On physical problems that are slightly more difficult than $QMA$

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Abstract

We study the complexity of computational problems from quantum physics. Typically, they are studied using the complexity class $QMA$ (quantum counterpart of $NP$) but some natural computational problems appear to be slightly harder than $QMA$. We introduce new complexity classes consisting of problems that are solvable with a small number of queries to a $QMA$ oracle and use these complexity classes to quantify the complexity of several natural computational problems (for example, the complexity of estimating the spectral gap of a Hamiltonian).

1 Introduction

Quantum Hamiltonian complexity [30] is a new field that combines quantum physics with computer science, by using the notions from computational complexity to study the complexity of problems that appear in quantum physics.

One of central notions of Hamiltonian complexity is the complexity class $QMA$ [25, 24, 40, 21, 3] which is the quantum counterpart of $NP$. $QMA$ consists of all computational problems whose solutions can be verified in polynomial time on a quantum computer, given a quantum witness (a quantum state on a polynomial number of qubits).

$QMA$ captures the complexity of several interesting physical problems. For example, estimating the ground state energy of a physical system (described by a Hamiltonian) is a very important task in quantum physics. We can characterize the complexity of this problem by showing that it is $QMA$-complete, even if we restrict it to natural classes of Hamiltonians.

One such natural restriction is to assume that the Hamiltonian is a sum of terms in which each term is determined by interaction among at most $k$ particles, for some small $k$. Estimating the ground state energy of such a Hamiltonian is known as the $k$-local Hamiltonian problem [22, 21]. This problem is $QMA$-complete for any $k \geq 2$ [21]. $QMA$-completeness also holds if we assume a natural geometric structure on the particles, with particles arranged on a grid and each particle interacting with its nearest neighbours [29] or restrict the Hamiltonian to certain natural interactions between qubits [5].
QMA-completeness has been used to characterize the complexity of many computational problems in quantum physics. (A number of other QMA-complete problems are given in [6].) But some natural physical problems seem to have a complexity that is slightly above QMA. For example, one such problem is estimating the spectral gap of a Hamiltonian $H$. The spectral gap of $H$ is the difference $\lambda_2 - \lambda_1$ between the energy $\lambda_1$ of the ground state and the energy $\lambda_2$ of the state with the next smallest energy. To verify that $H$ has a spectral gap that is at least $\lambda$, one has to verify two statements:

(a) The ground state energy $\lambda_1$ is at most $a$, for some $a$;

(b) Any state that is orthogonal to the ground state has the energy at least $a + \lambda$.

The first statement can be verified by a quantum algorithm $V$ that takes the ground state $|\psi\rangle$ and estimates its energy. However, the second statement is hard to verify: a quantum algorithm can verify the existence of a state with energy at most $a + \lambda$ but not its non-existence!

In classical complexity theory, problems of similar nature are studied using generalizations of NP such as:

- $DP$, the class of “differences” of two NP-complete problems, introduced by Papadimitriou and Yannakakis [33].
- The Boolean hierarchy, a sequence of complexity classes defined by taking intersections and unions of sets in $NP$ and $coNP$ [11, 41, 38, 9, 10].
- $P^{NP[\log n]}$, the class of problems that are solvable in polynomial time, if the algorithm is allowed to make $O(\log n)$ queries to an NP oracle [8, 39].

There is a rich theory of such complexity classes and a number of natural computational problems have been shown to be complete for one of them (e.g., [37, 32, 12, 18, 17, 27]).

In this paper, we connect this theory with quantum Hamiltonian complexity, by introducing $DQMA$ and $P^{QMA[\log n]}$, the quantum counterparts of $DP$ and $P^{NP[\log n]}$. It turns out that these complexity classes are exactly the right tool for characterizing the complexity of natural computational problems (such as the spectral gap problem mentioned above) in quantum physics!

Namely, we have:

- The problem of determining whether the ground state energy of a local Hamiltonian is close to a given value $a$ (as opposed to being substantially larger or substantially smaller) is $DQMA$-complete;

- The ground state simulation problem[30] in which we are given a Hamiltonian $H$ and an observable $A$ and have to distinguish whether the expectation of $A$ in the ground state of $H$ is at least $a + \epsilon$ or at most $a - \epsilon$ is $P^{QMA[\log n]}$-complete.
Among these two problems, the second one is particularly interesting: determining the expectation of an observable $A$ in a ground state of a Hamiltonian $H$ is important in many situations in quantum physics. It was known that this problem is QMA-hard [30] but our result shows that it is probably harder than that (unless $P^{QMA[\log n]} = QMA$ which is unlikely).

For the problem of estimating the spectral gap of a Hamiltonian, we show that it is in $P^{QMA[\log n]}$ and it is hard for a smaller complexity class, $P^{UQMA[\log n]}$ where queries to the QMA oracle must be instances of QMA with either a unique witness or with no witness. It is not clear whether it is complete for any of these two classes.

Our results show that the complexity classes slightly above QMA (which have not studied before) are quite useful for analyzing computational problems in quantum physics. We expect that continuing this line of research could lead to other interesting discoveries.

1.1 Related work

While QMA has been studied in detail, there has been fairly little work on generalizations of QMA in directions similar to one that is considered in this paper.

The two main exceptions as as follows. First, Brown et al. [7] and Shi and Zhang [35] have studied the complexity class $\#QMA$ which is the quantum counterpart of $\#P$. The starting point for this work consists of two computational questions from quantum physics:

- Determining how degenerate is the ground state of a Hamiltonian $H$ (determining the dimensionality of the eigenspace with the smallest eigenvalue);
- Density of states problem: determine the number of eigenvalues of $H$ in a given interval $[\lambda_1, \lambda_2]$ (allowing to miscount the eigenvalues in the intervals $[\lambda_1, \lambda_1 + \frac{1}{n^c}]$ and $[\lambda_2 - \frac{1}{n^c}, \lambda_2]$ around the endpoints of $[\lambda_1, \lambda_2]$).

Brown et al. [7] show that both of those problems are complete for $\#QMA$ and that the class $\#QMA$ is equivalent to $\#P$ (i.e. $P^{\#P} = P^{\#QMA}$). The second result has been obtained independently by Shi and Zhang [35].

Our problem of estimating the spectral gap is related to the degeneracy problem in [7]: if the ground state is degenerate, the spectral gap is 0. The degeneracy problem is, however, much more general and, because of that, it has much higher complexity ($\#QMA = \#P$) than the problems in this paper (which are solvable with a small number of queries to a QMA oracle). As a result, the generalizations of QMA in [7] and in the current paper are completely different.

Second, Gharibian and Kempe [15] have studied a complexity class $cc - \Sigma_2$ which generalizes the classical class $\Sigma_2^p = NP^NP$. A problem is in $cc - \Sigma_2$ if, for any YES instance $x$, there exists a polynomial sized classical proof $y$ such that for all polynomial size quantum proofs $|\psi\rangle$, the verifier accepts $x, y$ and $|\psi\rangle$. Gharibian and Kempe [15] then show $cc - \Sigma_2$ hardness for several quantum counterparts of classical $\Sigma_2^p$-complete problems.

It is easy to see that $cc - \Sigma_2$ contains our class $DQMA$. The relation between $cc - \Sigma_2$ and $P^{QMA[\log n]}$ is unclear: $cc - \Sigma_2$ can be viewed as an NP algorithm which is allowed to
make one QMA query. This is stronger than \( P^{QMA[\log n]} \) in terms of the classical part (\( NP \) instead of \( P \)) but only allows one query to QMA.

Apart from [7, 35, 15], we are not aware of any work that is more than distantly related. [26, 1, 16] and many others have studied QMA\((k)\), a generalization of QMA in which we are given several witness states \(|\psi_1\rangle, \ldots, |\psi_k\rangle\) with a promise that they are not entangled. Both QMA\((k)\) and the complexity classes in the current paper are larger than QMA but, apart from that, they do not seem to be related.

The complexity of spectral gap has also been studied in the context when the number of qubits grows to infinity (and the Hamiltonian is translationally invariant and, hence, can be described by a finite number of qubits) [13]. In this case, estimating the spectral gap becomes undecidable. This is somewhat similar to the undecidable tiling problems in which one has to decide whether it is possible to tile an infinite plane using a finite set of tiles [4] and the proof of undecidability of the spectral gap [13] uses the undecidability of the tiling problem. The setting of this work is completely different from ours (in which every instance of the spectral gap has a fixed number of qubits \( n \)) and there is no relation between the results.

2 Technical preliminaries

2.1 Notation

We assume that we have a physical system consisting of \( n \) qubits. The evolution of a physical system is described by a Hamiltonian \( H \) which is a Hermitian operator acting on the state-space of the system. If \(|\psi(t)\rangle\) is the state of the system at time \( t \), then we have

\[
\frac{d|\psi(t)\rangle}{dt} = H|\psi(t)\rangle.
\]

In principle, any Hermitian \( H \) can be a Hamiltonian of a physical system. On the other hand, Hamiltonians of actual physical systems usually satisfy various locality constraints.

For example, a Hamiltonian may be formed by a combination of interactions, each of which involves at most \( k \) particles (qubits). Such Hamiltonians are called \( k \)-local. More formally, \( H \) is \( k \)-local if we can express it as \( H = \sum_i H_i \), with each \( H_i \) depending only on at most \( k \) qubits. Throughout this paper, we assume that Hamiltonians \( H \) are scaled so that all eigenvalues of \( H \) are between 0 and \( O(n^c) \) for some \( c \) that is independent of \( n \).

