The QMA-hard (and also hard) Local Hamiltonian Ground State Problem

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This paper introduces the quantum local Hamiltonian ground state problem and its relationship with the problem class Quantum Merlin Arthur (QMA). Derivation regarding the QMA-hardness for 5-local Hamiltonian problem is shown to some extent.

INTRODUCTION

The computation of ground state energy of a Hamiltonian has always been a hot topic due to its applications in areas such as solid state physics. And we expect to apply quantum computing to this type of problem, making use of its great potential in calculations. This paper introduces the classical complexity theory first. Then, the quantum Hamiltonian problem and its problem class QMA are introduced. Then, we show that QMA problems can reduce to 5-local Hamiltonian problem, which means that 5-local Hamiltonian problem is QMA-hard. At the end, we briefly mentioned some results from other paper regarding QMA-completeness and 2-local Hamiltonian problem.

CLASSICAL COMPLEXITY

Computation complexity measures how hard a certain computational task is. And two complexity classes, P and NP, are of interest here (since the QMA problems depend on the quantum analog of NP classes.) Decision problems such that some algorithm can provide answer in polynomial time belongs to class P. And if the problem's answer cannot be found quickly, but it is possible to verify an answer within polynomial time, then that problem is in class NP [4]. A problem L is NP-complete if it is in class NP and every other NP-problem can be reduced to L. This means that by solving only one L efficiently, all NP-problems are solved efficiently as well [3]. This shows why we are interested in such problems, and also their quantum analogs.

Classical local Hamiltonian ground state

A type of problem, k-SAT is related to our discussion of local Hamiltonian. Here, the k indicates the number of literals in each clause, where a literal means a variable or its negation and a clause is a disjunction of literals. For a k-SAT problem, we have a CNF formula f (consists of AND's of several clause) in which each clause has exactly k literals, and we need to decide whether or not f is satisfiable [3]. k-SAT with $k \geq 3$ problems are shown to be NP-complete by Cook-Levin Theorem. And if we replace each clause with a classical 3-local Hamiltonian, 3-SAT problem reduces to a classical 3-local Hamiltonian ground state problem. The task of finding a 3-local Hamiltonian is at least as hard as 3-SAT and any problems in class NP, which makes it NP-hard.

QUANTUM HAMILTONIAN PROBLEM AND QMA

The difficulty even for classical case is apparent – there are many local energy minima for each local Hamiltonian that do not minimize energy globally. And as we can predict, the quantum version only gets worse since local Hamiltonians might not commute with each other. We begin defining the quantum analog of NP class, followed by the quantum Hamiltonian problem.

QMA class

The quantum analog of NP class is called QMA. And the following definition of QMA is adapted and combined from [3] and [2]:

A language L is in QMA if there exists a uniform quantum circuit family V and a single qubit measurement $\{E_0,E_1\}$ such that

1. V has polynomial size.
2. If $x \in L$, then there exists a quantum witness $|\psi\rangle_x$ such that $|\psi\rangle = V(|\psi\rangle_x \otimes |x\rangle \otimes |0\rangle^*)$ such that probability of V accepts the input is Pr[accept]$= \langle\psi|E_1|\psi\rangle \geq 1 - \epsilon$ (Completeness).
3. If $x \notin L$, then Pr[accept]$= \langle\psi|E_1|\psi\rangle \leq \epsilon$ for all potential witnesses $|\psi\rangle_x$ (Soundness).

Here, $V = U_T U_{T-1} ... U_1$ where U_t are local elementary gates, $|x\rangle$ is the input, and $|0\rangle^*$ is a collection of scrap qubits initialized in zero-state, and we take $|\psi_0\rangle = |\psi\rangle_x \otimes |x\rangle \otimes |0\rangle^*$

Quantum k-local Hamiltonian problem

The definition of k-local Hamiltonian problem is (from [3] and [2]):

> Assume we have a n-qubit Hamiltonian, $H = \Sigma_a H_a$, where H_a acts on at most k qubits. Given two numbers E_{low}, and E_{high} where $E_{\text{high}} - E_{\text{low}} > \frac{1}{\text{poly(n)}}$. The local Hamiltonian problem decides if there exists ground state energy $E_0 \leq E_{\text{low}}$ or $E_0 > E_{\text{high}}$. So we can determine E_0 up to the accuracy of $\frac{1}{\text{poly(n)}}$.

k-local Hamiltonian problem is QMA-hard

In this section, we want to show that k-local Hamiltonian problem is QMA-hard based on their definition in the previous section, i.e. any QMA problems can be reduced into a local Hamiltonian problem.

