Title: The Bose-Hubbard model is QMA-complete

Date: Dec 18, 2013 04:00 PM

URL: http://pirsa.org/13120067

Abstract: <span>The Bose-Hubbard model is a system of interacting bosons that live on the vertices of a graph. The particles can move between adjacent vertices and experience a repulsive on-site interaction. The Hamiltonian is determined by a choice of graph that specifies the geometry in which the particles move and interact. We prove that approximating the ground energy of the Bose-Hubbard model on a graph at fixed particle number is QMA-complete. In our QMA-hardness proof, we encode the history of an n-qubit computation in the subspace with at most one particle per site (i.e., hard-core bosons). This feature, along with the well-known mapping between hard-core bosons and spin systems, lets us prove a related result for a class of 2-local Hamiltonians defined by graphs that generalizes the XY model. By avoiding the use of perturbation theory in our analysis, we circumvent the need to multiply terms in the Hamiltonian by large coefficients. This is joint work with Andrew Childs and Zak Webb.</span>

# The Bose-Hubbard model is QMA-complete

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arXiv: 1311.3297

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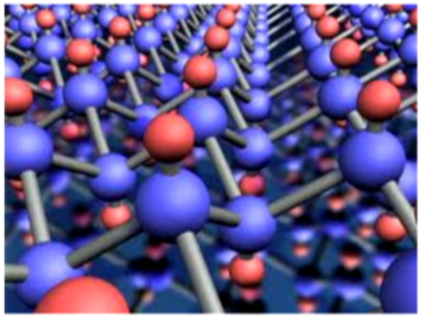

What can we compute with it?
What can we compute about it?

Image source: http://www.condmat.physics.manchester.ac.uk/imagelibrary/

## Aside: Classes of computational problems

Efficient algorithm to solve

| | |
|---|---|
| **P** | Problems which can be solved efficiently with a classical computer. |
| **BQP** | Problems which can be solved efficiently with a quantum computer. |

# Aside: Classes of computational problems

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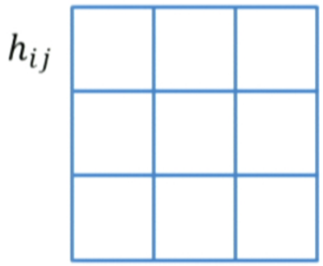
| Efficient algorithm to solve | **P** | Problems which can be solved efficiently with a classical computer. |
| | **BQP** | Problems which can be solved efficiently with a quantum computer. |
| Efficient algorithm to verify solution | **NP** | Problems whose solutions can be verified efficiently with a classical computer. |
| | **QMA** | Problems whose solutions can be verified efficiently with a quantum computer. |

| Class of Hamiltonians | Ground energy problem | Complexity |
| --- | --- | --- |
| Local | k-local Hamiltonian problem | QMA-complete for $k \geq 2$<br>[Kempe, Kitaev, Regev 2006] |
| Frustration-free | Quantum k-SAT<br>(testing frustration-freeness) | Contained in P for $k = 2$<br>$QMA_1$-complete for $k \geq 3$<br>[Bravyi 2006] [G. , Nagaj 2013 ] |
| Stoquastic<br>(no "sign problem") | Stoquastic k-local Hamiltonian problem | Contained in AM<br>MA-hard<br>[Bravyi et. al. 2006] |
| Fermions or Bosons | | QMA-complete<br>[Liu, Christandl, Verstraete 2007]<br>[Wei, Mosca, Nayak 2010] |




2-local Hamiltonian on a 2D grid [Oliveira Terhal 2008]


2-local Hamiltonian on a line with qudits
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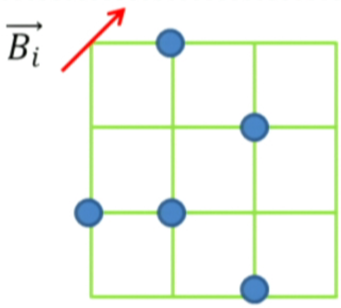


Hubbard model on a 2D grid with site-dependent magnetic field [Schuch Verstraete 2009].

Versions of the XY, Heisenberg, and other models with adjustable coefficients
[Cubitt Montanaro 2013]

E.g.,

$$\sum_{ij} \alpha_{ij} ({\sigma_x}^i {\sigma_x}^j + {\sigma_y}^i {\sigma_y}^j)$$


$h_{ij}$
2-local Hamiltonian on a 2D grid [Oliveira Terhal 2008]
$H_{i,i+1}$
2-local Hamiltonian on a line with qudits
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$\vec{B_i}$
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- Hamiltonians with no sign problem for Quantum Monte Carlo have a special status
- Systems with QMA-complete ground energy problems can be deceptively simple!

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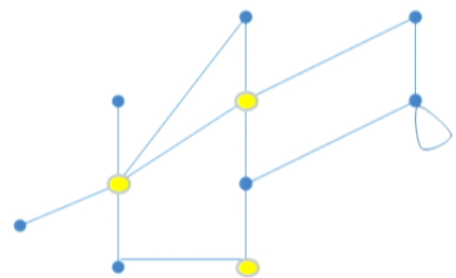
- The complexity of many simple models from condensed matter physics remains unknown.

- Many of the previous QMA-completeness results allow the coefficients in the Hamiltonian to grow with the system size. This is an undesirable feature (and is related to the use of perturbation theory in the analysis).

## Our work

**Bose-Hubbard model:** bosons move and interact on the vertices of a graph.



The system is defined by a graph and a number of particles (no adjustable coefficients).

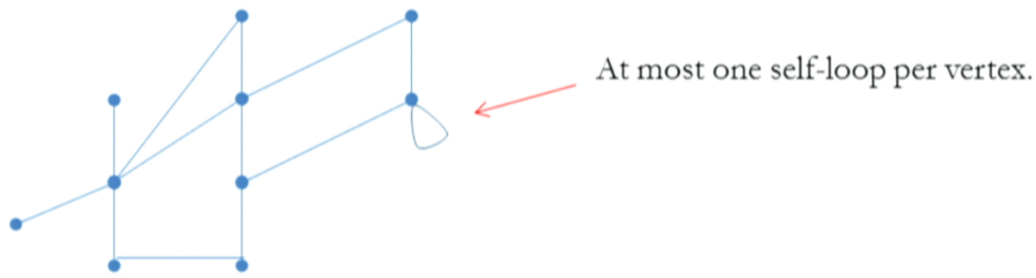
Overview of results

QMA-completeness for ground energy problems
(general strategy and example)

Our strategy for the Bose-Hubbard model

# Bose-Hubbard model on a graph

**Graph:** described by its adjacency matrix $A(G)$, a symmetric 0-1 matrix.




**Hamiltonian**

$$H_G = \underbrace{\sum_{i,j\in V} A(G)_{ij} a_i^\dagger a_j}_{\text{Movement}} + \underbrace{\sum_{k\in V} n_k(n_k - 1)}_{\text{On-site interaction}}$$

# Other choices

We fixed the coefficients in front of the movement and interaction terms

$$t \sum_{i,j \in V} A(G)_{ij} a_i^\dagger a_j + U \sum_{k \in V} n_k (n_k - 1)$$

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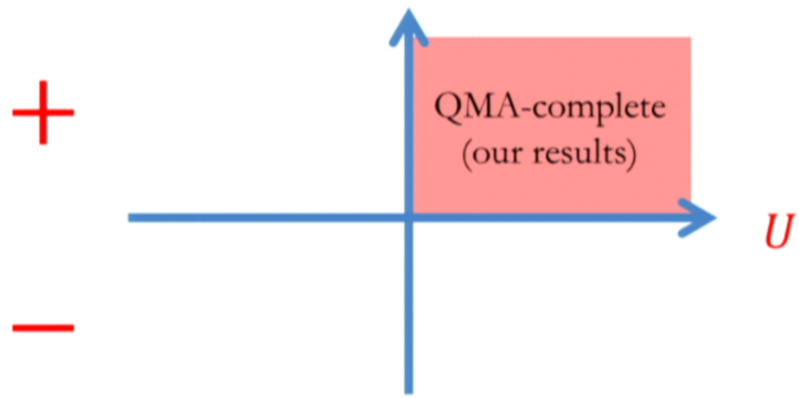

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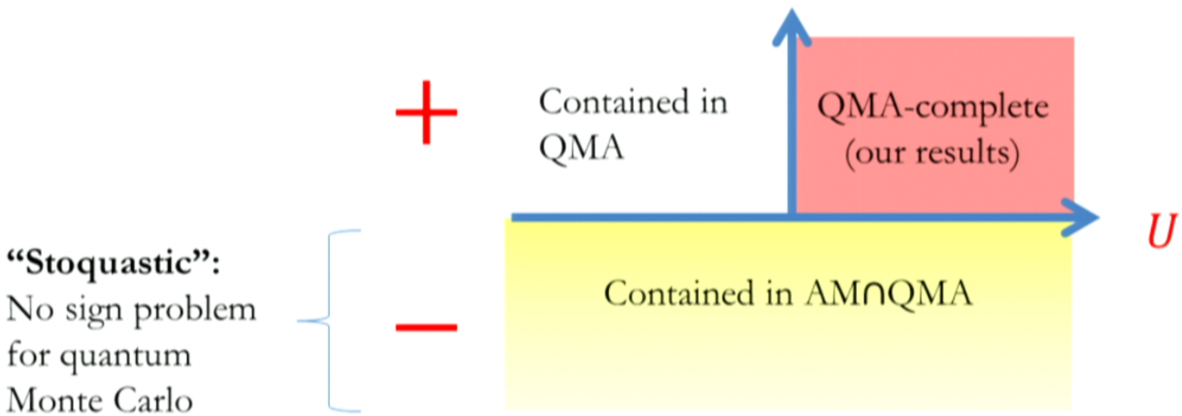

Why does our proof apply to the problem with any repulsive interaction strength?

$$\underbrace{\sum_{i,j\in V} A(G)_{ij} a_i^\dagger a_j}_{\geq N\mu(G)} + U \sum_{k\in V} n_k(n_k - 1)$$

$\mu(G)$= smallest eigenvalue of $A(G)$

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$\mu(G)$= smallest eigenvalue of $A(G)$

If the ground energy is $N\mu(G)$ we say the **groundspace is frustration-free.**

⟺

1) Each particle is in a groundstate of $A(G)$
2) Each vertex is occupied by $\leq 1$ particles

Any state with these properties is a ground state for all $U > 0$

**The main step in our QMA-hardness proof**: we design a graph so that the frustration-free ground states encode the history of a computation (works for all $U > 0$)

**When $U \to \infty$ the Hamiltonian is equivalent to a spin model…**

# A related spin model

Graph $G$ with vertex set $V$ $\longrightarrow$ $|V|$-qubit Hamiltonian $O_G$


$\longrightarrow$ $\left(|01\rangle\langle 10| + |10\rangle\langle 01|\right)_{ij}$


$\longrightarrow$ $|1\rangle\langle 1|_i$

# A related spin model

$$O_G = \sum_{\substack{A(G)_{ij}=1 \\ i\neq j}} \big(|01\rangle\langle 10| + |10\rangle\langle 01|\big)_{ij} + \sum_{A(G)_{ii}=1} |1\rangle\langle 1|_i$$

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

Conserves total magnetization (Hamming weight)

Write $\Theta_G^N$ for the smallest eigenvalue of $O_G$ within the sector with magnetization N.

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**XY Hamiltonian problem**

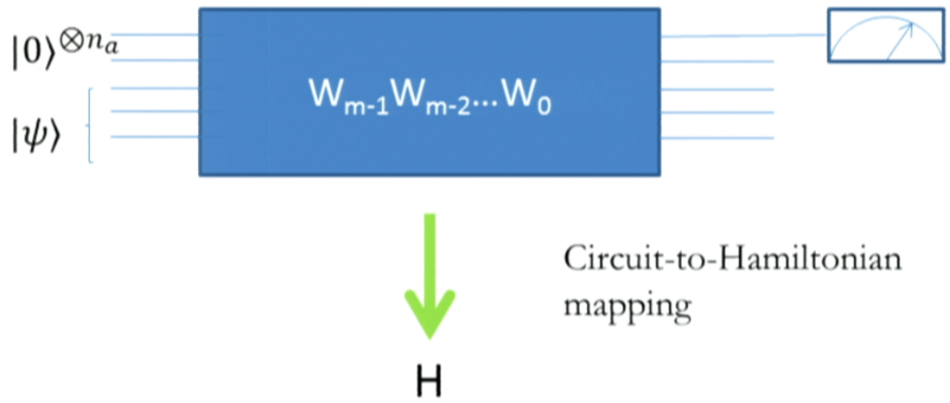
**Input:**

- Graph $G$
- Magnetization $N$
- Energy threshold $c$
- Precision parameter $\epsilon$

**Problem**: Is $\Theta_G^N$ at most $c$, or at least $c + \epsilon$ ? (promised one of these conditions holds)


QMA
An instance x of a problem in QMA has an efficiently computable verification circuit
$|0\rangle^{\otimes n_a}$
$|\psi\rangle$
$W_{m-1}W_{m-2}\cdots W_0$
Circuit "accepts" $|\psi\rangle$ iff output is 1.
If x is a yes instance there exists $|\psi\rangle$ (a witness) which is accepted with high probability.

# One way to prove QMA-hardness



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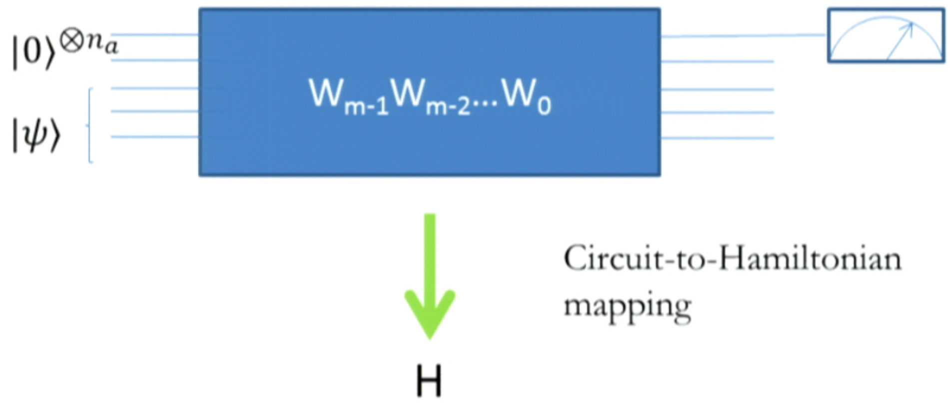


**x is a yes instance:** the ground energy of H is less than $c$.

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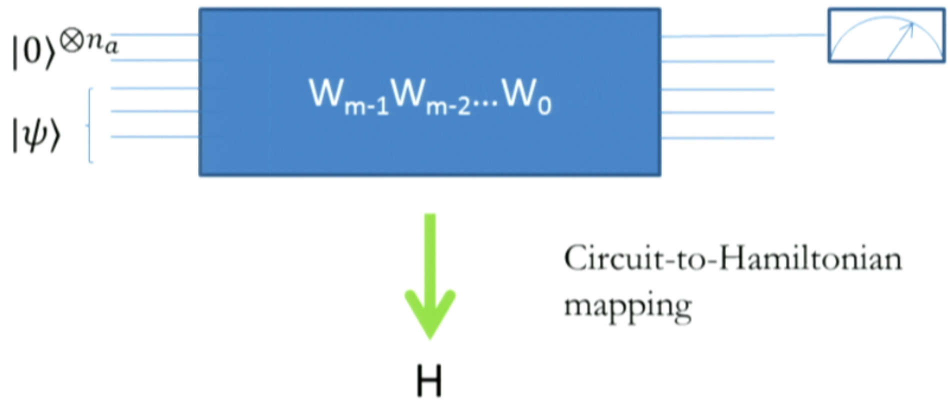


**x is a yes instance:** the ground energy of H is less than $c$.

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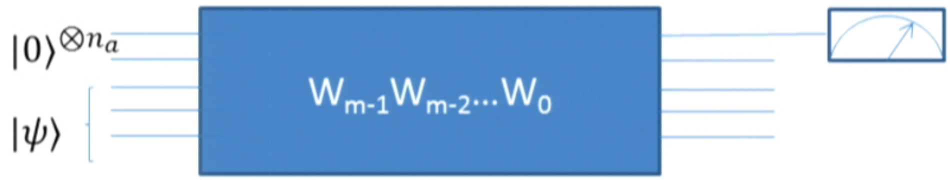
Computing the ground energy of $H$ lets you solve the instance x of the QMA problem.

# Example: Feynman/Kitaev




**Step 1:** A Hamiltonian with ground states which encode the computational history.

$H_1$ has ground states:

$$|\text{Hist}(\phi)\rangle = \frac{1}{\sqrt{m+1}}\left(|\phi\rangle|0\rangle + W_0|\phi\rangle|1\rangle + W_1W_0|\phi\rangle|2\rangle + ... + W_{m-1}W_{m-2}...W_0|\phi\rangle|m\rangle\right)$$

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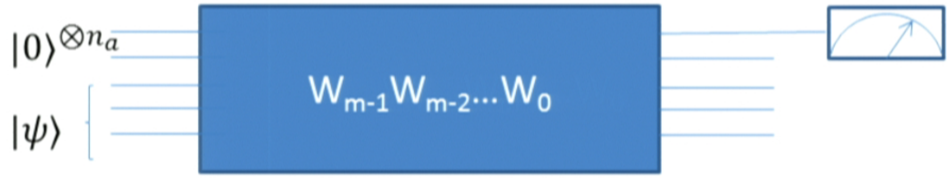


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**Step 2:** Add a term $H_2$ which penalizes states where $|\phi\rangle$ has low acceptance probability or where the ancillas are not initialized correctly.

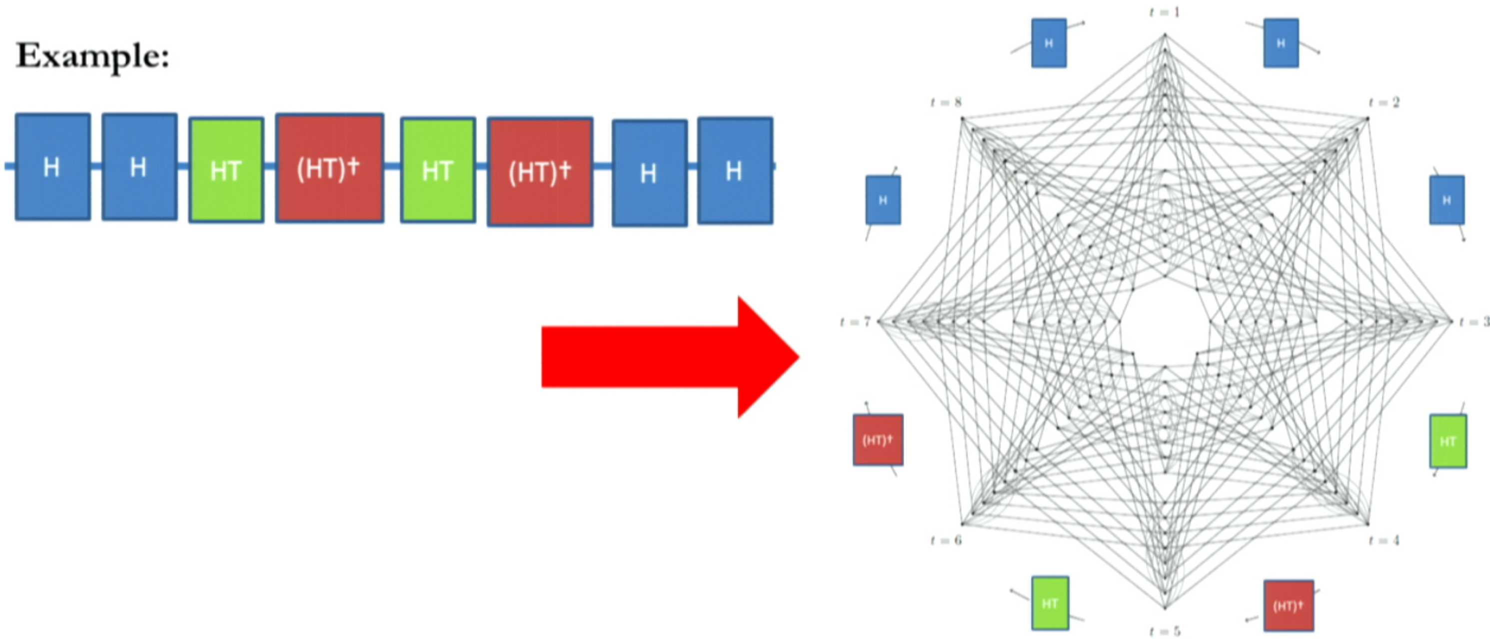
$$H = H_1 + H_2$$

**Challenge:** encode the history of an $n$-qubit, $g$-gate computation in the groundspace of the $n$-particle Bose-Hubbard model on a graph with $poly(n, g)$ vertices.

# Encoding one qubit with one particle ($n = 1$)

We use a variant of the Feynman-Kitaev circuit-to-Hamiltonian mapping where the Hamiltonian is a symmetric 0-1 matrix.

**Example:**



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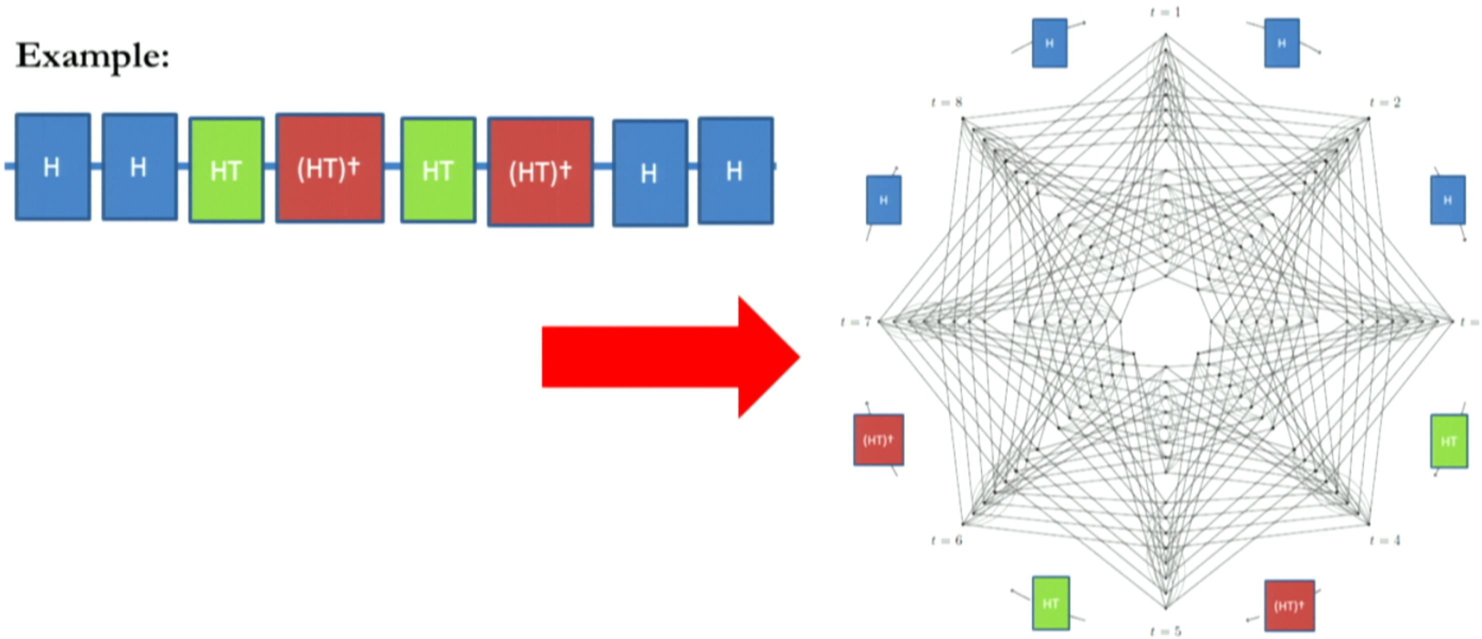


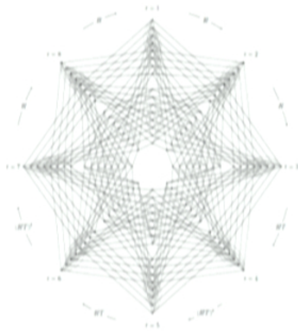
# More particles ($n > 1$)

With more than one particle, the interaction term plays a role.

$$H_G = \sum_{i,j \in V} A(G)_{ij} a_i^\dagger a_j + \sum_{k \in V} n_k(n_k - 1)$$

We use a class of graphs where we can analyze the **frustration-free** $n$-particle ground states.

The graphs we use are built from multiple copies of



# Graphs for two-qubit gates

**Two qubit gate *U***  **A graph shaped like this**


**Single-particle ground states** encode a qubit and one out of four possible locations

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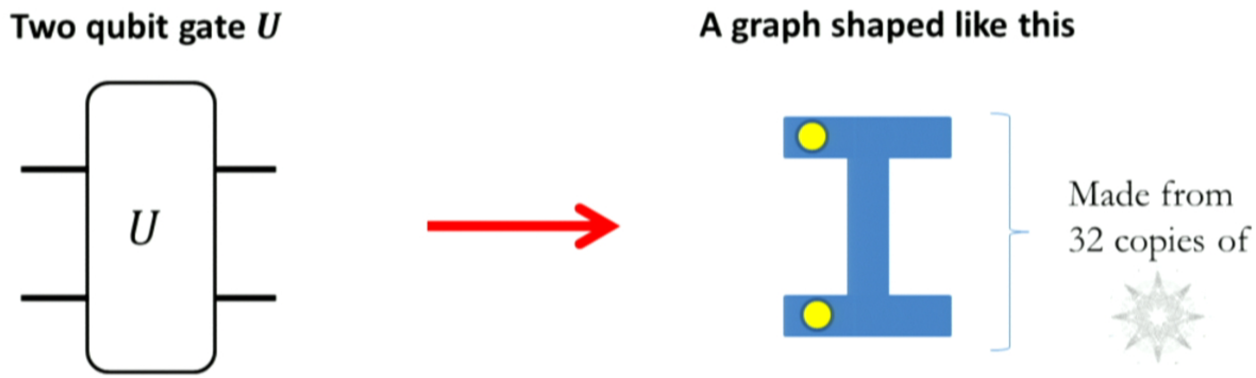
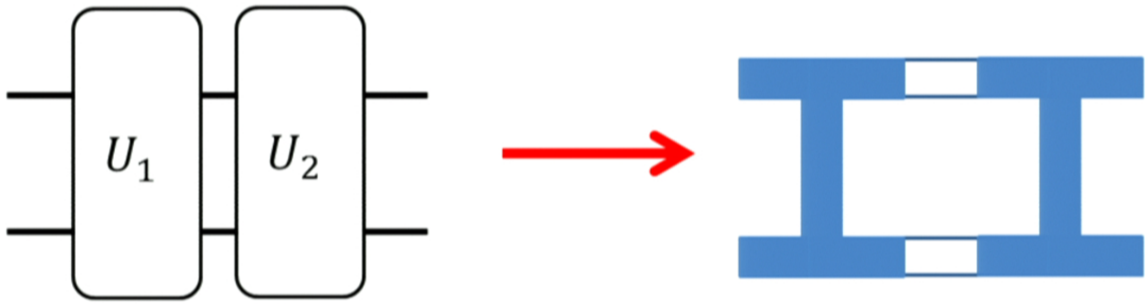



**Single-particle ground states** encode a qubit and one out of four possible locations

**Two-particle frustration-free ground states** have the form

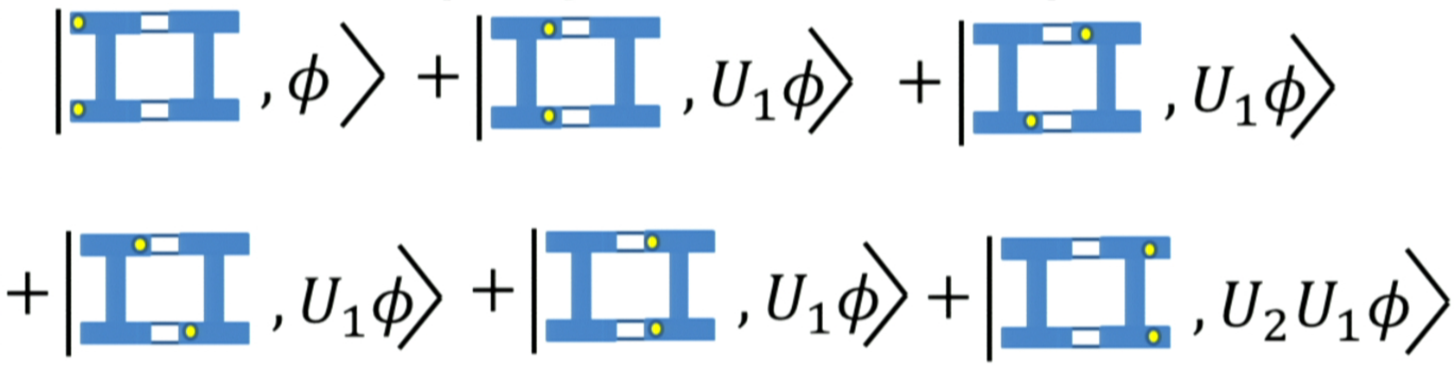
$$\frac{1}{\sqrt{2}}|\text{both particles on the left}, \phi\rangle + \frac{1}{\sqrt{2}}|\text{both particles on the right}, U\phi\rangle$$

# Connecting them together

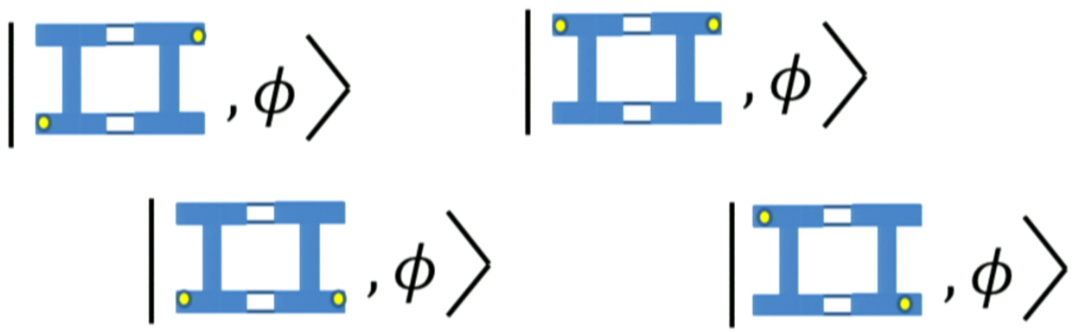



Subgraphs for $U_1$ and $U_2$ are connected (in some way)

**Good news:** there are two-particle ground states which encode computations



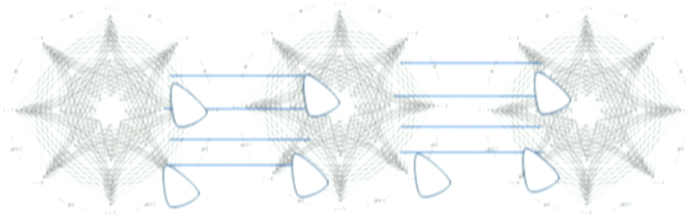
**Bad news:** there are also two-particle ground states which don't encode computations



We develop a general method for enforcing constraints on the locations of particles.
We use this "Occupancy Constraints Lemma" to get rid of the bad states.

