The Bose-Hubbard and XY models are QMA-complete

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Hamiltonian complexity

Classical constraint satisfaction:
How hard is it to determine whether a Boolean formula has a satisfying assignment (or find minimum number of violated clauses)?

\[(x_1 \lor \bar{x}_2 \lor x_5) \land (x_{17} \lor x_{22} \lor \bar{x}_{25}) \land \cdots \land (\bar{x}_2 \lor \bar{x}_{25} \lor x_{99})\]

Quantum analog:
How hard is it to (approximately) compute the smallest eigenvalue of a Hermitian matrix?

\[H = \sum_j H_j\quad \text{each term } H_j \text{ acts on } k \text{ qubits}\]
Quantum Merlin-Arthur

QMA: the quantum analog of NP

Merlin wants to prove to Arthur that some statement is true.

- If the statement is true, there exists a $|\psi\rangle$ that Arthur will accept with probability at least 2/3.
- If the statement is false, any $|\psi\rangle$ will be rejected by Arthur with probability at least 2/3.
Complexity of ground energy problems

- $k$-Local Hamiltonian problem: QMA-complete for $k \geq 2$ [Kitaev 99; Kempe, Kitaev, Regev 06]
- Quantum $k$-SAT (is there a frustration-free ground state?): in P for $k=2$; QMA$_1$-complete for $k \geq 3$ [Bravyi 06; Gosset, Nagaj 13]
- Stoquastic $k$-local Hamiltonian problem: in AM [Bravyi, DiVincenzo, Oliveira, Terhal 06]
- Fermion/boson problems: QMA-complete [Liu, Christandl, Verstraete 07; Wei, Mosca, Nayak 10]
- 2-local Hamiltonian on a grid: QMA-complete [Oliveira, Terhal 08]
- 2-local Hamiltonian on a line of qudits: QMA-complete [Aharonov, Gottesman, Irani, Kempe 09]
- Hubbard model on a 2d grid with a site-dependent magnetic field: QMA-complete [Schuch, Verstraete 09]
- Heisenberg and XY models with site-dependent couplings: QMA-complete [Cubitt, Montanaro 13]
Dynamics are universal; ground states are hard

**Theorem:** The Schrödinger dynamics generated by time-independent local Hamiltonians can perform universal quantum computation. [Feynman 85]

\[ H = \sum_j (U_j \otimes |j + 1\rangle\langle j| + U_j^\dagger \otimes |j\rangle\langle j + 1|) \]

**Theorem:** Local Hamiltonian is QMA-complete. [Kitaev 99]

**Theorem:** The dynamics generated by the adjacency matrix of an unweighted sparse graph (i.e., a continuous-time quantum walk) can perform universal quantum computation. [C 09]

**Theorem:** Approximating the smallest eigenvalue of an unweighted sparse graph is QMA-complete. [CGW 14]
Dynamics are universal; ground states are hard

**Theorem:** Any $n$-qubit, $g$-gate quantum circuit can be simulated by a Bose-Hubbard model with $n + 1$ particles interacting for time $\text{poly}(n, g)$ on an unweighted $\text{poly}(n, g)$-vertex graph. [CGW 13]

**Consequences:**
- Architecture for a quantum computer with no time-dependent control
- Simulating dynamics of interacting many-body systems is BQP-hard (e.g., Bose-Hubbard model on a sparse, unweighted, planar graph)

**Theorem:** Approximating the ground energy of the $n$-particle Bose-Hubbard model on a graph is QMA-complete. [CGW 14]

**Consequences:**
- Computing the ground energy of the Bose-Hubbard model is (probably) intractable
- New techniques for quantum Hamiltonian complexity
... but not always

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Bose-Hubbard model

Consider $n$ distinguishable particles:

- **states:** $|v_1, \ldots, v_n\rangle \quad v_i \in V(G)$
- **Hilbert space dimension:** $|V(G)|^n$

**Hamiltonian:**

$$H^{(n)}_G = t_{\text{hop}} \sum_{i=1}^{n} A(G)_i + \mathcal{U}$$

**Indistinguishable bosons: symmetric subspace**

**On-site interaction:**

$$\mathcal{U} = J_{\text{int}} \sum_{v \in V(G)} \hat{n}_v (\hat{n}_v - 1)$$

$$\hat{n}_v = \sum_{i=1}^{n} |v\rangle \langle v|_i$$

**Second-quantized notation:**

$$H_G = t_{\text{hop}} \sum_{u,v \in V(G)} A(G)_{uv} a_u^\dagger a_v + J_{\text{int}} \sum_{v \in V(G)} \hat{n}_v (\hat{n}_v - 1)$$

$$\hat{n}_v = a_v^\dagger a_v$$
Bose-Hubbard Hamiltonian is QMA-complete

Bose-Hubbard model on $G$:

$$H_G = t_{\text{hop}} \sum_{u,v \in V(G)} A(G)_{uv} a_u^\dagger a_v + J_{\text{int}} \sum_{v \in V(G)} \hat{n}_v (\hat{n}_v - 1)$$

**Theorem:** Determining whether the ground energy for $n$ particles on the graph $G$ is less than $n e_1 + \epsilon$ or more than $n e_1 + 2\epsilon$ is QMA-complete, where $e_1$ is the 1-particle ground energy.

