Classical approximation algorithms for quantum constraint satisfaction problems

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1. Intro: Local Hamiltonians
2. Existing Results
3. Approximating the quantum Heisenberg model
4. Conclusions
1 Intro: Local Hamiltonians
2 Existing Results
3 Approximating the quantum Heisenberg model
4 Conclusions
How quickly can we compute properties of physical quantum systems?
Focus

Our focus: Low temperature properties of local Hamiltonian systems
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Local Hamiltonians?
Govern time evolution of quantum systems via local interactions or “constraints”.

- Ice melts: 273K
- Nitrogen liquifies: 77K
- Outer space: 2.7K
- Helium-4 becomes superfluid: 2.17K
- World record (1999): 0.0000000001K, nuclear spins in rhodium metal
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Boolean constraint satisfaction

and

local Hamiltonians
Constraint satisfaction

Max-$k$-Constraint Satisfaction Problem (MAX-$k$-CSP)

Given a set of boolean constraints on $k$ boolean variables each, e.g.

$$x_1 \lor x_2 \quad \overline{x_2} \land x_4 \quad x_2$$

(here, $k = 2$)

what is the maximum number of constraints we can satisfy with an assignment to the $x_i \in \{0, 1\}$?

Generalizes: MAX-3-SAT, MAX-CUT, etc...
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Generalizes: MAX-3-SAT, MAX-CUT, etc.

Question

What if we talk about quantum constraints on quantum bits?
Quantum bits and constraints?

A classical 2-bit system takes values in \{00, 01, 10, 11\}.

A quantum 2-qubit system takes linear combinations of these values,

e.g. \[ \frac{1}{2}|00\rangle + \frac{1}{2}|01\rangle + \frac{1}{2}|10\rangle + \frac{1}{2}|11\rangle, \]

where \{\langle 00\rangle, \langle 01\rangle, \langle 10\rangle, \langle 11\rangle\} denote the standard basis for \(\mathbb{C}^4\).
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A quantum constraint thus asks:

“I want qubits 1 and 2 to lie in a certain subspace, e.g. to lie in the span of \(|00\rangle\) and \(|11\rangle\).”
Local Hamiltonians

2-Local Hamiltonian
A Hermitian operator \( H = \sum_{ij} H_{ij} \) acting on \( n \) qubits, such that:

- \( H \) is a \( 2^n \times 2^n \) matrix with description of size \( O(\text{poly}(n)) \).
- Each \( H_{ij} \) is a “quantum constraint” acting on qubits \( i \) and \( j \),
- Each \( H_{ij} \) is a \( 4 \times 4 \) complex positive semidefinite matrix, e.g.
  \[
  H_{12} = |00\rangle\langle00| + |11\rangle\langle11| = \begin{pmatrix}
  1 & 0 & 0 & 0 \\
  0 & 0 & 0 & 0 \\
  0 & 0 & 0 & 0 \\
  0 & 0 & 0 & 1
\end{pmatrix}.
  
- Implicitly, each local term is really \( H_{ij} \otimes I_{[n]\setminus\{i,j\}} \).
Local Hamiltonians

2-Local Hamiltonian
A Hermitian operator $H = \sum_{ij} H_{ij}$ acting on $n$ qubits, such that:

- $H$ is a $2^n \times 2^n$ matrix with description of size $O(\text{poly}(n))$.
- Each $H_{ij}$ is a “quantum constraint” acting on qubits $i$ and $j$,
- Each $H_{ij}$ is a $4 \times 4$ complex positive semidefinite matrix, e.g.

$$H_{12} = |00\rangle\langle 00| + |11\rangle\langle 11| = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$ 

- Implicitly, each local term is really $H_{ij} \otimes I_{[n] \setminus \{i,j\}}$.

2-local Hamiltonian problem (2-LH)
Given a 2-local Hamiltonian $H = \sum_{ij} H_{ij}$, what is $\lambda_{\min}(H)$?
Why should we care?

To a physicist:
2-LH is the task of estimating energy of a physical system at low temperature.

To a computer scientist:
2-LH generalizes MAX-2-CSP. Moreover:

- **2-local** Hamiltonian is QMA-complete
  [Kitaev 1999, Kempe, Kitaev, Regev 2006].

- 2-local Hamiltonian with qubits on a **2D lattice** is QMA-complete
  [Oliveira, Terhal 2008].

- 2-local Hamiltonian with 12-dimensional systems on the line is QMA-complete
  [Aharonov, Gottesman, Irani, Kempe, 2009].

- Quantum 2-SAT is in **P**
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The case for approximating $k$-LH

What the physicists have been up to: Heuristics!

Density Matrix Renormalization Group (DMRG) [W92,W93]
“Local update” heuristic for 1D gapped local Hamiltonian systems.
Approximability in a quantum world

Trivial observations:

- A “random assignment” yields a $\frac{1}{2^k}$-approximation for $k$-LH.
- UGC-hard to do better than 0.878 for 2-LH [Khot, Kindler, Mossel, O’Donnell, 2005].
- UGC-hard to do better than $(k + 1)/2^{k-1}$ for $k$-LH for $k \geq 3$ [Samorodnitsky, Trevisan, 2006].
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Algorithms:

- PTAS for 2-LH on planar graphs of bounded degree [Bansal, Bravyi, Terhal 2009].
- $\frac{1}{2^{k-1}}$-approximation algorithm for dense $k$-LH [G, Kempe 2011].
- PTAS for $k$-LH on planar, dense, or low threshold-rank graphs [Brandão, Harrow, 2013].
- FPRAS for partition function of ferromagnetic Transverse Ising Model [Bravyi 2013].
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Hardness results:
- Quantum Succinct Set Cover is $c_{q}-\Sigma_2$-hard to approximate within $n^{1-\epsilon}$ for any fixed $\epsilon > 0$ [G, Kempe 2012].
(Very) high-level techniques

PTAS for 2-LH on planar graphs of bounded degree [BBT09]

- Partition graph into $O(1)$-size pieces, solve each piece optimally via brute force

$\frac{1}{2^{k-1}}$-approximation algorithm for dense $k$-LH [GK11], PTAS for $k$-LH on planar, dense, or low threshold-rank graphs [BH13]

- “Mean field ansatz”, or optimize over product quantum states

FPRAS for partition function of ferromagnetic Transverse Ising Model [B13]

- Apply “quantum-to-classical” mapping to map a $d$-dimensional quantum system to a $d + 1$-dimensional classical system
Optimizing over product states

Problem
An assignment $|\psi\rangle$ on $n$ qubits for $k$-LH generally requires $O(2^n)$ bits to describe classically.

Notes:
• Optimizing over product states is NP-complete! (Could solve MAX-$k$-CSP.)
• Product states ignore quantum correlations, i.e. entanglement. (Nevertheless, the mean field ansatz is physicist-approved.)
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*Luckily, some assignments have succinct representations...*

A **product** state is of the form $|\psi_{\text{prod}}\rangle = |\psi_1\rangle \otimes \cdots \otimes |\psi_n\rangle$ for $|\psi_i\rangle \in \mathbb{C}^2$. 
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Why physicist approved?

1. A local Hamiltonian $H$ does not (cannot) in general accurately model all physical parameters of a system.
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2. Rather, $H$ is a phenomenological object, which up to minor corrections, models certain local properties of a system (e.g. values of local measurements).
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Rather, $H$ is a phenomenological object, which up to minor corrections, models certain local properties of a system (e.g. values of local measurements).

Local properties are often of interest — in such cases, one need not accurately obtain the entire ground state of $H$. Rather, an ansatz (such as mean field) may approximate the local property sufficiently well.
Results for product states

Theorem 1 [G, Kempe, 2011]
For any $k$-local Hamiltonian instance $H$, there exists a product state assignment achieving a $\left(\frac{1}{2k-1}\right)$-approximation.
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Remarks:

- For 2-local Hamiltonian, we get a $\frac{1}{2}$-approximation. This is tight.
- For $k$-local Hamiltonian, we can show upper bound on ratio of $\frac{1}{2^{\lceil k/2 \rceil}}$.
- No quantum PCP theorem for $r < \frac{1}{2k-1}$ unless $\text{NP} = \text{QMA}$. 
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Open Question:
Is there an efficient $1/2$-approximation algorithm for 2-LH?
(Subtlety: Recall cannot simply optimize over product states, NP-hard.)
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Theorem 2 [G, Kempe, 2011]
For any $\epsilon > 0$ and $k$-local Hamiltonian instance $H$ on $n$ qubits, there exists a deterministic poly-time algorithm outputting a product state $|\psi\rangle$ satisfying

\[
\text{Tr}(H|\psi\rangle\langle\psi|) \geq \text{OPT}_{\text{prod}} - \epsilon n^k.
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Here, $\text{OPT}_{\text{prod}}$ is optimal product state assignment value.
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**Implication:**
For any $\epsilon > 0$, there exists a $\left(\frac{1}{2^{k-1}} - \epsilon\right)$-algorithm for dense $k$-LH.
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Implication:
For any $\epsilon > 0$, there exists a $\left(\frac{1}{2^{k-1}} - \epsilon\right)$-algorithm for dense $k$-LH.

Question:
Can one obtain a PTAS in the dense case?
Results for product states

Theorem [Brandão, Harrow, 2013]
Let $G = (V, E)$ be $D$-regular graph on $n$ vertices. For any $n$-qubit quantum state $\rho$, there exists $n$-qubit fully separable state $\sigma$ such that

$$\mathbb{E}_{(i,j) \in E} \| \rho_{ij} - \sigma_{ij} \|_{tr} \leq 12 \left( \frac{4 \ln(2)}{D} \right)^{1/3}.$$
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Corollary [Brandão, Harrow, 2013, using G, Kempe, 2011]
The dense $k$-LH problem admits a PTAS.
The [GK11] algorithm uses technique of “exhaustive sampling” of [Arora, Karger, Karpinski, 1999].

This technique can arguably be seen as a “rigorous formulation” of mean field theory (!).

**Moral of the story:** Computer scientists and physicists get along.
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2 Existing Results

3 Approximating the quantum Heisenberg model

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The quantum Heisenberg model

MAX CUT
Given a simple, undirected graph $G = (V, E)$, find a cut of maximum size, i.e. $S \subseteq V$ maximizing number of edges between $S$ and $[n] \setminus S$.

The 2-local Hamiltonian encoding MAX CUT is $H = \sum_{(i,j) \in E} Z_i \otimes Z_j$ for Pauli

$$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$
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In the quantum setting, there are additional degrees of freedom:

$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$.
Quantum Heisenberg anti-ferromagnet

\[ H = \sum_{(i,j) \in E} H_{ij} \quad \text{for} \quad H_{ij} = X_i \otimes X_j + Y_i \otimes Y_j + Z_i \otimes Z_j. \]

- **Intuition:** A quantum “analogue” of MAX CUT.
Quantum Heisenberg anti-ferromagnet

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- **Rank** \( H_{ij} \) = 3.
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- **Intuition:** A quantum “analogue” of MAX CUT.
- **Rank:** \( \text{Rank}(H_{ij}) = 3. \)
- **Unique vector in null space:**
  \[ |\psi^-\rangle = \frac{1}{\sqrt{2}} (|01\rangle - |10\rangle) \]  ("singlet" or antisymmetric state)
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- **Two sources of “frustration”:**
  - Neighboring spins should be “anti-aligned”.
  - Monogamy of entanglement (target state \(|\psi^-\rangle\) is maximally entangled).
Let us convert this to a weighted maximization problem:

\[ H = \sum_{(i,j) \in E} w_{ij} H_{ij} \]

for \( H_{ij} = I - X_i \otimes X_j - Y_i \otimes Y_j - Z_i \otimes Z_j = 4\psi^\dagger\psi \) and \( w_{ij} \geq 0 \) \( \forall i, j \).

**Goal:** Compute \( \lambda_{\text{max}}(H) \). Call this problem AFH.
Our setup

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What is known about this problem?

