

A convergent hierarchy of spectral gap certificates for qubit Hamiltonians

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Abstract

We give a convergent hierarchy of SDP certificates for bounding the spectral gap of local qubit Hamiltonians from below. Our approach is based on the NPA hierarchy applied to a polynomially-sized system of constraints defining the universal enveloping algebra of the Lie algebra $\mathfrak{su}(2^n)$, as well as additional constraints which put restrictions on the corresponding representations of the algebra. We also use as input an upper bound on the ground state energy, either using a hierarchy introduced by Fawzi, Fawzi, and Scalet, or an analog for qubit Hamiltonians of the Lasserre hierarchy of upper bounds introduced by Klep, Magron, Massé, and Volčič. The convergence of the certificates does not require that the Hamiltonian be frustration-free.

We prove that the resulting certificates have polynomial size at fixed degree and converge asymptotically (in fact, at level n), by showing that all allowed representations of the algebra correspond to the second exterior power $\wedge^2(\mathbb{C}^{2^n})$, which encodes the sum of the two smallest eigenvalues of the original Hamiltonian. We also give an example showing that for a commuting 1-local Hamiltonian, the hierarchy certifies a nontrivial lower bound on the spectral gap.

1 Introduction and motivation

Certifying the presence of a nonzero spectral gap for local quantum qubit Hamiltonians a fundamental problem in quantum many-body physics. A positive gap controls correlation decay and stability of phases. For 1D and 2D systems in particular, the existence of a gap can imply strong properties about entanglement in the system, such as the existence of an area law. Such properties are relevant for the design of algorithms for many-body systems, which in some cases use limitations on entanglement in the ground state to output good classical approximations.

However, proving rigorous lower bounds on the spectral gap is often difficult. From a computational complexity viewpoint, Gharibian and Yirka proved that computing the spectral gap of a local qubit Hamiltonian is hard for the complexity class $\mathsf{P}^{\mathsf{UQMA}[\log]}$ [GY19]. In certain models of infinite-size systems, computing the spectral gap is known to be undecidable [CPW15; Bau+20]. From a condensed matter physics viewpoint, several well-known open problems, such as the Haldane conjecture [Hal83a; Hal83b; Hal16], amount to showing that particular quantum systems are either gapped or gapless.

The goal of this paper is to present a *convergent* hierarchy of semidefinite programming (SDP) certificates that can be used to certify lower bounds on spectral gaps of qubit Hamiltonians which may be frustrated. The hierarchy is constructed from a noncommutative polynomial system which bounds the sum of the first two eigenvalues of a given local Hamiltonian. We also use a family of upper-bound SDPs to bound the first eigenvalue of the Hamiltonian from above. We then deduce lower bounds on the spectral gap by combining the bounds output by the two hierarchies.

1.1 Previous work

There has been some recent work on approaches for giving SDP-based bounds on the spectral gap of spin systems. The spectral bootstrap method of [NX23] uses an approach inspired by the bootstrap method in conformal field theory to give *upper* bounds on the spectral gaps of translationally-invariant qubit systems. The approach allows one to more generally deduce constraints on the matrix elements of local operators expanded in the eigenbasis of the system.

A recent SDP hierarchy for producing *lower* bounds on gaps of frustration-free Hamiltonians was proposed in [Rai+24]. If the exact ground energy $\lambda_0(H)$ of the Hamiltonian is known, then a gap of at least γ is equivalent to the operator $(H - \lambda_0(H))(H - \gamma - \lambda_0(H))$ being positive. One can then try to certify a lower bound on the spectral gap by searching over low-degree sum-of-squares certificates that this operator is positive. If $\lambda_0(H)$ is known, then the left-hand side becomes linear in γ and thus amenable to SDP approaches based on the noncommutative sum-of-squares hierarchy. The same work also proposed several approximations and simplifications for translationally-invariant qubit systems on a lattice.

1.2 Results

We propose a hierarchy of SDP-based certificates for proving lower bounds on the spectral gaps of quantum qubit systems on a finite lattice. We first define a noncommutative polynomial optimization problem whose optimal value is equal to the sum of the first two eigenvalues of a given local qubit Hamiltonian, which can then be approximated using the NPA hierarchy [PNA10; NPA12]. We then use a variant of the Lasserre hierarchy of upper bounds on polynomial minimization problems, introduced by Klep, Magron, Massé, and Volčič in [Kle+25], to bound the ground state energy of a local Hamiltonian from above. Taking an appropriate linear combination then gives a certified lower bound on the spectral gap of the Hamiltonian.

We prove both asymptotic convergence of the hierarchy and note that standard arguments imply that convergence in fact occurs at level n . The proof that the noncommutative polynomial system encodes the desired problem is quite involved, and uses a number of facts about the Lie algebra $\mathfrak{su}(2^n)$ and its representations.

1.3 Further directions

The size of the noncommutative polynomial system we construct is polynomial in n but it is still rather large, with roughly $O(n^2)$ variables and $O(n^8)$ constraints and nontrivial constant factors. Thus the main question is whether there is a simpler polynomial system for which one still has asymptotic convergence of the hierarchy to the true spectral gap. It seems unclear if it is possible to use the same approach of defining generators and relations for $\mathfrak{su}(2^n)$ as a Lie algebra, since the proof strategy in this paper seems to rely on all of the relations included in the system. But it is still possible that there is some other set of constraints which may suffice to give complete certificates of lower bounds on the spectral gap.

Our hierarchy also suggests an approach to compute bounds on the first k eigenvalues of H for constant values of k . This would require finding constraints which characterize the higher exterior powers $\wedge^k(\mathbb{C}^{2^n})$ as representations of $\mathfrak{su}(2^n)$ beyond $k = 2$, although even for $k = 2$ the constraints we give here are already rather complicated.

2 Technical overview

Here we summarize the construction of the two SDP hierarchies we use to certify spectral gaps and give an idea of the techniques used in the proof of convergence.

2.1 Reduction to two SDP hierarchies

Our approach combines an SDP hierarchy of *lower bounds* on the sum of the smallest two eigenvalues of a local Hamiltonian H , obtained from noncommutative sum-of-squares (SOS) proofs in an algebra defined by suitable generators and relations, and an SDP family of *upper bounds* on ground energy coming from a noncommutative analog of the Lasserre hierarchy of upper bounds which is connected to approximate ground-space projectors (AGSPs). The two bounds are then combined as

$$\lambda_2(H) - \lambda_1(H) \geq A - 2B$$

where $A \leq \lambda_1(H) + \lambda_2(H)$ is a certified lower bound and $B \geq \lambda_1(H)$ is a certified upper bound.

2.2 Hierarchy for lower bounds

The lower-bound SDP hierarchy is built from a noncommutative $*$ -algebra on a finite set of generators (with variables denoted S_i^a and T_{ij}^{ab}), together with the explicit relations recorded in (1) and also the spectral and representation-theoretic constraints in (2). Intuitively, S_i^a is meant to correspond to a 1-local Pauli operator, and T_{ij}^{ab} corresponds to a 2-local Pauli operator.

Concretely, we first define the algebra $\mathbb{C}\langle V_n \rangle / \mathcal{I}$ where $\mathcal{I}$ is the two-sided $*$ -ideal generated by the relations (1). These relations enforce certain commutation relations which characterize the universal enveloping algebra of the Lie algebra $\mathfrak{su}(2^n)$. Its representations then correspond to irreducible Lie algebra representations of $\mathfrak{su}(2^n)$, of which one is the antisymmetric subspace $\wedge^2(\mathbb{C}^{2^n})$. The action of H on the antisymmetric subspace has $\lambda_1(H) + \lambda_2(H)$ as its lowest eigenvalue, though there are other representations. The definitions of the generators and relations and proof that these characterize $\mathfrak{su}(2^n)$ are in Section 5.

We then impose additional noncommutative polynomial constraints and inequalities to rule out representations other than the antisymmetric subspace. For example, in (2) there are constraints on the eigenvalues of S_i^a , which then force the irreducible representation of $\mathfrak{su}(2^n)$ to correspond to one of five particular Young diagrams. Additional constraints then rule out each of the four remaining irreducible representations other than $\wedge^2(\mathbb{C}^{2^n})$. The exact definitions of these additional constraints, as well as the proof that they rule out all other irreducible representations, appear in Section 6.

One slightly subtle point is that the additional two-site variables T_{ij}^{ab} are needed to encode higher-locality interactions. Specifically, any k -local term in a Hamiltonian can be expressed as a Lie polynomial (which can be expanded to a noncommutative polynomial) in the chosen generators. The action of H on a representation of the algebra we define is then that of the Lie algebra representation, which is the intended operator for $\wedge^2(\mathbb{C}^{2^n})$. However, writing the Hamiltonian as a noncommutative polynomial in the S_i^a would not give a correctly converging hierarchy of lower bounds on $\lambda_1(H) + \lambda_2(H)$.

2.3 Hierarchy of upper bounds

One hierarchy of upper bounds uses the noncommutative version of the Lasserre hierarchy introduced in [Kle+25]. Concretely, one optimizes over positive noncommutative polynomials P of bounded degree and forms the reweighted state $\psi_P(\cdot) = \frac{\varphi(P \cdot)}{\varphi(P)}$ where φ is a fixed reference state. Minimizing the expectation $\psi_P(H)$ over such P yields a sequence of upper bounds B_d on the ground energy which can be computed using an SDP. The resulting sequence of upper bounds decreases with d and converges to the true ground energy. We give slightly more background in this hierarchy in Section 4.1.

Another is based on the KMS conditions for thermal states at inverse temperature β [FFS24], in the limit $\beta \rightarrow \infty$. The conditions contain a family of scalar inequalities indexed by observables of the system, and after truncating to a finite-dimensional space of observables one can re-encode the family of scalar constraints by an SDP constraint [FFS24], assuming that the $\beta \rightarrow \infty$ limit is taken. (For general β one can instead use a constraint which is convex but non-SDP, as done in [FFS24].)

2.4 Example of a certificate

To illustrate the hierarchy we include an explicit example in Section 7. For the trivial 1-local Hamiltonian $H_n = -\sum_i Z_i$ we show that a degree-4 SOS constructed using the system presented here certifies the optimal lower bound on the sum of the first two energy levels.

3 Preliminaries

3.1 Noncommutative polynomial optimization problems

A **noncommutative polynomial optimization problem** is defined by a finite set of noncommuting variables

$$X_1, \dots, X_n$$

along with a set of relations $q_1, \dots, q_m$, which are polynomials in the X_i and X_i^* , together with a Hermitian polynomial $p(X_1, \dots, X_n)$ satisfying $p^* = p$. The goal is to maximize (or minimize) the expectation value of p over all Hilbert space representations of the variables that satisfy the relations, with respect to some quantum state ρ . Concretely, the value of the problem is

$$\inf_{\rho, \{X_i\}} \text{Tr}(\rho p(X_1, \dots, X_n))$$

where $\mathcal{H}$ is a fixed, infinite-dimensional separable Hilbert space, ρ is a density operator on $\mathcal{H}$, and the supremum ranged over bounded operators $X_i : \mathcal{H} \rightarrow \mathcal{H}$ such that $q_j(X_1, \dots, X_n) = 0$ for all $j \in [m]$.

3.1.1 The NPA hierarchy

The NPA hierarchy [PNA10; NPA12] gives a hierarchy of semidefinite programs which approximate the value of a noncommutative polynomial optimization problem. Specifically, one considers

$$\min E[p]$$

$$\begin{aligned}
& \text{s.t. } E : \mathbb{R}\langle X_1, \dots, X_n \rangle_{\leq k} \rightarrow \mathbb{C} \\
& 0 \leq E[q^*q] \quad 2 \deg q \leq k \\
& 0 = E[q_i q] \quad i \in [m], \deg q_i + \deg q \leq k
\end{aligned}$$

where k is an integer parameter and E is defined on all noncommutative $*$ -polynomials of degree at most k . In [PNA10], it is proven that as $k \rightarrow \infty$, the value of these SDP converges monotonically to the true value of the noncommutative polynomial optimization problem.

3.2 Algebras and Lie algebras defined by generators and relations

The proof of asymptotic convergence will work with a Lie algebra defined by generators and relations, and show that it is isomorphic to $\mathfrak{su}(2^n)$. Recall that a $*$ -algebra A is **free** on n generators $x_1, \dots, x_n$ if it satisfies the following initiality (or universality) property: for any n elements $b_1, \dots, b_n$ of a $*$ -algebra B , there is a unique $*$ -homomorphism $A \rightarrow B$ sending x_i to b_i . Similarly, A is defined by n generators satisfying a set of relations if the same property holds for any elements $b_1, \dots, b_n$ which satisfy the same relations. To construct a $*$ -algebra which is free, one can take the ring of noncommutative $*$ -polynomials in a set of n variables. To impose relations, one can take the quotient of the free $*$ -algebra by a two-sided $*$ -ideal generated by the given relations.

Similar versions of these constructions can be given for Lie algebras, which we will use later. The definition of quotient Lie algebras is relatively standard, but the construction of free Lie algebras is more involved. One can use *Lyndon words* to construct an explicit basis, similar to the set of all words used for associative $*$ -algebras [Reu93]. We will only use the existence of these constructions and the corresponding initiality/universality properties, and so do not give the full explicit construction here.

3.3 Facts from representation theory

The proof of convergence of our hierarchy uses a number of facts from representation theory, whose full proofs would be too lengthy to repeat here. Instead, we briefly state a number of the most important facts and refer the reader to the references [Bum13; DK00; Zhe73] for more detail.

Definition 1. A (finite-dimensional) **representation** of a Lie group G is a homomorphism

$$\pi : G \rightarrow GL(V)$$

from G into the group of invertible linear transformations on a complex vector space V . The dimension of V is called the dimension of the representation. A representation is *irreducible* (an *irrep*) if V has no nontrivial proper subspace which is invariant under all $\pi(g)$.

A representation of a Lie algebra $\mathfrak{g}$ is a Lie algebra homomorphism

$$\rho : \mathfrak{g} \rightarrow \mathfrak{gl}(V)$$

into the Lie algebra of endomorphisms of a vector space V , satisfying $\rho([X, Y]) = [\rho(X), \rho(Y)]$. Irreducibility is defined analogously.

Correspondence between representations of Lie groups and Lie algebras. Every finite-dimensional irreducible representation of a compact connected Lie group G , such as $SU(m)$, can be restricted to a Lie algebra $\mathfrak{g}$ by differentiating (in a suitable sense) the homomorphism $G \rightarrow GL(V)$, and remains irreducible. Conversely, every finite-dimensional irreducible representation of $\mathfrak{g}$ can be integrated uniquely to an irreducible representation of G . Thus we may freely identify irreps of $SU(m)$ with irreps of $\mathfrak{su}(m)$. Concretely, the Lie algebra $\mathfrak{su}(m)$ is the space of all skew-Hermitian matrices in $\mathbb{C}^{m \times m}$, and the Lie bracket is given by taking commutators.

Definition 2. If (π, V) and (π', W) are representations of a Lie group G , their tensor product is the representation

$$\begin{aligned}\pi \otimes \pi' : G &\rightarrow GL(V \otimes W) \\ (\pi \otimes \pi')(g) &= \pi(g) \otimes \pi'(g).\end{aligned}$$

Similarly, if (ρ, V) and (ρ', W) are representations of a Lie algebra $\mathfrak{g}$, their tensor product is

$$\begin{aligned}\rho \otimes \rho' : \mathfrak{g} &\rightarrow \mathfrak{gl}(V \otimes W) \\ (\rho \otimes \rho')(X) &= \rho(X) \otimes I_W + I_V \otimes \rho'(X).\end{aligned}$$

The tensor product is associative up to a canonical isomorphism.

Example 3. Let $V = \mathbb{C}^m$ be the defining (fundamental) representation of $SU(m)$. For each $k = 1, \dots, m$, the k -th exterior power

$$\wedge^k V := \{v \in V^{\otimes k} : \sigma \cdot v = \text{sgn}(\sigma)v\}$$

is a subspace of the k -fold tensor product $V^{\otimes k}$ consisting of antisymmetric tensors, where a permutation $\sigma \in S_k$ acts on $V^{\otimes k}$ by permuting indices. The action of $SU(m)$ on $V^{\otimes k}$ is given by

$$g \cdot (v_1 \otimes \dots \otimes v_k) = (gv_1) \otimes \dots \otimes (gv_k),$$

For the Lie algebra $\mathfrak{su}(m)$ one has

$$X \cdot (v_1 \otimes \dots \otimes v_k) = \sum_{i=1}^k v_1 \otimes \dots \otimes (Xv_i) \otimes \dots \otimes v_k.$$

It can be checked that the action is again well-defined on the space of antisymmetric tensors. Each $\wedge^k V$ is an irreducible representation of $SU(m)$ with highest weight equal to the k -th fundamental weight. Its dimension is

$$\dim(\wedge^k V) = \binom{m}{k}.$$

Some standard special cases include

- the defining representation $\wedge^1 V \cong V$
- the two-index antisymmetric irrep $\wedge^2 V$
- the determinant representation $\wedge^m V \cong \mathbb{C}$, which is isomorphic to the trivial irrep for $SU(m)$.

Remark 4. If H is a quantum Hamiltonian, where we think of $iH \in \mathfrak{su}(m)$, then the action of H on the two-index antisymmetric irrep gives another Hamiltonian acting on a different space whose smallest eigenvalue is $\lambda_1(H) + \lambda_2(H)$, which is the sum of the two smallest eigenvalues of H .

Definition 5. We denote by ϵ_{abc} the Levi-Civita symbol in three indices:

$$\epsilon_{abc} = \begin{cases} +1 & \text{if } (a, b, c) \text{ is an even permutation of } (1, 2, 3), \\ -1 & \text{if } (a, b, c) \text{ is an odd permutation of } (1, 2, 3), \\ 0 & \text{if any two indices coincide.} \end{cases}$$

The Lie bracket of $\mathfrak{su}(2)$ can be written as $[\sigma^a, \sigma^b] = 2i \epsilon_{abc} \sigma^c$.

Schur–Weyl duality for $SU(m)$. Let $V = \mathbb{C}^m$ be the defining representation of $SU(m)$. The tensor power $V^{\otimes n}$ carries commuting actions of $SU(m)$ and the symmetric group S_n , which have both been defined above. Schur–Weyl duality states that

$$V^{\otimes n} \cong \bigoplus_{\substack{\lambda \vdash n \\ \ell(\lambda) \leq m}} V_\lambda \otimes W_\lambda,$$

where the sum is over partitions λ of n with at most m parts, W_λ is the irreducible $SU(m)$ representation with highest weight λ , and V_λ is the corresponding irreducible representation of S_n , both sets of which exhaust all irreducible representations of the two groups. We will sometimes denote the irreducible representation W_λ by $S_\lambda(V)$.

Young tableau bases for irreducible representations of $SU(m)$. Let $\lambda = (\lambda_1, \lambda_2, \dots, \lambda_\ell)$ be a Young diagram of m boxes. A *semistandard Young tableau* (SSYT) of shape λ with entries in $\{1, \dots, m\}$ is a filling of the boxes of λ with numbers from $\{1, \dots, m\}$ such that the entries are weakly increasing along each row and strictly increasing down each column. The irreducible representation W_λ has a distinguished basis indexed by semistandard Young tableaux of shape λ . For a tableau T , let

$$c_i(T) := \#\{\text{boxes of } T \text{ filled with } i\}$$

so that $\sum_{i=1}^m c_i(T) = |\lambda|$. For $g = \text{diag}(t_1, \dots, t_m) \in GL(m, \mathbb{C})$ we have

$$g \cdot v_T = \left(\prod_{i=1}^m t_i^{c_i(T)} \right) v_T.$$

Similarly, for the Lie algebra action we have that for $H = \text{diag}(h_1, \dots, h_m) \in \mathfrak{gl}(m, \mathbb{C})$,

$$H \cdot v_T = \left(\sum_{i=1}^m c_i(T) h_i \right) v_T.$$

The weight of v_T is $\text{wt}(v_T) = \sum_{i=1}^m c_i(T) e_i$, where e_i is the i -th standard basis vector. The highest weight of V^λ corresponds to the partition λ itself.

The Young tableau basis is constructed from a fixed ordered basis $(e_1, \dots, e_m)$ of the defining representation $\mathbb{C}^m$. A box filled with i in a tableau corresponds e_i . In particular, different choices of basis of $\mathbb{C}^m$ give different Young tableau bases of each V^λ .

Casimir operators for $SU(m)$. Let $\mathfrak{su}(m)$ have Killing form $\kappa(X, Y) = 2m \operatorname{Tr}(XY)$ on traceless matrices. Choose a basis $\{X_i\}$ of $\mathfrak{su}(m)$ and a dual basis $\{X^i\}$ with respect to κ . The quadratic Casimir element is

$$C = \sum_i X_i X^i \in U(\mathfrak{su}(m)),$$

where $U(\mathfrak{su}(m))$ denotes the universal enveloping algebra. The Casimir element is in the center of $U(\mathfrak{su}(m))$ and hence acts as a scalar on every irreducible representation. If V_λ is the irrep of $SU(m)$ (or $\mathfrak{su}(m)$) with highest weight $\lambda = (\lambda_1, \dots, \lambda_{m-1})$, then C acts on V_λ by

$$C \cdot v = (\langle \lambda, \lambda + 2\rho \rangle) v$$

where ρ is the Weyl vector, which is half the sum of positive roots, and $\langle \cdot, \cdot \rangle$ is the standard inner product on weights.

4 Upper bounds for ground energies of qubit Hamiltonians

The main part of our hierarchy will give lower bounds $A \leq \lambda_1(H) + \lambda_2(H)$ for a local Hamiltonian H . To deduce bounds on the spectral gap, one then needs an **upper** bound $B \geq \lambda_1(H)$, from which we get

$$\lambda_2(H) - \lambda_1(H) = \lambda_2(H) + \lambda_1(H) - 2\lambda_1(H) \geq A - 2B.$$

The simplest way to obtain such an upper bound B would be to have some ansatz of states which are easy to optimize over with respect to the expectation value of H . Keeping with the spirit of this paper, we will describe an approach based on SDP hierarchies.

4.1 The Lasserre hierarchy of upper bounds

The earliest such hierarchy is due to Lasserre [Las11], in the classical/commutative setting, and starts by fixing a reference measure μ on the feasible set with known moments. The ansatz of states considered is the set of probability distributions $p d\mu$, where p ranges over low-degree sum-of-squares polynomials such that $\int p d\mu = 1$. Concretely, we have the sequence of upper bounds which can be defined as

$$f^{(d)} = \inf_{\substack{p \in \Sigma[x] \\ \deg p \leq 2d}} \frac{\int f(x) p(x) d\mu(x)}{\int p(x) d\mu(x)}$$

and computed using an SDP. Knowledge of the moments of μ is required to be able to efficiently check the normalization for a given polynomial, as well as to be able to compute $\int f p d\mu$ where f is the objective function.

4.1.1 Noncommutative version of the Lasserre hierarchy of upper bounds

In [Kle+25], a noncommutative version of the Lasserre hierarchy of upper bounds was introduced. Here one considers a unital $*$ -algebra $\mathcal{A}$ generated by noncommuting elements $X_1, \dots, X_m$ with known relations, together with a fixed reference state φ on $\mathcal{A}$. For degree bound $2d$, one optimizes over noncommutative sums of squares $P \in \Sigma\langle X \rangle$ of degree at most $2d$, forming the reweighted state

$$\psi_P(a) := \frac{\varphi(Pa)}{\varphi(P)}.$$

Given a Hermitian polynomial $f \in \mathcal{A}$, the level- d bound is

$$f^{(d)} := \inf_{\substack{P \in \Sigma\langle X \rangle \\ \deg P \leq 2d}} \frac{\varphi(Pf)}{\varphi(P)}.$$

As in the commutative case, knowledge of the noncommutative $*$ -moments of φ is required to be able to efficiently check the normalization condition and compute the expectation of f , and the constraint $P \in \Sigma\langle X \rangle$ is semidefinite representable. The sequence of bounds decreases with d and converges to the true minimum of f over all representations compatible with φ in sufficiently nice cases.

4.1.2 Upper bounds for ground energies of qubit Hamiltonians

For quantum local Hamiltonians, one can consider a straightforward noncommutative analog of the Lasserre hierarchy following the previous general outline. The algebra is the one $\mathcal{B}(\mathbb{C}^{2^n})$ of operators on $\mathbb{C}^{2^n}$, which is generated by Pauli matrices X_i, Y_i, Z_i subject to standard commutation relation. The natural choice of a state is the maximally mixed state, for which the expectation of A is given by $2^{-n} \text{Tr}(A)$. The moments in terms of the Pauli matrices are all 0, except for the expectation of the identity operator (which is 1).

Approximate ground space projectors (AGSPs) are operators which are meant to approximate the true projector onto the ground space projector but have controlled complexity, and are often used in proofs of area laws for geometrically local Hamiltonians [Ara+13; LVV15; AAG22]. In the SDP hierarchy for qudit systems, the reweighting polynomial P plays the role of such an operator. Specifically, the normalized state $\psi(a) = \varphi(Pa)/\varphi(P)$ concentrates weight near the ground space. As an operator on $\mathbb{C}^{2^n}$ it can be seen as an approximate ground space projector, and the degree of the polynomial can be seen as measuring its complexity.

4.2 Hierarchy based on entropy-energy balance conditions

As introduced by [FFS24] in the context of optimization hierarchies, one has the following characterization of a thermal state ϕ of a Hamiltonian H at inverse temperature β :

$$\begin{aligned} \phi([H, a]) &= 0 \\ \phi(a^*[H, a]) &\geq \frac{1}{\beta} \phi(a^*a) \log \left(\frac{\phi(a^*a)}{\phi(aa^*)} \right) \end{aligned}$$

where a in both constraints ranges over all observables (here we only consider Hamiltonians on a finite number of qubits). In the limit as $\beta \rightarrow \infty$, which corresponds to the ground state of H , the second constraint becomes $\phi(a^*[H, a]) \geq 0$, which is equivalent to the matrix $[\phi(a_i^*[H, a_j])]_{i,j}$ being positive semidefinite for a linear basis $\{a_i\}$ of the space of observables.

