Computational Complexity of Spectral Gaps

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December 11, 2015

1 Introduction

In this report we survey some results on the complexity of finding the *spectral gap* of a quantm Hamiltonian. First, let us review some basic definitions. A *k-local Hamiltonian* acting on a system of n qudits with local dimension d is a Hermitian positive semidefinite operator H with a decomposition

$$H = \sum_{i=1}^{m} h_i$$

of *local terms* h_i, where each term satisfies $\|h_i\| \leq 1$ and only acts nontrivially on at most k qudits. Physically, the Hamiltonian representes the energy of the system. The *spectral gap* of a Hamiltonian H is defined to be the difference $\Delta(H) \equiv \lambda_2 - \lambda_1 \geq 0$ of its smallest two eigenvalues.

2 Finite systems

The first setting we study is the case of finite system sizes. This case has been most fully investigated by Ambainis [Amb14]. This work studies the following decision problem:

Definition 1. *Given a local Hamiltonian H over n qudits, and an error parameter $\epsilon(n) > 0$, the problem SPECTRAL-GAP is to decide whether the spectral gap $\Delta(H)$ is either (i) $\leq \epsilon(n)$ or (ii) $\geq 2\epsilon(n)$, promised that one two cases holds.*

We restrict our attention to the case where $\epsilon(n) = \Omega(1/\operatorname{poly}(n))$. Ambainis relates the complexity of this problem to two classes $P^{\mathrm{QMA}[\log(n)]}$ and $P^{\mathrm{UQMA}[\log(n)]}$. The class $P^{\mathrm{QMA}[\log(n)]}$ is the class of polynomial-time machines that are allowed to make $O(\log(n))$ queries to an oracle for QMA. The definition of $P^{\mathrm{UQMA}[\log(n)]}$ is similar, but with queries to an oracle for UQMA: this is a class similar to QMA but with the added promise that in the YES instance, there is a *unique* satisfying witness state. The following two theorems are the main results achieved by Ambainis.

Theorem 2. *SPECTRAL-GAP for $O(\log(n))$-local Hamiltonians is contained in $P^{\mathrm{QMA}[\log(n)]}$.*

Proof. Let the given Hamiltonian be H, and let the Hilbert space it acts on be $\mathcal{H}$. Then we use $O(\log(n))$ queries to QMA oracle to determine by binary search a constant a such that the minimum energy λ_1 of H lies in the interval $[a, a+\epsilon/4]$. Next, we call the QMA oracle on the following measurement acting on a state in $\mathcal{H} \otimes \mathcal{H}$:

1. First, project the input state to the antisymmetric subspace of $\mathcal{H} \otimes \mathcal{H}$. If the measurement succeeds, then the post-measurement state must have the form

$$|\Psi\rangle = \sum_{ij} c_{ij}(|\psi_i\rangle|\phi_j\rangle - |\phi_j\rangle|\psi_i\rangle), \tag{1}$$

where $\{|\psi_i\rangle\}$ is an orthonormal basis of $\mathcal{H}$; without loss of generality, we can choose this basis to consist of eigenstates of H.

2. Next, estimate the value of $H \otimes I + I \otimes H$[1] on the post-measurement state using phase estimation, up to precision $\epsilon/5$. Accept if the value is below $2a + \frac{7\epsilon}{4}$, and reject otherwise.

It is easy to show that the state of the form (1) that minimizes the expectation value of $H \otimes I + I \otimes H$ is the state

$$|\Psi\rangle = \frac{1}{\sqrt{2}}(|\psi_1\rangle|\psi_2\rangle - |\psi_2\rangle|\psi_1\rangle),$$

where ψ_1 and ψ_2 are the two lowest-energy eigenstates of H, with eigenvalues λ_1 and λ_2 respectively. This state $|\Psi\rangle$ is in turn an eigenstate of $H \otimes I + I \otimes H$ with eigenvalue $\lambda_1 + \lambda_2$. Thus, in the YES case, the result of phase estimation will be below $(a + \epsilon/4) + (a + 5\epsilon/4) = a + \frac{3\epsilon}{2}$ with high probability, and in the NO case, the result of phase estimation will be above $2a + 2\epsilon$ with high probability, thus establishing completeness and soundness. □

Theorem 3. *SPECTRAL-GAP* for $O(\log(n))$-local Hamiltonians *is hard for* $P^{\text{UQMA}[\log(n)]}$.

