Quantum Complexity, Statistical Physics, and Combinatorial Optimization

Project Report for 6.S899: Seminar on Computation and Physics

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December 11, 2015

Finding quantum analogues of well-known computational problems is a possible way to enrich the study of quantum computational complexity, which in turn can give us new insights into physical systems. In the other direction, tools from statistical mechanics have been used to study the complexity of NP-complete problems. Here we briefly survey some of these quantum analogues along with the statistical physics of SAT and its quantum version, QSAT, while highlighting very recent work.

1. Introduction

Physics and combinatorial optimization have interacted in at least two ways. On one hand, the k-local Hamiltonian (k-LH) problem, a quantum analogue of MAX-k-CSP, started a field at the boundary of computer science and condensed matter physics called Quantum Hamiltonian Complexity [1]. From a computational perspective, Kitaev initiated the study of QMA-completeness with a proof that 5-LH is QMA-complete, much like the Cook-Levin theorem started the study of NP-complete problems. From the physics side, physicists are interested in understanding different properties of local Hamiltonians. For example, they want to know how hard or feasible it is to compute ground state properties, the correlations or entanglement present in the eigenstates of these Hamiltonians, and their time evolution, among other things. It is natural to ask: what other problems have interesting quantum analogues? In section 2, we will briefly review the quantum versions of k-SAT and MaxFlow-MinCut.

On the other hand, tools from statistical mechanics have been successfully applied to study the 'typical' computational complexity of NP-complete problems. Fu and Anderson[2] realized that the hardness in the complexity of NP-complete problems corresponds to the amount of 'glassiness' exhibited by spin-glasses in statistical physics. Roughly speaking, the hard instances of an NP- complete problem are found when the corresponding spin-glass is at a phase transition. While computational complexity does a good job of classifying problems according to their worst-case complexity, i.e by how well algorithms perform on every instance of a problem, in most practical cases we are interested in efficient performance of an algorithms on a typical or average instance of a problem. In section 3, we will review the ideas of using statistical physics to study typical instances before surveying recent results on the statistical physics of k-SAT and its quantum analogue.

These are not the only ways in which combinatorial optimization and physics communicate with each other. For example, the study of classical and quantum simulated annealing [3][4], quantum adiabatic optimization [5][6], or Ising models [7] are already big enough to deserve their own survey. The goal of this paper is to give the reader an overview of recent results at the boundary of combinatorial optimization, statistical physics, and quantum computational complexity.

2. Quantum Analogues

Quantum Satisfiability— Bravyi [8] defined the quantum satisfiability problem (k-QSAT) as the quantum version of k-SAT. The problem is defined as follows.

Problem 2.1. [8] **(k-QSAT)** Given $n \in \mathbb{N}$, $\epsilon \geq 1/poly(n)$, and k-local projectors $\{\Pi_1, ..., \Pi_M\}$ acting on n-qubits states, decide whether there is $|\Psi\rangle$ s.t $\Pi_i|\Psi\rangle = 0$ for all $i \in [M]$ or if for all states $|\Psi\rangle$ we have that $\sum_i \langle\Psi|\Pi_i|\Psi\rangle \geq \epsilon$, promised that one of this is the case.

When the projectors are diagonal in the computational basis, the problem reduces to k-SAT. The quantum-classical relation, in a sense, maps the NP-completenes of MAX-2-SAT to the QMA-completeness of 2-LH. Contrary to MAX-2-SAT which is NP-complete, there is a linear time algorithm to decide 2-SAT. Wondering if this was also the case for 2-QSAT, Bravyi found a polynomial time algorithm for 2-QSAT. In the same paper, Bravyi introduced the complexity class QMA_1, QMA with one sided error, and showed that k-QSAT is QMA_1-complete for $k \geq 4$. More recently, Gosset and Nagaj showed that 3-QSAT is also QMA_1-complete [9]. The analogy between 2-SAT and 2-QSAT was completed recently when two different groups [10], [11] found linear time algorithms for 2-QSAT.

Quantum Max-Flow— Very recently, Cui et al. [12] used tensor networks to define the Quantum Max Flow (QMF). The Hilbert space of a large number of particles, say spins on a lattice, is exponentially big, making efficient computational simulation of many-body quantum states a difficult task. Quantum states are tensor networks, and many numerical methods have been develop to simulate certain types of tensor networks efficiently. In particular, the entanglement properties of a many-body quantum state result from the underlying tensor network, so they can be seen as networks transporting entanglement.

An instance of QMF is given by an undirected graph $G = (V, E)$, two disjoint sets S and T of open edges (edges adjacent to only one vertex), and a capacity function $C : S \cup T \cup E \to \mathbb{N}$. Given the above as input, the authors in [12] map G into a tensor network in the following way:

1. For every vertex v, find a local ordering of the adjacent vertices $1, 2, ..., d_v$ where d_v is the degree of v. If the vertex has an open edge, label the open end as if it was an adjacent vertex. Denote by $e(v, i) \in S \cup T \cup E$ the edge between vertex v and the vertex labeled by i in the local ordering of v.

2. To each edge $e \in S \cup T \cup E$ append a Hilbert space $\mathcal{H}_e := \mathbb{C}^{C(e)}$ of dimension $C(e)$.

3. Assign a tensor $\mathcal{T}_v \in \mathcal{H}_{e(v,1)} \otimes ... \otimes \mathcal{H}_{e(v,d_v)}$ to every vertex $v \in V$. Denote the total assignment by $\mathcal{T}$.

4. Contract tensors according to the edges of the graph.

The result of this mapping is a tensor network, and following [12] we will denote it by $G \mapsto N(G, C; \mathcal{T})$. Fixing basis over the Hilbert spaces of the open edges we have that $N(G, C; \mathcal{T})$ defines a state $|N(G, C; \mathcal{T})\rangle \in (\underset{e\in S}{\otimes} \mathcal{H}_e) \otimes (\underset{e\in T}{\otimes} \mathcal{H}_e)$ given by

$$|N(G, C; \mathcal{T})\rangle = \sum_{i_1,...,i_{|S|},j_1,...j_{|T|}} N(G, C; \mathcal{T})_{i_1,...,i_{|S|},j_1,...j_{|T|}} |i_1, ..., i_{|S|}\rangle \otimes |j_1, ..., j_{|T|}\rangle. \tag{1}$$

Definition 2.2. [12] Consider the following linear map $\beta(G, C; \mathcal{T}) : \underset{e\in S}{\otimes} \mathcal{H}_e \to \underset{e\in T}{\otimes} \mathcal{H}_e$ acting on the basis vectors as

$$\begin{aligned}\beta(G, C; \mathcal{T})|i_1, i_2, ..., i_{|S|}\rangle &:= (\langle i_1, i_2, ..., i_{|S|}| \otimes I)|N(G, C; \mathcal{T})\rangle \\ &= \sum_{j_1,...j_{|T|}} N(G, C; \mathcal{T})_{i_1,...,i_{|S|},j_1,...j_{|T|}} |j_1, ..., j_{|T|}\rangle\end{aligned} \tag{2}$$

The S, T-**quantum flow** of $\mathcal{T}$ is the rank of $\beta(G, C; \mathcal{T})$. The S, T-**quantum max-flow** of G with capacity C is

$$QMF_{S,T}(G, C) := \max_{\mathcal{T}} \ \mathrm{rank}(\beta(G, C; \mathcal{T})). \tag{3}$$

In summary, given a graph G with open edges S and T, we assigned Hilbert spaces H_S and H_T that are tensor products of the Hilbert spaces in edges of S and T respectively. The graph structure allows for the construction of a tensor network $N \in H_S \otimes H_T$, which in turn defines a map $H_S \to H_T$. The rank of this map is the quantum flow of the tensor network N. Maximizing over all tensor networks, gives you the quantum max-flow. With this definition of quantum flow as the rank of a linear map, an edge cut R in a the network allows us to interpret the total map as a composition $H_S \to H_R \to H_T$. The quantum max-flow measures, more or less, the ability of a graph to transport Hilbert space dimensions between the source edges S and the sink edges T.

The decision version of the problem can be stated as:

Problem 2.3. (QMF) Given a number k, an undirected graph $G = (V, E)$, two disjoint sets S and T of open edges, and a capacity function $C : S \cup T \cup E \to \mathbb{N}$, is $QMF_{S,T}(G, C) \leq k$?

Cui et al. also defined the quantum cut between two subsets of vertices A and B, as the product (instead of the sum as in the classical cut) of the capacities of the edges in an edge cut set of A and B. They found that the Max-Flow/Min-Cut result of classical computation does not hold in general for the quantum versions, but in fact that the S,T-QMF is always less than or equal to the minimum quantum cut (QMC) between S and T. However, they find that if there is a constant $d > 0$ such that the capacity of each edges is equal to some power of d, then the QMF equals the QMC. Although the existent efficient algorithms for classical min-cut would also find the quantum min-cut, Cui et al. do not give any efficient algorithm to calculate QMF. They do not address the computational complexity of QMF.

Consider the entanglement entropy between S and T subsystems in a state given by Eq. (1), and denote it as $S_{S,T}(G, C; \mathcal{T})$. Cui et al. proved that

$$\max_{\mathcal{T}} S_{S,T}(G, C; \mathcal{T}) \leq \log QMF_{S,T}(G, C), \tag{4}$$

and that equality holds under the same condition for which they showed that QMF equals QMC.

Finally, they showed how there are graphs for which randomly/generically choosing projectors to generate QSAT instances that are equivalent to QMF instances on some other graphs. A complete reduction from QSAT to QMF or vice versa is not known. They end the paper with an interesting conjecture:

$$\lim_{n \to \infty} QMF_{S,T}(G, nC) = QMC_{S,T}(G, nC). \tag{5}$$

As will be seen in the next section, this conjecture is similarly spirited to a conjecture in [13]. They both say that some sort of quantumness is disappearing in the large system limit.

Other Quantum Analogues— Surprisingly, there are not many known quantizations of well-known combinatorial optimization problems in the literature. Beigi and Shor[14] introduced the quantum version of the clique (or maximum independent set) problem, and showed its QMA-completeness. Gharibian and Kempe[15] defined the quantum version of succinct set cover in connection to their generalization of the polynomial hierarchy to a quantum/classical hierarchy and the hardness of approximating quantum problems. Gurvits [16],[17] used tools from quantum information to obtain complexity results for generalizations to Edmond's matching problem, and he generalized the concept of perfect matching to what he called a quantum perfect matching. It is in [17] that he showed the NP-hardness of the separability problem of bipartite density matrices. There are many problems, such as knapsack, steiner tree, graph partitioning, closest lattice vector, among many others that could be 'quantized'. As with QMF and QSAT, it might be the case that the generalizations to some of these problems will have non-trivial things to say about entanglement.

3. Statistical Physics of QSAT

Phase Transitions and Computational Hardness— The idea from statistical physics is to assign a parametrized measure to the space of instances of a particular problem, and to analyze the typical cases arising from this measure. By tuning the parameter, it is expected that we can obtain information/structure about which instances are hard to solve and which ones are easy. For example, if the parameter represents the number of random constraints, as it increases, we expect that the problem will have less and less solutions, and, in most cases, they will be harder to find. In general, the harder instances of a problem are found near the phase transition from a phase with solutions to a phase without them. It is at this point, for problems like SAT for which such a phase transition is believed to exist, that there are some solutions that are hard to find. Intuitively, any local search will not find solutions because most solutions are far apart (say in Hamming distance). This method of attacking computational problems have been successful in developing heuristic algorithms, like Belief propagation, to deal with the harder instances encountered. [18], [19]

Random SAT— Perhaps, the most studied ensemble for k-SAT is random k-SAT [19]. Given numbers $n, m \in \mathbb{N}$, an instance of random k-SAT is generated by choosing uniformly at random m clauses over k-variables out of the n possible variables. The parameter $\alpha := m/n$ characterizes the solution space of random k-SAT. Intuitively, the more clauses there are, the higher the chance that the formula will be unsatisfiable, and in the limit $\alpha \to \infty$ the probability of a formula from random k-SAT to be satisfiable becomes 0, since with probability 1, a clause and its negation will appear in the formula. Let $p(\alpha, k)$ be the probability that a randomly chosen formula from random k-SAT with m clauses over n variables is satisfiable. The threshold conjecture states that for any $k \geq 2$, there is a threshold β_k, s.t in the thermodynamic limit $n \to \infty$, we have that $p(\alpha < \beta_k, k) = 1$ and that $p(\alpha > \beta_k, k) = 0$. In other words, that the random k-SAT ensemble exhibits a phase transition (in the thermodynamic limit) from SAT to UNSAT as the parameter α increases. Last year, Ding, Sly, and Sun [20] proved that there is a constant k_0 s.t the conjecture holds for $k \geq k_0$. They also found an explicit asymptotic formula for the value of the threshold as a function of k.

Random QSAT— Motivated by the study of random k-SAT, and in order to find insights into the hard instances of QSAT, Laumann et al. [21] introduced random k-QSAT.

Definition 3.1. Consider n vertices V. For all $I \subseteq [n]$ with $|I| = k$, let $\{v_i\}_{i \in I} \in E$ with probability $\alpha / \binom{n}{k}$. This way, we construct a hypergraph uniformly at random, with expected $m = \alpha n$ number of hyperedges. Then, for each hyperedge $e \in E$, uniformly at random (from the Haar measure) choose projectors of the form $\Pi_e = |\psi_e\rangle\langle\psi_e|$ where $|\psi_e\rangle$ is a state in the 2^k dimensional Hilbert space of the k -qubits on the vertices incident on e. This generates an instance of **random k-QSAT** over n variables with projector density parameter α. The question is then the same as in QSAT, with $H = \sum_e \Pi_e$.

One of their main results is the geometrization theorem. Roughly stated, it says that the projectors average out, and that the satisfiability of the particular instance depends only on the interaction graph. It says that given a fixed graph G, for almost every choice of projector, $\dim(kerH) = D$ for some particular value D with probability 1; furthermore, this value D is minimal with respect to the choice of projectors. Using the geometrization theorem, they bounded the SAT phase for any k. Given a graph G, any classical choice of projector is a particular choice of projectors, and the minimality condition on the geometrization theorem implies that the dimensions of the satisfying space of this classical choice upper bounds the SAT phase with probability 1. This means that finding the number of SAT assignments of the most constrained k-SAT instance over G serves as an upper bound for the SAT phase for k-QSAT with graph G. Using this approach and AdSAT (adversarial SAT problem), Bardoscia, Nagaj, and Scardicchio [22] were able to find an upper bound for 3-QSAT SAT/UNSAT transition of about $\alpha_q \leq 1.5$, improving upon the bound of Bravyi, Moore, and Russell [23] which was 3.59.

Laumann et al. [21] also found a phase transition for 2-QSAT at $\alpha = \frac{1}{2}$, and show the existence of both a SAT and an UNSAT phase for $k \geq 3$. To prove the existence of a SAT phase, they constructed satisfiable product states using Bravyi's transfer matrices [8]. To show the existence of an UNSAT phase, they upper bounded the dimensions of satisfying manifolds, and using the upper bound showed that for $\alpha > -1/\log_2(1 - 2^{-k})$ the instances from random k-QSAT are almost always (as $n \to \infty$) not satisfiable. Although the bounds from [21], [23] on the SAT phase are done by constructing product states, by proving a quantum version of Lovász local lemma, Ambainis, Kempe, and Sattath improved the SAT phase bound by showing the onset of an entangled SAT phase in between the product SAT bounds and the UNSAT phase for $k \geq 13$ [24]. At this entangled phase region, the techniques from [21] and [23] could not say anything.

2-SAT/2-QSAT Ensemble— The geometrization theorem raises questions about the role of quantumness on QSAT. If the graph characterizes the problem, then where does the difference between the quantum and classical cases come from? To study this classical-quantum interplay, Potirniche, Laumann, and Sondhi introduced the SAT/QSAT ensemble [25]. They focused on the 2-SAT/QSAT ensemble.

Definition 3.2. [25] Given n vertices V , generate a random graph $G = (V, E)$ in which for any pair $v, w \in V$, $(v, w) \in E$ with probability $\alpha n/\binom{n}{2}$. Then, for all $e \in E$, label e as Q (quantum) with probability β and C (classical) with probability $1 - \beta$. To each edge labeled as Q, assign a quantum projector chosen uniformly as random as in the QSAT case. In the same way, assign a classical projector (a diagonal projector) chosen uniformly at random to the edges labeled by C. The result is an instance from the **(α, β)-2-SAT/QSAT ensemble**.

Similarly, one could construct a k-SAT/QSAT ensemble by generalizing to hypergraphs. In that paper, the authors proved the existence of a phase transition boundary in the (α, β) plane of random 2-SAT/QSAT. They showed that the phase transition from SAT to UNSAT (in terms of increasing α) occurs precisely at:

$$\alpha_C(\beta) = \frac{2}{1 + \beta + \sqrt{-7\beta^2 + 10\beta + 1}}. \tag{6}$$

To show this, they proved that the formula above is both the lower and the upper bound for the phase transition. Perhaps, the interpolation between classical-quantum will allow us to understand better the role of entanglement shedding light on open problems like the quantum PCP conjecture [25].

When is QSAT satisfiable?— Is there a sufficient condition determining whether a QSAT instance is satisfiable? Sattath et al.[13] found this to be the case. A k-local Hamiltonian $H = \sum_i H_i$ is said to be frustration-free if any ground state of H is also a ground state of H_i for all i. When the ground states have 0 energy and H_i are projectors, determining whether H is frustration free is equivalent to k-QSAT. The authors of [13] found a combinatorial criterion that is sufficient to determine if a Hamiltonian is frustration free. Interestingly enough, they found a lower bound for the dimension of $\ker(H)$ in terms of the partition function of a hardcore gas.

Definition 3.3. Given a k-local projector Hamiltonian H, let $Z(G_H, \lambda)$ be the partition function of a hardcore lattice gas with fugacity λ and with the particles living on the hyperedges of G, where G_H is the interaction graph of H. Z is given by

$$Z(G_H, \lambda) = \sum_{\{n_i\}} \lambda^{\sum_i n_i} \prod_{\langle i,j \rangle} (1 - n_i n_j) \tag{7}$$

where $\{n_i\}$ are the occupation number of the particles (hardcore gas means that $n_i = 0, 1$ for all i), and the product is over all projectors sharing qubits.

Their main result is the following theorem:

Theorem 3.4. *[13] Given a k-local projector Hamiltonian $H = \sum_i \Pi_i$ acting on n-qudit Hilbert space $\mathcal{H}$, with G_H interaction graph and $p = \frac{\dim ker(\Pi_i)}{\dim \mathcal{H}}$ for all i, if $Z(G_H, -p') > 0$ for all $0 \leq p' \leq p$, then $\frac{\dim ker(H)}{\dim \mathcal{H}} \geq Z(G_H, p) > 0$.*

Sattath et al. noted that there are cases for which this inequality is strict, but they conjecture that for d- dimensional qudits, as $d \to \infty$, the inequality becomes tight. In particular, this result, along with the geometrization theorem, give an almost complete classical characterization of QSAT. For large local dimensions, and in the thermodynamic limit, the 'quantumness' of the problem seems to disappear. This conjecture is along the same lines of the conjecture from [12] on the equality of QMF and QMC of large systems.

By using this theorem, and cavity methods calculations, they found evidence for the appearance of the entangled SAT phase at $k \geq 7$, improving on the bound by [24].

4. Beyond QSAT

The random ensemble method can be applied to problems outside of QMA and outside of NP. One could ask, on a typical case of SAT, how many satisfying assignments would there be? This is random #SAT, the counting version of random SAT.

#2-QSAT— Like SAT, 2-QSAT has a counting problem version, #2-QSAT, that is #P-complete. #P-hardness follows from the #P-hardness of #SAT. That #2-QSAT is in #P was shown in [26]. The problem is to determine the total number of satisfying assignments. De Beaudrap [27] showed that the typical instances in the random version of #2-QSAT are 'easy' to solve. Formally, random #2-QSAT is defined as the problem of determining the degeneracy of a local Hamiltonian sampled from random 2-QSAT. The arguments through which [21] showed that 2-QSAT has a phase transition can be used to find instances in which #2-QSAT are easy to solve. For a fix graph G over n vertices with no loops, the degeneracy of the satisfying space is $n+1$. If G has one loop, the degeneracy is 2, and if it has 2 or more loops, it is 0. This happen with probability 1 in the thermodynamic limit. Intuitively, the Haar measure picks projectors onto entangled states, so the constraints are somewhat long-ranged, and the graph becomes over-constrained when too many loops are present. But what happens if we forget about the Haar measure? De Beaudrap [27] asked the question: under which distributions or family of graphs will #2-QSAT instances be hard? He found that, with probability 1 in the thermodynamic limit, for uniformly randomly chosen (Erdos-Renyi) graphs with discrete distributions over product states projectors (in between #SAT and #QSAT) the instances are still efficiently solvable, and that only when #2-QSAT cases resemble monotone #2-SAT instances is that the problem becomes difficult. This suggests that the hardness of #QSAT comes only from the hardness of #SAT, but that typical quantum cases are easily solvable. This point of view if a very interesting one. It seems as if the quantumness washes out the complexity of the typical instances.

5. Summary & Discussion

In this paper we have collected many of the recent results at the boundary of statistical physics, quantum complexity, and computation. We have seen the interplay between the quantum and classical aspects of some computational problems and the interesting results that quantumness seems to vanish in the thermodynamic limit of typical instances. Cui et al. [12] made this connection in terms of entanglement of a tensor network and the quantum min-cut, and Sattath et al. [13] in terms of a classical characterization of QSAT through the partition function of a hardcore gas. Along the same lines, De Beaudrap [27] showed that the difficult instances of #2-QSAT seem to be only the ones coming from the hard instances of #2-SAT. With all of these results, it is intriguing to wonder about the phenomena possibly exhibited in classical-quantum ensembles for $k \geq 3$ [25]. What more can statistical mechanics and physics tell us about computation? In turn, would computation tell us more about the nature of entanglement?

Perhaps, there are quantum results with no classical analogues (a hopeful candidate would be Shor's algorithm); in addition, there might be classical aspects of computation with no interesting quantum version. Yet we have learned that there is a fascinating world in between the classical and quantum aspects of computation, and that physics has much to contribute to it. For example, this boundary between classical and quantum could help our approach to prove or disprove the quantum PCP conjecture. What features make approximating the solution to a quantum problem hard? At least in the results we discussed here, the role of quantumness is still not very well understood; nevertheless, in a sense, there is an underlying classical characterization of the quantum problems. Are there cases for which the complexity of typical instances in a quantum problem arise solely because of entanglement? Connecting statistical physics to quantum computing might be the way to go.

Acknowledgement

I would like to thank Prof. Aaronson for a very interesting and enlightening course.

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