Improved Approximations for Extremal Eigenvalues of Sparse Hamiltonians

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─── **Abstract** ───

We give a classical $1/(qk+1)$-approximation for the maximum eigenvalue of a k-sparse fermionic Hamiltonian with strictly q-local terms, as well as a $1/(4k+1)$-approximation when the Hamiltonian has both 2-local and 4-local terms. More generally we obtain a $1/O(qk^2)$-approximation for k-sparse fermionic Hamiltonians with terms of locality at most q. Our techniques also yield analogous approximations for k-sparse, q-local qubit Hamiltonians with small hidden constants and improved dependence on q.

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Table 1 Main results contrasted with the previous state of the art.

	Hamiltonian	Our result	Previous result
fermionic	k-sparse, strictly q-local fermionic	$1/(qk+1)$	$1/\mathcal{O}(q^2k^2)$[5]
	k-sparse, $4, 2$-local	$1/(4k+1)$	$1/\mathcal{O}(k^2)$[5]
	k-sparse, q-local	$1/\mathcal{O}(qk^2)$	N/A
qubit	k-sparse, strictly q-local	$1/(qk+1)$	$3^{-q/2}/(4qk)$[3]
	k-sparse, 2-local	$1/(2k+1)$	$1/(24\mathrm{k})$[3]
	k-sparse, q-local	$1/\mathcal{O}(qk^2)$	$3^{-q/2}/(4qk)$[3]

1 Introduction

Finding the ground state energy of systems of particles is a fundamental problem of quantum mechanics. Finding the ground state energies of local Hamiltonians is believed to be difficult for both classical and quantum computers [7, 8]. Instead, it is often easier to find classical and quantum approximations to these ground state energies. In this paper, we consider approximations to the extremal eigenvalues of a local, k-sparse fermionic Hamiltonian:

$$H = \sum_{\Gamma} H_{\Gamma} c^{\Gamma}.$$

Here H is a fermionic Hamiltonian with real coefficients H_{Γ}, where ignoring phase factors, each term c^{Γ} is a product of q Majorana operators (i.e., H is q-local with q even) and each Majorana operator appears in at most k non-zero terms (i.e., H is k-sparse). We let $m = \sum_{\Gamma} |H_{\Gamma}|$.

Our main technical contribution is a carefully designed graph G, whose vertices correspond to the terms in H. We are able to construct states that achieve better approximations than in previous works by finding a suitably large independent set in G. This work is similar to (but distinct from) recent work by Herasymenko, Stroeks, Helsen, and Terhal [5] in which a similar graph is used to find *diffuse sets* of Majorana monomials from which they construct a state. Herasymenko et al. also work with a graph whose vertices correspond to the terms in H; however, their edge set is different. Our new edge set also allows us to generalize our results beyond the $q = 4, 2$ case handled by Herasymenko et al., and to prove better approximation ratios.

Table 1 summarizes our main results. We also list the previously known best results. The table is split into two sections: (1) fermionic Hamiltonians and (2) qubit Hamiltonians. Although our work does not focus on qubit Hamiltonians, our proof ideas furnish results that improve upon the previously known best results (see Sections 2 and 6).

2 Contextualizing our results

Bravyi, Gosset, Koenig, and Temme [2] were the first to suggest approximation algorithms for the largest eigenvalue of fermionic Hamiltonians using fermionic Gaussian states, achieving a $1/\mathcal{O}(n \log(n))$-approximation ratio for generic 4-local fermionic Hamiltonians. They also asked whether Gaussian states might provide a constant-factor approximation. Among other results, Hastings and O'Donnell [4] subsequently demonstrated that Gaussian states offer at best a $1/\Omega(\sqrt{n})$-approximation for a class of 4-local fermionic Hamiltonians, known as the Sachdev-Ye-Kitaev (SYK) model. Hamiltonians in the SYK model are dense 4-local Hamiltonians, hence the work of Hastings and O'Donnell left open the possibility of a

constant-factor Gaussian approximation algorithm for models with sparse Hamiltonians. Sparse Hamiltonians are a natural class of Hamiltonians to study. Examples, such as the Fermi-Hubbard model, are ubiquitous [6].

Recent work by Herasymenko, Stroeks, Helsen, and Terhal [5] proves the existence of such constant-factor approximations. They show that $\lambda_{\max}(H) \geq m/Q$, where $\lambda_{\max}(H)$ is the largest eigenvalue of H and $Q = q(q-1)(k-1)^2 + q(k-1) + 2$ for a k-sparse strictly q-local fermionic Hamiltonian. Herasymenko et al. also prove an improved ratio of $Q = 12(k+1)^2 + 4(k-1) + 2$ when specializing to k-sparse, $4,2$-local fermionic Hamiltonians. Our work directly improves upon these results (see Table 1). Our work also removes the conditions on system size present in Herasymenko et al. This leads to immediate improvements in Herasymenko et al.'s work on the sparse SYK model. All of the above results are obtained by efficient classical algorithms producing descriptions of Gaussian states. We refer the reader to [5] for further background, motivation, and applications to the SYK model. Finally, Herasymenko et al.'s result do not extend to k-sparse, q-local fermionic Hamiltonians (i.e., where all terms have locality *at most q*). To our knowledge, our $1/\mathcal{O}(qk^2)$ approximation is the first of this kind. It remains an open question whether this may be improved to $1/\mathcal{O}(qk)$.

