The Bose-Hubbard Model is QMA-complete*

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Abstract. 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.

1 Introduction

The problem of approximating the ground energy of a given Hamiltonian is a natural quantum analog of classical constraint satisfaction. Many authors have considered the computational complexity of such quantum ground state problems. For a variety of classes of Hamiltonians and a suitable notion of approximation, this task is complete for the complexity class QMA, the quantum version of NP with two-sided error (see reference [2] for a recent review). These results provide evidence that approximating the ground energy of such quantum systems is intractable.

The first such example is the Local Hamiltonian problem introduced by Kitaev [3]. A k-local Hamiltonian acts on a system of n qubits and can be written as a sum of terms, each acting nontrivially on k qubits. The k-Local Hamiltonian problem is a promise problem related to the task of approximating the ground energy of a k-local Hamiltonian. Given such a Hamiltonian and two thresholds a and b, one is asked to determine if the ground energy is below a or above b (promised that one of these conditions holds). Kitaev's original work showed that 5-local Hamiltonian is QMA-complete [3]; subsequent works proved QMA-completeness of the 3-local Hamiltonian problem [4], the 2-local Hamiltonian

* Reference [1] is a detailed technical version of this extended abstract.

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problem [5], and the 2-local Hamiltonian problem with interactions between qubits restricted to a two-dimensional lattice [6].

The complexity of similar computational problems related to other classes of Hamiltonians has also been considered. These include Hamiltonians in one dimension [7, 8], frustration-free Hamiltonians [9, 10], and stoquastic Hamiltonians (Hamiltonians with no "sign problem") [11, 12], among others.

The QMA-hardness of ground energy problems for local Hamiltonians acting on qubits has implications for Hamiltonians acting on indistinguishable particles (bosons or fermions) due to formal mappings between these systems. By applying such mappings to the Local Hamiltonian problem, one can show that certain bosonic [13] and fermionic [14] Hamiltonian problems are QMA-hard. A more restrictive class of QMA-complete fermionic Hamiltonians was considered by Schuch and Verstraete, who showed that the Hubbard model with a site-dependent magnetic field is QMA-complete [15]. This is a specific model of interacting electrons (i.e., spin-$\frac{1}{2}$ fermions) on a two-dimensional lattice, with a magnetic field that may take different values and point in different directions (in three dimensions) at distinct sites of the lattice.

Many of the QMA-complete problems considered previously have the property that the form of the terms in the Hamiltonian is part of the specification of the instance. For example, a 2-local Hamiltonian is specified by a graph, indicating pairs of qubits where terms in the Hamiltonian act, along with a 2-local Hermitian operator for each edge. In the Hubbard model considered in reference [15], there is a similar freedom in the choice of magnetic field at each site. A recent classification of local Hamiltonian problems [16] likewise applies only to models with adjustable coefficients. In fact, these results typically require coefficients that grow with the problem size.

In contrast, here we consider a system of interacting bosons with fixed movement and interaction terms. Specifically, we consider the Bose-Hubbard model, which has one of the simplest interactions between particles that conserves total particle number. Although the Bose-Hubbard model is traditionally defined on a lattice and with negative hopping strength [17], here we consider its extension to a general graph, with positive hopping strength.

We consider undirected graphs without multiple edges and with at most one self loop per vertex. Any such graph G (with vertex set V) can be specified by its adjacency matrix, a symmetric 0-1 matrix denoted $A(G)$. The Bose-Hubbard model on G with hopping strength t_{hop} and interaction strength J_{int} has the Hamiltonian

$$H_G = t_{\text{hop}} \sum_{i \in V} \sum_{j \in V} A(G)_{ij}\, a_i^\dagger a_j + J_{\text{int}} \sum_{k \in V} n_k(n_k - 1) \tag{1.1}$$

where $a_i^\dagger$ creates a boson at vertex i and $n_i = a_i^\dagger a_i$ counts the number of bosons at vertex i. Our results apply to the Bose-Hubbard model for any fixed positive hopping strength $t_{\text{hop}} > 0$ and any fixed positive (i.e., repulsive) interaction strength $J_{\text{int}} > 0$. Unlike other QMA-hardness results, in our work the coefficients $t_{\text{hop}}, J_{\text{int}}$ are not inputs to the problem; rather, each fixed choice defines a computational problem and we prove QMA-completeness for each of them.

