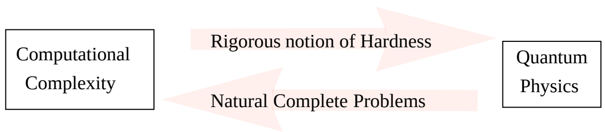
Overview of Hamiltonian Complexity



"How hard is it to simulate a physical system?"

(Jun 2011) Hamiltonian Complexity
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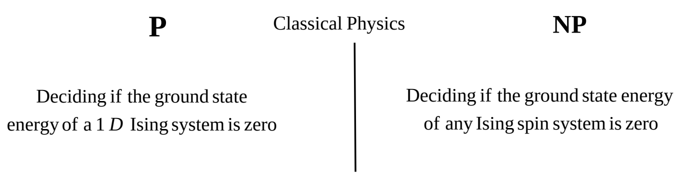
Classical Complexity

Informally, **P** is the set of decision problems (i.e. yes/no questions) that can be answered by a deterministic classical computer in an amount of time that scales polynomially with the input size. **NP** is the set of decision problems for which "yes" instances have a proof that can be checked in polynomial time.



Any problem in **P** is also in **NP**, but **NP** also contains hard-to-solve problems with easy-to-check answers, like decisions based on the energy of an unknown ground state.

To isolate the most difficult problems in **NP**, we say that a problem is **NP**-hard if solving it in polynomial time would lead to a polynomial time solution to every problem in **NP**. In other words, a problem S is **NP**-hard if any other problem in **NP** can be efficiently reduced to deciding S.

An **NP**-hard problem that is also in **NP** is called **NP**-complete. The complete problems are the ones that characterize the difficulty of the class **NP**.

Boolean Satisfiability

Boolean formulas are made out of boolean variables ("bits"), $x_i \in \{0, 1\}$ for $i \in [n]$, joined together by operations like AND ("$\wedge$") and OR ("$\vee$"). Two or more bits joined by an OR is called a clause, and a series of clauses connected by AND is the general type of formula we will consider:

$$(x_2 \vee x_5 \vee x_7) \wedge (x_1 \vee x_5 \vee x_6) \wedge (x_3 \vee x_4 \vee x_7)$$

Any boolean formula can be written in this disjunctive normal form (DNF). We say a formula is satisfiable if there is some choice for the $\{x_i\}$ that makes the formula true.

k-SAT: Given a DNF boolean formula with n variables, having k variables per clause, and $m = \text{poly}(n)$ number of clauses, determine whether the formula has a satisfying assignment.

Theorem (Cook-Levin). 3-SAT is **NP**-complete.

k-SAT is in **NP**, since if there is a satisfying assignment it can be checked in polynomial time. To show that *k*-SAT is **NP**-hard, the trick is to show that the steps of any computation can be turned into the clauses in a boolean formula, so the question of whether the computation outputs "yes" is equivalent to asking whether that boolean formula has a satisfying assignment.

Local Hamiltonian Problem

A Hamiltonian H acting on n qubits is called k-local if it is the sum of terms $H_1, \ldots, H_m$ that each act on k qubits of the system. Here the H_i are positive semi-definite with bounded norm, $\| H_i \| \leq 1$.

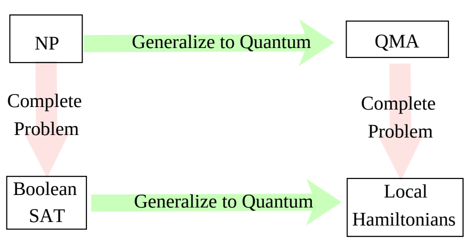
Informally, the ***k*-local Hamiltonian problem** is to decide whether the ground state energy is zero. More precisely, we are given real numbers a, b such that $b - a \geq 1/\text{poly}(n)$, and we need to decide whether the ground state energy is less than a or greater than b.

