

Quantum Hamiltonian Complexity

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Abstract

Constraint satisfaction problems are a central pillar of modern computational complexity theory. This survey provides an introduction to the rapidly growing field of Quantum Hamiltonian Complexity, which includes the study of quantum constraint satisfaction problems. Over the past decade and a half, this field has witnessed fundamental breakthroughs, ranging from the establishment of a “Quantum Cook-Levin Theorem” to deep insights into the structure of 1D low-temperature quantum systems via so-called area laws. Our aim here is to provide a computer science-oriented introduction to the subject in order to help bridge the language barrier between computer scientists and physicists in the field. As such, we include the following in this survey: (1) The motivations and history of the field, (2) a glossary of condensed matter physics terms explained in computer-science friendly language, (3) overviews of central ideas from condensed matter physics, such as indistinguishable particles, mean field theory, tensor networks, and area laws, and (4) brief expositions of selected computer science-based results in the area. For example, as part of the latter, we provide a novel information theoretic presentation of Bravyi’s polynomial time algorithm for Quantum 2-SAT.

1

Introduction

“Computers are physical objects, and computations are physical processes. What computers can or cannot compute is determined by the laws of physics alone. . . .”

— *David Deutsch [125]*

The Cook-Levin Theorem [53, 111], which states that the SATISFIABILITY problem is NP-complete, is one of the cornerstones of modern computational complexity theory [22]. One of its implications is the following simple, yet powerful, statement: Computation is, in a well-defined sense, *local*. Yet, as David Deutsch’s quote above perhaps foreshadows, this is not the end of the story, but rather its beginning. Indeed, just as a sequence of computational steps on a Turing machine can be encoded into local classical constraints (as in the Cook-Levin theorem), the quantum world around us also evolves “locally”, and this quantum evolution can be encoded into an analogous notion of local *quantum* constraints. The study of such quantum constraint systems underpins an emerging field at the intersection of condensed matter physics, computer science, and mathematics, known as *Quantum Hamiltonian Complexity (QHC)*.

At the heart of QHC lies a central object of study: The notion of a *local Hamiltonian* H , which can intuitively be thought of as a quantum constraint system (in this introduction, we will keep our discussion informal in order to convey high-level ideas; all formal definitions, including an introduction to quantum information, are given in Chapter 2). To introduce local Hamiltonians, we begin with the fact that the state of a quantum system S on n qudits is described by some d^n -dimensional complex unit vector $|\psi\rangle \in (\mathbb{C}^d)^{\otimes n}$. How can we describe the evolution of the state $|\psi\rangle$ of S as time elapses? This is given by the Schrödinger equation, which says that after time t , the new state of our system is $e^{-iHt}|\psi\rangle$, where H is a $d^n \times d^n$ -dimensional complex (more precisely, Hermitian) operator called a *Hamiltonian*. Here, the precise definition of the matrix exponential e^{iHt} is irrelevant; what *is* important is the dependence of the Schrödinger equation on H . In other words, Hamiltonians are intricately tied to the evolution of quantum systems. We thus arrive at a natural question: Which classes of Hamiltonians correspond to *actual* quantum evolutions for systems occurring in nature? It turns out that typically, only a special class of Hamiltonians is physically relevant: These are known as *local* Hamiltonians.

Roughly, a k -local Hamiltonian is a Hermitian matrix which has a succinct representation of the form

$$H = \sum_i H_i,$$

where each H_i acts “non-trivially” only on some subset of k qudits. Here, each H_i should be thought of as a “quantum constraint” or “clause”, analogous to the notion of a k -local clause in classical constraint satisfaction problems. For example, just as a classical clause such as $(x_i \vee x_j \vee x_k)$ for $x_i, x_j, x_k \in \{0, 1\}$ forces its bits to lie in set $x_i x_j x_k \in \{001, 010, 011, 100, 101, 110, 111\}$ (where \vee denotes logical OR), a quantum clause H_i restricts the state of the k qudits it acts on to lie in a certain *subspace* of $(\mathbb{C}^d)^{\otimes k}$. Moreover, each clause H_i requires $O(k)$ bits express (assuming all matrix entries are specified to constant precision). This is because each H_i is given as a $d^k \times d^k$ complex matrix (this is made formal in Section 2.2). As a result, although H itself is a matrix of dimension $d^n \times d^n$, i.e. H has dimension exponential in n the

number of qudits, the description of H in terms of local clauses $\{H_i\}$ has size *polynomial* in n .

Since local Hamiltonians are intricately tied to the time evolution of quantum systems in nature, the goal of QHC is to study properties of local Hamiltonians H . Common computational tasks include estimating the *ground state energy* (smallest eigenvalue) of H , or computing features of H 's *ground state* (eigenvector corresponding to the smallest eigenvalue). Intuitively, the ground state can be thought of as the vector $|\psi\rangle$ which “maximally satisfies” the constraints $\{H_i\}$ (i.e. the “optimal solution” to the quantum constraint system), and is of particular interest as it encodes the state of the corresponding quantum system when cooled to low temperature. In fact, any classical Constraint Satisfaction Problem (CSP) of arity k can be embedded into a k -local Hamiltonian, such that determining the ground state of the Hamiltonian yields the optimal solution to the CSP. (This connection is made explicit in §2.2.) Thus, ground states are interesting from a complexity theoretic perspective.

Let us also motivate ground states from a physics perspective. Consider the case of helium-4: When cooled to near absolute zero, helium-4 relaxes to a state $|\psi\rangle$ which is the ground state of some local Hamiltonian H (the precise form of H is beyond the scope of this introduction). This ground state exhibits an exotic phase of matter known as *superfluidity* — it acts like a fluid with zero viscosity. (See [1] for a video demonstrating this remarkable phenomenon.) Ideally, we would like to understand the properties of the superfluid phase demonstrated by $|\psi\rangle$, so that, for example, we can in turn use this knowledge to design new, advanced materials. In this direction, QHC might ask questions such as: Which quantum systems in nature have a ground state with a succinct classical representation? Can we run efficient classical simulations to predict when a quantum system will exhibit interesting phenomena, such as a phase transition? Can we quantify the hardness of determining certain properties of local Hamiltonians by establishing connections to computational complexity theory? In the context of helium-4, for example, the first of these questions is particularly relevant — to the best of our knowledge, a closed form for the ground state energy or

the ground state of helium-4 remain elusive. (Heuristic approximations based on variational methods, however, have long been known; see, e.g. [139].)

This state of affairs illustrates the formidable challenge facing QHC: Namely, we are interested in computing properties of k -local Hamiltonians H , which are matrices of dimension $d^n \times d^n$, whereas an efficient algorithm must run in time polynomial in n , the number of qudits H acts on. Despite this challenge, QHC has proven a very fruitful area of research. For example, in 1999 Kitaev established [106] a quantum version of the celebrated Cook-Levin theorem [53, 111] for local Hamiltonian systems. In 2006, Bravyi gave a polynomial time algorithm for solving the quantum analogue of 2-SATISFIABILITY, known as Quantum 2-SAT [38]. And though the heuristic approach of White [168, 169] (known as “Density Matrix Renormalization Group”) was known to solve 1-dimensional (gapped) Hamiltonians in practice efficiently, Hastings’ 1D area law in 2007 [88] helped explain the efficacy of this heuristic by strongly characterizing the entanglement structure of such 1-dimensional systems. This survey aims to review a select subset of such fundamental results in QHC.

To help make this survey accessible to computer scientists with little or no background in quantum information, we begin in §2.1 with a review of basic quantum information. We next establish some of the fundamental definitions of QHC in §2.2, including an explicit sketch of how an instance of 3-CSP can be encoded into a local Hamiltonian. With this basic background in place, we finally proceed in Chapter 3 to give a roadmap for the remainder of this survey.

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