Proof. This proof uses a "history state" construction, which each time step in the "history" corresponds to a single oracle query. Suppose we are given a machine in $P^{\text{UQMA}[\log(n)]}$. This machine makes a series of $T = O(\log(n))$ queries to a UQMA oracle. It is fairly straightforward to show that a complete problem for UQMA is to find a low energy state of a Hamiltonian H promised that at most one such state exists. Thus, every query to the UQMA oracle is specified by a Hamiltonian obeying this promise. We denote the answer to the i-th oracle query by y_i, and the Hamiltonian sent as the i-th query by $H_{i|y_1 y_2 \dots y_{i-1}}$, acting on a Hilbert space $\mathcal{H}$—the notation reminds us that the i-th query is allowed to depend on the results of the previous queries. At the end, the machine decides to accept or reject based on the answers to its oracle queries. We construct a new Hamiltonian H whose spectral gap will encode whether the given machine accepts or rejects. This Hamiltonian acts on an enlarged Hilbert space $\mathcal{H}' = \mathbb{C}^2 \otimes (\mathbb{C}^2 \otimes \mathcal{H})^{\otimes T}$, and consists of two terms:

$$H = I \otimes H_{\text{accepting history}} + \epsilon|0\rangle\langle 0| \otimes H_{\text{query}},$$

where the first term in the tensor product acts on the first qubit register in the Hilbert space. The term $H_{\text{accepting history}}$ enforces that the sequence of answers to the oracle queries cause the $P^{\text{UQMA}[\log(n)]}$ machine to accept; it is given by

$$H_{\text{accepting history}} = \sum_{y_1 \dots y_T \text{ rejecting}} |y_1\rangle\langle y_1| \otimes I_{\mathcal{H}} \otimes |y_2\rangle\langle y_2| \otimes I_{\mathcal{H}} \otimes \cdots \otimes |y_T\rangle\langle y_T| \otimes I_{\mathcal{H}}.$$

[1] In [Amb14] this is written as $H \otimes H$, which is presumably a typo

The other term H_{query} enforces that the answers in the history state are correct for the queries issued by the machine. It is given by

$$H_{\text{query}} = \sum_{i=1}^{T} \frac{1}{4^{i-1}} \sum_{y_1 \cdots y_{i-1}} |y_1\rangle\langle y_1| \otimes I_{\mathcal{H}} \otimes \cdots \otimes |y_{i-1}\rangle\langle y_{i-1}| \otimes I_{\mathcal{H}} \\ \otimes \Big(|0\rangle\langle 0| \otimes (H_0) + |1\rangle\langle 1| \otimes H_{i|y_1 \cdots y_{i-1}}\Big) \otimes I \otimes I_{\mathcal{H}} \otimes \ldots,$$

where H_0 is a certain fixed Hamiltonian. It is shown by Ambainis that if the $P^{\mathrm{UQMA}[\log n]}$ machine accepts, then the spectral gap of H is 0–i.e. there exist two orthogonal degenerate ground states, and if the machine rejects, then the spectral gap is at least $\epsilon/4^T$, where ϵ is a constant related to the completeness-soundness gap for the Hamiltonians sent to the UQMA oracle. The intuition is that in the accepting case, the "accepting history" term and "query" term will both be satisfied by the *same* history state $|\psi\rangle$, so $|0\rangle \otimes |\psi\rangle$ and $|1\rangle \otimes |\psi\rangle$ will both be ground states of H; in the rejecting case, this degeneracy is broken. □

Ambainis' results show that the problem SPECTRAL-GAP is closely related to the class QMA, for which many interesting questions remain open. Any progress on QMA would also tell us about the complexity of SPECTRAL-GAP. Below, we list some other open questions of interest.

