Near-optimal ground state preparation

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arXiv:2002.12508

1 Overview

Preparing the ground state of a given Hamiltonian and estimating its ground energy are important but computationally hard tasks. However, given some additional information, these problems can be solved efficiently on a quantum computer. We assume that an initial state with non-trivial overlap with the ground state can be efficiently prepared, and the spectral gap between the ground energy and the first excited energy is bounded from below. With these assumptions we design an algorithm that prepares the ground state when an upper bound of the ground energy is known, whose runtime has a logarithmic dependence on the inverse error. When such an upper bound is not known, we propose a hybrid quantum-classical algorithm to estimate the ground energy, where the dependence of the number of queries to the initial state on the desired precision is exponentially improved compared to the current state-of-the-art algorithm proposed in [Ge et al. 2019]. These two algorithms can then be combined to prepare a ground state without knowing an upper bound of the ground energy. We also prove that our algorithms reach the complexity lower bounds by applying it to the unstructured search problem and the quantum approximate counting problem.

2 Background

Estimating ground energy and obtaining information on the ground state of a given quantum Hamiltonian are of immense importance in condensed matter physics, quantum chemistry, and quantum information. Classical methods suffer from the exponential growth of the size of Hilbert space, and therefore quantum computers are expected to be used to overcome this difficulty. However even for quantum computer, estimating the ground energy is a hard problem: deciding whether the smallest eigenvalue of a generic local Hamiltonian is greater than b or smaller than a for some $a < b$ is QMA-complete [1, 8, 9, 14].

Therefore to make the problem efficiently solvable we need more assumptions. We denote the Hamiltonian we are dealing with by H, and consider its spectral decomposition $H = \sum_k \lambda_k |\psi_k\rangle \langle\psi_k|$ where $\lambda_k \leq \lambda_{k+1}$. The key assumption is that we have an initial state $|\phi_0\rangle$ which can be efficiently prepared by an oracle U_I, and has some overlap with the ground state $|\psi_0\rangle$ lower bounded by γ. This is a reasonable assumption in many practical scenarios. For instance, even for strongly-correlated molecules in quantum chemistry, there is often a considerable overlap between the true ground state and the Hartree-Fock state. The latter can be trivially prepared in the molecular orbital basis, and efficiently prepared in other basis [10]. For the moment we also assume the spectral gap is bounded from below: $\lambda_1 - \lambda_0 \geq \Delta$.

With these assumptions we can already use phase estimation coupled with amplitude amplification [5] to prepare the ground state, if we further know the ground energy to high precision. To our knowledge, the most comprehensive work on ground state preparation and ground state energy estimation was done by Ge *et al.* [6], which provided detailed complexity estimates for well-known methods such as phase estimation, and proposed new methods based on the recently developed linear combination of unitaries (LCU) technique. As analyzed in [6, Appendix A], in order to prepare the ground state to fidelity[1] $1 - \epsilon$, the runtime of the

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[1] In this work, the fidelity between states $|x\rangle, |y\rangle$ is defined to be $|\langle x|y\rangle|$.

controlled-time-evolution of the Hamiltonian is $\widetilde{\mathcal{O}}(1/(\gamma^2\Delta\epsilon))$ [2] , and the number of queries to U_I is $\widetilde{\mathcal{O}}(1/\gamma)$, assuming the spectral norm of H is bounded by a constant. This is however far from optimal. Poulin and Wocjan [15] proposed a method that, by executing the inverse of phase estimation to filter out the unwanted components in the initial state, can prepare a state whose energy is in a certain given range. A different choice of parameters yields a way to prepare the ground state to fidelity $1-\epsilon$ by running the controlled-time-evolution of the Hamiltonian with $\widetilde{\mathcal{O}}(1/(\gamma\Delta)\log(1/\epsilon))$ runtime, and using $\widetilde{\mathcal{O}}(1/\gamma)$ queries to U_I [6, Appendix C]. Using LCU, Ge *et al.* proposed a new method to filter the initial state by applying a linear combination of time-evolutions of different time length [6], which achieves the same complexity, up to logarithmic factors, as the modified version of Poulin and Wocjan's method discussed above.

