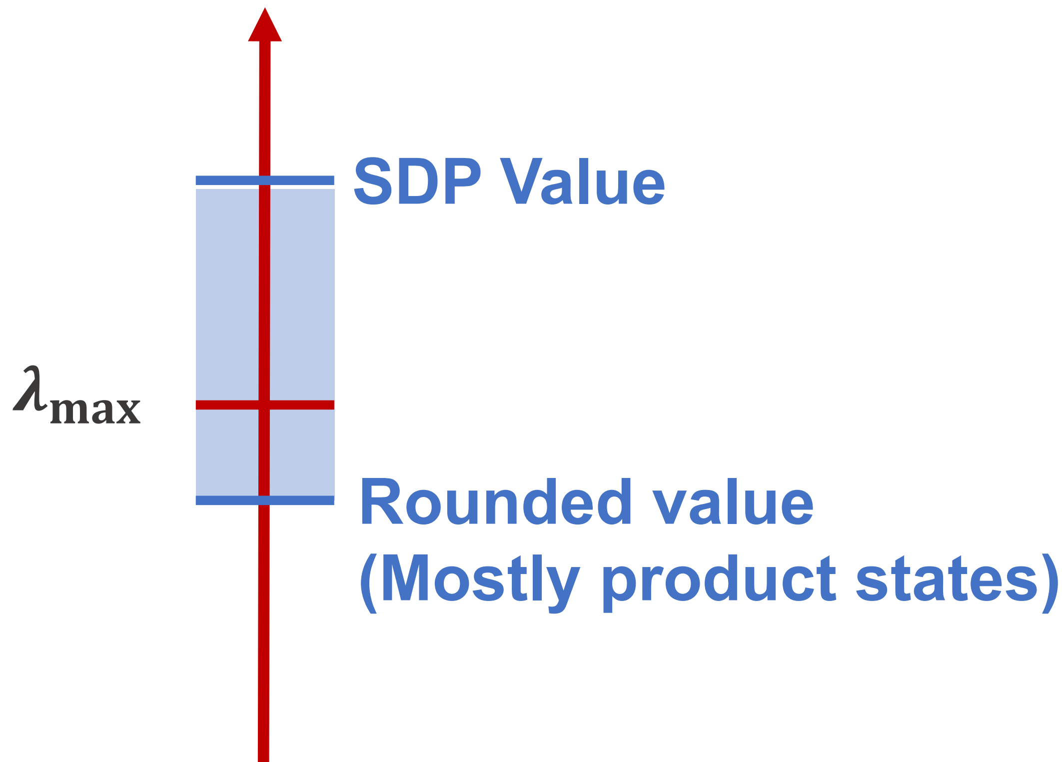

Open questions

- **Rounding to entangled states in SDP relaxations?**

  [Parekh, Thompson 2020, Anshu, Gosset, Morenz Korol 2020]

- **More theoretical study of near-term algorithms for estimating ground-state energy**

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