Hamiltonian Complexity: Part 2

Based on Henry Yuen's Lectures on Advanced Topics in QI Theory

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k-Local Hamiltonians

A k-local Hamiltonian is the analogue of a k-local CSP. Such a Hamiltonian:
(a) Acts on n qubits.
(b) Consists of m Hamiltonian terms $H_1, \ldots, H_m$ where each H_i is a Hermitian matrix defined over $(\mathbb{C}^2)^{\otimes n}$. Each H_i can be written in the form

$$H_i = h_i \otimes \underbrace{I \otimes I \cdots \otimes I}_{n-k'}$$

where each h_i is a Hermitian matrix defined on $(\mathbb{C}^2)^{\otimes k'}$. Conceptually, each H_i acts non-trivially on k' qubits (with $k' \leq k$), and acts on the remaining $n - k'$ qubits with identity. As in the table, each Hamiltonian term corresponds to a constraint in a CSP.

Note: This notation can be misleading, because it seems to suggest that the Hamiltonian term H_i acts nontrivially on the *first* k-qubits (if we were to arrange the qubits on a line). However, h_i may act on some other subset of k qubits, and so the reader will have to look for where this is specified. For example sometimes for a two-local Hamiltonian, we will write $H_{i,j}$ to indicate a Hamiltonian term that acts nontrivially on qubits i and j, where the qubits have some numbering. Sometimes we may write something like $H_i = (h_i)|_S \otimes I_{[n]\setminus S}$ to indicate that h_i acts on a subset of qubits S.

To get a full constraint satisfaction problem from these Hamiltonian terms, consider the full Hamiltonian

$$H = H_1 + H_2 + \cdots + H_m$$

Since we're adding up a bunch of Hermitian matrices together, H is a Hermitian matrix acting on n qubits. Since H is Hermitian, by the Spectral Theorem we can diagonalize it:

$$H = \sum_i \lambda_i |\psi_i\rangle\langle\psi_i|$$

where $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_N$ (for $N = 2^n$) are real eigenvalues and $|\psi_i\rangle$ is the i-th eigenvector of H with eigenvalue λ_i.

A k-local Hamiltonian acting on n-qubits assigns every state $|\varphi\rangle \in (\mathbb{C}^2)^{\otimes n}$ an *energy*, which is given by

$$\langle\varphi|H|\varphi\rangle = \sum_i \lambda_i \langle\varphi| \cdot |\psi_i\rangle\langle\psi_i| \cdot |\varphi\rangle = \sum_i \lambda_i |\langle\varphi|\psi\rangle|^2$$

which is a real number. Going back to our dictionary, if we think of a Hamiltonian H as a CSP and a state $|\varphi\rangle$ as assignment to the variables, the energy of the state $|\varphi\rangle$ is like how many clauses are violated by the assignment (though it needn't be an integer value).

The state $|\varphi\rangle$ that *minimizes* the energy of H is called a *ground state* of the Hamiltonian H. It's the analogue of having an optimal assignment (one that violates the fewest constraints).

It's a standard fact in linear algebra that a ground state of a Hamiltonian is equivalently an eigenvector with the smallest eigenvalue. So the eigenvalue λ_1 is the minimum energy of H. There may be multiple eigenvectors with the same eigenvalue (this is the case when $\lambda_1 = \lambda_2 = \cdots$), we say then that H has a *degenerate ground space*, which is the space of states spanned by all ground states.

When modelling a physical system, a local Hamiltonian describes a system that has only local interactions. For instance, consider a lattice shown in figure 1.

