Lecture 3

Classification of local hamiltonian problems

Scribe: Zijing Di

3.1 Perturbation theory

Our goal in this section is to finish the proof of Theorem 2.4 that 2LH is QMA-complete. We have shown in the last lecture that 3LH is QMA-complete, and we are left to prove that the ground energy of every 3LH can be approximated with the ground energy of a 2LH.

To solve it, we will introduce a powerful technique called perturbation theory, which is used to analyze the spectrum of the sum of two Hamiltonians when one of them has small norm while the spectrum of the other one has large gap. This can give a better approximation than the projection lemma (Lemma 2.6) because we consider higher order terms in the approximation. Interestingly, as a byproduct, we will see how the higher order terms create 3-local Hamiltonian from 2-local Hamiltonians, and this will be crucial in simulating 3-local Hamiltonians with 2-local Hamiltonians.

Given a sum of two Hamiltonians $H = H_0 + V$ (we treat the norm of V as small and the spectrum gap of H_0 as large), define Π_- as the projection onto the span of eigenvectors of H_0 whose eigenvalues are smaller than $\frac{J}{2}$ and $\Pi_+ = \mathrm{Id} - \Pi_-$. Then for every operator A, define $A_+ = \Pi_+ A \Pi_+$, $A_{-+} = \Pi_- A \Pi_+$, $A_{+-} = \Pi_+ A \Pi_-$, and $A_- = \Pi_- A \Pi_-$. We also define Π'_- to be the projection onto the low-energy space of H (the span of eigenvectors of H whose eigenvalues are smaller than $\frac{J}{2}$). Let $G^H(z) = (z \cdot \mathrm{Id} - H)^{-1}$ and $\Sigma_-(z) = z \cdot \mathrm{Id}_- - (G^H_-(z))^{-1}$, where $G^H_-(z) = \Pi_- G^H(z) \Pi_-$.

Theorem 3.1. *Assume all of H_0's eigenvalues are in $(-\infty, 0] \cup [J, +\infty)$ and $\|V\| < J/2$. Suppose there exists an effective Hamiltonian H_{eff} such that $Spec(H_{eff}) \subseteq [-c, c]$ (eigenvalues of H_{eff} lie in the range $[-c, c]$). If $\|\Sigma_-(z) - H_{eff}\| \le \epsilon$ for some $c < \frac{J}{2} - \epsilon$ and all $z \in [-c-\epsilon, c+\epsilon]$, then for each j, the j^{th} eigenvalue of H_{eff} is ϵ-close to the j^{th} eigenvalue of $\Pi'_- H \Pi'_-$.*

Remark 3.2. $\lambda_{min}(\Pi'_- H \Pi'_-)$ is the same as the ground energy of H since Π'_- projects H into its low-energy space. Then this lemma says the ground energy of H_{eff} is ϵ-close to that of H if $\|\Sigma_-(z) - H_{eff}\| \le \epsilon$.

We will only give the intuition behind the proof. Intuitively, when we project H onto $\Pi_- H \Pi_-$, the spectrum often changes and eigenvalues are not preserved. Instead, we encode eigenvalues of H in the poles of $G^H(z)$ at z being eigenvalues of H. Since poles are preserved under projection, small eigenvalues of H are also poles of G^H_-. With some effort we can show z is the pole of G^H_- if and only if it is an eigenvalue of $\Sigma_-(z)$. Then if the ground energy of $\Sigma_-(z)$ is ϵ-close to that of H_{eff}, we will have that the ground energy of H is ϵ-close to H_{eff}.

This theorem is particularly useful when $\|V\|$ is close to $\sqrt{J}$. For example, consider the following 2×2 matrices,

$$H_0 = \begin{pmatrix} J & 0 \\ 0 & 0 \end{pmatrix}, V = \begin{pmatrix} 0 & \delta \\ \delta & \epsilon \end{pmatrix}, H = H_0 + V = \begin{pmatrix} J & \delta \\ \delta & \epsilon \end{pmatrix}.$$

The smallest eigenvalue of H is $\frac{1}{2}\left(J + \epsilon - \sqrt{(J-\epsilon)^2 + 4\delta^2}\right)$. This is close to $\lambda_{min}(V|_S) \approx \epsilon$ if $\delta^2 \ll J$ where S is the null space of H_0, but is very different otherwise.

Next, we will show how to use Theorem 3.1 to obtain 2-local Hamiltonians from 3-local Hamiltonians.

Given a 3-local Hamiltonian H_{target}, assume that we can write $H_{target} = A \otimes B \otimes C + H_{else}$ where A, B, C are 1-local Hamiltonians and H_{else} is a 2-local Hamiltonian. In general, we can always write a 3-local Hamiltonian as $\sum_i A_i \otimes B_i \otimes C_i + H_{else}$ and the proof generalizes.

