COMPLEXITY OF THE BOSE-HUBBARD MODEL ON SIMPLE GRAPHS

ANDREW M. CHILDS[1,2,3], DAVID GOSSET[1,2], AND ZAK WEBB[2,4]

Approximating the ground energy of a Hamiltonian is a quantum constraint satisfaction problem. Beginning with Kitaev's seminal work on the Local Hamiltonian problem [5], many examples of such ground energy problems have been shown complete for the complexity class QMA. For example, the Local Hamiltonian problem remains QMA-complete with reduced locality [4, 3] and a simplified interaction graph [7]. Further work has considered other restrictions on the form of the Hamiltonian (see, e.g., [1]).

In this and in previous work [2], we consider the complexity of approximating the ground energy of the Bose-Hubbard model on a graph. For a given graph G, the Bose-Hubbard Hamiltonian is

$$H_G = \underbrace{\sum_{i,j\in V(G)} A(G)_{ij} a_i^\dagger a_j}_{H_G^{\text{move}}} + \underbrace{J_{\text{int}} \sum_{i\in V(G)} n_i(n_i-1)}_{H_G^{\text{int}}}$$

where $a_i^\dagger$ is a bosonic creation operator and $n_i = a_i^\dagger a_i$ counts the number of bosons at vertex i. The first term moves particles between adjacent vertices, while the second provides an energy penalty when multiple particles occupy the same vertex.

In previous work [2], we showed that approximating the ground energy of such a Hamiltonian at fixed particle number on an unweighted graph with at most one self-loop per vertex is QMA-complete. (Using a simple reduction from the Bose-Hubbard model, we also established QMA-completeness of a related class of spin models on graphs that generalize the XY model.) The proof of our main result was based on a reduction from quantum circuit satisfiability. In our reduction, quantum circuits are mapped to a special type of graph called gate graphs.

In our present work, we show that this problem is QMA-complete even on simple graphs, i.e., unweighted graphs without self-loops. Observe that in a sector with fixed particle number, adding or removing self-loops from *all* vertices of the underlying graph corresponds to an overall constant shift in the energy spectrum (i.e., adding a multiple of the identity). Hence, we can exchange the problem of removing self-loops with the problem of adding self-loops. Our proof proceeds by taking a gate graph G and defining a related graph G^{SL} with a self-loop on every vertex. We relate the eigenvalue promise gap of the Bose-Hubbard model on G^{SL} to that on G using the special relationship between the two graphs and extensively applying the nullspace projection lemma [6, 2].

We aim to modify a gate graph G without greatly changing its ground energy, but ensuring that every vertex of the modified graph has a self-loop. To do this, we take two copies of the graph G, and for any vertex $v \in V(G)$ without a self-loop, we add an edge between the two copies of v and a self-loop to each of the two copies of v. By construction, the new graph G^{SL} has a self-loop on every vertex, so it suffices to show that the ground energy is not significantly changed. While the eigenvalue promise gap for an arbitrary graph would not be preserved by this construction, we can make use of the restricted form of a gate graph.

[1] Department of Combinatorics & Optimization, University of Waterloo
[2] Institute for Quantum Computing, University of Waterloo
[3] Department of Computer Science, Institute for Advanced Computer Studies, and Joint Center for Quantum Information and Computer Science, University of Maryland
[4] Department of Physics & Astronomy, University of Waterloo
E-mail addresses: amchilds@umd.edu, dngosset@gmail.com, zakwwebb@gmail.com.

In particular, this construction does not significantly alter the single-particle ground space of a gate graph. The first step of our proof is to show that for any gate graph, the ground space of $A(G)$ is isomorphic to $A(G^{\mathrm{SL}})$, and that states in the two spaces are identified in a natural way. We then use the nullspace projection lemma [6, 2] from our previous work to bound the eigenvalue gap of $A(G^{\mathrm{SL}})$ in terms of the eigenvalue gap of $A(G)$. These results generalize directly to multiple non-interacting bosons with Hamiltonian given by the movement term of the Bose-Hubbard model: the ground spaces of H_G^{move} and $H_{G^{\mathrm{SL}}}^{\mathrm{move}}$ are isomorphic and we obtain a bound on the eigenvalue gap of the latter Hamiltonian.

The next step in our proof is to consider the restriction of the interaction term to the ground space of the movement term. We use the isomorphism between the two ground spaces to show that $H_{G^{\mathrm{SL}}}^{\mathrm{int}}$ restricted to the ground space of $H_{G^{\mathrm{SL}}}^{\mathrm{move}}$ is equal to $\frac{1}{2}H_G^{\mathrm{int}}$ restricted to the ground space of H_G^{move} (the constant $\frac{1}{2}$ is not essential to the result).

To combine these two results, we use the nullspace projection lemma [6, 2] to give a bound on the promise gap for our modified construction, G^{SL}, in terms of the bound for G. We then shift the energy scale by removing the self-loops from the graph G^{SL} and thereby give the same bound on the promise gap for a simple graph. Thus we prove that approximating the ground energy of the Bose-Hubbard model on a simple graph (at fixed particle number) is at least as hard as approximating the ground energy of the Bose-Hubbard model on a gate graph, which is QMA-hard.

An immediate open question is the complexity of the XY model on a simple graph. We expect that our results can be used to show QMA-completeness of this model (at fixed magnetization) without much additional work. Along similar lines, one might investigate the complexity of the Heisenberg model on a simple graph at fixed magnetization. A more challenging research direction is to generalize our results to the case of unconstrained particle number (or for spin models, unconstrained magnetization). It remains unclear how to remove the restriction to fixed particle number using our current approach, so resolving this question will likely require new proof techniques.

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