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LECTURE #15: HAMILTONIAN COMPLEXITY THEORY

In the last lecture, we started by reviewing some of the important classical complexity classes like $\mathbf{P}, \mathbf{NP}, \mathbf{BPP}$, and introduced our first quantum complexity class $\mathbf{BQP}$. We saw that $\mathbf{BQP}$ is the quantum analogue for $\mathbf{BPP}$. A natural question would be: what is the quantum analogue for the class $\mathbf{NP}$?

We also reviewed the notion of $\mathbf{NP}$-completeness. Another question is the following: are there natural quantum information tasks which are intractable task for quantum computers, the way $\mathbf{SAT}$ is hard for the classical computers?

In this lecture, first we are going to introduce Hamiltonians, which describe the laws of a physical system. We then propose calculating low-energy states of Hamiltonians as a quantum analogue to $\mathbf{SAT}$ problem for classical computers. Finally, we are going to introduce the class $\mathbf{QMA}$ as a quantum analogue for the classical complexity class $\mathbf{MA}$.

1 Hamiltonians

1.1 What is a Hamiltonian?

In both classical and quantum physics, a **Hamiltonian** captures the physical characteristics of a system. In particular, it specifies how a collection of particles (in isolation) interact with each other over time.

In quantum physics, the allowed energies of a system comprise *discrete* energy levels; this is in stark contrast with classical physics, where we view energy as a *continuous* parameter.

Hamiltonians allow us to derive important properties of quantum mehcanical systems, such as:

- the allowed energy levels of the system;
- the stationary states/eigenstates of the system;
- how the system evolves in time;
- how particles interact with each other.

Now we give the mathematical definition for a Hamiltonian.

Definition 1.1 (Hamiltonian)**.** *A **Hamiltonian** is a hermitian operator H which characterizes the total energy of the system. If H describes a system of n qubits, then $H \in \mathbb{C}^{2^n \times 2^n}$ is a hermitian matrix*

$$H = \sum_{i=0}^{2^n-1} E_i \left|\psi_i\right\rangle \left\langle\psi_i\right|$$

In particular, for any eigenstate $|\psi_i\rangle$, we have $H|\psi_i\rangle = E_i|\psi_i\rangle$.

Let us now make a few remarks about the *spectrum* of the Hamiltonian. We call the states $|\psi_i\rangle$ the stationary states (or eigenstates) of H, and we say that E_i the corresponding energy of the eigenstate $|\psi_i\rangle$. Note that since H is a hermitian matrix, E_i is always a real number.

1.2 Physical Interpretation

A Hamiltonian H assigns an average energy to any state $|\psi\rangle$. By the spectral theorem, we know that the eigenstates of H form an orthonormal basis, and hence we can expand any state $|\psi\rangle$ in this basis:

$$|\psi\rangle = \sum_{i=0}^{2^n-1} \alpha_i |\psi_i\rangle .$$

Now, the average energy for $|\psi\rangle$ with respect to H is defined as

$$\text{(average energy)} \qquad \langle\psi| H |\psi\rangle .$$

The reason that we call this quantity average energy is because of the following characterization as an expectation value:

$$\langle\psi| H |\psi\rangle = \langle\psi| \left(\sum_{i=0}^{2^n-1} E_i |\psi_i\rangle \langle\psi_i| \right) |\psi\rangle = \sum_{i=0}^{2^n-1} E_i \cdot |\alpha_i|^2 = \mathop{\mathbb{E}}_{i \sim |\alpha_i|^2} [E_i].$$

Because $|\psi\rangle$ is a normalized state with $\||\psi\rangle\| = 1$, the squared amplitudes serve as probabilities with $\sum_{i=0}^{2^n-1} |\alpha_i|^2 = 1$, and this justifies why we think of the above as an expectation value.

Definition 1.2 (Ground Energy)**.** *The smallest eigenvalue E_{min} of H is called **ground energy** of H. The states $|\psi\rangle$ with average energy of E_{min} are called **ground states**.*

Since average energy is a weighted average of the energy levels, we can see that ground states have to be eigenvectors corresponding to E_{min}.
The problem that we are interested in here is to find the ground energy, and the corresponding ground states. At first glance it may look like that this is an easy problem since we only need to compute the smallest eigenvalue of a matrix, but H is a $2^n \times 2^n$ matrix and classical linear algebra algorithms would take exponential time to find E_{min}. Nevertheless, we are interested in finding the ground states of a system because they are the most stable configurations of the system.

1.3 k-local Hamiltonians

In physics the laws of nature are inherently local as particles interact with nearby ones. Just like how quantum circuits consist of local gates acting on one or two qubits at a time, the interesting Hamiltonians in physics are built out of local terms. We say a Hamiltonian H is **k-local**, if we can write it as

$$H = H_1 + \cdots + H_m$$

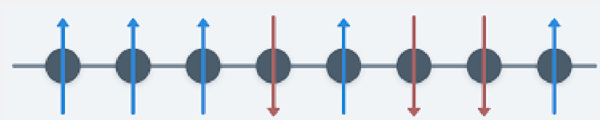
where each H_i only touches at most k qubits; for example, H_i could be an operator of the form

$$H_i = \underbrace{h_i}_{\text{acting on } k \text{ qubits}} \otimes \underbrace{I \otimes \cdots \otimes I}_{\text{acting on } n-k \text{ qubits}} .$$

We now examine two examples of Hamiltonians, and discuss what their ground states look like.

