When a local Hamiltonian must be frustration-free

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A broad range of quantum optimization problems can be phrased as the question of whether a specific system has a ground state at zero energy, i.e., whether its Hamiltonian is frustration-free. Frustration-free Hamiltonians, in turn, play a central role for constructing and understanding new phases of matter in quantum many-body physics. Unfortunately, determining whether this is the case is known to be a complexity-theoretically intractable problem. This makes it highly desirable to search for efficient heuristics and algorithms to, at least, partially answer this question. Here we prove a general criterion—a sufficient condition—under which a local Hamiltonian is guaranteed to be frustration-free by lifting Shearer’s theorem from classical probability theory to the quantum world. Remarkably, evaluating this condition proceeds via a fully classical analysis of a hardcore lattice gas at negative fugacity on the Hamiltonian’s interaction graph, which, as a statistical mechanics problem, is of interest in its own right. We concretely apply this criterion to local Hamiltonians on various regular lattices, while bringing to bear the tools of spin glass physics that permit us to obtain new bounds on the satisfiable to unsatisfiable transition in random quantum satisfiability. We are then led to natural conjectures for when such bounds will be tight, as well as to a novel notion of universality for these computer science problems. Besides providing concrete algorithms leading to detailed and quantitative insights, this work underscores the power of marrying classical statistical mechanics with quantum computation and complexity theory.

quantum satisfiability | local Hamiltonian | hardcore lattice gas | critical exponents | universality

An overwhelming majority of systems of physical interest can be described via local Hamiltonians:

$$H = \sum_{i=1}^{M} \Pi_i$$

[1] Here, the “$k$-local” operator $\Pi_i$ acts on a $k$-tuple of the microscopic degrees of freedom, best thought of as qudits for the computer scientists among our readers or spins for the physicists. The $M$ operators define an interaction (hyper)graph $G$, displayed in Fig. 1.

A surprisingly diverse and important class of such model Hamiltonians is defined by the additional property of being “frustration-free”: The ground state $|\psi\rangle$ of $H$ is a simultaneous ground state of each and every $\Pi_i$. This class comprises both commuting Hamiltonians—for which $[\Pi_i, \Pi_j] = 0 \forall i,j$—such as the toric code, general quantum error correcting codes, and Levin–Wen models (1–3), and noncommuting ones, such as the Affleck-Kennedy-Lieb-Tasaki (AKLT) and Rokhsar–Kivelson models (4–6). Their particular usefulness is also related to the fact that many of these examples can be viewed as “local parent Hamiltonians” for generalized matrix product states (7). In general, frustration-free conditions provide analytic control of ground state properties in otherwise largely inaccessible quantum problems.

Determining whether a given Hamiltonian $H$ is frustration-free is well known in quantum complexity theory as the quantum satisfiability (QSAT) problem. QSAT is widely believed to be intractable, in the sense that no general purpose classical or quantum algorithm can efficiently determine whether a given Hamiltonian is frustration-free (“satisfiable”). The technical statement is that QSAT is complete for the Quantum Merlin Arthur complexity class (QMA$_c$-complete) (8), even when restricted to qudits and $k = 3$ (9) or when the interaction is between neighboring qudits on a line (10).

Fortunately, such hardness results apply only in the worst case. For instance, in contrast to the hardness result, it is immediately obvious that a fully disconnected interaction graph $G$ can be analyzed efficiently by considering each term $\Pi_i$ individually.

The central result reported here is a sufficient combinatorial criterion for a local Hamiltonian $H$ to be frustration-free. In fact, we provide a lower bound for the dimension of the satisfying subspace. This amounts to a generalization of Shearer’s theorem (11) from classical probability theory to the quantum world.

We first formulate the result in Theorem 1, followed by an intuitive explanation of its content, with a technical proof relegated to SI Appendix. We then turn to applying Theorem 1, for which we enlist the results available on statistical mechanics of hardcore objects with negative fugacity on the interaction graph to deduce statements regarding QSAT, producing new bounds on the satisfiability threshold for a large class of 1D, 2D, and 3D interaction graphs. With the help of the cavity method, we are able to conjecture improved lower bounds for the satisfiability of QSAT on regular and Erdős–Rényi random graphs, canonical models for quantum constraint optimization problems. These statement hold just as well for classical satisfiability—but for some of these classical models better bounds are known (12, 13).

We close with an outlook, including a discussion of the role of a universality that emerges in our analysis, as well as conjectures on when our results are exact or tight.

Theorem 1. Given a local projector Hamiltonian $H$ as in Eq. 1 with interaction graph $G$ and relative projector rank $p = \text{R} (\text{Im} \: \Pi_i)$ for all $i$, then

$$R (\ker H) \geq Z (G, -p) > 0$$

if $Z (G, -p') > 0$ for all $0 \leq p'$ $\leq p$.

Significance

Quantum computers promise computational power qualitatively superior to that achievable classically. This power will not be unlimited: Beyond much-touted applications, such as breaking encryption schemes, entire classes of problems are known to be intractable even for quantum computers. This work addresses a question of great practical relevance: In between these two extremes of certain (in)tractability, how can one efficiently diagnose the nature and properties of a given problem instance? To achieve this, we adopt a strategy of transferring insights from statistical physics and classical computing into the quantum realm. This provides a new perspective on the complexity of quantum problems and allows us to analyze a canonical class of quantum optimization problems in unprecedented explicit detail.

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The area covered by the bubbles is largest if they do not overlap, corresponding to a large number of violating configurations; we thus expect a lower bound on $R(\ker H)$ when they are fully disjoint. To calculate this lower bound, we expand the product in Eq. 3 and introduce a collection of occupation variables $n_i = 0,1$ that indicate the presence of $\Pi_i$ in each term of the expansion,

$$R(\ker H) = \sum_{\{n_i\}} (-1)^{\sum_i n_i} \prod_{j=1}^M (1-p_{ij}).$$

If two dependent projectors, $\Pi_i$ and $\Pi_j$, are thus occupied, then that term is zero when their bubbles are made disjoint. Otherwise, it is given by $p\sum_{n_i}$. Thus,

$$R(\ker H) \geq \sum_{\{n_i\}} (-p)^{\sum_i n_i} \prod_{i} (1-n_i n_j) \equiv Z(G, -p),$$

where $i \leftrightarrow j$ runs over projectors that share qudits.

We have derived inequality [5] under the assumption that it is possible to make the dependent bubbles disjoint. If $p$ is small enough, this is always the case; in the Venn diagram, the bubbles can be made disjoint without covering more area than the total space contains. Shearer (11, 14) showed that the above intuitive bound is correct for classical projectors as long as $p \leq p_c$, where $p_c$ is the first zero of $Z(G, -p)$. This is the classical analog of our quantum generalization, Theorem 1.

The classical sketch above makes little sense for noncommuting quantum projectors. In the language of probability, this reflects the failure of the inclusion–exclusion principle (Eq. 4) for the relative dimension of vector spaces. Nonetheless, the result holds; the proof—our fundamental technical advance—is provided in SI Appendix, Proof of Theorem 1.

Statistical Mechanical Transcription

A remarkable aspect of Theorem 1 is that it maps the quantum satisfiability problem onto the classical statistical mechanical problem of determining the position of the first negative fugacity zero $\lambda(G)$ of the partition function $Z(G, \lambda)$. In general, evaluating $Z$ is computationally hard, but for many infinite graphs it may nonetheless be accomplished in a satisfactory manner using statistical mechanical tools. [Technically, computing $Z$ is #P-hard almost everywhere (15).] In the thermodynamic limit (number of qudits $N \to \infty$), the first zero $\lambda(G)$ can be identified with a well-known critical point $\lambda(H_{\infty})$ of the hardcore lattice gas mapping, each square may be occupied by a particle covering also the adjacent circles (shaded blobs), on which it must not overlap with another particle. (Right) A $k = 6$ interaction graph forming a triangular lattice of the operators $\Pi_i$. The corresponding hardcore lattice gas corresponds to the hard hexagon model, which is exactly solvable.

![Fig. 1. (Left) The interaction graph of a $k = 3$-local Hamiltonian. The degrees of freedom, qudits, are denoted by circles; the squares, which indicate the operators $\Pi_i$ appearing in $H$, are joined to the qudits on which they act. In the hardcore lattice gas mapping, each square may be occupied by a particle covering also the adjacent circles (shaded blobs), on which it must not overlap with another particle. (Right) A $k = 6$ interaction graph forming a triangular lattice of the operators $\Pi_i$. The corresponding hardcore lattice gas corresponds to the hard hexagon model, which is exactly solvable.](image)

![Fig. 2. Shearer bound for dependent projectors. Projectors are independent if they do not share any qudit (Top Left), and there will always exist configurations violating any combination of such projectors simultaneously. In the Venn diagram (Top Right), this is represented by the mutual intersections of the shaded circles, each of which denotes the fraction of configuration space “knocked out” by a projector, with overlapping bubbles representing configurations multiply penalized by the corresponding projectors.](image)
the hardcore lattice gas referred to as the hardcore singularity. The critical fugacity $\lambda_c(G_{\infty})$ upper bounds the $\lambda_c$ of any finite subgraph by monotonicity (11). Thus, Theorem 1 implies that all subgraphs of $G_{\infty}$ are frustration-free as long as the relative rank of the projectors satisfies $p < -\lambda_c(G_{\infty})$.

The hardcore singularity has been studied extensively in the statistical mechanical literature (16–25) and its location is known for many infinite lattices. Table 1 summarizes some of these critical values and indicates their translation into QSAT interaction graphs.

In addition, there exist rigorous bounds on $\lambda_c$ that may be efficiently calculated on any sufficiently simple lattice (16). The singularity exhibits universal features just like standard phase transitions. In particular, the free energy density $f(\lambda) = (1/N)\log Z(\lambda)$ near the critical point $\lambda_c$ has universal exponents (21, 22) due to its connection with the so-called Yang-Lee edge singularity (24–28). Technically, this means that the leading nonanalytic part of the free energy $f \sim (\lambda - \lambda_c)^\phi(\lambda)$ near $\lambda_c$, where $\phi_D$ is a noninteger critical exponent that depends only on the spatial dimension $D$ of the lattice (21, 22, 24). It is known analytically that $\phi_L = 1/2$, $\phi_2 = 5/6$ (20, 29, 30), and $\phi_D = 3/2$ for $D$ above the upper critical dimension $D_C = 6$ (24).

The critical exponents control the lower bounds on the dimension of the ground space of Hamiltonians close to the critical threshold. Indeed, by Theorem 1, $R(\ker H) \geq \exp(\lambda)\alpha(\lambda)$ for $\lambda > \lambda_c$, so the critical exponents show up directly—and perhaps somewhat unexpectedly—as anomalous growth laws in $D = 1,2$ (SI Appendix, Improved Bounds Using the Critical Exponents). In the following, observation of the expected exponent in the random $k$-QSAT ensemble helps confirm the validity of the nonrigorous cavity analysis.

### Examples

As a first application of Theorem 1, we calculate the critical threshold $\lambda_c$ for several infinite graphs. We do this using the cavity method, a well-known technique for studying statistical (31) and quantum (32–34) models on infinite graphs that are locally tree-like. On trees and chains, the results are rigorously exact whereas on infinite random graphs they are less rigorous, but often just as exact.

The heart of the cavity method is to introduce an auxiliary system of messages that propagate in both directions between the hyperedges and the nodes of the interaction graph $G$. For the model given by Eq. 2, the derivation is straightforward and quite intuitive at positive fugacity where the cavity messages correspond to marginal distributions that may be efficiently calculated (22). Theorem 1 of the ground space of Hamiltonians close to the critical threshold.

Given a solution of the BP equations, the cavity estimate of the free energy $F = \log Z$ of the system is given by a sum of the free energies associated to the addition of individual elements of the interaction graph; i.e.,

$$F = \sum_a F_a + \sum_i F_i - \sum_{(ai)} F_{ai},$$

where $F_a, F_i,$ and $F_{ai}$ correspond to the change in free energy due to the addition of sites $a$, hyperedges $i$, and the links $ai$ between them, respectively. The full expressions may be found in SI Appendix, The Cavity Derivations.