- Easy cases:
  - In 1D, can be handled via Bethe ansatz [Bethe, 1931].
  - On complete graphs and complete bipartite graphs (Lieb-Mattis model) can be solved via theory of spin.
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\[ MA \subseteq \text{StoqMA} \subseteq \text{AM} \subseteq \text{PH} \quad [\text{BDOT06}] \]
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  $$\text{MA} \subseteq \text{StoqMA} \subseteq \text{AM} \subseteq \text{PH} \quad \text{[BDOT06]}$$
- QMA-complete in general [Piddock, Montanaro, 2015].
Strategy

\[
\text{OPT} := \max_{|\psi\rangle \in (\mathbb{C}^2)^\otimes n} \text{Tr}(H|\psi\rangle\langle\psi|)
\]

\[
\text{OPT}_{\text{prod}} := \max_{|\psi_{\text{prod}}\rangle = |\psi_1\rangle \otimes \cdots \otimes |\psi_n\rangle} \text{Tr}(H|\psi_{\text{prod}}\rangle\langle\psi_{\text{prod}}|).
\]

\[
\text{MAXCUT} := \max_{x \in \{1,-1\}^n} \frac{1}{2} \sum_{(i,j) \in E} w_{ij}(1 - x_i x_j).
\]

1. Use “mean field” ansatz, i.e. optimize over product states.
2. Use Goemans-Williamson framework to compute “good” product state solutions.
3. Show tight bounds between OPT and MAXCUT to relate OPT to OPT_{\text{prod}}.
Lemma
For any AFH instance,

\[ 2 \cdot \text{MAXCUT} \leq \text{OPT}_{\text{prod}} \leq \text{OPT} \leq 4 \cdot \text{MAXCUT}. \]
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Proof.
(\(2 \cdot \text{MAXCUT} \leq \text{OPT}_{\text{prod}}\)) Consider optimal MAX CUT assignment.
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(\(\text{OPT} \leq 4 \cdot \text{MAXCUT}\)) Define \(\Pi_{ij} := (|01\rangle\langle 01| + |10\rangle\langle 10|)\), i.e. MAX CUT constraints. Then,

\[ H_{ij} = 4|\psi^-\rangle\langle \psi^-| \leq 4\Pi_{ij} = 4(|01\rangle\langle 01| + |10\rangle\langle 10|). \]
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Both inequalities are tight:
- (OPT \leq 4 \cdot \text{MAXCUT}) Consider since unit weight constraint.
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Implication: For any AFH instance, \( \text{OPT}_{\text{prod}} \geq \frac{1}{2} \text{OPT} \).

Both inequalities are tight:
- (OPT \leq 4 \cdot \text{MAXCUT}) Consider since unit weight constraint.
- (2 \cdot \text{MAXCUT} \leq \text{OPT}_{\text{prod}}) Consider any “superdense” graph. Proof uses quantum de Finetti theorem and \( U \otimes U \) invariance of \( |\psi^-\rangle \).
The algorithm

Theorem
There exists a polynomial-time classical algorithm $A$ for AFH on interaction graph $G$ such that:

- For arbitrary $G$, $A$ is $0.478$-algorithm.
- For $D$-regular $G$, let $\Delta := m / (\sum_{ij} w_{ij})$ and $w_{\text{max}} := \max_{ij} w_{ij}$. Then, $A$ has approximation ratio

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- Recall for general 2-LH, don’t have even 1/2-approximation.
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- **Surprise:** Cannot approximate MAX CUT better than $0.878 + O(\frac{1}{\sqrt{D}})$ (UGC) or $0.941 + O(\frac{1}{\sqrt{D}})$ ($P \neq NP$).
Key observation: Work in Bloch vector picture.

Any single qubit state $\rho$ is characterized by *Bloch vector* $r \in \mathbb{R}^3$ such that

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\rho = \frac{1}{2} \left( I + r_1 X + r_2 Y + r_3 Z \right) \text{ for } \|r\|_2 \leq 1.
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$$\text{Tr}((I - XX - YY - ZZ)_{ij} \rho_i \otimes \rho_j) = 1 - \langle r_1, r_2 \rangle.$$
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Thus,

$$\text{OPT}_{\text{prod}} = \max \quad \frac{1}{2} \sum_{(i,j) \in E} w_{ij} (1 - \langle v_i, v_j \rangle)$$

s.t.  

$$\langle v_i, v_i \rangle \leq 1$$

$$v_i \in \mathbb{R}^3 \quad \text{for} \quad 1 \leq i \leq n.$$
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SDP relaxation:

$$S = \max \frac{1}{2} \sum_{(i,j) \in E} w_{ij}(1 - X_{ij})$$

s.t. $X_{ii} \leq 1$ for $1 \leq i \leq n$

$X \succeq 0$. 
The algorithm

• Input: Graph $G = (V, E)$ and weights $\{w_{ij} \geq 0\}$ on $n$ vertices.
• Output: Product state $\rho_{\text{prod}} = \rho_1 \otimes \cdots \otimes \rho_n$.

1. Solve semidefinite program $S$, obtaining solution $X$.
2. Take the Cholesky decomposition of $X$ in order to extract a set of vectors $\{x_i\} \subseteq \mathbb{R}^n$.
3. Select random $P = (P_{ij}) \in \mathbb{R}^{3 \times n}$ with each entry $P_{ij} \sim \mathcal{N}(0, 1)$.
4. Return $\rho_{\text{prod}} = \rho_1 \otimes \cdots \otimes \rho_n$ for $\rho_i$ with Bloch vector $P x_i / \|P x_i\|_2$.
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Remarks:

- Steps 3 and 4 are higher dimensional analogue of Goemans-Williamson rounding [Briët, de Oliveira Filho, Vallentin, 2010].
- Rounding obtains 0.9563-approximation to $\text{OPT}_{\text{prod}}$ [BoFV,2010].
- Combining this with our $\text{OPT}_{\text{prod}} \geq \frac{1}{2} \text{OPT}$ bound yields 0.478-algorithm.
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What about the second claim? Show using:

**Theorem [Brandão, Harrow, 2013]**
Let $G = (V, E)$ be $D$-regular graph on $n$ vertices. For any $n$-qubit quantum state $\rho$, there exists $n$-qubit fully separable state $\sigma$ such that

$$\mathbb{E}_{(i,j) \in E} \| \rho_{ij} - \sigma_{ij} \|_{\text{tr}} \leq 12 \left( \frac{4 \ln(2)}{D} \right)^{1/3}.$$
Recall for $D$-regular $G$, $A$ has approximation ratio

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Need $D \geq 1033890$ before improving on $0.478$ (assume unit weights).
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**Conjecture**

Let $G = (V, E)$ be an interaction graph with average degree $d_{\text{avg}} > 0$. Define $w_{\text{max}} := \max_{ij} w_{ij}$. Then,

$$2 \cdot \text{MAXCUT} \leq \text{OPT} \leq 2w_{\text{max}} \left( 1 + \frac{1}{\sqrt{d_{\text{avg}}}} \right) \cdot \text{MAXCUT}.$$
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**Corollary:** For an instance of AFH on graph $G$, algorithm $A$ achieves ratio

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Can prove conjecture for bipartite graphs using Coffman-Kundu-Wootters inequality.
More work in progress

Similar algorithmic techniques apply to Heisenberg XY model:

\[ H = \sum_{(i,j) \in E} H_{ij} \quad \text{for} \quad H_{ij} = X_i \otimes X_j + Y_i \otimes Y_j. \]

Theorem
Let \( R := m/\text{MAXCUT} \). There exists poly-time algorithm \( A \) for the XY model such that:

1. For arbitrary \( G \), \( A \) yields an approximation ratio of \( \left( \frac{2}{2+R} \right) \cdot 0.9563 \).
2. For \( D \)-regular \( G \), let \( \Delta := m/(\sum_{ij} w_{ij}) \) and \( w_{\text{max}} := \max_{ij} w_{ij} \). Then, \( A \) has ratio
   \[ 0.9563 \cdot \max \left( \frac{2}{2+R}, 1 - 36\Delta w_{\text{max}} \left( \frac{4 \ln(2)}{D} \right)^{1/3} \right). \]

Remarks:
- For any \( G \), one has \( 1 \leq R \leq 2 \).
- Conjecture: Can replace \( R \) with 1 above.
1. Intro: Local Hamiltonians
2. Existing Results
3. Approximating the quantum Heisenberg model
4. Conclusions
Conclusions

Recap

- Local Hamiltonians (“quantum CSPs”) are physically well-motivated.
- Physics community has traditionally relied on heuristics.
- Study of approximation algorithms for LH in infancy.
- Goemans-Williamson relaxation can be used to approximate Heisenberg model.

Open Questions

- 1/2-approximation algorithm for 2-LH on general graphs?
- Similar techniques to approximate other QMA-complete problems?
- Approximation algorithms for optimizations over tensor networks?
Thank you for your attention!

Thanks to NSERC Banting Fellowship program.

For more on Quantum Hamiltonian Complexity, see: