CMSC 858L: Quantum Complexity

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15 QMA-Completeness of LOCAL HAMILTONIAN

15.1 References

For QMA-completeness of the local Hamiltonian problem, see chapter 14 of Kitaev, Shen, and Vyalyi, *Classical and Quantum Computation*.

15.2 Completeness of $O(\log n)$-LOCAL HAMILTONIAN

One exception to the last statement is when the Hamiltonian is $O(\log n)$-local rather than k-local for constant k. That is, the Hamiltonian is a sum of terms, each of which acts on $O(\log n)$ qubits, where n is the total number of qubits in the system. The instance size is polynomial in n, so we could equally have said logarithmic in the instance size. In this case, the "local" matrices are still polynomial in size and there is still an efficient quantum simulation. This is convenient, because it is a bit easier to prove that the $O(\log n)$-LOCAL HAMILTONIAN problem is QMA-complete.

The main technique for proving QMA-completeness of local Hamiltonian problems is the *history state*. The idea is construct hard subsets of instances by designing a Hamiltonian whose ground state represents the history of some circuit. Given a circuit with T gates, let $|\psi_0\rangle$ be the initial state of the circuit and $|\psi_t\rangle$ ($t = 1, \dots, T$) be the state of the circuit after the ith gate. Then, at its simplest, the *history state* of this circuit is the state

$$\sum_{t=0}^{T} |\psi_t\rangle|t\rangle. \tag{1}$$

That is, the history state has two registers, one containing the state of the circuit at time t and the other a *clock register* containing the time, and then we have a superposition over all times.

We can create a Hamiltonian that has history states as ground states by including terms that cause transitions between $|\psi_{t-1}\rangle|t-1\rangle$ and $|\psi_t\rangle|t\rangle$.

Lemma 1. *If a circuit consists of a sequence of gates U_t, $t = 1, \dots, T$, then the Hamiltonian*

$$H_P = \frac{1}{2}\sum_{t=1}^{T}\Big[I \otimes (|t\rangle\langle t| + |t-1\rangle\langle t-1|) - U_t \otimes |t\rangle\langle t-1| - U_t^\dagger \otimes |t-1\rangle\langle t|\Big] \tag{2}$$

has as 0 energy states all states of the form $\sum_{t=0}^{T} |\psi_t\rangle|t\rangle$ for arbitrary initial states $|\psi_0\rangle$ and no other states. The eigenvalues of H_P are $1 - \cos(\pi k/(T+1))$ for $k = 0, \dots, T$.

We need the $U_t^\dagger \otimes |t-1\rangle\langle t|)$ term to ensure that the Hamiltonian is Hermitian.

Proof. Let us calculate what the Hamiltonian does to any history state $\sum_{t=0}^{T} |\psi_t\rangle|t\rangle$. First consider the action of a single term:

$$I \otimes |t\rangle\langle t| \left(\sum_{t=0}^{T} |\psi_t\rangle|t\rangle \right) = |\psi_t\rangle|t\rangle \tag{3}$$

$$(U_t \otimes |t\rangle\langle t-1|) \left(\sum_{t=0}^{T} |\psi_t\rangle|t\rangle \right) = U_t|\psi_{t-1}\rangle|t\rangle = |\psi_t\rangle|t\rangle \tag{4}$$

$$(U_t^\dagger \otimes |t-1\rangle\langle t|) \left(\sum_{t=0}^{T} |\psi_t\rangle|t\rangle \right) = U_t^\dagger|\psi_t\rangle|t-1\rangle = |\psi_{t-1}\rangle|t-1\rangle. \tag{5}$$

Then

$$H_P \left(\sum_{t=0}^{T} |\psi_t\rangle|t\rangle \right) = \frac{1}{2} \sum_{t=1}^{T} \left[(|\psi_t\rangle|t\rangle + |\psi_{t-1}\rangle|t-1\rangle) - |\psi_t\rangle|t\rangle - |\psi_{t-1}\rangle|t-1\rangle \right] = 0. \tag{6}$$

Thus, all history states are eigenstates of 0 eigenvalue.

To understand the other eigenvalues, note that for any specific $|\psi_0\rangle$, all terms in the Hamiltonian preserve the subspace spanned by states of the form $|\psi_t\rangle|t\rangle$ for the specific value of $|\psi_t\rangle$ derived from $|\psi_0\rangle$:

$$|\psi_t\rangle = \prod_{i=t}^{1} U_i|\psi_0\rangle. \tag{7}$$

Thus, any eigenvectors are superpositions of states of this form. Let us look at this subspace and consider the basis $\{|v_t\rangle = |\psi_t\rangle|t\rangle\}$ for $t = 0, \ldots, T$. Using this basis, what does the Hamiltonian look like? The diagonal terms are $\frac{1}{2}|v_0\rangle\langle v_0| + \sum_{t=1}^{T-1} |v_t\rangle\langle v_t| + \frac{1}{2}|v_T\rangle\langle v_T|$ (since the middle terms $|v_t\rangle\langle v_t|$ get $\frac{1}{2}$ contributions from the t and $t+1$ terms in the Hamiltonian, whereas the first and last terms only get one such contribution, from either the $t = 1$ or $t = T$ term). The off-diagonal terms are $-\frac{1}{2} \sum_{t=1}^{T}(|v_t\rangle\langle v_{t-1}| + |v_{t-1}\rangle\langle v_t|)$. We can write this as a matrix too:

$$H_P = \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} & 0 & 0 & 0 \\ -\frac{1}{2} & 1 & -\frac{1}{2} & 0 & 0 \\ 0 & -\frac{1}{2} & 1 & -\frac{1}{2} & 0 \\ 0 & 0 & -\frac{1}{2} & 1 & -\frac{1}{2} \\ 0 & 0 & 0 & -\frac{1}{2} & \frac{1}{2} \end{pmatrix}. \tag{8}$$

We can recognize this as a quantum walk on a line. A prospective eigenvector will be a wave along the line:

$$|\phi\rangle = \sum_{t=0}^{T} (\alpha e^{i\omega t} + \beta e^{-i\omega t})|v_t\rangle. \tag{9}$$

To see when something of this form is an eigenvector, compute

$$\begin{aligned} H_P|\phi\rangle = & \frac{1}{2}(\alpha + \beta - \alpha e^{i\omega} - \beta e^{-i\omega})|v_0\rangle + \sum_{t=1}^{T-1} (\alpha e^{i\omega t} + \beta e^{-i\omega t})(1 - \frac{1}{2}e^{i\omega} - \frac{1}{2}e^{-i\omega})|v_t\rangle \\ & + \frac{1}{2} \left[\alpha e^{i\omega T}(1 - e^{-i\omega}) + \beta e^{-i\omega T}(1 - e^{i\omega}) \right] |v_T\rangle \qquad (10) \\ = & \, i(-\alpha e^{i\omega/2} + \beta e^{-i\omega/2}) \sin\omega/2|v_0\rangle + \sum_{t=1}^{T-1} (\alpha e^{i\omega t} + \beta e^{-i\omega t})(1 - \cos\omega)|v_t\rangle \\ & + i(\alpha e^{i\omega(T-1/2)} - \beta e^{-i\omega(T-1/2)}) \sin\omega/2|v_T\rangle. \qquad (11) \end{aligned}$$

We have eigenvalue λ if:

$$i(-\alpha e^{i\omega/2} + \beta e^{-i\omega/2}) \sin \omega/2 = \lambda(\alpha + \beta) \tag{12}$$

$$(\alpha e^{i\omega t} + \beta e^{-i\omega t})(1 - \cos \omega) = \lambda(\alpha e^{i\omega t} + \beta e^{-i\omega t}) \tag{13}$$

$$i(\alpha e^{i\omega(T-1/2)} - \beta e^{-i\omega(T-1/2)}) \sin \omega/2 = \lambda(\alpha e^{i\omega T} + \beta e^{-i\omega T}) \tag{14}$$

The equations for $t = 1, \ldots, T-1$ tell us $\lambda = 1 - \cos \omega = 2\sin^2 \omega/2$. Thus, to satisfy the equations for $t = 0$ and $t = T$, we need that

$$\frac{i}{2}(-\alpha e^{i\omega/2} + \beta e^{-i\omega/2}) = \sin \omega/2(\alpha + \beta) \tag{15}$$

$$\frac{i}{2}(\alpha e^{i\omega(T-1/2)} - \beta e^{-i\omega(T-1/2)}) = \sin \omega/2(\alpha e^{i\omega T} + \beta e^{-i\omega T}). \tag{16}$$

The first can be solved by letting $\alpha = e^{i\omega}\beta$ since then we have

$$e^{i\omega} e^{i\omega/2} - e^{-i\omega/2} = (e^{i\omega/2} - e^{-i\omega/2})(e^{i\omega} + 1). \tag{17}$$

The last equation then becomes

$$e^{i\omega(T+1/2)} - e^{i\omega(T-1/2)} = -(e^{i\omega/2} - e^{-i\omega/2})(e^{i\omega(T+1)} + e^{-i\omega T}) \tag{18}$$

$$= -e^{i\omega(T+3/2)} + e^{i\omega(T+1/2)} - e^{-i\omega(T-1/2)} + e^{-i\omega(T+1/2)}, \tag{19}$$

or

$$e^{i\omega(T+3/2)} = e^{-i\omega(T+1/2)} \tag{20}$$

This means that $2\omega(T+1)$ is an integer multiple of 2π, or $\omega = \pi k/(T+1)$ for integer k.