All of the above methods prepare the ground state assuming the ground energy is known to high precision. When the ground energy is unknown, Ge *et al.* proposed a method to estimate the ground energy using a search method called minimum label finding [6]. This method can estimate the ground energy to precision h by running the controlled-time-evolution of the Hamiltonian for $\widetilde{\mathcal{O}}(1/(\gamma h^{3/2}))$ [3], and querying U_I $\widetilde{\mathcal{O}}(1/(\gamma\sqrt{h}))$ times. It is worth noting that their method requires $h = \widetilde{\mathcal{O}}(\Delta)$, and therefore is very expensive when the gap is extremely small. When the ground energy is not known *a priori* , Ge *et al.* proposed a method to first estimate the ground energy and then apply the LCU approach.

3 Main results

Below we discuss our main results regarding estimating the ground energy and preparing the ground state of a Hamiltonian $H = \sum_k \lambda_k |\psi_k\rangle \langle\psi_k| \in \mathbb{C}^{N\times N}$, where $\lambda_k \leq \lambda_{k+1}$, given through its $(\alpha, m, 0)$-block-encoding U_H (the definition of block-encoding will be provided later). Also suppose we have an initial state $|\phi_0\rangle$ prepared by circuit U_I. We will selectively assume that we are given one or more of the following promises in different settings:

(P1) Lower bound for the overlap: $|\langle\phi_0|\psi_0\rangle| \geq \gamma$,

(P2) Bounds for the ground energy and spectral gap: $\lambda_0 \leq \mu - \Delta/2 < \mu + \Delta/2 \leq \lambda_1$.

(P2') Bound for the spectral gap: $\lambda_1 - \lambda_0 \geq \Delta$.

The following are our main results:

Ground state preparation with *a priori* ground energy bound (Theorem 4): Suppose we are given promises (P1) and (P2). Then the ground state $|\psi_0\rangle$ can be prepared to fidelity $1-\epsilon$ with $\widetilde{\mathcal{O}}(\frac{\alpha}{\gamma\Delta}\log(\frac{1}{\epsilon}))$ queries to U_H and $\widetilde{\mathcal{O}}(\frac{1}{\gamma})$ queries to U_I.

Ground energy (Theorem 6): Suppose we are given the promise (P1). Then the ground energy can be estimated to precision h with probability $1-\vartheta$ with $\widetilde{\mathcal{O}}\left(\frac{\alpha}{\gamma h}\log\left(\frac{1}{\vartheta}\right)\right)$ queries to U_H and $\widetilde{\mathcal{O}}\left(\frac{1}{\gamma}\log\left(\frac{\alpha}{h}\right)\log\left(\frac{1}{\vartheta}\right)\right)$ queries to U_I.

Ground state preparation without *a priori* bound (Corollary 7): Suppose we are given the promises (P1) and (P2'). Then the ground state can be can be prepared to fidelity $1-\epsilon$ with probability $1-\vartheta$ with $\widetilde{\mathcal{O}}\left(\frac{\alpha}{\gamma\Delta}\log\left(\frac{1}{\vartheta\epsilon}\right)\right)$ queries to U_H and $\widetilde{\mathcal{O}}\left(\frac{1}{\gamma}\log\left(\frac{\alpha}{\Delta}\right)\log\left(\frac{1}{\vartheta}\right)\right)$ queries to U_I.

The main improvements in our approach are in ground energy estimation. Compared to the phase estimation algorithm, whose complexity is analyzed in [6, Appendix A], our algorithm improved the dependence in the number of queries to U_H on the overlap γ from γ^{-3} to γ^{-1}. Compared to the algorithm proposed by Ge *et al.* [6, Theorem 4], our algorithm the dependence in the number of queries to U_H and U_I on the precision h, from $h^{-3/2}$ and $h^{-1/2}$, to h^{-1} and $\log(h^{-1})$ respectively. These improvements result in corresponding improvements in the algorithm to prepare the ground state without *a priori* ground energy

[2] In this work the notation $\widetilde{\mathcal{O}}(f)$ means $\mathcal{O}(f \operatorname{poly}\log(f))$ unless otherwise stated.

[3] In [6], the meaning of the notation $\widetilde{\mathcal{O}}(\cdot)$ is different from that in our work. In particular, $\widetilde{\mathcal{O}}(\cdot)$ in [6] hides all factors that are poly-logarithmic in $1/h$, $1/\epsilon$, $1/\gamma$, and $1/\Delta$, regardless of what is inside the parentheses. We preserve their notation when citing their results since these factors do not play an important role when comparing the complexities of our methods.

bound. A side-by-side comparison of the query complexities of the algorithms in our work and those in Ref. [6] is provided in Table 1 in our work. It is also worth noting that [6, Theorem 4] assumes the precision $h = \widetilde{\mathcal{O}}(\Delta)$, while in our algorithm no such assumption is needed. This makes our algorithm far more efficient when the spectral gap Δ is small but we only need to estimate the ground energy to precision h much larger than Δ. Moreover, our algorithms also use significantly fewer ancilla qubits outside of those needed for block-encoding than both the phase estimation algorithm and the algorithms in Ref. [6].

Optimality of our algorithms (Theorems 8 and 9): Besides the complexity upper bound above we also provided lower bounds in our work to show our ground state preparation algorithms achieve essentially the optimal dependence on γ and Δ (Theorem 8) in the number of queries to both U_H and U_I. For the ground energy estimation problem our result is less complete. We proved that the dependence on the precision h in the number of queries to U_H is near-optimal (Theorem 9). This result can also be derived from the proof of the optimality of the phase estimation algorithm [4].

4 Methodology

The basic tools we use to perform non-unitary operations are block-encoding [3, 7, 12] and quantum signal processing (QSP) [7, 11]. We briefly discuss them below.

Block-encoding and quantum signal processing: A matrix $A \in \mathbb{C}^{N\times N}$ where $N = 2^n$ can be encoded in the upper-left corner of an $(m+n)$-qubit unitary matrix if $\|A - \alpha(\langle 0^m| \otimes I)U(|0^m\rangle \otimes I)\| \leq \epsilon$. In this case we say U is an (α, m, ϵ)-block-encoding of A. Many matrices of practical interests can be efficiently block-encoded. In particular we discuss the block-encoding of Hamiltonians of physical systems in Section 7. With the block-encoding of a Hermitian matrix we can implement polynomial eigenvalue transformations of this matrix through QSP, which is also known as quantum singular value transformation.

With these tools we can solve the ground energy estimation and ground state preparation problems through the following procedure.

Implementation of the reflection and projection operators: Since we assume the block-encoding of the Hamiltonian H is given, we use QSP to implement the reflection and projection operators associated with the low-energy subspace (Lemma 3). This requires a polynomial approximation of the sign function (Lemma 2). The application of the projction operator directly enables us the prepare the ground state under assumptions (P1) and (P2), which leads to Theorem 4.

The binary search procedure: With the projection, and using amplitude estimation, for any x we can output either $\lambda_0 > x - h$ or $\lambda_0 < x + h$ correctly with high probability. The success probability can be made at least $1 - \delta$ with only $\log(\delta^{-1})$ query complexity overhead using a procedure we call binary amplitude estimation (Lemma 5). This enables us to perform a binary search to locate the ground energy λ_0 as shown in Algorithm 1. The above procedure enables us to estimate the ground energy under assumption (P1), which leads to Theorem 6. We can couple the ground energy estimation algorithm with the ground state preparation algorithm to obtain the ground state without knowing an upper bound for the ground energy, which gives us Corollary 7.

The unstructured search problem and the approximate counting problem: In order to show the optimality of our algorithms we consider the unstructured search problem and the approximate counting problem, whose complexity lower bounds have been extensively studied [2, 13]. We convert the unstructured search problem to several different ground state preparation problems, creating trade-offs between the spectral gap and the overlap, and in this way prove the optimality of the dependence on the spectral gap Δ and the overlap γ in our ground state preparation algorithm (Theorem 8). Similarly we convert the approximate counting problem into a ground energy estimation problem and prove the optimal dependence on the precision (Theorem 9).

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