Mathematically, we can regard a Hamiltonian \( H \) as a \( D \times D \) Hermitian matrix. The ground state of a Hamiltonian is just the eigenstate \(|\psi\rangle\): \( H|\psi\rangle = \lambda|\psi\rangle \) with the smallest eigenvalue \( \lambda \). In physics terminology, the eigenvalue \( \lambda \) is often called the energy of the state \(|\psi\rangle\). The degeneracy of the ground state is the dimension of the subspace consisting of all \(|\psi\rangle\): \( H|\psi\rangle = \lambda|\psi\rangle \) with the smallest \( \lambda \).

An observable is a Hermitian operator (which can be described by a Hermitian matrix) which corresponds to a quantity of a physical system that can be measured. The value of an observable \( O \) on a state \(|\psi\rangle\) is just \langle \psi | O | \psi \rangle\). Often, observables are also \( k \)-local.
2.2 Background on QMA

We define the complexity class $QMA(c, s)$ to consist of all promise problems $L$ for which there exists a polynomial-time quantum algorithm $M(x, |\psi\rangle)$ such that:

- if $L(x) = 1$, there exists $|\psi\rangle$ such that $M(x, |\psi\rangle)$ outputs 1 with probability at least $c$;
- if $L(x) = 0$, then for any $|\psi\rangle$, $M(x, |\psi\rangle)$ outputs 1 with probability at most $s$.

We define $QMA = QMA(2/3, 1/3)$. It is known that the definition is robust w.r.t. choice of $c$ and $s$:

**Theorem 1** [24] $QMA = QMA(c, s)$ for any $c$ and $s$ such that $c \leq 1 - 2^{-p(x)}$, $s \geq 2^{-p(x)}$ and $c - s \geq \frac{1}{p(x)}$ for some polynomial $p(x)$.

$QMA$ is sometimes called “Quantum NP” and was first introduced by Kitaev [23, 24] as a quantum counterpart of the classical complexity class $NP$. Instead of a classical witness and a classical verification algorithm in the definition of $NP$, we have a quantum state $|\psi\rangle$ as a witness and a quantum algorithm for verifying this witness. Since the output of a quantum algorithm is probabilistic, it is natural to allow a small probability of error, making the definition of $QMA$ similar to the classical complexity class $MA$.

$QMA$ includes many natural computational problems from quantum physics. A prototypical $QMA$-complete problem is $k$-LOCAL HAMILTONIAN($H, a, b$). In this problem, we are given a Hamiltonian $H$ (which can be expressed as $H = \sum_i H_i$ with each $i$ being $k$-local for a constant $k$) acting on $n$ qubits and real numbers $a, b$: $b \geq a + \frac{1}{p(x)}$ (where $c$ is a fixed constant). The task is to distinguish between the two cases:

- $k$-LOCAL HAMILTONIAN($H, a, b$) = 0: the ground state energy of $H$ is at least $b$;
- $k$-LOCAL HAMILTONIAN($H, a, b$) = 1: the ground state energy of $H$ is at most $a$ under a promise that one of those two cases occurs.

We can always modify the Hamiltonian $H$ so that it has a state with energy exactly $b$. Therefore, we can modify the promise to “the ground state energy is either at most $a$ or is exactly $b$”.

**Theorem 2** [21] 2-LOCAL HAMILTONIAN is $QMA$-complete.

**Closure properties** $QMA$ satisfies closure properties that are similar to the closure properties of NP. Let $L_1$ and $L_2$ be two promise problems. We define $L = L_1 \land L_2$ by $L(x) = L_1(x) \land L_2(x)$ and $L = L_1 \lor L_2$ by $L(x) = L_1(x) \lor L_2(x)$. (In both cases, if one of $L_1(x)$ and $L_2(x)$ is undefined, $L(x)$ is undefined as well.) It is easy to show

**Theorem 3** If $L_1 \in QMA$, $L_2 \in QMA$, then $L_1 \land L_2 \in QMA$ and $L_1 \lor L_2 \in QMA$. 

2.3 QMA with unique witnesses

UQMA is a variant of QMA in which we require the quantum witness $|\psi\rangle$ to be unique in the $L(x) = 1$ case. It is non-trivial to define when a quantum witness is “unique” because the space of all witnesses $|\psi\rangle$ is continuous. Therefore, if $M(x, |\psi\rangle)$ outputs 1 with a probability $p > 2/3$, then $M(x, |\psi'\rangle)$ will also output 1 with probability at least $2/3$ whenever $|\psi'\rangle$ is sufficiently close to $|\psi\rangle$.

The solution to this problem is as follows. We say that a quantum witness $|\psi\rangle$ is unique if $M$ rejects any $|\psi'\rangle \perp |\psi\rangle$ with a high probability. Then, the only witnesses $|\phi\rangle$ that are accepted are the ones that have a sufficiently high overlap with $|\psi\rangle$.

**Definition 1** [2] The complexity class $UQMA(c, s)$ consists of all promise problems $L$ for which there exists a polynomial-time quantum algorithm $M(x, |\psi\rangle)$ such that:

- if $L(x) = 1$, there exists $|\psi\rangle$ such that
  - (a) $M(x, |\psi\rangle)$ outputs 1 with probability at least $c$;
  - (b) If $|\psi'\rangle \perp |\psi\rangle$, then $M(x, |\psi'\rangle)$ outputs 1 with probability at most $s$.
- if $L(x) = 0$, then for any $|\psi\rangle$, $M(x, |\psi\rangle)$ outputs 1 with probability at most $s$.

Classically, we can reduce general instances of problems in $NP$ to instances with a unique witness (this is the well-known Valiant-Vazirani theorem [37]). It is not known whether a similar result is true in the quantum case [2, 20].

An example of a problem in $UQMA$ is UNIQUE $k$-LOCAL HAMILTONIAN($H, a, b$) in which $H, a, b$ are similar to $k$-LOCAL HAMILTONIAN and the task is to distinguish between the two cases:

- UNIQUE $k$-LOCAL HAMILTONIAN($H, a, b$) = 0: the ground state energy of $H$ is at least $b$;
- UNIQUE $k$-LOCAL HAMILTONIAN($H, a, b$) = 1: the ground state energy of $H$ is at most $a$ and any other eigenstate of $H$ has the energy at least $b$.

under a promise that one of those two cases occurs.

$UQMA$-complete problems have not been studied before but we can show that this problem is complete for $UQMA$, similarly to how $k$-LOCAL HAMILTONIAN is $QMA$-complete.

**Theorem 4** $UNIQUE 3$-LOCAL HAMILTONIAN is $UQMA$-complete.

The theorem follows by adapting the proof that 3-LOCAL HAMILTONIAN is $QMA$-complete by Kempe and Regev [22]. We include it in appendix B.

It is plausible that the proof of $QMA$-completeness of 2-LOCAL HAMILTONIAN by Kitaev, Kempe and Regev [21] can be adapted to show that $UNIQUE 2$-LOCAL HAMILTONIAN is $UQMA$-complete but we have not verified that.
3 Our results

3.1 Problems slightly beyond QMA

We now consider three problems whose true complexity seems to be slightly beyond QMA.

1. Given a Hamiltonian $H$, is it true that its ground state energy is close to a given number $a$?

**Definition 2** \textsc{Exact $k$-Local Hamiltonian} $(H, a, \epsilon, \delta)$.

Given a Hamiltonian $H$ and real numbers $a, \epsilon, \delta$: $\epsilon \geq \frac{1}{n^c}, \delta \geq \frac{1}{n^c}$, distinguish between the following two cases:

- \textsc{Exact $k$-Local Hamiltonian} $(H, a, \epsilon, \delta) = 0$: the ground state energy of $H$ is in the interval $[a - \epsilon, a + \epsilon]$;
- \textsc{Exact $k$-Local Hamiltonian} $(H, a, \epsilon, \delta) = 1$: the ground state energy of $H$ does not belong to the interval $[a - \epsilon - \delta, a + \epsilon + \delta]$.

2. Given a Hamiltonian $H$, estimate its spectral gap: the difference $\lambda_2 - \lambda_1$ where $\lambda_1$ and $\lambda_2$ are the two smallest eigenvalues of $H$.

The spectral gap $\lambda_2 - \lambda_1$ is an important physical quantity in several contexts. In the context of quantum computing, it is related to the running time of adiabatic quantum algorithms [14] which roughly scales as $\frac{1}{(\lambda_2 - \lambda_1)^2}$. To estimate the running time, we are interested in distinguishing whether the spectral gap is small (close to 0) or large. We can formalize this as

**Definition 3** \textsc{Spectral Gap} $(H, \epsilon)$.

Given a Hamiltonian $H$ and a real number $\epsilon \geq \frac{1}{n^c}$, distinguish between two cases:

- \textsc{Spectral Gap} $(H, \epsilon) = 1$: $\lambda_2 - \lambda_1 \leq \epsilon$;
- \textsc{Spectral Gap} $(H, \epsilon) = 0$: $\lambda_2 - \lambda_1 \geq 2\epsilon$.

3. In the ground state simulation problem [30], we are given a Hamiltonian $H$ (we assume that $H$ is $k$-local) and a physical quantity described by an observable $A$ (we also assume that $A$ is $k$-local). The task is to estimate $\langle \psi | A | \psi \rangle$ where $| \psi \rangle$ is the ground state of $H$. We can turn this into a (promise) decision problem in a standard way: we define that the task is to output 1 if $\langle \psi | A | \psi \rangle \leq \alpha_1$ and to output 0 if $\langle \psi | A | \psi \rangle \geq \alpha_2$ for some $\alpha_1, \alpha_2$: $\alpha_1 < \alpha_2$, $\alpha_2 - \alpha_1 = \Omega(1/n^c)$.

We can study this problem in two versions: exact or approximate:

**Definition 4** \textsc{Exact-Simulation} $(H, A, \alpha_1, \alpha_2)$.

Given a Hamiltonian $H$, an observable $A$ and numbers $\alpha_1, \alpha_2$ with $\alpha_2 - \alpha_1 \geq \frac{1}{n^c}$ (where $n$ is the input size), distinguish between the following two cases:
• $\text{EXACT-SIMULATION} = 1$ if $H$ has a ground state $|\psi\rangle$ with $\langle \psi | A | \psi \rangle \leq \alpha_1$;

• $\text{EXACT-SIMULATION} = 0$ if $H$ has no ground state $|\psi\rangle$ with $\langle \psi | A | \psi \rangle \leq \alpha_2$.

Definition 5 $\text{APPROX-SIMULATION}(H, A, \alpha_1, \alpha_2, \epsilon)$.

Given a Hamiltonian $H$, an observable $A$ and numbers $\alpha_1, \alpha_2, \epsilon$ with $\alpha_2 - \alpha_1 \geq \frac{1}{n^c}$, $\epsilon \geq \frac{1}{n^c}$, distinguish between the following two cases:

• $\text{APPROX-SIMULATION} = 1$ if $H$ has a ground state $|\psi\rangle$ with $\langle \psi | A | \psi \rangle \leq \alpha_1$;

• $\text{APPROX-SIMULATION} = 0$ if, for any $|\psi\rangle$ with $\langle \psi | H | \psi \rangle \leq \lambda + \epsilon$ (where $\lambda$ is the smallest eigenvalue of $H$), we have $\langle \psi | A | \psi \rangle \geq \alpha_2$.

In this paper, we study $\text{APPROX-SIMULATION}$ because it is more similar in spirit to the other problems that we consider. We also think that it may be more natural because it is more robust w.r.t. small perturbations in the Hamiltonian $H$.

For all of these 3 problems, to verify that $P = 1$ we must verify a combination of a statement that involves existence of a quantum state with certain properties with a statement that involves non-existence of a quantum state. For example, for $\text{EXACT } k\text{-LOCAL HAMILTONIAN}$, we have to verify that

(a) There exists a state $|\psi\rangle$ such that $\langle \psi | H | \psi \rangle \leq a + \epsilon$;

(b) There is no state $|\psi\rangle$ such that $\langle \psi | H | \psi \rangle \leq a - \epsilon - \delta$.

The first statement can be verified in $\text{QMA}$ but the second statement is an opposite of what can be verified in $\text{QMA}$.

3.2 Complexity results

In classical complexity theory [31, Chapter 17.1], such problems are characterized using complexity classes that are slightly above $\text{NP}$. One such class is $\text{DP}$ [33] which consists of all languages $L$ such that $L = L_1 \cap L_2$, $L_1 \in \text{NP}$, $L_2 \in \text{coNP}$. Examples of problems belonging to $\text{DP}$ are:

• $\text{EXACT TSP}$: we are given an instance of traveling salesman problem (TSP) and have to determine if the shortest TSP tour has the length exactly $k$;

• $\text{UNIQUE SAT}$: we have to determine whether a SAT formula has exactly one satisfying assignment

• $\text{CRITICAL SAT}$: we have to determine whether it is true that a SAT formula is unsatisfiable but removing an arbitrary clause from it would result in a satisfiable formula.
In all of those cases, it is easy to show that the problem is in DP, by expressing it as a combination of two statements, one of which can be verified in NP and the other is a negation of a statement that can be verified in NP. Interestingly, all 3 of those problems are also DP-complete (as shown by Papadimitriou and Yannakakis [33], Valiant and Vazirani [37] and Papadimitriou and Wolfe [32], respectively).

We can characterize the complexity of EXACT k-LOCAL HAMILTONIAN by a new quantum complexity class DQMA (which is a quantum counterpart of DP).

**Definition 6** DQMA is a class consisting of all promise problems L for which we have $L_1, L_2 \in QMA$ such that:

- If $L(x) = 1$ then $L_1(x) = 1$ and $L_2(x) = 0$;
- If $L(x) = 0$ then $L_1(x)$ and $L_2(x)$ are both defined and either $L_1(x) = 0$ or $L_2(x) = 1$.

**Theorem 5** EXACT 3-local HAMILTONIAN is DQMA-complete.

**Proof:** In section A.1.

The other two problems (APPROX-SIMULATION and SPECTRAL GAP) are more difficult. If we are given a QMA oracle, we can solve APPROX-SIMULATION with $O(\log n)$ queries to the oracle, in a following way:

1. We use the QMA oracle and binary search to obtain an estimate $a$ for $\lambda_1$ (the smallest eigenvalue of $H$) such that $\lambda_1 \in [a, a + \epsilon/2]$;
2. We use one more query to the QMA oracle to verify the statement: “there exists $|\psi\rangle$ which is a linear combination of eigenvectors of $H$ with eigenvalues in $[a, a + \epsilon/2]$ and satisfies $\langle \psi | A | \psi \rangle \leq \alpha_1$”.

For the first step, we need $O(\log \frac{1}{\epsilon}) = O(\log n)$ queries to obtain an estimate $a$ with a sufficient precision. The second step requires 1 query.

This shows that APPROX-SIMULATION belongs to a complexity class $P^{QMA[\log n]}$ in which a polynomial time classical algorithm $M$ is allowed to make $O(\log n)$ queries to an oracle solving a promise problem in QMA. APPROX-SIMULATION is also complete for this complexity class.

**Theorem 6** APPROX-SIMULATION is $P^{QMA[\log n]}$-complete.

**Proof:** In section A.2.

SPECTRAL GAP also belongs to $P^{QMA[\log n]}$ (by a similar binary search argument) but it is not clear whether it is $P^{QMA[\log n]}$-complete.

The reason why it is difficult to show $P^{QMA[\log n]}$-hardness of SPECTRAL GAP is as follows. We assume that we are trying to embed a computation consisting of $O(\log n)$ queries to a QMA oracle into one instance of SPECTRAL GAP. We can assume that the queries are to an oracle solving k-LOCAL HAMILTONIAN problem. Then, it could be the
case that the Hamiltonians $H$ in the queries have very small spectral gaps (of the order smaller than $1/n^c$ for any fixed $c$). In this case, it is difficult to expect that the Hamiltonian for SPECTRAL GAP obtained by combining them would have a larger spectral gap of order $\Omega(1/n^c)$, as required in the case when SPECTRAL GAP=0.

If this problem does not arise (i.e., if all queries are to instances of UNIQUE $k$-LOCAL HAMILTONIAN), we can embed a computation involving $O(\log n)$ queries to a QMA oracle into an instance of SPECTRAL GAP. Since UNIQUE $k$-LOCAL HAMILTONIAN is $UQMA$-complete, this gives us

**Theorem 7**  
(a) $\text{SPECTRAL GAP} \in P^{QMA[\log n]}$;  
(b) $\text{SPECTRAL GAP}$, for $O(\log n)$-local Hamiltonians, is $P^{UQMA[\log n]}$-hard.

**Proof:** In section A.3

We note that SPECTRAL GAP is probably not in $P^{UQMA[\log n]}$, for the following reason. Let $H$ be the Hamiltonian that is the input for the SPECTRAL GAP problem. If the spectral gap of $H$ is small, then it is likely that the query Hamiltonians (which are produced from $H$) will also have a small spectral gap and, thus, they will not be instances of a $UQMA$ problem.

### 4 Conclusion

In this paper, we have connected complexity classes defined using a small number of queries to an $NP$ oracle with quantum Hamiltonian complexity, by introducing $DQMA$ and $P^{QMA[\log n]}$, the quantum counterparts of $DP$ and $P^{NP[\log n]}$. We then used the new complexity classes to characterize the complexity of several natural computational problems (such as simulation problem and spectral gap) in quantum physics.

Some of the problems that we study have been known to be $QMA$-hard but not in $QMA$. Yet, the possibility of capturing the complexity of these problems via complexity classes slightly above $QMA$ was not noticed before.

We think that this is just the beginning for a new research area further work in this direction can lead to other interesting discoveries. Some specific open questions resulting from our work are:

1. Can we quantify the complexity of SPECTRAL GAP more precisely?

2. What can we prove about the complexity of EXACT-SIMULATION? Intuitively, it should be much harder than APPROX-SIMULATION because very small changes to the Hamiltonian $H$ can change an instance with $\text{EXACT-SIMULATION}(H) = 1$ into an instance with $\text{EXACT-SIMULATION}(H) = 0$.

3. Our hardness results use 3-local Hamiltonians for EXACT $k$-LOCAL HAMILTONIAN and $O(\log n)$-local Hamiltonians for APPROX-SIMULATION and SPECTRAL-GAP.
Since most of Hamiltonians which actually occur in nature obey quite strong locality constraints (typically, they are $k$-local for quite small constant $k$), it would be interesting to know whether one can achieve similar hardness results using $k$-local Hamiltonians for smaller $k$.

More general topics for future research are:

1. Quantifying the complexity of other physical problems through the complexity classes $DQMA$, $P^{QMA[log n]}$ and other similar complexity classes;

2. Developing a quantum theory of classes “slightly above $QMA$”, along the lines of the classical theory of classes “slightly above $NP$”.

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A Proofs of our main results

A.1 Complexity of EXACT HAMILTONIAN

In this section, we prove Theorem 5.

To show that \( \text{EXACT } k\)-local HAMILTONIAN \( \in \text{DQMA} \), we observe that computing \( E = \text{EXACT } k\)-local HAMILTONIAN\( (H, a, e, \delta) \) reduces to computing \( E_1 = k\)-local HAMILTONIAN\( (H, a + e, a + e + \delta) \) and \( E_2 = k\)-local HAMILTONIAN\( (H, a - e - \delta, a - e) \).

If \( E = 1 \), then \( E_1 = 1 \) and \( E_2 = 0 \). If \( E = 0 \), then both \( E_1 \) and \( E_2 \) are defined and either \( E_1 = 0 \) or \( E_2 = 1 \).

To show the completeness, let \( L \in \text{DQMA} \) and \( L_1, L_2 \) be the corresponding problems from QMA. By Theorem 2, we can reduce both \( L_1 \) and \( L_2 \) to 2-LOCAL HAMILTONIAN with the same \( a \) and \( b \) in both cases. We also assume that \( a = e, b = 2e \).

Let \( H_1 \) and \( H_2 \) be the two instances of 2-local Hamiltonian problem produced by our reduction from \( L_1(x) \) and \( L_2(x) \). We assume that both \( H_1 \) and \( H_2 \) are Hamiltonians on \( m \) qubits and define an \( m + 1 \) qubit Hamiltonian

\[
H = |0\rangle\langle 0| \otimes H_1 + 3|1\rangle\langle 1| \otimes H_2 + 4|0\rangle\langle 0| \otimes I.
\]

We claim that \( L(x) \) is equivalent to \( \text{EXACT } 3\)-LOCAL HAMILTONIAN\( (H, 4.5e, e/2, e) \).

Let \( \mathcal{H}_0 (\mathcal{H}_1) \) be the subspace consisting of all states with the first qubit being \( |0\rangle \) \( (|1\rangle) \) and let \( \lambda_0, \lambda_1 \) be the lowest energies of \( H_1 \) and \( H_2 \). Then, the lowest energy state of \( H \) on the subspace \( \mathcal{H}_0 \) has the energy \( \lambda_0 + 4e \) and the lowest energy state on \( \mathcal{H}_1 \) has the energy \( 3\lambda_1 \).

We consider three cases:

1. \( L(x) = 1 \), \( \lambda_0 \in [0, e] \) and \( \lambda_0 + 4e \in [4e, 5e] \). The lowest energy state on the subspace \( \mathcal{H}_0 \) has the energy at least \( 3\lambda_1 \geq 6e \) (since \( L_2(x) = 0 \)).

2. \( L(x) = 0 \) and \( L_2(x) = 1 \). Then, the lowest energy state on \( \mathcal{H}_1 \) has the energy \( 3\lambda_1 \leq 3e \) (since \( L_2(x) = 1 \)).

3. \( L(x) = 0 \) and \( L_1(x) = L_2(x) = 0 \). Then, the lowest energy state on \( \mathcal{H}_0 \) has the energy \( \lambda_1 + 4e \geq 6e \) (since \( L_2(x) = 0 \)), and the lowest energy state on \( \mathcal{H}_1 \) has the energy at least \( 6e \) (similarly to the first case).

A.2 Complexity of APPROX-SIMULATION

In this section, we prove Theorem 6.

**Part 1:** \( \text{APPROX-SIMULATION} \in \text{PQMA}[\log n] \). As we already described in section 3.2, the algorithm consists of two steps:
1. We use the $QMA$ oracle and binary search to obtain an estimate $a$ for $\lambda$ (the smallest eigenvalue of $H$) such that $\lambda \in [a,a + \epsilon/2]$;

2. We use one more query to the $QMA$ oracle to verify the statement: “there exists $|\psi\rangle$ which is a linear combination of eigenvectors of $H$ with eigenvalues in $[a,a + \epsilon/2]$ and satisfies $\langle \psi | A | \psi \rangle \leq \alpha_1$”.

The first step is performed as follows:

1. Let $\delta = \epsilon/2$.
2. Start with $[a, b] = [0,1]$.
3. As long as $b - a > \frac{\epsilon}{4}$, repeat:
   
   (a) Query $k$-LOCAL HAMILTONIAN($H, \frac{a+b}{2} - \frac{\delta}{4}, \frac{a+b}{2} + \frac{\delta}{4}$).
   
   (b) Depending on the answer, set $[a, b] = [a, \frac{a+b}{2} + \frac{\delta}{4}]$ or $[a, b] = [\frac{a+b}{2} - \frac{\delta}{4}, b]$.

Each repetition decreases the size of the interval $[a, b]$ by almost a half and, after $O(\log \frac{1}{\epsilon}) = O(\log n)$ repetitions, we have $b - a \leq \frac{\epsilon}{4}$.

For the second step, we query the $QMA$ oracle whether there exists a state $|\psi\rangle$ which is accepted (with a high probability) by a following quantum algorithm $M$. (Formally, this can be done by reducing the existence of such $|\psi\rangle$ to an instance of $k$-LOCAL HAMILTONIAN and querying the oracle for $k$-LOCAL HAMILTONIAN.)

Let $H$ be the Hilbert space on which $H$ acts. The input space of $M$ is $(\mathcal{H})^{\otimes k}$ for sufficiently large $k = poly(n)$. $M$ first performs eigenvalue estimation for operator $H$ on each copy of $\mathcal{H}$ with precision $\epsilon/4$ (and sufficiently small error). If at least one of estimates for eigenvalues is more than $a + \frac{\epsilon}{4}$, $M$ outputs 0. Otherwise, it uses $k$ copies of $\mathcal{H}$ to estimate the average of $\langle \psi | A | \psi \rangle$ over all $k$ registers with a precision $\delta < \frac{\epsilon}{8k}$. (Since $\delta = \Omega(\frac{1}{\sqrt{n}})$, such precision can be achieved using $k = poly(n)$ copies.) If the resulting estimate is at most $\alpha_1 + \delta$, $M$ outputs 1. Otherwise, $M$ outputs 1.

If APPROX-SIMULATION=1, then the smallest eigenvalue of $H$ is $\lambda \leq a + \frac{\epsilon}{4}$ and the corresponding eigenvector $|\psi\rangle$ satisfies $\langle \psi | A | \psi \rangle \leq \alpha_1$. Then, inputting $|\psi\rangle^{\otimes k}$ to $M$ results in $M$ outputting 1 with a high probability.

If APPROX-SIMULATION=0, we would like to show that there is no $|\psi\rangle \in (\mathcal{H})^{\otimes k}$ for which $M$ outputs 1 with a substantial probability. We first note that any $|\psi\rangle \in (\mathcal{H})^{\otimes k}$ can be expressed as a linear combination of $|\psi_1\rangle \otimes |\psi_2\rangle \otimes \ldots \otimes |\psi_k\rangle$ where each $|\psi_i\rangle$ is an eigenstate of $H$. We express $|\psi\rangle = |\psi_+\rangle + |\psi_-\rangle$, with $|\psi_+\rangle$ being the part of $|\psi\rangle$ consisting of $|\psi_1\rangle \otimes |\psi_2\rangle \otimes \ldots \otimes |\psi_k\rangle$ where each $|\psi_i\rangle$ has the the eigenvalue that is at most $a + \epsilon$ and $|\psi_-\rangle$ consisting of all other $|\psi_1\rangle \otimes |\psi_2\rangle \otimes \ldots \otimes |\psi_k\rangle$.

On $|\psi_-\rangle$, the eigenvalue estimation part of $H$ results in $M$ outputting 0 with a high probability. Conditional on $|\psi\rangle$ not being rejected, the remaining state is close to $|\psi_+\rangle$. However, $\langle \psi_+ | A | \psi_+ \rangle \geq \alpha_2$ for any $|\psi_+\rangle$ that is a linear combination of eigenvectors of $H$ with eigenvalues at most $\lambda + \epsilon > a + \epsilon$. Therefore, estimating the average of $\langle \psi_+ | A | \psi_+ \rangle$ results in an estimate that is at least $\alpha_2 - \delta$, with a high probability (and the same happens
when, instead of \(|\psi_+\rangle\), we estimate \(\langle \psi| A| \psi \rangle\) for a state \(|\psi\rangle \approx |\psi_+\rangle\). In this case, \(M\) also outputs 0.

**Part 2:** APPROX-SIMULATION is \(P^{QMA[\log n]}\)-hard. By Theorem 2, we assume that queries are to an oracle \(O\) for 2-LOCAL HAMILTONIAN problem, with \(a = \epsilon \) and \(b = 3\epsilon\) where \(\epsilon = 1/n^c\).

Let \(M\) be a polynomial time classical algorithm that makes \(O(\log n)\) queries to a \(QMA\) oracle. Given an input \(x\), we can simulate \(M(x)\) for all possible combinations of answers by oracle \(O\). Let \(d\) be the maximum number of queries made by \(M(x)\). Then, we have \(d \leq c \log n\) for some \(c\). Therefore, there are \(O(n^c)\) possible sequences of answers and this simulation runs in a polynomial time. Let \(H_{y_1\ldots y_\ell}^{(i)}\) be the Hamiltonian that is asked by \(M(x)\) in the \(i\)th query, if the answers to the previous queries are \(y_1, \ldots, y_{i-1}\). We can assume that all of those Hamiltonians act on the same Hilbert space \(\mathcal{H}\) consisting of the same number of qubits. Let \(\text{ans}_{y_1\ldots y_\ell}\) be the answer output by \(M(x)\), if the answers to \(M\)'s queries are \(y_1\ldots y_\ell\).

We take a bigger Hilbert space \(\mathcal{H}' = \otimes_{i=1}^d \mathcal{H}_{i,1} \otimes \mathcal{H}_{i,2}\) where \(\mathcal{H}_{i,1}\) is the Hilbert space for one qubit and \(\mathcal{H}_{i,2}\) is isomorphic to \(\mathcal{H}\). We let the Hamiltonians \(H_{y_1\ldots y_\ell}^{(i)}\) act on \(\mathcal{H}_{i,2}\). We consider the Hamiltonian

\[
H_t = \sum_{i=1}^{t} \frac{1}{4^{i-1}} \sum_{y_1\ldots y_{i-1}} \otimes_{j=1}^{i-1} |y_j\rangle \langle y_j| \mathcal{H}_{j,1} \otimes \left(2\epsilon|0\rangle \langle 0| \mathcal{H}_{i,1} + |1\rangle \langle 1| \mathcal{H}_{i,1} \otimes H_{y_1\ldots y_{i-1}}^{(i)}\right).
\]

**Claim 1** Let \(y_1\ldots y_\ell\) be the correct answers to queries made by \(M(x)\). The ground state of \(H_t\) is in the subspace

\[
\mathcal{H}_{y_1\ldots y_\ell} = \otimes_{i=1}^d |y_i\rangle \langle y_i| \otimes \mathcal{H}_{i,2}.
\]

Let \(\lambda_t\) be the ground state energy of \(H_t\). Then, energy of any state in \(\mathcal{H}_{y'_1\ldots y'_\ell}\), for any \(y'_1\ldots y'_\ell \neq y_1\ldots y_\ell\), is at least \(\lambda_t + \frac{\epsilon}{4^{t-1}}\).

This claim reduces the problem solved by \(M\) to APPROX-SIMULATION in a following way. We take the Hamiltonian \(H_d\) and define the observable \(A\) as the sum of \(\otimes_{i=1}^d |y_i\rangle \langle y_i| \mathcal{H}_{i,1}\) over all \(y_1\ldots y_\ell\) such that \(M(x)\) outputs 1 if the answers to queries are \(y_1, \ldots, y_\ell\). Then, \(M(x) = 1\) is equivalent to APPROX-SIMULATION\((H_d, A, 0, 1, \epsilon/4^{d-1}) = 1\).

**Proof:** [of Claim] By induction over \(t\). We assume that the claim is true for \(H_{t-1}\) and prove that it is also true for \(H_t\). For each term of the form

\[
\otimes_{j=1}^{i-1} |y_j\rangle \langle y_j| \mathcal{H}_{j,1} \otimes \left(2\epsilon|0\rangle \langle 0| \mathcal{H}_{i,1} + |1\rangle \langle 1| \mathcal{H}_{i,1} \otimes H_{y_1\ldots y_{i-1}}^{(i)}\right),
\]

its ground state has the energy between 0 and \(3\epsilon\). Therefore, the lowest energy of a state in \(\mathcal{H}_{y_1\ldots y_{t-1}}\) is at most

\[
E = \lambda_{t-1} + \frac{1}{4^{t-1}} \cdot 3\epsilon
\]

and the lowest energy of a state in any other \(\mathcal{H}_{y'_1\ldots y'_{t-1}}\) is at least

\[
\lambda_{t-1} + \frac{\epsilon}{4^{t-2}} = E + \frac{\epsilon}{4^{t-1}}.
\]
This means that the ground state of $H_t$ must lie in $H_{y_1...y_{t-1}}$. On this subspace, $H_t$ acts in the same way as
\[ H_{t-1} + \frac{1}{4^{t-1}} \left( 2\epsilon |0\rangle \langle 0|_{H_{t-1}} + |1\rangle \langle 1|_{H_{t-1}} H_{y_1...y_{t-1}}^{(t)} \right) \]  
(1)
Since the two terms of (1) act on different qubits, the ground state is the tensor product of their ground states. We have two cases:

1. If $y_t = 0$, the ground state of the second term is any state that has $|0\rangle$ in $H_{t-1}$, with the energy $2\epsilon$. Therefore, the overall ground state is in $H_{y_1...y_{t-1}}$, with the energy $\lambda_t = \lambda_{t-1} + \frac{3\epsilon}{4^{t-1}}$. Any state in $H_{y_1...y_{t-1}}$ must have energy at least
\[ \lambda_{t-1} + \frac{3\epsilon}{4^{t-1}} = \lambda_t + \frac{\epsilon}{4^{t-1}}. \]

2. If $y_t = 1$, the ground state of the second term is a state of the form $|1\rangle \otimes |\psi\rangle$, with $|\psi\rangle$ being the ground state of $H_{y_1...y_{t-1}}^{(t)}$. This state has energy at most $a = \epsilon$. Hence, the ground state of $H_t$ is in $H_{y_1...y_{t-1}}$, with energy $\lambda_t \leq \lambda_{t-1} + \frac{1}{4^{t-1}} \epsilon$. Any state in $H_{y_1...y_{t-1}}$ must have energy at least
\[ \lambda_{t-1} + \frac{2\epsilon}{4^{t-1}} = \lambda_t + \frac{\epsilon}{4^{t-1}}. \]

### A.3 Complexity of SPECTRAL GAP

In this section, we prove Theorem 7.

(a) SPECTRAL GAP can be solved by a following algorithm:

1. Use binary search with $O(\log n)$ queries to the QMA oracle to determine an interval $[a, a + \epsilon/4]$ such that $\lambda \in [a, a + \epsilon/4]$ where $\lambda$ is the smallest eigenvalue of $H$.

2. Use the QMA oracle to determine if there exists a quantum state $|\psi\rangle$ accepted by the following algorithm $M$:

   (a) The input to $M$ is a quantum state in $H' = H \otimes H$ where $H$ is the Hilbert space on which $H$ acts.

   (b) Let $H_-$ by the antisymmetric subspace of $H'$ (the subspace spanned by the states of the form $|\varphi\rangle \otimes |\varphi'\rangle - |\varphi'\rangle \otimes |\varphi\rangle$).

   (c) $M$ measures whether the input state $|\psi\rangle$ belongs to $H_-$ or the subspace $H_+ \perp$ which is perpendicular to $H_-$ and rejects if the answer is $H_+ \perp$.

   (d) If the answer is $H_-$, $M$ performs eigenvalue estimation for $H \otimes H$ on the state $|\psi\rangle$, with precision $\epsilon/5$. $M$ outputs 1 if the estimate for the eigenvalue is at most $2a + \frac{7}{4} \epsilon$ and 0 otherwise.
To analyze the algorithm, we first observe that, restricted to $\mathcal{H}_-$, eigenstates of $H \otimes H$ are of the form

$$|\psi_i\rangle \otimes |\psi_j\rangle - |\psi_j\rangle \otimes |\psi_i\rangle$$

where $|\psi_i\rangle$ and $|\psi_j\rangle$ are eigenstates of $H$.

If the spectral gap of $H$ is at most $\epsilon$, let $|\psi_1\rangle$ and $|\psi_2\rangle$ be two eigenstates with the smallest eigenvalues $\lambda_1$ and $\lambda_2$. Then, $|\psi_1\rangle \otimes |\psi_2\rangle - |\psi_2\rangle \otimes |\psi_1\rangle$ is an eigenstate of $H \otimes H$ with an eigenvalue

$$\lambda_1 + \lambda_2 \leq \left( a + \frac{\epsilon}{4} \right) + \left( a + \frac{\epsilon}{4} \right) + \epsilon = 2a + \frac{3}{2}\epsilon.$$

If the spectral gap of $H$ is $2\epsilon$ or more, let $|\psi\rangle$ be an eigenstate of $H \otimes H$. Then, $|\psi\rangle$ is of the form (2). Let $\lambda_i$ and $\lambda_j$ be the eigenvalues of $|\psi_i\rangle$ and $|\psi_j\rangle$. Then, the eigenvalue of $|\psi\rangle$ is

$$\lambda_i + \lambda_j \geq a + (a + 2\epsilon) = 2a + 2\epsilon.$$

In both cases, estimating the eigenvalue with precision $\epsilon/5$ will give the right answer.

(b) We assume that queries are to an oracle $O$ for 2-LOCAL HAMILTONIAN problem, with $a = \epsilon$ and $b = 3\epsilon$ where $\epsilon = 1/n^c$, with a promise that the spectral gap of the Hamiltonians that are being queried is at least $\epsilon$.

Without a loss of generality, we assume that $M(x)$ always makes the maximum number of questions $d$ to the oracle $O$. Similarly to the proof of Theorem 6, we simulate $M(x)$ for all possible combinations of answers by $O$ and let $H_{y_1...y_i-1}^{(i)}$ be the Hamiltonian that is asked by $M(x)$ in the $i^{th}$ query, if the answers to the previous queries are $y_1, \ldots, y_{i-1}$.

Let $H_0$ be any fixed Hamiltonian (on $\mathcal{H}$) with the following properties:

- $H_0$ has a unique ground state with an eigenvalue $2\epsilon$;
- All other eigenvalues of $H_0$ are at least $3\epsilon$.

We build a sequence of Hamiltonians $H_1, \ldots, H_d$ where

$$H_t = \sum_{i=1}^{t} \sum_{j=1}^{t-1} y_1...y_{t-1} \otimes \otimes^{t-1} |y_j\rangle \langle y_j| H_{y_1} \otimes (|0\rangle \langle 0| H_{i,1} \otimes (H_0) H_{i,2}$$

$$+ |1\rangle \langle 1| H_{i,1} \otimes H_{y_1...y_{t-1}}^{(i)}).$$

Similarly to Claim 1, the ground state of $H_t$ lies in the subspace $\mathcal{H}_{y_1...y_t}$. Moreover, we have

Claim 2 As a Hamiltonian on $\otimes_{i=1}^{t} H_{i,1} \otimes H_{i,2}$, $H_t$ has a unique ground state and spectral gap of at least $\frac{\epsilon}{4T}$.

Proof: By induction. We assume that $H_{t-1}$ satisfies the claim and show that this assumption implies that $H_t$ also satisfies the claim. (The base case for $H_1$ follows by slightly modifying the proof of the inductive case.)

The eigenstates of $H_t$ can be expressed as $|\psi\rangle \otimes |y\rangle \otimes |\phi\rangle$ where
\[ |\psi\rangle \in \bigotimes_{i=1}^{t} H_{i,1} \otimes H_{i,2} \text{ is an eigenstate of } H_{t-1}; \]
\[ y \in \{0, 1\}; \]
\[ |\phi\rangle \text{ is an eigenstate of } H_0 \text{ (if } y = 0) \text{ or } H_{y_1 \ldots y_{t-1}}^{(i)} \text{ (if } y = 1). \]

The eigenvalue of this state is \( \lambda_{t-1} + \Delta \) where \( \lambda_{t-1} \) is the eigenvalue of \( |\psi\rangle \) (as an eigenstate of \( H_{t-1} \)) and \( \Delta \) is the eigenvalue of \( |\phi\rangle \) (as an eigenstate of \( \frac{1}{4} H_0 \) or \( \frac{1}{4} H_{y_1 \ldots y_{t-1}}^{(i)} \)). To minimize this, \( \lambda_{t-1} \) and \( \Delta \) must both be the smallest eigenvalues of the respective Hamiltonians. Let \( |\psi\rangle \otimes |y\rangle \otimes |\phi\rangle \) be the corresponding eigenvector.

Let \( |\psi'\rangle \otimes |y'\rangle \otimes |\phi'\rangle \) be any other eigenstate of \( H_{t-1} \). If \( |\psi'\rangle \neq |\psi\rangle \), then \( \lambda_t \) is larger by at least \( \epsilon \) (from the inductive assumption). If \( |\psi\rangle = |\psi'\rangle \), we have two cases:

1. If \( y = y' \), the eigenvalue \( \Delta \) for \( |\phi'\rangle \) is larger than \( \Delta \) for \( |\phi\rangle \) by at least \( \frac{\epsilon}{4} \) (for \( y = 0 \), this is true because we choose a Hamiltonian with the spectral gap \( \epsilon \) as \( H_0 \); for \( y = 1 \), it follows from the promise about the spectral gap of the Hamiltonians that we are querying).

2. If \( y \neq y' \), then one of \( |\phi\rangle, |\phi'\rangle \) is an eigenvector of \( H_0 \) and the other is an eigenvector of \( H_{y_1 \ldots y_{t-1}}^{(i)} \). Since the smallest eigenvalue of \( H_0 \) is at most \( a = \epsilon \) and the smallest eigenvalue of \( H_{y_1 \ldots y_{t-1}}^{(i)} \) is either at most \( a = \epsilon \) or at least \( b = 3 \epsilon \), this results in a difference of at least \( \frac{\epsilon}{4} \) between the corresponding eigenvalues \( \Delta \).

We now define
\[
H' = \sum_{y_1 \ldots y_d} \bigotimes_{i=1}^{d} |y_i\rangle \langle y_i| H_{i,1}
\]
with the summation over all \( y_1, \ldots, y_d \) such that \( M(x) \) outputs 0 if the answers to queries are equal to \( y_1, \ldots, y_d \). We then add an extra qubit \( B \) to the system and define
\[
H_{\text{final}} = I_B \otimes H_d + \epsilon |0\rangle \langle 0|_B \otimes H'.
\]
We claim that \( M(x) = 1 \) is equivalent to \( \text{SPECTRAL GAP}(H_{\text{final}}, \epsilon/4^d) \):

1. If \( M(x) = 1 \), the spectral gap is 0 because \( H_{\text{final}} \) has 2 orthogonal states with the smallest eigenvalue: \( |0\rangle \otimes |\psi\rangle \) and \( |1\rangle \otimes |\psi\rangle \) where \( |\psi\rangle \) is the ground state of \( H \);

2. If \( M(x) = 0 \), the state with the smallest eigenvalue is \( |1\rangle \otimes |\psi\rangle \). Its eigenvalue differs from the eigenvalue of \( |0\rangle \otimes |\psi\rangle \) by \( \epsilon \) (because of the \( |0\rangle \langle 0|_B \otimes H' \) term in \( H_{\text{final}} \)) and from any other eigenvalue by at least \( \frac{\epsilon}{4^d} \) (because of the spectral gap of \( H_d \)).
B UQMA-completeness of UNIQUE $k$-LOCAL HAMILTONIAN

B.1 Background on QMA-completeness of LOCAL HAMILTONIAN

We can reduce $L$ to 3-LOCAL HAMILTONIAN using the reduction of Kitaev and Regev [22]. We claim that this is actually a reduction to UNIQUE 3-LOCAL HAMILTONIAN.

This reduction works as follows. We first amplify the success probability of the verifier $M$ to $1 - \frac{1}{2^n}$, using the error reduction for $QMA/UQMA$ described in the next subsection. We then represent the verifier circuit $M$ as a sequence of quantum gates acting on 1 or 2 qubits: $U_1, U_2, \ldots, U_T$. We can then construct a reduction of $L$ to $O(\log n)$-LOCAL HAMILTONIAN. To do that, we introduce an $\left\lceil \log_2(T+1) \right\rceil$ qubit register $C$ with basis states $|0\rangle, \ldots, |T\rangle$. Let $A_i$ (for $i = 1, \ldots, m$) be the ancilla qubits (which must be initialized to $|0\rangle$ at the beginning) and $O$ be the output qubit of $M$. We define a Hamiltonian

$$H_1 = H_{in} + H_{out} + H_{prop}$$

where

$$H_{in} = \sum_{i=1}^{m} |1\rangle_{A_i} \otimes |0\rangle_C,$$

$$H_{out} = |0\rangle_O \otimes |T\rangle_C,$$

$$H_{prop} = \sum_{t=0}^{T-1} H_{prop,i},$$

$$H_{prop,i} = \frac{1}{2} \left( I \otimes |t\rangle\langle t| + I \otimes |t-1\rangle\langle t-1| - U_t \otimes |t\rangle\langle t-1| - U_t^\dagger \otimes |t-1\rangle\langle t| \right).$$

To obtain a reduction to 3-LOCAL HAMILTONIAN, we use the unary representation for $C$, representing $|i\rangle_C$ as

$$|0\ldots01\ldots1\rangle_i \quad (3)$$

and choose $H$ as

$$H_2 = H'_{in} + H'_{out} + H'_{prop} + H_{clock}$$

where

$$H_{clock} = T^6 \sum_{i=1}^{T-1} |1\rangle_i \otimes |0\rangle_{i+1}$$

is a Hamiltonian that penalizes the states of $C$ that are not valid unary representations and $H'_{in}, H'_{out}, H'_{prop}$ are 3-local Hamiltonians that satisfy the following requirements:

- $H_{in} = \Pi H'_{in} \Pi$, $H_{out} = \Pi H'_{out} \Pi$, $H_{prop} = \Pi H'_{prop} \Pi$ where $\Pi$ is the projection to the subspace $\mathcal{H}_{\text{legal}}$ consisting of the states in which $C$ is in one of valid unary states of form (3);
\[
\|H'_\text{in} + H'_\text{out} + H'_\text{prop}\| = O(T).
\]

Then, we have

**Theorem 8** \[22\]

1. If \( M \) accepts \( |\psi\rangle \otimes |0^m\rangle \) for some \( |\psi\rangle \) with probability more than \( 1 - \epsilon \), \( H_2 \) has an eigenvalue that is smaller than \( \frac{\epsilon}{T+1} \).

2. If \( M \) accepts \( |\psi\rangle \otimes |0^m\rangle \) with any \( |\psi\rangle \) with probability at most \( \epsilon \) on any \( |\psi\rangle \), \( H_2 \) has no eigenvalue that is smaller than \( \frac{c}{T^3} \) for some constant \( c > 0 \).

To show that this is also a reduction from \( L \in UQMA \) to UNIQUE 3-LOCAL HAMILTONIAN, we need to show

**Lemma 1** Assume that there is a state \( |\psi\rangle \) such that \( M \) accepts \( |\psi\rangle \otimes |0^m\rangle \) with probability at least \( 1 - \epsilon \) and accepts any \( |\phi\rangle \otimes |0^m\rangle \), \( |\phi\rangle \perp |\psi\rangle \) with probability at most \( \epsilon \). Then, the second smallest eigenvalue of \( H_2 \) is at least \( \frac{c}{T^3} \) for an appropriately chosen \( c > 0 \).

**B.2 Error reduction**

Let \( L \in UQMA \). Because of the error reduction for \( UQMA \) (Theorem 2 of [20] which builds on a similar result for QMA by Marriott and Watrous) we can build a verifier \( M \) with the following properties:

- If \( L(x) = 1 \), there is a state \( |\psi\rangle \) such that \( M \) accepts \( |\psi\rangle \otimes |0^m\rangle \) with probability at least \( 1 - \epsilon \) and accepts any \( |\phi\rangle \otimes |0^m\rangle \), \( |\phi\rangle \perp |\psi\rangle \) with probability at most \( \epsilon \);

- If \( L(x) = 0 \), \( M \) accepts any \( |\phi\rangle \otimes |0^m\rangle \) with probability at most \( \epsilon \);

where \( \epsilon = \frac{1}{2^n} \) and both the number of ancilla qubits \( m \) and the running time of the verifier \( T \) are \( \text{poly}(n) \). We observe that this implies the following.

