QMA-complete problems for stoquastic Hamiltonians and Markov matrices

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Definition: stoquastic Hamiltonian
a Hermitian matrix in which all off-diagonal entries are non-positive

- In physics not all bases are created equal!
- Basis of unentangled states is easy to prepare and measure
- We use $\sigma_z$ basis but results hold for any basis of tensor product states
Some stoquastic Hamiltonians:
- ferromagnetic Heisenberg model
- transverse Ising model
- adiabatic optimization algorithms
- Josephson junction flux qubits
Problem: LOCAL HAMILTONIAN
Input: Hamiltonian $H$ on $n$ qubits
parameters $a < b$ with $b-a > 1/poly(n)$
Output: YES if ground energy is $< a$
NO if ground energy is $> b$
Promise: ground energy not between $a$ and $b$
k-Local: each term acts on at most $k$ qubits
- **NP**: proof (bit string) is efficiently verifiable on classical computer
- **MA**: proof (bit string) is efficiently verifiable on randomized classical computer, $p(\text{error})$ small
- **QMA**: proof (quantum state) is efficiently verifiable on quantum computer

$k$-LOCAL HAMILTONIAN is QMA-complete for any $k > 1$
• Stoquastic LOCAL HAMILTONIAN $\in$ AM
  – probably not QMA-complete!
• Stoquastic adiabatic computation $\in$ $\mathsf{BPP}_{\text{path}}$
  – probably not universal!  

[Bravyi, et al.]

However:

• Approximating highest energy of stoquastic Hamiltonian is QMA-complete
• Adiabatic computation in highest eigenstate of stoquastic Hamiltonian is universal
Actually, we prove QMA-completeness and adiabatic universality for a more restricted class of Hamiltonians:

**Definition:** stochastic Hamiltonian
- symmetric matrix
- all entries real and nonnegative
- sum of entries in any row (or column) is 1
- also called Markov

If $H$ is stochastic, $-H$ is stoquastic
Intuition

• By Perron-Frobenius: highest eigenvector of stochastic matrix is probability distribution
  – lowest eigenvector of stoquastic Hamiltonian is a probability distribution
  – QMA $\rightarrow$ AM

• Other eigenstates have amplitudes of both signs
Stochastic LOCAL HAMILTONIAN is QMA-complete

**Proof:** Begin by using result of Biamonte & Love:

For a Hamiltonian of the form:

\[
H_{XZ} = \sum_i d_i X_i + \sum_i h_i Z_i + \sum_{i,j} K_{ij} X_i X_j + \sum_{i,j} J_{ij} Z_i Z_j
\]

LOCAL HAMILTONIAN is QMA-complete
Proof strategy:

- **given** $H_{XZ}$ construct a stochastic Hamiltonian $\bar{H}$ whose spectrum relates to that of $H_{XZ}$ in a known way

- By calculating ground energy of $\bar{H}$ we learn ground energy of $H_{XZ}$

- $H_{XZ}$ QMA-hard $\implies$ $\bar{H}$ QMA-hard
Main trick:

- We want to get rid of negative matrix elements
- So, we represent the group \( \mathbb{Z}_2 = \{1, -1\} \) by \[ \left\{ \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \right\} \]
- $H_{XZ}$ is of the form:

$$H_{XZ} = \sum_{k} \alpha_k S_k$$

where each coefficient $\alpha_k$ is positive and each $S_k$ is one of $\pm X, \pm Z, \pm X_i X_j, \pm Z_i Z_j$

- All entries in $S_k$ are $+1$, $-1$, or $0$

- Make the replacements

$$1 \rightarrow \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad -1 \rightarrow \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad 0 \rightarrow \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}.$$

Call the result $\tilde{S}_k$
• By the replacement:

\[ 1 \rightarrow \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad -1 \rightarrow \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad 0 \rightarrow \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}. \]

each \( \tilde{S}_k \) is a permutation matrix

• Hence

\[ H_{XZ} = \sum_k \alpha_k S_k \quad \rightarrow \quad \tilde{H}_{XZ} = \frac{1}{\sum k \alpha_k} \sum_k \alpha_k \tilde{S}_k \]

yields stochastic Hamiltonian
\[ H_{XZ} = \sum_{k} \alpha_k \mathcal{S}_k \text{ acts on } n \text{ qubits} \]

\[ \tilde{H}_{XZ} = \frac{1}{\sum_k \alpha_k} \sum_k \alpha_k \tilde{\mathcal{S}}_k \text{ acts on } n+1 \text{ qubits} \]

The 2x2 blocks from the replacement:

\[
1 \rightarrow \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad -1 \rightarrow \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad 0 \rightarrow \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}.
\]

act on the extra qubit
• If the ancilla is \( \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \) then the blocks act like the original scalars.

• If the ancilla is \( \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \) then the blocks replacing +1 and -1 both act like +1.

\[
1 \rightarrow \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad -1 \rightarrow \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad 0 \rightarrow \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}.
\]
Thus:

\[ \tilde{H}_{XZ} = \frac{1}{\sum_k \alpha_k} \left( H_{XZ} \otimes \langle - \rangle \langle - \rangle + H'_{XZ} \otimes \langle + \rangle \langle + \rangle \right) \]

where \( H'_{XZ} \) is the entrywise absolute value of \( H_{XZ} \).

Next we penalize the \( |+\rangle \) subspace

\[ \bar{H} = (1 - p)X_{n+1} + p\tilde{H}_{XZ} \]

QED
- How about highest eigenvalue of stochastic Hamiltonian?
- Always 1, can't be QMA-complete.
- Proof fails at penalty step:

\[ \tilde{H} = (1 - p)X_{n+1} + p\tilde{H}_{XZ} \]

- Proof fails for ground energy of stoquastic H
• Besides application to stoquastic Hamiltons:
  - we have QMA-completeness for a “classical” problem
  - exponentially large stochastic matrices arise in Markov chains
  - natural tensor product structure:
    \[ p_{t+1} = M p_t \]
    \[ q_{t+1} = N q_t \]
    joint probability evolves with \( M \otimes N \)
Adiabatic Quantum Computing

Hamiltonian: $H(0) \quad \longrightarrow \quad \text{smoothly} \quad \longrightarrow \quad H(T)$

ground state: $\lvert 000... \rangle \quad \longrightarrow \quad \lvert \text{answer} \rangle$

If $\left| \frac{dH}{dt} \right|$ is sufficiently small compared to the eigenvalue gap then the system will track the ground state.
Adiabatic Quantum Computing

- Originally proposed by Farhi et al. as a method for solving satisfiability problems (e.g. 3-SAT)

- Can be simulated by quantum circuits using standard Trotterization

- Can simulate quantum circuits [Aharonov et al.]
• Adiabatic quantum computation with 5-local Hamiltonians is universal \cite{Aharonov et al}
• 3-local is universal \cite{Kempe, Kitaev, Regev}
• XZ is universal \cite{Biamonte & Love}
• Stoquastic is universal (in excited states)
QMA-completeness of LOCAL-HAMILTONIAN

Universality of adiabatic quantum computation

- 5-local \cite{Aharonov et al, Kitaev}
- 3-local \cite{Kempe & Regev}
- 2-local \cite{Kempe Kitaev & Regev}
- XZ \cite{Biamonte & Love}
- stoquastic

why?
• **Proof techniques:**
  
  – **Quantum circuit** $U$:
    \[
    |\psi_0\rangle \rightarrow U_1|\psi_1\rangle \rightarrow U_2U_1|\psi_0\rangle \rightarrow \ldots
    \]
  
  – **Construct** $H_U$ **with ground state**:
    \[
    \frac{1}{\sqrt{n+1}} (|\psi_0\rangle |0\rangle + U_1|\psi_0\rangle |1\rangle + U_2U_1|\psi_0\rangle + \ldots)
    \]
  
  – **LOCAL HAMILTONIAN**: add energy penalty against “NO” outcomes
  
  – **adiabatic computation**: find $H(s)$ such that $H(0)$ has a simple ground state, $H(1) = H_U$, and gap is polynomial
Adiabatic Quantum Computation with 3-local Stochastic Hamiltonians is Universal

Proof sketch:

• Adiabatic QC is universal with a Hamiltonian of the form $H_{XZ}(t)$ [Biamonte, Love]
• Apply our construction to each instantaneous Hamiltonian $H_{XZ}(t) \rightarrow \bar{H}(t)$
• By construction $\bar{H}_{XZ}(1)$ has the desired ground state
• $\bar{H}(t)$ is smoothly varying
• gap is smaller by factor of $\sum_k \alpha_k$ QED
Adiabatic Quantum Computation with 3-local \textbf{Stoquastic} Hamiltonians is Universal

- Proof #1: use $-\bar{H}(t)$

- We can do better:
  - only do this:
    \[
    1 \rightarrow \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad -1 \rightarrow \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad 0 \rightarrow \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}.
    \]
  - no rescaling by $\sum_k \alpha_k$ and no penalty against $|+\rangle$
  - universality in $|\_\rangle$ subspace
  - no overhead
Gadgets

to simulate:

\[ H^{\text{comp}} = \sum_{s=1}^{r} c_s H_s \]

\[ H_s = \sigma_{s,1} \sigma_{s,2} \cdots \sigma_{s,k} \]

\[ \sigma_{s,j} = \hat{n}_{s,j} \cdot \vec{\sigma}_{s,j} \]

use:

\[ H^{\text{gad}} = \sum_{s=1}^{r} H_s^{\text{anc}} + \lambda \sum_{s=1}^{r} \sqrt{c_s} V_s \]

\[ H_s^{\text{anc}} = \sum_{1 \leq i < j \leq k} \frac{1}{2} (I - Z_{s,i} Z_{s,j}) \]

\[ V_s = \sum_{j=1}^{k} \sigma_{s,j} \otimes X_{s,j} \]
Applications & Open Problems

• Antiapplication: can't efficiently compute highest energy of stoquastic Hamiltonians
  - other excited states?
• Adiabatic computation with Josephson junctions
  - 2-local?
  - protection against decay into lower energies?
• Complexity theory
  - QMA-complete problem regarding Markov chains
  - QMA-completeness of mixing time?
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Thank You