Problem 4. *What is the complexity of SPECTRAL-GAP for Hamiltonians of constant locality? Recent unpublished work of Wu et al. shows that $P^{\mathrm{UQMA}[\log(n)]} = P^{\mathrm{QMA}[\log(n)]}$ but this does not completely resolve the question. Can perturbative gadgets be used to reduce the locality of the history state Hamiltonian?*

Problem 5. *Can we put SPECTRAL-GAP in* $\mathrm{QMA}(2)$*? Since coNP $\in P^{\mathrm{UQMA}[\log(n)]}$, and it's not even known whether coNP $\in$* $\mathrm{QMA}(2)$*, this problem may be intractable with present knowledge.*

Problem 6. *Is the SPECTRAL-GAP problem for frustration-free Hamiltonians any easier? Could results analogous to Ambainis's be found relating SPECTRAL-GAP for such Hamiltonians to $P^{\mathrm{QMA}_1[\log(n)]}$?*

3 Translation-invariant infinite systems

The second setting in which the complexity of finding spectral gaps has been studied is the limit of infinitely many particles. In this case, in order for the input size of the computational problem to be finite, we restrict our attention to *translation-invariant* Hamiltonians acting on qudits laid out spatially in a lattice. The decision problem we solve is to determine whether a given translation-invariant Hamiltonian H has a spectral gap $\Delta \to 0$ as the system size n tends to ∞ (this limit is known as the *thermodynamic limit*). If the gap tends to 0, the system is called *gapless*; otherwise, it is called *gapped*. In a tour-de-force result, it was shown by Cubitt, Perez-Garcia, and Wolf [CPGW15] that this problem is in fact *undecidable* for qudits on a 2D lattice, with local dimension above a certain universal constant. Their construction encodes the specification of a classical Turing machine into the entries of a local term in the Hamiltonian. The ground state of the overall Hamiltonian is a history state for quantum Turing machine that first applies phase estimation to read out the input, and then applies a universal classical Turing machine on the input string. Thus, the halting problem is embedded into the spectral properties of this Hamiltonian. The full construction is quite involved for several technical reasons; most importantly, in order to achieve a spectral gap in the thermodynamic limit, the Hamiltonian must be "composed" with another Hamiltonian encoding a classical tiling problem. The ground state of the combined Hamiltonian consists of a pattern of tiles, with copies of the quantum history state along edges of the tiles.

Problem 7. *Can the construction of [CPGW15] be improved to 1D chains? How low can we reduce the local dimension?*

From the other end, recent work of Bravyi and Gosset [BG15] has shown that the thermodynamic-spectral gap question *is* decidable for a restricted set of Hamiltonians with the important property of being *frustration free*. For our purposes frustration-free Hamiltonian is one that can be written as a sum of local projectors, such that the ground energy is 0. Bravyi and Gossett analyze frustration-free Hamiltonians on 1D chains of qubits, and provide a simple criterion for whether the Hamiltonian is gapped or gapless in the thermodynamic limit. (In fact, their criterion implies that the spectral gap problem for these Hamiltonians is not only decidable but also solvable in polynomial time.)

Theorem 8 ([BG15])**.** *Let H be a translation-invariant Hamiltonian acting on a 1D chain of n qubits with the form*

$$H = \sum_{i=1}^{n-1} |\psi\rangle_{i,i+1}\langle\psi|_{i,i+1},$$

where $|\psi\rangle \in \mathbb{C}^2 \otimes \mathbb{C}^2$ is a fixed two-qubit state; by construction, this Hamiltonian is frustration free. Then the spectral gap of H goes to 0 as $n \to \infty$ iff the eigenvalues of the matrix

$$T_\psi = \begin{pmatrix} \langle\psi|0,1\rangle & \langle\psi|1,1\rangle \\ -\langle\psi|0,0\rangle & -\langle\psi|1,0\rangle \end{pmatrix}$$

have equal non-zero absolute vaue.