**Claim 3** Let \( |\psi_1\rangle \perp |\psi_2\rangle \). Then, for at least one of \( i \in \{1, 2\} \), \( M \) accepts \( |\psi_i\rangle \otimes |0^m\rangle \) with probability at most \( \frac{1+\sqrt{\epsilon}}{2} \).

**Proof:** Since \( |\psi_1\rangle \perp |\psi_2\rangle \), the angle between one of \( |\psi_i\rangle \) and \( |\psi\rangle \) is at least \( \frac{\pi}{4} \). Therefore,

\[
|\psi_i\rangle = \alpha|\psi\rangle + \beta|\psi^\perp\rangle
\]

where \( |\psi^\perp\rangle \perp |\psi\rangle \), \( |\alpha| \leq \frac{1}{\sqrt{2}} \). Since \( |\psi\rangle \) is accepted with probability at most 1 and \( |\psi^\perp\rangle \) with probability at most \( \epsilon \), the claim follows.
B.3 Useful facts from linear algebra

We use two facts from linear algebra:

**Lemma 2** ([Corollary 7.7.4]) Let $H, H'$ be Hermitian matrices such that $H \succeq H'^1$. Let $\lambda_1 \geq \lambda_2 \geq \ldots$ and $\lambda'_1 \geq \lambda'_2 \geq \ldots$ be the eigenvalues of $H$ and $H'$, respectively. Then, $\lambda_i \geq \lambda'_i$ for all $i$.

**Lemma 3** Let $H = \Pi + \Pi'$ where $\Pi$ and $\Pi'$ are two projections acting on the same Hilbert space $\mathcal{H}$. Then, we can decompose $\mathcal{H}$ into a direct sum of 1-dimensional and 2-dimensional subspaces $\mathcal{H}_i$ such that each $H(\mathcal{H}_i) \subseteq \mathcal{H}_i$, with

(a) each 1-dimensional subspace spanned by $|\psi\rangle$ that is an eigenvector of both $\Pi$ and $\Pi'$;

(b) each 2-dimensional subspace spanned by two eigenvectors of $\Pi$, one with eigenvalue 1 and one with eigenvalue 0 (and, similarly, by two eigenvectors of $\Pi'$).

A consequence of this lemma is that we can determine the smallest eigenvalue of $H$ by looking at each subspace separately. Each one dimensional subspace $\mathcal{H}_i$ is spanned by one eigenstate $|\psi_i\rangle$. Therefore, we either have $\Pi|\psi_i\rangle = |\psi_i\rangle$ or $\Pi|\psi_i\rangle = 0$ (and similarly for $\Pi'$).

Hence, the eigenvalue of $|\psi_i\rangle$ is 0, 1 or 2.

For two-dimensional subspaces $\mathcal{H}_i$, each of them is spanned by two eigenstates $|\psi_{i,1}\rangle$ and $|\psi_{i,2}\rangle$ of $\Pi$ and two eigenstates $|\phi_{i,1}\rangle$ and $|\phi_{i,2}\rangle$ of $\Pi'$. If both $|\psi_{i,1}\rangle$ and $|\psi_{i,2}\rangle$ have the same eigenvalue, then $\mathcal{H}_i$ decomposes into a sum of two one-dimensional subspaces, spanned by $|\phi_{i,1}\rangle$ and $|\phi_{i,2}\rangle$. Hence, we can assume that $\Pi|\psi_{i,1}\rangle = |\psi_{i,1}\rangle$ and $\Pi|\psi_{i,2}\rangle = 0$. Similarly, $\Pi'|\phi_{i,1}\rangle = |\phi_{i,1}\rangle$ and $\Pi'|\phi_{i,2}\rangle = 0$. We assume that the phases of $|\phi_{i,1}\rangle$ have been chosen so that $\langle \psi_{i,1}|\phi_{i,1}\rangle$ is a non-negative real. Then, the eigenstates of $H = \Pi + \Pi'$ on $\mathcal{H}_i$ are

$$|\varphi_{i,1}\rangle = |\psi_{i,1}\rangle + |\phi_{i,1}\rangle$$

and $|\varphi_{i,2}\rangle \perp |\varphi_{i,1}\rangle$, with eigenvalues $2\cos^2 \frac{\alpha}{2}$ and $2\sin^2 \frac{\alpha}{2}$ where $\alpha$ is the angle between $|\psi_{i,1}\rangle$ and $|\phi_{i,1}\rangle$. Since $\langle \psi_{i,1}|\phi_{i,1}\rangle$ is a non-negative real, we have $\alpha \in [0, \frac{\pi}{2}]$ and, hence, $\cos^2 \frac{\alpha}{2} \geq \frac{1}{2} \geq \sin^2 \frac{\alpha}{2}$.

B.4 Analysis of Hamiltonian $H_1$

We first analyze the Hamiltonian $H_1$. The counterpart of Lemma 1 is

**Lemma 4** Assume that there is a state $|\psi\rangle$ such that $M$ accepts $|\psi\rangle \otimes |0\rangle^{\otimes m}$ with probability at least $1 - \epsilon$ and accepts any $|\phi\rangle \otimes |0\rangle^{\otimes m}$, $|\phi\rangle \perp |\psi\rangle$ with probability at most $\epsilon$. Then, the second smallest eigenvalue of $H_1$ is at least $\frac{1}{c}$, for an appropriately chosen $c > 0$.

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In this paper, $A \succeq B$ means that $A - B$ is positive semidefinite.
Proof: We express \( H_1 = H_{\text{prop}} + H_{\text{other}} \) where \( H_{\text{other}} = H_{\text{in}} + H_{\text{out}} \). The smallest non-zero eigenvalue of \( H_{\text{other}} \) is 1 because all terms of \( H_{\text{other}} \) are diagonal in the computational basis and the smallest non-zero eigenvalue of each term is 1. The smallest non-zero eigenvalue of \( H_{\text{prop}} \) is \( \lambda = \Omega(1/T^2) \) [22]. By Lemma 2, we can replace \( H_1 \) with \( \lambda(\Pi_{\text{other}} + \Pi_{\text{prop}}) \) where \( \Pi_{\text{other}} \) and \( \Pi_{\text{prop}} \) are projections to the subspaces spanned by all eigenvectors of \( H_{\text{other}} \) and \( H_{\text{prop}} \) with non-zero eigenvalues.

Let \( \delta \) be the second smallest eigenvalue of \( H' = \Pi_{\text{other}} + \Pi_{\text{prop}} \). We will show that \( \delta > \frac{c}{T+1} \) for some constant \( c \). This implies that the second smallest eigenvalue of \( H_1 \) is at least \( c\lambda = \Omega(1/T^3) \).

The zero eigenspace of \( \Pi_{\text{prop}} \) consists of all the “history states” of the form

\[
\frac{1}{\sqrt{T+1}} \sum_{i=0}^{T} |\psi_i\rangle \otimes |i\rangle
\] (4)

where \( |\psi_i\rangle \) is the state of the verifier \( M \) after \( i \) steps (given that the starting state is \( |\psi_0\rangle \)).

We consider the decomposition of \( H' = \Pi_{\text{other}} + \Pi_{\text{prop}} \) given by Lemma 3. We claim that:

- (a) Each subspace \( H_i \) contains at most one eigenvector of \( H' \) with an eigenvalue less than 1.
- (b) If \( H_i \) contains an eigenvector with eigenvalue at most \( \delta < 1 \), it also contains a history state such that

\[
\|\Pi_{\text{in}}|\psi_0\rangle + \Pi_{\text{out}}|\psi_T\rangle\| \leq \sqrt{2(T+1)}\delta.
\] (5)

If \( H_i \) is one-dimensional, the first part is obvious. For the second part, let \( |\psi\rangle \in H_i \). If \( H_i \) is one-dimensional, then \( |\psi\rangle \) must be an eigenvector of both \( \Pi_{\text{other}} \) and \( \Pi_{\text{prop}} \) and, if the eigenvalue of \( |\psi\rangle \) is at most \( \delta < 1 \), then \( \Pi_{\text{other}}|\psi\rangle = \Pi_{\text{prop}}|\psi\rangle = 0 \). \( \Pi_{\text{prop}}|\psi\rangle = 0 \) means that \( |\psi\rangle \) is a “history state” of the form (4). \( \Pi_{\text{other}}|\psi\rangle = 0 \) means that \( \Pi_{\text{in}}|\psi\rangle = \Pi_{\text{out}}|\psi\rangle = 0 \), implying that (5) is satisfied.

If \( H_i \) is 2-dimensional, it must contain one eigenvector of \( \Pi_{\text{prop}} \) with eigenvalue 1 and one eigenvector of \( \Pi_{\text{other}} \) with eigenvalue 1. If \( \lambda_1 \) and \( \lambda_2 \) are the eigenvalues of \( H' \) for the two eigenvectors in \( H_i \), then

\[
\lambda_1 + \lambda_2 = Tr(H'\Pi_{H_i}) = Tr(\Pi_{\text{prop}}\Pi_{H_i}) + Tr(\Pi_{\text{other}}\Pi_{H_i}) = 2.
\]

This means that at most one of \( \lambda_1 \), \( \lambda_2 \) can be less than 1. For the part (b), let \( |\psi_1\rangle \) and \( |\psi_2\rangle \) be the 1-eigenvectors of \( \Pi_{\text{prop}} \) and \( \Pi_{\text{other}} \) in \( H_i \). We assume that the phases of \( |\psi_1\rangle \) and \( |\psi_2\rangle \) have been chosen so that \( \langle \psi_1 | \psi_2 \rangle \) is a positive real. Then, the eigenvectors of \( H' \) are \( |\psi_1\rangle + |\psi_2\rangle \) and \( |\psi_1\rangle - |\psi_2\rangle \) with eigenvalues \( 2\cos^2 \frac{\beta}{2} \) and \( 2\sin^2 \frac{\beta}{2} \) where \( \beta \) is such that \( \cos \beta = \langle \psi_1 | \psi_2 \rangle \). The smallest of those eigenvalues is \( 2\sin^2 \frac{\beta}{2} \).

We now express the left hand side of (5) through \( \beta \). The history state \( |\psi_{\text{hist}}\rangle \) contained in \( H_i \) is a 0-eigenstate of \( \Pi_{\text{prop}} \). Therefore, it is orthogonal to \( |\psi_1\rangle \). Since all those states
lie in a 2-dimensional subspace $\mathcal{H}_t$, this means that $\langle \psi_2 | \psi_{\text{hist}} \rangle = \sin \beta$. $\langle \psi_2 | \psi_{\text{hist}} \rangle$ is also the length of the projection of $|\psi_{\text{hist}}\rangle$ to $|\psi_2\rangle$. This projection is the same as

$$
\Pi_{\text{other}} |\psi_{\text{hist}}\rangle = \frac{1}{\sqrt{T+1}} \Pi_{\text{in}} |\psi_0\rangle + \frac{1}{\sqrt{T+1}} \Pi_{\text{out}} |\psi_T\rangle.
$$

Therefore, we have $\|\Pi_{\text{in}} |\psi_0\rangle + \Pi_{\text{out}} |\psi_T\rangle\| = \sin \beta$. If $2 \sin^2 \frac{\beta}{2} \leq \delta$, then

$$
\sin \beta = 2 \sin \frac{\beta}{2} \cos \frac{\beta}{2} \leq 2 \sqrt{\frac{\delta}{2}}(1 - \frac{\delta}{2}) \leq \sqrt{2\delta}.
$$

Hence, if the 2nd smallest eigenvalue of $H'$ is $\delta$, then we have two orthogonal history states $|\psi_{\text{hist},1}\rangle$ and $|\psi_{\text{hist},2}\rangle$ satisfying the condition (5).

For each of those history states, we define a new history state $|\psi'_{\text{hist},i}\rangle$ in the following way. Let $|\psi_{i,0}\rangle$ denote the starting state $|\psi_0\rangle$ that is used to define $|\psi_{\text{hist},i}\rangle$. Since $|\psi_{\text{hist},1}\rangle$ and $|\psi_{\text{hist},2}\rangle$ are orthogonal, $|\psi_{1,0}\rangle$ and $|\psi_{2,0}\rangle$ must be orthogonal, as well. Let

$$
|\psi'_{i,0}\rangle = \frac{|\psi_{i,0}\rangle - \Pi_{\text{in}} |\psi_{i,0}\rangle}{\| |\psi_{i,0}\rangle - \Pi_{\text{in}} |\psi_{i,0}\rangle \|}.
$$

Because of (5), we have

$$
\| |\psi_{i,0}\rangle - |\psi'_{i,0}\rangle \| \leq \sqrt{2(T+1)}\delta + o(\sqrt{(T+1)}\delta). \tag{6}
$$

Let $\alpha$ be the angle between $|\psi'_{i,0}\rangle$ and $|\psi'_{2,0}\rangle$. Because of $|\psi_{1,0}\rangle \perp |\psi_{2,0}\rangle$ and (6), we have $\alpha \leq 2 \sqrt{2(T+1)}\delta + o(\sqrt{(T+1)}\delta)$. We take the plane spanned by $|\psi'_{i,0}\rangle$ for $i \in \{1, 2\}$ and in this plane choose $|\psi''_{i,0}\rangle$ so that the angle between $|\psi'_{i,0}\rangle$ and $|\psi''_{i,0}\rangle$ is $\frac{\pi}{2} - \frac{\alpha}{2}$ and $|\psi''_{1,0}\rangle \perp |\psi''_{2,0}\rangle$. Then,

$$
\| |\psi''_{i,0}\rangle - |\psi'_{i,0}\rangle \| \leq \sqrt{2(T+1)}\delta + o(\sqrt{(T+1)}\delta). \tag{7}
$$

We have $\Pi_{\text{in}} |\psi''_{i,0}\rangle = 0$ (because $\Pi_{\text{in}} |\psi'_{i,0}\rangle = 0$ for both $i \in \{1, 2\}$ and $|\psi''_{i,0}\rangle$ are in the plane spanned by $|\psi'_{i,0}\rangle$). Let $|\psi_{i,T}\rangle (|\psi''_{i,T}\rangle)$ be the final states of the computation if we start it in the state $|\psi_{i,0}\rangle (|\psi''_{i,0}\rangle)$. Because of (6), (7) and unitary transformations being length-preserving, we have

$$
\| |\psi_{i,T}\rangle - |\psi''_{i,T}\rangle \| \leq 2 \sqrt{2(T+1)}\delta + o(\sqrt{(T+1)}\delta). \tag{8}
$$

Also, because of (5), we have $\|\Pi_{\text{out}} |\psi_{i,T}\rangle\| \leq \sqrt{2(T+1)}\delta$. Together with (8), this means

$$
\|\Pi_{\text{out}} |\psi''_{i,T}\rangle\| \leq 3 \sqrt{2(T+1)}\delta + o(\sqrt{(T+1)}\delta).
$$

Moreover, if we have some other starting state $|\psi_0\rangle$ in the plane spanned by $|\psi''_{i,0}\rangle$, then

$$
|\psi_0\rangle = \alpha |\psi''_{1,0}\rangle + \beta |\psi''_{2,0}\rangle.
$$

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For the corresponding final state $|\psi_T\rangle$, we have
\[
\|\Pi_{\text{out}}|\psi_T\rangle\| \leq (|\alpha| + |\beta|)3\sqrt{2(T + 1)}\delta + o(\sqrt{T + 1})
\leq 6\sqrt{(T + 1)}\delta + o(\sqrt{T + 1}).
\]
Hence, any state $|\psi_0\rangle$ in the plane spanned by $|\psi_{1,0}\rangle$ is accepted with probability at least $1 - 36(T + 1)\delta - o((T + 1)\delta)$. Because of Claim 3, we must have $(T + 1)\delta \geq c$ for some constant $c > 0$. Then, $\delta \geq \frac{c}{T+1}$.

**B.5 Analysis of Hamiltonian $H_2$**

We now complete the proof of Lemma 1. Similarly to the previous case, we show that, if the Hamiltonian $H_2$ has two eigenstates with small eigenvalues, then there must be a two-dimensional subspace such that the verifier accepts any state in this subspace with a probability close to 1.

We express $H_2 = H'_\text{clock} + H'_\text{other}$ where $H'_\text{other} = H'_\text{in} + H'_\text{out} + H'_\text{prop}$. Let $|\psi_1\rangle, |\psi_2\rangle$ be two eigenstates of $H_2$ with eigenvalues $\lambda_i$ less than $\frac{\delta}{T^3}$. We will prove that $\delta > c$ for an appropriately chosen $c > 0$.

For each $i \in \{1, 2\}$, we express $|\psi_i\rangle = |\psi_{i,1}\rangle + |\psi_{i,2}\rangle$

with $|\psi_{i,1}\rangle \in \mathcal{H}_{\text{legal}}, |\psi_{i,2}\rangle \perp \mathcal{H}_{\text{legal}}$. Because of
\[
\lambda_i = \langle \psi_i | H_2 | \psi_i \rangle \geq \langle \psi_i | H'^{\text{clock}} | \psi_i \rangle = T^6 \| \psi_i \|^2
\]
must have $\| \psi_{i,2} \|^2 \leq \frac{\delta}{T^3}$.

Since $\langle \psi_i | H'_\text{other} | \psi_i \rangle \leq \frac{\delta}{T^3}, \| \psi_{i,2} \|^2 \leq \frac{\delta}{T^3}$ and $\| H'_\text{other} \| = O(T)$, we have
\[
\langle \psi_{i,1} | H'_\text{other} | \psi_{i,1} \rangle \leq \frac{\delta + o(1)}{T^3}.
\]
Moreover, since $\| \psi_{i,2} \|^2 \leq \frac{\delta}{T^3}$, we have $\| \psi_{i,1} \| \geq 1 - \sqrt{\frac{\delta}{T^3}}$ and $|\langle \psi_{1,1} | \psi_{2,1} \rangle| = O(\frac{1}{T^{3/2}})$. Hence, we can replace $|\psi_{i,1}\rangle$ by $|\psi'_{i,1}\rangle$ such that $\| \psi'_{i,1} \| = 1$ and $|\psi'_{i,1}\rangle \perp |\psi'_{2,1}\rangle$ and we still have
\[
\langle \psi'_{i,1} | H'_\text{other} | \psi'_{i,1} \rangle \leq \frac{\delta + o(1)}{T^3}.
\]
Since $|\psi'_{i,1}\rangle \in \mathcal{H}_{\text{legal}}$, we have
\[
\langle \psi'_{i,1} | H'_\text{other} | \psi'_{i,1} \rangle = \langle \psi'_{i,1} | \Pi_{\text{legal}} H'_\text{other} \Pi_{\text{legal}} | \psi'_{i,1} \rangle.
\]
This means that the Hamiltonian $\Pi_{\text{legal}} H'_\text{other} \Pi_{\text{legal}}$ has two eigenvalues that are at most $\frac{\delta + o(1)}{T^3}$.

We now recall that, on the subspace $\mathcal{H}_{\text{legal}}$, terms of $\Pi_{\text{legal}} H'_\text{other} \Pi_{\text{legal}}$ act in the same way as the terms of $H_1$. Therefore, we can now use the proof from the previous subsection.