Beating Random Assignment for Approximating Quantum 2-Local Hamiltonian Problems

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Abstract

The quantum k-Local Hamiltonian problem is a natural generalization of classical constraint satisfaction problems (k-CSP) and is complete for QMA, a quantum analog of NP. Although the complexity of k-Local Hamiltonian problems has been well studied, only a handful of approximation results are known. For Max 2-Local Hamiltonian where each term is a rank 3 projector, a natural quantum generalization of classical Max 2-SAT, the best known approximation algorithm was the trivial random assignment, yielding a 0.75-approximation. We present the first approximation algorithm beating this bound, a classical polynomial-time 0.764-approximation. For strictly quadratic instances, which are maximally entangled instances, we provide a 0.801 approximation algorithm, and numerically demonstrate that our algorithm is likely a 0.821-approximation. We conjecture these are the hardest instances to approximate. We also give improved approximations for quantum generalizations of other related classical 2-CSPs. Finally, we exploit quantum connections to a generalization of the Grothendieck problem to obtain a classical constant-factor approximation for the physically relevant special case of strictly quadratic traceless 2-Local Hamiltonians on bipartite interaction graphs, where a inverse logarithmic approximation was the best previously known (for general interaction graphs). Our work employs recently developed techniques for analyzing classical approximations of CSPs and is intended to be accessible to both quantum information scientists and classical computer scientists.

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1 Introduction

The design and analysis of approximation algorithms [37,38] is an extensively studied area in theoretical computer science. In this setting, we are given some (generally NP-hard) optimization problem, and we are tasked with producing a valid (feasible) solution with objective within some provable factor of the optimal objective value. To understand this formally imagine we are given some optimization problem \mathcal{P} , which corresponds to an infinite set of problem instances $\{P_i\}$. Each problem instance corresponds to a triple $P_i = (f_i, \mathcal{T}_i, n_i)$ where $n_i \in \mathbb{N}_+$, $\mathcal{T}_i \subseteq \{0, 1\}^{n_i}$, and $f_i : \mathcal{T}_i \to \mathbb{R}_+$ is an objective function. This gives rise to an optimization problem of the form: $OPT_i = \max_{s \in \mathcal{T}_i} f_i(s)$.

An approximation algorithm \mathcal{A} acts on an efficient description of an instance to produce some feasible solution to the problem: $\mathcal{A}(f_i, \mathcal{T}_i, n_i) = \bar{s}_i \in \mathcal{T}_i$ in time polynomial in the instance size (polynomial in n_i). It is said that algorithm has approximation factor α for $0 < \alpha \le 1$ if in the worst-case (over all instances), the solution produced by the algorithm is a factor of α off of the optimal answer:

$$\min_{i} \frac{f_i(\bar{s}_i)}{OPT_i} \ge \alpha.$$

Since we should not expect to solve NP-hard problems in polynomial time, an interesting question is then the approximability of NP-hard optimization problems, or the study of which approximation factors α are obtainable for different problems. As one might expect, approximability is highly problem sensitive and there are many classes of natural problems with widely varying approximability [15, 17, 23, 37, 38].

2-Local Hamiltonian. In stark contrast, although QMA-hard quantum optimization problems arise naturally through well-known physically motivated problems [5, 35], they have very few known approximation algorithms with provable approximation factors [2, 4, 8, 11, 18, 19, 21, 22, 31]¹. The QMA-hard optimization studied in these works, as well as the problem we sill study here, is the 2-Local Hamiltonian problem [24, 25].

An instance of this problem is specified by a problem size, n, as well as a set of 2-local interactions (i.e., interactions on pairs of qubits), $\{H_{ij}\}_{ij\in E}$. Each $H_{ij}\in\mathbb{C}^{2^n\times 2^n}$ is some local Hamiltonian which can be written as the tensor product of n-2 identity terms with some nontrivial operator, $\mathcal{O}_{ij}\in\mathbb{C}^{4\times 4}$, that acts on at most 2 qubits, i.e. $H_{ij}=\mathcal{O}_{ij}\otimes\mathbb{I}_{[n]\setminus\{i,j\}}\in\mathbb{C}^{2^n\times 2^n}$ (see Section 2.1 for notation). The optimization problem corresponding to a particular instance is to find the smallest or largest eigenvalue, λ_{\min} or λ_{\max} , of $H=\sum_{ij\in E}H_{ij}$.

▶ **Problem 1** (QLH: Quantum Max 2-Local Hamiltonian). Given a problem size, n, as well as a classical description of a set of 2-local terms $\{H_{ij} = \mathcal{O}_{ij} \otimes \mathbb{I}_{[n]\setminus\{i,j\}}\}_{ij\in E}$ with $H_{ij} \in \mathbb{C}^{2^n \times 2^n}$ Hermitian, find:

$$\lambda_{\max}(H) := \max_{|\phi\rangle \in (\mathbb{C}^2)^{\otimes n}} \langle \phi | H | \phi \rangle = \max_{\substack{\rho \in \mathbb{C}^{2^n} \times \mathbb{C}^{2^n} \\ \operatorname{Tr}(\rho) = 1, \ \rho \succeq 0}} \operatorname{Tr}\left[H\rho\right], \ where \ H := \sum_{ij \in E} H_{ij}.$$

Ideally, an algorithm solving this problem would also produce a description of or access to a corresponding eigenvector. We will focus on approximating λ_{\max} for special cases of 2-local Hamiltonian. Although exactly computing $\lambda_{\max}(H)$ is equivalent to computing $\lambda_{\min}(-H)$, the approximability of these problems can differ. An approximation algorithm, \mathcal{A} , acts on the description of the local Hamiltonians $\{H_{ij}\}$ to produce a classical description of a valid quantum state, $\bar{\rho}$. Once again we say that the algorithm achieves approximation factor α if:

$$\frac{\operatorname{Tr}\left[\left(\sum_{ij} H_{ij}\right) \bar{\rho}\right]}{\lambda_{\max}\left(\sum_{ij} H_{ij}\right)} \geq \alpha, \text{ for all instances.}$$

¹ Here and throughout this paper we mean a *classical* algorithm which takes as input a classical description of a quantum problem and produces a classical description of a quantum state. An approximation algorithm for a QMA-hard problem can have several natural meanings distinct from this (quantum input, quantum algorithm which produces classical output, etc.).

Generally we assume some property of the Hamiltonian which forces $\lambda_{\max}(H) > 0$ so that this is a sensible definition. A common assumption [18,21,24] is that the terms H_{ij} are positive semi-definite (PSD) and nonzero. We note that when all of the terms H_{ij} are taken to be diagonal projectors (in say, the standard computational basis), the corresponding instance of 2-Local Hamiltonian corresponds precisely to an instance of the classical 2-Constraint-Satisfaction problem (2-CSP). In this case, the 4 diagonal entries of \mathcal{O}_{ij} correspond to the $\{0,1\}$ output values of a Boolean function on variables x_i and x_j corresponding to i and j. See Appendix E in [30] for more details as well as a classical motivation for 2-Local Hamiltonian. In addition Table 1 highlights classical 2-CSP specializations of quantum Max 2-local Hamiltonian problems for which approximation algorithms are known.

The 2-Local Hamiltonian problem is interesting in many different contexts of physics and quantum information [24,25,29]. This problem is manifestly interesting to physicists because the 2-local nature of the problem matches the local nature of many physical systems (spin chains, Ising model, etc.). Hence, the study of eigenstates and energies is of utmost importance, and has been since the beginnings of quantum mechanics itself [6]. From a theoretical computer science perspective, the 2-Local Hamiltonian problem is interesting for the same reasons that classical approximation algorithms are interesting. Under standard complexity theoretic assumptions, we should not expect to be able to efficiently solve the problem, so the interesting direction is the study of the approximability of the problem. Can we find rigorous approximation algorithms, and how well can we expect to be able to approximate the answer? Moreover, which classes of instances admit constant-factor approximation algorithms? Akin to the classical PCP Theorem, the potential inapproximability of local Hamiltonian problems to within constant factors is known as the Quantum PCP Conjecture. The resolution of the conjecture would yield insight into properties of quantum mechanics and entanglement (e.g., Section 1.3 in [1]).

