The Bose-Hubbard model is QMA-complete

Andrew M. Childs
David Gosset
Zak Webb

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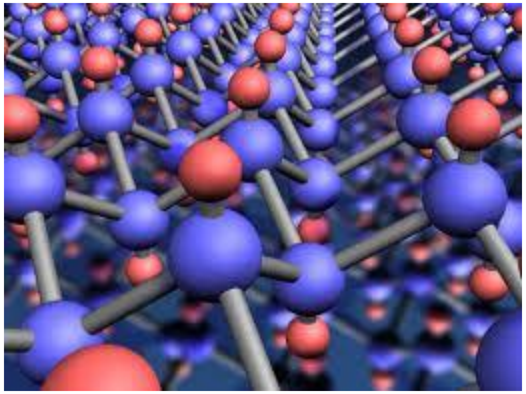

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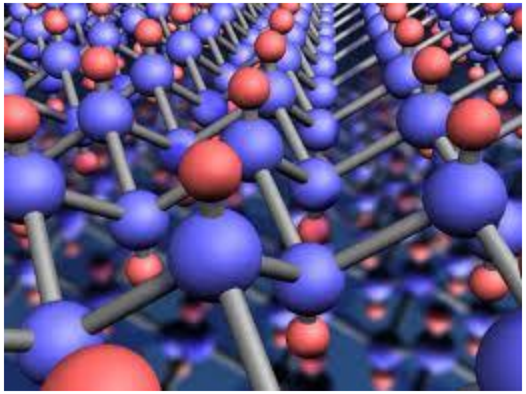

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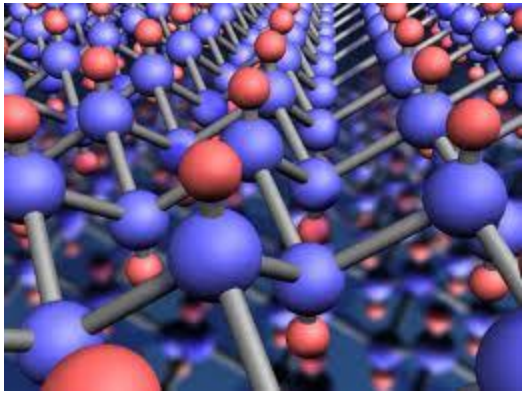

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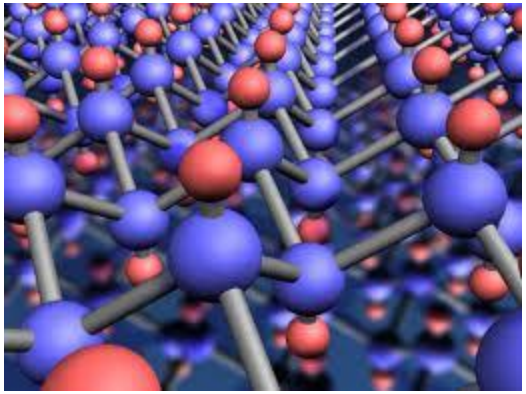

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This talk is about the computational difficulty of computing the ground energy.

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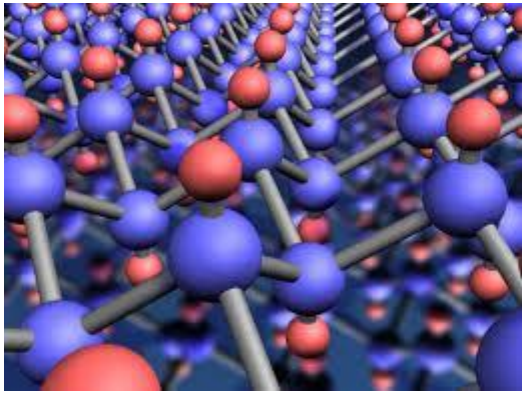

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This talk is about the computational difficulty of computing the ground energy.

To assess computational difficulty, we use complexity theory…

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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.

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The computational difficulty of computing the ground energy has been studied for many types of Hamiltonians…

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

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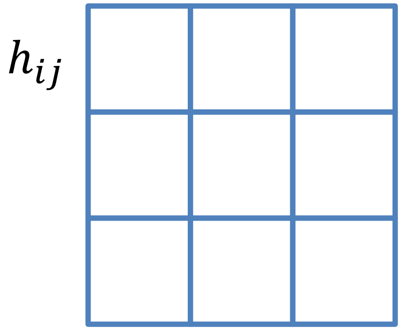
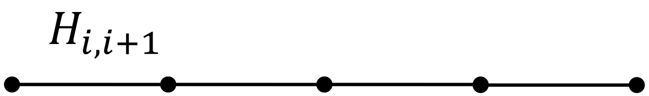
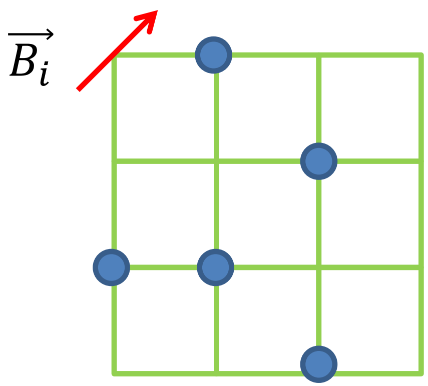
Even very simple systems have QMA-complete ground energy problems…



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



2-local Hamiltonian on a line with qudits
[Aharonov et. al 2009] [Gottesman Irani 2009]



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.,

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

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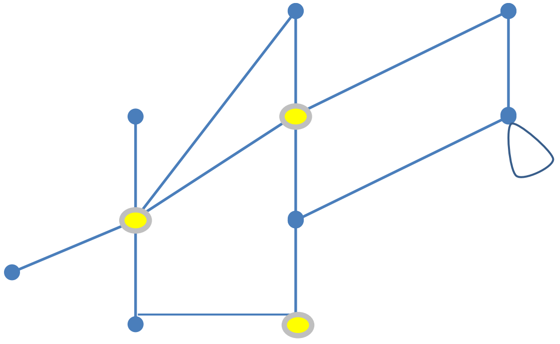
- The complexity of many simple models from condensed matter physics remains unknown.

- 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.



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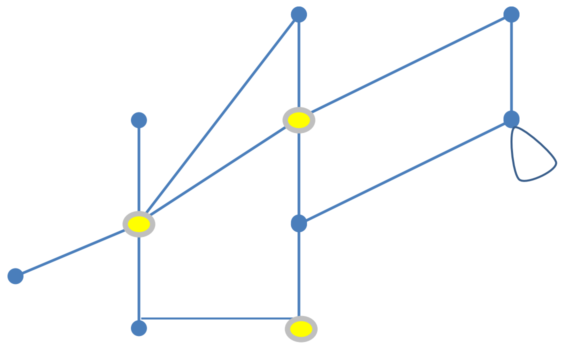

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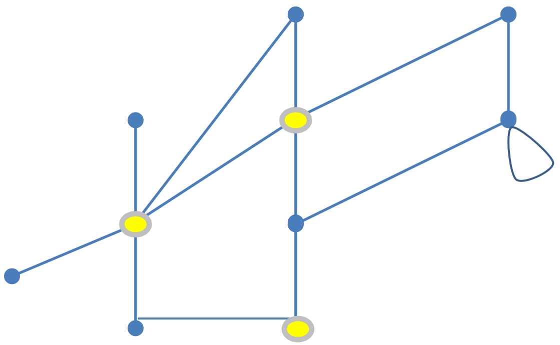

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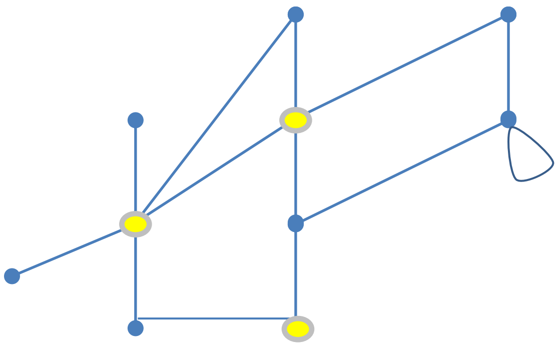

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We don't use perturbation theory in our analysis.

Our result holds for any repulsive interaction strength.

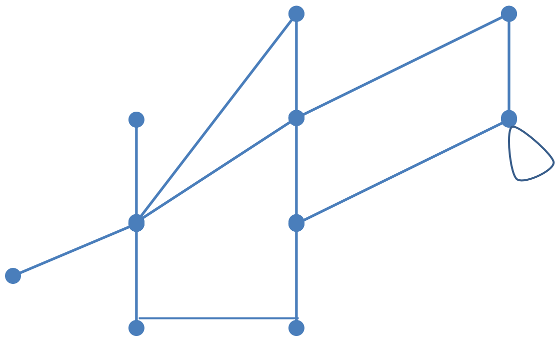
Overview of results

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.



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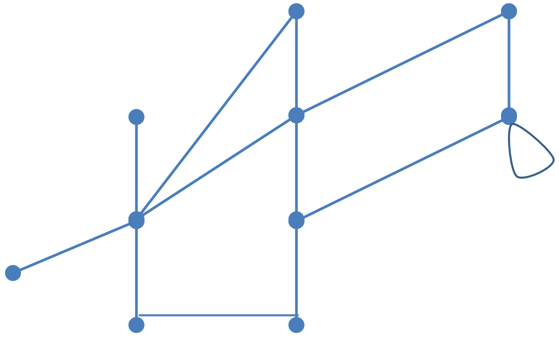

Hamiltonian

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

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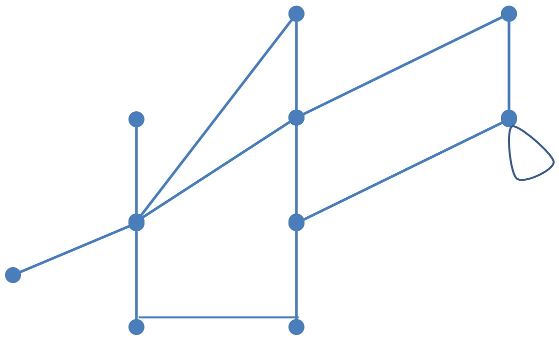

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Movement — On-site interaction

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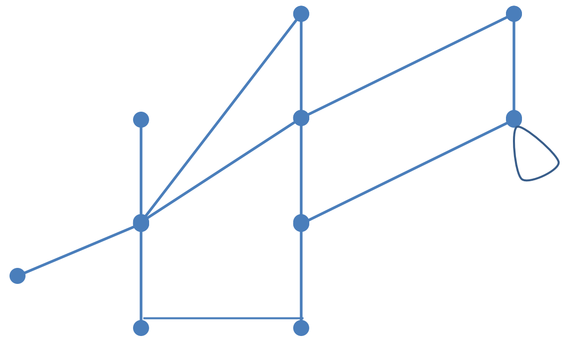

Hamiltonian

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

Write $\overline{H}_G^N$ for the Hamiltonian within the N-particle sector.

Bose-Hubbard Hamiltonian problem

Input:
- Graph G
- Number of particles N
- Energy threshold c
- Precision parameter ϵ

Problem: Is the ground energy of $\overline{H}_G^N$ at most c, or at least $c + \epsilon$?
(promised that one of these conditions holds)

Our main result: Bose-Hubbard Hamiltonian is QMA-complete

Other choices

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

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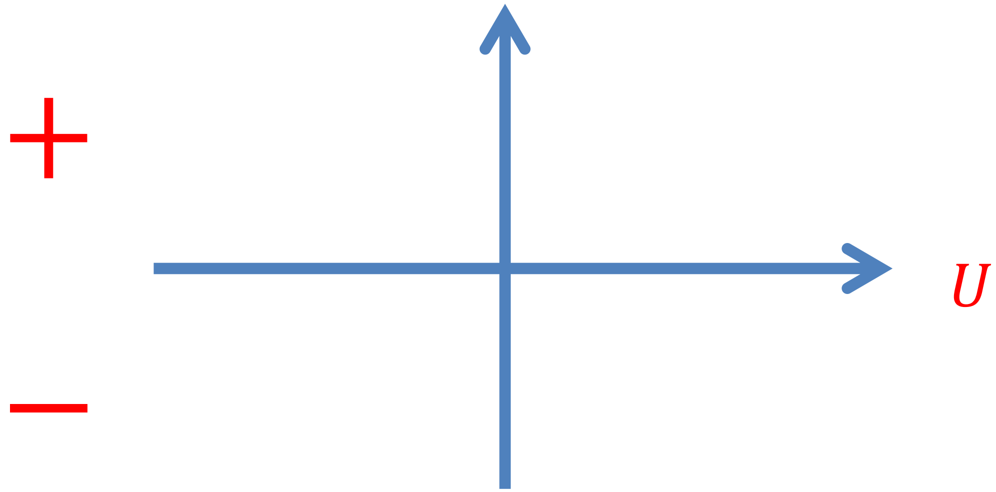

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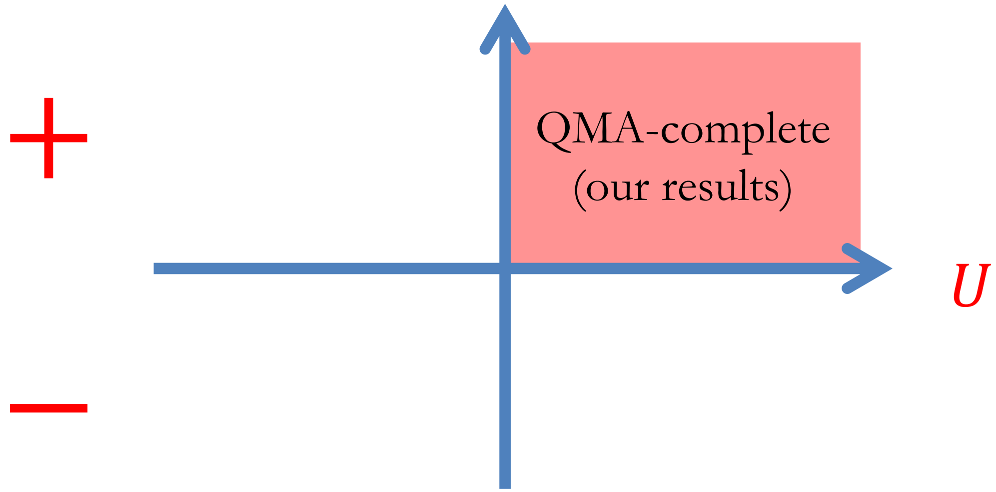

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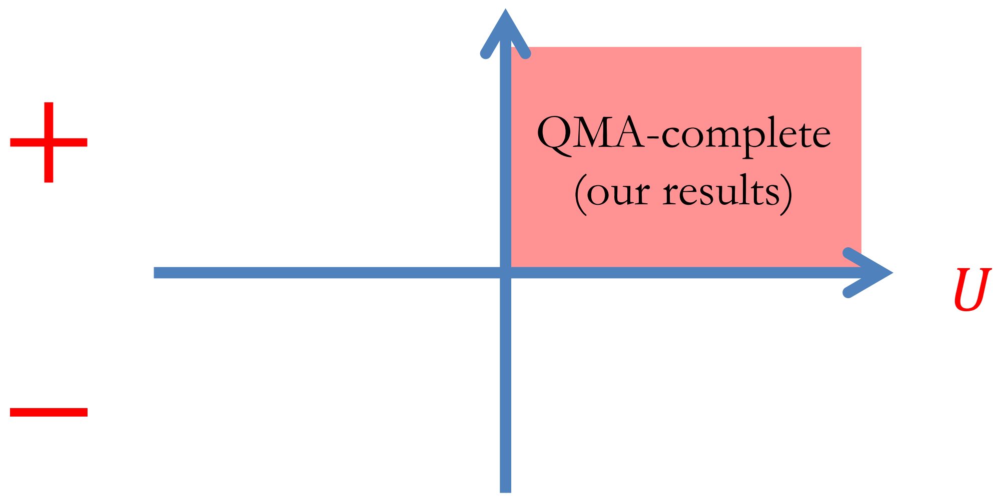

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No sign problem for quantum Monte Carlo

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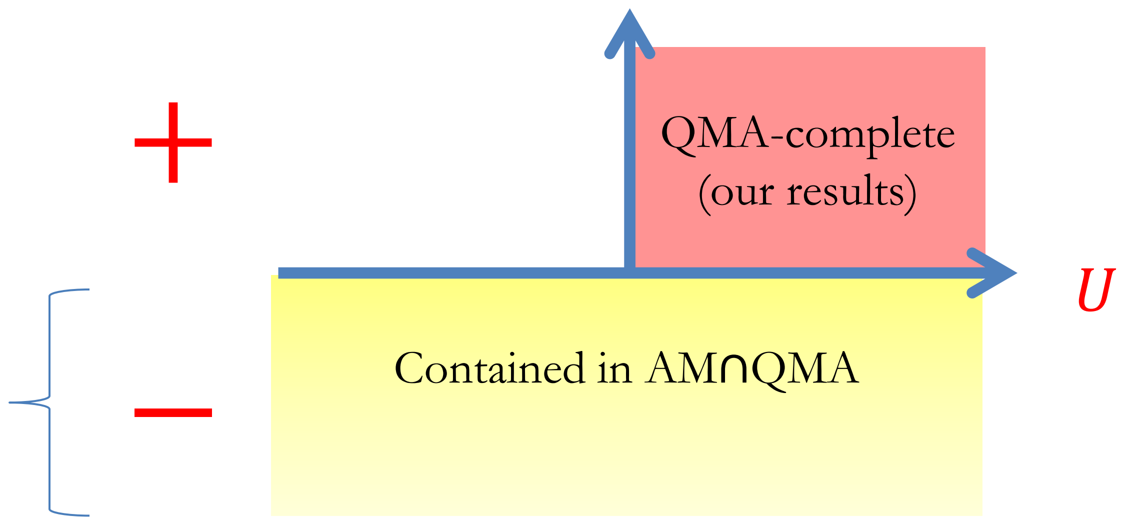

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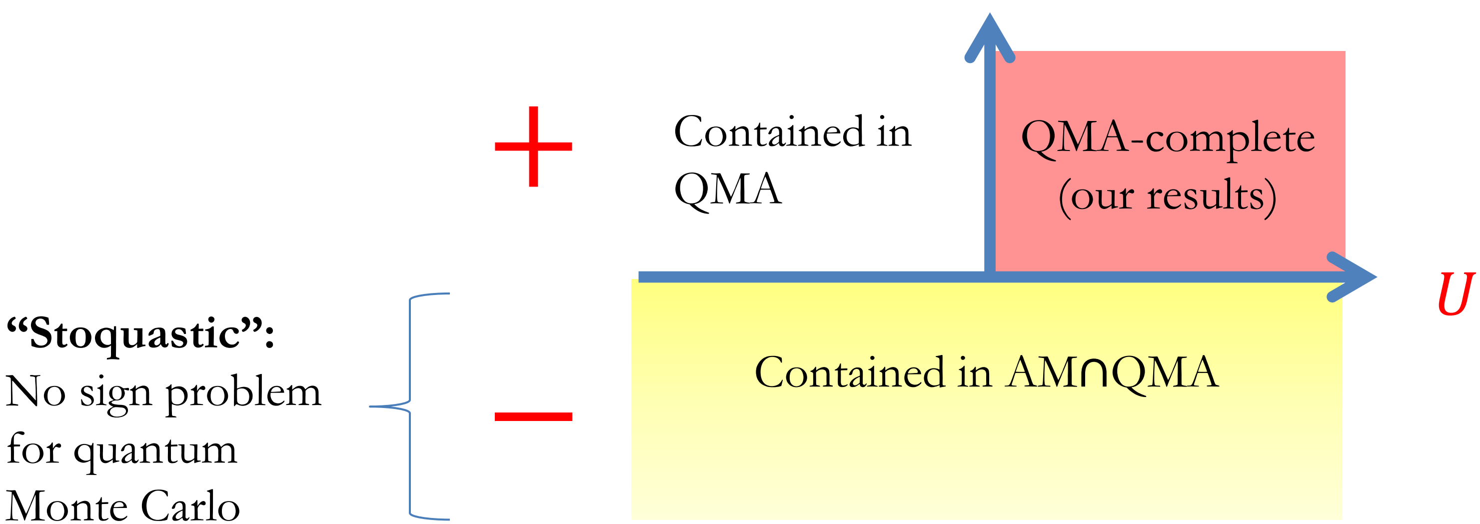

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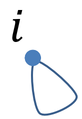
When $U \to \infty$ the Hamiltonian is equivalent to a spin model…

A related spin model

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

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



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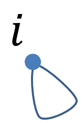

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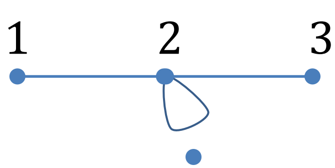
Example



→ $|01\rangle\langle 10|_{12} + |10\rangle\langle 01|_{12} + |01\rangle\langle 10|_{23} + |10\rangle\langle 01|_{23} + |1\rangle\langle 1|_2$

A related spin model

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

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

Conserves total magnetization (Hamming weight)

Write Θ_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 ϵ

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

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We prove XY Hamiltonian is QMA-complete.

Overview of results

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

Our strategy for the Bose-Hubbard model

How can one prove QMA-completeness for these types of problems?

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A generic ground energy problem

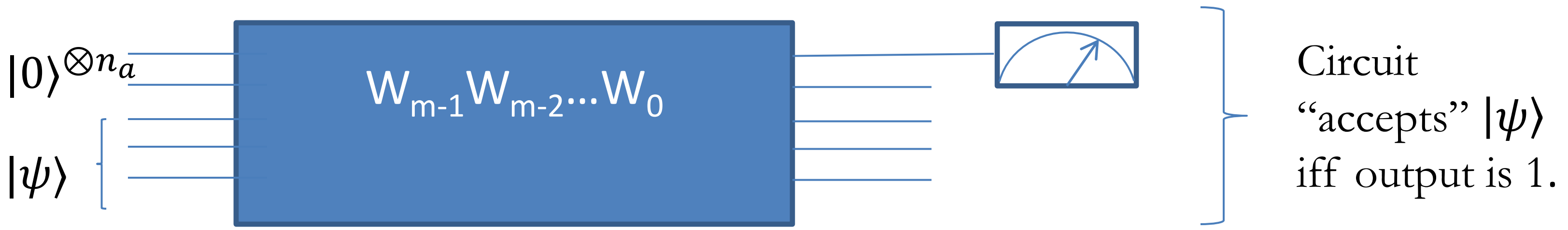
Input:

- A Hamiltonian H from some allowed set
- Energy threshold c
- Precision parameter ϵ

Problem: Is the ground energy of H at most c, or at least $c + \epsilon$?
(promised that one of these conditions holds)

QMA

An instance x of a problem in QMA has an efficiently computable verification circuit



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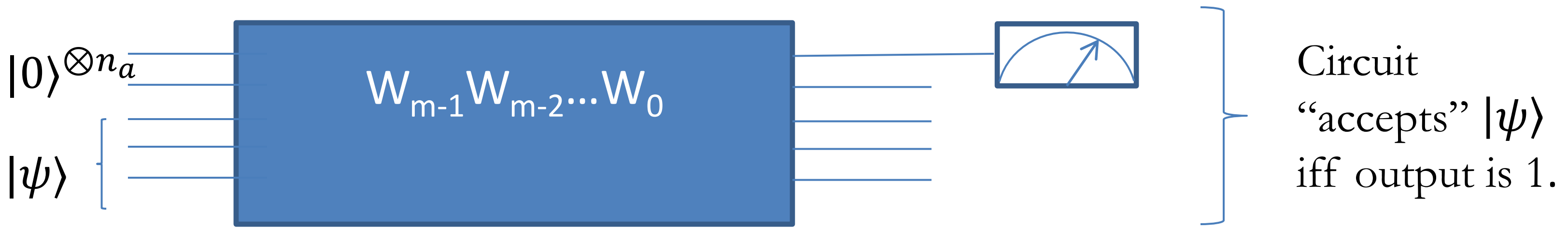

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QMA

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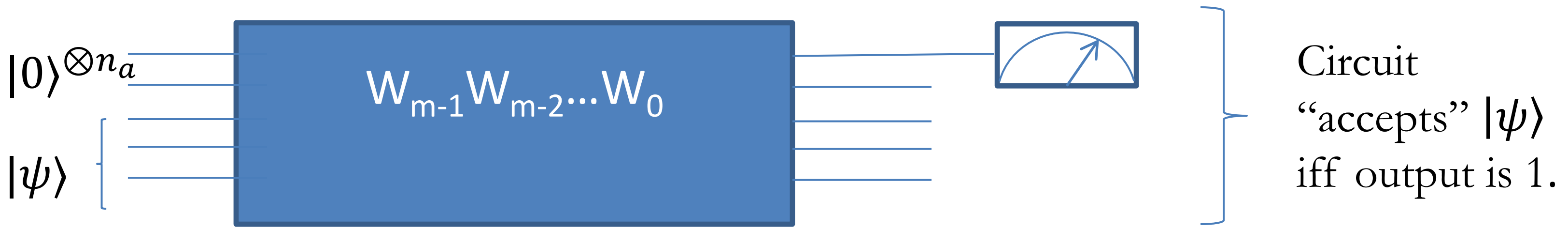

If x is a yes instance there exists $|\psi\rangle$ (a witness) which is accepted with high probability.

If x is a no instance every state has low acceptance probability.

Ground energy problems are usually contained in QMA.

The witness is the ground state and the verification circuit is a measurement of the energy.

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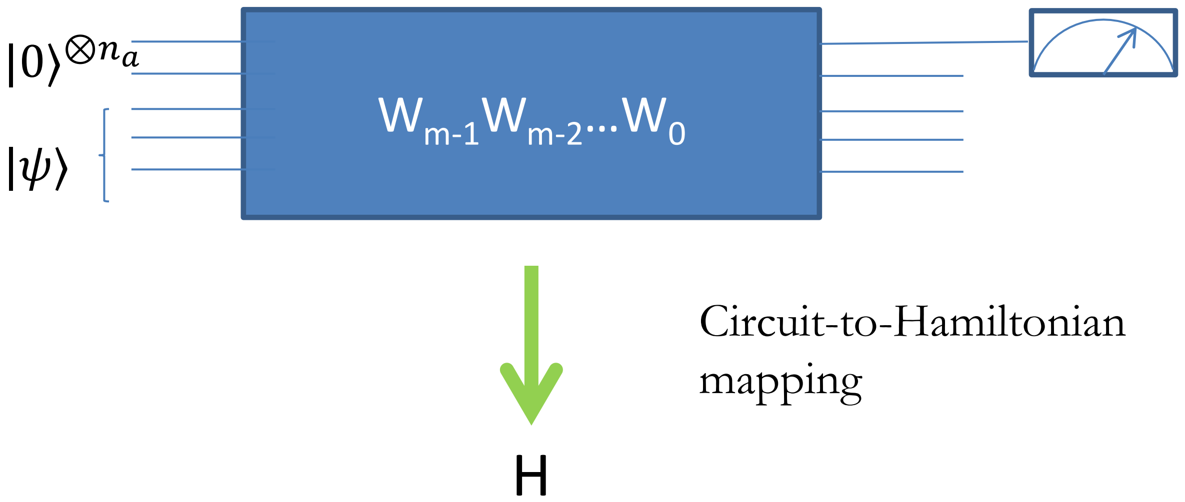
The witness is the ground state and the verification circuit is a measurement of the energy.

To prove QMA-completeness one must also show the problem is QMA-hard.
i.e., an instance of any problem in QMA can be efficiently mapped into an instance of the ground energy problem.

One way to prove QMA-hardness



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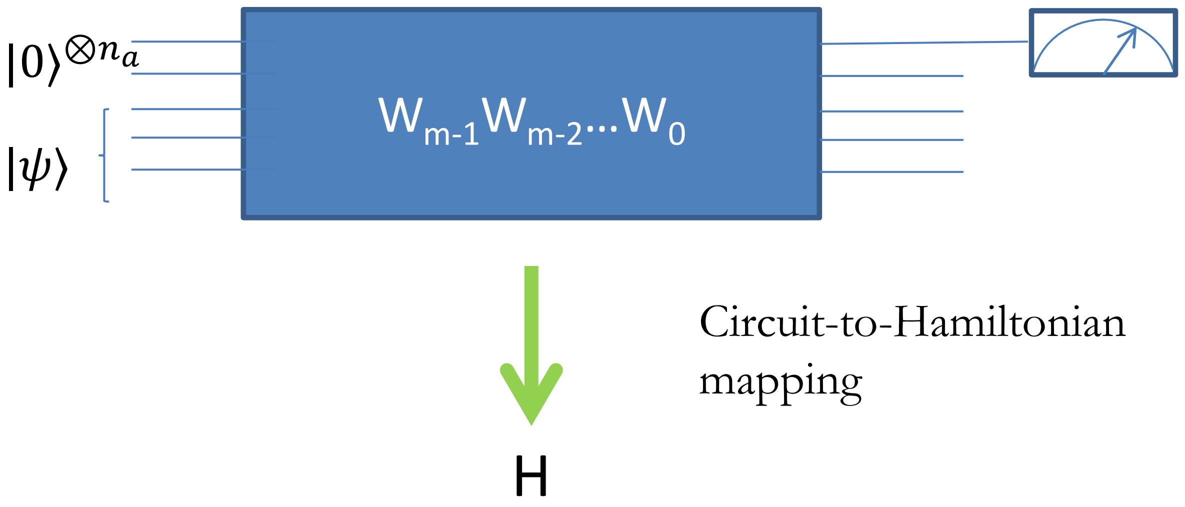

Circuit-to-Hamiltonian mapping

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

x is a no instance: the ground energy of H is greater than $c + \epsilon$.

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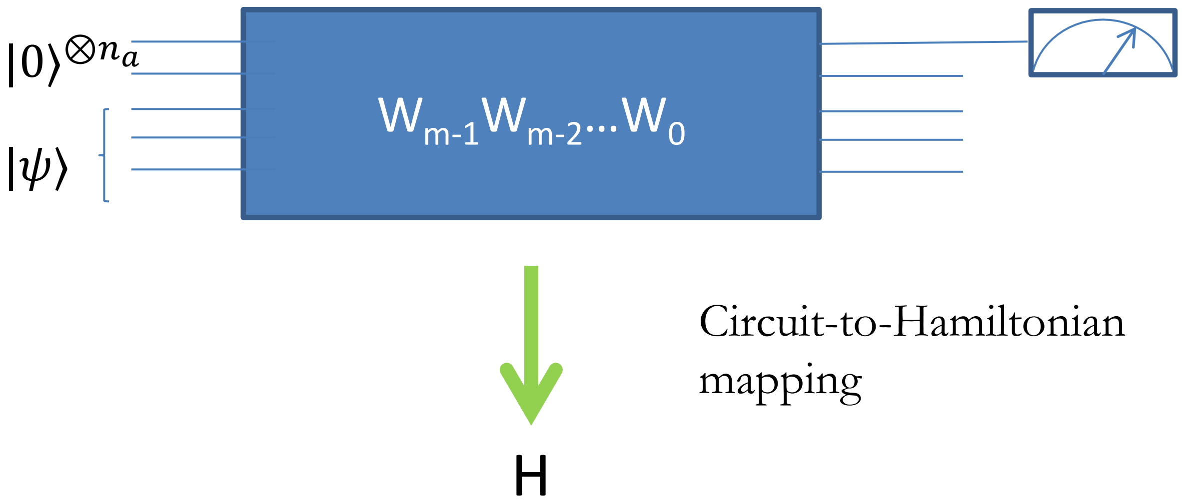

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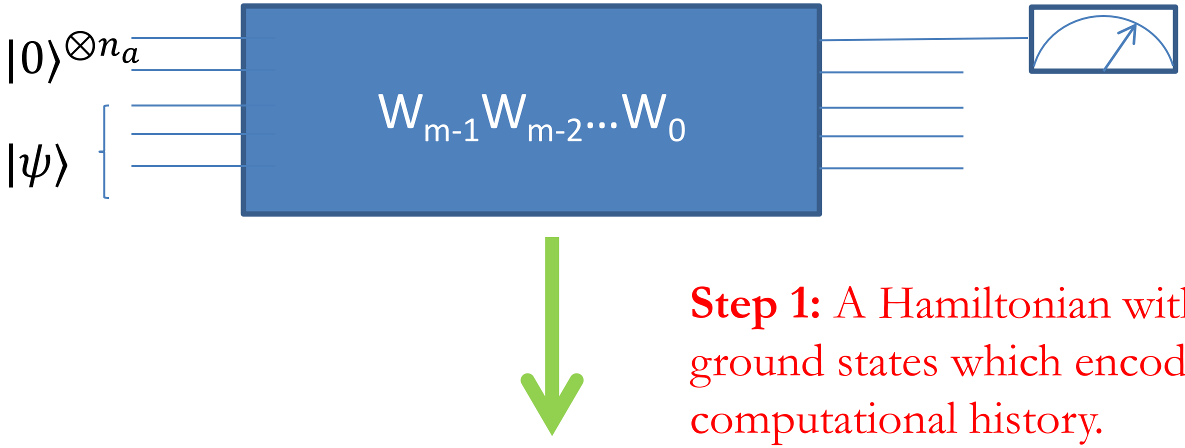
Computing the ground energy of H lets you solve the instance x of the QMA problem.

Example: Feynman/Kitaev



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

H_1 has ground states:

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

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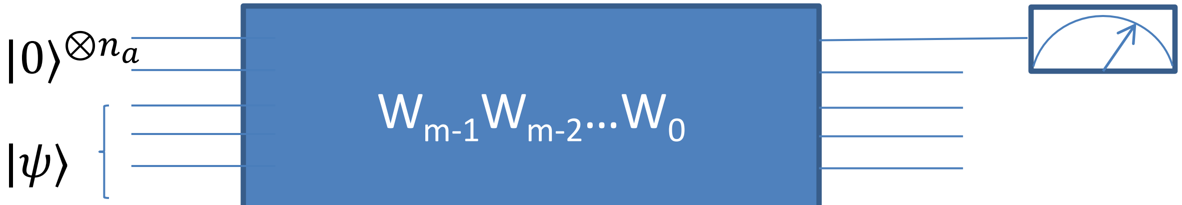

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Step 2: Add a term H_2 which penalizes states where $|\phi\rangle$ has low acceptance probability or where the ancillas are not initialized correctly.

$$H = H_1 + H_2$$

Overview of results

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

Our strategy for the Bose-Hubbard model

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.

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When $n = 1$ the Hamiltonian is just the adjacency matrix of the graph…

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.

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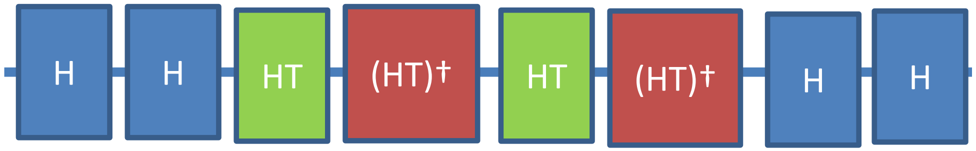

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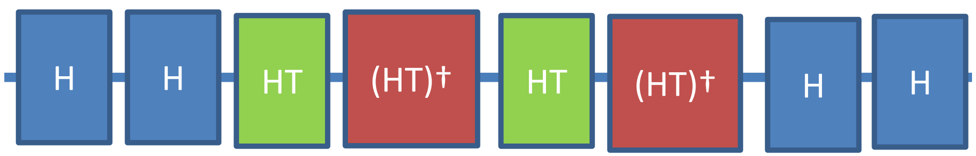

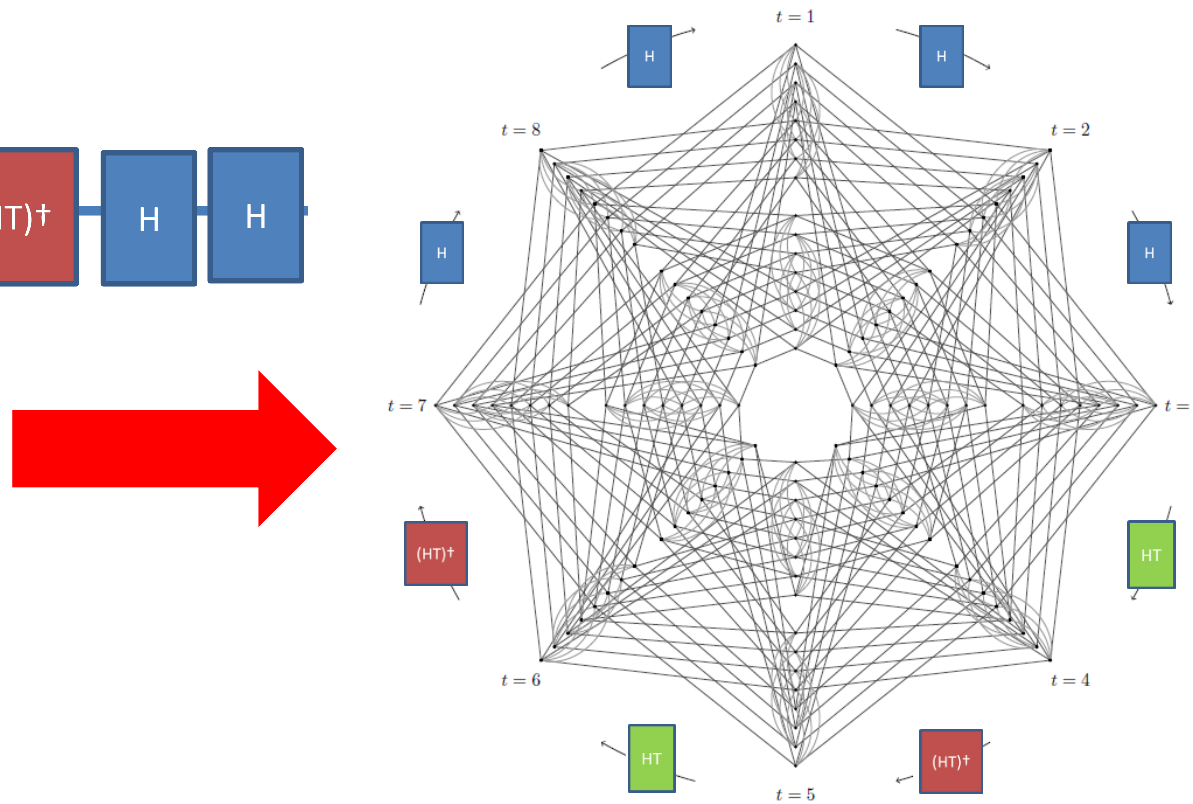

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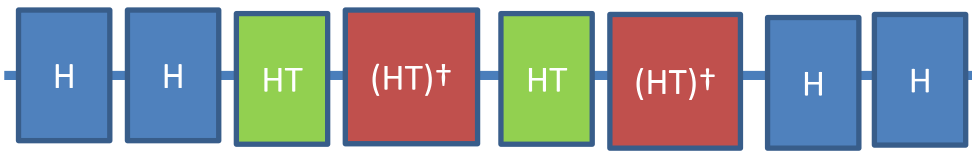

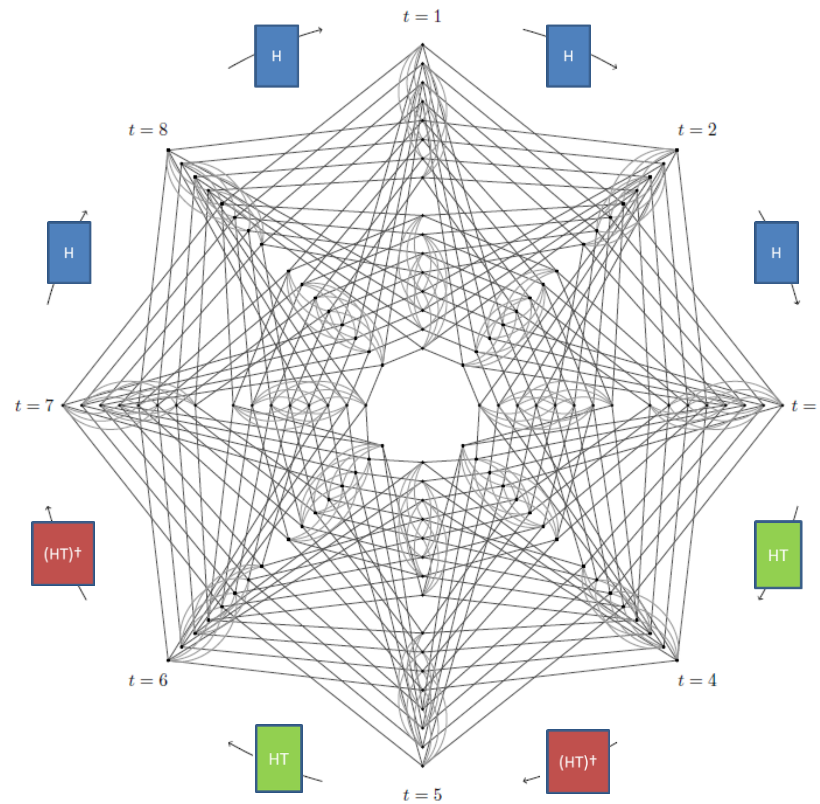

Groundstates of the adjacency matrix:

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

a specific state

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

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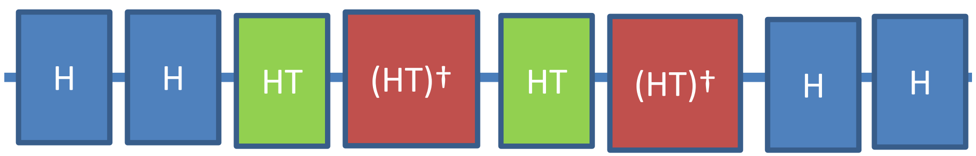

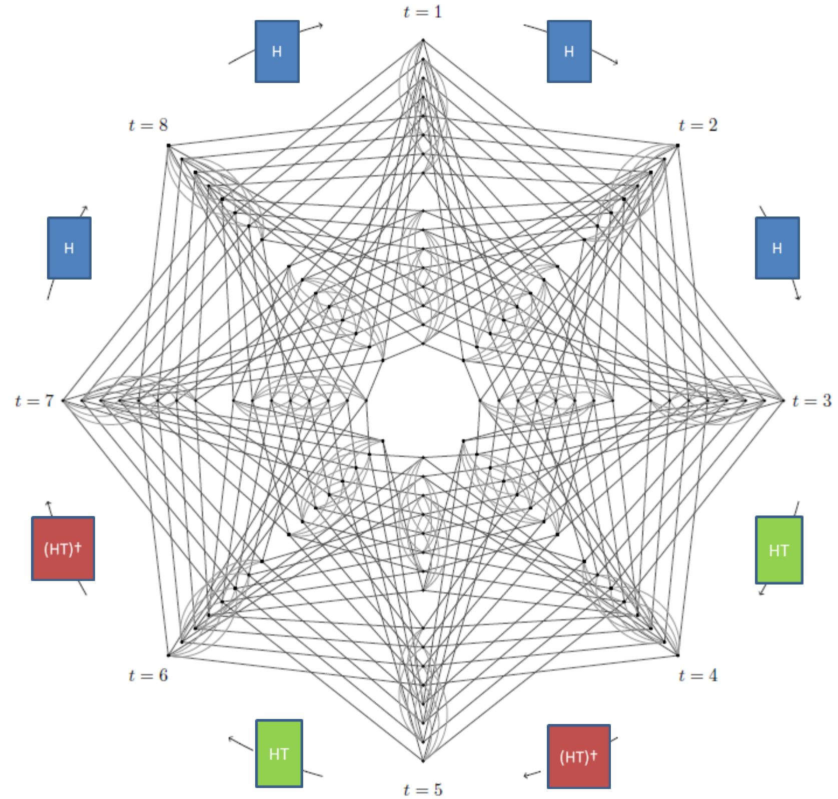

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encodes the computation where the circuit is complex-conjugated

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.

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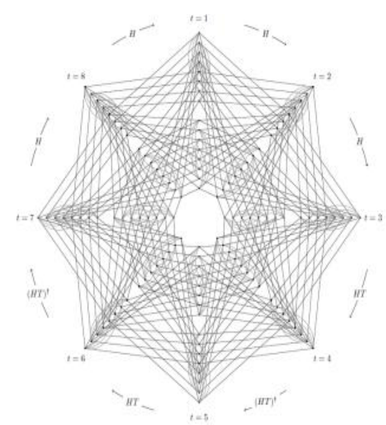
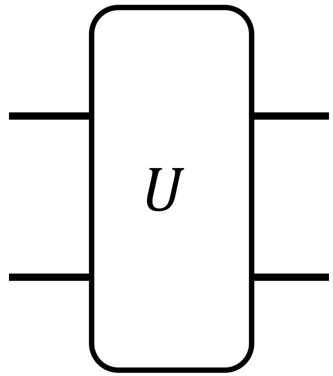
The graphs we use are built from multiple copies of

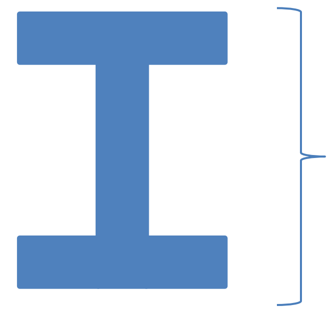


Graphs for two-qubit gates

Two qubit gate U



A graph shaped like this



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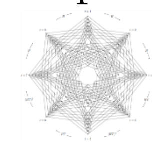

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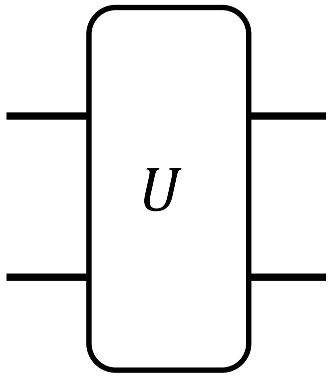

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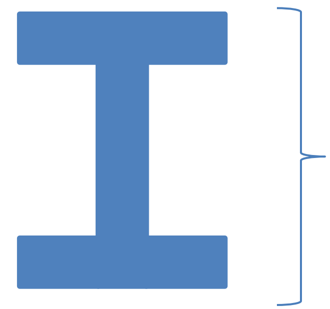

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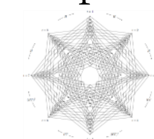

Single-particle ground states encode a qubit and one out of four possible locations

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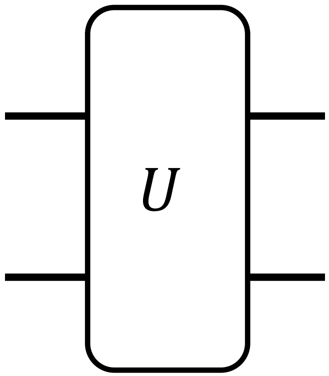

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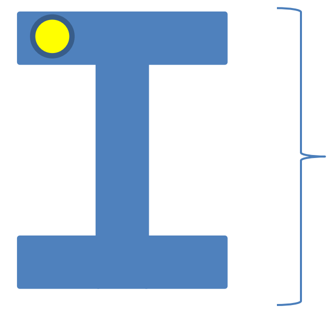

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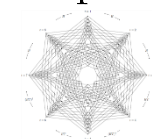

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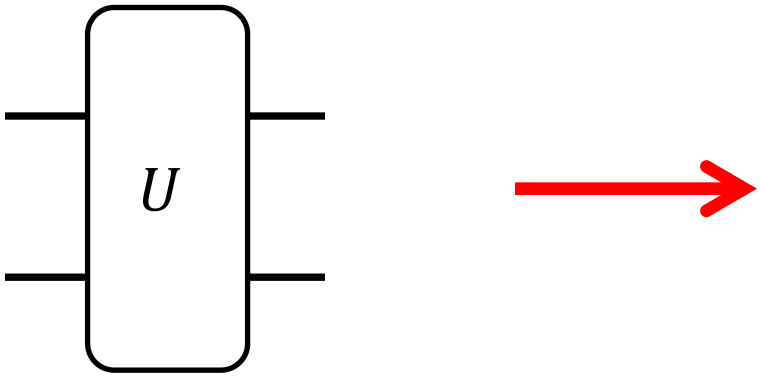

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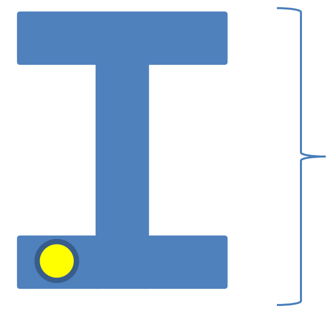

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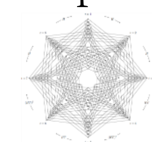

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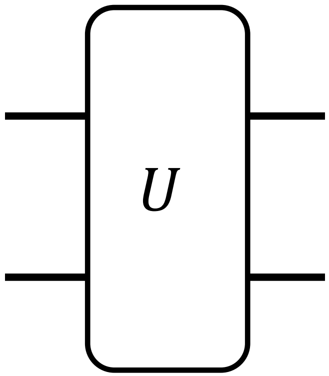

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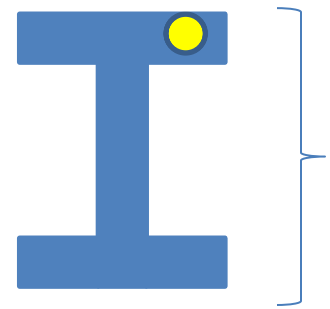

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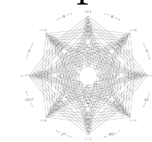

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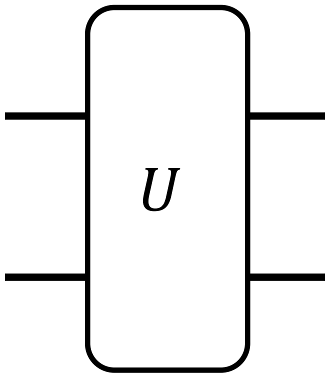

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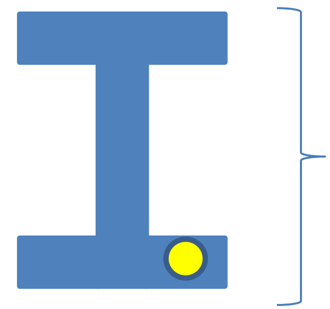

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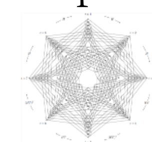

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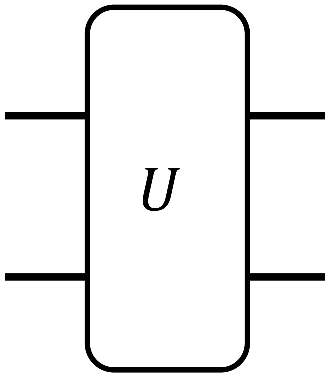

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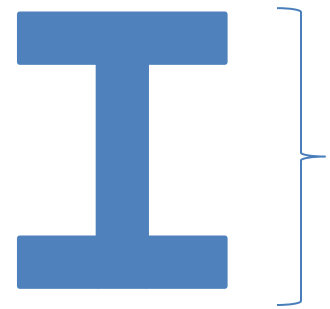

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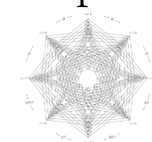

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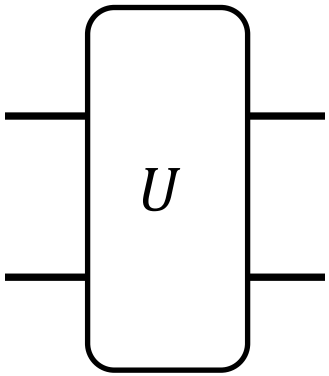

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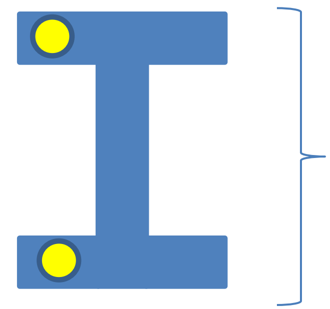

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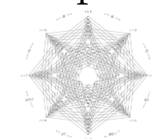

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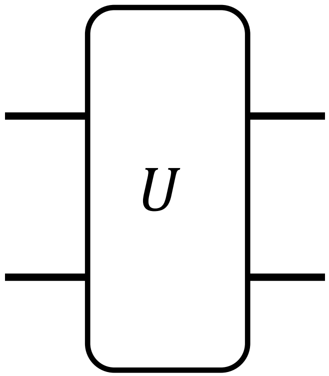

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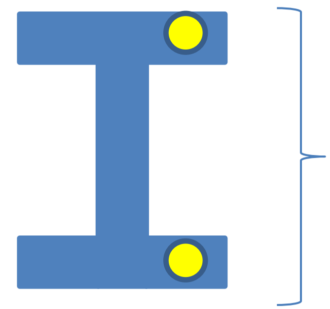

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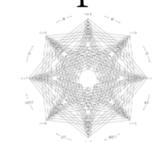

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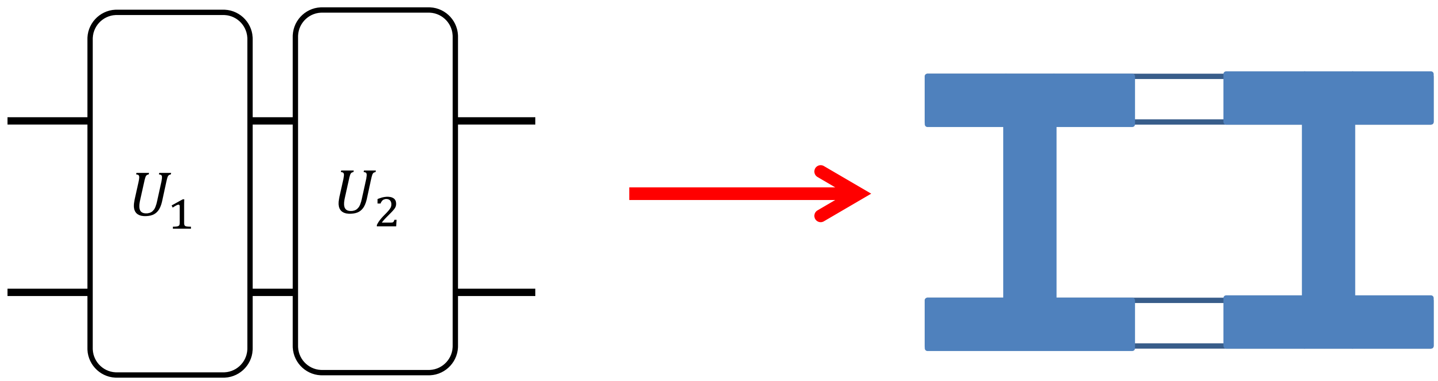

Subgraphs for U_1 and U_2 are connected (in some way)

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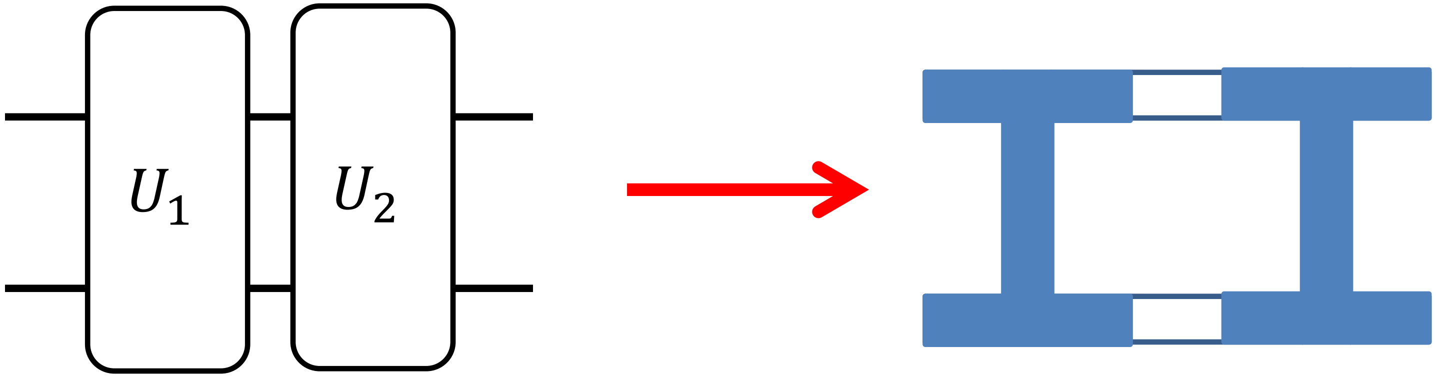

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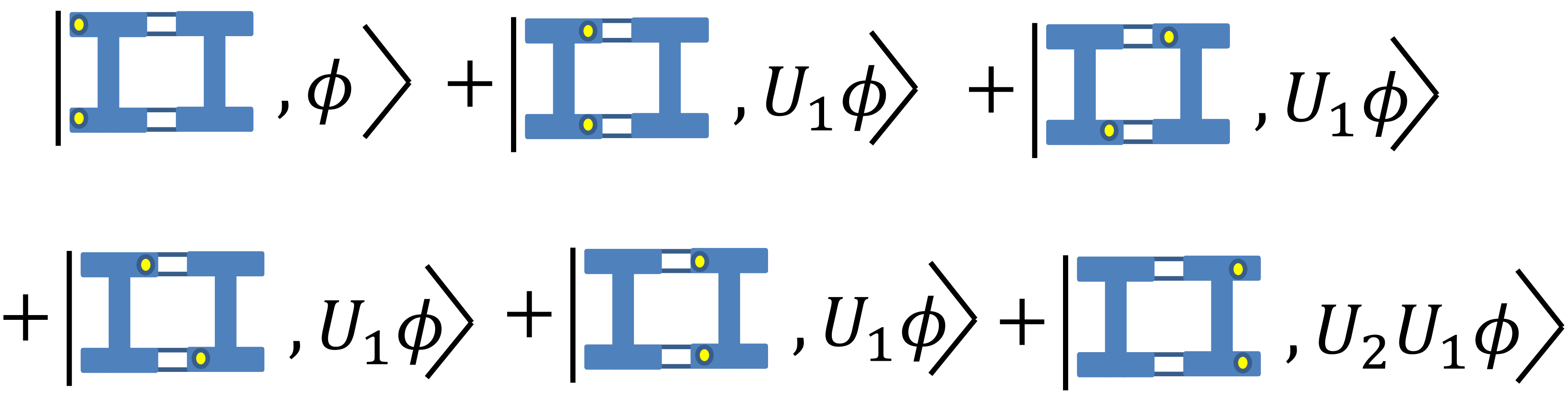
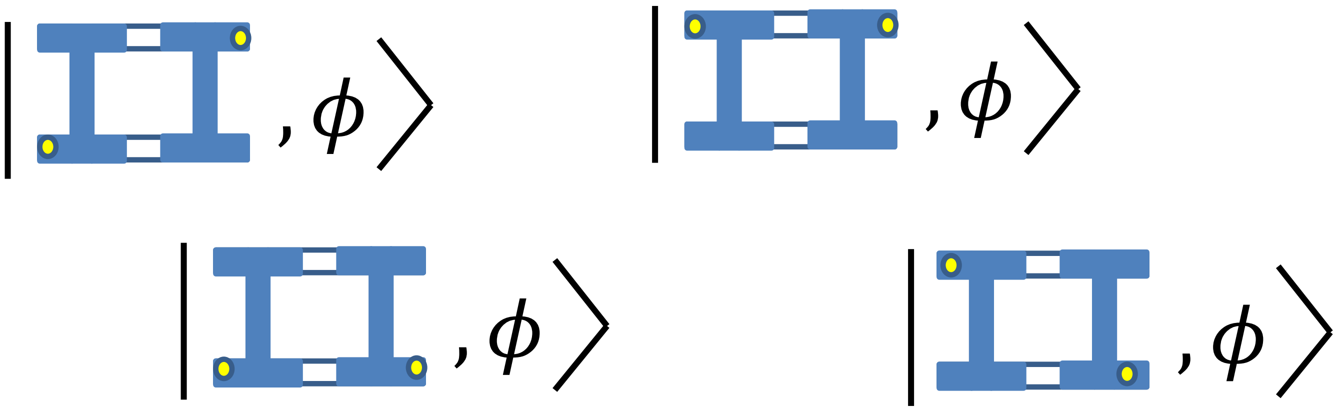
Good news: there are two-particle ground states which encode computations



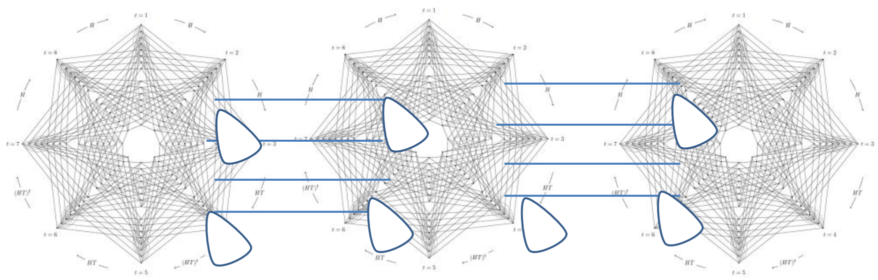
Bad news: there are also two-particle ground states which don't encode computations



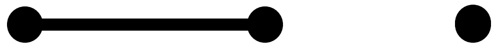
We develop a general method for enforcing constraints on the locations of particles.
We use this "Occupancy Constraints Lemma" to get rid of the bad states.

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.

Occupancy Constraints Lemma

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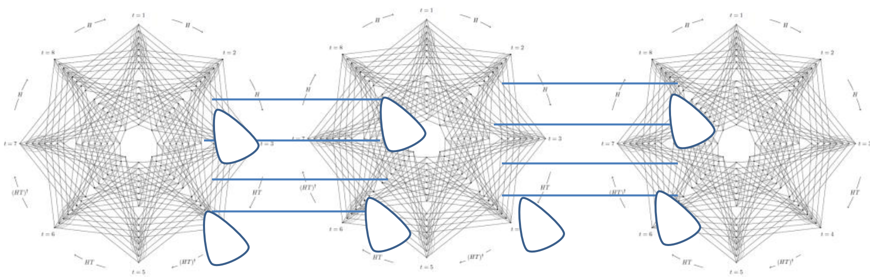

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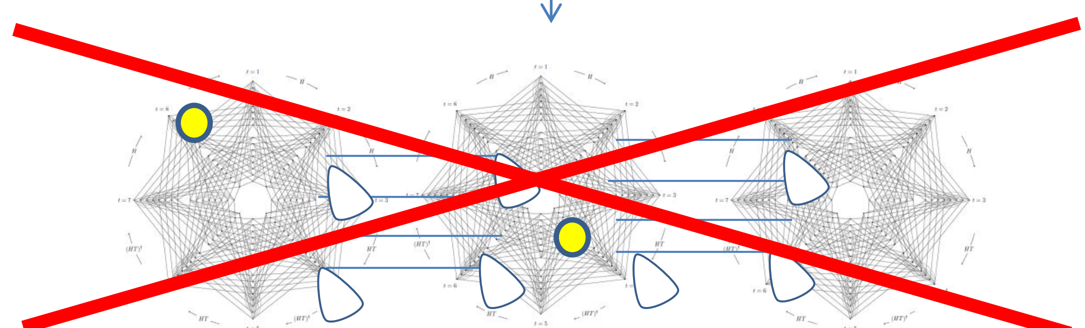

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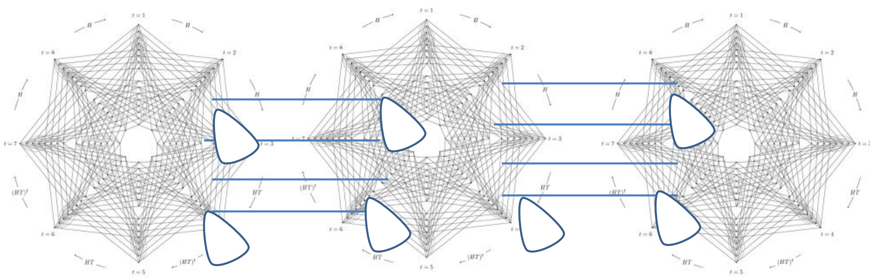

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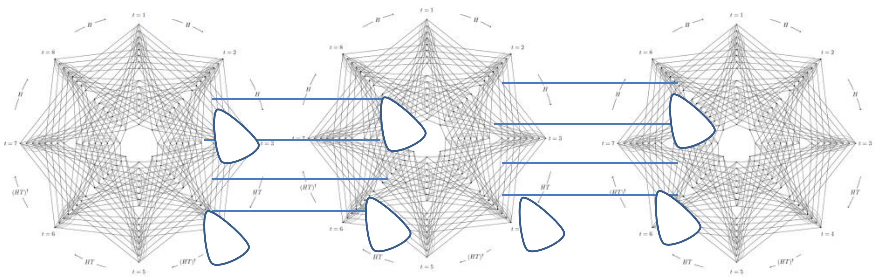

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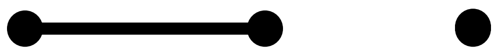

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Good states: The frustration-free states of G which live in the subspace where the occupancy constraints are satisfied.

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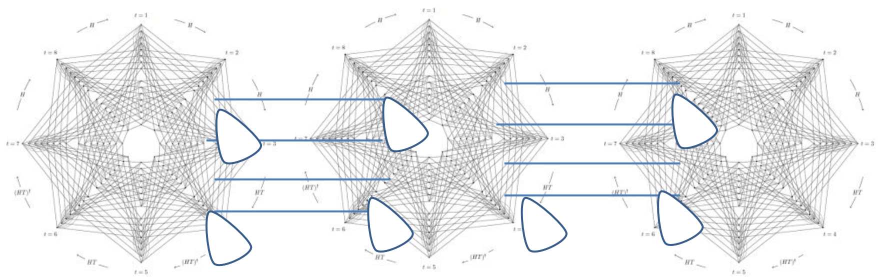


Occupancy constraints graph G_{occ}

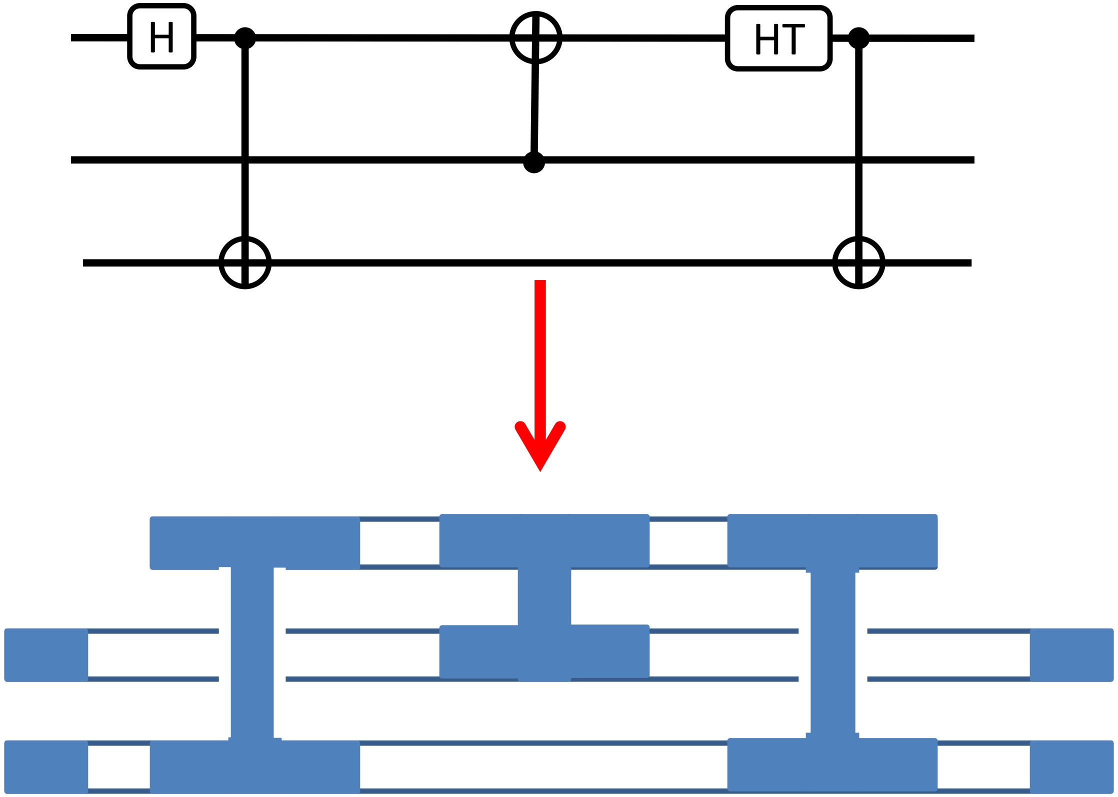
Each edge indicates two copies of the basic subgraph that we don't want simultaneously occupied.

Good states: The frustration-free states of G which live in the subspace where the occupancy constraints are satisfied.

(G, G_{occ}) → Occupancy Constraints Lemma → G'

The frustration-free states of G' are in 1-1 correspondence with the "good states".

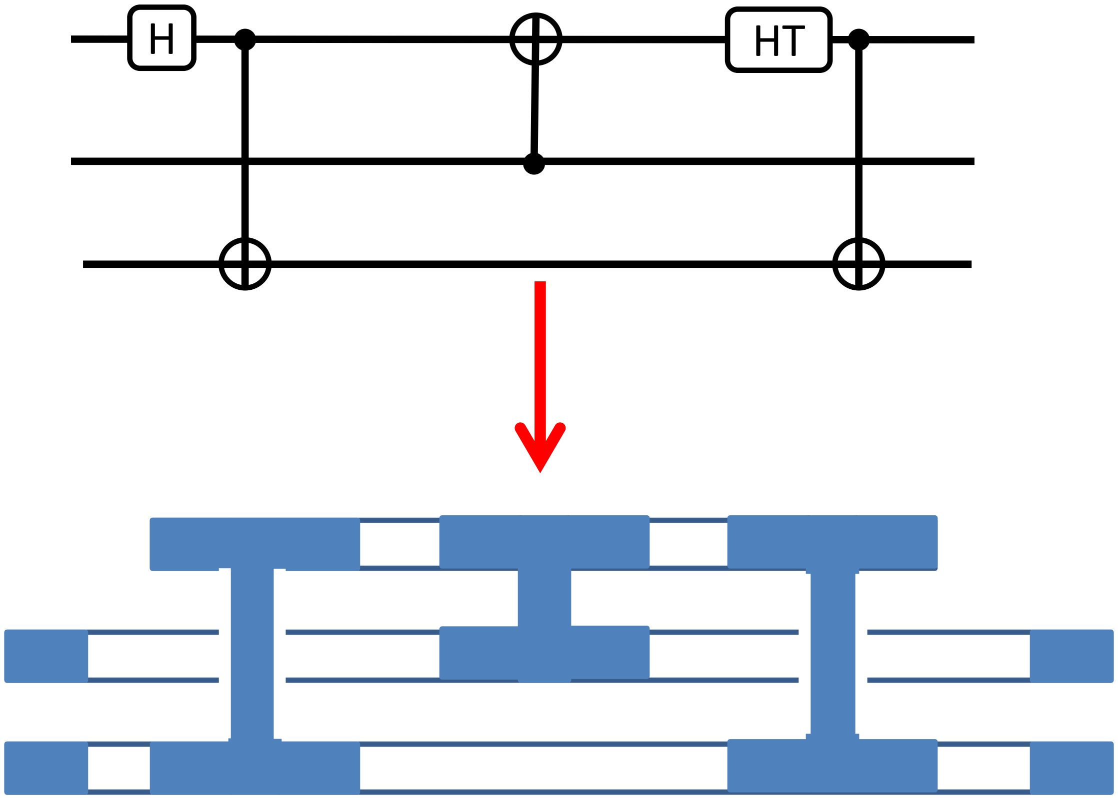
Overview of our strategy



n qubits, g gates

$O(g+n)$ vertices

Overview of our strategy

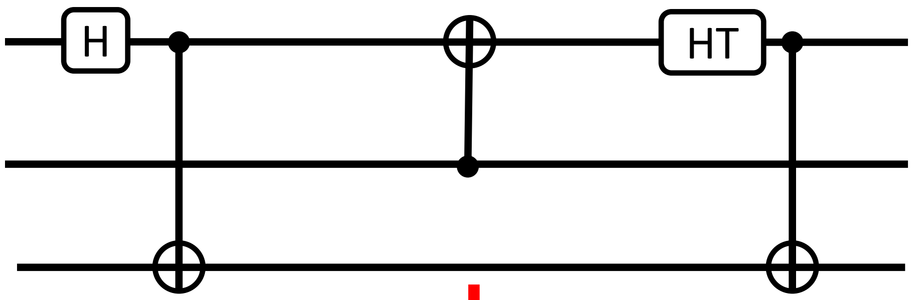


n qubits, g gates

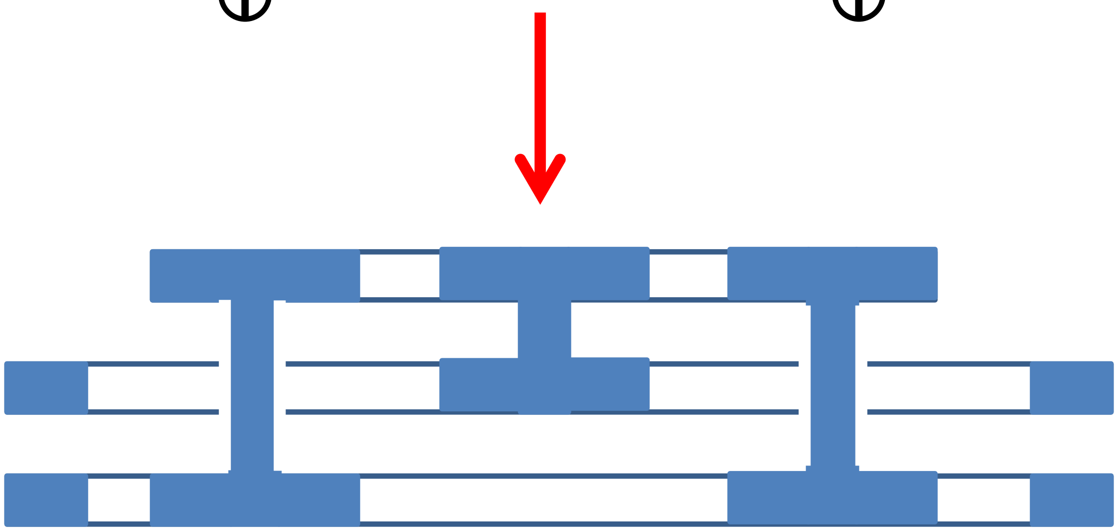
$O(g + n)$ vertices

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

Overview of our strategy



n qubits, g gates



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Then we apply the Occupancy Constraints Lemma with constraints designed to eliminate groundstates that do not encode computations. This outputs a graph with $O\left((g+n)^2\right)$ vertices where every n-particle groundstate encodes a computation.

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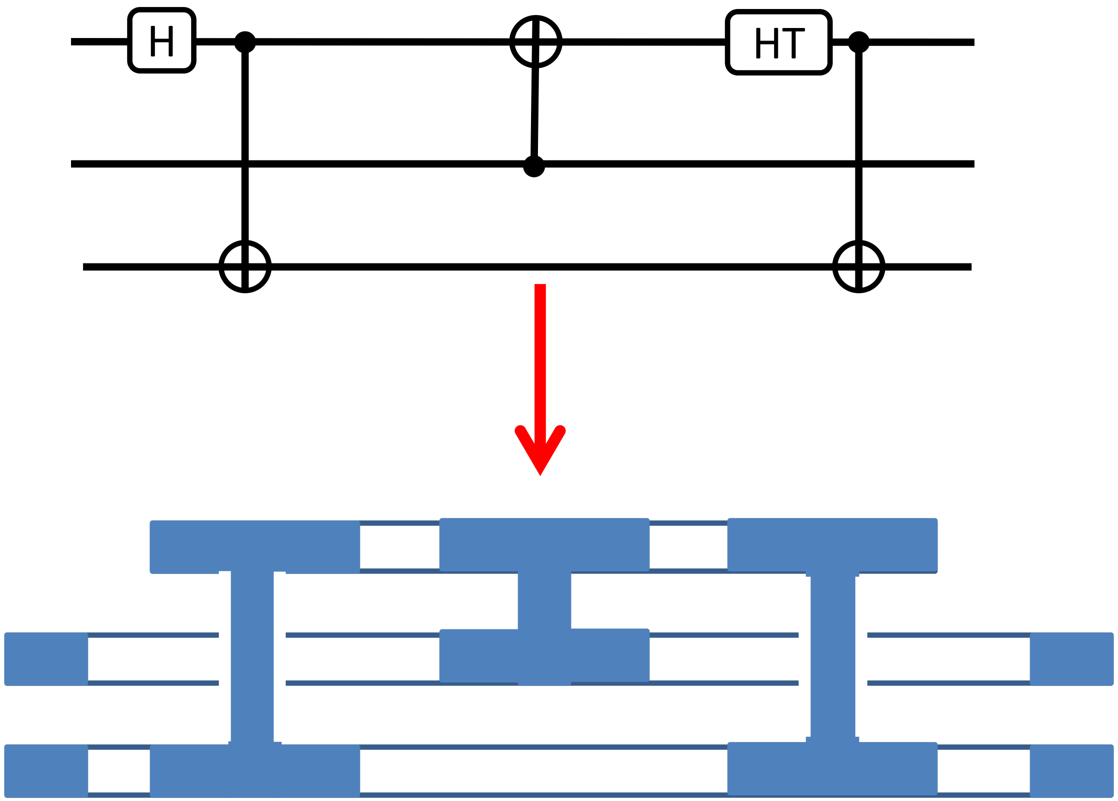

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To prove our result we establish spectral bounds **without using perturbation theory.**

Extensions and open questions

- Using our circuit-to-graph mapping, we prove that the problem of approximating the smallest eigenvalue of a sparse, efficiently row computable graph is QMA-complete.

- In arXiv 1503.07083 we strengthen the QMA-completeness results for the Bose-Hubbard model and the XY model, and prove that they hold for simple graphs (without self-loops).

- 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?