This gives $T+1$ eigenvalues $1 - \cos(\pi k/(T+1))$, which matches the dimension of the subspace, so these are all the eigenvalues. This argument also gives us the explicit eigenstates, and we can see that we don't get a proper history state unless $\omega = 0$; otherwise, we get a history state with some additional phases between terms. □

But how is this related to proving that the local Hamiltonian problem is QMA-complete? We can prove QMA-completeness by reducing from an arbitrary QMA language to $O(\log n)$-LOCAL HAMILTONIAN. What do we know about an arbitrary QMA language? It has an efficient checking circuit. We will therefore pick a Hamiltonian whose ground state is a history state for the language we are reducing from.

Theorem 1. *$O(\log n)$-LOCAL HAMILTONIAN is QMA-complete.*

Proof. We wish to reduce from a language L to $O(\log n)$-LOCAL HAMILTONIAN. Let C be the checking circuit for L for an instance of size n, and assume that the acceptance probability of this checking circuit has been amplified to close to 1 (we will need it to be polynomially close). We will discuss the best ways to do this later. We define a Hamiltonian H as follows:

$$H = H_P + H_i + H_f. \tag{21}$$

Here H_P is the Hamiltonian defined above whose ground states are history states for C.

$H_i = \sum_j |1\rangle_j\langle 1| \otimes |0\rangle\langle 0|$, where the sum is taken over all qubits j which are ancilla states for C and the second tensor factor is the clock register. This ensures that at time 0, the ancilla states for C start out in the $|0\rangle$ state; otherwise they will suffer an energy penalty. Note that we don't put a constraint on all the input qubits to C, since C also takes the witness as input, and we don't know what that is supposed to be.

$H_f = |0\rangle_0\langle 0| \otimes |T\rangle\langle T|$, where the first register is a projector on the output qubit of C and the second tensor factor is the clock register. This term gives an energy penalty if the output qubit of the circuit is 0, indicating that the checking circuit does not accept.

Note that each of H_P, H_i, and H_f are positive semi-definite. This means that the energy of a state for H is at least as large as the energy for each of the three pieces.

This Hamiltonian is $O(\log n)$-local, since each gate for C acts on a constant number of qubits. The clock requires $\log T$ qubits, and $T = O(\mathrm{poly} n)$, so the clock has $O(\log n)$ qubits in it. The Hamiltonian is the sum of terms each of which is an operator on the first register which acts on a constant number of qubits tensor an operator of the form $|t\rangle\langle t|$ or $|t\rangle\langle t'|$, which can potentially act on all qubits in the clock. Thus, each term of the Hamiltonian may act on up to $O(\log n)$ qubits.

Let us compute the energy of a history state $|\psi\rangle = \frac{1}{\sqrt{T+1}} \sum_t |\psi_t\rangle|t\rangle$ for C with correctly-initialized ancillas for some choice of witness. (I have normalized the state correctly since this will be important for our calculation.) $H_P|\psi\rangle = 0$ by lemma 1. Since the initial state $|\psi_0\rangle$ of the circuit has 0 for all ancilla qubits, $H_i|\psi\rangle = 0$ as well. However, H_f does not necessarily give 0 energy because the witness might not be accepted. Suppose the final state $|\psi_T\rangle$ for a particular witness is accepted with probability p. Then $|\psi_T\rangle = \sqrt{p}|1\rangle|\psi_T^1\rangle + \sqrt{1-p}|0\rangle|\psi_T^0\rangle$ and

$$H_f|\psi\rangle = \frac{1}{\sqrt{T+1}} \sum_{t=0}^{T} H_f|\psi_t\rangle|t\rangle \tag{22}$$

$$= \frac{1}{\sqrt{T+1}} (|0\rangle_0\langle 0| \otimes |T\rangle\langle T|)(\sqrt{p}|1\rangle|\psi_T^1\rangle + \sqrt{1-p}|0\rangle|\psi_T^0\rangle) \otimes |T\rangle \tag{23}$$

$$= \frac{1}{\sqrt{T+1}} \sqrt{1-p}|0\rangle|\psi_T^0\rangle \otimes |T\rangle \tag{24}$$

$$\langle\psi|H_f|\psi\rangle = \frac{1-p}{T+1}. \tag{25}$$

Thus, the energy of this state is not 0 unless the witness for L is accepted by C with probability 1. The history state is also not an eigenstate of H unless the witness is accepted with probability 1.