1.1 Our Contributions

The QLH problems we consider generalize a variety of classical optimization problems, including Max 2-SAT, Max Cut, general Max 2-CSP, and the Grothendieck problem (see Table 1 for our results). We focus on QLH where each term H_{ij} is a projector and the special case where each projector is strictly quadratic, both of which remain QMA-hard [32]. The strictly quadratic case precludes non-identity 1-local terms (i.e. $\mathcal{O}_i \otimes \mathbb{I}_{[n]\setminus\{i\}}$ with $\mathcal{O}_i \neq \mathbb{I}$) that may be implicit in a 2-local term (see Definition 8). In this case $\mathcal{O}_{ij} = w_{ij}P_{ij}$, where P_{ij} is a 2-qubit projector, and $w_{ij} \geq 0$ is a weight. There are three interesting cases, depending on the rank of P_{ij} . We will obtain approximation factors for each.

- ▶ Problem 2 (QLHP(k): Quantum Max 2-Local Hamiltonian on Projectors). Given a problem size, n, as well as a classical description of a set of 2-local terms $\{H_{ij} = w_{ij}P_{ij} \otimes \mathbb{I}_{[n]\setminus\{i,j\}}\}_{ij\in E}$ with $w_{ij} \geq 0$ and $P_{ij} \in \mathbb{C}^{4\times 4}$ a 2-qubit projector of rank at least k, find $\lambda_{\max}(\sum_{ij\in E} H_{ij})$.
- ▶ Remark 3. Although Problem 2 is formulated for a single term H_{ij} per pair of qubits i, j, our techniques apply when multiple terms are present per pair. Since any $\mathcal{O}_{ij} \succeq 0$ can be written as a positive combination of rank-1 projectors, the version of QLHP(1) we solve more generally captures instances of QLH where each $H_{ij} \succeq 0$.

▶ Theorem 4 (Informal). Given an instance of QLHP(k), $\{H_{ij} = w_{ij}P_{ij} \otimes \mathbb{I}_{[n]\setminus\{i,j\}}\}$, where all 2-local projectors P_{ij} are rank $k \in \{1,2,3\}$, we give a classical randomized polynomial-time algorithm with approximation ratio $\alpha(k)$, where

$$\alpha(k) = \begin{cases} 0.387 & \text{if } k = 1\\ 0.565 & \text{if } k = 2\\ 0.764 & \text{if } k = 3. \end{cases}$$

▶ **Theorem 5** (Informal). If in addition to the assumptions of Theorem 4, the terms H_{ij} are strictly quadratic, we give a classical randomized polynomial-time algorithm with approximation ratio $\alpha(k)$, where

$$\alpha(k) = \begin{cases} 0.467 & \text{if } k = 1\\ 0.639 & \text{if } k = 2\\ 0.805 & \text{if } k = 3. \end{cases}$$

The decision version of the problem we consider is known as Quantum-SAT and was introduced in 2006 by Bravyi [10], and the approximability of QLHP was first considered in 2011 by Gharibian and Kempe [18], who observed that the maximally mixed state trivially achieves an approximation ratio of k/4 for $k \in \{1,2,3\}$. The only nontrivial result previously known is a 0.328-approximation for the k=1 case by Hallgren, Lee, and Parekh [21]. In contrast to previous works [19,21], we are able to directly analyze the expected performance of our algorithm rather than appealing to known but weaker black-boxes.

Significance of our work. We give the first approximation algorithms beating random assignment for QLHP. We show how to move beyond numerical evaluation of approximation ratios for QLH, which is not as critical in the classical case that enjoys only a handful of parameters. This is accomplished by: (1) reducing the number of parameters for analysis of a single term from 18 to 3 (in the strictly quadratic case), and (2) explicitly computing the coefficients of a Hermite decomposition of a multivariate Gaussian expectation. The latter generalizes previous results of Briët, de Oliveira Filho, and Vallentin [13] employed in [19]. We are able to analyze a natural generalization of classical hyperplane rounding that we expect will enable approximation of other QLH problems.

Strictly quadratic instances. We believe the strictly quadratic case is an interesting special case for several reasons. As noted, one of the difficulties in analyzing rounding schemes for QLH is the sheer number of parameters involved. The quadratic case reduces the number of parameters to consider, while still including physically relevant QMA-hard instances such as the Max Heisenberg model that serves as a quantum generalization of Max Cut [19]. Indeed we believe that quadratic instances allow one to glean insights and develop techniques that might otherwise be obscured in more general instances. Some of the first rigorous approximation algorithms for QLH that go beyond product states were recently developed for quantum Max Cut [2,31]. Moreover, maximally entangled instances are strictly quadratic, and we conjecture these are the hardest cases to approximate.

Numerical results and upper bounds. We conjecture that the true performance of our algorithm for general QLHP, including linear terms, is:

▶ Conjecture 6. (Informal) Our rounding algorithm achieves approximation ratio:

$$\alpha(k) = \begin{cases} 0.498 & \text{if } k = 1\\ 0.653 & \text{if } k = 2\\ 0.821 & \text{if } k = 3, \end{cases}$$

and these quantities match the worst-case gap between OPT and our SDP upper bound.

We have indeed confirmed the approximation ratios in Conjecture 6 through numerical experiments. The difficulty in taking these encouraging results as fact is: (1) the increase in complexity for an exhaustive search as the number of parameters grows, and (2) although we do give series expansions for the expected performance of the algorithm, establishing smoothness of the expected performance is more difficult than for classical CSP approximation algorithms. Classical 2-CSP approximation factors are also established numerically; however, the performance is usually a well-behaved function of a single parameter, which makes exhaustive numerical search more plausible. There has been limited work on rigorous analysis of 2-CSP approximation guarantees [36]. We note that for the strictly quadratic case, our approach requires a search over only three parameters, rendering these numerical results more plausible. We also note that the performance of a similar approximation algorithm for quantum Max Cut, a special case of QLHP(1), is a hypergeometric function in one parameter, and the corresponding approximation guarantee is indeed 0.498 [19].

An upper bound on $\alpha(k)$ is given below for an instance of QLPH(k) on 2 qubits, with multiple edges that are each strictly quadratic rank-k projectors. These bounds are fairly close to the values in Conjecture 6.

▶ Theorem 7. There exist an instance of QLH on a single edge e, where $H_e \succeq 0$ is strictly quadratic, is a convex combination of rank-k projectors, and satisfies:

$$\max_{|\phi_{1}\rangle \in \mathbb{C}^{2}, |\phi_{2}\rangle \in \mathbb{C}^{2}} \langle \phi_{1}| \otimes \langle \phi_{2}| H_{e} |\phi_{1}\rangle \otimes |\phi_{2}\rangle \leq \beta(k) \cdot \lambda_{max} (H_{e}),$$

where
$$\beta(k) = \begin{cases} 1/2 & \text{if } k = 1\\ 2/3 & \text{if } k = 2\\ 5/6 & \text{if } k = 3. \end{cases}$$

Proof. The Bell states take their usual definition:

$$|\Phi^{+}\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}, \ |\Phi^{-}\rangle = \frac{|00\rangle - |11\rangle}{\sqrt{2}}, \ |\Psi^{+}\rangle = \frac{|01\rangle + |10\rangle}{\sqrt{2}}, \ \text{and} \ |\Psi^{-}\rangle = \frac{|01\rangle - |10\rangle}{\sqrt{2}}.$$

We define.

$$H_e(k) = \frac{k-1}{3} \mathbb{I} + \frac{4-k}{3} |\Psi^-\rangle \langle \Psi^-|.$$

Let $\mu(k) = \max_{|\phi_1\rangle \in \mathbb{C}^2, |\phi_2\rangle \in \mathbb{C}^2} \langle \phi_1 | \otimes \langle \phi_2 | H_e(k) | \phi_1 \rangle \otimes |\phi_2 \rangle$. From, e.g., [19], we know that $\mu(1) = 1/2$, while $\lambda_{max}(H_e(1)) = 1$ since $|\Psi^-\rangle$ is an eigenvector of the rank-1 projector $H_e(1)$. For k > 1 we have that

$$\mu(k) = \frac{k-1}{3} + \frac{4-k}{3}\mu(1) = \frac{k+2}{6}, \text{ and}$$
$$\lambda_{\max}(H_e(k)) = \frac{k-1}{3} + \frac{4-k}{3}\lambda_{\max}(H_e(1)) = 1,$$

