Obstacles to State Preparation and Variational Optimization from Symmetry Protection

Robert König

joint work with

Sergey Bravyi, Alexander Kliesch and Eugene Tang

arXiv:1910.08980



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Variational methods

How well do these methods perform?

(1) What is the best energy attained by a state from *S*(2) What is the best energy of a state that can be computed efficiently.



many-body Hamiltonian H





optimize over product states

mean-field theory

Variational methods

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Combinatorial optimization

Quantum approximate optimization (QAOA)

Combinatorial optimization

Given: A function $C: \{0,1\}^n \to \mathbb{R}$.

Goal: Find $x^* \in \{0,1\}^n$ such that $C(x^*)$ approximates the maximum

 $\max_{x\in\{0,1\}^n}C(x)$



Example: MaxCUT for G = (V, E)

$$C_G(x) = \frac{1}{2} \sum_{(u,v) \in E} (1 - (-1)^{x_u} (-1)^{x_v})$$

Computing maximum exactly Is NP-hard.

Figure of merit for an algorithm \mathcal{A} :

(expected) approximation ratio

$$\alpha(\mathcal{A}) = \frac{\mathbb{E}_{x^* \leftarrow \mathcal{A}}[C(x^*)]}{\max_{x \in \{0,1\}^n} C(x)}$$

A polynomial-time algorithm achieving $G\alpha$ (A) ≥ 0.878 for every graph G ! W

Goemans and Williamson (1995)

Assuming the unique games conjecture andS. Khot and $P \neq NP$ there is no polynomial-time algorithmN. Vishnoi, \mathcal{A} satisfying $\alpha(\mathcal{A}) > 0.878$ for every graph G.FOCS (2005)

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E. Farhi, J. Goldstone, S. Gutmann, arXiv:1411.4028.

$$H = \sum_{x \in \{0,1\}^n} C(x) |x\rangle \langle x|$$

 $|x\rangle = |x_1\rangle \otimes |x_2\rangle \otimes \cdots \otimes |x_n\rangle$

Level-p QAOA algorithm

1. Prepare state ψ^* such that $\langle \psi^* | H | \psi^* \rangle$ approximates

$$\max_{\psi} \quad \langle \psi | H | \psi \rangle$$



$$\psi(\beta, \gamma) = \prod_{k=1}^{p} e^{i\beta_k B} e^{i\gamma_k H} |+\rangle^{\otimes n}$$

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QAOA algorithm: Limitations on level p

- descriptive power of variational class of states increases with level p
- energy maximization becomes more challenging with increasing p
- NISQ implementation requires constant (small) p

Main question:Can constant-level QAOA outperform the best known classical
algorithm (i.e., Goemans-Williamson) for MAXCUT?

Main theme:Lower bounds on circuit-depth/circuit-rangenecessary to prepare low-energy statesusing symmetric unitary preparation circuits



Symmetric Hamiltonians/unitaries and states

A Hamiltonian *H* is \mathbb{Z}_2 -symmetric if $[H, X^{\otimes n}] = 0$.

Examples:

$$H_{TF} = -\sum_{k\in\mathbb{Z}_n} X_k$$

$$H_{Ising} = -\sum_{k \in \mathbb{Z}_n} Z_k Z_{k+1}$$

A state
$$\psi$$
 is \mathbb{Z}_2 -symmetric if $X^{\otimes n}\psi = \psi$ or $X^{\otimes n}\psi = -\psi$.

Examples: $|+\rangle^{\otimes n} = |+\rangle \otimes |+\rangle \otimes \cdots \otimes |+\rangle$ $|GHZ_n\rangle = \frac{1}{\sqrt{2}}(|0\rangle^{\otimes n} + |1\rangle^{\otimes n})$

A unitary U is \mathbb{Z}_2 -symmetric if $UX^{\otimes n} U^{\dagger} = X^{\otimes n}$.

Examples: $U = X^{\bigotimes n}$

any circuit U composed of \mathbb{Z}_2 -symmetric gates.

QAOA: a \mathbb{Z}_2 -symmetric circuit



$$H = \sum_{x \in \{0,1\}^n} C(x) |x\rangle \langle x| \qquad B = \sum_{j=1}^n X_j$$

 $|x\rangle = |x_1\rangle \otimes |x_2\rangle \otimes \cdots \otimes |x_n\rangle$

This circuit is \mathbb{Z}_2 -symmetric if

 $C(x) = C(\bar{x})$ where $\bar{x}_j = 1 - x_j$

e.g., for MAXCUT!