- Fixed movement and interaction terms ($A(G)$ is a 0-1 matrix)
- Applies for any fixed $t_{\text{hop}}, J_{\text{int}} > 0$
- It is QMA-hard even to determine whether the instance is approximately frustration free
- Analysis does not use perturbation theory
Dependence on signs of coefficients

\[ t_{\text{hop}} \]

\[ J_{\text{int}} \]

\[ \in \text{QMA} \]

\[ \in \text{AM} \cap \text{QMA} \]

stoquastic (no sign problem)
Frustration-freeness

\[ H_G = t_{\text{hop}} \sum_{u,v \in V(G)} A(G)_{uv} a_u^\dagger a_v + J_{\text{int}} \sum_{v \in V(G)} \hat{n}_v (\hat{n}_v - 1) \]

\[ \geq n \mu(G) \]

\[ \mu(G) = \text{smallest eigenvalue of } A(G) \]

If a ground state of \( H_G \) has energy \( t_{\text{hop}} n \mu(G) \), we call it frustration free.

We encode a computation in frustration-free states; this is why our result holds for any positive \( J_{\text{int}} \).
**XY model**

Frustration-free states have at most one boson per site (“hard-core bosons”)

Thus we can translate our results to spin systems, giving a generalization of the XY model on a graph:

\[
\sum_{A(G)_{ij}=1, \ i\neq j} \frac{\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y}{2} + \sum_{A(G)_{ii}=1} \frac{1 - \sigma_i^z}{2}
\]

**Theorem:** Approximating the ground energy in the sector with magnetization \(\sum_i \frac{1 - \sigma_i^z}{2} = n\) is QMA-complete.
Removing self-loops

In our original proof, the adjacency matrix can be any symmetric 0-1 matrix (i.e., the adjacency matrix of an undirected graph with at most one self-loop per vertex).

We improve this to show that the ground energy problems remain hard without self-loops.

Bose-Hubbard model:

\[ H_G = t_{\text{hop}} \sum_{u,v \in V(G)} A(G)_{uv} a_u^\dagger a_v + J_{\text{int}} \sum_{v \in V(G)} \hat{n}_v (\hat{n}_v - 1) \]

XY model:

\[ \sum_{u,v \in V(G')} A(G')_{uv} \frac{\sigma_x^u \sigma_x^v + \sigma_y^u \sigma_y^v}{2} \]
Containment in QMA

Ground energy problems are usually in QMA

Strategy:
• Merlin provides the ground state
• Arthur measures the energy using phase estimation and Hamiltonian simulation

Only one small twist for boson problems: project onto the symmetric subspace
The quantum Cook-Levin Theorem

**Theorem:** Local Hamiltonian is QMA-complete [Kitaev 99]

Consider a QMA verification circuit $U_t \ldots U_2 U_1$ with witness $|\psi\rangle$

The Feynman Hamiltonian

$$H = \sum_{j=1}^{t} (I \otimes |j\rangle\langle j| + I \otimes |j - 1\rangle\langle j - 1| - U_j \otimes |j\rangle\langle j - 1| - U_j^\dagger \otimes |j - 1\rangle\langle j|)$$

has ground states $|\text{hist}_\psi\rangle = \frac{1}{\sqrt{t + 1}} \sum_{j=0}^{t} U_j \ldots U_1 |\psi\rangle \otimes |j\rangle$

- Implement the “clock” using local terms
- Add a term penalizing states with low acceptance probability

Establish a promise gap:
- yes instances have ground energy $\leq a$
- no instances have ground energy $\geq b$
QMA-hardness for sparse graphs

Theorem: Approximating the smallest eigenvalue of an unweighted sparse graph is QMA-complete.

Use the Feynman-Kitaev Hamiltonian

\[-\sqrt{2} \sum_j (U_j \otimes |j + 1\rangle \langle j| + U_j^\dagger \otimes |j\rangle \langle j + 1|)\]

with gates \(\{H, HT, (HT)^\dagger, (H \otimes 1)\text{CNOT}\}\)

Then every nonzero matrix element is a power of \(\omega = e^{i\pi/4}\)

Replace \(\omega^k \mapsto S^k\) where \(S = \text{cyclic shift mod 8}\)

Penalty term \(S^3 + S^4 + S^5\) penalizes ancilla states with eigenvalues other than \(\omega\) or \(\omega^*\)
Single-qubit gates

Construct a graph encoding a universal set of single-qubit gates in the single-particle sector:

- Start from Feynman-Kitaev Hamiltonian for a particular sequence of gates
- Obtain matrix elements $\omega^j$ by careful choice of gate set and scaling
- Make all entries 0 or 1 using an ancilla

Ground state subspace is spanned by

$$|\psi_{z,0}\rangle = \frac{1}{\sqrt{8}} (|z\rangle(|1\rangle + |3\rangle + |5\rangle + |7\rangle)$$

$$+ H|z\rangle(|2\rangle + |8\rangle) + HT|z\rangle(|4\rangle + |6\rangle)) |\omega\rangle$$

$$|\psi_{z,1}\rangle = |\psi_{z,0}\rangle^*$$

For $z \in \{0, 1\}$

some ancilla state
Two-qubit gates

Two-qubit gate gadgets: 4096-vertex graphs built from 32 copies of the single-qubit graph, joined by edges and with some added self-loops

Single-particle ground states are associated with one of two input regions or one of two output regions:

(States also carry labels associated with the logical state & complex conjugation.)

Two-particle ground states encode two-qubit computations:

\[
\frac{1}{\sqrt{2}} \left( \left| \begin{array}{c}
\text{orange}
\end{array} \right\rangle \otimes |\psi\rangle + \left| \begin{array}{c}
\text{orange}
\end{array} \right\rangle \otimes U|\psi\rangle \right)
\]
Constructing a verification circuit

Connect two-qubit gate gadgets to implement the whole verification circuit, e.g.:

Some multi-particle ground states encode computations:

\[ |\psi\rangle + U_1|\psi\rangle + U_1|\psi\rangle + U_2U_1|\psi\rangle \]

But there are also ground states that do not encode computations (two particles for the same qubit; particles not synchronized).

To avoid this, we introduce a way of enforcing occupancy constraints, forbidding certain kinds of configurations. We establish a promise gap using nonperturbative spectral analysis (no large coefficients).
Spectral analysis

For $H \geq 0$, let $\gamma(H)$ denote the smallest nonzero eigenvalue of $H$.

Nullspace Projection Lemma: Let $H_A, H_B \geq 0$ and let $S$ denote the nullspace of $H_A$. Suppose $\gamma(H_B|_S) \geq c$ and $\gamma(H_A) \geq d$. Then

$$\gamma(H_A + H_B) \geq \frac{cd}{c + d + \|H_B\|}.$$ 

Using this repeatedly, we can establish a promise gap between yes and no instances.

Advantage over other techniques: we do not need to add terms with large coefficients (as with the KKR projection lemma or perturbative gadgets).
**Removing self-loops**

**Main idea:** Add a self-loop to every vertex (without significantly changing the ground energy). This is just an overall energy shift (in a sector with fixed particle number).

Make two copies of the graph. For every vertex without a self-loop, add a self-loop in each copy and an edge between the two copies.

\[
|+\rangle\langle+| = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}
\]

**Ground space:** States \(|\psi\rangle|\rightarrow\rangle\) where \(|\psi\rangle\) is an eigenstate of the original graph.

Also, the interaction term within the space of states \(|\psi\rangle|\rightarrow\rangle\) is just 1/2 times the usual interaction term.

Promise gap of the Bose-Hubbard model on the original graph \(\Rightarrow\) promise gap for the new graph.
Summary

Approximating the ground energy of the Bose-Hubbard model on a simple graph at fixed particle number is QMA-complete.

Consequently, approximating the ground energy of the XY model on a simple graph at fixed magnetization is QMA-complete.

A frustration-free encoding and the Nullspace Projection Lemma let us establish these results without using perturbation theory.
Open questions

• Related improvements for $\kappa$-local Hamiltonian
  - Constant-size coefficients
  - Finite set of allowed terms without variable coefficients
  - Instances of Local Hamiltonian defined entirely by a (hyper)graph

• Complexity of other models of multi-particle quantum walk
  - Attractive interactions
  - Negative hopping strength (stoquastic; is it AM-hard?)
  - Bosons or fermions with nearest-neighbor interactions
  - Unrestricted particle number

• Complexity of other quantum spin models defined on graphs
  - Antiferromagnetic Heisenberg model