We then construct a 2-local Hamiltonian $H = H_0 + V$ as follows. We add a new qubit w and define

$$\begin{aligned}
H_0 &= J|1\rangle\langle 1|_w \\
V &= \left(H_{else} + \frac{\alpha^2}{J}(-A+B)^2 + \frac{\alpha^2\beta}{J^2}\left(A^2+B^2\right)C\right) \otimes |0\rangle\langle 0|_w \\
&\quad + (\alpha(-A+B) \otimes X_w + \beta(-C) \otimes |1\rangle\langle 1|_w) \\
&= H'_{else} \otimes |0\rangle\langle 0|_w + V'
\end{aligned}$$

for some constants $\alpha, \beta \in \mathbb{R}$, where $H'_{else} = H_{else} + \frac{\alpha^2}{J}(-A+B)^2 + \frac{\alpha^2\beta}{J^2}\left(A^2+B^2\right)C$ and the rest of terms in V consist of V'. Observe that H_0 and V are 2-local. Our goal is to show $\lambda_{min}(H) \approx \lambda_{min}(H_{target})$ using Theorem 3.1.

First, we partition V by projectors $\Pi_- = |0\rangle\langle 0|_w$ and $\Pi_+ = |1\rangle\langle 1|_w$ as follows.

$$\begin{aligned}
V &= \begin{pmatrix} H'_{else} & \alpha(-A+B) \\ \alpha(-A+B) & \beta(-C) \end{pmatrix} \\
V_- &= H'_{else} \otimes |0\rangle\langle 0|_w \\
V_{-+} &= \alpha(-A+B) \otimes |0\rangle\langle 1|_w \\
V_{+-} &= \alpha(-A+B) \otimes |1\rangle\langle 0|_w \\
V_+ &= \beta(-C) \otimes |1\rangle\langle 1|_w
\end{aligned}$$

Let $G(z) = (z \cdot \mathrm{Id} - H_0)^{-1}$. We can compute $G_+(z) = \frac{1}{z-J}|1\rangle\langle 1|_w$. Since $z \ll J$ by assumption, $\frac{1}{z-J}$ is on the order of $\frac{1}{-J}$.

By Taylor expansion on G and Σ_-, we have

$$\begin{aligned}
\Sigma_-(z) &= V_- + V_{-+}G_+V_{+-} + V_{-+}G_+V_+G_+V_{+-} + \dots \\
&= H'_{else} \otimes |0\rangle\langle 0|_w + (-\frac{1}{J})\alpha^2(-A+B)^2 \otimes |0\rangle\langle 0|_w \\
&\quad + \left((-\frac{1}{J})^2\alpha^2(-A+B)^2\beta(-C)\right) \otimes |0\rangle\langle 0|_w + \dots \\
&= H_{else} \otimes |0\rangle\langle 0|_w + \frac{2\alpha^2\beta}{J^2}ABC \otimes |0\rangle\langle 0|_w + \dots
\end{aligned}$$

In the second equation, notice that $\frac{\alpha^2}{J}(-A+B)^2 \otimes |0\rangle\langle 0|_w$ in H'_{else} of the first term cancels out with the second term. The rest of the terms in the expansion is on the order $O(\frac{1}{J^{1/3}})$. Setting $\alpha = \frac{1}{\sqrt{2}}J^{2/3}$ and $\beta = J^{2/3}$,

$$\Sigma_-(z) = ABC \otimes |0\rangle\langle 0|_w + H_{else} \otimes |0\rangle\langle 0|_w + O(\frac{1}{J^{1/3}})$$

Setting $H_{eff} = (ABC + H_{else}) \otimes |0\rangle\langle 0|_w$, this implies that $\|\Sigma_-(z) - H_{eff}\| \leq \epsilon = O(\frac{1}{J^{1/3}})$. Then by Theorem 3.1, the j^{th} eigenvalue of H_{eff} is $O(\frac{1}{J^{1/3}})$-close to the j^{th} eigenvalue of $\Pi'_- H \Pi'_-$. With some extra effort, we can show that the smallest eigenvalue of H_{eff} is that of the initial 3-local Hamiltonian H_{target}, which concludes the proof that the 2-local Hamiltonian is QMA-complete.

3.2 Classification theorem

After learning the QMA-completeness of general 2LH, we introduce more restrictions and see how they affect the complexity of solving the Local Hamiltonian problem.

Definition 3.3. For a set S of local terms, $S -$ LH is the Local Hamiltonian problem with the restriction that all local terms are in S.

For example, for a set $S = \{Z \otimes Z, X\}$, the input Hamiltonian H of the $S -$ LH problem is specified by a space of n qubits and a collection of m local Hamiltonians H_j acting on the space such that H_j is in the form of $Z_{i_1} \otimes Z_{i_2}$ or X_i ($1 \leq i_1, i_2, i \leq n$). The $S\text{LH}_{a,b}$ problem is to decide between the following two cases:

- *(YES):* $\exists |\psi\rangle \in \mathbb{C}^{2^n}$, $\||\psi\rangle\| = 1$, such that $\langle\psi|H|\psi\rangle \leq a$
- *(NO):* $\forall |\psi\rangle \in \mathbb{C}^{2^n}$, $\||\psi\rangle\| = 1$, $\langle\psi|H|\psi\rangle \geq b$

What is the complexity of solving the $S -$ LH problem?

When $S = \{Z \otimes Z\}$, $S -$ LH is exactly the MAXCUT problem, which is NP-complete.

When $S = \{X \otimes X, X \otimes I, Z \otimes I, X \otimes Z, I \otimes I, Z \otimes Z\}$, $S -$ LH is QMA-complete. The reason is as follows. With some extra effort, we can see that we do not need complex numbers in the proof of QMA-completeness of 2LH. Since every 2-local Hamiltonian that does not contain complex numbers can be written as a linear combination of local terms from S (and $Y \otimes Y$, but it is not hard to see that such terms are not needed at any step), solving SLH implies solving a QMA-complete problem.

We have the following classification theorem to characterize the hardness of the $S -$ LH problem.

Theorem 3.4 (Classification theorem)**.** SLH *problem is:*

- *in* P *if S only has 1-local terms;*
- *otherwise* NP*-complete if there exists a unitary U on $\mathbb{C}^2$ such that for every Hamiltonian $h \in S$, $U^{\otimes 2} h \left(U^{\otimes 2}\right)^\dagger$ is diagonal;*
- *otherwise* StoqMA*-complete if there exists a unitary U on $\mathbb{C}^2$ such that for every Hamiltonian $h \in S$, $U^{\otimes 2} h \left(U^{\otimes 2}\right)^\dagger = \alpha Z \otimes Z + A \otimes I + I \otimes B$ (a diagonal term plus some 1-local terms);*
- QMA*-complete otherwise.*

The first point is easy to verify, as 1-local terms decouple and H can be diagonalized by diagonalizing the constraints on each qubit one at a time. For the second point, inclusion in NP is easy to see since eigenstates of H are computational basis states. NP-completeness requires more work, but can be shown using standard techniques in NP-completeness; essentially, a reduction from MAXCUT. The third bullet is more delicate. We will not define the class StoqMA here. It is an interesting class that lies between MA and AM, and as a consequence is believed to be strictly larger than NP, and strictly smaller than QMA. Finally, the last bullet is shown using a lot of perturbation theory. The significance of the theorem is that the complexity of $S-\mathrm{LH}$ can, overall, take only a small number of forms; at a high level the moral is that a family of local Hamiltonians is "hard unless it is obviously easy."

By setting $S=\{\frac{1}{4}(\mathrm{Id}-X\otimes X-Y\otimes Y-Z\otimes Z)\}$, we can obtain the following corollary.

Corollary 3.5. *Quantum MAXCUT problem is* QMA*-complete.*

We can also consider Hamiltonians with geometric locality. To be more specific, we can consider the Hamiltonians where the qubits are arranged in a geometric way (e.g. 1D line, 2D grid, 3D cube) and interactions can only occur between two adjacency nodes. This kind of Hamiltonians has motivations from physics. Again, most quantum mechanical systems exist in one, two or three-dimensional Euclidean space where interactions are geometrically local. We give figures for 1D LH and 2D LH problem.

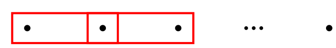

Figure 3.1: The 1D LH problem where each node is a qubit and each H_j acts on one edge where $H=\frac{1}{m}\sum_{j=1}^{m}H_j$

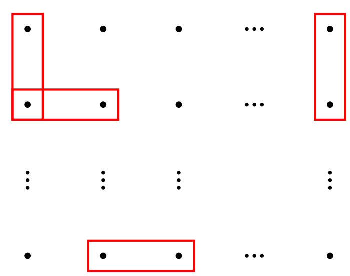

Figure 3.2: The 2D LH problem where each node is a qubit and each H_j acts on one edge where $H=\frac{1}{m}\sum_{j=1}^{m}H_j$

Surprisingly, the Local Hamiltonian problem is hard even when interactions are restricted to geometric locality.

Theorem 3.6. *The 2D Local Hamiltonian problem is* QMA*-hard.*

The proof of this theorem is not very difficult, and combines tools that we have already seen. Essentially, one has to go through all steps, from the circuit-to-Hamiltonian construction to perturbation theory, and revisit each step while having in mind a geometric location for the qubits, trying to ensure that qubits that participate in the same local constraint (such as a clock qubit and the qubits on which the gate at that time step acts) are always close by in Euclidean space. Then, one needs to deal with crossings, etc., which is done using perturbation theory.

Theorem 3.7. *The 1D Local Hamiltonian problem on 9-d qubits is* QMA*-hard.*

Furthermore, the Local Hamiltonian problem is hard even when the interactions satisfy translation invariance (TI). In this case, there is a single local Hamiltonian term which is copied on every edge, and the only variable parameter is the number of qubits of the line. So the input to the problem is the binary representation of an integer N, and yes (resp. no) instances are such that the smallest eigenvalue of the TI Hamiltonian on a line of N qubits is at most a (resp. at least b).

With this interpretation of the input the number of qubits is exponential in the input size, thus the natural quantum witness is exponential in the input size and the natural inclusion is that the 1D-TI LH problem is in $\mathrm{QMA}_{\mathrm{EXP}}$. In fact, the following theorem holds.

Theorem 3.8. *The 1D-TI Local Hamiltonian problem on 11-d qubits is* $\mathrm{QMA}_{\mathrm{EXP}}$*-complete.*