This initial state is \mathbb{Z}_2 -symmetric!

$$H_n = \sum_{k \in \mathbb{Z}_n} (I - Z_k Z_{k+1})$$

Conventions throughout this talk:

- $\{H_n\}_n$ family of local Hamiltonians with n = number of qubits
- Hamiltonians are sums of local terms of strength O(1)
- Ground state energy zero for every Hamiltonian: $min_{\psi} \langle \psi | H_n | \psi \rangle = 0$

$$H_n = \sum_{k \in \mathbb{Z}_n} (I - Z_k Z_{k+1})$$

Goal: prepare *a ground state* $|\psi\rangle = U|+\rangle^{\otimes n}$ from $|+\rangle^{\otimes n}$

What is the required circuit range for U?

U has

(backward) *range* R^{\leftarrow} if the backward light-cone of every output qubit *j* is contained in $(j - R^{\leftarrow}, j + R^{\leftarrow})$ (forward) **range** R^{\rightarrow} if the forward light-cone of every input qubit k is contained in $(k - R^{\rightarrow}, k + R^{\rightarrow})$

range $R = \max\{R^{\leftarrow}, R^{\rightarrow}\}.$



$$H_n = \sum_{k \in \mathbb{Z}_n} (I - Z_k Z_{k+1})$$

Goal: prepare *a ground state* $|\psi\rangle = U|+\rangle^{\otimes n}$ from $|+\rangle^{\otimes n}$

If U is arbitrary (**no symmetry**):

$$\begin{split} |\psi\rangle &= \alpha |0\rangle^{\otimes n} + \beta |1\rangle^{\otimes n}, \ \alpha,\beta \text{ arbitrary} \\ & \downarrow \\ \text{Choose } |\psi\rangle &= |0\rangle^{\otimes n} \text{ and } U = H^{\otimes n} \\ & \text{Easy! (range-1, local)} \end{split}$$

If U is Z₂-symmetric: $|\psi\rangle$ has to be $|GHZ_n\rangle = \frac{1}{\sqrt{2}}(|0\rangle^{\otimes n} + |1\rangle^{\otimes n})$ Need linear range!

This is a fundamental limitation of \mathbb{Z}_2 -symmetric circuits!

Circuit range lower bound for preparing $|GHZ_n\rangle$

Claim: Suppose a circuit *U* prepares $|GHZ_n\rangle$ from a product state, i.e., $|GHZ_n\rangle = U|+\rangle^{\bigotimes n}$. Then the range of *U* satisfies $R \ge \frac{n}{2}$.

$$|GHZ_{n}^{+}\rangle = \frac{1}{\sqrt{2}}(|0\rangle^{\otimes n} + |1\rangle^{\otimes n})$$
$$GHZ_{n}^{-}\rangle = \frac{1}{\sqrt{2}}(|0\rangle^{\otimes n} - |1\rangle^{\otimes n})$$

These two states are orthogonal, but *locally indistinguishable*: the reduced density operators on n-1 qubits are identical.

The observable UO_jU^{-1} distinguishes these two states.

 $U^{-1}|\mathbf{GHZ}_n^+\rangle = |+\rangle^{\otimes n}$

 $U^{-1}|GHZ_n^-\rangle$

These states are *locally distinguishable* because they are orthogonal and the first is a product state

There is a single-qubit observable O_j distinguishing these two states.

S. Bravyi, M. B. Hastings, and F. Verstraete, Phys. Rev. Lett. 97, 050401 (2006).

 $|+\rangle$ $|+\rangle$ $j - R^{\leftarrow}$ $j + R^{\leftarrow}$ 0_{j} $|+\rangle$ $|+\rangle$

Saturating the range lower bound: GHZ-preparing circuit



$$H_n = \sum_{k \in \mathbb{Z}_n} (I - Z_k Z_{k+1})$$

Goal: prepare *a ground state* $|\psi\rangle = U|+\rangle^{\otimes n}$ from $|+\rangle^{\otimes n}$

If U is arbitrary (no symmetry): (range-1 suffices)

If U is \mathbb{Z}_2 -symmetric:

Need linear range!



"Symmetry protection"

Haldane. PRL 50:1153-1156, 1983. Affleck, Kennedy, Lieb, Tasaki. PRL 59:799-802, 1987. Gu, Wen, PRB 80:155131, (2009) Pollmann, Turner, Berg, Oshikawa. PRB 81:054439 (2010) Haegeman, Perez-Garcia, Cirac, Schuch, PRL 102, 050402 (2012) Chiu, Teo, Schnyder, Ryu. Rev. Mod. Phys., 88:035005,2016.



Low-energy states of Ising model: Preparation with symmetry

$$H_n = \sum_{k \in \mathbb{Z}_n} (I - Z_k Z_{k+1})$$

Theorem: Suppose $|\psi\rangle = U|+\rangle^{\otimes n}$ where U has range R < n/4 and is \mathbb{Z}_2 -symmetric.

Then
$$\langle \psi | H_n | \psi \rangle \ge \frac{1}{2R+1} n$$

Preparing any state with an energy density lower than ε density requires $R = \Omega(1/\epsilon)$.

Symmetry obstructs the preparation of low-energy states!

also see G. Mbeng, R. Fazio, G. Santoro, arXiv:190608948 for QAOA

Toric code: no zero-energy trivial states

Geometrically local circuits require $\Omega(\sqrt{n})$ depth.

Bravyi, Hastings, Verstraete, PRL 97, 050401 (2006)

All toric code *zero-energy states* are *non-trivial* (topologically ordered).



Toric code: existence of low-energy trivial states

If $n \ge d^2$ the output state is NOT a ground state of H_n^{toric}

Bravyi, Hastings, Verstraete, PRL 97, 050401 (2006)

All toric code *zero-energy states* are *non-trivial* (topologically ordered).



constant-size patches of local ground states (can be created in parallel)



For every constant $\varepsilon > 0$ there is a **constant-depth** circuit U such that $\langle +|^{\otimes n}U^{\dagger}H_{n}^{toric}U|+\rangle^{\otimes n} \leq \varepsilon n$

The toric code has *low-energy states that are trivial.*

The NLTS conjecture

Freedman and Hastings, Quant. Inf. Comp. 14 (2014)

No low-energy trivial states (NLTS) property:

There is $\varepsilon > 0$ and a function $f: \mathbb{N} \to \mathbb{N}$ such that for any depth-d (local) circuit U

$$\langle +|^{\otimes n}U^{\dagger}H_{n}U|+\rangle^{\otimes n} > \varepsilon n$$
 for any $n \ge f(d)$

Conjecture: There is a family $\{H_n\}_n$ of local Hamiltonians that has the NLTS property.

The following families $\{H_n\}_n$ **do not** satisfy the NLTS property:

Hamiltonian family	Reference
toric code Hamiltonians	Freedman & Hastings 2014
2-local Hamiltonians on non-expanding graphs	Brandao and Harrow 2013
2-local Hamiltonians with commuting terms	Bravyi and Vyalyi 2005
3-qubit Hamiltonian with commuting terms	Aharonov and Eldar 2011
O(1)-local Hamiltonians with commuting terms with high local expansion	Aharonov and Eldar 2015
Sparse commuting O(1)-local Hamiltonians corresponding to graphs with high girth	Hastings 2012

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Conjecture: There is a family $\{H_n\}_n$ of local Hamiltonians that has the NLTS property.

Evidence for the NLTS conjecture:

- There is a family of toric-code like (CSS-stabilizer) Hamiltonians on simplicial complexes such that an NLTS-like statement holds *when one restricts to a certain subset of excited states*. (Freedman and Hastings)
- There is a family of Hamiltonians satisfying a related "*no lowerror trivial states property*" (Harrow and Eldar, FOCS 2017)

Main result: NLTS with symmetry protection

for a family

 $\{H_n\}_n$ of local \mathbb{Z}_2 -symmetric Hamiltonians No low-energy \mathbb{Z}_2 -trivial states property:

There is $\varepsilon > 0$ and a function $f: \mathbb{N} \to \mathbb{N}$ such that for any \mathbb{Z}_2 -symmetric depth-d (local) circuit U

$$\langle +|^{\otimes n}U^{\dagger}H_{n}U|+\rangle^{\otimes n} > \varepsilon n$$
 for any $n \ge f(d)$

Main result: Construction of a family $\{H_n\}_n$ of local Hamiltonians that has the NLZ₂TS property.



Symmetryprotected NLTS

 $\mathbf{NL} \mathbb{Z}_2 \mathbf{TS}$

Let $\{G_n\}_{n \in I}$ be an infinite family of *D*-regular graphs such that $h(G_n) \ge h$ for all $n \in I$

Graph
$$G = (V, E)$$
 given $S \subset V$ (edge) boundary $\partial(S) = \{e \in E \mid |e \cap S| = 1\}$ Cheeger constant of G : $h(G) = \min_{\substack{S \subseteq V \\ 0 < |S| \le |V|/2}} \frac{|\partial(S)|}{|S|}$

We need infinite families of D-regular graphs with $h = \Omega(1)$.

Ramanujan graphs:

- connected
- satisfy $h(G) \ge \frac{1}{2}(D 2\sqrt{D 1})$

There is an infinite family of *D*-regular Ramanujan graphs for every $D \ge 3$.

Marcus, Spielman, Srivastava, Annals of Mathematics 182, 307 (2015)

Let $\{G_n\}_{n \in I}$ be an infinite family of *D*-regular graphs such that $h(G_n) \ge h$ for all $n \in I$

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$$H_n = \frac{1}{2} \sum_{(u,v) \in E_n} (I - Z_u Z_v)$$



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Theorem:
$$(+|^{\otimes n}U^{\dagger}H_{n}U|+)^{\otimes n} > \binom{h}{6}n$$
for any $n > 24^{2}2^{4d/3}$ Image: and any \mathbb{Z}_{2} -symmetric depth- d (local) circuit U Image: and any \mathbb{Z}_{2} -symmetric depth- d (local) circuit U Proof: $|+\rangle - symmetric - circuit U$ Suppose $(+|^{\otimes n}U^{\dagger}H_{n}U|+)^{\otimes n} < \binom{h}{6}n$ Image: and any \mathbb{Z}_{2} -symmetric depth- d (local) circuit U Image: and any \mathbb{Z}_{2} -symmetric depth- d (local) circuit U Proof: $|+\rangle - symmetric - circuit U$ Image: and any \mathbb{Z}_{2} -symmetric depth- d (local) circuit U Image: and any \mathbb{Z}_{2} -symmetric depth d Image: and any \mathbb{Z}_{2} -symmetric depth- d (local) circuit U Image: and any \mathbb{Z}_{2} -symmetric depth d Image: and any \mathbb{Z}_{2} -symmetric depth- d (local) circuit U Image: and any \mathbb{Z}_{2} -symmetric depth d Image: and any \mathbb{Z}_{2} -symmetric depth- d (local) circuit U Image: and any \mathbb{Z}_{2} -symmetric depth d Image: and any \mathbb{Z}_{2} -symmetric depth- d (local) circuit U Image: and any \mathbb{Z}_{2} -symmetric depth d Image: and any \mathbb{Z}_{2} -symmetric depth d Image: an one of the transformation of

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"low energy configurations"



Let $\{G_n\}_{n \in I}$ be an infinite family of *D*-regular graphs such that $h(G_n) \ge h$ for all $n \in I$

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Theorem:
$$\langle +|^{\otimes n}U^{\dagger}H_{n}U|+\rangle^{\otimes n} > \left(\frac{h}{6}\right)n$$
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and any \mathbb{Z}_{2} -symmetric depth- d (local) circuit U Proof: $|+\rangle - symmetric - x_{1}$
 $|+\rangle - of depth d - x_{2}$
 $|+\rangle - of depth d - x_{n}$ Suppose $\langle +|^{\otimes n}U^{\dagger}H_{n}U|+\rangle^{\otimes n} < \left(\frac{h}{6}\right)n$
Consider the distribution
 $p(x) = |\langle x|U|+\rangle^{\otimes n}|^{2}$ where
 $x \in \{0,1\}^{n}$ by \mathbb{Z}_{2} -symmetry: $p(S_{0}) \ge 1/4$ and
 $p(S_{1}) \ge 1/4$ $p(S_{1}) \ge 1/4$ $p(S_{1}) \ge 1/4$