### The Chain

On the infinite chain, the BP equations can be solved by uniform messages $q_{b \rightarrow a} = q, l_{b \rightarrow a} = l$. After some algebra and taking the root of the BP equations corresponding to $q(\lambda = 0) = 0$, one finds

$$l = q = 1 + (1 - \sqrt{1 + 4l})/2l.$$

This expression suggests that $\lambda_c = -1/4$ as $q$ becomes complex for $\lambda < \lambda_c$. Indeed, it is easy to check that the free energy density $f = \log Z$ (Eq. 6) has the expansion near $\lambda_c$:

$$f = -\log 2 + 2(\lambda - \lambda_c)^{1/2} - 2(\lambda - \lambda_c) + \cdots.$$

The free energy goes complex for $\lambda < \lambda_c$, which reflects the accumulation of partition function zeros and indicates the failure of the lower bound.

The free energy precisely $-\log 2$ at the critical point. For qudits of local dimension $q$, this provides a lower bound on the dimension of the ground space $\dim(\ker H) = q^D R(\ker H) \geq (g/2)^N$.

In fact, careful application of Theorem 1 for finite chains agrees with the exact result $\dim(\ker H) = (g/2)^N(N + 1)$ for open chains derived using matrix-product techniques (37, 38). It is interesting to note that the entropy per site is zero for qubits at criticality, but has a finite value for larger $q$.

### Regular Trees

The BP equations on infinite regular trees with site degree $t$ and hyperedge degree $k$ can be solved under the ansatz that all messages $\alpha(a)$ have the form $\alpha(a) = \rho_{\alpha,a}(\lambda)$, where $\rho_{\alpha,a}(\lambda)$ is a noninteger critical exponent that depends only on the spatial dimension $D$ of the lattice (21, 22, 24). It is known analytically that $\phi_L = 1/2$, $\phi_2 = 5/6$ (20, 29, 30), and $\phi_D = 3/2$ for $D$ above the upper critical dimension $D_C = 6$ (24).

### Table 1. Summary of the critical threshold for various infinite interaction graphs

| Lattice          | $\rho_c$   | Qudits | Projectors | $k$ |
|------------------|------------|--------|------------|-----|
| 1D chain         | $1/3$      | Vertices, Edges | 2       |
| Triangular       | $5/6$      | Edges, Vertices | 6       |
| Square           | 0.1193     | Edges, Vertices | 4       |
| Square           | 0.0889     | Vertices, Edges | 2       |
| Checkerboard     | 0.0688     | Black, Red | 4       |
| Hexagonal        | 0.1547     | Edges, Vertices | 3       |
| Simple cubic     | 0.0744     | Edges, Vertices | 6       |
| t-regular tree   | $1$        | Vertices, Edges | 2       |

For $k = 2$-local trees, this agrees with previous results obtained by matrix product states on trees (39). As far as we are aware, Eq. 7 provides a strictly better lower bound on satisfiability of infinite random trees than any previous literature. The corresponding expansion of the free energy density is

$$f = f_0(t,k) + A(t,k)(\lambda - \lambda_c) + B(t,k)(\lambda - \lambda_c)^{3/2} + \cdots.$$  

We thus recover the expected nonanalyticity ($\phi = 3/2$) in the free energy density for the infinite-dimensional hardcore singularity (24).
Random $k$-QSAT

We now apply Theorem 1 to random $k$-QSAT. Random satisfiability has been a workhorse for the study of typical case complexity and heuristic algorithms. By tuning the density $\alpha = M/N$ of Erdős–Rényi-type random interaction graphs, a cornucopia of phases and phase transitions in the structure of the satisfying space has been discovered. In the quantum case, three phases for random $k$-QSAT on qubits and rank-1 projectors are believed to be (i) at low density, a product state satisfiable phase (PRODSAT); (ii) at intermediate densities for $k$ sufficiently large, a satisfiable phase in which all ground states are entangled (ENTSAT); and (iii) at high density, an unsatisfiable (UNSAT) phase. The arguably most interesting of these phases, ENTSAT, has been shown to exist using the quantum Lovász local lemma (QLLL) (40) for $k \geq 13$. The application of Theorem 1 to the Erdős–Rényi (ER) ensemble is not straightforward, as the interaction graphs exhibit an unbounded degree distribution, so that a strict application of Shearer’s theorem provides no useful information. However, as explained in SI Appendix, Local Degree Fluctuations for Random $k$-QSAT, such local degree fluctuations do not appear to be the source of unsatisfiability in $k$-QSAT for qubits.

Neglecting this local rare-region effect, we calculate the self-consistent solutions to the disorder-averaged cavity equations, using standard methods (population dynamics) (35). For $\lambda > \lambda_c$, this numerical technique converges to a population of messages that represents the distribution of $q$ and $f$ in the infinite random graph and from which we can directly estimate the disorder-averaged free energy $f$ and occupation number density $\langle n \rangle = \frac{df}{d\log \lambda}$. The latter is particularly useful, because as $\lambda \to \lambda_c$, we expect $\langle n \rangle$ to exhibit a square-root singularity by universality; i.e., $\langle n \rangle \sim (\lambda - \lambda_c)^{1/2}$. Observing this singularity allows us to estimate $\lambda_c$ accurately and confirms the validity of the numerical approach. By fitting these singularities, we extract a new and improved (lower) but nonrigorous threshold for the existence of an ENTSAT phase, $\lambda \geq 7$ (Fig. 3).

Conclusion and Open Questions

By extending the classical Shearer theorem to quantum mechanical systems, we have provided a new statistical mechanical criterion for determining whether a local Hamiltonian is frustration-free. We have applied this criterion to a large class of regular and random Hamiltonians. These instances cover many of the geometries that have been studied in quantum complexity and as parent Hamiltonians for wavefunction-based many-body physics. In the context of random satisfiability problems, we have provided a set of new lower bounds on the existence of the ENTSAT phase. In particular, these bounds suggest that the ENTSAT phase is eminently more reachable in simulations than previously established.

Theorem 1 depends on the dimension $p$ of the projectors $I_i$ relative to the Hilbert space dimension and not the absolute local dimension $d$ of the qudits. At small $p$ (e.g., qubits), there are many Hamiltonians where $R(\ker H)$ is strictly larger than the bound of Theorem 1 (compare the discussion of random $k$-QSAT). Nonetheless, for large $p$ we conjecture that Theorem 1 becomes tight. This is in sharp contrast to the classical case where the length-4 cycle (periodic chain) already provides a counterexample to the analogous statement (41). However, it is easy to show numerically that this counterexample breaks down for quantum projectors.

If, indeed, Theorem 1 is tight, there are several striking consequences. The geometrization theorem (37) states that $R(\ker H)$ is minimized by almost all choices of the $I_i$. Coupled with tightness, the lattice gas partition function $Z$ then provides a complete characterization of quantum satisfiability for almost all Hamiltonians with large enough qudits. It also directly lifts the universality of the lattice gas critical exponents to the counting of the ground state entropy of almost all quantum Hamiltonians in the frustration-free regime. In this sense, the conjecture amounts to an even larger scope of transferring insights from classical statistical mechanics into the quantum complexity domain.

Although Theorem 1 can guarantee the existence of zero energy states, it does not construct them. This is in contrast to classical SAT and commuting QSAT, where efficient constructive classical algorithms (under Lovász’s and Shearer’s assumptions) and quantum algorithms (under Lovász’s assumption) are known (41–44). Analogously constructing the wavefunctions corresponding to the solutions of the noncommuting quantum problem would represent a milestone for quantum complexity theory.

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Fig. 3. Our current understanding of the phase diagram of the random $k$-QSAT. For small $\alpha$, the instances are PRODSAT, with the transition out of PRODSAT approaching $\alpha \rightarrow 1$ from below as $k$ grows (45). For large $\alpha$, the instances are guaranteed to be UNSAT, with the best known upper bound (46) for the satisfiability transition at $\alpha^* = 0.573 - 2^{-k}$ at $k \geq 4$. In between, there may be an unsatisfiable phase if $\alpha < \alpha^*$. The best previous lower bound for the satisfiability transition, $\alpha_0$, was given by the quantum Lovász local lemma (QLLL, up triangles) (40) and is roughly exponential at large $k$. This work obtains a better lower bound through the Shearer criterion (squares), lowering the threshold for the existence of an ENTSAT phase from $k = 13$ to $k = 7$.

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