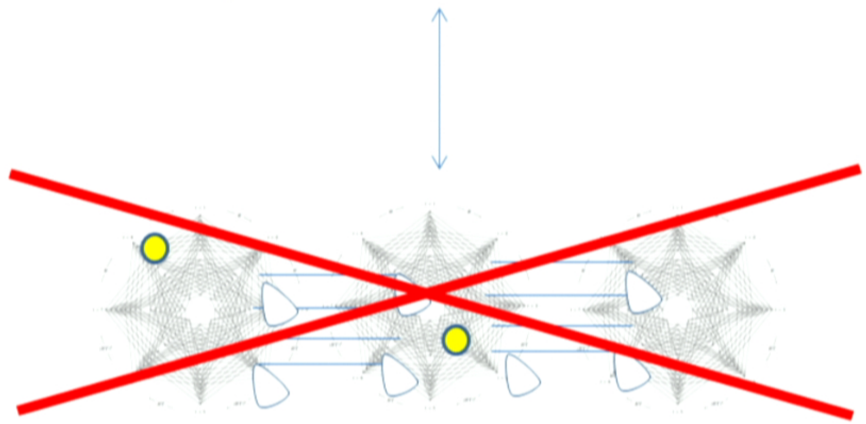
# Occupancy Constraints Lemma

**Graph $G$ (from the class we consider)**



**Occupancy constraints graph $G_{occ}$**

Each edge indicates two copies of the basic subgraph that we don't want simultaneously occupied.



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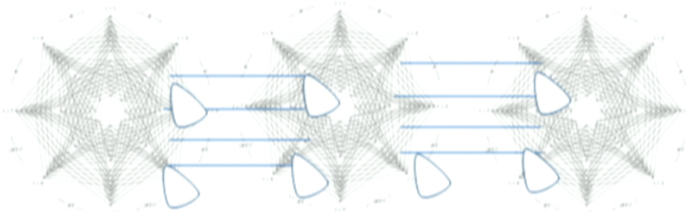

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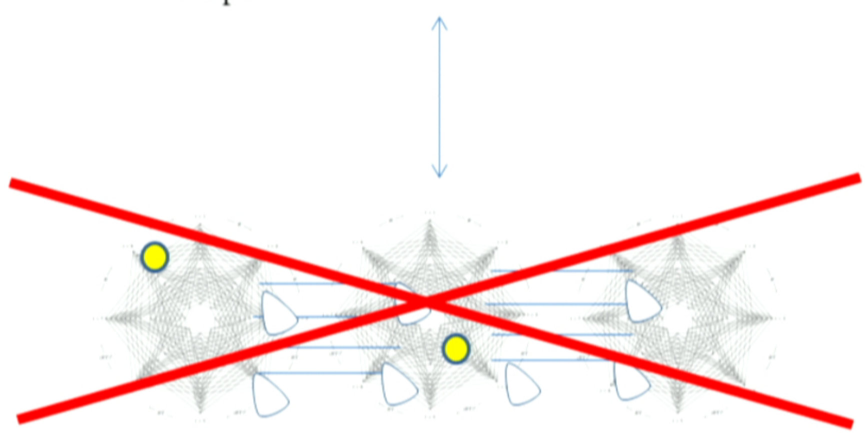
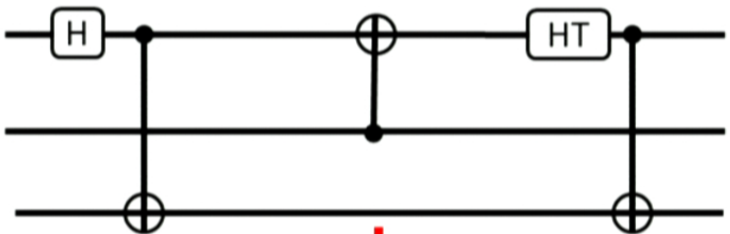
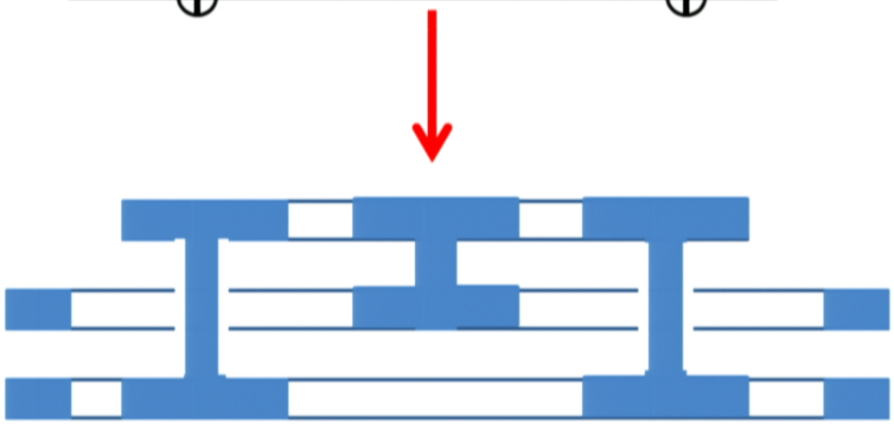


# Overview of our strategy




$n$ qubits, $g$ gates



$O(g + n)$ vertices

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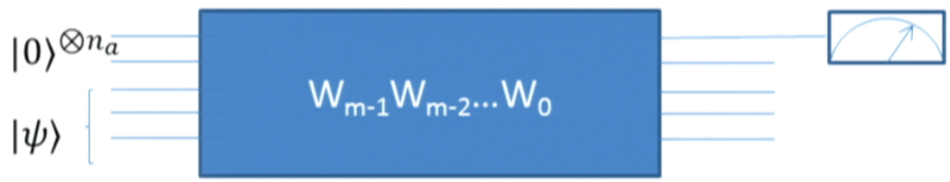


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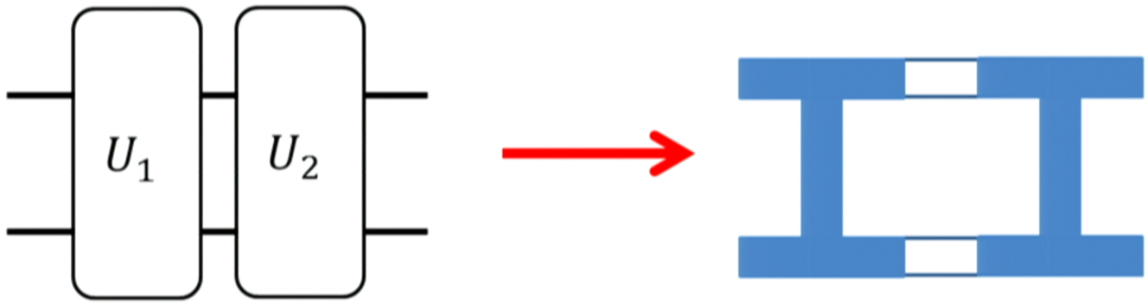


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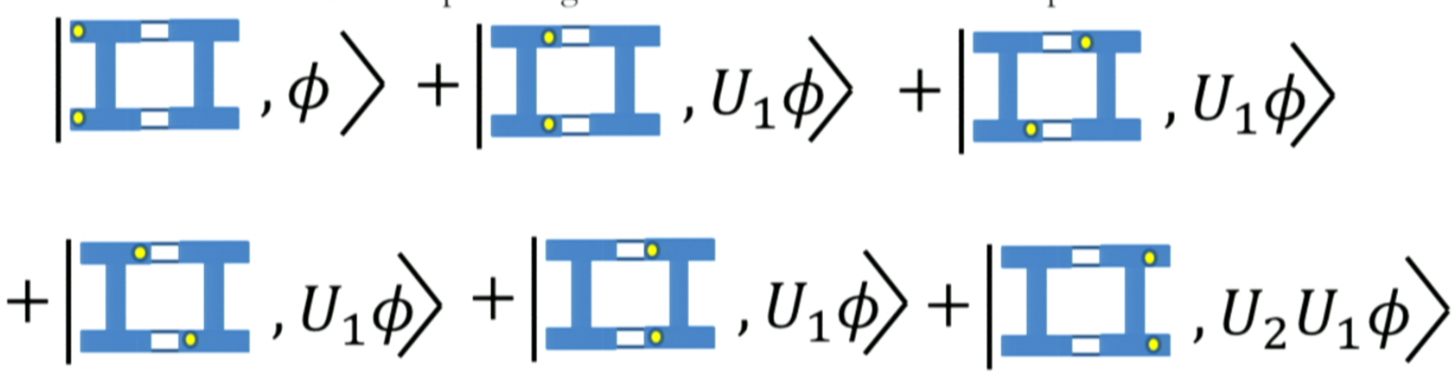

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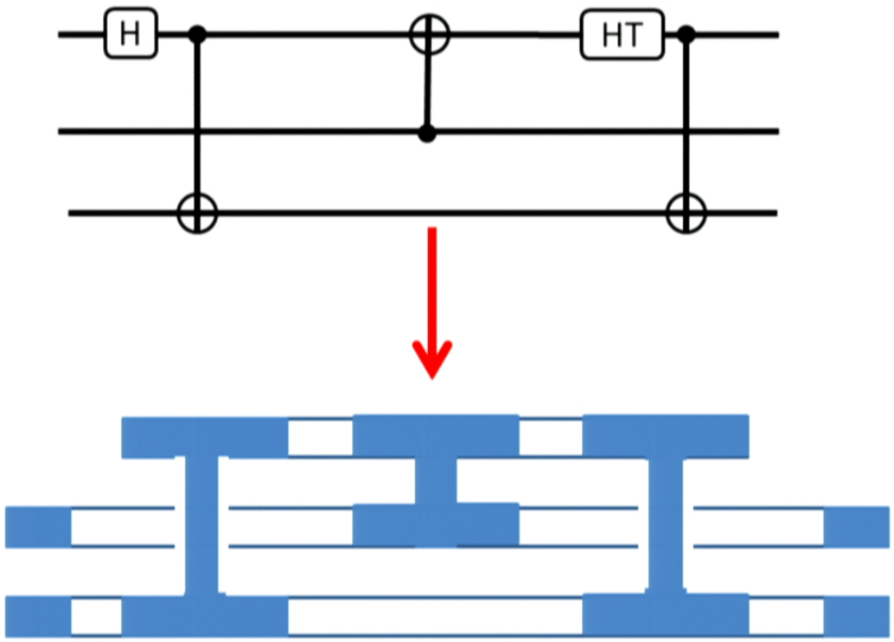


$n$ qubits, $g$ gates

$O(g+n)$ vertices

Some $n$-particle ground states encode computations, others don't.

# Open questions

- What is the complexity of the Bose-Hubbard model on **simple** graphs (i.e., no self-loops)?
- XY model on a (simple) graph?
- Can we remove restriction to fixed particle number?
- Other models of indistinguishable particles
  - bosons or fermions with nearest-neighbor interactions
  - Attractive interactions
  - Negative hopping strength
- Other spin models defined by graphs, e.g., the antiferromagnetic Heisenberg model?