Circuit depth lower bound for sampling from bimodal distributions

Theorem:

(Corollary 43, Eldar & Harrow, 2017) Let p(x) denote the output distribution of a depth-d quantum circuit U. Let $S_0, S_1 \subset \{0,1\}^n$ be such that $p(S_0) > 0$ and $p(S_1) > 0$. Then $\operatorname{dist} (S_0, S_1) \leq \frac{4n^{1/2}2^{3d/2}}{\min\{p(S_0), p(S_1)\}}$

A distribution produced by a shallow quantum circuit does not have large support on any two distant subsets of strings at the same time.



level-p QAOA variational state

$$\psi(\beta,\gamma) = \prod_{k=1}^{p} e^{i\beta_k B} e^{i\gamma_k H} |+\rangle^{\otimes n}$$



MAXCUT on graph	approximation ratio to classical algorithm	approximation ratio achieved by QAOA	required QAOA level p	
any		1	$p ightarrow \infty$	Farhi et al. 2014 Lloyd 2018
triangle-free D-regular graphs		$\frac{1}{2} + \frac{1}{2\sqrt{D}}(1 - \frac{1}{D})^{(D-1)/2}$	p = 1	Wang, Hadfield, Jiang, Rieffel, PRA 97, 022304 (2018) Ryan-Anderson, arXiv:1812.04735 (2018).

Sampling from the output distribution of (p = 1) –QAOA cannot be efficiently simulated classically unless the polynomial hierarchy collapses (Farhi & Harrow 2016)

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MAXCUT on graph	approximation ratio to classical algorithm	approximation ratio achieved by QAOA	required QAOA level p				
any		1	$p ightarrow \infty$	classical algorithm D 2 0.2500		classical algorithm C	
triangle-free D-regular graphs $D \le 1000$	numerically optimized local algorithm	$\frac{1}{2} + \frac{1}{2\sqrt{D}} (1 - \frac{1}{D})^{(D-1)/2}$	p = 1		3 0.187 4 0.140 5 0.156 6 0.122 7 0.128	75 96 92 91 92	0.1925 0.1624 0.1431 0.1294 0.1190
¹ Station Q, Microsoft ² Quantum Architectures and Compu- We consider some classical and depth. First, we define a class of "I step version of these algorithms can MAX-3-LIN-2. Second, we show tha considered in the literature[I], and a the single-step QAOA on all triang degree, existing single-step classical while for the remaining 4 choices we consider the QAOA and provide stro on MAX-3-LIN-2 on bounded degree	Bounded Depth Approximation Matthew B. Hastings ^{1, 2} Research, Santa Barbara, CA 93106-6105, <i>itation Group, Microsoft Research, Redmond</i> , quantum approximate optimization algorithm local" classical optimization algorithms and s in achieve the same performance as the sing at this class of classical algorithms generalizes also that a single step of the classical algorithm gle-free MAX-CUT instances. In fact, for all algorithms already outperform the QAOA is show that the generalization here outperfor- ing evidence that, for any fixed number of step be graphs cannot achieve the same scaling as	Algorithms USA WA 98052, USA ms with bounded how that a single le step QAOA on a class previously n will outperform l but 4 choices of on these graphs, ms it. Finally, we s, its performance can be done by a	XCUT on D-regular graph for $D \leq 1000$	ıs,	8 0.116 9 0.107 10 0.107 11 0.092 12 0.098 13 0.088 14 0.090 15 0.085 16 0.083 17 0.081 18 0.077 19 0.077	66 77 25 67 66 95 63 63 71 78	0.1108 0.1040 0.0984 0.0936 0.0894 0.0858 0.0825 0.0796 0.0770 0.0770 0.0747 0.0725 0.0705

class of "global" classical algorithms. These results suggest that such local classical algorithms are likely to be at least as promising as the QAOA for approximate optimization.

on MAX-3-LIN-2 on bounded degree graphs cannot achieve the same scaling as can be done by a

level-p QAOA variational state

$$\psi(\beta,\gamma) = \prod_{k=1}^{p} e^{i\beta_k B} e^{i\gamma_k H} |+\rangle^{\otimes n}$$



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triangle-free bipartite 3-regular graphs, o(n) squares	0.87856	0.756	p = 2	Farhi et al. 2014
	0.87856	?	WHAT ABOUT p > 1 ? (constant)	

Goemans and Williamson, 1995

Main result for MAXCUT-QAOA with p > 1

Theorem: For every $D \ge 3$ there is an infinite family of *D*-regular bipartite graphs $\{G_n\}_{n \in I}$ such that

$$\alpha(QAOA_p) \le \frac{5}{6} + \frac{\sqrt{D-1}}{3D}$$
 if $p \le D^{-1}(\frac{1}{3}\log_2 n - 4)$

In particular:

 $\alpha(QAOA_p) < 0.87856 = \alpha$ (Goemans-Williamson) if $D \ge 54$

The best classical polynomial-time algorithm (Goemans-Williamson) beats QAOA for any constant level p

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Proof: Take $\{G_n\}_n$ to be family of D-regular bipartite Ramanujan graphs. (Marcus, Spielman, Srivastava 2015)

$$\max_{\psi} \langle \psi | H_n | \psi \rangle = |E_n|$$

$$H_n = \frac{1}{2} \Sigma_{(u,v) \in E_n} (I - Z_u Z_v)$$
because G_n is bipartite.
$$\max_{(\beta,\gamma)} \langle \psi(\beta,\gamma) | H_n | \psi(\beta,\gamma) \rangle = \frac{|E_n|}{2} + \max_{(\beta,\gamma)} \langle \widehat{\Psi}(\beta,\gamma) | \widehat{H}_n | \widehat{\Psi}(\beta,\gamma) \rangle \quad \widehat{H}_n = \frac{1}{2} \Sigma_{(u,v) \in E_n} Z_u Z_v$$

NL \mathbb{Z}_2 **TS:** $\langle \widehat{\Psi}(\beta,\gamma) | \widehat{H}_n | \widehat{\Psi}(\beta,\gamma) \rangle < \frac{|E_n|}{2} - \frac{hn}{6}$ because $\prod_{k=1}^p e^{i\beta_k B} e^{i\gamma_k H_n}$ is \mathbb{Z}_2 -symmetric depth, depth $d \leq p D$

The **best classical polynomial-time algorithm** (Goemans-Williamson) beats QAOA for any constant level p

level-p QAOA variational state

$$\psi(\beta,\gamma) = \prod_{k=1}^{p} e^{i\beta_k B} e^{i\gamma_k H} |+\rangle^{\otimes \gamma}$$



MAXCUT on graph	approximation ratio to classical algorithm	approximation ratio achieved by QAOA	required QAOA level p	
any		1	$p ightarrow \infty$	Farhi et al. 2014 Lloyd 2018
triangle-free D-regular graphs $D \le 1000$	numerically optimized local algorithm	$\frac{1}{2} + \frac{1}{2\sqrt{D}} (1 - \frac{1}{D})^{(D-1)/2}$	p = 1	Wang, Hadfield, Jiang, Rieffel, PRA 97, 022304 (2018) Ryan-Anderson, arXiv:1812.04735 (2018 Hastings 2019 (based on Hirvonen et al. 2014)
triangle-free bipartite 3-regular graphs, o(n) squares	0.87856	0.756	<i>p</i> = 2	Farhi et al. 2014
D -regular bipartite expander graphs	0.87856	$\leq \frac{5}{6} + \frac{\text{const}}{\sqrt{D}} \to 0.8333$ $(D \to \infty)$	1	Goemans and Williamson, 1995 THIS WORK

The best classical polynomial-time algorithm (Goemans-Williamson) beats QAOA for any constant level p

Conclusions and open problems

- \mathbb{Z}_2 -symmetric No Low Energy Trivial States (NLTS) property for a family of Ising models on expander graphs
 - Other symmetries?
 - General NLTS conjecture still open
- Limitations to quantum approximate optimization algorithm (QAOA): Efficient (i.e., constant-level) QAOA underperforms compared to the best classical polynomial-time algorithm (Goemans-Williamson)
 - Comparison for generic instances (instead of worst-case)? Finding independent sets in random graphs:

The Quantum Approximate Optimization Algorithm Needs to See the Whole Graph: A Typical Case

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- Non-local modifications of QAOA/RQAOA: some evidence for their suitability:
 - More extensive benchmarks/case studies?