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).

Keywords—quantum computing, $QMA$, complexity of physical problems, quantum Hamiltonian complexity

I. Introduction

Quantum Hamiltonian complexity [31] 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 $QMA$ [26], [25], [41], [22], [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 [23], [22]. This problem is $QMA$-complete for any $k \geq 2$ [22]. $QMA$-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 [30] or restrict the Hamiltonian to certain natural interactions between qubits [6].

$QMA$-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 [7].) 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 [34].
- The Boolean hierarchy, a sequence of complexity classes defined by taking intersections and unions of sets in \( NP \) and \( coNP \) [12], [42], [39], [10], [11].
- \( P^{NP[\log n]} \), 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 [9], [40].

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., [38], [33], [13], [19], [18], [28]).

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 [31] 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 [31] 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.

A. 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. [8] and Shi and Zhang [36] 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 \([\lambda_1, \lambda_1 + \frac{\epsilon}{n^c}]\) and \([\lambda_2 - \frac{\epsilon}{n^c}, \lambda_2]\) around the endpoints of \([\lambda_1, \lambda_2]\)).

Brown et al. [8] 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 [36].

Our problem of estimating the spectral gap is related to the degeneracy problem in [8]: 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 [8] and in the current paper are completely different.

Second, Gharibian and Kempe [16] have studied a complexity class \( cc - \Sigma_2 \) which generalizes the classical class \( \Sigma_2^P = NP^N \). 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 [16] then show $cc - \Sigma_2$ hardness for several quantum counterparts of classical $\Sigma^p_2$-complete problems.

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

Apart from [8], [36], [16], we are not aware of any work that is more than distantly related. Many researchers ([27], [1], [17] and 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.

Cubitt et al. [14] have studied the complexity of spectral gap 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). 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 [5] and the proof of undecidability of the spectral gap of [14] 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.

II. TECHNICAL PRELIMINARIES

A. 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.

B. 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: [25] $QMA = QMA(c, s)$ 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 [24], [25] 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 \( a,b; \ b \geq a + \frac{1}{n^c} \) (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.

In our constructions (where we combine several instances of \( k \)-LOCAL HAMILTONIAN), it is helpful to have a slightly different promise “the ground state energy is either at most \( a \) or is exactly \( b' \). One can ensure that this promise is satisfied by modifying the Hamiltonian \( H \) so that it always has a state with energy exactly \( b \).

**Theorem 2:** [22] \( 2 \)-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 \( L(x) = L_1(x) \ AND \ L_2(x) \) and \( L = L_1 \lor L_2 \) by \( L(x) = L_1(x) \ OR \ L_2(x) \). (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 \( L_1 \lor L_2 \in QMA \).

C. \( UQMA \) 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 \( M(x, |\psi'|) \) will also output 1 with probability at least 2/3 whenever \( |\psi'| \) 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 \( |\psi'| \perp |\psi\rangle \) 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 \( |\psi'| \perp |\psi\rangle \), then \( M(x, |\psi'|) \) 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 [38]). It is not known whether a similar result is true in the quantum case [2], [21].

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 [23]. We omit it for the space constraints but it can be found in the full version of the paper on arxiv [4].
It is plausible that the proof of QMA-completeness of 2-LOCAL HAMILTONIAN by Kitaev, Kempe and Regev [22] can be adapted to show that UNIQUE 2-LOCAL HAMILTONIAN is UQMA-complete but we have not verified that.

III. Our Results

A. 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: 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:

- **EXACT $k$-LOCAL HAMILTONIAN($H, a, \epsilon, \delta$) = 0:** the ground state energy of $H$ is in the interval $[a - \epsilon, a + \epsilon]$;
- **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 [15] 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: SPECTRAL GAP($H, \epsilon$).

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

- **SPECTRAL GAP($H, \epsilon$) = 1:** $\lambda_2 - \lambda_1 \leq 2\epsilon$;
- **SPECTRAL GAP($H, \epsilon$) = 0:** $\lambda_2 - \lambda_1 \geq 2\epsilon$.

3) In the ground state simulation problem [31], 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: 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:

- **EXACT-SIMULATION= 1** if $H$ has a ground state $| \psi \rangle$ with $\langle \psi | A | \psi \rangle \leq \alpha_1$;
- **EXACT-SIMULATION= 0** if $H$ has no ground state $| \psi \rangle$ with $\langle \psi | A | \psi \rangle \leq \alpha_2$.

Definition 5: 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:

- **APPROX-SIMULATION= 1** if $H$ has a ground state $| \psi \rangle$ with $\langle \psi | A | \psi \rangle \leq \alpha_1$;
- **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 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 EXACT $k$-LOCAL HAMILTONIAN, we have to verify that

(a) There exists a state $| \psi \rangle$ such that $\langle \psi | H | \psi \rangle \leq
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 the 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 B.

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

**Proof:** In section C

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.

IV. 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. Complexity of EXACT HAMILTONIAN

In this section, we prove Theorem 5. To show that $\text{EXACT } k\text{-local HAMILTONIAN} \in DQMA$, we observe that computing $E = \text{EXACT } k\text{-local HAMILTONIAN}(H, a, \epsilon, \delta)$ reduces to computing $E_1 = k\text{-local HAMILTONIAN}(H, a + \epsilon, a + \epsilon + \delta)$ and $E_2 = k\text{-local HAMILTONIAN}(H, a - \epsilon - \delta, a - \epsilon)$. 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 $L \in DQMA$ 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 $a = \epsilon$, $b = 2\epsilon$.

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

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

We claim that $L(x)$ is equivalent to $\text{EXACT } 3\text{-LOCAL HAMILTONIAN}(H, 4.5\epsilon, \epsilon/2, \epsilon)$. 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 $\lambda_0 + 4\epsilon$ and the lowest energy state on $\mathcal{H}_1$ has the energy $3\lambda_1$.

We consider three cases:

1) $L(x) = 1$. $\lambda_0 \in [0, \epsilon]$ and $\lambda_0 + 4\epsilon \in [4\epsilon, 5\epsilon]$. The lowest energy state on the subspace $\mathcal{H}_0$ has the energy at least $3\lambda_1 \geq 6\epsilon$ (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 $3\lambda_1 \leq 3\epsilon$ (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 $\lambda_1 + 4\epsilon \geq 6\epsilon$ (since $L_2(x) = 0$), and the lowest energy state on $\mathcal{H}_1$ has the energy at least $6\epsilon$ (similarly to the first case).

B. Complexity of APPROX-SIMULATION

In this section, we prove Theorem 6. Part 1: APPROX-SIMULATION $\in P^{QMA[logn]}$. As we already described in section III-B, 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 $b - a > \frac{\epsilon}{2}$, repeat:
   a) Query $k$-LOCAL HAMILTONIAN($H, a^2 + b^2 - \frac{\delta}{4}$).
   b) Depending on the answer, set $[a, b] = [a, \frac{a^2 + \delta}{4}]$ or $[a, b] = [\frac{a^2 + \delta}{4}, b]$.
Each repetition decreases the size of the interval $[a, b]$ by almost a half and, after $O(\log \frac{1}{\delta}) = O(\log n)$ repetitions, we have $b - a \leq \frac{\epsilon}{4}$.

For the second step, we query the \textit{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 $k = \text{poly}(n)$. $M$ 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 $a + \frac{\epsilon}{2}$, $M$ 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 $\delta < \frac{\alpha_2 - \alpha_1}{2}$. (Since $\delta = \Omega(\frac{1}{\sqrt{n}})$, such precision can be achieved using $k = \text{poly}(n)$ 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 $\lambda \leq a + \frac{\epsilon}{2}$ 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 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.

\textbf{Part 2:} APPROX-SIMULATION is $\text{PQMA}[\log n]$-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 $H_{y_1,\ldots,y_{i-1}}^{(i)}$ be the Hamiltonian that is asked by $M(x)$ in the $i^{th}$ query, if the answers to the previous queries are $y_1, \ldots, y_{i-1}$. We can assume that all of those Hamiltonians act on the same Hilbert space $\mathcal{H}$ consisting of the same number of qubits. Let $\text{ans}_{y_1,\ldots,y_d}$ be the answer output by $M(x)$, if the answers to $M$‘s queries are $y_1 \ldots y_d$.

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 $H_{y_1,\ldots,y_{i-1}}^{(i)}$ act on $\mathcal{H}_{i,2}$. We consider the Hamiltonian

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

\textbf{Claim 1:} Let $y_1 \ldots y_d$ be the correct answers to queries made by $M(x)$. The ground state of $H_t$ is in the subspace $\mathcal{H}_{y_1,\ldots,y_d} = \otimes_{i=1}^t |y_i\rangle \langle y_i| \otimes \mathcal{H}_{i,2}$.

Let $\lambda_i$ be the ground state energy of $H_t$. Then, energy of any state in $\mathcal{H}_{y_1,\ldots,y_d}$, for any $y'_1 \ldots y'_t \neq y_1 \ldots y_t$, is at least $\lambda_t + \frac{\epsilon}{4^t}\tau$. 
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 $y_1, \ldots, y_d$ such that $M(x)$ outputs 1 if the answers to queries are $y_1, \ldots, y_d$. Then, $M(x) = 1$ is equivalent to APPROX-SIMULATION($H_d, A, 0, 1, \epsilon/4^{d-1}$) $= 1$.

Proof: 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

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

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 $\mathcal{H}_{y_1, \ldots, y_{t-1}}$. On this subspace, $H_t$ acts in the same way as

$$H_{t-1} + \frac{1}{4^{t-1}} (2\epsilon |0\rangle \langle 0|_{\mathcal{H}_{t-1}} + |1\rangle \langle 1|_{\mathcal{H}_{t-1}} H(i)_{y_1, \ldots, y_{t-1}})$$

(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 $\mathcal{H}_{t-1}$, with the energy $2\epsilon$. Therefore, the overall ground state is in $\mathcal{H}_{y_1, \ldots, y_{t-1}}$, with the energy $\lambda_t = \lambda_{t-1} + \frac{2\epsilon}{4^{t-1}}$. Any state in $\mathcal{H}_{y_1, \ldots, y_{t-1}}$ 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 $H(i)_{y_1, \ldots, y_{t-1}}$. This state has energy at most $a = \epsilon$. Hence, the ground state of $H_t$ is in $\mathcal{H}_{y_1, \ldots, y_{t-1}}$, with energy $\lambda_t \leq \lambda_{t-1} + \frac{\epsilon}{4^{t-1}}$. Any state in $\mathcal{H}_{y_1, \ldots, y_{t-1}}$ must have energy at least

$$\lambda_{t-1} + \frac{2\epsilon}{4^{t-1}} = \lambda_t + \frac{\epsilon}{4^{t-1}}.$$

C. 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 $\mathcal{H}' = \mathcal{H} \otimes \mathcal{H}$ where $\mathcal{H}$ is the Hilbert space on which $H$ acts.

b) Let $\mathcal{H}_-$ by the antisymmetric subspace of $\mathcal{H}'$ (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 $\mathcal{H}_-$ or the subspace $\mathcal{H}_+$ which is perpendicular to $\mathcal{H}_-$ and rejects if the answer is $\mathcal{H}_+$.

d) If the answer is $\mathcal{H}_-$, $M$ 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 $2a + 7\epsilon$ and 0 otherwise.

To analyze the algorithm, we first observe that, restricted to $\mathcal{H}_-$, eigenstates of $H \otimes H$ are of the form

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

(2)

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

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

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 $H_{y_1 \ldots y_{t−1}}$ be the Hamiltonian that is asked by $M(x)$ in the $i^{th}$ query, if the answers to the previous queries are $y_1, \ldots, y_{t−1}$.

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

$$H_t = \sum_{i=1}^{t} \frac{1}{4t-1} \sum_{y_1 \ldots y_{t−1}} \otimes_{j=1}^{t−1} |y_j\rangle\langle y_j|_{\mathcal{H}_{i,j}} \otimes (|0\rangle\langle 0|_{\mathcal{H}_{i,1}} \otimes (H_0)_{\mathcal{H}_{i,2}} + |1\rangle\langle 1|_{\mathcal{H}_{i,1}} \otimes H^{(i)}_{y_1 \ldots y_{t−1}}).$$

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

**Claim 2**: As a Hamiltonian on $\otimes_{i=1}^{d} \mathcal{H}_{i,1} \otimes \mathcal{H}_{i,2}$, $H_t$ has a unique ground state and spectral gap of at least $\frac{4\epsilon}{7t}$.

**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

- $|\psi\rangle \in \otimes_{i=1}^{d} \mathcal{H}_{i,1} \otimes \mathcal{H}_{i,2}$ is an eigenstate of $H_{t−1}$;
- $y \in \{0, 1\}$;
- $|\phi\rangle$ is an eigenstate of $H_0$ (if $y = 0$) or $H^{(i)}_{y_1 \ldots y_{t−1}}$ (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 $\frac{1}{\epsilon}H_0$ or $\frac{1}{\epsilon}H^{(i)}_{y_1 \ldots y_{t−1}}$). 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 $\frac{4\epsilon}{7t}$ (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 $\frac{4\epsilon}{7t}$ (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 $H^{(i)}_{y_1 \ldots y_{t−1}}$. Since the smallest eigenvalue of $H_0$ is $2\epsilon$ and the smallest eigenvalue of $H^{(i)}_{y_1 \ldots y_{t−1}}$ is either at most $a = \epsilon$ or at least $b = 3\epsilon$, this results in a difference of at least $\frac{4\epsilon}{7t}$ between the corresponding eigenvalues $\Delta$.

We now define

$$H' = \sum_{y_1 \ldots y_d} \otimes_{i=1}^{d} |y_i\rangle\langle y_i|_{\mathcal{H}_{i,1}},$$

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

$$H_{final} = I_B \otimes H_d + \epsilon|0\rangle\langle 0|_B \otimes H'.$$

We claim that $M(x) = 1$ is equivalent to SPECTRAL GAP($H_{final}, \epsilon/4^d$):  

1) If $M(x) = 1$, the spectral gap is 0 because $H_{final}$ 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 $H_I$;

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 $H_{final}$) and from any other eigenvalue by at least $\frac{4\epsilon}{7t}$ (because of the spectral gap of $H_d$).