Just as "yes" instances of NP problems have proofs that are easy to check, any "yes" instance of LH has a proof that is easy to check on a quantum computer, the proof being a description of the quantum ground state.

It might seem like the requirement of k-locality comes from physical considerations for realistic quantum architectures, but in fact it is for a deeper computational reason. Any question about the satisfiability of a boolean formula can be transformed into a question about the ground state of a local Hamiltonian:

$$\underset{\text{is satisfiable}}{(x_1 \vee x_3) \wedge (x_1 \vee x_2)} \quad \Longleftrightarrow \quad \underset{\text{has ground state energy zero}}{(1 - Z_1)(1 - Z_3) + (1 - Z_1)(1 - Z_2)}$$

This correspondence means that the 3-local Hamiltonian problem is **NP**-hard. Since the proof for "yes" instances is easy to check on a quantum computer, but not necessarily easy to check on a classical computer, it suggests a quantum generalization of **NP** which Kitaev called **QMA**.



Future Topics: Stoquastic Hamiltonians

A Hamiltonian H with real entries on the diagonal and negative entries off-diagonal is called stoquastic. Such Hamiltonians are thought to have intermediate complexity between classical and quantum. Note that if $c = \| H \|$ then $G = I - H/c$ is entry-wise positive and satisfies the Perron-Frobenius theorem, from which it follows that that the ground state has all non-negative coefficients.

The matrix G is sub-stochastic, which leads to the construction of various markov chains that are known as Quantum Monte Carlo methods. Stoquastic Hamiltonians also include the Hamiltonians used in quantum adiabatic optimization, so it is of both theoretical and practical interest to know whether these Hamiltonians can be efficiently simulated classically.

Future Topics: Detectability Lemma

The detectability lemma is a recent result that yields a local operator that approximates the ground state projector of a local frustration-free Hamiltonian.

Let $H = \sum H_i$ be a local Hamiltonian with ground state $|\Omega\rangle$ and energy gap ϵ to the first excited state. Assume H is frustration-free so that $H_i |\Omega\rangle = 0$ for each i, and let P_i be the projection onto the ground state of H_i. Define Π_{odd} to be the product of all odd terms P_1, P_3, ... and Π_{even} the product of all even terms. Finally, define $A = \Pi_{\text{odd}} \Pi_{\text{even}}$ and let H' be the orthogonal compliment of the ground space, then in 1D the detectability lemma says:

$$\| A|_{H'} \| \leq \frac{1}{(\epsilon/2+1)^{1/3}}$$

Future Topics: Entanglement Entropy

Although the constraints in the local Hamiltonian problem are local, the solution depends on the global ground state. One way to characterize the amount of local vs global structure in a ground state is to look at its entanglement entropy. Certain classes of states with a low amount of entanglement entropy can be efficiently approximated on a classical computer (e.g. matrix product states).

It's conjectured that the entanglement entropy in the ground state of any gapped local Hamiltonian obeys an **area law**, meaning that the entropy scales as L^{D-1} with system size L in D dimensions. The conjecture has been proven in 1D by Hastings, who used the Lieb-Robinson bound to construct a local approximate projector onto the ground state, recently there has been an alternative proof of the 1D area law based on the detectability lemma.

Future Topics: Quantum PCP Conjecture

Recall that the local Hamiltonian requires deciding if the ground state energy is less than a, or greater than b, where $b - a \geq 1/\text{poly}(n)$. It's natural to ask if the problem gets any easier when we only wish to decide the ground state energy to within a constant fraction c of the number of interaction terms m, $b - a \geq c\, m$.

In the classical setting, the surprising answer is that even this approximation to within a constant factor is NP-complete. This is based on the classical PCP theorem which says every problem in NP has a probabilistically checkable proof.

By analogy, the quantum PCP conjecture would state that even deciding the local Hamiltonian problem within a constant factor is QMA-complete. Interest in the conjecture has been sparked recently because the detectability lemma is seen as a quantum analogue to a major step called gap amplification in a classical proof of the PCP theorem.