When H is local, one can then obtain an SDP hierarchy of outer approximations to the singleton set containing the ground state by only considering a of bounded locality and replacing ϕ by a pseudo-state $\tilde{\phi}$ defined only on operators of bounded locality. By maximizing $\tilde{\phi}(H)$ subject to these constraints one can then obtain a hierarchy of upper bounds on the ground state energy of H . In some cases this can give more useful or tighter bounds compared to the noncommutative analog of the Lasserre hierarchy of upper bounds, as it will for the example we given in Section 7.

5 Generators and relations for $\mathfrak{su}(2^n)$

In this section, we give a set of generators of $\mathfrak{su}(2^n)$ as a Lie algebra and determine a complete set of relations which these generators satisfy. The proof starts by first defining the generators, of which there are $O(n^2)$. Then for each k -local Pauli operator $O \in \mathfrak{su}(2^n)$ we define a canonical Lie polynomial in generators which is sent to O . We then define a set of relations in the generators such that any Lie polynomial in the generators is equivalent to a linear combination of the expressions corresponding to k -local Pauli operators defined previously. The proof amounts to a series of induction arguments which iteratively rewrite a given Lie polynomial into a normal form.

Warning 6. In this section (and only in this section), we adopt the convention that the Pauli matrices are given by

$$\sigma^1 = \frac{i}{2}X \qquad \sigma^2 = \frac{i}{2}Y \qquad \sigma^3 = \frac{i}{2}Z$$

so that the commutation relations $[\sigma^a, \sigma^b]$ satisfy commutation relations only involving ± 1 , without additional factors of i or 2 . This simplifies the notation in our proof, which is already quite dense. Later sections defining the full hierarchy will use the usual convention for the Pauli matrices, while referring back to the Lie algebra relations defined here (which must be taken with the appropriate constant factors included).

5.1 Definition and set-up

Let $n \geq 1$ be an integer.

Definition 7. Denote by $\mathfrak{f}_n$ the free Lie algebra generated by the symbols S_i^a and T_{ij}^{ab} for $1 \leq i < j \leq n$ and $a, b \in \{1, 2, 3\}$. We define a Lie algebra homomorphism $f_n : \mathfrak{f}_n \rightarrow \mathfrak{su}(2^n)$ by

$$f_n(S_i^a) = \sigma_i^a \qquad f_n(T_{ij}^{ab}) = \sigma_i^a \sigma_j^b.$$

Our goal in this section is to determine the kernel of the homomorphism f_n , or in other words to determine all Lie algebra relations satisfied by the images of the generators of $\mathfrak{f}_n$ in $\mathfrak{su}(2^n)$. To this end, we will define a set of distinguished elements of $\mathfrak{f}_n$, along with a linear map $g_n : \mathfrak{su}(2^n) \rightarrow \mathfrak{f}_n$ which is a one-sided inverse of f_n , that is $f_n \circ g_n = \text{id}_{\mathfrak{su}(2^n)}$. After defining g_n , we will show that there is a set of relations of polynomial size such that the quotient of $\mathfrak{f}_n$ by these relations is isomorphic to $\mathfrak{su}(2^n)$, with the isomorphisms being given by the induced maps of f_n and g_n .

Definition 8. We define A_n to be the set containing each S_i^a for $1 \leq i \leq n$, and all expressions of the form

$$[[\dots [[S_{i_1}^{b_1}, T_{i_1 i_2}^{a_1 b_2}], T_{i_2 i_3}^{a_2 b_3}], \dots], T_{i_{m-1} i_m}^{a_{m-1} b_m}]$$

where $i_1 < i_2 < \dots < i_m$ and b_i is always before a_i in the cyclic order on $\{1, 2, 3\}$, or equivalently $(b_i, a_i) \in \{(1, 2), (2, 3), (3, 1)\}$. We define a linear map $g_n : \mathfrak{su}(2^n) \rightarrow \mathfrak{f}_n$ by first defining

$$g_n(\sigma_i^a) = S_i^a$$

$$g_n(\sigma_{i_1}^{c_1} \dots \sigma_{i_m}^{c_m}) = [[\dots [[S_{i_1}^{b_1}, T_{i_1 i_2}^{a_1 b_2}], T_{i_2 i_3}^{a_2 b_3}], \dots], T_{i_{m-1} i_m}^{a_{m-1} b_m}]$$

for all $i_1 < i_2 < \dots < i_m$, where $b_m = c_m$, and (a_j, b_j) is the unique element of $\{(1, 2), (2, 3), (3, 1)\}$ not containing c_j . The definition of g_n is then extended linearly. We also define g'_n similarly by $g'_n(\sigma_i^a) = S_i^a$ and

$$g'_n(\sigma_{i_1}^{c_1} \dots \sigma_{i_m}^{c_m}) = [[\dots [[T_{i_1 i_2}^{c_1 b_2}, T_{i_2 i_3}^{a_2 b_3}], T_{i_3 i_4}^{a_3 b_4}], \dots], T_{i_{m-1}, i_m}^{a_{m-1} b_m}]$$

For completeness, we include the following proof that f_n is surjective. The proof is likely standard and is similar to the proof that quantum circuits built from 1- and 2-local unitary gates can approximate any n -qubit unitary.

Proposition 9. *For any element $x \in \mathfrak{su}(2^n)$, we have $f_n(g_n(x)) = x$ and $f_n(g'_n(x)) = x$.*

Proof. By linearity, it suffices to check the statement for Pauli strings. We prove the statement by induction on the cardinality m of the support of a given Pauli string. The base case $m = 1$ is clear. For the induction step, let $\sigma_{i_1}^{c_1} \dots \sigma_{i_m}^{c_m}$ be a given Pauli string. Let $(b_{m-1}, a_{m-1}) \in \{(1, 2), (2, 3), (3, 1)\}$ such that neither are equal to c_{m-1} . Applying the induction hypothesis to $\sigma_{i_1}^{c_1} \dots \sigma_{i_{m-2}}^{c_{m-2}} \sigma_{i_{m-1}}^{b_{m-1}}$ gives

$$f_n([\dots [[S_{i_1}^{b_1}, T_{i_1 i_2}^{a_1 b_2}], T_{i_2 i_3}^{a_2 b_3}], \dots], T_{i_{m-2}, i_{m-1}}^{a_{m-2} b_{m-1}}]) = \sigma_{i_1}^{c_1} \dots \sigma_{i_{m-2}}^{c_{m-2}} \sigma_{i_{m-1}}^{b_{m-1}}$$

so

$$\begin{aligned} & f_n([\dots [[S_{i_1}^{b_1}, T_{i_1 i_2}^{a_1 b_2}], T_{i_2 i_3}^{a_2 b_3}], \dots], T_{i_{m-1}, i_m}^{a_{m-1} c_m}) \\ &= [f_n([\dots [[S_{i_1}^{b_1}, T_{i_1 i_2}^{a_1 b_2}], T_{i_2 i_3}^{a_2 b_3}], \dots], T_{i_{m-2}, i_{m-1}}^{a_{m-2} b_{m-1}}]), f_n(T_{i_{m-1}, i_m}^{a_{m-1} c_m})] \\ &= [\sigma_{i_1}^{c_1} \dots \sigma_{i_{m-2}}^{c_{m-2}} \sigma_{i_{m-1}}^{b_{m-1}}, \sigma_{i_{m-1}}^{a_{m-1}} \sigma_{i_m}^{c_m}] \\ &= \sigma_{i_1}^{c_1} \dots \sigma_{i_{m-2}}^{c_{m-2}} [\sigma_{i_{m-1}}^{b_{m-1}}, \sigma_{i_{m-1}}^{a_{m-1}}] \sigma_{i_m}^{c_m} \\ &= \sigma_{i_1}^{c_1} \dots \sigma_{i_m}^{c_m} \end{aligned}$$

finishing the induction step. A similar induction argument shows that $f_n(g'_n(x)) = x$. $\square$

We can now use g_n and g'_n to define the relations we will use.

Definition 10. Define the following system of noncommutative polynomial equations in the generators of $\mathfrak{f}_n$, which is also a system of Lie polynomial equations:

$$[S_i^a, S_j^b] = \delta_{ij} \sum_c \epsilon_{abc} S_i^c \tag{1a}$$

$$[S_i^a, T_{ij}^{bc}] = \delta_{ij} \sum_d \epsilon_{abd} T_{jk}^{dc} + \delta_{ik} \sum_d \epsilon_{acd} T_{jk}^{dc} \tag{1b}$$

$$[T_{ij}^{ab}, T_{kl}^{cd}] = \begin{cases} -[T_{kj}^{cb}, T_{il}^{ad}] & i = k, j \neq l \\ -[T_{ik}^{ac}, T_{jl}^{bd}] & j = k, i \neq l \\ -[T_{il}^{ad}, T_{kj}^{cb}] & j = l, i \neq k \end{cases} \tag{1c}$$

$$[T_{ij}^{ab}, T_{kl}^{cd}] = \begin{cases} \sum_e \epsilon_{bde} S_j^e & i = k, j = l, a = c, b \neq d \\ \sum_e \epsilon_{ace} S_i^e & i = k, j = l, a \neq c, b = d \\ 0 & \text{otherwise} \end{cases} \tag{1d}$$

$$[[T_{ij}^{ab}, T_{kl}^{cd}], T_{rs}^{ef}] = g'_n(f_n([T_{ij}^{ab}, T_{kl}^{cd}], T_{rs}^{ef})) \quad (1e)$$

$$[[[T_{ij}^{ab}, T_{kl}^{cd}], T_{rs}^{ef}], T_{tu}^{gh}] = g'_n(f_n([[[T_{ij}^{ab}, T_{kl}^{cd}], T_{rs}^{ef}], T_{tu}^{gh}])) \quad (1f)$$

$$[[S_i^a, T_{jk}^{bc}], T_{lr}^{de}] = g_n(f_n([S_i^a, T_{jk}^{bc}], T_{lr}^{de})). \quad (1g)$$

Remark 11. The first four families of relations can also be written as $x = g_n(f_n(x))$ or $x = g'_n(f_n(x))$ for a given element $x \in \mathfrak{f}_n$, but for clarity we have chosen to write them out explicitly.

Definition 12. We denote by $\mathfrak{g}_n$ the Lie algebra which is the quotient of $\mathfrak{f}_n$ by the relations in Equation 1.

While the relations defined in Equation 1 may be difficult to read, the proof that the homomorphism f_n is well-defined will help motivate where each of the relations comes from.

Proposition 13. *The homomorphism $f_n : \mathfrak{f}_n \rightarrow \mathfrak{su}(2^n)$ induces a well-defined homomorphism $\mathfrak{g}_n \rightarrow \mathfrak{su}(2^n)$.*

Proof. It suffices to check that f_n sends both sides of each relations to the same element of $\mathfrak{su}(2^n)$. The relation in Equation 1a states that $[\sigma_i^a, \sigma_j^b]$ is 0 if $i \neq j$ and otherwise the appropriate Pauli operator on site i . The relation in Equation 1b states that the commutator of a 1-local and a 2-local Pauli operator is 0 if they commute, and otherwise the other 2-local Pauli operator if the supports intersect each other.

The relation in Equation 1c states that the commutator of two 2-local Pauli operators can be written as another commutator of two 2-local Pauli operators when the supports intersect on a single site; in this case we have

$$[\sigma_i^a \sigma_j^b, \sigma_j^c \sigma_k^d] = \sigma_i^a [\sigma_j^b, \sigma_j^c] \sigma_k^d = -\sigma_i^a [\sigma_j^c, \sigma_j^b] \sigma_k^d = -[\sigma_i^a \sigma_j^c, \sigma_j^b \sigma_k^d]$$

and similarly for the other cases. When both supports are the same, as in Equation 1d, either the two operators commute or on one of the sites the operators are the same and on the other they are different; in the first case the commutator is zero, and in the second we have

$$[\sigma_i^a \sigma_j^b, \sigma_i^a \sigma_j^c] = (\sigma_i^a)^2 \sigma_j^b \sigma_j^c - (\sigma_i^a)^2 \sigma_j^c \sigma_j^b = [\sigma_j^b, \sigma_j^c]$$

which is a 1-local Pauli operator.

For the final relation in Equation 1e, we have $f_n(g'_n(f_n(x))) = f_n(x)$ by applying Proposition 9. (The same argument works for the other relations if they are written in a similar manner.) $\square$

5.2 Proof of completeness of the relations

The following lemma is standard, but we prove it for completeness.

Lemma 14. *If $x, y \in \mathfrak{f}_n$, then $[x, y]$ can be written as a linear combination of expressions of the form $[\dots [x, z_1], z_2], \dots, z_m]$ where $z_1, \dots, z_m$ are one of the generators of $\mathfrak{f}_n$.*

Proof. The element $y \in \mathfrak{f}_n$ can be written as a Lie polynomial in the generators, which is an expression constructed inductively as either one of the generators or a commutator of two such expressions. We use induction on the depth of the expression to prove the lemma. The base case

is when y itself is a generator, which holds vacuously. For the induction step, let $y = [y_1, y_2]$. Then the Jacobi identity gives

$$\begin{aligned} [x, y] &= [x, [y_1, y_2]] \\ &= [[x, y_1], y_2] - [[x, y_2], y_1]. \end{aligned}$$

For the first term, the induction hypothesis allows us to write $[x, y_1]$ as a linear combination of terms of the form $x_i = [\cdots [[x, z_1], z_2], \dots, z_{m'}]$. The induction hypothesis can then be applied to each $[x_i, y_2]$ and y_2 , and taking an appropriate linear combination shows that $[[x, y_1], y_2]$ can be written as an expression of the desired form. A similar argument holds for $[[x, y_2], y_1]$. $\square$

Our goal is to show that any element in $\mathfrak{g}_n$ is equal to a linear combination of elements of A under the relations from Equation 1. We will split the proof into several lemmas.

Lemma 15. *Let $x \in A$ be a given element written as*

$$x = [[\cdots [[S_{i_1}^{b_1}, T_{i_1 i_2}^{a_1 b_2}], T_{i_2 i_3}^{a_2 b_3}], \dots], T_{i_{m-1} i_m}^{a_{m-1} b_m}].$$

Let g be a given generator and k be the largest index such that i_k is equal to a subscript of g . If such a k does not exist then in $\mathfrak{g}_n$ we have that $[x, g] = 0$ and otherwise

$$[x, g] = [[\cdots [[[[\cdots [[S_{i_1}^{b_1}, T_{i_1 i_2}^{a_1 b_2}], T_{i_2 i_3}^{a_2 b_3}], \dots], T_{i_k i_{k+1}}^{a_k b_{k+1}}], g], T_{i_{k+1} i_{k+2}}^{a_{k+1} b_{k+2}}], \dots], T_{i_{m-1} i_m}^{a_{m-1} b_m}].$$

Proof. We use induction. The Jacobi rule shows for any elements x, y, z that

$$[x, [y, z]] = [[x, y], z] + [y, [x, z]].$$

In particular, if $[x, y] = 0$ then $[x, [y, z]] = [y, [x, z]]$. From the relations in Equation 1 we see that if g and h are generators where the indices in the subscripts are disjoint, then $[g, h] = 0$. Inductively applying this equality then proves the lemma. $\square$

Lemma 16. *Suppose a given expression x contains only indices strictly less than some integer M and that $i < j \leq k < l$ with $k > M$. Then*

$$[[x, y], T_{kl}^{cd}] = [x, [y, T_{kl}^{cd}]].$$

Proof. We have

$$\begin{aligned} [[x, y], T_{kl}^{cd}] &= [[x, T_{kl}^{cd}], y] + [x, [y, T_{kl}^{cd}]] \\ &= [x, [y, T_{kl}^{cd}]] \end{aligned}$$

since the first term is zero by Lemma 15 and the assumption that $k > M$. $\square$

Lemma 17. *Suppose a given expression x contains only indices strictly less than some integer M and that $i < j \leq k < l$ with $k > M$. Then*

$$[[x, T_{ij}^{ab}], T_{jk}^{cd}] = -[[x, T_{ij}^{ac}], T_{jk}^{bd}]$$

Proof. Using Lemma 16, we have

$$\begin{aligned} [[x, T_{ij}^{ab}], T_{jk}^{cd}] &= [x, [T_{ij}^{ab}, T_{jk}^{cd}]] \\ &= [x, -[T_{ij}^{ac}, T_{jk}^{bd}]] \\ &= -[[x, T_{ij}^{ac}], T_{jk}^{bd}] \end{aligned}$$

using Equation 1c in the second line and Lemma 16 again in the third. $\square$

Lemma 18. *If $x \in A$, then $[x, S_i^a]$ is a linear combination of elements from A .*

Proof. If i does not appear in any subscript in the expression for x , then by Lemma 15 the commutator is 0. If it appears as the smallest index, then by Lemma 15 we can write

$$[x, S_i^a] = [[\dots [[S_{i_1}^{b_1}, S_{i_1}^a], T_{i_1 i_2}^{a_1 b_2}], T_{i_2 i_3}^{a_2 b_3}], \dots], T_{i_{m-1} i_m}^{a_{m-1} b_m}].$$

We can then apply Equation 1a to simplify the innermost commutator. If the cyclic ordering condition does not hold for the resulting innermost commutator, we can apply Equation 1b so that it does, possibly negating the expression.