Now, let us consider a "yes" instance of L. Then there exists a witness that is accepted with probability $p \geq 1 - O(1/\mathrm{poly}(n))$. Therefore, we can construct a history state using that witness and the expectation value of its energy for H is $(1-p)/(T+1) \leq O(1/[(T+1)\mathrm{poly}(n)]) = E$. While this history state is not an eigenstate, there must be a ground state and its energy must be less than or equal to that of the history state, so in particular, we see that the ground state energy is at most E.

For a "no" instance of L, we can make a history state out of any witness, but C will always accept with probability $p \leq O(1/\mathrm{poly}(n))$. This implies that the energy of that history state is at least $(1 - O(1/\mathrm{poly}(n))/(T+1) = E + c_1/(T+1)$ for some constant c_1. We want this to be a "no" instance of $O(\log n)$-LOCAL HAMILTONIAN, which means that the energy of every eigenstate is at least $E + \Delta$. This is equivalent to saying that all states have their energy at least this big. However, so far we have only checked history states formed with initial states with correctly initialized ancillas. What about states that are not of this form?

For instance, consider a history state $|\psi\rangle$ with one or more incorrectly initialized ancillas. Then

$$\langle\psi|H|\psi\rangle \geq \langle\psi|H_i|\psi\rangle = \frac{1}{T+1} \sum_j \langle\psi_0|1\rangle_j\langle 1|\psi_0\rangle \otimes \langle 0|0\rangle = \frac{d}{T+1}, \tag{26}$$

where d is the number of incorrectly initialized ancillas. This is greater than E by at least $c_2/(T+1)$ for some constant c_2. Let $c = \min(c_1, c_2)$.

But what if we don't have a history state at all? Such a state will be penalized by H_P, but how much? We will determine this using a lemma by Kitaev:

Lemma 2. *Let K_1, K_2 be positive semi-definite operators with no shared 0 eigenstates and suppose that all eigenstates of both K_1 and K_2 with nonzero eigenvalue have eigenvalue at least v. Let θ be the minimum angle between $|\psi_1\rangle$ and $|\psi_2\rangle$ where $|\psi_i\rangle$ is an eigenstate of K_i with eigenvalue 0. Then*

$$\langle\phi|(K_1 + K_2)|\phi\rangle \geq 2v \sin^2\theta/2 \tag{27}$$

for all state $|\phi\rangle$.

We will apply this lemma by letting $K_1 = H_P$ and $K_2 = H_i + H_f$. The 0 eigenstates of H_P are the history states and the arguments above show that for any history state $|\psi_1\rangle$,

$$\langle\psi_1|H_i + H_f|\psi_1\rangle \geq E + \frac{c}{T+1}. \tag{28}$$

Thus, K_1 and K_2 have no shared 0 eigenstates. By lemma 1, the smallest non-zero eigenvalue of $K_1 = H_P$ is $1 - \cos(\pi/(T+1)) = \Theta(1/T^2)$. $H_i + H_f$ is easy to diagonalize, and we see that the smallest non-zero eigenvalues are 1.

To determine the angle between 0 eigenstates of K_1 and K_2, let $|\psi_1\rangle$ be a history state, a 0 eigenstate of K_1, and let $|\psi_2\rangle$ be a 0 eigenstate of K_2. Choose $|\psi_1\rangle$ and $|\psi_2\rangle$ that achieve the minimum angle θ. Then

$$\cos\theta = \langle\psi_1|\psi_2\rangle = \langle\psi_1|(I - K_2)|\psi_2\rangle. \tag{29}$$

Now,

$$\|(I - K_2)|\psi_1\rangle\| = \sqrt{\langle\psi_1|(I - K_2)|\psi_1\rangle} \leq \sqrt{1 - (E + c/(T+1))} \tag{30}$$

since K_2 is a projector and $I - K_2$ is a projector onto the orthogonal space. Then

$$\cos\theta \leq \|(I - K_2)|\psi_1\rangle\| \leq 1 - \Omega(1/T) \tag{31}$$

and $\sin^2\theta/2 = \Omega(1/T)$. By lemma 2, we then have that

$$\langle\phi|H|\phi\rangle \geq 2\Theta(1/T^2)\Omega(1/T) = \Omega(1/\mathrm{poly}(n)) = \Delta. \tag{32}$$

Thus, the instance (H, E, Δ) is a "no" instance. It follows that we have a reduction from L to $O(\log n)$-LOCAL HAMILTONIAN for arbitrary $L \in$ QMA, and therefore $O(\log n)$-LOCAL HAMILTONIAN is QMA-complete. $\square$