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yielding the desired values of $\beta(k)$. We give explicit descriptions of $H_e(k)$ as convex combinations of rank-k projectors for k = 2, 3:

$$\begin{split} H_{e}(2) = &\frac{1}{3}(\left|\Psi^{-}\right\rangle\left\langle\Psi^{-}\right| + \left|\Phi^{+}\right\rangle\left\langle\Phi^{+}\right|) + \frac{1}{3}(\left|\Psi^{-}\right\rangle\left\langle\Psi^{-}\right| + \left|\Phi^{-}\right\rangle\left\langle\Phi^{-}\right|) \\ &+ \frac{1}{3}(\left|\Psi^{-}\right\rangle\left\langle\Psi^{-}\right| + \left|\Psi^{+}\right\rangle\left\langle\Psi^{+}\right|), \text{ and} \\ H_{e}(3) = &\frac{1}{3}\left(\mathbb{I} - \left|\Phi^{+}\right\rangle\left\langle\Phi^{+}\right|\right) + \frac{1}{3}\left(\mathbb{I} - \left|\Phi^{-}\right\rangle\left\langle\Phi^{-}\right|\right) + \frac{1}{3}\left(\mathbb{I} - \left|\Psi^{+}\right\rangle\left\langle\Psi^{+}\right|\right). \end{split}$$

1.2 Related Work

In the interest of classical approximations of a 2-Local Hamiltonian instance H, let $OPT := \lambda_{\max}(H)$ and define

$$OPT_{\operatorname{prod}} := \max_{\substack{|\phi_1\rangle, \dots, |\phi_n\rangle \\ \in \mathbb{C}^2}} \left\langle \phi_1 | \otimes \dots \otimes \left\langle \phi_n | H \left| \phi_1 \right\rangle \otimes \dots \otimes \left| \phi_n \right\rangle \right.$$

to be the product state² with the largest objective value or energy.

Approximations for QLH generally make assumptions on the form of the terms H_{ij} . One common assumption is on the geometry of the interactions in E. Bansal, Bravyi, and Terhal show that 2-Local Hamiltonian on bounded-degree planar graphs admits a polynomial-time approximation scheme³ (PTAS) [4], and Brandão and Harrow generalize this to arbitrary planar graphs [8]. On the other end, for k-Local Hamiltonian on dense graphs, Gharibian and Kempe give a PTAS with respect to OPT_{prod} [18], and Brandão and Harrow extend this result to obtain a PTAS for dense graphs with respect to OPT [8]. Brandão and Harrow also show the existence of product-states with energy nearly that of OPT or give product-state approximations for a variety of graph classes [8].

Bravyi, Gosset, König, and Temme give an $\Omega(\frac{1}{\log n})$ - approximation for traceless ⁴ QLH [11]. This case is general enough to capture classical problems with no constant-factor approximations [3]. Harrow and Montanaro give an approximation algorithm for traceless k-Local Hamiltonian with respect to the maximum degree and size of the interaction hypergraph [22]. Note that approximating traceless QLH generalizes all problems considered in this paper, since adding copies of the identity only improves the approximation factor; however there is no reason to expect such analysis could be used to prove constant factor approximations for the classes we study.

A unifying theme among recent approaches (see Table 1 for approximation guarantees) is employing a semi-definite program (SDP) to provide an upper bound on OPT and then using generalization of some classical randomized rounding scheme to produce a product state [11,19,21]. Such an approach was first carried out by Brandão and Harrow [8]. Gharibian and Parekh [19] consider a QMA-hard rank-1 QLHP problem that is a generalization of the classical Max Cut problem. Hallgren, Lee, and Parekh [21] study QLHP and give the first approximation beating random assignment for rank-1 QLHP. They also provide

As is suggested by the expression, a product state is a quantum state which factors according to tensor product of individual quantum states. Such states have no entanglement and are considered "classical" states.

³ This is an approximation algorithm that for a constant $\varepsilon > 0$, allows a 1- ε approximation factor at the expense of a runtime that depends on $1/\varepsilon$.

⁴ A traceless instance is one with Tr[H] = 0. Alternatively, when expressed as a polynomial in the Pauli basis, H is traceless if it has no identity term.

approximations when each term is a product term, $H_{ij} = H_i \otimes H_j$, which is a QMA-hard class of QLH. An approximation result of [8] leverages the quantum Lasserre hierarchy of SDPs. The first level of this hierarchy yields a natural SDP relaxation that is employed by [11] and [19]. Our work adopts the approach of [21] and strengthens the natural SDP relaxation with additional constraints related that enforce positivity of 2-qubit marginals. Both [19] and [21] appeal to approximation results of Briët, de Oliveira Filho, and Vallentin [12, 13] to analyze the expected performance of their rounding algorithms. The rounding scheme of [11] is a generalization of a classical approximation by Charikar and Wirth [14].

Beyond product states. Gharibian and Parekh [19] give a 0.498-approximation for their quantum generalization of Max Cut, where $\frac{1}{2}$ is the best possible approximation by product states (see Theorem 7). Anshu, Gosset, and Morenz [2] demonstrate that it is possible to beat a $\frac{1}{2}$ -approximation for quantum Max Cut by furnishing a classical randomized approximation that outputs a description of a tensor product of 1- and 2-qubit states rather than product states, which are tensor products of 1-qubit states. This result does not rely on an SDP as an upper bound on OPT, instead appealing to well-known monogamy of entanglement bounds for the Heisenberg model. Parekh and Thompson [31] observe that a similar type of approximation is possible using the second level of the quantum Lasserre hierarchy and obtain a slight improvement over the approximation ratio of [2].

Although these results may seem to suggest that the future of approximation algorithms for QLH should look beyond product states, a solid understanding of the approximability of product states is likely necessary for any type of general approximation algorithm for QLH. Brandão and Harrow [8] show that for (certain generalizations of) regular graphs, OPT_{prod} approaches OPT as the degree increases. Indeed, trading off product-state approximations with more general quantum states is a key ingredient in both [2] and [31].

2 Semidefinite Relaxation and Rounding Approach

In this section we present a rigorous but high-level overview of our approach, with technical lemmas deferred to later sections. We define the main problems considered and our semidefinite relaxation and rounding algorithm. We conclude by motivating the analysis that will occur in detail in the full version of this paper, [30].

2.1 Preliminaries

Quantum information notation. We adopt some standard notations used in quantum information [28]. The $kets |0\rangle := [0,1]$ and $|1\rangle := [1,0]$ represent the standard basis vectors for \mathbb{C}^2 , while the $bras \langle 0|$ and $\langle 1|$ represent their conjugate transposes. The $d \times d$ identity matrix is denoted by \mathbb{I}_d , and the subscript will be omitted when redundant. We obtain the standard bases for \mathbb{C}^{2^n} as $|b_1b_2 \dots b_n\rangle := |b_1\rangle |b_2\rangle \dots |b_n\rangle := |b_1\rangle \otimes |b_2\rangle \otimes \dots \otimes |b_n\rangle$, with $b_i \in \{0,1\}$. The Pauli matrices will have the usual definition:

$$\sigma^0 = \mathbb{I} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \sigma^1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma^2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \text{ and } \quad \sigma^3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$
 (1)

We will generally use subscripts to indicate quantum subsystems. If ρ is a density matrix on n qubits, for instance, ρ_{ij} will correspond to the marginal density matrix on qubits i and j, i.e. the partial trace $\rho_{ij} = \mathrm{Tr}_{[n] \setminus \{i,j\}}[\rho]$ (e.g. [28], Section 2.4.3). Similarly, σ_i^j corresponds to Pauli j on qubit i. Subscripts will supercede position in many cases in the paper, for instance $\sigma_i^1 \otimes \sigma_j^2 \otimes \mathbb{I}_{[n] \setminus \{i,j\}}$ is meant as $\mathbb{I} \otimes \mathbb{I} \otimes \ldots \otimes \sigma^1 \otimes \ldots \otimes \mathbb{I} \otimes \sigma^2 \otimes \ldots \otimes \mathbb{I}$ where σ^1 is at

Table 1 Approximation algorithms for Max 2-local Hamiltonian problems. The number of qubits or Boolean variables is n, and the set of pairwise constraints is E. For readability in the table below, we omit weights $w_{ij} \geq 0$ that may be present in both 2-local Hamiltonian (2-LH) and related classical constraint satisfaction (2-CSP) problems. [30] provides more details on the relationship between 2-LH and 2-CSP, as well as definitions for X_i, Y_i, Z_i . An "N" denotes a numerical result; the classical results are implicitly numerical since they are obtained by numerically finding the worst-case ratio over a range of parameters. The abbreviation "quad." refers to strictly quadratic instances.

| Max 2-LH problem (QMA-hard) | Max 2-CSP specialization (NP-hard) | Classical approx. for 2-CSP | Classical approx. for 2-LH problem (product state) |
|--|--|-----------------------------------|--|
| $\begin{array}{l} \textbf{Traceless} \\ \sum_{ij \in E} H_{ij} \otimes \mathbb{I}_{[n] \setminus \{ij\}} \\ H_{ij} \text{ has no } \mathbb{I} \text{ terms} \end{array}$ | Classical Ising $\max -\sum_{ij \in E} z_i z_j$ $z_i \in \{\pm 1\}$ | $\Omega(\frac{1}{\log n}) \ [14]$ | $\Omega(\frac{1}{\log n})^{\dagger}[11]$ |
| $\begin{array}{l} \textbf{Bipartite Traceless} \\ \sum_{e \in E} H_{ij} \otimes \mathbb{I}_{[n] \setminus \{ij\}} \\ H_{ij} \text{ has no } \mathbb{I} \text{ terms} \\ E \text{ bipartite} \end{array}$ | $egin{aligned} \mathbf{Grothendieck} \ \max &- \sum_{ij \in E} z_i z_j \ z_i \in \{\pm 1\} \ E \ \mathrm{bipartite} \end{aligned}$ | $0.561 + \varepsilon [9]$ | $0.187^{\dagger}({ m quad.})$ |
| Positive/Rank 1 $\sum_{ij \in E} H_{ij} \otimes \mathbb{I}_{[n] \setminus \{ij\}}$ $\mathbb{I} \succeq H_{ij} \succeq 0$ $(\equiv H_{ij} \text{ rank 1 projector})$ | Max 2-CSP (≡ 1 satisfying assignment per clause) | 0.874 [27] | 0.25 (random) 0.328 [21] 0.387 0.467 (quad.) 0.498 (quad., N) 0.5 (upper bound) |
| Max Heisenberg $\sum_{ij \in E} \mathbb{I} - X_i X_j - Y_i Y_j - Z_i Z_j$ (special case of above) | Max Cut $\max \sum_{ij \in E} 1 - z_i z_j$ $z_i \in \{\pm 1\}$ | 0.878 [20] | 0.25 (random) 0.498 [19] 0.5 (upper bound) 0.53*[2] 0.533*[31] |
| Rank 2 $\sum_{ij \in E} H_{ij} \otimes \mathbb{I}_{[n] \setminus \{ij\}} \\ H_{ij} \text{ rank 2 projector}$ | Max 2-CSP with 2 satisfying assignments/clause | 0.874 [27] | 0.5 (random) 0.565 0.639 (quad.) 0.653 (quad., N) 0.667 (upper bound) |
| 2-QSAT $\sum_{ij \in E} H_{ij} \otimes \mathbb{I}_{[n] \setminus \{ij\}} \\ H_{ij} \text{ rank 3 projector}$ | Max 2-SAT (≡ 3 satisfying assignments/clause) | 0.940 [27] | 0.75 (random) 0.764 0.805 (quad.) 0.821 (quad., N) 0.834 (upper bound) |

^{*} This exceeds the product-state upper bound because it is achieved by a classical approximation algorithm that rounds to a description of a non-product state.

[†] For any traceless 2-LH problem, we obtain a product-state approximation ratio that is $\frac{1}{3}$ of an approximation ratio for a related classical CSP, using the appropriate classical approximation algorithm as a black box (see Appendix F in the extended version of this article [30]). This also gives another algorithm and proof for the result of [11] in the first row.

the *i*th position and σ^2 is at the *j*th position. We encourage readers familiar with classical constraint satisfaction problems to consult Appendix E in [30], which casts such problems as quantum local Hamiltonian problems.

2-local Hamiltonian. Our approxiations for QLHP allow multiedges, i.e. distinct edges e and e' on the same pair of qubits i, j. For the sake of exposition, we generally ignore this possibility and conduct our analysis assuming we have a single term H_{ij} for each $ij \in E$. However, when necessary, we will use the notation e_1 and e_2 to refer to the qubits on which an edge e acts. In this context a term H_e is 2-local if it can be written in the form $H_e = \mathcal{O}_e \otimes \mathbb{I}_{[n] \setminus \{e_1, e_2\}}$. Local Hamiltonians have polynomially-sized descriptions which can be given in terms of the local operators \mathcal{O}_e , but for our purposes the details of the description will not be important. We will use $rank(H_e)$ to mean $rank(\mathcal{O}_e)$. The actual rank of H_e is $rank(\mathcal{O}_e)2^{n-2}$, but for ease of exposition we will say that the "rank" of a 2-local term is equal to the rank of its non-trivial part.

The bulk of our work focuses on strictly quadratic instances of QLHP, allowing us to express our main ideas more clearly. The strictly quadratic case precludes non-identity 1-local terms (i.e. $\mathcal{O}_i \otimes \mathbb{I}_{[n] \setminus \{i\}}$ with $\mathcal{O}_i \neq \mathbb{I}$) that may be implicit in a 2-local term.

▶ **Definition 8** (Strictly Quadratic). Let H_e be a 2-local term on n qubits. Write $H_e = \mathcal{O}_e \otimes \mathbb{I}_{[n] \setminus \{e_1, e_2\}}$ for some nontrivial operator \mathcal{O}_e . Express \mathcal{O}_e in the Pauli basis as:

$$\mathcal{O}_e = \sum_{k,l=0}^3 \alpha_{k,l} \sigma^k \otimes \sigma^l. \tag{2}$$

We say that H_e is a strictly quadratic if $\alpha_{k,0} = 0$ for all $k \neq 0$, and $\alpha_{0,l} = 0$ for all $l \neq 0$. Note that the coefficients in Equation (2) may be obtained as $\alpha_{k,l} = \text{Tr}[(\sigma^k \otimes \sigma^l)\mathcal{O}_e]/4$ and are real since \mathcal{O}_e is Hermitian.

Example. An example of a strictly quadratic instance of QLH is quantum Max Cut [19], where for all $ij \in E$, $\mathcal{O}_{ij} = \frac{1}{4}(\mathbb{I} - \sigma^1 \otimes \sigma^1 - \sigma^2 \otimes \sigma^2 - \sigma^3 \otimes \sigma^3)$. In this case $\mathcal{O}_{ij} = |\Psi^-\rangle \langle \Psi^-|$, with $|\Psi^-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$, so that \mathcal{O}_{ij} has rank 1. In general, any maximally entangled pure state on 2 qubits gives rise to a rank-1 strictly quadratic term, since such states must have maximally mixed reduced density matrices.

2.2 Semidefinite Relaxation

We employ a semidefinite programming relaxation for QLH (Problem 1) that is a refinement of the now standard SDP relaxation that has been used in designing approximation algorithms [8, 11,19]. Our relaxation is related to one used by Hallgren, Lee, and Parekh [21] and may be viewed as a specialization of noncommutative Lasserre hierarchies proposed for quantum information applications [16,31,34].

In this section we assume, for the sake of exposition, that there is a single edge ij on any pair of qubits $i, j \in [n]$; however, the relaxation and rounding algorithm may be readily extended to handle general instances of QLH with multiedges. Suppose we have an instance of QLH on n qubits. The first set of variables in our SDPs will be marginal density matrices $\{\rho_{ij}\}$. Since there are n qubits, there are $\binom{n}{2}$ many of these, and each of them is a 4×4 Hermitian matrix. While we cannot impose global consistency, we can force each ρ_{ij} to be a valid density matrix on its own: $\text{Tr}[\rho_{ij}] = 1$ and $\rho_{ij} \succeq 0$ for all $i, j \in [n]$. We could also explicitly force overlapping marginals to be consistent on single qubit density matrices, however this will be implicit through our use of moment matrices.

Moment matrices. Suppose we have a quantum state on n qubits $|\psi\rangle \in \mathbb{C}^{2^n}$. Consider the 1-local Pauli operators, $\mathcal{M} = \{\mathbb{I}\} \cup \{\sigma_i^k \otimes \mathbb{I}_{[n] \setminus \{j\}} \mid k \in [3], i \in [n]\}$. We apply each of the 3n+1Pauli operators $\mathcal{O} \in \mathcal{M}$ on $|\psi\rangle$ to obtain columns of a matrix $V = \{\mathcal{O} | \psi\rangle\}_{\mathcal{O} \in \mathcal{M}} \in \mathbb{C}^{2^n \times (3n+1)}$. We call $M := V^{\dagger}V \in \mathbb{C}^{(3n+1)\times(3n+1)}$ the moment matrix of $|\psi\rangle$ with respect to \mathcal{M} ; note that M is Hermitian and $M \succeq 0$ by construction. The notation $M(\mathcal{O}, \mathcal{P})$ refers to the entry of M at the row and column corresponding to $\mathcal{O}, \mathcal{P} \in \mathcal{M}$ respectively. We have $M(\mathcal{O}, \mathcal{P}) = \langle \psi | \mathcal{OP} | \psi \rangle$, for all $\mathcal{O}, \mathcal{P} \in \mathcal{M}$, so that M captures all the 2-local Pauli statistics of $|\psi\rangle$. In particular the quantity $\langle\psi|H|\psi\rangle$ is a linear function of the entries of M for a 2-local Hamiltonian H. If we let \mathcal{M}_k consist of all the k-local tensor products of Paulis, instead of just the 1-local ones, the corresponding moment matrix M_k , of size $O(n^k)$ by $O(n^k)$, includes all the 2k-local Pauli statistics. We may obtain SDP relaxations for QLH problems by constructing a relaxed $M_k \succeq 0$ that satisfies linear constraints of the form $\text{Tr}[AM_k] = b$, that a true moment matrix would satisfy. This corresponds to the kth level of noncommutative Lasserre hierarchies introduced for quantum information [16,31,34]. Our approach relaxes \mathcal{M}_1 and adds additional constraints enforcing positivity of 2-local marginals; the relaxation we obtain sits between the k=1 and k=2 levels of the noncommutative Lasserre hierarchy.

SDP Relaxation. We define a (relaxed) moment matrix M, which will track local statistics of the set of marginals $\{\rho_{ij}\}$. Let M be a symmetric, $(3n+1)\times(3n+1)$ real matrix whose rows and columns correspond to operators in \mathcal{M} . Entries of M will correspond to coefficients of the marginal density matrices $\{\rho_{ij}\}$ in the Pauli basis. We use the notation $M(\sigma_i^k, \sigma_j^l)$ to refer to entries of M for $i, j \in [n]$ and $k, l \in [3]$; in addition we have a row and column of M indexed by \mathbb{I} . We set $M(\sigma_i^k, \sigma_j^l) = \text{Tr}[\sigma^k \otimes \sigma^l \ \rho_{ij}]$ for (i, k), (j, l) in $[n] \times [3]$. In addition we set $M(\mathbb{I}, \mathbb{I}) = 1$, and $M(\sigma_i^k, \mathbb{I}) = \text{Tr}[\sigma^k \otimes \mathbb{I} \ \rho_{ij}]$ for all $(i, k) \in [n] \times [3]$ and $j \in [n]$. Note that this constraint forces consistent single-qubit marginals since

$$\operatorname{Tr}_{u}[\rho_{iu}] = \operatorname{Tr}_{v}[\rho_{iv}] \Leftrightarrow \operatorname{Tr}[\sigma^{l} \otimes \mathbb{I} \ \rho_{iu}] = \operatorname{Tr}[\sigma^{l} \otimes \mathbb{I} \ \rho_{iv}] \ \forall l.$$

Since M contains all local information of $\{\rho_{ij}\}$, we can use M to evaluate the objective of our SDP. In this direction, we will define a weight matrix for each edge $H_{ij} = w_{ij} \mathcal{O}_{ij} \otimes \mathbb{I}_{n \setminus \{i,j\}}$, where $\mathcal{O}_{ij} \in \mathbb{C}^{4\times 4}$, and w_{ij} is a scalar weight. We define the $(3n+1) \times (3n+1)$ matrix C_{ij} , which contains the coefficients of \mathcal{O}_{ij} in the Pauli basis:

$$C_{ij}(\sigma_i^k, \sigma_j^l) = C_{ij}(\sigma_j^l, \sigma_i^k) = Tr[\sigma^k \otimes \sigma^l \ \mathcal{O}_{ij}]/8 \quad \forall k, l \in [3],$$

$$C_{ij}(\sigma_i^k, \mathbb{I}) = C_{ij}(\mathbb{I}, \sigma_i^k) = Tr[\sigma^k \otimes \mathbb{I} \ \mathcal{O}_{ij}]/8 \quad \forall k \in [3],$$

$$C_{ij}(\sigma_j^l, \mathbb{I}) = C_{ij}(\mathbb{I}, \sigma_j^l) = Tr[\mathbb{I} \otimes \sigma^l \ \mathcal{O}_{ij}]/8 \quad \forall l \in [3],$$
(3)

and all other entries of C_{ij} are 0. To illustrate application of the matrix C_{ij} , suppose \mathcal{O}_{ij} and the marginal density matrix ρ_{ij} have Pauli decompositions:

$$\mathcal{O}_{ij} = \sum_{k,l=0}^{3} \alpha_{kl} \sigma^k \otimes \sigma^l$$
 and $\rho_{ij} = \frac{1}{4} \sum_{k,l=0}^{3} \beta_{kl} \sigma^k \otimes \sigma^l$.

Since, for $k, l \ge 0$, $(\sigma^k)^2 = \mathbb{I}$ and $\text{Tr}[\sigma^k \sigma^l] = 0$ when $k \ne l$, the value we gain from edge ij, ignoring the weight w_{ij} , is written as:

$$\operatorname{Tr}[\mathcal{O}_{ij}\rho_{ij}] = \alpha_{00}\beta_{00} + \sum_{\substack{k,l:\\(k\neq 0)\vee(l\neq 0)}} \alpha_{kl}\beta_{kl} = \frac{\operatorname{Tr}[\mathcal{O}_{ij}]}{4} + \operatorname{Tr}[C_{ij}M]. \tag{4}$$

With these facts in hand, we may finally give the main SDP relaxation in this work:

▶ **Problem 9.** Given an instance of QLH (Problem 1) on n qubits with local terms $\{H_{ij} = w_{ij}\mathcal{O}_{ij} \otimes \mathbb{I}_{[n]\setminus\{i,j\}}\}$, let C_{ij} be defined according to Equation (3) for each $ij \in E$. Solve the following SDP:

$$\max \sum_{ij \in E} w_{ij} \left(\frac{Tr[\mathcal{O}_{ij}]}{4} + Tr[C_{ij}M] \right)$$
 (5)

$$s.t. M(\mathbb{I}, \mathbb{I}) = 1, (6)$$

$$M(\sigma_i^k, \sigma_i^k) = 1 \qquad \forall i \in [n] \text{ and } k \in [3], \tag{7}$$

$$M(\sigma_i^k, \sigma_i^l) = 0 \qquad \forall i \in [n] \text{ and } k \neq l \in [3], \tag{8}$$

$$M(\sigma_i^k, \sigma_j^l) = Tr[\sigma^k \otimes \sigma^l \ \rho_{ij}] \quad \forall ij \in E \ and \ k, l \in [3], \tag{9}$$

$$M(\sigma_i^k, \mathbb{I}) = Tr[\sigma^k \otimes \mathbb{I} \ \rho_{ij}] \quad \forall ij \in E \ and \ k \in [3],$$
 (10)

$$M(\sigma_i^l, \mathbb{I}) = Tr[\mathbb{I} \otimes \sigma^l \ \rho_{ij}] \quad \forall ij \in E \ and \ l \in [3],$$
 (11)

$$Tr[\rho_{ij}] = 1 \qquad \forall ij \in E,$$
 (12)

$$\mathcal{H}(\mathbb{C}^{4\times 4}) \ni \rho_{ij} \succeq 0 \qquad \forall ij \in E, \tag{13}$$

$$\mathcal{S}(\mathbb{R}^{(3n+1)\times(3n+1)}) \ni M \succeq 0,\tag{14}$$

where $S(\cdot)$ and $\mathcal{H}(\cdot)$ refer to the symmetric and Hermitian matrices, respectively.

▶ **Theorem 10.** The mathematical program of Problem 9 is an efficiently computable semidefinite program that provides an upper bound on $\lambda_{max}(\sum_{ij\in E} H_{ij})$.

Proof. Constraints (6)–(12) are linear equalities on the entries of PSD matrices M and ρ_{ij} $\forall ij \in E$, hence we do indeed have an SDP. Since there are polynomially many variables of polynomial size, the usual considerations show computational efficiency, i.e. the program can be solved to arbitrary additive precision in polynomial time.

A larger matrix $X \succeq 0$, consisting of M and the ρ_{ij} as its diagonal blocks may be used to put the SDP into a more standard form (e.g. [7], Section 4.6.2). Although the ρ_{ij} are complex, the SDP may be solved as a real SDP by appealing to the standard approach of tracking the real and imaginary parts separately and observing $X \succeq 0$ if and only if

$$\begin{bmatrix} \operatorname{Re}(X) & -\operatorname{Im}(X) \\ \operatorname{Im}(X) & \operatorname{Re}(X) \end{bmatrix} \succeq 0.$$

Let $|\psi\rangle$ be an eigenvector corresponding to $\lambda_{max}(\sum_{ij\in E} H_{ij})$, and let ρ_{ij}^* , $\forall ij\in E$, be the 2-qubit marginal density matrices of $\rho = |\psi\rangle\langle\psi|$, so that Constraints (12) and (13) are satisfied for the ρ_{ij}^* . In addition consider the moment matrix M for $|\psi\rangle$ with respect to \mathcal{M} , as described above. The matrix M satisfies Constraints (6), (7), (9)–(11), and (14) by the definition of a moment matrix, since

$$\langle \psi | \sigma_i^k \otimes \sigma_i^l \otimes \mathbb{I}_{[n] \setminus \{i,j\}} | \psi \rangle = \text{Tr}[\sigma^k \otimes \sigma^l \ \rho_{ij}^*], \text{ for } 0 \le k, l \le 3.$$
 (15)

Constraint (8) is the only one that remains. Note that the real part of $M, M^* := \operatorname{Re}(M) \succeq 0$ since $M \succeq 0$. By Equation (15), for any $j \in [n]$ and $k \neq l \in [3], M(\sigma_i^k, \sigma_i^l) = \pm i \operatorname{Tr}[\sigma^m \otimes \mathbb{I} \ \rho_{ij}^*]$, where $m \in [3] \setminus \{k, l\}$. The quantities in Equation (15) are real since tensor products of Pauli operators are Hermitian. This implies that $M(\sigma_i^k, \sigma_i^l)$ for $k \neq l \in [3]$ is imaginary and more generally that M^* and the ρ_{ij}^* satisfy all the constraints.

Consider the objective value for this solution, $\sum_{ij\in E} w_{ij} (\text{Tr}[\mathcal{O}_{ij}]/4 + \text{Tr}[C_{ij}M^*]) =$

$$\sum_{ij \in E} w_{ij} \operatorname{Tr}[\mathcal{O}_{ij} \rho_{ij}^*] = \operatorname{Tr}\left[\sum_{ij \in E} H_{ij} \ \rho\right] = \lambda_{max} \left(\sum_{ij \in E} H_{ij}\right),$$

where the first equality follows from Equation (4). It follows that the optimal solution to Problem 9 has value at least that of the optimal solution of QLH.

2.3 Rounding Approach and Formal Statement of Results

Overview. In classical SDP-based rounding schemes, one typically seeks to randomly "round" unit vectors $\mathbf{v}_i \in \mathbb{R}^d$ to scalars $z_i \in \{\pm 1\}$ so that the expected value of $z_i z_j$ approximates $\mathbf{v}_i \cdot \mathbf{v}_j$. The seminal hyperplane rounding scheme of Goemans and Williamson [20] achieves this by selecting a random unit vector $\mathbf{r} \in \mathbb{R}^d$ and setting $z_i = \mathbf{r} \cdot \mathbf{v}_i/|\mathbf{r} \cdot \mathbf{v}_i|$.

Rounding solutions from SDP relaxations for QLH to product states generalizes this approach. Recall that a product state has the form $|\psi\rangle = |\psi_1\rangle \otimes \ldots \otimes |\psi_n\rangle$ where each $|\psi_i\rangle \in \mathbb{C}^2$ is a local state on qubit i. We obtain a density matrix $\rho = |\psi\rangle \langle \psi| = |\psi_1\rangle \langle \psi_1| \otimes \ldots \otimes |\psi_n\rangle \langle \psi_n|$, which is a tensor product of single-qubit density matrices $\rho_i := |\psi_i\rangle \langle \psi_i|$. Any such ρ_i may be expressed in the Pauli basis as $\rho_i = \frac{1}{2}(\mathbb{I} + \theta_{i1}\sigma^1 + \theta_{i2}\sigma^2 + \theta_{i3}\sigma^3)$, where $\theta_{ik} = \mathrm{Tr}[\sigma^k\rho_i] \in \mathbb{R}$ and $\sum_{k \in [3]} \theta_{ik}^2 = 1$. In particular, product states with $\theta_{i1} = \theta_{i2} = 0$ and $\theta_{i3}^2 = 1$ correspond precisely to the classical setting (see Appendix E in [30] for an explicit connection between the two). Product states exhibit no entanglement, and we may specify θ_{ik} independently for each qubit i. However, instead of producing a single $z_i^2 = 1$ as in the classical case, we must produce a unit vector $\theta_i = [\theta_{i1}, \theta_{i2}, \theta_{i3}] \in \mathbb{R}^3$ for each $i \in [n]$. Briët, de Oliveira Filho, and Vallentin were the first to consider such generalizations of scalars to unit vectors, in the context of the Grothendieck problem [12, 13], and their analysis has fueled recent approximation algorithms for QLH [19, 21].

The classical Goemans-Williamson rounding scheme obtains the unit vectors \mathbf{v}_i from a Cholesky decomposition of a PSD matrix $V^TV = R \succeq 0$. Taking the \mathbf{v}_i to be columns of V yields $R_{i,j} = \mathbf{v}_i \cdot \mathbf{v}_j$. Recent approximation algorithms [11, 19, 21] for QLH have mimicked this approach, as do we. Let $M^* \succeq 0$ be an optimal solution to Problem 9 (the ρ_{ij}^* are not necessary to describe the rounding algorithm). We find a Cholesky decomposition $V^TV = M^*$, and let $\mathbf{v}_{ik} \in \mathbb{R}^d$ be the column of V associated with σ_i^k for $i \in [n], k \in [3]$; we may assume $d \leq 3n + 1$. In addition we let \mathbf{v}_0 be the column of V corresponding to \mathbb{I} . These are unit vectors as a consequence of Constraints (6) and (7).

We will employ the same rounding algorithm for both the general and strictly quadratic cases. While previous related works [11, 19, 21] have in some cases had to rely on more sophisticated rounding schemes because they have been amenable to analysis, we are able to shed light on what is arguably the most natural generalization of the Goemans-Williamson approach. We draw $\mathbf{r} \sim \mathcal{N}(0, \mathbb{I}_d)$, i.e. a multivariate distribution over d independent and standard Gaussian variables. For each qubit, we obtain the desired vector $\theta_i = [\theta_{i1}, \theta_{i2}, \theta_{i3}]$ as:

$$[\mathbf{v}_{i1} \cdot \mathbf{r}, \ \mathbf{v}_{i2} \cdot \mathbf{r}, \ \mathbf{v}_{i3} \cdot \mathbf{r}]/Q_i,$$

where
$$Q_i := \sqrt{(\mathbf{v}_{i1} \cdot \mathbf{r})^2 + (\mathbf{v}_{i2} \cdot \mathbf{r})^2 + (\mathbf{v}_{i3} \cdot \mathbf{r})^2}$$
 is a normalization.

The classical Max Cut problem corresponds to a strictly quadratic Hamiltonian (see Appendix E in [30] for justification); however, classical Max 2-SAT and more general Max 2-CSP have 1-local terms (i.e., linear terms in $\{\pm 1\}$ variables). In contrast, strictly quadratic instances of QLHP serve as a quantum generalization of Max 2-SAT and Max 2-CSP that have no 1-local terms. In order to obtain effective classical approximations in the presence of 1-local terms, an additional vector \mathbf{v}_0 is necessary, representing (scalar) identity. Generally, the vector \mathbf{v}_0 is used in conjunction with more sophisticated rounding schemes (e.g. [27]) to obtain positive expectation from the 1-local terms. For the quantum case, relatively simple approaches suffice to get good approximations [21]. Using the vector \mathbf{v}_0 is not necessary for the strictly quadratic case, and including it does not affect its approximation.

Rounding algorithm. The rounding approach described above produces single-qubit density matrices:

$$\rho_i = \frac{1}{2} \left(\mathbb{I} + \frac{\mathbf{v}_{i1} \cdot \mathbf{r}}{Q_i} \sigma^1 + \frac{\mathbf{v}_{i2} \cdot \mathbf{r}}{Q_i} \sigma^2 + \frac{\mathbf{v}_{i3} \cdot \mathbf{r}}{Q_i} \sigma^3 \right).$$

Hence, on any 1-local term, $\mathbb{E}[\text{Tr}[\sigma^k \rho_i]] = \mathbb{E}[\mathbf{v}_{ik} \cdot \mathbf{r}/Q_i] = 0$ since Q_i is an even function and $\mathbf{v}_{ik}\cdot\mathbf{r}$ is an odd function in each entry of \mathbf{r} . Thus, in order to get a nontrivial approximation on 1-local terms, we will use the vector \mathbf{v}_0 to globally flip the sign of the θ_i vectors of all qubits, i.e. $\mathbf{v}_{ik} \cdot \mathbf{r}/Q_i \to sign(\mathbf{v}_0 \cdot \mathbf{r})(\mathbf{v}_{ik} \cdot \mathbf{r}/Q_i)$. Since $sign(\mathbf{v}_0 \cdot \mathbf{r}) \in \{\pm 1\}$, for quadratic objective terms this factor will cancel out, but for 1-local terms we will gain additional objective from the correlation of $\mathbf{v}_0 \cdot \mathbf{r}$ and $\mathbf{v}_{ik} \cdot \mathbf{r}$. Formally, we can state the rounding algorithm, which applies to any instance of QLH, in Algorithm 1.

Algorithm 1 Hyperplane rounding for 2-Local Hamiltonian.

- 1. Given some instance of Problem 1 formulate and solve the corresponding instance of Problem 9. Let M^* be the optimal moment matrix obtained from Problem 9.
- 2. Find the Cholesky decomposition of M^* , obtaining Cholesky vectors $\mathbf{v}_0 \in \mathbb{R}^d$ and $\{\mathbf{v}_{ik} \in \mathbb{R}^d\}$ such that $M^*(\sigma_i^k, \sigma_i^l) = \mathbf{v}_{ik} \cdot \mathbf{v}_{jl}$ and $M^*(\mathbb{I}, \sigma_i^k) = \mathbf{v}_0 \cdot \mathbf{v}_{ik}$ for $i, j \in [n]$ and $k, l \in [3].$
- 3. Let \mathbf{r} be a random vector with $\mathbf{r} \sim \mathcal{N}(0, \mathbb{I}_d)$. 4. For each qubit i, set $Q_i = \sqrt{(\mathbf{v}_{i1} \cdot \mathbf{r})^2 + (\mathbf{v}_{i2} \cdot \mathbf{r})^2 + (\mathbf{v}_{i3} \cdot \mathbf{r})^2}$, and set $\theta_{ik} = sign(\mathbf{v}_0 \cdot \mathbf{r})$ \mathbf{r})($\mathbf{v}_{ik} \cdot \mathbf{r}/Q_i$) for $k \in [3]$.
- **5.** Output the (pure) state:

$$\rho = \bigotimes_{i=1}^{n} \frac{1}{2} (\mathbb{I} + \theta_{i1}\sigma^{1} + \theta_{i2}\sigma^{2} + \theta_{i3}\sigma^{3}).$$

We will give the following approximation guarantees for QLHP:

▶ **Theorem 11.** Fix $k \in \{1, 2, 3\}$. Suppose we are given an instance of QLHP (Problem 2), $\{H_e\}$ where $H_e = w_e P_e \otimes \mathbb{I}_{[n] \setminus \{e_1, e_2\}}$ for $w_e \geq 0$ and P_e a projector of rank at least k, for all $e \in E$. Let M^* be the optimal moment matrix for the corresponding SDP relaxation, Problem 9, and let ρ be the random output of Algorithm 1. Then,

$$\mathbb{E}\left[\operatorname{Tr}\left[\sum_{e\in E}H_e\ \rho\right]\right]\geq \alpha(k)\left(\sum_{e\in E}w_e\left(\frac{\operatorname{rank}(P_e)}{4}+\operatorname{Tr}[C_eM^*]\right)\right)\geq \alpha(k)\,\lambda_{\max}\left(\sum_{e\in E}H_e\right),$$

where

$$\alpha(k) = \begin{cases} 2/\pi - 1/4 \approx 0.387 & \text{if } k = 1\\ 16/(9\pi) \approx 0.565 & \text{if } k = 2\\ 3/8 + 11/(9\pi) \approx 0.764 & \text{if } k = 3. \end{cases}$$

Theorem 12. If, in addition to the assumptions of Theorem 11, the P_e are strictly quadratic projectors, then the random output of Algorithm 1 satisfies:

$$\mathbb{E}\left[\operatorname{Tr}\left[\sum_{ij\in E}H_{ij}\rho\right]\right]\geq\alpha(k)\lambda_{max}\left(\sum_{ij\in E}H_{ij}\right),$$

where

$$\alpha(k) = \begin{cases} 22/(15\pi) \approx 0.467 & \text{if } k = 1\\ 1/3 + 24/(25\pi) \approx 0.639 & \text{if } k = 2\\ 1/2 + 388/(405\pi) \approx 0.804 & \text{if } k = 3. \end{cases}$$

The above results are rigorous, but non-optimal. The quadratic analysis depends crucially on an expansion of a particular expectation in Hermite polynomials. One can consider a higher order Hermite series to more accurately capture the expectation and achieve a better approximation factor. We have such results, but opt to not include them in the interest of the reader. Higher orders bring increased tedium, and our technique should be clear enough at the end of the paper that an interested reader could do the higher order calculation.

One can ask, why not include a high enough order that the result becomes essentially optimal? The issue is that polynomial expansions often converge slowly in the presence of discontinuities [33]. Indeed, computationally we have determined that to get essentially optimal results one would need to go to high enough order that the polynomial expansion would become intractable. One can determine the optimal approximation factor by using a high order expansion and numerically optimizing or simply by randomly sampling over some "net" of the parameter space. Our observed approximation factors under these approaches are stated in Conjecture 6. Proving an approximation factor as large as the observed performance of our algorithm is the subject of future work.

2.4 Analysis Overview

We present an overview of our analysis for the strictly quadratic case, which will also carry over to the general case with additional bookkeeping and bounding for the 1-local terms. Suppose we are given an instance of QLHP (Problem 2) on which we execute Algorithm 1 to produce a random solution ρ . For $i, j \in [n]$, the 2-qubit marginals of ρ are

$$\rho_{ij} = \frac{1}{4} (\mathbb{I} + \theta_{i1}\sigma^1 + \theta_{i2}\sigma^2 + \theta_{i3}\sigma^3) \otimes (\mathbb{I} + \theta_{j1}\sigma^1 + \theta_{j2}\sigma^2 + \theta_{j3}\sigma^3), \tag{16}$$

and the objective value of ρ is $\sum_{ij\in E} \operatorname{Tr}[H_{ij}\rho] = \sum_{ij\in E} w_{ij}APX_{ij}$, where $APX_{ij} := \operatorname{Tr}[P_{ij}\rho_{ij}]$ is the unweighted contribution to the objective value from edge ij. Let M^* and ρ_{ij}^* for $ij \in E$ be the SDP solution obtained by Algorithm 1, and let $SDP_{ij} := \operatorname{Tr}[P_{ij}\rho_{ij}^*]$ be the unweighted contribution to the SDP objective value from edge ij. The approximation ratio, which we seek to bound from below, is consequently:

$$\alpha = \mathbb{E}\left[\frac{\sum_{ij \in E} w_{ij} APX_{ij}}{\sum_{ij \in E} w_{ij} SDP_{ij}}\right] = \frac{\sum_{ij \in E} w_{ij} \mathbb{E}[APX_{ij}]}{\sum_{ij \in E} w_{ij} SDP_{ij}}.$$

Observe that $APX_{ij} \geq 0$ and $SDP_{ij} \geq 0$ since P_{ij} , ρ_{ij} , and ρ_{ij}^* are all PSD. Since all the terms in the denominator are nonnegative, it follows from an elementary argument that

$$\alpha \geq \frac{\sum_{ij \in E} w_{ij} \mathbb{E}[APX_{ij}]}{\sum_{ij \in E} w_{ij} SDP_{ij}} \geq \min_{ij \in E} \frac{\mathbb{E}[APX_{ij}]}{SDP_{ij}}.$$

Thus it suffices to bound the approximation ratio for the worst case occurring on a single edge.

Bounding a worst-case edge. We now focus our attention on a single edge e=12 on qubits 1, 2. We collect the vectors \mathbf{v}_{ik} , obtained from a Cholesky decomposition of the SDP solution M^* , into matrices $V_i = [\mathbf{v}_{i1}, \mathbf{v}_{i2}, \mathbf{v}_{i3}] \in \mathbb{R}^{d \times 3}$, for i=1,2. We define an objective matrix $C \in \mathbb{R}^{3 \times 3}$, containing scaled 2-local Pauli-basis coefficients of P_{12} , in the vein of Equation (3): $C(\sigma_1^k, \sigma_2^l) := \text{Tr}[\sigma^k \otimes \sigma^l \ P_{12}]$, for $k, l \in [3]$ (note that C is not symmetric). With these definitions in hand, observe that $V_i^T V_i = \mathbb{I}_3$, by the SDP constraints (7) and (8), and that $4\text{Tr}[C_{12}M^*] = \text{Tr}[V_1CV_2^T]$. The hyperplane rounding produces unit vectors $\theta_i^T = [\theta_{i1}, \theta_{i2}, \theta_{i3}] = \mathbf{r}^T V_i / ||V_i^T \mathbf{r}||$. In terms of these variables, we have:

$$SDP_{e} = \text{Tr}[P_{12}\rho_{12}^{*}] = \frac{1}{4} \left(rank(P_{12}) + \text{Tr}[V_{1}CV_{2}^{T}] \right), \text{ and}$$

$$\mathbb{E}[APX_{e}] = \mathbb{E}[\text{Tr}[P_{12}\rho_{12}]] = \frac{1}{4} \left(rank(P_{12}) + \mathbb{E}\left[\theta_{1}^{T}C\theta_{2}\right] \right) = \frac{1}{4} \left(rank(P_{12}) + \mathbb{E}_{\mathbf{r}}\left[\frac{\mathbf{r}^{T}V_{1}CV_{2}^{T}\mathbf{r}}{||V_{1}^{T}\mathbf{r}|| ||V_{2}^{T}\mathbf{r}||} \right] \right),$$

by Equation (4) and because $Tr[P_{12}] = rank(P_{12})$, since P_{12} is a projector. Thus, setting $k = rank(P_{12})$, the quantity we seek to bound is

$$\alpha \geq \min_{V_1, V_2, C} \frac{k + \mathbb{E}_{\mathbf{r}} \left[\frac{\mathbf{r}^T V_1 C V_2^T \mathbf{r}}{||V_1^T \mathbf{r}|| \ ||V_2^T \mathbf{r}||} \right]}{k + \text{Tr}[V_1 C V_2^T]}.$$

The bulk of our analysis lies in (i) simplifying the above to reduce the number of parameters in the minimization and expectation (Appendix B in [30]), and (ii) deriving analytical bounds on the expectation (Appendix C in [30]).

Simplifying the Gaussian expectation. The first simplification follows from observing that $V_i^T \mathbf{r} \in \mathbb{R}^3$ are multivariate Gaussians for i = 1, 2 since they are linear combinations of Gaussians, $\mathbf{r} \sim \mathcal{N}(0, \mathbb{I})$. If we let $\mathbf{z}^T = [z_1, z_2, z_3] = \mathbf{r}^T V_1$ and $(\mathbf{z}')^T = [z'_1, z'_2, z'_3] = \mathbf{r}^T V_2$, then $[\mathbf{z}, \mathbf{z}'] \sim \mathcal{N}(0, \Sigma)$, where

$$\Sigma = \begin{bmatrix} \mathbb{I} & V_1^T V_2 \\ V_2^T V_1 & \mathbb{I} \end{bmatrix} \in \mathbb{R}^{6 \times 6}.$$

The Gaussians z_i are mutually independent as well as the z_i' , and the covariance between \mathbf{z} and \mathbf{z}' is given by $M = V_1^T V_2 \in \mathbb{R}^{3\times 3}$. Our bound now depends on a constant number of parameters, the 18 entries of C and M:

$$\alpha \ge \min_{M,C} \frac{k + \mathbb{E}_{\mathbf{z},\mathbf{z}'} \left[\frac{\mathbf{z}^T C \mathbf{z}'}{||\mathbf{z}|| \, ||\mathbf{z}'||} \right]}{k + \text{Tr}[C^T M]}.$$
(17)

For classical hyperplane rounding algorithms, C and M simply reduce to scalars, and one may resort to a numerical argument to furnish the desired bound. However, in the case of QLH above, numerical bounds exhibit poor precision or convergence due to the number of parameters. Thus we press on, and our next observation is that only the singular values of M matter for the analysis. The above arguments are detailed in Lemma 15 in [30], which also shows that we may assume:

$$C = \begin{bmatrix} p & 0 & 0 \\ 0 & q & 0 \\ 0 & 0 & r \end{bmatrix} \text{ and } M = \begin{bmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{bmatrix},$$
 (18)

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where a, b, c are the singular values of $V_1^T V_2$. This reduction to 6 parameters puts analysis of α within reach. The special case when a = b = c turns out to be equivalent to the recently studied quantum analog of Max Cut related to the quantum Heisenberg model [2, 19]. For this case, a representation of the expectation,

$$\mathbb{E}_{\mathbf{z},\mathbf{z}'}\left[\frac{\mathbf{z}^T C \mathbf{z}'}{||\mathbf{z}|| \, ||\mathbf{z}'||}\right] \tag{19}$$

as a hypergeometric function follows from work of Briët, de Oliveira Filho, and Vallentin (the expectation ends up being equivalent to the one in Lemma 2.1 from [13], when $\mathbf{u} \cdot \mathbf{v}$ in the lemma equals a = b = c). To the best of our knowledge, no elementary representation is known when a, b, c may be distinct. We appeal to Hermite analysis to express the expectation (19) as a polynomial that we are subsequently able to bound; this is carried out in Lemmas 17-18/Appendix C of [30].

Introducing constraints from positivity. The matrices C and M from (18) are related to the quadratic Pauli-basis coefficients of P_{12} and ρ_{12}^* , respectively. The other ingredient of our analysis of the bound (17) is restricting C and M based on the facts that $P_{12} \succeq 0$ and $\rho_{12}^* \succeq 0$, which is undertaken in Appendix B.1 and Lemma 14 of [30]. This is where the SDP constraint (13) is used. The bound we obtain is

$$\alpha \ge \min_{\substack{[a,b,c] \in \mathcal{S}\\ [p,a,r] \in \mathcal{P}_{k}}} \frac{k + \mathbb{E}_{\mathbf{z},\mathbf{z}'} \left[\frac{pz_1 z_1' + qz_2 z_2' + rz_3 z_3'}{\sqrt{(z_1^2 + z_2^2 + z_3^2)((z_1')^2 + (z_2')^2 + (z_3')^2)}} \right]}{k + ap + bq + cr},$$
(20)

where S and \mathcal{P}_k are specific polytopes (S is a simplex as is \mathcal{P}_k for $k \neq 2$) derived from the positivity of P_{12} and ρ_{12}^* . We further observe in Lemma 34 in [30] that p, q, r may be fixed (e.g., for k = 3, we may take p = q = r = 1). Finally, Lemmas 17 and 18 in [30] derive the bounds in the main theorems 11 and 12, respectively.

Analysis Highlights. We utilize Hermite polynomials to evaluate the expectation given in Equation (20). As the natural set of polynomials orthogonal under the expectation of Gaussian variables, [26], we obtain an expression for the expectation in terms of a convergent series which we can then truncate and bound to get rigorous results. Obtaining the coefficients in this series requires some additional facts about Hermite polynomials, and some combinatorial identities.

3 Conclusion

In this work we have demonstrated several new approximation algorithms for interesting cases of the Max 2-Local Hamiltonian problem. As is the theme in many works [4,8,18], we have given evidence that the geometry of 2-Local interactions can drastically effect approximability for traceless Hamiltonians since we demonstrate the bipartite case has a constant factor approximation algorithm and the unconstrained case is known to have no constant factor algorithm [11]. In addition to this, we have given a novel approximation algorithm and analysis for 2-Local Hamiltonian with local terms that are also projectors. This is especially interesting given the the scarcity of approximation algorithms for quantum problems. Indeed, the rank 3 case, has been open for some time [18,21]. Furthermore, we have provided new techniques for rounding to product states that we believe will have additional applications

in quantum information. Our rounding algorithm is quite natural given the solution of the SDP, and the ability to understand the expectation through Hermite polynomial analysis seems likely to extend to other kinds of Hamiltonians or problems.

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