If i appears as the largest index, then similarly we can write $x = [x', T_{ji}^{bc}]$ and get

$$\begin{aligned} [x, S_i^a] &= [[x', T_{ji}^{bc}], S_i^a] \\ &= [[x', S_i^a], T_{ji}^{bc}] + [x', [T_{ji}^{bc}, S_i^a]] \\ &= [x', [T_{ji}^{bc}, S_i^a]] \end{aligned}$$

which can then be simplified using Equation 1b. If it appears as some index which is neither the smallest nor largest, then we apply Lemma 15. Working just with the part of the expression with the commutator involving S_i^a , we have a commutator of the form

$$\begin{aligned} &[[[x', T_{ji}^{bc}], T_{ik}^{de}], S_i^a] \\ &= [[x', T_{ji}^{bc}], [T_{ik}^{de}, S_i^a]] + [[x', [T_{ji}^{bc}, S_i^a]], T_{ik}^{de}] + [[[x', S_i^a], T_{ji}^{bc}], T_{ik}^{de}] \\ &= [[x', T_{ji}^{bc}], [T_{ik}^{de}, S_i^a]] + [[x', [T_{ji}^{bc}, S_i^a]], T_{ik}^{de}] \end{aligned}$$

applying Lemma 15 again. By applying Equation 1b both of the resulting expressions can be simplified, and by Lemma 17 we can guarantee the cyclic ordering condition holds. Since the bracket is bilinear, we can apply the same argument when the part of the expression outside of the commutator involving S_i^a is included. $\square$

Lemma 19. *If $x \in A$ and T_{ij}^{ab} is such that only i and not j appears in a subscript in the expression for x , then $[x, T_{ij}^{ab}]$ is a linear combination of elements of A .*

Proof. If i appears as the largest index, then the lemma follows directly. Thus we assume that i does not appear as the largest index.

Applying Lemma 15, we use induction on the number of commutators outside the position where T_{ij}^{ab} was put. For the case when T_{ij}^{ab} is put at the innermost level, we apply Equation 1g. Otherwise, working just with the commutator involving T_{ij}^{ab} , we have an expression of the form

$$[[[x', T_{ki}^{cd}], T_{il}^{ef}], T_{ij}^{ab}] = [[x', [T_{ki}^{cd}, T_{il}^{ef}]], T_{ij}^{ab}]$$

$$= [x', [[T_{ki}^{cd}, T_{il}^{ef}], T_{ij}^{ab}]]$$

by applying Lemma 16 twice. Applying Equation 1e, the second factor in the commutator can be rewritten so that the indices in the subscripts appear in order. Then applying Lemma 16 twice again in reverse, we obtain an expression which is a linear combination of elements of A .

For the commutators at the outer levels, we do the following. Suppose using the notation of Lemma 15 that T_{ij}^{ab} was put at level k . Then, after having applied the above rewriting, $T_{i_{k+1}, i_{k+2}}^{a_{k+1}, b_{k+2}}$ has its first subscript included in the rewritten expression and not the second subscript. Concretely, including the commutator at level $k+1$ we have either an expression of the form

$$[[[x', T_{ki}^{ab}], T_{ij}^{cd}], T_{jl}^{ef}], T_{lr}^{gh}]$$

if $j < l$, or

$$[[[x', T_{ki}^{ab}], T_{il}^{cd}], T_{lj}^{ef}], T_{lr}^{gh}]$$

if $j > l$, where l, r, g, h are chosen such that $T_{lr}^{gh} = T_{i_{k+1}, i_{k+2}}^{a_{k+1}, b_{k+2}}$. Thus the same rewriting can be applied inductively to $T_{i_{k+1}, i_{k+2}}^{a_{k+1}, b_{k+2}}$ and the rewritten expression, with the base case being that T_{ij}^{ab} was put at the outermost level to begin with. $\square$

Lemma 20. *If $x \in A$ and T_{ij}^{ab} is such that only j and not i appears in a subscript in the expression for x , then $[x, T_{ij}^{ab}]$ is a linear combination of elements of A .*

Proof. Let k be such that $i_k < i < i_{k+1}$. We use induction on the number of indices in between i_k and the position where j appears in the expression for x . For the case when j is already the smallest index appearing in x , we can apply Equation 1g. Otherwise we have an expression of the form

$$\begin{aligned} [[x', T_{rj}^{ab}], T_{jl}^{cd}], T_{ij}^{ef}] &= [[x', [T_{rj}^{ab}, T_{jl}^{cd}]], T_{ij}^{ef}] \\ &= [x', [[T_{rj}^{ab}, T_{jl}^{cd}], T_{ij}^{ef}]] \end{aligned}$$

by applying Lemma 16 twice. Applying Equation 1e, the second factor can be rewritten so that the indices in the subscripts appear in order. Then applying Lemma 16 twice again in reverse, we get an expression of the form

$$[[[x', T_{ir}^{ab}], T_{rj}^{cd}], T_{jl}^{ef}]$$

and can then apply the induction hypothesis to T_{ir}^{ab} and x' . The base case is when the commutator involving j already included i , in which case one can apply Equation 1d.

For the outer commutators which are outside the position where index j appears, applying Lemma 15 and bilinearity of the Lie bracket then finishes the proof of the lemma. $\square$

Lemma 21. *If $x \in A$ and T_{ij}^{ab} is such that both i and j appear in a subscript in the expression for x , then $[x, T_{ij}^{ab}]$ is a linear combination of elements of A .*

Proof. We use induction on the number of indices in between i and j which appear in the expression for x . For the base case when there are no such indices, using Lemma 15 to work just with the relevant inner part gives an expression of the form

$$[[[x', T_{ki}^{cd}], T_{ij}^{ef}], T_{jl}^{gh}], T_{ij}^{ab}] = [[x', [T_{ki}^{cd}, T_{ij}^{ef}]], T_{jl}^{gh}], T_{ij}^{ab}]$$

$$\begin{aligned}
&= [[x', [[T_{ki}^{cd}, T_{ij}^{ef}], T_{jl}^{gh}], T_{ij}^{ab}] \\
&= [x', [[[[T_{ki}^{cd}, T_{ij}^{ef}], T_{jl}^{gh}], T_{ij}^{ab}]]
\end{aligned}$$

applying Lemma 16 three times. Then using Equation 1f and applying Lemma 16 three times again in reverse gives an expression which is a linear combination of elements of A .

For the induction step, we use Lemma 16 twice to combine the commutators where i and j appear, obtaining an expression of the form

$$[[\cdots [x', [T_{ki}^{cd}, T_{il}^{ef}]], \cdots], [T_{rj}^{gh}, T_{js}^{\alpha\beta}]]$$

ignoring the parts of the expression involving indices larger than j . By the Jacobi rule and Lemma 15, taking the commutator of this expression with T_{ij}^{ab} gives an expression of the form

$$[\cdots [x', [[T_{ki}^{cd}, T_{il}^{ef}], T_{ij}^{ab}]], \cdots] + [\cdots [x', [T_{ki}^{cd}, T_{il}^{ef}]], \cdots], [[T_{rj}^{gh}, T_{js}^{\alpha\beta}], T_{ij}^{ab}].$$

We inductively rewrite the two terms separately. For the second, we again use Equation 1e similarly as in the induction steps of Lemma 19 and Lemma 20, along with Lemma 16 used in reverse twice to obtain an expression of the form

$$[[[[\cdots [x', [T_{ki}^{cd}, T_{il}^{ef}]], \cdots], T_{ir}^{ab}], T_{rj}^{cd}], T_{js}^{ef}]$$

and then the induction hypothesis can be applied to the inner expression and T_{ir}^{ab} . For the first term, we apply a similar argument to obtain an expression of the form

$$[[[x', T_{ki}^{ab}], T_{il}^{ef}], T_{lj}^{gh}]$$

in the inner part, after which the same argument can be applied inductively with T_{lj}^{gh} and the rest of the expression on the outside. $\square$

Proposition 22. *The kernel of the homomorphism $\mathfrak{g}_n \rightarrow \mathfrak{su}(2^n)$ induced by f_n is 0.*

Proof. From Proposition 13, we know that the induced map is surjective. Thus it suffices to show that the dimension of $\mathfrak{g}_n$ as a vector space is finite and bounded above by $\dim \mathfrak{su}(2^n) = 4^n - 1$. To this end, we claim that any element of $\mathfrak{g}_n$ is a linear combination of elements from the set A , each of which are written in a particular normal form. Concretely, each element of A is the image of a Pauli operator under g_n , and is sent to an m -local Pauli operator under f_n .

As in Lemma 14, we use induction on the depth of the Lie polynomials defining the given elements. The base case is when the expression is one of the generators. For the induction step, we consider a commutator of the form $[x, y]$. The induction hypothesis implies that x and y are equal to linear combinations of elements of A . By linearity, it then suffices to consider the commutator of two elements of A . We proceed by cases on the type of element of A . The commutator of two generators of the form S_i^a and S_j^b is another such generator or 0.

For the second case, we consider the commutator of S_i^a and an element of A . Then Lemma 18 shows that this is a linear combination of elements of A .

Finally, we consider the commutator of two elements of A which are both not generators. Then Lemma 14 implies that it suffices to consider the commutator of an element of A with a generator T_{ij}^{ab} or S_i^a . The second case follows from Lemma 18 as before, and the first follows from either Lemma 15, Lemma 20, Lemma 19, or Lemma 21 depending on whether i or j are included in the subscripts in the element of A or not. $\square$

Combining the two propositions gives the following theorem.

Theorem 23. *The homomorphism f_n induces an isomorphism of Lie algebras $\mathfrak{g}_n \cong \mathfrak{su}(2^n)$.*

6 The hierarchy

We will define an SDP hierarchy of lower bounds on $\lambda_1(H) + \lambda_2(H)$ as the NPA hierarchy associated to a given system of noncommutative polynomial equations. The set of variables is

$$V_n := \{S_i^a : i \in [n], a \in [3]\} \cup \{T_{ij}^{ab} : i, j \in [n], a, b \in [3]\}$$

subject to the noncommutative constraints

$$\text{all Lie algebra relations from Equation 1} \tag{2a}$$

$$(S_i^a)^* = S_i^a \tag{2b}$$

$$0 = S_j^a(S_j^a - 2)(S_j^a + 2) \tag{2c}$$

$$C_4 \geq \sum_{a,b \in [3]} (T_{ij}^{ab})^* T_{ij}^{ab} \tag{2d}$$

$$8(n-1) \geq \sum_{i=1}^n \sum_{a=1}^3 (S_i^a)^* S_i^a \tag{2e}$$

where C_4 is the eigenvalue of the quadratic Casimir operator, acting on the irreducible representation $\wedge^2(\mathbb{C}^4)$ of $SU(4)$.

6.1 Encoding a higher-locality Hamiltonian

Encoding a k -local Hamiltonian for $k \geq 3$ is somewhat more nontrivial than in the usual case. For computing ground energies of local Hamiltonians, one typically thinks of $\mathcal{B}(\mathbb{C}^{2^n})$ as being generated by 1-local Pauli operators satisfying certain relations, and then a k -local Hamiltonian can be written as a degree- k noncommutative polynomial in the 1-local Pauli generators.

In our hierarchy, while there do exist generators S_i^a corresponding in some sense to 1-local Pauli operators, thinking of a k -local Hamiltonian H as a polynomial in the S_i^a will not give the correct result. The final goal is to bound the action $P_{\wedge^2(\mathbb{C}^{2^n})}(H \otimes I + I \otimes H)P_{\wedge^2(\mathbb{C}^{2^n})}$ of H on the antisymmetric subspace, which is general not equal to a noncommutative polynomial in the S_i^a even if H is. One instead needs to write H as a linear combination of Pauli terms, and then use either the map g_n or g'_n to write each Pauli term as an expression involving commutators in the S_i^a and T_{ij}^{ab} . For Hamiltonians with only 1- and 2-local terms, which are some of the most common and important examples, the resulting expressions end up just being linear combinations of the generators S_i^a and T_{ij}^{ab} .

More conceptually, the action of H on the antisymmetric subspace is given by a representation of the Lie algebra $\mathfrak{su}(2^n)$. In order to write this in a “low-degree” way, one should write H as an element of $\mathfrak{su}(2^n)$ using its generators and the Lie bracket, which when combined with the other relations implies that one gets the corresponding action of H on the antisymmetric subspace. In contrast, writing it as a noncommutative polynomial in the S_i^a treats the underlying algebra as the $*$ -algebra of operators on $\mathbb{C}^{2^n}$, which does not give the Lie algebra action on the antisymmetric subspace.

6.2 Proof of asymptotic convergence

To prove asymptotic convergence of the hierarchy, it suffices (by asymptotic convergence of the general NPA hierarchy) to consider irreducible representations of the $*$ -algebra defined by the generators in V and corresponding relations. The proof will consist of using the Lie algebra relations to show that any irreducible representation of this algebra is also canonically an irreducible representation of the Lie algebra $\mathfrak{su}(2^n)$, and then using the following propositions to deduce which irreducible representation it must be.

Proposition 24. *Consider $\mathbb{C}^{2^n}$ as the tensor product of the standard representations of n copies of $SU(2)$. Then we have*

$$\begin{aligned}\mathrm{Sym}^2(\mathbb{C}^{2^n}) &\cong \bigoplus_{\substack{v \in \{0,2\}^n \\ |v|=n \pmod 2}} \bigotimes_{i=1}^n \mathrm{Sym}^{v_i}(\mathbb{C}^2) \\ \wedge^2(\mathbb{C}^{2^n}) &\cong \bigoplus_{\substack{v \in \{0,2\}^n \\ |v|=n-1 \pmod 2}} \bigotimes_{i=1}^n \mathrm{Sym}^{v_i}(\mathbb{C}^2)\end{aligned}$$

as representations of $SU(2)^n$, where $|v|$ denotes the L^1 -norm of an integer vector, and $\bigotimes_{i=1}^n V_i$ denotes the $SU(2)^n$ representation which is the tensor product of n representations V_i of $SU(2)$.

Proof. By Schur-Weyl duality, we have

$$V^{\otimes 2} \cong 1_{S_2} \otimes \mathrm{Sym}^2(V) \oplus \mathrm{sgn}_{S_2} \wedge^2(V)$$

where 1_{S_2} and sgn_{S_2} denote the trivial and sign representations of S_2 . When $V \cong \mathbb{C}^2$ we have $\wedge^2(V) \cong 1 \cong \mathrm{Sym}^0(\mathbb{C}^2)$, the trivial representation of $SU(2)$. This gives

$$\begin{aligned}\mathrm{Sym}^2(\mathbb{C}^{2^n}) &\cong \left(\left(\bigotimes_{i=1}^n \mathbb{C}^2 \right)^{\otimes 2} \otimes 1_{S_2} \right)^{S_2} \\ &\cong \left(1_{S_2} \otimes \bigotimes_{i=1}^n (\mathbb{C}^2)^{\otimes 2} \right)^{S_2} \\ &\cong \left(1_{S_2} \otimes \bigotimes_{i=1}^n (1_{S_2} \otimes \mathrm{Sym}^2(\mathbb{C}^2) \oplus \mathrm{sgn}_{S_2} \otimes \mathrm{Sym}^0(\mathbb{C}^2)) \right)^{S_2} \\ &\cong \left(\bigoplus_{v \in \{0,2\}^n} \mathrm{sgn}_{S_2}^{|v|/2} \otimes \bigotimes_{i=1}^n \mathrm{Sym}^{v_i}(\mathbb{C}^2) \right)^{S_2} \\ &\cong \bigoplus_{\substack{v \in \{0,2\}^n \\ |v|=n \pmod 2}} \bigotimes_{i=1}^n \mathrm{Sym}^{v_i}(\mathbb{C}^2).\end{aligned}$$

Similarly, we have

$$\begin{aligned}\wedge^2(\mathbb{C}^{2^n}) &\cong \left(\text{sgn}_{S_2} \otimes \bigotimes_{i=1}^n (1_{S_2} \otimes \text{Sym}^2(\mathbb{C}^2) \oplus \text{sgn}_{S_2} \otimes \text{Sym}^0(\mathbb{C}^2)) \right)^{S_2} \\ &\cong \bigoplus_{\substack{v \in \{0,2\}^n \\ |v|=n-1 \pmod 2}} \bigotimes_{i=1}^n \text{Sym}^{v_i}(\mathbb{C}^2).\end{aligned}$$

□

Proposition 25. *Suppose $\mathcal{H}$ is a Hilbert space with a unitary action of the Lie group $SU(2^n)$. Consider the associated action of the Lie algebra $\mathfrak{su}(2^n)$ and the restriction to the 1- and 2-local Pauli operators in the image of f_n . If the corresponding actions of the generators in V_n satisfy Equation 2, then $\mathcal{H} \cong \mathcal{H}' \otimes \wedge^2(\mathbb{C}^{2^n})$ as representations of $SU(2^n)$, where $\mathcal{H}'$ has the trivial action.*

Proof. We first consider the case where $\mathcal{H}$ is an irreducible representation of $SU(2^n)$. It suffices to prove the result in this case, since otherwise we can decompose $\mathcal{H}$ into irreducible representations and then deduce that no others can occur besides $\wedge^2(\mathbb{C}^{2^n})$. Thus let λ be a partition with at most $2^n - 1$ rows indexing the irreducible representation isomorphic to $\mathcal{H}$.

For notational convenience, let $m = 2^n$. We first claim that Equation 2c implies that λ is either (2) , $(1, 1)$, (1^{m-2}) , $(2, 1^{m-2})$, or (2^{m-1}) . (The notation 1^k or 2^k indicates that the corresponding partition has k rows of size 1 or 2, respectively.) To show this, let λ have C columns with $c_1, \dots, c_C$ boxes. On $\mathbb{C}^m$ the eigenvalues of S_i^a are ± 1 each with multiplicity $m/2$. The irreducible representation $S_\lambda(\mathbb{C}^m)$ has a basis indexed by semistandard Young tableaux T of shape λ and maximum entry 2^n , where each basis element is an eigenvector of the action of S_i^a and the corresponding eigenvalue is $\sum_{i \in T} \lambda_i$, where λ_i is the i -th eigenvalue of S_i^a acting on $\mathbb{C}^m$. In T the entries in each column must be strictly increasing and thus distinct, so the number of entries in column i contributing $+1$ is at most $\min(c_i, m/2)$ and the contribution to a possible eigenvalue of T is at most

$$\min(c_i, m/2) - (c_i - \min(c_i, m/2)) = 2 \min(c_i, m/2) - c_i.$$

Moreover, one can see that such a contribution is always possible by taking the entries in each column i to be consecutive integers from 1 to c_i . In particular, if there are $C \geq 3$ or more columns then there is an eigenvalue at least 3, contradicting Equation 2c, so there are at most 2 columns. For the maximum eigenvalue to be exactly 2 we must have that either one column contributes 2 to the sum, which means λ is either $(1, 1)$ or (1^{m-2}) , or there are two columns each contributing 1, so λ is either (2) , $(2, 1^{m-2})$, or (2^{m-1}) .

We now claim that Equation 2e implies that λ cannot be (2) or (2^{m-1}) . The highest weights of the two corresponding representations of $SU(m)$ differ by a vector whose entries are all m , so they give dual representations of $SU(m)$. The restrictions to $SU(2)^n$ are then isomorphic, and since Equation 2e only depends on the $SU(2)^n$ (or equivalently $\mathfrak{su}(2)^{\oplus n}$) action it suffices to just consider (2) . The right-hand side of Equation 2e acts as the scalar $\sum_{i=1}^n v_i/2$ on the $SU(2)^n$ irrep $\bigotimes_{i=1}^n \text{Sym}^{v_i}(\mathbb{C}^2)$, so by Proposition 24 it will have an eigenvalue of n on $S_{(2)}(\mathbb{C}^m) \cong \text{Sym}^2(\mathbb{C}^m)$.

We claim that a similar argument shows that λ cannot be $(2, 1^{m-2})$. It suffices to show that $S_{(2, 1^{m-2})}(\mathbb{C}^m)$ contains a copy of $\bigotimes_{i=1}^n \text{Sym}^2(\mathbb{C}^2)$. To prove this, it suffices to give a vector which is a simultaneous $+1$ eigenvector of S_i^1 for all $i \in [n]$, which is then a corresponding highest weight vector. Since the S_i^1 are simultaneously diagonalizable on $\mathbb{C}^m$, we can take the basis element

indexed by the Young tableau containing all elements but the simultaneous -1 eigenvector of the S_i^1 in the first column, and in the second column contains the simultaneous $+1$ eigenvector.

We finally claim that Equation 2d implies that λ cannot be (1^{m-2}) . To show this, we consider $S_{(1^{m-2})}(\mathbb{C}^m) \cong \wedge^{m-2}(\mathbb{C}^m)$ as a representation of $SU(4)^{n_1} \times SU(2)^{n_0}$, where $n = 2n_1 + n_0$ and $n_0 \in \{0, 1\}$. A similar argument as in the previous paragraph shows that it contains irreps where one of the tensor factors is an $SU(4)$ irrep with degree strictly greater than 2, implying that the Casimir operator of $SU(4)$ acts as a scalar with constant strictly greater than C_4 on that subspace, and so λ cannot be (1^{m-2}) . $\square$

The final step in the proof of asymptotic convergence is given by the following proposition.

Proposition 26. *Any irreducible representation of the algebra generated by the variables V_n satisfying the relations in Equation 2 is isomorphic to $\wedge^2(\mathbb{C}^{2^n})$, where the action of each of the variables S_i^a and T_{ij}^{ab} comes from the map $f_n : \mathfrak{f}_n \rightarrow \mathfrak{su}(2^n)$ and the Lie algebra action of $\mathfrak{su}(2^n)$ on $\wedge^2(\mathbb{C}^{2^n})$.*

Proof. Let $\mathcal{H}$ be a Hilbert space and identify each variable in V_n with an operator acting on $\mathcal{H}$, which together satisfy the constraints of Equation 2. Then by Theorem 23, there exists a unique Lie algebra homomorphism $\rho : \mathfrak{su}(2^n) \rightarrow \mathcal{H}$ such that $\rho \circ f$ sends each variable to its original action on $\mathcal{H}$ and such that $\rho(g)$ is anti-self-adjoint for each $g \in \mathfrak{su}(2^n)$. Such irreps are in bijection with irreps of $SU(2^n)$, and the action of each generator S_i^a or T_{ij}^{ab} is the corresponding Lie algebra action. The action of any Lie polynomial in the generators is again the Lie algebra action, since the generators generate all of $\mathfrak{su}(2^n)$. By Proposition 25, the additional constraints force the irrep of $\mathfrak{su}(2^n)$ to be the antisymmetric subspace $\wedge^2(\mathbb{C}^{2^n})$. $\square$

Remark 27 (Finite convergence). While above we have applied the standard proof of asymptotic convergence of the NPA hierarchy, it is in fact true that the hierarchy converges at a finite level. One can see this by noting that generating $\mathfrak{su}(2^n)$ using our given generating set uses only commutators of depth at most n , and such commutators expand to noncommutative polynomials of degree at most n . In particular, a linear basis for the $*$ -algebra defined by our generators is given by such commutator expressions, and standard argument then imply that the hierarchy must converge at level n .

7 Using the hierarchy to certify a nontrivial bound

In this section, we show that the hierarchy can certify a nontrivial lower bound on the spectral gap of the 1-local frustration-free Hamiltonian

$$H_n := - \sum_{i=1}^n Z_i.$$

Of course, this particular Hamiltonian is explicitly diagonalizable on the standard basis, with any standard basis vector of Hamming weight k having eigenvalue $n - 2k$, and the spectral gap is easily seen to be 2. We use it simply as an example where the hierarchy gives a nontrivial (that is, nonzero) lower bound on the spectral gap.

First, note that the constraint $Z_i(Z_i - 2)(Z_i + 2) = 0$ implies that any univariate polynomial in a single Z_i is a degree-4 SOS up to the given relations if it is positive on the set $\{-2, 0, 2\}$, using standard facts about univariate polynomials. In particular, $Z_i^* Z_i - 2Z_i$ is a degree-4 SOS.

Next, we have

$$\begin{aligned}
(X_j + iY_j)^*(X_j + iY_j) &= X_j^*X_j + Y_j^*Y_j + iX_j^*Y_j - iY_j^*X_j \\
&= X_j^*X_j + Y_j^*Y_j + i[X_j, Y_j] \\
&= X_j^*X_j + Y_j^*Y_j - 2Z_j
\end{aligned}$$

again using the given relations, thus the right-hand side is a degree-2 SOS. (Very pedantically, we have

$$X_j^*X_j + Y_j^*Y_j - 2Z_j = (X_j + iY_j)^*(X_j + iY_j) + i(X_j - X_j^*)Y_j - i(Y_j - Y_j^*)X_j + i(2iZ_j - [X_j, Y_j])$$

as an explicit SOS expression for the right-hand side, using the given relations.) Summing the two inequalities over all n gives that

$$\begin{aligned}
&8(n-1) + 4H_n \\
&= 8(n-1) - 4 \sum_{j=1}^n Z_j \\
&= 8(n-1) - \sum_{j=1}^n (X_j^*X_j + Y_j^*Y_j + Z_j^*Z_j) + \sum_{j=1}^n (X_j^*X_j + Y_j^*Y_j - 2Z_j) + \sum_{j=1}^n (Z_j^*Z_j - 2Z_j)
\end{aligned}$$

is a degree-4 SOS. In particular, the hierarchy certifies that the action of H_n on the antisymmetric subspace has lowest eigenvalue at least $-2(n-1)$, matching the true value of $-n - (n-2)$.

To completely certify the bound, one should also bound the ground energy of H_n from above. There are a few options for doing this. The Lasserre hierarchy of upper bounds seems to have particularly slow convergence in this example, but at a sufficiently high level will certify a tight enough upper bound to obtain a nontrivial lower bound on the spectral gap. If one is willing to assume an exact upper bound for frustration-free Hamiltonians, as is done in [Rai+24], then combining it with the previous argument shows that the degree-4 relaxation certifies an exact lower bound on the spectral gap.

Alternatively, one can use the hierarchy of outer approximations to the singleton containing the ground state described in [FFS24]. Concretely, it is known that the hierarchy converges exactly at a finite level depending on the number of qubits. Since the given Hamiltonian is a sum of 1-local terms, taking a constant finite level of the hierarchy will give both exact upper and lower bounds on the ground state energy, which then gives an exact lower bound on the spectral gap when combined with the previous argument.

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