An Approximation Algorithm for the MAX-2-Local Hamiltonian Problem

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—— **Abstract** ——

We present a classical approximation algorithm for the MAX-2-Local Hamiltonian problem. This is a maximization version of the QMA-complete 2-Local Hamiltonian problem in quantum computing, with the additional assumption that each local term is positive semidefinite. The MAX-2-Local Hamiltonian problem generalizes NP-hard constraint satisfaction problems, and our results may be viewed as generalizations of approximation approaches for the MAX-2-CSP problem. We work in the product state space and extend the framework of Goemans and Williamson for approximating MAX-2-CSPs. The key difference is that in the product state setting, a solution consists of a set of normalized 3-dimensional vectors rather than boolean numbers, and we leverage approximation results for rank-constrained Grothendieck inequalities. For MAX-2-Local Hamiltonian we achieve an approximation ratio of 0.328. This is the first example of an approximation algorithm beating the random quantum assignment ratio of 0.25 by a constant factor.

1 Introduction

The k-Local Hamiltonian problem is the most studied QMA-complete problem in quantum computing [19] and generalizes classical constraint satisfaction problems (CSPs). It is physically motivated, asking about the ground state energy of a system specified by its Hamiltonian, or equivalently the minimum eigenvalue of an exponentially large Hermitian

matrix. Even though the matrix is exponentially large in the number of qubits, it can be succinctly described as a sum of matrices that are each a tensor product of a $2^k \times 2^k$ Hermitian matrix and the $2^{n-k} \times 2^{n-k}$ identity matrix, where n is the size of the whole matrix, and k is some constant given by a problem instance (called locality). Note that one only needs to describe the $2^k \times 2^k$ matrices to describe the whole problem. A precise definition will be given later. There are many variations depending on the locality, the number of levels each particle has (instead of 2 for the qubit case above), and other assumptions that can be made on the Hamiltonian. The class QMA has also been well-studied, and a large set of problems has been shown to be QMA-complete [6].

There has been much less progress in finding approximation algorithms for these problems. One difference arising in the quantum case is that classical algorithms cannot efficiently represent arbitrary solutions, which in general are entangled quantum states and thus reside in an exponentially large space (2^n dimensional). One approach to circumvent this problem is to only consider product state solutions, which are a subset of quantum states that exhibit no entanglement and admit efficient classical descriptions. Bansal, Bravyi, and Terhal [5] proved that a polynomial time approximation scheme (PTAS) (a polynomial-time algorithm that offers an arbitrarily good approximation at the expense of increase in run time) exists for Quantum Ising Spin Glass when assuming the underlying graph describing the interaction of the qubits is planar with bounded degree. Brandão and Harrow [7] analyze the D-regular case and give an additive approximation algorithm.

Another issue in the design of approximation algorithms is ensuring that problems have well-defined approximations. For general Hamiltonians, which are Hermitian, the spectrum can include positive and negative numbers, so it is difficult to define a meaningful approximation ratio. Gharibian and Kempe [12] defined the MAX-k-Local Hamiltonian problem and analyze the dense case. Their definition requires the k-local terms of the Hamiltonian to be positive semidefinite, so that meaningful approximations exist. This case is still QMA-hard and includes the classical constraint satisfaction problem, MAX-k-CSP as a special case.

The Max-2-Local Hamiltonian problem

In this paper we give a randomized classical approximation algorithm for the MAX-2-Local Hamiltonian (MAX-2-LH) problem on qubits. MAX-2-LH is QMA-hard, so approximation algorithms are a natural solution strategy. The problem is NP-hard because it includes MAX-2-CSP as a special case. To see that it is QMA-hard requires relating it to the decision (promise) k-Local Hamiltonian problem, defined on n qubits. In this problem, $2^k \times 2^k$ Hermitian matrices H_S are given for each subset $S \subseteq [n]$ of size k, together with real numbers a and b with $b - a \geq 1/poly(n)$. The H_S are called k-local terms and may be viewed as quantum generalizations of classical boolean constraints on k variables. The promise on the input is that either some eigenvalue of the Hamiltonian $H := \sum_S H_S \otimes I_{[n]\setminus S}$ is less than a, or all eigenvalues are greater than b (the notation $H_S \otimes I_{[n]\setminus S}$ signifies that H_S acts on the k qubits of S and is tensored with identity on the other $n - k$ qubits). The QMA witness for the yes case is a quantum state that is an eigenstate with eigenvalue less that a, and a quantum algorithm can verify in polynomial time whether its eigenvalue is less than a or larger by $1/poly(n)$. The QMA-hard 2-Local Hamiltonian problem may be reduced to the optimization problem, MAX-2-LH by negating H (since MAX-2-LH is a maximization problem) and adding identity terms, if necessary, to ensure that each 2-local term is positive semidefinite. MAX-2-LH also generalizes the NP-hard MAX-2-CSP problem, which is illustrated in Section 2.2.

For MAX-2-LH, we assume an edge set E over the vertex set $[n]$ and a set of 4×4 positive semidefinite Hermitian matrices $\{H_{pq}\}_{(p,q)\in E}$ are given. The goal is to compute the maximum eigenvector of $H := \sum_{(p,q)\in E} H_{pq} \otimes I_{[n]\setminus\{p,q\}}$. The Hermitian matrix H acts on n qubits, and each term H_{pq} acts on the two qubits p, q and as the identity on the remaining $n - 2$ qubits. More precisely, $H_{pq} : \mathcal{H}_p \otimes \mathcal{H}_q \to \mathcal{H}_p \otimes \mathcal{H}_q$, where for all $p \in [n]$, $\mathcal{H}_p$ is the 2 dimensional complex Hilbert space, representing the qubit p, and $I_{[n]\setminus\{p,q\}}$ is the identity matrix on $\bigotimes_{i\in[n]\setminus\{p,q\}} \mathcal{H}_i$. The input matrices $\{H_{pq}\}_{(p,q)\in E}$ therefore implicitly describe the $2^n \times 2^n$ Hermitian matrix H, whose maximum eigenvector we wish to compute.

Related work

Other generalizations of classical problems to physically motivated Local Hamiltonian problems have been studied, but the exact relationship to well-studied classical problems such as MAX-2-SAT, MAX-CUT, and MAX-2-AND depends on which variant of the Local Hamiltonian problem is being considered. Gharibian and Parekh [14] study a maximization problem on 2-Local Hamiltonians for the Heisenberg model, which is a physically motivated generalization of MAX-CUT. These have the form $H = \sum_{(p,q)\in E} w_{pq} H_{pq}$ for $w_{pq} \geq 0$, where $H_{pq} = I - \alpha X_p X_q - \beta Y_p Y_q - \gamma Z_p Z_q$, for $\alpha, \beta, \gamma \in \{0, 1\}$, where X_p, Y_p, Z_p are the Pauli matrices on qubit p (e.g., X_p is a $2^n \times 2^n$ matrix formed by taking the 2×2 Pauli X matrix on qubit p tensored with identity on all the other $n - 1$ qubits). They get approximation ratios 0.498 (when $\alpha + \beta + \gamma = 3$), 0.649 (when $\alpha + \beta + \gamma = 2$), or 0.878 (when $\alpha + \beta + \gamma = 1$). Furthermore, they show that their ratios are almost tight in the product state space. In particular they give a simple instance on which a product state cannot provide an approximation ratio better than 0.5, for the $\alpha + \beta + \gamma = 3$ case. This case of their problem is a special case of MAX-2-LH, hence 0.5 is also an upper bound on the best attainable approximation ratio for MAX-2-LH using product states. Anshu, Gosset, and Morenz [2] have very recently demonstrated that it is possible for a classical algorithm to provide an approximation ratio better than 0.5 for this problem, by outputting descriptions of relatively simple entangled states.

Bravyi, Gosset, König, and Temme [8] consider traceless 2-local Hamiltonians. This generalizes the Maximum Quadratic Programming problem (MAX-QP) where the diagonal entries are zero [10, 3]. In addition to generalizing MAX-QP, it also captures a variety of physical quantum models. They give a randomized classical algorithm that outputs a product state with expected energy OPT $/O(\log n)$, where OPT is the maximum eigenvalue of the input Hamiltonian.

Our results

In this paper we achieve an approximation ratio of 0.328 for MAX-2-LH. The approximation algorithm for MAX-2-LH that picks a random assignment (i.e., the fully mixed quantum state) achieves ratio 0.25. Ours is the first example of an approximation algorithm for this problem that beats the trivial bound by a constant. It is also possible to achieve a ratio of $0.25 + 1/O(\log(n))$ by taking the input instance, shifting each term H_i so that it is traceless, and using the result in [8]. In MAX-2-LH each local term, acting on 2 qubits, is a rank 1 projector. In the special case when each local term is a rank 1 projector that is a product of two rank 1 projectors, one on each qubit, we get a better ratio of 0.40. This special case is detailed in Section 4. It is QMA-hard to find the maximum eigenvalue of this special type of Hamiltonian by Theorem 7 in [11].

In terms of techniques, we follow the framework that was first introduced by Goemans and Williamson. We first formulate a semidefinite program (SDP) whose optimal objective value provides an upper bound on the maximum energy of a given 2-local Hamiltonian. We can solve the SDP to arbitrary precision in polynomial time. Then we randomly round the solution, which resides in a larger space, down to the original solution space. Analyzing the randomized rounding is considerably more complicated than in the classical setting, because we need to round the solutions to a continuous 3-dimensional space, whereas the solution space is the boolean space for classical cases. We build upon a rounding procedure analyzed for generalizing the positive-semidefinite Grothendieck problem to a rank-constrained setting, by Briët, de Oliveira Filho, and Vallentin [9].

Even with this rounding procedure, obtaining a multiplicative bound that outperforms a random assignment for MAX-2-LH is a nontrivial task. In particular, our analysis takes the 1-local part of the input Hamiltonian explicitly into account. Ours is the first work of its kind to do so. Bravyi, Gosset, König, and Temme [8] showed that in the context of their problem, 1-local terms could be ignored without loss of generality, while Gharibian and Parekh [14] considered a problem without 1-local terms.

It is natural to consider SDP relaxations for our problem, because most approximation algorithms for classical MAX-2-CSP employ SDP rounding [15, 23, 22, 20]. Our SDP formulation is similar to that of [14, 8]; however, we must use additional constraints to handle the 1-local part. We also consider a different SDP formulation in order to get an improved approximation ratio in the special case where each local term is a product projector. The alternative formulation is described in Section 4. An advantage of the first SDP formulation is that the optimal value of the program provides an upper bound on OPT itself (the maximum eigenvalue of the Hamiltonian), whereas the optimal value of the alternative program gives an upper bound on OPT_{prod}, the objective value achieved by the best product state.

Open questions

There are several open questions. Is it possible to close the gap between 0.328 that we achieve and the 0.5 upper bound for product states? Is it possible to beat the uniformly random assignment when each term is a rank 3 projector, which is a quantum generalization of the classical Max 2-SAT problem? Is it possible to use more general states than product states, for example, as in the recent developments of Anshu, Gosset, and Morenz [2]? Does the approximation algorithm shed any light on the quantum PCP theorem?

2 Background

2.1 Approximating quantum problems

We first define the MAX-2-Local Hamiltonian problem.

▶ **Definition 1** (MAX-2LH). *An instance is given as a set of Hamiltonians $\{H_{pq} : (p,q) \in E\}$, for some edge set $E \subseteq [n] \times [n]$, where $H_{pq} \otimes I_{[n]\setminus\{p,q\}}$ is positive semidefinite and operates non-trivially on qubits p and q. Given such a list of Hamiltonians on 2 qubits, the goal of the problem is to find the largest eigenvalue of $H = \sum_{(p,q)\in E} H_{pq} \otimes I_{[n]\setminus\{p,q\}}$, which we denote as OPT.*

To simplify notation we will write $H = \sum_{pq} H_{pq}$, where terms H_{pq} for $(p,q) \notin E$ are the zero matrix (so have rank 0). Also, let OPT_{prod} denote the maximum energy achievable over the set of product states, i.e., $\text{OPT}_{\text{prod}} = \max_{|\phi_1\rangle\cdots|\phi_n\rangle}\langle\phi_1|\cdots\langle\phi_n|H|\phi_1\rangle\cdots|\phi_n\rangle$.

Since the 2-Local Hamiltonian problem can be reduced to the MAX-2-Local Hamiltonian problem, this problem is QMA-hard. So instead, we turn to approximating OPT with a multiplicative error. The goal of this paper is to beat the trivial approximation for the maximum eigenvalue of 2-local Hamiltonians presented in the following theorem.

▶ **Theorem 2.** *Given a 2-local Hamiltonian $H = \sum_{pq} H_{pq} \otimes I_{[n] \setminus \{p,q\}}$ with local terms that are rank r projectors, H_{pq} ($r \in \{1, 2, 3\}$), if the maximum eigenvalue (energy) of H is OPT, then the uniformly random product state achieves energy at least $r/4 \cdot$ OPT .*

Proof. Consider the contribution of the local term H_{pq} to the energy. Since we are assigning the uniformly random product state, the qubit p, q is assigned

$$\rho_{pq} := \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} \otimes \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} = I/4$$

jointly. The energy contribution of H_{pq} is then $\mathrm{Tr}(H_{pq}\rho_{pq}) = \mathrm{Tr}(H_{pq})/4 = r/4$, because H_{pq} is a rank r projector. Therefore if ρ_n is the uniformly random product state on n qubits, the total energy is $\mathrm{Tr}(H\rho_n) = rm/4$ where m is the number of local terms. We know that $m \geq$ OPT. So $\mathrm{Tr}(H\rho_n) \geq r/4 \cdot$ OPT . ◀

Harrow and Montanaro [16] consider approximation of the minimum and maximum eigenvalue of local Hamiltonians where each qubit can appear in at most D local terms. They give an algorithm with approximation ratio $c + \Omega(1/\sqrt{D})$, where c is the ratio achieved by uniformly random assignment. More related to the problem we consider, Gharibian and Kempe [12] consider approximating the maximum eigenvalue of a k-local Hamiltonian with positive semidefinite local terms.

▶ **Theorem 3** ([12]). *For a k-local Hamiltonian H on n, d-dimensional qudits with positive semidefinite local terms and maximum eigenvalue (energy) OPT, there exists a product state assignment with energy of OPT $/d^{k-1}$.*

We are interested in the case of $(d, k) = (2, 2)$ in this paper. In this case, the above theorem implies there exists a product state with energy OPT $/2$ and this means $\mathrm{OPT}_{\mathrm{prod}} \geq \mathrm{OPT}/2$; however, finding such a product state is NP-hard in general. They also give an approximation algorithm achieving a constant approximation ratio for dense instances.

▶ **Theorem 4** ([12]). *For any k-local Hamiltonian H on n qubits, there exists a deterministic poly-time algorithm outputting a product state achieving $\langle \psi | H | \psi \rangle > \mathrm{OPT}_{\mathrm{prod}} - \epsilon n^k$. $\mathrm{OPT}_{\mathrm{prod}}$ is the highest energy that can be achieved by a product state.*

In the case of $k = 2$, this implies a product state with energy $\mathrm{OPT}_{\mathrm{prod}} - \epsilon n^2$ can be efficiently found. If the constraint graph is dense, combining the two gives a $(1/2 - \epsilon')$-approximation algorithm. With a dense constraint graph, we know that $\mathrm{OPT}_{\mathrm{prod}} = \Theta(n^2)$ (by assigning a random product state). So $\mathrm{OPT}_{\mathrm{prod}} - \epsilon n^2 = \mathrm{OPT}_{\mathrm{prod}} - c\epsilon \, \mathrm{OPT}_{\mathrm{prod}} = (1 - c\epsilon) \, \mathrm{OPT}_{\mathrm{prod}}$, for some constant c. By Theorem 3, we know that this value is at least $(1/2 - c\epsilon/2) \, \mathrm{OPT}$.

Brandão and Harrow's result [7] also says that product states do better on regular constraint graphs as the degree increases.

▶ **Theorem 5** ([7]). *Suppose a 2-local Hamiltonian H on qudits has non-trivial terms on a D-regular graph. For all edges (p, q) on the graph, suppose the local term H_{pq} satisfies $\|H_{pq}\| \leq 1$. Then there exists a product state $|\psi\rangle$ such that $\langle \psi | H | \psi \rangle \geq \mathrm{OPT} - 12 \frac{nD}{2} (\frac{d^2 \ln d}{D})^{1/3}$, where OPT is the largest eigenvalue of H.*

The above theorems imply that there exists a product state that achieves approximation ratio of $1 - 12 (\frac{d^2 \ln d}{D})^{1/3}$ when the constraint graph is D-regular.

More recent and closely related work is that of Gharibian and Parekh [14] and Bravyi, Gosset, König, and Temme [8]. These works and our work all aim to optimize 2-local Hamiltonians in the product state space, and they all use SDP to do so. The work [14] considers a specialization of Max-2-LH; however, a key difference is that their main target Hamiltonian is more restricted and physically motivated, a maximization version of the quantum Heisenberg model. The special case they consider is qualitatively simpler in some sense, as their Hamiltonian does not have any 1-local terms, which present an additional complication in our work. They also consider additional Hamiltonians that do not have PSD local terms, which are not special cases of MAX-2-LH. Another difference is in the SDP relaxations employed. We must use additional constraints yielding a strengthened SDP relaxation to obtain our results. They get the following results.

▶ **Theorem 6** ([14]). *Consider a local Hamiltonian $H = \sum_{(p,q) \in E} w_{pq} H_{pq}$ for $w_{pq} \geq 0$, where $H_{pq} = I - \alpha X_p X_q - \beta Y_p Y_q - \gamma Z_p Z_q$, for $\alpha, \beta, \gamma \in \{0, 1\}$. There exists a randomized classical approximation algorithm with approximation ratio 0.498 (when $\alpha + \beta + \gamma = 3$), 0.649 (when $\alpha + \beta + \gamma = 2$), or 0.878 (when $\alpha + \beta + \gamma = 1$).*

The $\alpha + \beta + \gamma = 3$ case of the above problem is when H_{pq} is a rank 1 projector onto the Bell state $|\Psi^-\rangle = |01\rangle - |10\rangle$, on qubits p and q. Thus this case is an instance of MAX-2-LH.

The work [8] uses similar techniques for a slightly different problem. They consider the problem of approximating the maximum eigenvalue of traceless 2-local Hamiltonians on n qubits. They give a randomized classical approximation algorithm that outputs a product state with expected energy OPT $/O(\log n)$ where OPT is the maximum eigenvalue of the input Hamiltonian. They use the same SDP relaxation as [14] for the maximum eigenvalue, but they use a different rounding technique from [14] or this work; as with [14], being able to ignore 1-local terms simplifies their algorithm and analysis relative to this work.

Another related work is by Bansal, Bravyi, and Terhal, where they prove that a PTAS (an algorithm that runs in polynomial time in problem size and $1/\epsilon$ where ϵ is an arbitrarily small approximation ratio) exists [5] for Quantum Ising Spin Glass defined over a planar interaction graph with bounded degree, where the goal is to find the minimum eigenvalue of Hamiltonians of form $H = \sum_{(u,v) \in E} c_{uv} L_{uv} + \sum_u L_u$, where L_{uv} is quadratic in Pauli matrices and L_u is linear.

There are limited results on the hardness of approximation of quantum problems. Gharibian and Kempe introduce a quantum version of Σ_2^p called cq-Σ_2 [13]. They prove that QSSC and QIRR, defined in the paper, are cq-Σ_2-hard to approximate to certain ratios. Moreover, they also show that it is QCMA-hard to approximate Quantum Monotone Minimum Satisfying Assignment, defined in their paper, to approximation ratio $N^{1-\epsilon}$ for all $\epsilon > 0$, where N is the size of instance.

2.2   Reducing Max-2-CSP to Max-2-LH

MAX-2-CSP is reduced to MAX-2-Local Hamiltonian as follows. Suppose we are given a MAX-2-CSP instance on n boolean variables $x_1, x_2, \ldots, x_n \in \{0, 1\}$, a set of edges E between the x_i's, and functions $f_{ij} : \{0, 1\}^2 \rightarrow \{0, 1\}$ on (x_i, x_j) for $(i, j) \in E$. The question is to compute the quantity $\text{OPT}_{\text{CSP}} = \max_{x_1, \ldots, x_n} \sum_{(i,j) \in E} f_{ij}(x_i, x_j)$. We can reduce this instance to a MAX-2-LH instance on n qubits $q_1, q_2, \ldots, q_n$ with projectors $P_{ij} := \sum_{(x_i, x_j) \in \text{Supp}(f_{ij})} |x_i x_j\rangle \langle x_i x_j|$ on qubit i, j for $(i, j) \in E$, where $\text{Supp}(f_{ij}) = \{(x_i, x_j) \mid f_{ij}(x_i, x_j) = 1\}$. To see that this is a correct reduction, consider an optimizer $|\phi\rangle = \sum_{x \in \{0,1\}^n} c_x |x\rangle$ to the MAX-2-LH instance. The energy of $|\phi\rangle$ is $\langle \phi | \sum_{(i,j) \in E} P_{ij} | \phi \rangle = \sum_{x \in \{0,1\}^n} |c_x|^2 \langle x | \sum_{(i,j) \in E} P_{ij} | x \rangle$. Measuring $|\phi\rangle$ in the computational basis and using it as

an assignment for the original instance, we satisfy $\sum_{x \in \{0,1\}^n} |c_x|^2 \sum_{(i,j) \in E} f_{ij}(x_i, x_j)$ constraints in expectation, which coincides with the energy of $|\phi\rangle$. So MAX-2-Local Hamiltonian on qubits is NP-hard. Then MAX-k-Local Hamiltonian with $k > 2$ on qudits is also NP-hard because MAX-2-LH on qubits is a special case of MAX-k-LH on qudits, when each projector acts non-trivially on 2 locations within an embedded 2 dimensional space.

2.3 Approximating 2-CSPs using SDP

SDP has been a major tool for approximating 2-CSP problems since Goemans and Williamson used semidefinite programming to obtain a 0.878-approximation for MAX-CUT and MAX-2-SAT, as well as a 0.796-approximation for a MAX-DICUT [15].

There had been gradual improvements in the approximation ratio [23, 22], and finally [20] obtained the best approximation ratios to date, 0.94016 for MAX-2-SAT and 0.87401 for MAX-DICUT. All of the papers mentioned above employ SDP rounding techniques.

On the other hand, [17] showed that the approximation ratio 0.878 for MAX-CUT is tight and the approximation ratio for MAX-DICUT is upper bounded by 0.878, assuming that the Unique Game Conjecture (UGC) is true. Austrin proved that the approximation ratio 0.94016 is tight for MAX-2-SAT and the approximation ratio for MAX-2-AND is upper bounded by 0.87435, assuming the UGC [4]. More details about CSP approximation can be found in a recent survey by Makarychev and Makarychev [21].

2.4 Lemmas on randomized rounding

We use the following lemmas without proof. The inequalities are special cases of more general "Grothendieck inequalities." Grothendieck inequalities have begun playing an important role in theoretical computer science with a variety of applications. For more details see a survey by Khot and Naor [18].

The first two lemmas below are given by Goemans and Williamson with which they prove approximation ratios for their MAX-CUT and MAX-2SAT algorithms respectively, namely, Theorem 3.3 and Lemma 7.3.2 in [15].

▶ **Lemma 7** ([15]). *Let $u, v \in S^N$ be unit vectors in $\mathbb{R}^{N+1}$ for $N \geq 2$, and let $x = \operatorname{sgn}(u \cdot r), y = \operatorname{sgn}(v \cdot r)$ for a uniformly random vector $r \in S^N$. Then*

$$\mathbb{E}_r[1 \pm xy] \geq \alpha_1(1 \pm u \cdot v),$$

where $\alpha_1 = \frac{2}{\pi} \min_{0 < \theta < \pi} \frac{\theta}{1 - \cos \theta} = 0.878\ldots$.

▶ **Lemma 8** ([15]). *Let $u, v, w \in S^N$ be unit vectors in $\mathbb{R}^{N+1}$ for $N \geq 2$, and let $x = \operatorname{sgn}(u \cdot r), y = \operatorname{sgn}(v \cdot r), z = \operatorname{sgn}(w \cdot r)$, for a uniformly random vector $r \in S^N$. Then*

$$\mathbb{E}_r[1 \pm xy \pm xz + yz] \geq \alpha_2(1 \pm u \cdot v \pm u \cdot w + v \cdot w),$$

where $\alpha_2 = \min_{0 < \theta < \arccos(-1/3)} \frac{2}{\pi} \frac{2\pi - 3\theta}{1 + 3 \cos \theta} = 0.796\ldots$.

We will also use the following lemma, obtained by Briët, de Oliveira Filho, and Vallentin [9] in considering a rank-constrained version of the Grothendieck problem, to bound randomized rounding for positive semidefinite matrices.

▶ **Lemma 9** ([9]). *Let A be a $m \times m$ real-valued positive semidefinite matrix and $u_1, \ldots, u_m$ be unit vectors in S^N for an integer $N \geq m$. For all $1 \leq i \leq m$, let $x_i = \text{sgn}(r \cdot u_i)$ for a uniformly random vector $r \in S^N$. Then*

$$\mathbb{E}\left[\sum_{1 \leq i,j \leq m} A_{ij} x_i x_j\right] \geq \frac{m}{\pi} \left(\frac{\Gamma(m/2)}{\Gamma((m+1)/2)}\right)^2 \sum_{1 \leq i,j \leq m} A_{ij} u_i \cdot u_j.$$

The coefficient $\frac{m}{\pi}\left(\frac{\Gamma(m/2)}{\Gamma((m+1)/2)}\right)^2$ is asymptotically $2/\pi + \Theta(1/m)$. We will use the lemma for $m = 6$, which has associated constant $\alpha_7 := \frac{6}{\pi}\left(\frac{\Gamma(3)}{\Gamma(3.5)}\right)^2 = \frac{6}{\pi}\left(\frac{2}{15\sqrt{\pi}/8}\right)^2 = 0.691 \cdots$.

Since Lemma 9 is not explicitly stated in the form of a theorem in [9], we give a brief description about how to piece the statements in [9] together. This lemma follows from the analysis in [9], where they give an approximation algorithm for the Grothendieck problem. In particular, Lemma 1 and the argument surrounding Equation (3) are used as follows. Using their notation, let $E_1(t) = \frac{2}{\pi} \arcsin t$ and let $\widetilde{E}_1(t) = \frac{2}{\pi} \arcsin t - \frac{2}{\pi}\frac{t}{\gamma(m)}$. It turns out that the functions only depend on the inner product between two vectors, so $E_1(u_i, u_j)$ means $E_1(t)$, where $t = u_i \cdot u_j$. Lemma 1 states that $\widetilde{E}_1(t)$ is of positive type for S^{m-1}. This means that for any vectors $u_1, \ldots, u_m \in S^{m-1}$, the matrix $\left(\widetilde{E}_1(u_i, u_j)\right)_{1 \leq i,j \leq m}$ is positive semidefinite. Since A is also positive semidefinite, it holds that $\sum_{i,j=1}^m A_{ij}\left(\frac{2}{\pi}\arcsin u_i \cdot u_j - \frac{2}{\pi}\frac{u_i \cdot u_j}{\gamma(m)}\right) = \sum_{i,j=1}^m A_{ij}\widetilde{E}_1(u_i, u_j) \geq 0$. Therefore $\sum_{ij} A_{ij}\frac{2}{\pi}\arcsin u_i \cdot u_j \geq \sum_{ij} A_{ij}\frac{2}{\pi}\frac{u_i \cdot u_j}{\gamma(m)}$. Finally, use the fact that $\mathbb{E}\left[\text{sgn}(r \cdot u_i)\text{sgn}(r \cdot u_j)\right] = \frac{2}{\pi}\arcsin u_i \cdot u_j$, and the fact that $\frac{2}{\pi}\frac{1}{\gamma(m)}$ is equal to the factor given in the lemma above, as in Theorem 2 in [9].

2.5 Notation

▶ **Definition 10** (Pauli matrices). *We denote the Pauli matrices on a qubit as $W_0 := I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, $W_1 := X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $W_2 := Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, and $W_3 := Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. On n qubits, we write $W_{pi} := W_i \otimes I_{[n]\setminus\{p\}}$, where W_i is on the qubit p, and $I_{[n]\setminus\{p\}}$ is the identity on the rest of the qubits.*

3 The algorithm and analysis

The setup

A 2-local Hamiltonian is given as a set of Hamiltonians $\{H_{pq} : (p,q) \in E\}$, for some edge set $E \subseteq [n] \times [n]$, where H_{pq} operates on qubits p and q. This means H_{pq} is a 4×4 matrix on the Hilbert space $\mathcal{H}_p \otimes \mathcal{H}_q$ that represents the joint space of qubits p, q. Given such a list of Hamiltonians on 2 qubits, the goal is to approximate the maximum eigenvalue of $H := \sum_{(p,q) \in E} H_{pq} \otimes I_{[n]\setminus\{p,q\}}$. In this paper we assume each term H_{pq} is a PSD matrix. We will decompose H_{pq} using its eigenvectors $H_{pq} = \sum_{t=1}^4 w_{pq,t}|\gamma_{pq,t}\rangle\langle\gamma_{pq,t}|$, where $w_{pq,i} \geq 0$ for all p, q, t.

Let OPT denote the maximum eigenvalue of H over quantum states. Stated in terms of energy, $\text{OPT} = \max_{|\phi\rangle}\langle\phi|H|\phi\rangle$. We seek to produce an approximately optimal state; however, since our approximation algorithms are classical polynomial-time algorithms, we output an efficient representation of such a state. Our approach is to formulate an SDP that upper-bounds the maximum energy of the given Hamiltonian. We then randomly round the solution vectors of the SDP to real numbers to get a product quantum state, admitting a polynomial-size representation, with a relatively high energy.

A semidefinite program relaxation

We start with an SDP relaxation that gives an upper bound on the optimal energy. By "relaxation", we mean an SDP for which each quantum state generates a feasible solution, with objective function value matching its energy. This way, we know that the value of the SDP is at least the highest energy possible by a physical state.

For each pair of qubits $(p, q) \in E$ (E consists of ordered pairs pq with $p < q$), we have a local Hamiltonian $H_{pq} = \sum_{t=1}^{4} w_{pq,t} |\gamma_{pq,t}\rangle \langle \gamma_{pq,t}|$. We denote the Pauli decomposition of the local terms $C_{pqij} = \text{Tr}(H_{pq}(W_i \otimes W_j))/4$. Note that the matrix $C_{pq} = (C_{pqij})_{ij}$ is real for all $(p, q) \in E$, since tensor products of Pauli matrices form a real-coefficient basis for the Hermitian matrices. Consider the SDP:

$$\text{Maximize} \quad \sum_{(p,q) \in E} \sum_{i,j=0}^{3} C_{pqij} v_{pi} \cdot v_{qj} \qquad (S1)$$

subject to:
$$||v_0|| = 1$$
$$||v_{pi}|| = 1, \ \forall p, i$$
$$v_0 \cdot v_{p0} = 1, \ \forall p$$
$$v_{pi} \cdot v_{pj} = 0, \ \forall p, \ i, j > 0 : i \neq j$$
$$v_0, v_{pi} \in \mathbb{R}^N, \ \forall p, i$$
$$\sum_{i,j=0}^{3} C_{pqij} v_{pi} \cdot v_{qj} \leq \sum_{t=1}^{4} w_{pq,t}, \ \forall (p, q) \in E.$$

and N can be taken to be the total number of vectors, v_0 and the v_{pi} in the program, which is $4n+1$. The motivation for this relaxation is that, for any quantum state $|\phi\rangle$, we may construct additional complex unit vectors by applying tensor products of Pauli matrices to $|\phi\rangle$. In particular, setting $v_0 := |\phi\rangle$, and $v_{pi} := W_{pi}|\phi\rangle$, for all p and i, yields a solution that is "almost" feasible for the above SDP. The first three constraints are satisfied, noting that $W_{p0} = W_0 = I$ for all p. For the fourth constraint, we have that $v_{pi} \cdot v_{pj} = \langle \phi | W_{pi} W_{pj} | \phi \rangle = -\langle \phi | W_{pj} W_{pi} | \phi \rangle$, since distinct nontrivial Pauli matrices anticommute. This implies that $\text{Re}(v_{pi} \cdot v_{pj}) = 0$. Indeed, we obtain a true solution to the SDP by modifying the vectors so that the imaginary part of their inner products is discarded. This is formalized in the claim below.

▶ **Remark 11.** The complex vectors v_{pi}, as constructed above from $|\phi\rangle$, suggest a complex SDP relaxation; however, the real version, $(S1)$ is simpler and equivalent in terms of optimal objective value. The relationship $v_{pi} \cdot v_{qj} = \langle \phi | W_{pi} W_{qj} | \phi \rangle$ connects 2-moments of the state $|\phi\rangle$ to SDP relaxations. Considering higher-order moments leads to larger but stronger SDP relaxations, and considering n-moments leads to an exact SDP formulation of exponential size. Restricting the moments considered to products over only $W_{p3} = Z_p$ for different p yields an SDP hierarchy equivalent to the celebrated classical Lasserre hierarchy.

▷ **Claim 12.** This SDP is a relaxation, i.e., there is a mapping from pure quantum states to vectors such that objective value is the energy of the state.

Proof. Let $|\phi\rangle$ be a quantum state, and let $v_0 := (\text{Re}(|\phi\rangle), \text{Im}(|\phi\rangle))$, and $v_{pi} := (\text{Re}(W_{pi}|\phi\rangle), \text{Im}(W_{pi}|\phi\rangle))$, for $p \in [n], i \in \{0, 1, 2, 3\}$. Here $\text{Re}(u) := (\text{Re}(u_i))_{i \in [d]}$, $\text{Im}(u) := (\text{Im}(u_i))_{i \in [d]}$ for a d-dimensional complex vector u.

To check the SDP constraints, first note the v_0 has norm 1, and $v_0 = v_{p0}$ for all p. Next, each vector v_{pi} has norm 1, and two different vectors on qubit p are orthogonal:

$$v_{pi} \cdot v_{pj} = (\mathrm{Re}(W_{pi}|\phi\rangle), \mathrm{Im}(W_{pi}|\phi\rangle)) \cdot (\mathrm{Re}(W_{pj}|\phi\rangle), \mathrm{Im}(W_{pj}|\phi\rangle))$$
$$= \mathrm{Re}(\langle\phi|W_{pi}W_{pj}|\phi\rangle) = \delta_{ij},$$

for all $i, j \in \{1, 2, 3\}$, $p \in [n]$. This follows from the Pauli matrices anticommutation relations $W_i W_j + W_j W_i = 2\delta_{ij} I$.

Next, we consider two vectors on different qubits. Let $\rho := |\phi\rangle\langle\phi|$. Then

$$v_{pi} \cdot v_{qj} = (\mathrm{Re}(W_{pi}|\phi\rangle), \mathrm{Im}(W_{pi}|\phi\rangle)) \cdot (\mathrm{Re}(W_{qj}|\phi\rangle), \mathrm{Im}(W_{qj}|\phi\rangle))$$
$$= \mathrm{Re}(\langle\phi|W_{pi}W_{qj}|\phi\rangle) = \mathrm{Re}(\mathrm{Tr}(W_{pi}W_{qj}\rho)),$$

for all $p \neq q$, and $i, j \in \{0, 1, 2, 3\}$. This follows from the fact that two Pauli matrices commute when they act on different qubits.

The SDP objective is therefore equal to the enegy of the state:

$$\sum_{(p,q)\in E} \sum_{i,j=0}^{3} C_{pqij} v_{pi} \cdot v_{qj} = \sum_{(p,q)\in E} \sum_{i,j=0}^{3} \frac{1}{4} \mathrm{Tr}(H_{pq}(W_i \otimes W_j)) \mathrm{Re}(\mathrm{Tr}(W_{pi}W_{qj}\rho))$$

$$= \mathrm{Re}\left(\sum_{(p,q)\in E} \sum_{i,j=0}^{3} \frac{1}{4} \mathrm{Tr}(H_{pq}(W_i \otimes W_j)) \mathrm{Tr}((W_i \otimes W_j)\rho_{pq}) \right)$$

$$= \sum_{(p,q)\in E} \mathrm{Tr}(H_{pq}\rho_{pq}) = \mathrm{Tr}(H\rho),$$

where ρ_{pq} is the reduced density matrix of ρ onto qubits $\{p, q\}$. The second last equality is because the Pauli matrices form an orthogonal basis. The last constraint of $(S1)$ asserts that the energy contribution from the site (p, q) should not exceed the sum of the eigenvalues of (p, q). The seemingly unnecessary last constraint will be useful in the analysis. ◁

We can solve the SDP to arbitrary multiplicative quality $1 - \epsilon$ using existing SDP solvers (for example, [1]), in time polynomial to the size of the program and $\log(1/\epsilon)$. This gives us a solution of quality $\mathrm{OPT}_{\mathrm{SDP}}(1 - \epsilon)$, where $\mathrm{OPT}_{\mathrm{SDP}}$ is the optimal value of the SDP. We will ignore $(1 - \epsilon)$ factor because it can be absorbed into our approximation ratio.

The algorithm and analysis

■ **Algorithm 1** MAX-2-Local Hamiltonian with PSD local terms.

1: Input: $\{H_{pq} : (p, q) \in E\}, E \subseteq [n] \times [n]$.
2: Calculate $(C_{pqij} := \mathrm{Tr}(H_{pq}(W_i \otimes W_j))/4)_{pqij}$.
3: Solve the SDP $(S1)$, and get $(v_0, (v_{pi})_{pi})$.
4: Pick a uniformly random unit vector $r \in \mathbb{R}^N$ (use $N := 4n + 1$).
5: Set $(x_0, (x_{pi})_{pi}) := (\mathrm{sgn}(v_0 \cdot r), (\mathrm{sgn}(v_{pi} \cdot r))_{pi})$.
6: If $\sum_{(p,q)\in E} \left(\sum_{i=1}^{3} C_{pqi0} x_{pi} x_0 + \sum_{j=1}^{3} C_{pq0j} x_0 x_{qj} \right) < 0$, set $\widetilde{x}_{pi} := -x_{pi}x_0$ for all p and $1 \leq i \leq 3$. Otherwise set $\widetilde{x}_{pi} := x_{pi}x_0$ for all p, $1 \leq i \leq 3$.
7: Output state $\rho := \bigotimes_{p=1}^{n} \rho_p$, where $\rho_p := \frac{1}{2}I + \frac{1}{2}\sum_{i=1}^{3} \frac{1}{\sqrt{3}} \widetilde{x}_{pi} W_i$

Algorithm 1 describes our rounding procedure. Let $C_{pq} \in \mathbb{R}^{4 \times 4}$ refer to the matrix $(C_{pqij})_{ij}$, let $c_{pq} := C_{pq00} = \frac{1}{4} \sum_{t=1}^{4} w_{pq,t}$, let $a_{pq} \in \mathbb{R}^3$ refer to the vector $(C_{pqi0})_{i:i>0}$, and $b_{pq} := (C_{pq0j})_{j:j>0}$ is defined analogously. Finally $\bar{C}_{pq} \in \mathbb{R}^{3 \times 3}$ is $(C_{pqij})_{ij:i,j>0}$. So we have

$$
C_{pq} = \left[\begin{array}{cc} c_{pq} & b_{pq}^T \\ \\ a_{pq} & \bar{C}_{pq} \end{array} \right].
$$

To apply the bound from [9], we need a symmetrized and PSD version of C_{pq}, so define

$$
C_{pq}^{+} = \left[\begin{array}{ccc} c_{pq} & a_{pq}^T & b_{pq}^T \\ \\ a_{pq} & c_{pq}I & \bar{C}_{pq} \\ \\ b_{pq} & \bar{C}_{pq}^T & c_{pq}IW_{pqi} \end{array} \right] \in \mathbb{R}^{7 \times 7}.
$$

The matrix C_{pq}^{+} is clearly symmetic. To see that $C_{pq}^{+} \succeq 0$, use the fact that $H_{pq} = \sum_{t=1}^{4} w_{pq,t} |\gamma_{pq,t}\rangle\langle\gamma_{pq,t}|$ for non-negative $w_{pq,t}$'s, and get

$$
4W_{pqj}C_{pqij}^{+} = \sum_{t=1}^{4} w_{pq,t} \mathrm{Re}\left(\mathrm{Tr}\left[|\gamma_{pq,t}\rangle\langle\gamma_{pq,t}| W_{pqi} W_{pqj} \right] \right)
$$

$$
= \sum_{t=1}^{4} w_{pq,t} (\mathrm{Re}(W_{pqi}|\gamma_{pq,t}\rangle), \mathrm{Im}(W_{pqi}|\gamma_{pq,t}\rangle)) \cdot (\mathrm{Re}(W_{pqj}|\gamma_{pq,t}\rangle), \mathrm{Im}(W_{pqj}|\gamma_{pq,t}\rangle)),
$$

where $(W_{pqi})_{0 \leq i \leq 6} := (I, W_1 \otimes I, W_2 \otimes I, W_3 \otimes I, I \otimes W_1, I \otimes W_2, I \otimes W_3)$. Since C_{pq}^{+} is therefore a non-negative-weighted sum of Gram matrices, it is PSD. Now we state the main theorem.

▶ **Theorem 13.** *Algorithm 1 runs in polynomial time and outputs a product state with expected energy at least* $0.328\,\mathrm{OPT}$, *where* OPT *is the maximum energy of the 2-local Hamiltonian* $H = \sum_{(p,q) \in E} H_{pq} \otimes I_{[n] \setminus \{p,q\}}$ *where* H_{pq} *is PSD for all* $(p,q) \in E$.

Proof. Algorithm 1 outputs a product state, whose reduced part on p and q is

$$
\rho_p \otimes \rho_q = \frac{1}{4} \left(I + \frac{\widetilde{x}_{p1}}{\sqrt{3}} W_1 + \frac{\widetilde{x}_{p2}}{\sqrt{3}} W_2 + \frac{\widetilde{x}_{p3}}{\sqrt{3}} W_3 \right) \otimes \left(I + \frac{\widetilde{x}_{q1}}{\sqrt{3}} W_1 + \frac{\widetilde{x}_{q2}}{\sqrt{3}} W_2 + \frac{\widetilde{x}_{q3}}{\sqrt{3}} W_3 \right).
$$

Thus the total energy of the approximate solution is $\mathbb{E}_r \left[\sum_{(p,q) \in E} \mathrm{Tr}(H_{pq}(\rho_p \otimes \rho_q)) \right]$, which is equal to

$$
\mathbb{E}_r \sum_{(p,q) \in E} \left[c_{pq} + \frac{\sum_{i=1}^{3} a_{pqi} \widetilde{x}_{pi} + \sum_{j=1}^{3} b_{pqj} \widetilde{x}_{qj}}{\sqrt{3}} + \frac{\sum_{i,j=1}^{3} \bar{C}_{pqij} \widetilde{x}_{pi} \widetilde{x}_{qj}}{3} \right]. \tag{1}
$$

Meanwhile, the SDP objective value is

$$
\sum_{(p,q) \in E} \left[c_{pq} + \sum_{i=1}^{3} a_{pqi} v_{pi} \cdot v_0 + \sum_{j=1}^{3} b_{pqj} v_0 \cdot v_{qj} + \sum_{i,j=0}^{3} \bar{C}_{pqij} v_{pi} \cdot v_{qj} \right]. \tag{2}
$$

Fix an edge $(p, q) \in E$, and let $v_{pq} := (v_0, v_{p1}, v_{p2}, v_{p3}, v_{q1}, v_{q2}, v_{q3})$. By applying Lemma 9 to C_{pq}^+ and v_{pq}, we get

$$
\mathbb{E}_r \left[7c_{pq} + 2\sum_{i=1}^{3} a_{pqi} x_{pi} x_0 + 2\sum_{j=1}^{3} b_{pqj} x_0 x_{qj} + 2\sum_{i,j=1}^{3} \bar{C}_{pqij} x_{pi} x_{qj} \right] \geq
$$
$$
\alpha_7 \left(7c_{pq} + 2\sum_{i=1}^{3} a_{pqi} v_{pi} \cdot v_0 + 2\sum_{j=1}^{3} b_{pqj} v_0 \cdot v_{qj} + 2\sum_{i,j=1}^{3} \bar{C}_{pqij} v_{pi} \cdot v_{qj} \right). \tag{3}
$$

The coefficients 7 and 2 above come from how many times each parts are in C_{pq}^+. We would like to compare the energy of our solution (1) against the SDP objective (2) using the inequality (3). For the series of inequalities that will appear below, we define some short-hand:

$$
L_x := \sum_{(p,q) \in E} \left[\sum_{i=1}^{3} a_{pqi} x_{pi} x_0 + \sum_{j=1}^{3} b_{pqj} x_0 x_{qj} \right],
$$
$$
Q_x := \sum_{(p,q) \in E} \left[\sum_{i,j=1}^{3} \bar{C}_{pqij} x_{pi} x_{qj} \right],
$$
$$
L_v := \sum_{(p,q) \in E} \left[\sum_{i=1}^{3} a_{pqi} v_{pi} \cdot v_0 + \sum_{j=1}^{3} b_{pqj} v_0 \cdot v_{qj} \right],
$$
$$
Q_v := \sum_{(p,q) \in E} \left[\sum_{i,j=1}^{3} \bar{C}_{pqij} v_{pi} \cdot v_{qj} \right],
$$
$$
\widetilde{L}_x := \sum_{(p,q) \in E} \left[\sum_{i=1}^{3} a_{pqi} \widetilde{x}_{pi} + \sum_{j=1}^{3} b_{pqj} \widetilde{x}_{qj} \right],
$$
$$
\widetilde{Q}_x := \sum_{(p,q) \in E} \left[\sum_{i,j=1}^{3} \bar{C}_{pqij} \widetilde{x}_{pi} \widetilde{x}_{qj} \right],
$$
$$
c := \sum_{(p,q) \in E} c_{pq}.
$$

After summing the inequality (3) over the edges and moving the terms, we get

$$
\mathbb{E}_r \left[c + \frac{L_x + Q_x}{3} \right] \geq \frac{\alpha_7 (\frac{7}{2} c + L_v + Q_v) - \frac{1}{2} c}{3}. \tag{4}
$$

Because $\widetilde{L}_x \geq 0$ (Step 6 of Algorithm 1), and $\widetilde{L}_x + \widetilde{Q}_x \geq L_x + Q_x$ for every r, we can bound the energy of the approximate solution:

$$
\mathbb{E}_r \left[c + \frac{\widetilde{L}_x}{\sqrt{3}} + \frac{\widetilde{Q}_x}{3} \right] \geq \mathbb{E}_r \left[c + \frac{\widetilde{L}_x + \widetilde{Q}_x}{3} \right] \geq \mathbb{E}_r \left[c + \frac{L_x + Q_x}{3} \right] \geq \frac{\alpha_7 (\frac{7}{2} c + L_v + Q_v) - \frac{1}{2} c}{3},
$$

where the last inequality follows from (4). We can now bound the approximation factor,

$$
\frac{\mathbb{E}_r \left[c + \frac{\widetilde{L}_x}{\sqrt{3}} + \frac{\widetilde{Q}_x}{3} \right]}{c + L_v + Q_v} \geq \frac{\alpha_7 (\frac{7}{2} c + L_v + Q_v) - \frac{1}{2} c}{3(c + L_v + Q_v)} = \frac{\alpha_7 (\frac{7}{2} c + S) - \frac{1}{2} c}{3(c + S)},
$$

letting $S := L_v + Q_v$ for convenience. The value of the SDP $(S1)$ is $c + S$ and the energy of the maximally mixed state is $c = \sum_{(p,q) \in E} c_{pq}$. The SDP value $c + S$ should at least be the energy of the maximally mixed state, so $c + S \geq c$. This implies that $S \geq 0$. By summing the last constraint of $(S1)$ over the edges, we get $c + S \leq \sum_{(p,q) \in E, 1 \leq t \leq 4} w_{pq,t} = 4c$. Therefore, the approximation ratio is at least

$$\min_{S \in [0,3c]} \frac{\alpha_7(\frac{7}{2}c + S) - \frac{1}{2}c}{3(c+S)} \geq \frac{\alpha_7(\frac{13}{8}) - \frac{1}{8}}{3} = 0.328 \ldots .$$

The min occurs at $S = 3c$ since $\frac{\alpha_7(\frac{7}{2}c+S) - \frac{1}{2}c}{3(c+S)} = \frac{\alpha_7(c+S) + \alpha_7\frac{5}{2}c - \frac{1}{2}c}{3(c+S)} = \frac{\alpha_7}{3} + \frac{5\alpha_7 - 1}{6(c+S)}c$ is decreasing for $c + S \geq 0$. ◀

4 Improved approximation in for tensor product projectors using a different SDP and rounding

In this section we show that a better approximation factor is possible when each local term is a rank 1 projector that is a product of 2 rank 1 projectors on a qubit. Namely, $H_{pq} = H_{pq,p} \otimes H_{pq,q}$, and $H_{pq,p}, H_{pq,q}$ are rank 1 projectors on qubit p, q respectively for all $(p,q) \in E$. The algorithm is similar to the previous one in that Goemans-Williamson approach is used. This time, however, we formulate the SDP and round the vector solution in a different way: we first formulate a quadratic programming (QP) in the real space that has the highest energy by a product state as the objective value, and relax the QP to an SDP. The previous rounding reduced the norms of the solution vectors by $1/\sqrt{3}$, but here we will keep the norms. The first observation we make is that the value of the following quadratic program (Q) is the maximum energy achieved by a product state.

Quadratic program for MAX-2-Local Hamiltonian over product states:

$$\text{Maximize } 4 \sum_{pq} \sum_{i,j=0}^{3} C_{pqij} x_{pi} x_{qj} \qquad (Q)$$

subject to:

$$x_{p0} = \frac{1}{2}, \ \forall p$$

$$\sum_{i=0}^{3} x_{pi}^2 = \frac{1}{2}, \ \forall p$$

$$x_{pi} \in \mathbb{R}, \ \forall p, i.$$

The Pauli coefficients C_{pqij} are the same as defined previously. The constraints will restrict us to the set of quantum states that are product states. We use the Pauli basis so that all numbers we solve for are real valued. Representing qubits as density matrices, let $\Phi_p := |\phi_p\rangle\langle\phi_p|$ for all p.

For any density matrix, there exists a unique decomposition into Pauli matrices. So we can write $\Phi_p = \sum_{i=0}^{3} x_{pi} W_i$, and $H_{pq} = \sum_{i,j=0}^{3} C_{pqij} W_i \otimes W_j$. Moreover, we know that $\text{Tr}[\Phi_p] = 1$ because the state $|\phi_p\rangle$ is norm 1, and also $\text{Tr}[\Phi_p^2] = 1$ if we assume, without loss of generality, that the state $|\phi_p\rangle$ is pure. This implies that (i) $x_{p0} = \frac{1}{2}$ for all p, (ii) $\sum_i x_{pi}^2 = \frac{1}{2}$ for all p, (iii) $C_{pq00} = \frac{1}{4}$ for all p, q, and (iv) $\sum_{ij} C_{pqij}^2 = \frac{1}{4}$ for all p, q.

The reverse process also works: Given real numbers $(x_{p0}, x_{p1}, x_{p2}, x_{p3})$ as a part of a feasible solution to (Q), one can construct a state $|\phi_p\rangle$ such that $|\phi_p\rangle\langle\phi_p| = \sum_{i=0}^{3} x_{pi} W_i$.

This is because of the properties of the Pauli basis:

$$\Phi_p^2 = \sum_{i,j=0}^{3} x_{pi}x_{pj}W_iW_j = x_{p0}^2 W_0^2 + 2\sum_{i=0}^{3} x_{pi}x_{p0}W_i + \sum_{i,j=1}^{3} x_{pi}x_{pj}W_iW_j$$

$$= \frac{1}{4}W_0 + \sum_{i=0}^{3} x_{pi}W_i + \sum_{i=1}^{3} x_{pi}^2 W_i^2 + \sum_{1 \le i,j \le 3, i \ne j} x_{pi}x_{pj}W_iW_j$$

$$= \frac{1}{4}W_0 + \sum_{i=0}^{3} x_{pi}W_i + \sum_{i=1}^{3} x_{pi}^2 W_0 + \sum_{1 \le i < j \le 3} x_{pi}x_{pj}(W_iW_j + W_jW_i)$$

$$= \frac{1}{4}W_0 + \sum_{i=0}^{3} x_{pi}W_i + \frac{1}{4}W_0 + 0 = \Phi_p.$$

The fact that $\Phi_p^2 = \Phi_p$ implies that Φ_p is a projector, and $\operatorname{Tr}\Phi_p = 1$ implies that it is a rank 1 projector. So there exists a vector $|\phi_p\rangle$ such that $|\phi_p\rangle\langle\phi_p| = \Phi_p = \sum_{i=0}^{3} x_{pi}W_i$.

Exactly solving this program is NP-hard, because as noted in Section 2.2, MAX-2-CSP can be cast as an instance of MAX-2-LH. Additionally, an optimum solution to such a MAX-2-LH instance is always, without loss of generality, a product state. We can, however, solve this approximately by first relaxing the program to an SDP, solving the SDP in polynomial time, and performing randomized rounding to the SDP solution we get to obtain a valid solution to the original program. Below is the SDP to which we relax. The coefficients C_{pqij}'s are given as constants.

SDP relaxation for MAX-2-Local Hamiltonian over product states:

Maximize $4\sum_{pq}\sum_{i,j=0}^{3} C_{pqij}v_{pi} \cdot v_{qj}$ $\hspace{3cm}$ (S2)

subject to:

$$\|v_0\| = \frac{1}{2}$$

$$\|v_{p0}\| = \frac{1}{2}, \ \forall p$$

$$v_0 \cdot v_{p0} = \frac{1}{4}, \ \forall p$$

$$\sum_{i=0}^{3} \|v_{pi}\|^2 = \frac{1}{2}, \ \forall p$$

$$v_0 \in \mathbb{R}^N$$

$$v_{pi} \in \mathbb{R}^N, \ \forall p, i.$$

The first three conditions simply force that for all p, $v_{p0} = v_0$. The SDP is in fact a relaxation of the quadratic program in the sense that given a solution x_{pi}, for all p, i, to the first program, the vector solution $v_0 := (1, 0, \ldots, 0)$, $v_{pi} := x_{pi}v_0$, for all p, i, is a feasible solution to the SDP that achieves the same objective value. Therefore the value of the SDP is at least the value of the first program. Algorithm 2 details our approach.

▶ **Theorem 14.** *Given a local Hamiltonian on n qubits $H = \sum_{pq} P_{pq}$, where P_{pq} is a product of a rank 1 projector on qubit p and a rank 1 projector on qubit q, Algorithm 2 outputs a product state that has an expected energy of at least $\alpha_2 \cdot \mathrm{OPT}_{\mathrm{prod}}$, where $\alpha_2 = 0.796\ldots$, and $\mathrm{OPT}_{\mathrm{prod}} = \max_{|\phi_1\rangle,\ldots,|\phi_n\rangle}\langle\phi_1|\ldots\langle\phi_n|H|\phi_1\rangle\ldots|\phi_n\rangle.$*

Algorithm 2 MAX-2-local Hamiltonian with PSD local terms.

1: Input: $\{H_{pq} : (p,q) \in E\}, E \subseteq [n] \times [n]$.
2: Calculate $(C_{pqij} := \mathrm{Tr}(H_{pq}(W_i \otimes W_j))/4)_{pqij}$.
3: Solve the SDP $(S2)$, and get $(v_0, (v_{pi}))$.
4: Pick a random unit vector $r \in \mathbb{R}^N$ (use $N := 4n+1$).
5: For all $p \in [n]$ and $i \in \{0,1,2,3\}$, assign $x_{pi} := \|v_{pi}\| \, \mathrm{sgn}(v_0 \cdot r) \, \mathrm{sgn}(v_{pi} \cdot r)$.
6: Output $\Phi_p := \bigotimes_{p=1}^{n} \sum_{i=0}^{3} x_{pi} W_i$ as the resulting product state assignment.

Proof. We express the rank 1 projector H_{pq} as $|\gamma_{pq}\rangle\langle\gamma_{pq}|$ for some state $|\gamma_{pq}\rangle$. $\mathrm{OPT}_{\mathrm{prod}}$ is the value of the program (Q). We relax the program (Q) to the SDP $(S2)$ and get v_{pi} for all p, i as a solution to the SDP. To get real-valued x_{pi}, we perform randomized rounding reminiscent of the Goemans-Williamson algorithm: $x_{pi} = \|v_{pi}\| \, \mathrm{sgn}(v_0 \cdot r) \, \mathrm{sgn}(v_{pi} \cdot r)$. The x_{pi} are used in Step 6 of the algorithm to produce a product state; these variables constitute a feasible solution to (Q) because $x_{p0} = \|v_{p0}\| \, \mathrm{sgn}(v_0 \cdot r) \, \mathrm{sgn}(v_{p0} \cdot r) = \frac{1}{2} \, \mathrm{sgn}(v_0 \cdot r)^2 = \frac{1}{2}$, and

$$\sum_{i=0}^{3} x_{pi}^2 = \sum_{i=0}^{3} \|v_{pi}\|^2 \, \mathrm{sgn}(v_0 \cdot r)^2 \, \mathrm{sgn}(v_{pi} \cdot r)^2 = \sum_{i=0}^{3} \|v_{pi}\|^2 = \frac{1}{2}.$$

We apply Lemma 16 below to analyze the performance of the rounding term by term to yield:

$$\mathbb{E}\left[4 \sum_{pq} \sum_{i,j=0}^{3} C_{pqij} x_{pi} x_{qj} \right] \geq \alpha_2 4 \sum_{pq} \sum_{i,j=0}^{3} C_{pqij} v_{pi} \cdot v_{qj} = \alpha_2 \, \mathrm{OPT}_{\mathrm{SDP}} \geq \alpha_2 \, \mathrm{OPT}_{\mathrm{prod}} . \blacktriangleleft$$

▶ **Corollary 15.** *Algorithm 2 outputs a product state achieving* $0.40 \cdot \mathrm{OPT}$.

Proof. By Theorem 14 the algorithm outputs a state achieving $0.796 \cdot \mathrm{OPT}_{\mathrm{prod}}$, which is at least $0.40 \cdot \mathrm{OPT} / 2$ by Theorem 3. ◀

Note that we have not yet used the assumption that H_{pq} is a tensor product of rank 1 projectors. In this case we have that $|\gamma_{pq}\rangle\langle\gamma_{pq}| = H_{pq} = H_{pq,p} \otimes H_{pq,q} = |\gamma_p\rangle\langle\gamma_p| \otimes |\gamma_q\rangle\langle\gamma_q| = (|\gamma_p\rangle \otimes |\gamma_q\rangle)(\langle\gamma_p| \otimes \langle\gamma_q|)$, for some states $|\gamma_p\rangle$ and $|\gamma_q\rangle$. Consequently $|\gamma_{pq}\rangle = |\gamma_p\rangle \otimes |\gamma_q\rangle$ is a product state, and the Pauli coefficients are $C_{pqij} = \mathrm{Tr}(|\gamma_{pq}\rangle\langle\gamma_{pq}| W_i \otimes W_j)/4 = \mathrm{Tr}((|\gamma_p\rangle\langle\gamma_p| \otimes |\gamma_q\rangle\langle\gamma_q|)(W_i \otimes W_j))/4 = \mathrm{Tr}(|\gamma_p\rangle\langle\gamma_p| W_i) \mathrm{Tr}(|\gamma_p\rangle\langle\gamma_p| W_i)/4 = C_{pi} C_{qj}$. So for all i, j, $C_{pqij} = C_{pi} C_{qj}$. Note that since $|\gamma_p\rangle$ is a 1 qubit state, $C_{p0}^2 = (\frac{1}{2})^2 = \sum_{i=1}^{3} C_{pi}^2$. To conclude our analysis, we leverage this structure in the lemma below.

▶ **Lemma 16.** *Let* $u_0, \ldots, u_3, v_0, \ldots, v_3 \in \mathbb{R}^N$ *be vectors such that* $u_0 = v_0$, $\|u_0\| = \|v_0\| = 1/2$, *and* $\sum_{i=0}^{3} \|u_i\|^2 = \sum_{i=0}^{3} \|v_i\|^2 = 1/2$. *Let* $x_i = \|u_i\| \, \mathrm{sgn}(u_0 \cdot r) \, \mathrm{sgn}(u_i \cdot r)$, $y_j = \|v_j\| \, \mathrm{sgn}(v_0 \cdot r) \, \mathrm{sgn}(v_j \cdot r)$ *be the rounding of the vectors with respect to a uniformly random vector* $r \in S^{N-1}$. *Let* $C_{ij} = C_i D_j$ *where* $C_i, D_j \in \mathbb{R}$ *such that* $C_0^2 = \sum_{i=1}^{3} C_i^2 = D_0^2 = \sum_{i=1}^{3} D_i^2$. *Then*

$$\alpha_2 \sum_{i,j=0}^{3} C_{ij} u_i \cdot v_j \leq \mathbb{E}\left[\sum_{i,j=0}^{3} C_{ij} x_i y_j \right], \text{ where } \alpha_2 = \min_{0 < \theta < \arccos -1/3} \frac{2}{\pi} \frac{2\pi - 3\theta}{1 + 3\cos\theta} = 0.796 \ldots .$$

Proof. The proof is by applying Lemma 7, Lemma 8, and the Cauchy-Schwarz inequality. Let $U_i = \text{sgn}(u_i \cdot r)$ and $V_i = \text{sgn}(v_i \cdot r)$ and note that $U_0 = V_0$. Also for convenience, set

$$A_0 := C_0\|u_0\| - \sum_{i=1}^{3}|C_i|\|u_i\|, \quad A_1 := \sum_{i=1}^{3}|C_i|\|u_i\|(1 + \text{sgn}(C_i)U_0U_i),$$

$$B_0 := D_0\|v_0\| - \sum_{j=1}^{3}|D_j|\|v_j\|, \quad B_1 := \sum_{i=1}^{3}|C_i|\|u_i\|(1 + \text{sgn}(C_i)U_0U_i)$$

$$\mathbb{E}\left[\sum_{i,j=0}^{3}C_{ij}x_iy_j\right] = \mathbb{E}\left[\sum_{i,j=0}^{3}C_iD_j\|u_i\|U_0U_i\|v_j\|V_0V_j\right]$$

$$= \mathbb{E}\left[\sum_{i=0}^{3}C_i\|u_i\|U_0U_i\sum_{j=0}^{3}D_j\|v_j\|V_0V_j\right]$$

$$= \mathbb{E}\left[\left(C_0\|u_0\| + \sum_{i=1}^{3}C_i\|u_i\|U_0U_i\right)\left(D_0\|v_0\| + \sum_{j=1}^{3}D_j\|v_j\|V_0V_j\right)\right]$$

$$= \mathbb{E}\left[(A_0 + A_1)(B_0 + B_1)\right]$$

$$= A_0B_0 + \mathbb{E}\left[A_1B_0\right] + \mathbb{E}\left[A_0B_1\right] + \mathbb{E}\left[A_1B_1\right].$$

For convenience, set

$$A_0' := A_0, \quad A_1' := \sum_{i=1}^{3}|C_i|\|u_i\|(1 + \text{sgn}(C_i)\frac{u_0 \cdot u_i}{\|u_0\|\|u_i\|}),$$

$$B_0' := B_0, \quad B_1' := \sum_{i=1}^{3}|D_i|\|v_i\|(1 + \text{sgn}(D_i)\frac{u_0 \cdot v_i}{\|u_0\|\|v_i\|}).$$

From Lemma 7,

$$\mathbb{E}\left[1 + \text{sgn}(C_i)\text{sgn}(u_0 \cdot r)\text{sgn}(u_i \cdot r)\right] \geq \alpha_1\left(1 + \text{sgn}(C_i)\frac{u_0 \cdot u_i}{\|u_0\|\|u_i\|}\right)$$

for all i. Therefore $\mathbb{E}\left[A_1\right] \geq \alpha_1 A_1'$ and $\mathbb{E}\left[B_1\right] \geq \alpha_1 B_1'$.

Using the fact that either exactly one of $\text{sgn}(C_i)$, $\text{sgn}(D_j)$, or $\text{sgn}(C_i)\text{sgn}(D_j)$ is positive, or all three are, Lemma 8 implies

$$\mathbb{E}\left[(1 + \text{sgn}(C_i)\text{sgn}(u_0 \cdot r)\text{sgn}(u_i \cdot r))(1 + \text{sgn}(D_j)\text{sgn}(v_0 \cdot r)\text{sgn}(v_j \cdot r))\right] \geq$$

$$\alpha_2\left(1 + \text{sgn}(C_i)\frac{u_0 \cdot u_i}{\|u_0\|\|u_i\|} + \text{sgn}(D_j)\frac{v_0 \cdot v_j}{\|v_0\|\|v_j\|} + \text{sgn}(C_iD_j)\frac{u_i \cdot v_j}{\|u_i\|\|v_j\|}\right)$$

for all i, j. Therefore $\mathbb{E}\left[A_1B_1\right] \geq \alpha_2 A_1'B_1'$.

From Cauchy-Schwarz we have $A_0, B_0 \geq 0$, and using this inequality we can bound

$$\mathbb{E}\left[\sum_{i,j=0}^{3} C_{ij} x_i y_j\right]$$

$$= A_0 B_0 + \mathbb{E}[A_1 B_0] + \mathbb{E}[A_0 B_1] + \mathbb{E}[A_1 B_1].$$

$$\geq A_0 B_0 + \alpha_1 A_1' B_0' + \alpha_1 A_0' B_1' + \alpha_2 A_1' B_1'$$

$$\geq \alpha_2 A_0 B_0 + \alpha_2 A_1' B_0' + \alpha_2 A_0' B_1' + \alpha_2 A_1' B_1'$$

$$= \alpha_2 (A_0' + A_1')(B_0' + B_1')$$

$$= \alpha_2 \sum_{i,j=0}^{3} C_i D_j u_i \cdot v_j = \alpha_2 \sum_{i,j=0}^{3} C_{ij} u_i \cdot v_j. \qquad \blacktriangleleft$$

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