The proof of both directions of this result is quite nontrivial. One of the key tools used in this proof is a remarkable result of Knabe [Kna88], which relates the spectral gap in the thermodynamic limit to spectral gaps of *fixed* finite size.

Lemma 9 ([Kna88])**.** *Let Π be a projector acting on two qudits, and consider the translation-invariant Hamiltonians H_n° and H_n given by*

$$H_n = \sum_{i=1}^{n-1} \Pi_{i,i+1}, \qquad H_n^\circ = H_n + \Pi_{n,1}.$$

(We refer to H_n as the Hamiltonian over an n-qudit chain with open *boundary conditions, and H_n° as the Hamiltonian for* periodic *boundary conditions). Further suppose that H_n and H_n° are frustration free for all n. Then for all $m \geq n \geq 2$, it holds that*

$$\Delta(H_m^\circ) \geq \frac{n-1}{n-2}\Big(\Delta(H_n) - \frac{1}{n-1}\Big).$$

Note that the right-hand side of the bound is *independent* of m. Thus, any value of n for which $\Delta(H_n) > \frac{1}{n-1}$ would be a certificate that H_n° is gapless in the thermodynamic limit. A recent work of Gosset and Mozgunov [GM15] improves this result by replacing $\frac{1}{n-1}$ with $\frac{6}{n(n-1)}$, and shows that this is asymptotically tight by finding examples of gapless systems where $\Delta(H_n) = \Omega(\frac{1}{n^2})$. The same work also establishes a variant of this lemma for 2D lattices.

The proofs of the original lemma of Knabe and its extensions all proceed by establishing the positivity of a polynomial function of the Hamiltonians H°_m and H_n by decomposing it as a sum of squared terms. For instance, in the original Knabe lemma, it is shown that

$$(H^\circ_m)^2 + \frac{1}{n-2} H^\circ_m \succeq \frac{1}{n-2} \sum_{k=1}^{m} A^2_{n,k},$$

where $A^2_{n,k}$ is a copy of H_n acting on the subchain of the system starting from index k. To complete the proof, one uses the fact that for a frustration-free Hamiltonian H, $H^2 \geq \epsilon H \Leftrightarrow \Delta(H) \geq \epsilon$ to bound the $A^2_{n,k}$ terms on the RHS. After some simple manipulations, one obtains

$$(H^\circ_m)^2 \succeq \frac{n-1}{n-2}\Big(\Delta(H_n) - \frac{1}{n-1}\Big) H^\circ_m,$$

which establishes the desired bound on the spectral gap of H°_m. The extensions of [GM15] are proved by modifying the sum of squares decomposition that is used. While this approach seems to be inherently limited to frustration-free systems (since lower bounds on H^2 do not imply anything the gap for a general Hamiltonian H), there is scope to achieve better results for other lattice configurations than those studied to date.

Problem 10. *Can an improved Knabe-type lemma be found for other lattices besides the 1D chain and 2D square lattice?*

Moreover, the Knabe lemma is only one of several crucial ingredients for the result of [BG15], and generalizing their whole result to even the case of 1D qudits with local dimension $d > 2$ would be significant progress.

Problem 11. *Can the classification of gapped and gapless phases of frustration-free systems in [BG15] be extended to beyond the case of 1D chains of qubits?*

Finally, the frustrated case remains wide open.

Problem 12. *Is there a criterion for gapped and gapless phases of 1D qubit chains with* non-*frustration-free Hamiltonians?*

4 Acknowledgements

The author thanks David Gosset and Xiaodi Wu for helpful discussions, and for sharing unpublished results.

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