Example 1: 1D-ISING MODEL

1D-Ising model is an important model of magnetism in physics. It is a chain of n spins, where each particle is a magnet that points up $|0\rangle$ or points down ($|1\rangle$). Neighboring magnets want to **anti-align**. There is also a **global magnetic field** that encourages all magnets to point in a specific direction.



The Hamiltonian for the 1D-Ising model can be written as follows:

$$H = \sum_{i=1}^{n-1} (Z_i \otimes Z_{i+1}) + \mu \sum_{i=1}^{n} Z_i$$

where $\mu \in \mathbb{R} \setminus \{0\}$ is the magnetic field strength parameter, and $Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. We let

$$Z_i \otimes Z_{i+1} = I \otimes \cdots \otimes I \otimes Z \otimes Z \otimes I \otimes \cdots \otimes I$$

where the two Z matrices are in the i-th and $(i+1)$-th positions. Similarly

$$Z_i = I \otimes \cdots \otimes I \otimes Z \otimes I \otimes \cdots \otimes I$$

where the Z is in the i-th position. In particular,

- μZ_i captures the global magnetic field on the i-th qubit, it contributes

$$\text{energy} = \begin{cases} +\mu, & \text{if the } i\text{-th qubit is } |0\rangle \\ -\mu, & \text{if the } i\text{-th qubit is } |1\rangle \end{cases}$$

  thus if $\mu > 0$ the i-th qubit *prefers* to be in the lower energy state $|1\rangle$, else if prefers $|0\rangle$

- $Z_i \otimes Z_{i+1}$ captures anti-alignment interactions between neighboring qubits. By expansion,

$$Z_i \otimes Z_{i+1} = |00\rangle \langle 00|_{i,i+1} + |11\rangle \langle 11|_{i,i+1} - |01\rangle \langle 01|_{i,i+1} - |10\rangle \langle 10|_{i,i+1}$$

  Thus, the term favors configurations where neighboring qubits have opposite spins.

These two parts of the Hamiltonians compete with each other. If $|\mu|$ were very large, then the magnetic field is very strong, and the $Z_i \otimes Z_{i+1}$ terms do not have much influence on the ground energy, and all of the particles tend to spin in one direction. On the other hand, if $|\mu|$ were very small, then the magnetic force would be very weak, and the decisive part would be the anti-alignment part, and the states with opposite neighboring spins would have a lower energy.

As we can see, the Ising Hamiltonian is a sum of **2-local** Hamiltonians.

Since the 1D Ising Hamiltonian is diagonal in the standard basis, the ground states are not in superposition, and they are completely classical. In the next example, the ground states are in superposition, and in fact they are highly entangled.

Example 2: TRANSVERSE FIELD ISING MODEL

The *Transverse Field Ising Model* Hamiltonian is another 2-local Hamiltonian of the form

$$H = J\sum_{i=1}^{n-1} Z_i \otimes Z_{i+1} + g\sum_{i=1}^{n} X_i$$

where $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ is the Pauli-X operator, and $J \in \mathbb{R} \setminus \{0\}$ is the anti-alignment parameter and $g \in \mathbb{R} \setminus \{0\}$ is a magnetic coupling parameter.

In this model, the ground states are highly entangled and non-classical.

2 Complexity: QMA

Now we are finally going to answer the questions we asked in the beginning of the lecture.

2.1 k-CSP

Constraint satisfaction problems are the natural complete problems for **NP**. First, we are going to introduce the **k-CSP** problem.

Problem 1: k-CSP

Input: We are given as input

- Variables $x_1, \ldots, x_n$
- Constraints $C_1, \ldots, C_m$ where C_i can depend on at most k variables at a time.

Output: The task is to output YES if there exists an assignment $(x_1^*, \cdots, x_n^*) \in \{0,1\}^n$ of variables which satisfies all of the constraints, and NO otherwise.

3-SAT is and example of **3-CSP**, and it is **NP**-complete.

Now we give the natural complete problem in the quantum world.

2.2 Local Hamiltonian Problem

We now introduce a quantum analog of the k-CSP problem—the k-local Hamiltonian problem. First, let us briefly recall the *operator norm* of a hermitian matrix (i.e., the largest eigenvalue); namely,

$$\|H\| = \max_{|\psi\rangle : \|\psi\| = 1} \langle\psi|H|\psi\rangle.$$

Problem 2: k-LOCAL HAMILTONIAN PROBLEM

Given a k-local Hamiltonian $H = \sum_{i=1}^{m} H_i$ on n qubits with $m = \text{poly}(n)$ and $\|H\| \leq \text{poly}(n)$ as well $a, b \in \mathbb{R}$ such that $0 < a < b$, and $|b - a| \geq 1/\text{poly}(n)$, output

- YES, if $E_{\min}(H) < a$
- NO, if $E_{\min}(H) \geq b$

(with the promise that one these is the case)

Here is a dictionary of analogies between classical **CSP** and Quantum Hamiltonians:

Classical CSP	**Quantum Hamiltonians**
Variables	Qubits
Constraints	Hamiltonian Terms
Assignments	Quantum States
$\#$ of unsatisfied constraints	Energy

2.3 QMA

Definition 2.1 (class **QMA**(Quantum-Merlin-Arthur))**.** **QMA** *is the class of desicision problems for which the YES instances admit polynomial-sized quantum proofs that convince a polynomial-time verifier with probability* $> \frac{2}{3}$.
Moreover if the instance is a NO instance the verifier rejects any state with high probability $> \frac{2}{3}$

Fact 1. *The k-local Hamiltonian Problem is* **QMA***-complete for* $k \geq 2$.

Here is a landscape of our complexity classes: