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)?

$$(x_1 \vee \bar{x}_2 \vee x_5) \wedge (x_{17} \vee x_{22} \vee \bar{x}_{25}) \wedge \cdots \wedge (\bar{x}_2 \vee \bar{x}_{25} \vee x_{99})$$

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

$$H = \sum_j H_j$$

each term H_j acts on k qubits

Quantum Merlin-Arthur

QMA: the quantum analog of NP

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

Merlin

quantum proof $|\psi\rangle$

Arthur

efficient quantum verification circuit

- 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]

$$H = \sum_j \left(U_j \otimes |j+1\rangle\langle j| + U_j^\dagger \otimes |j\rangle\langle j+1| \right)$$

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 $\mathrm{poly}(n,g)$ on an unweighted $\mathrm{poly}(n,g)$-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

model	dynamics	ground energy
Local Hamiltonians	BQP-complete	QMA-complete
Sparse adjacency matrices	BQP-complete	QMA-complete
Bose-Hubbard model (positive hopping)	BQP-complete	QMA-complete
stoquastic Local Hamiltonians	BQP-complete	AM
Bose-Hubbard model (negative hopping)	BQP-complete	AM
ferromagnetic Heisenberg model on a graph	BQP-complete	trivial

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

Indistinguishable bosons: symmetric subspace

On-site interaction: $\mathcal{U} = J_{\text{int}} \sum_{v \in V(G)} \hat{n}_v(\hat{n}_v - 1) \qquad \hat{n}_v = \sum_{i=1}^{n} |v\rangle\langle v|_i$

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

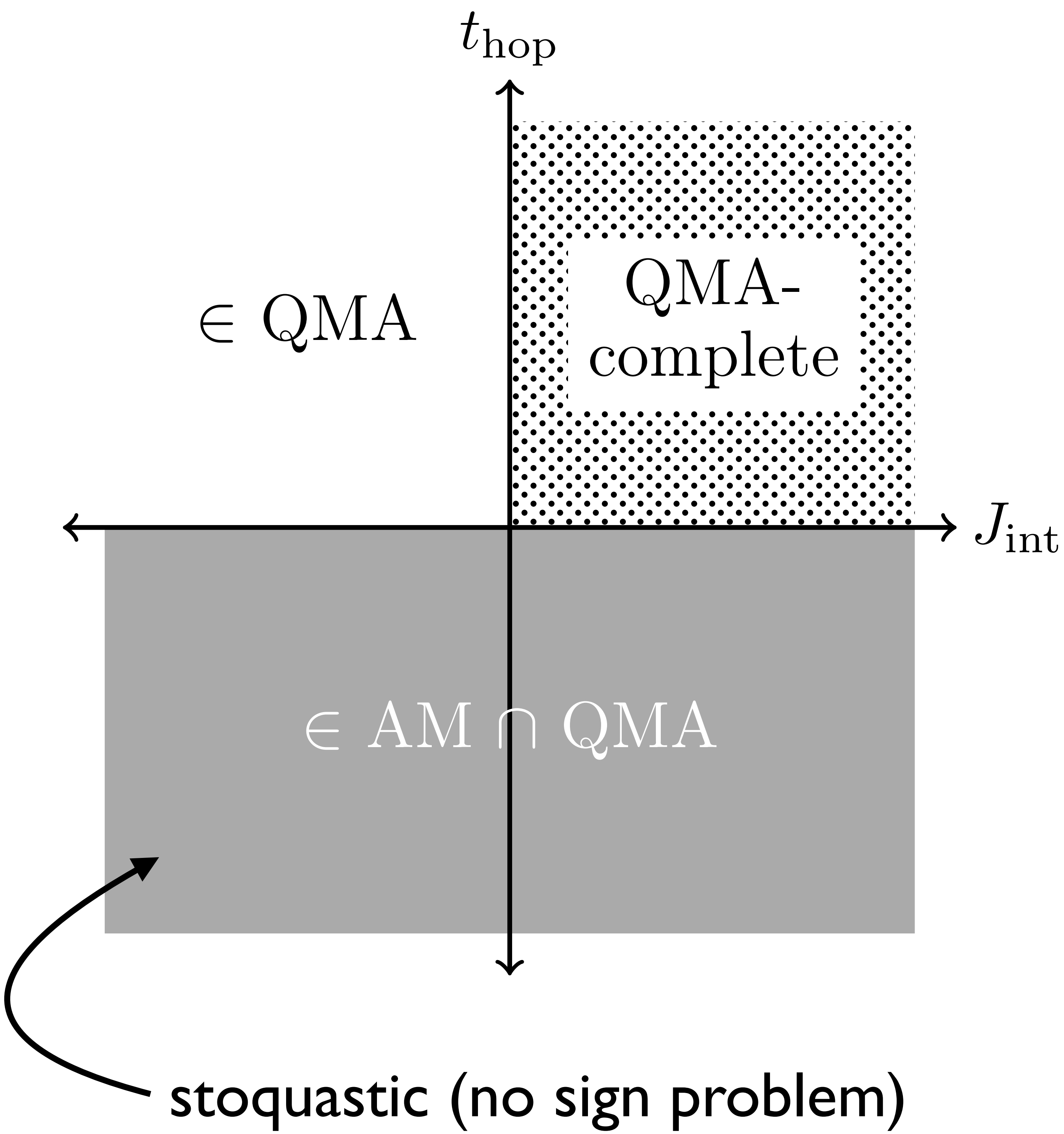
Bose-Hubbard model on G:

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

Theorem: Determining whether the ground energy for n particles on the graph G is less than $ne_1 + \epsilon$ or more than $ne_1 + 2\epsilon$ 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



Frustration-freeness

$$H_G = t_{\text{hop}} \underbrace{\sum_{u,v \in V(G)} A(G)_{uv} a_u^\dagger a_v}_{\geq n\,\mu(G)} + J_{\text{int}} \underbrace{\sum_{v \in V(G)} \hat{n}_v(\hat{n}_v - 1)}_{\geq 0}$$

$\mu(G)$ = 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_{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:

$$\sum_{\substack{A(G)_{ij}=1 \\ i\neq j}} \frac{\sigma_x^i \sigma_x^j + \sigma_y^i \sigma_y^j}{2} + \sum_{A(G)_{ii}=1} \frac{1-\sigma_z^i}{2}$$

Theorem: Approximating the ground energy in the sector with magnetization $\sum_i \frac{1-\sigma_z^i}{2} = n$ 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 $|\mathrm{hist}_\psi\rangle = \frac{1}{\sqrt{t+1}} \sum_{j=0}^{t} U_j \ldots U_1 |\psi\rangle \otimes |j\rangle$

- 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

$$-\sqrt{2}\sum_j \left(U_j \otimes |j+1\rangle\langle j| + U_j^\dagger \otimes |j\rangle\langle j+1|\right)$$

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

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

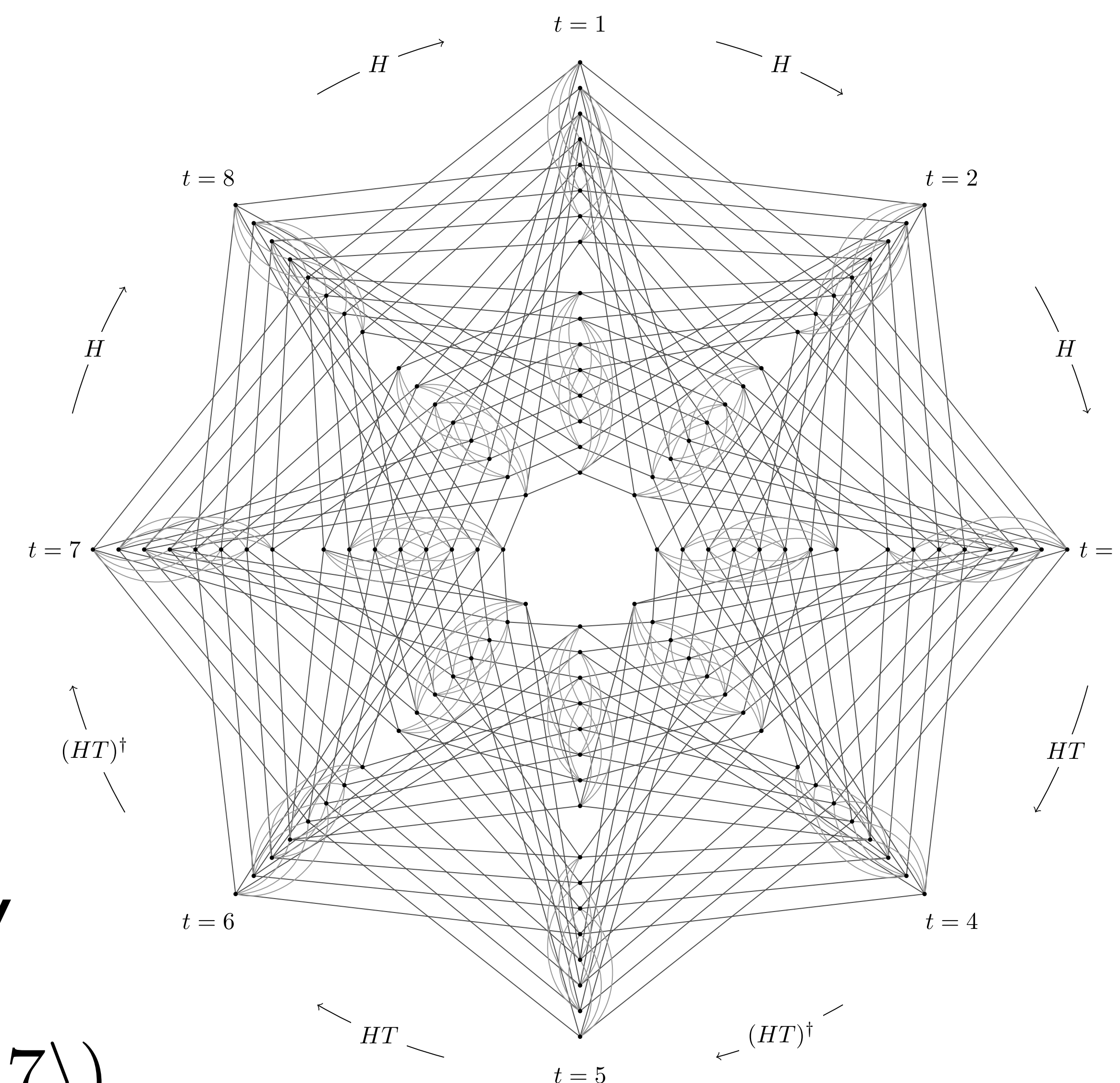
Replace $\omega^k \mapsto S^k$ where S = cyclic shift mod 8

Penalty term $S^3 + S^4 + S^5$ penalizes ancilla states with eigenvalues other than ω or ω^*

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 ω^j by careful choice of gate set and scaling
- Make all entries 0 or 1 using an ancilla



Ground state subspace is spanned by

$$|\psi_{z,0}\rangle = \frac{1}{\sqrt{8}}\Big(|z\rangle(|1\rangle + |3\rangle + |5\rangle + |7\rangle) + H|z\rangle(|2\rangle + |8\rangle) + HT|z\rangle(|4\rangle + |6\rangle)\Big)|\omega\rangle$$

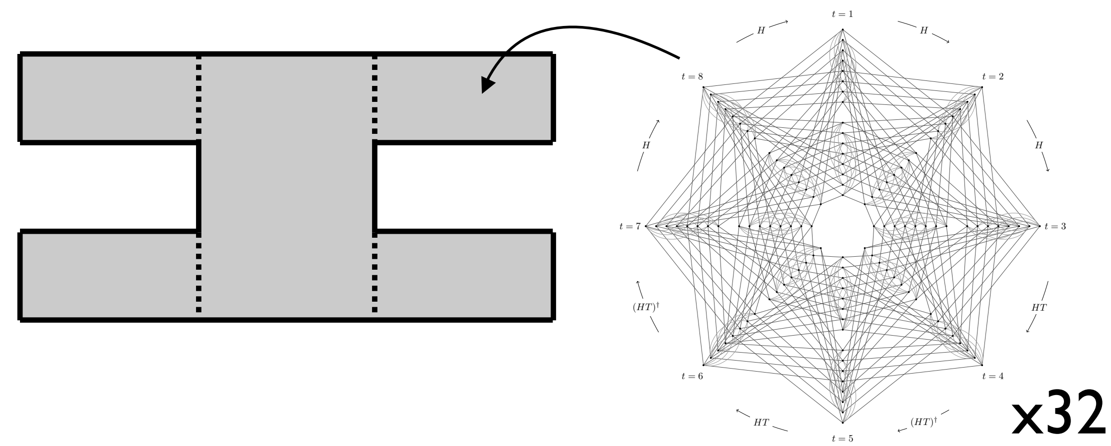
some ancilla state

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

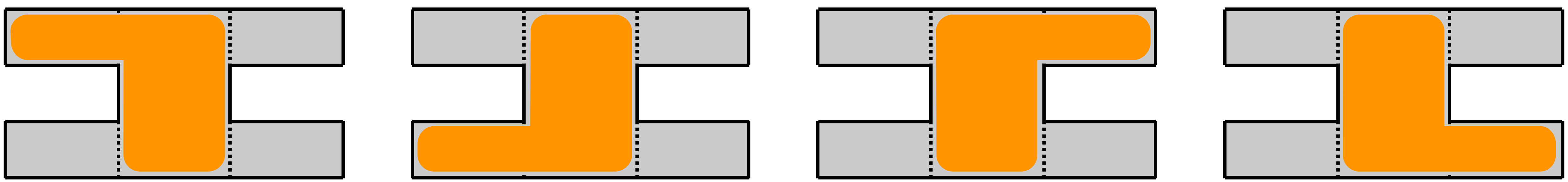
for $z \in \{0,1\}$

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

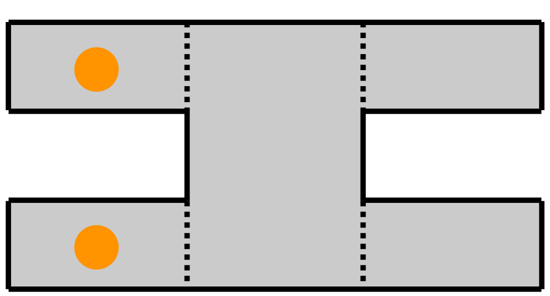
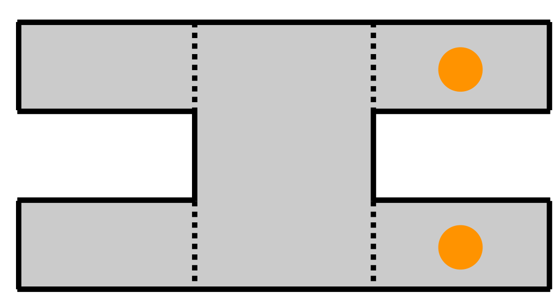


Single-particle ground states are associated with one of two input regions or one of two output regions:



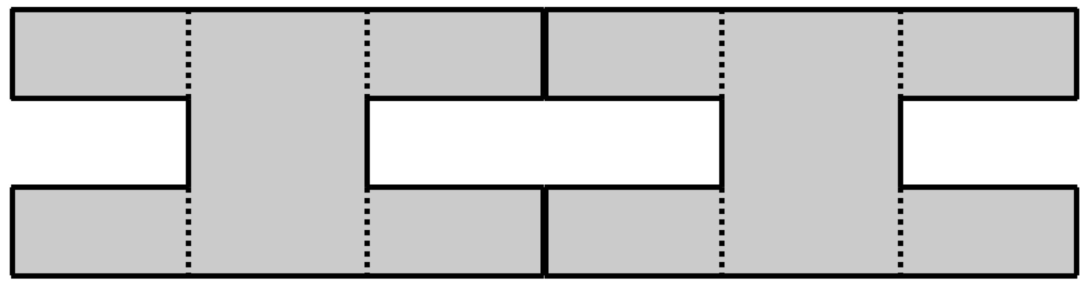
(States also carry labels associated with the logical state & complex conjugation.)

Two-particle ground states encode two-qubit computations:

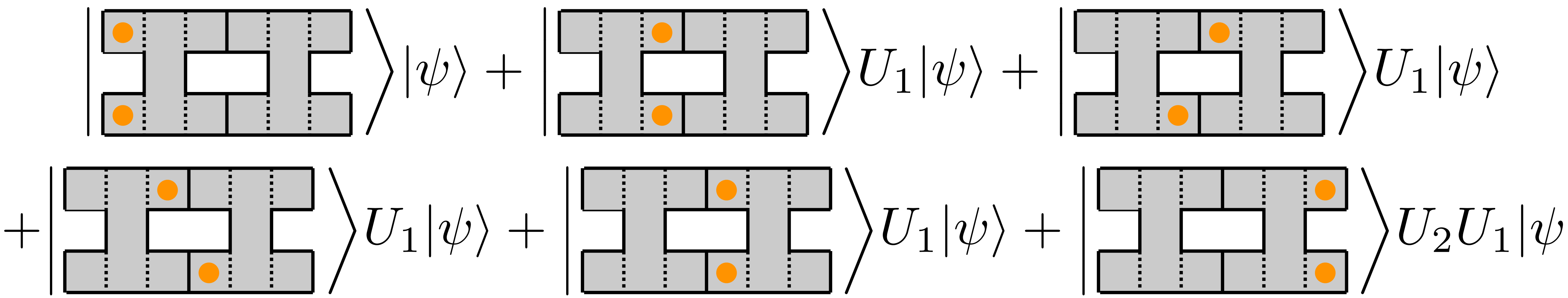
$\frac{1}{\sqrt{2}}\Bigg(\Bigg|$  $\Bigg\rangle \otimes |\psi\rangle + \Bigg|$  $\Bigg\rangle \otimes U|\psi\rangle\Bigg)$

Constructing a verification circuit

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



Some multi-particle ground states encode computations:



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

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

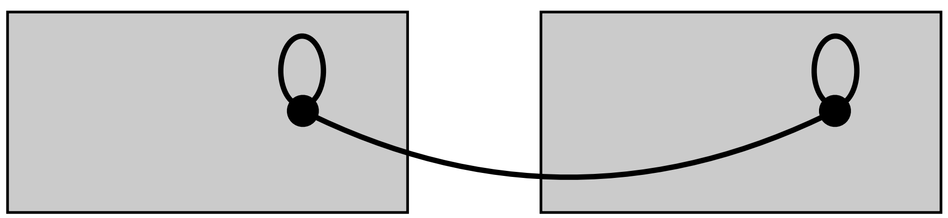
Using this repeatedly, we can establish a promise gap between yes and no instances.

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 $|\psi\rangle|-\rangle$ where $|\psi\rangle$ is an eigenstate of the original graph.

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

Promise gap of the Bose-Hubbard model on the original graph ⇒ 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 k-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