Based on the definition of QMA, we construct [3]

$$|\eta\rangle = \frac{1}{\sqrt{T+1}} \Sigma_{t=0}^{T} |\psi(t)\rangle \otimes |t\rangle \,, |\psi(t)\rangle = (U_t U_{t-1} ... U_0) |\psi_0\rangle \,,$$

as a quantum witness for the entire procedure. $|\psi(t)\rangle$ is the state after t steps of the quantum circuit, and $|t\rangle$ (clock register) records the time flow where $t \in \{0, 1, ..., T\}$.

Next, we define a Hamiltonian $H = H_{\text{in}} + H_{\text{out}} + H_{\text{prop}} + H_{\text{clock}}$ which checks the history. And $|\eta\rangle$ is in a low energy state of H if and only if the history is valid and accepts the witness. The purpose of H_{in} is to check whether the input qubits are properly initialized. For each qubit that is not properly initialized, the Hamiltonian adds an "energy penalty" of 1. Similarly, H_{out} adds energy penalty of 1 if the output qubit at time T is $|0\rangle$ instead of $|1\rangle$. H_{prop} checks if every step of V is executed correctly. And H_{clock} enforces encoding of clock (the definition in [3] and [2] differs, [2] does not include the term H_{clock}).

Completeness gives E_{low}

If we were to live in a perfect world that V accepts the input with probability of 1 when $x \in L$, then H_{out} incurs zero penalty. However, from the definition of QMA completeness, we see that Pr[accept] is $1-\epsilon$ which means that we might end up with $|0\rangle$ at time T with a probability ϵ. So we have $E_0(x \in L) \leq \langle\eta|H_{\text{out}}|\eta\rangle = \frac{\epsilon}{T+1}$.

Soundness gives E_{high}

The QMA soundness gives E_{high} and ensures the gap between E_{high} and E_{low}. Due to the complication of the calculation, I only briefly outlined the procedure, the detailed calculation is shown in [3].

- Apply change of basis to H_{prop} and then diagonalize the matrices by Fourier transform. The Hamiltonian has a spectral gap of $\frac{\pi^2}{2(T+1)^2}$
- Diagonalizing $H' = H_{\text{in}} + H_{\text{out}}$, and since the energy penalty is at least 1, so the total Hamiltonian has a spectral gap of 1.
- Since there is a small probability ϵ of wrongly accepting a computation, so we can assume there is a large relative angle between the null spaces of H' and H_{prop}. By considering the projection of $H' + H_{\text{prop}}$ onto null spaces and relative geometry between null spaces (and pages of algebra), we get a relationship that $E_0(x \notin L) \geq \frac{1-\sqrt{\epsilon}}{(T+1)^3}$

To conclude, we start from QMA problem conditions and show that they can be reduced to a problem of determining whether the ground state energy of a Hamiltonian is below a value E_{low} or above a value E_{high}. This is getting close to the definition of local Hamiltonian problem!

Complication of locality

To fully analyze the Hamiltonian H, we need to consider H_{clock} and its locality. One simple way of constructing the $|t\rangle$ states is to have $|t=0\rangle = |00...0\rangle \,, |t=1\rangle = |10...0\rangle \,, |t=2\rangle = |11...0\rangle \,, ..., |t=T\rangle = |11...1\rangle$. The Hamiltonian is defined as $H_{\text{clock}} = \Sigma_{t=1}^{T-1} (|01\rangle \langle 01|)_{t,t+1}$ [3] so that only strings that do not have 0 followed by 1 are valid representations. In H_{prop}, there is a tensor product of the form $U_t \otimes |t\rangle \langle t-1|$. The term $|t\rangle \langle t-1|$ acts on 3 qubits, and U_t acts on 2 qubits by definition. The other Hamiltonians only involve terms acting on less than 5 qubits. This means that our Hamiltonian is a 5-local Hamiltonian, and we conclude that 5-local Hamiltonian is QMA-hard.

RELATED CONCLUSIONS FOR QMA-COMPLETENESS AND k-LOCAL HAMILTONIAN

Going beyond QMA-hard for 5-local Hamiltonian, if we wish to prove QMA-completeness, we need to show that the local Hamiltonian problem is in QMA other than showing it is QMA-hard. For this proof, I would like to redirect readers to Proposition 14.2 in [2].

QMA-completeness for $k \geq 3$ has been known for a while before the publication of the milestone paper by Kempe, Kitaev and Regev [1]. The authors proved that 2-local Hamiltonian problem is also QMA-complete using two independent methods. The first method is based on projection lemma, which allows us to successively cut out parts of the Hilbert space by giving them large penalty. The second method relies on third order perturbation theory. Both methods are rather long and complicated, and I would like to revisit this paper when I have the chance.

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