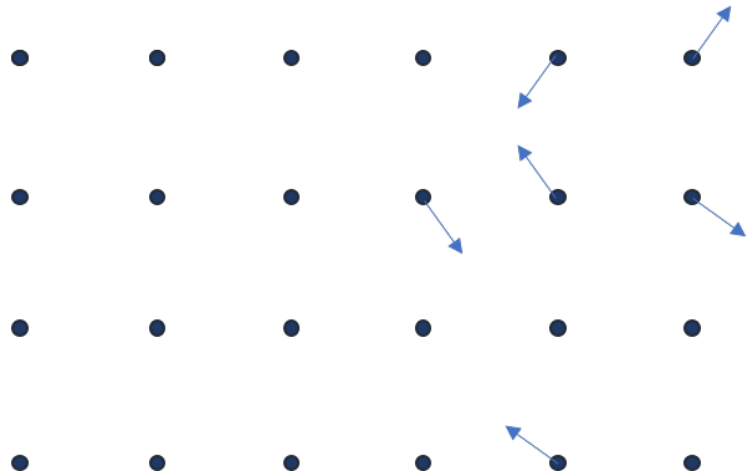

Figure: A lattice (e.g. of atoms). Considering the system to model the spin of each atom, with the arrows indicating the direction of spin, there will be an energy penalty (i.e. constraint violation) for misalignment of neighboring pairs. Similarly, one could use this picture to model macroscopic bar magnets, for which the energy penalty occurs when neighboring pairs *do* align: such a model is more similar to max-cut, as neighboring lattice-points need to have opposite orientation.

Each particle feels some individual force (e.g. if the entire setup is in some external potential), together with forces from all neighboring particles. The more distant interactions between non-neighboring particles are generally negligible, giving rise to a *local* Hamiltonian.

Often in such systems, physicists are interest in how the system evolves with time (its dynamics - in quantum mechanics this is given by the Schrodinger equation), as well as with the properties of low-energy or ground states (for instance, magnets are modelled as such a system of spins, and the low energy state might correspond to all aligning along one axis).

Max-Cut - the Classical Ising Model

Let $G = (V, E)$ be a graph with n vertices. Consider n qubits, one for each vertex. Let Z_u be the Pauli Z operator acting on the u-th qubit.

Then the Hamiltonian corresponding to Max-Cut is

$$H = \sum_{e=(u,v)\in E} Z_u \otimes Z_v$$

where we leave off the identity matrices to make the notation more understandable. The claim is that the ground energy of this Hamiltonian is achieved by state $|x\rangle$ where $x \in \{0,1\}^n$ is an optimal solution to the Max-Cut problem.

We see that $Z_u \otimes Z_v$, written in this way, is already diagonalized, and we can read off what the eigenvalues and eigenvectors are: the $+1$ eigenvectors are when the u and v qubits are in the state $|0,0\rangle$ or $|1,1\rangle$ and the -1 eigenvectors are when the u and v qubits are in the state $|1,0\rangle$ or $|0,1\rangle$.

Therefore, the minimum energy states of qubits u and v, at least with respect to the Hamiltonian term $Z_u \otimes Z_v$, are the ones where u and v have opposite classical values assigned to them (corresponding to eigenvalue -1). This is the precisely the constraint that we want u and v to be on opposite sides of the cut. If the qubits u and v have matching values, then $Z_u \otimes Z_v$ assigns a $+1$ energy penalty.

If $c(x)$ denotes the number of satisfied constraints (a number between 0 and m), then upon some simplification, H can be expressed as

$$H = \sum_{x \in \{0,1\}^*} \big(m - 2c(x)\big)|x\rangle\langle x|$$

Note that this is a diagonalization of H, where the vector $|x\rangle$ is an eigenvector with eigenvalue $m - 2c(x)$. Here we're explicitly including all the other qubits - x includes the states for all of them. Thus the state $|x\rangle$ that has minimum eigenvalue – or, equivalently, the maximum number of satisfied constraints – is a ground state of H. Furthermore, $|x\rangle$ is a classical state that indicates how to partition the vertices.

It's important to note that it's possible that there are several different ground states that give the same ground state energy - i.e. there may be multiple $|x\rangle$ all with the same maximum eigenvalue. Each would correspond to a solution to the max-cut problem.

Thus, the ground-space (the space spanned by the states with maximum eigenvalue) is spanned by optimal solutions to the max-cut problem, since each ground state eigenvector of H is corresponds to one such solution.

Coming Up Next: The Quantum Ising Model

We'll just mention the Quantum Ising Model, and discuss it further next week. Consider n qubits arranged on a ring. Then the Transverse Field Ising Model is the family of Hamiltonians composed of terms with the form:

$$H(g) = -\sum_i Z_i \otimes Z_{i+1} - g \sum_i X_i$$

where g is a real number, Z_i and Z_{i+1} indicate the Pauli Z matrix acting on qubits i and $i+1$ (we consider $N+1$ to be the same as 1), and X_i is the Pauli X matrix acting on the i-th qubit. So for every value g there is a corresponding Hamiltonian with different properties.

The End!