Observe that the Bose-Hubbard Hamiltonian (1.1) conserves the total number of particles $N = \sum_{k \in V} n_k$. We focus on the space of N-particle states, which can be identified with the symmetric subspace of $(\mathbb{C}^{|V|})^{\otimes N}$ (as we discuss in more detail in Section 3). The first term in (1.1) allows particles to move between vertices; the second term is an interaction between particles that assigns an energy penalty for each vertex that is occupied by more than one particle. The Bose-Hubbard model is an example of a multi-particle quantum walk, a generalization of quantum walk to systems with more than one walker.

Recently we showed that the Bose-Hubbard model on a graph can perform efficient universal quantum computation [18]. Sometimes universality goes hand-in-hand with QMA-completeness, e.g., for local Hamiltonians, whose dynamics are BQP-complete [19] and whose ground energy problem is QMA-complete [3]. However, not all classes of Hamiltonians with universal dynamics have QMA-complete ground energy problems. For example, the dynamics of stoquastic local Hamiltonians are BQP-complete (as follows from [20] and time reversal), whereas the corresponding ground energy problem is in AM [11] and hence unlikely to be QMA-hard. Similarly, the ground energy problem for a Bose-Hubbard model with $t_{\text{hop}} < 0$ is also in AM [11], whereas the dynamics of such Hamiltonians are universal [18]. The ferromagnetic Heisenberg model on a graph provides an even starker contrast: its dynamics are BQP-complete (as can be inferred from [18] using a correspondence between spins and hard-core bosons) but its ground energy problem is trivial since the ground space is the symmetric subspace.

2 Overview of Results and Techniques

In this paper we define the Bose-Hubbard Hamiltonian problem and characterize its complexity. In this problem one is given a graph G and a number of particles N and asked to approximate the ground energy of the Bose-Hubbard Hamiltonian (1.1) in the N-particle sector (in a precise sense described in Section 3). We prove that this problem is QMA-complete.

To prove QMA-hardness of the Bose-Hubbard Hamiltonian problem, we show that in fact a notable special case of this problem, called Frustration-Free Bose Hubbard Hamiltonian, is QMA-hard. In this problem one is asked (roughly) to determine if the ground energy of the Bose-Hubbard Hamiltonian (1.1) in the N-particle sector is close to N times its single-particle ground energy (i.e., N times the smallest eigenvalue of the adjacency matrix $A(G)$). This is always a lower bound on the N-particle energy, and when it is achieved we say the N-particle ground states are frustration free. A frustration-free state has the special property that it has minimal energy for both terms in (1.1), and in particular it is annihilated by the interaction term. Frustration-free states therefore live in the subspace of *hard-core* bosons, with at most one boson per vertex.

Furthermore, we prove a reduction from Frustration-Free Bose-Hubbard Hamiltonian to an eigenvalue problem for a class of 2-local Hamiltonians defined by graphs. The two problems are related by a well-known mapping between

hard-core bosons and spin systems. Specifically, given a graph G (with vertex set V) we consider the Hamiltonian

$$O_G = \sum_{\substack{A(G)_{ij}=1 \\ i \neq j}} \frac{\sigma_x^i \sigma_x^j + \sigma_y^i \sigma_y^j}{2} + \sum_{A(G)_{ii}=1} \frac{1 - \sigma_z^i}{2} \tag{2.1}$$

where $\sigma_x, \sigma_y, \sigma_z$ are the Pauli matrices. Note that this Hamiltonian commutes with the magnetization operator $M_z = \sum_{i=1}^{|V|} \frac{1-\sigma_z^i}{2}$ and has a sector for each of its eigenvalues $M_z \in \{0, 1, \ldots, |V|\}$. We reduce Frustration-Free Bose-Hubbard Hamiltonian (with N particles on a graph G) to the problem of approximating the smallest eigenvalue of (2.1) within the sector with magnetization $M_z = N$. We call this the XY Hamiltonian problem because of its connection to the XY model from condensed matter physics. Since this problem is contained in QMA, our reduction shows it to be QMA-complete.

We also obtain another result that may be of independent interest. In Appendix A of [1] we give a self-contained proof that computing the smallest eigenvalue of a sparse, efficiently row-computable [21] symmetric 0-1 matrix (the adjacency matrix of a graph) is QMA-complete. This can alternatively be viewed as a result about the QMA-completeness of a single-particle quantum walk on a graph with at most one self-loop per vertex. To prove this, we use a mapping from circuits to graphs that is also used in our main result. Note that Janzing and Wocjan used a similar construction to design a BQP-complete problem [20].

Proof Techniques

We prove our main result by direct reduction from quantum circuit satisfiability. We introduce several new techniques in order to do this using the Bose-Hubbard model on an unweighted graph.

Kitaev's original proof of QMA-hardness of the Local Hamiltonian problem encodes a QMA verification circuit using ideas from a computationally universal Hamiltonian proposed by Feynman [19]. This Hamiltonian uses a "clock register" to record the progress of the computation; in an appropriate basis, the Hamiltonian is a quantum walk on a path whose vertices represent the steps of the computation. Other proofs of QMA-hardness have used other encodings of the temporal structure of a verification circuit into a quantum state. In our construction, we encode the history of an n-qubit verification circuit in the state of n interacting particles on a graph, where each particle encodes a single qubit.

Our construction uses a class of graphs we define called *gate graphs*. Gate graphs are built from a basic subgraph whose single-particle ground states encode the history of a simple single-qubit computation. By combining copies of this basic unit, we define gadgets with other functionality. (Note that these gadgets realize some desired behavior exactly; they are not "perturbative gadgets" in the sense of [5, 22].) In particular, we design gadgets for two-qubit gates such that each ground state of the two-particle Bose-Hubbard model encodes a two-qubit

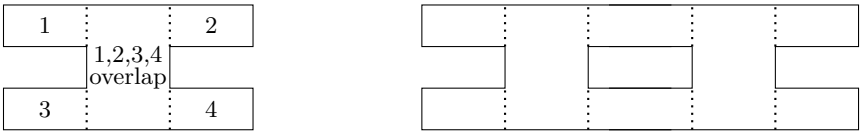

Fig. 2.1. We design graphs for two-qubit gates with overlapping regions as in (A). Regions 1 and 2 are associated with the first encoded qubit and regions 3 and 4 with the second encoded qubit. One could imagine designing a graph for a circuit with two-qubit gates U_1 followed by U_2 by connecting the corresponding gadgets as in (B). In the text we describe a challenge with this approach.

computation. We now give a high-level description of how these gadgets work and how we use them to construct a graph for a QMA verification circuit.

For each two-qubit gate U from a fixed universal set, we design a graph G_U that can be divided into four overlapping regions as shown schematically in Figure 2.1(a). (The specific graphs we use for two-qubit gates each have 4096 vertices and are described using the gate graph formalism.) The two-particle Bose-Hubbard model on this graph has ground states that encode the two-qubit computation. To describe them it is helpful to first consider the single-particle ground states, i.e., the ground states of the adjacency matrix $A(G_U)$. This matrix has 16 orthonormal single-particle ground states $|\rho^{i,U}_{z,a}\rangle$. Each index $i \in \{1,2,3,4\}$ is associated with the corresponding region in the graph, as $|\rho^{i,U}_{z,a}\rangle$ is supported entirely within region i. The index $z \in \{0,1\}$ corresponds to the computational basis states of a single encoded qubit. Note that, since $A(G_U)$ is a real matrix, the complex conjugate of any eigenstate is also an eigenstate with the same eigenvalue. The index $a \in \{0,1\}$ is associated with this freedom, i.e., $|\rho^{i,U}_{z,1}\rangle = |\rho^{i,U}_{z,0}\rangle^*$. The ground space of the two-particle Bose-Hubbard model on G_U is spanned by 16 states, indexed by two choices $z_1, z_2 \in \{0,1\}$ of computational basis states for the encoded qubits and two bits $a_1, a_2 \in \{0,1\}$ associated with complex conjugation. These states can be represented as symmetric states in the Hilbert space $\mathbb{C}^{4096} \otimes \mathbb{C}^{4096}$; they are

$$\frac{1}{2}(|\rho^{1,U}_{z_1,a_1}\rangle|\rho^{3,U}_{z_2,a_2}\rangle + |\rho^{3,U}_{z_2,a_2}\rangle|\rho^{1,U}_{z_1,a_1}\rangle)$$
$$+ \frac{1}{2}\sum_{x_1,x_2\in 0,1} U(a_1)_{x_1,x_2,z_1,z_2}(|\rho^{1,U}_{x_1,a_1}\rangle|\rho^{3,U}_{x_2,a_2}\rangle + |\rho^{3,U}_{x_2,a_2}\rangle|\rho^{1,U}_{x_1,a_1}\rangle)$$

where $U(0) = U$ is the two-qubit gate of interest and $U(1) = U^*$ is its elementwise complex conjugate. Observe that each of these states is a superposition of a term where both particles are on the left-hand side of the graph, encoding a two-qubit input state $|z_1\rangle|z_2\rangle$, and a term where both particles are on the right-hand side of the graph, encoding the two-qubit output state $U(a_1)|z_1\rangle|z_2\rangle$ where either U or its complex conjugate has been applied. While we might prefer the ground states to only encode the computation corresponding to U, we must

include the possibility of U^* because the Hamiltonian is real. The same issue arises for n-qubit verification circuits. Fortunately, the complex conjugate of a circuit is equally useful for QMA verification.

It is natural to attempt to construct a graph for an n-qubit verification circuit by combining gadgets for each of the two-qubit gates. However, there is an obstacle to this approach, as illustrated by the example of a two-qubit circuit consisting of only two gates U_1 and U_2. One could construct a graph for such a circuit as shown schematically in Figure 2.1(b), where the two-qubit gadgets for U_1 and U_2 are connected in some unspecified way in the middle. However, not every ground state of the two-particle Bose-Hubbard model on such a graph encodes a computation. For example, there could be a ground state where one of the particles is in the single-particle state $|\rho_{z,a}^{1,U_1}\rangle$ localized on the left side of the graph and the other particle is in the state $|\rho_{z,a}^{2,U_2}\rangle$ with support on a disjoint region of the graph on the right-hand side. To eliminate such spurious ground states, we develop a method to enforce *occupancy constraints* on the locations of particles in gate graphs using the Bose-Hubbard interaction. Although this interaction only directly penalizes simultaneous occupation of the same vertex, we show how to simulate terms that penalize simultaneous occupation of different regions of the graph. We formalize this method by proving an "Occupancy Constraints Lemma" for gate graphs.

In summary, our construction of the graph for an n-qubit verification circuit proceeds in two steps. We first construct a graph G by connecting two-qubit gadgets for each of the gates in the circuit. As discussed above, the ground space of the n-particle Bose-Hubbard model on G includes a subspace of states that encode computations and a subspace of states that do not. We construct a set of occupancy constraints that are only satisfied by states in the former subspace. We then apply the Occupancy Constraints Lemma to obtain another gate graph where each N-particle ground state encodes a computation.

Unlike many previous works, we do not use perturbation theory in our analysis. Instead, we use a "Nullspace Projection Lemma" (used implicitly in [23]) that characterizes the smallest nonzero eigenvalue of a sum of two positive semidefinite matrices $H_A + H_B$ in terms of the smallest nonzero eigenvalue of H_A and the smallest nonzero eigenvalue of H_B restricted to the nullspace of H_A. This Lemma allows us to establish an eigenvalue promise gap (i.e., to bound the ground energies of yes instances away from those of no instances) without having to multiply terms in the Hamiltonian by large coefficients, something that is not allowed in the setting of the Bose-Hubbard model on a graph. Whereas QMA-hardness proofs such as those of [4, 5, 6, 15, 16] require multiplying terms in the Hamiltonian by unphysical, problem-size dependent coefficients, our approach avoids this. To the best of our knowledge, our proof would not be much simpler if we only demanded constant-size coefficients; the further restriction that the model is defined entirely by a graph is an extra benefit with little additional cost.

3 Definitions and Results

In this Section we introduce the Bose-Hubbard model and a related spin model, and formally state our results.

3.1 The Bose-Hubbard Model on a Graph

We consider the Bose-Hubbard model on a graph G, where the Hamiltonian is given by (1.1). While our complexity-theoretic results apply to the Bose-Hubbard model for any strictly positive hopping and interaction strengths, we set $t_{\text{hop}} = J_{\text{int}} = 1$ for convenience.

In the second-quantized formulation of the Bose-Hubbard model used in (1.1), the Hamiltonian H_G acts on the Fock space with orthonormal basis vectors specified by the number of bosons at each vertex. For our purposes, it will be more convenient to work in an equivalent (first-quantized) basis.

Consider the Hilbert space $(\mathbb{C}^{|V|})^{\otimes N}$ where each basis state $|i_1\rangle \dots |i_N\rangle$ corresponds to an N-tuple of vertices $(i_1, ..., i_N) \in V^N$. Define the linear operator Sym that symmetrizes over all $N!$ permutations of the N particles:

$$\text{Sym}(|i_1\rangle \dots |i_N\rangle) = \frac{1}{\sqrt{N!}} \sum_{\pi \in S_N} |i_{\pi(1)}\rangle \dots |i_{\pi(N)}\rangle.$$

Every state in the Fock space can be uniquely paired with a state in

$$\mathcal{Z}_N(G) = \text{span}\{\text{Sym}(|i_1, \dots, i_N\rangle) \colon i_1, \dots, i_N \in V\}$$

since the two spaces have the same dimension. A natural bijection sends a basis state $\text{Sym}(|i_1\rangle \dots |i_N\rangle)$ to the Fock state with $|\{j \colon i_j = v\}|$ bosons at each vertex v.

If we restrict our attention to the N-particle sector, then the Bose-Hubbard Hamiltonian (with $t_{\text{hop}} = J_{\text{int}} = 1$) acts as the operator

$$H_G^N = \sum_{w=1}^{N} A(G)^{(w)} + \sum_{k \in V} \hat{n}_k \left(\hat{n}_k - 1\right) \tag{3.1}$$

on the space $\mathcal{Z}_N(G)$, where the number operator is $\hat{n}_i = \sum_{w=1}^{N} |i\rangle\langle i|^{(w)}$ (see for example [24, §64]). Here a superscript (w) indicates that an operator acts nontrivially on subsystem w.

While H_G^N is defined as a $|V|^N \times |V|^N$ matrix in the space $(\mathbb{C}^{|V|})^{\otimes N}$, we consider its restriction

$$\bar{H}_G^N = H_G^N \Big|_{\mathcal{Z}_N(G)}$$

to the bosonic N-particle subspace $\mathcal{Z}_N(G)$. It is convenient to add a term proportional to the identity to obtain a positive semidefinite operator. Letting $\mu(G)$ denote the smallest eigenvalue of the adjacency matrix $A(G)$, we consider

$$H(G, N) = \bar{H}_G^N - N\mu(G)$$

and we write $\lambda_N^1(G)$ for the smallest eigenvalue of $H(G,N)$. Clearly $\lambda_N^1(G) \geq 0$ since the interaction term is positive semidefinite. Also note that, given the graph G, the smallest eigenvalue $\mu(G)$ of its adjacency matrix can be efficiently approximated using a classical polynomial-time algorithm, so the complexity of approximating $\lambda_N^1(G)$ is equivalent to the complexity of approximating the ground energy of $\bar{H}_G^N$. (Note that here the graph is specified explicitly by its adjacency matrix. In other contexts one might consider a graph specified compactly, e.g., by a circuit that computes rows of its adjacency matrix. Then the situation is more complex since the input size can be much smaller than the number of vertices in the graph. Indeed, we prove in Appendix A of [1] that approximating the smallest eigenvalue of such a graph is QMA-complete.)

When $\lambda_N^1(G) = 0$, the ground energy of the N-particle Bose-Hubbard model $\bar{H}_G^N$ is equal to N times the one-particle energy $\mu(G)$. Then we say that the N-particle Bose-Hubbard model is *frustration free*.

3.2 Complexity of the Bose-Hubbard Model

Given a K-vertex graph G and a number of particles N, how hard is it to approximate the ground energy of the N-particle Bose-Hubbard model $\bar{H}_G^N$ on G? We consider the following decision version of this computational problem.

*Problem 1 (**Bose-Hubbard Hamiltonian**).* We are given a K-vertex graph G, a number of particles N, a real number c, and a precision parameter $\epsilon = \frac{1}{T}$. The positive integers N and T are provided in unary; the graph is specified by its adjacency matrix, which can be any $K \times K$ symmetric 0-1 matrix. We are promised that either the smallest eigenvalue of $\bar{H}_G^N$ is at most c (yes instance) or is at least $c + \epsilon$ (no instance) and we are asked to decide which is the case.

In this problem c is provided in a straightforward manner, with enough precision to resolve ϵ, i.e., using $\mathcal{O}(\log|c| + \log T)$ bits. The input size is therefore $\Theta(K^2 + T + N + \log|c|)$ bits. We prove that this problem is QMA-complete, providing evidence that approximating the ground energy of the N-particle Bose-Hubbard model on a graph G is intractable.

Theorem 1. *Bose-Hubbard Hamiltonian is QMA-complete.*

The proof of this Theorem has two parts.

The easy part is to show that Bose-Hubbard Hamiltonian is contained in QMA. The basic strategy of Arthur's verification protocol is to measure the energy of the Bose-Hubbard Hamiltonian in the state given to him by Merlin, using phase estimation and Hamiltonian simulation. Arthur accepts if the energy is small enough and rejects otherwise. We give a more detailed description of the verification procedure in Section 3 of [1].

The more involved part is to show that Bose-Hubbard Hamiltonian is QMA-hard. For this we show that any instance of a QMA problem can be converted

(in deterministic polynomial time on a classical computer) into an equivalent instance of Bose-Hubbard Hamiltonian. In fact, our reduction proves a slightly stronger result, namely that a notable extremal case of Bose-Hubbard Hamiltonian is already QMA-hard. We now discuss this special case.

Recall from the previous section that the ground energy of the N-particle Bose-Hubbard model is at least N times the single-particle ground energy $\mu(G)$, i.e., $\lambda_N^1(G) \geq 0$. We can ask if this inequality is close to equality, i.e., is the N-particle Bose-Hubbard model close to being frustration free?

*Problem 2 (**Frustration-Free Bose-Hubbard Hamiltonian**).* We are given a K-vertex graph G, a number of particles $N \leq K$, and a precision parameter $\epsilon = \frac{1}{T}$. The integer $T \geq 4K$ is provided in unary; the graph is specified by its adjacency matrix, which can be any $K \times K$ symmetric 0-1 matrix. We are promised that either $\lambda_N^1(G) \leq \epsilon^3$ (yes instance) or $\lambda_N^1(G) \geq \epsilon + \epsilon^3$ (no instance) and we are asked to decide which is the case.

For concreteness, we have made some specific choices in defining this problem. Our proof that it is QMA-hard also applies, for example, to variants of the problem where ϵ^3 is replaced (in both places it appears) by ϵ^α for any constant $\alpha \in \{1, 2, 3, \ldots\}$. We use the version with $\alpha = 3$ as stated above to facilitate a reduction to the XY Hamiltonian problem.

The requirement $T \geq 4K$ ensures that ϵ is small so that, for a yes instance, the system is very close to being frustration free. We choose the specific threshold $4K$ for concreteness.

The restriction $N \leq K$ is without loss of generality since the problem is trivial otherwise. To see this, note that any state with more than K particles is orthogonal to the nullspace of the interaction term since there are always two or more particles located at one vertex; hence $\lambda_N^1(G) \geq 2$ whenever $N \geq K + 1$.

Frustration-Free Bose-Hubbard Hamiltonian is a special case of Bose-Hubbard Hamiltonian with $c = N\mu(G) + \epsilon^3$. To prove that Bose-Hubbard Hamiltonian is QMA-hard, it therefore suffices to prove that Frustration-Free Bose-Hubbard Hamiltonian is QMA-hard. The bulk of our technical work [1] is concerned with the proof of this fact, following the strategy outlined in Section 2.

3.3 Complexity of the XY Hamiltonian Problem

We reduce Frustration-Free Bose-Hubbard Hamiltonian to an eigenvalue problem for a class of 2-local Hamiltonians defined by graphs. The reduction is based on a well-known mapping between hard-core bosons and spin systems.

We define the subspace $\mathcal{W}_N(G) \subset \mathcal{Z}_N(G)$ of N hard-core bosons on a graph G to consist of the states where each vertex of G is occupied by either 0 or 1 particle, i.e.,

$$\mathcal{W}_N(G) = \text{span}\{\text{Sym}(|i_1, \ldots, i_N\rangle) \colon i_j \in V,\, i_j \neq i_k \text{ for distinct } j, k \in [N]\}.$$

A basis for $\mathcal{W}_N(G)$ is the subset of Fock states with at most one particle per vertex, which can be labeled by bit strings with Hamming weight N. The space

$\mathcal{W}_N(G)$ can thus be identified with the weight-N subspace

$$\mathrm{Wt}_N(G) = \mathrm{span}\{|z\rangle : z \in \{0,1\}^{|V|}, \textstyle\sum_i z_i = N\}$$

of a $|V|$-qubit Hilbert space. We consider the restriction of H_G^N to the space $\mathcal{W}_N(G)$, which can equivalently be written as the $|V|$-qubit Hamiltonian O_G from equation (2.1) restricted to the space $\mathrm{Wt}_N(G)$.

Note that the Hamiltonian O_G conserves the total magnetization (Hamming weight) $M_z = \sum_{i=1}^{|V|} \frac{1-\sigma_z^i}{2}$ along the z axis. We define $\theta_N(G)$ to be the ground energy of O_G in the sector with magnetization N. We show that approximating this quantity is QMA-complete.

*Problem 3 (**XY Hamiltonian**).* We are given a K-vertex graph G, an integer $N \leq K$, a real number c, and a precision parameter $\epsilon = \frac{1}{T}$. The positive integer T is provided in unary; the graph is specified by its adjacency matrix, which can be any $K \times K$ symmetric 0-1 matrix. We are promised that either $\theta_N(G) \leq c$ (yes instance) or else $\theta_N(G) \geq c + \epsilon$ (no instance) and we are asked to decide which is the case.

Theorem 2. *XY Hamiltonian is QMA-complete.*

We prove QMA-hardness of XY Hamiltonian by reduction from Frustration-Free Bose-Hubbard Hamiltonian. The proof of Theorem 2 appears in Appendix B of [1].

4 Extensions and Open Questions

Our result shows that approximating the ground energy of the Bose-Hubbard model on a graph at fixed particle number is likely intractable. In showing this, we introduce techniques that we expect will be useful in other contexts. Here we briefly discuss some related questions for future work.

One might consider the complexity of variants of the Bose-Hubbard Hamiltonian problem. For example, one could consider the problem with negative hopping (i.e., $t_{\mathrm{hop}} < 0$), with attractive interactions (i.e., $J_{\mathrm{int}} < 0$), or both. For negative hopping, the results of [11] show that the problem is in AM; we do not know if it is AM-hard. For attractive interactions, the problem is clearly in QMA (the verification procedure described in Section 3 of [1] applies independent of the signs of $t_{\mathrm{hop}}, J_{\mathrm{int}}$), but again we do not know the true complexity.

One can define other variants of the Bose-Hubbard Hamiltonian problem by lifting the restriction to fixed particle number.

One could also consider other classes of graphs. The graphs we consider in this paper are described by symmetric 0-1 matrices and have at most one self-loop per vertex. We do not know if the model remains QMA-hard on simple graphs, i.e., without any self-loops.

There are many open questions concerning the complexity of the ground energy problem for other quantum systems defined by graphs. For example,

one could consider fermions or bosons on a graph with nearest-neighbor interactions. One could also consider quantum spin models defined on graphs such as the XY model or the antiferromagnetic Heisenberg model. Both of these examples correspond to Hamiltonians that conserve magnetization, so one could consider the ground energy problem with or without a restriction to a fixed-magnetization sector. This would complement existing results about the complexity of computing the lowest-energy configuration of classical spin models defined by graphs (for example, the antiferromagnetic Ising model on a graph is NP-complete, as it is equivalent to max cut).

As emphasized previously, the Hamiltonians we consider are determined entirely by a choice of graph, with the same type of movement and interaction terms applied throughout the graph. It might be interesting to find other QMA-complete problems with similar features, such as a version of Local Hamiltonian with only one type of local term. Analogous classical constraint satisfaction problems with a fixed type of constraint are well known (e.g., Exact Cover and Not-All-Equal SAT) and have been widely studied. Along similar lines, it might be interesting to understand when local Hamiltonian problems remain QMA-hard with constant-size coefficients. Nagaj and Mozes have shown that the 3-local Hamiltonian problem has this property [25], but whether the same holds for the 2-local Hamiltonian problem remains open.

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