Results of the above flavor were obtained for traceless k-sparse qubit Hamiltonians with constant locality by Harrow and Montanaro [3], who show that $\lambda_{\max}(H) \geq \Omega(m/k)$ using product states, where k-sparse and m are defined analogously as above; bounds upon which our ideas give a constant-factor improvement (see Table 1). They also give an improved bound with respect to the operator norm instead of the maximum eigenvalue: $\|H\| \geq \Omega(m/\sqrt{k})$. In the fermionic case, we give a 2-local example with $\lambda_{\max}(H) = \|H\| = \Theta(m/k)$, showing that such an improvement is not possible (see Section 7) and that our result for the strictly q-local case is tight. As noted in Table 1, our techniques also apply to the Hamiltonians considered by Harrow and Montanaro, yielding approximation guarantees with small hidden constants and improved dependence on q.

3   Preliminaries

In this section, we provide the necessary preliminaries for the rest of the work. We begin with an overview of fermionic Hamiltonians before providing the necessary background on Gaussian states. This section draws upon [5, 4, 1].

3.1   Fermionic Hamiltonians

Fermionic Hamiltonians describe systems of fermionic particles, such as electrons. For our purposes, it is easiest to express a fermionic Hamiltonian in terms of Majorana operators. Throughout, we use the notation $[n] := \{1, \ldots, n\}$. We also use the notation $\mathcal{E} = \{\Gamma \subseteq [n] \mid H_\Gamma \neq 0\}$ to denote the set of non-zero terms in a Hamiltonian.

▶ **Definition 1.** *Given n fermionic modes, a set of $2n$ traceless and Hermitian operators $\{c_i\}_{i=1}^{2n}$ are Majorana operators if they satisfy $c_i c_j + c_j c_i = 2\delta_{ij}$ for all $i, j \in [2n]$.*

▶ **Definition 2.** *Let $\{c_i\}$ be a collection of $2n$ Majorana operators endowed with an ordering (say the lexicographic ordering). A fermionic Hamiltonian has the form:*

$$H = \sum_{\Gamma \subseteq [2n]} H_\Gamma c^\Gamma, \tag{1}$$

where $\Gamma \subseteq [2n]$ has even order, c^Γ is the product of Majorana operators appearing in Γ (ordered lexicographically), and the $H_\Gamma \in \mathbb{R}$. Note that c^Γ may contain an additional pre-factor of i in order to satisfy hermiticity (e.g., when $|\Gamma| = 2$).

▶ **Definition 3.** *If H is a fermionic Hamiltonian defined in terms of $2n$ Majorana operators, then H is q-local if there exists $q \in \mathbb{N}$ such that each non-zero term in H has locality at most q, that is, for all $\Gamma \subseteq [2n]$ with $H_\Gamma \neq 0$, $|\Gamma| \leq q$. H is strictly q-local if $|\Gamma| = q$ for all non-zero summands.*

▶ **Definition 4.** *Let H be a fermionic Hamiltonian on $2n$ Majorana operators. Then H is k-sparse if each Majorana operator c_i appears in at most k non-zero terms, that is, for all $i \in [2n]$, $|\{\Gamma \in \mathcal{E} \mid i \in \Gamma\}| \leq k$.*

3.2   Gaussian states

First note that for any real, orthogonal matrix $R \in O(2n)$, the transformation

$$\tilde{c}_i = \sum_{j=1}^{2n} R_{ij} c_j, \tag{2}$$

gives rise to a new set of $[2n]$ Majorana operators $\{\tilde{c}_i\}$.

▶ **Definition 5.** *Let $\{c_i\}$ be a set of $[2n]$ Majorana operators, $R \in O(2n)$, and $\{\tilde{c}_i\}$ defined as in 2. For any assignment $\lambda_1, \ldots, \lambda_n \in [-1, 1]$, the following state is a (mixed) fermionic Gaussian state:*

$$\rho = \frac{1}{2^n} \prod_{j=1}^{n} \left(\mathbb{I} + i\lambda_j \tilde{c}_{2j-1} \tilde{c}_{2j} \right) \tag{3}$$

The state ρ is pure when $\lambda_j \in \{\pm 1\}$ for all $j \in [n]$.

Fermionic Gaussian states exhibit several nice properties. Not only are they the ground states of homogeneous 2-local fermionic Hamiltonians [1], but their higher-order correlates are efficiently computable from their *correlation matrix*. If ρ is defined as in Definition 5, then the correlation matrix M of ρ is the real, antisymmetric $2n \times 2n$ matrix with entries defined as:

$$M_{ij} = \frac{i}{2} Tr(\rho[c_i, c_j]). \tag{4}$$

The higher-order correlates of ρ can be computed via Wick's formalism:

$$Tr(c^\Gamma \rho) = Pf(M_\Gamma), \tag{5}$$

where M_Γ is the $|\Gamma| \times |\Gamma|$ submatrix of M containing only the ordered rows and columns in Γ and $Pf(\cdot)$ is the matrix Pfaffian. Finally, for any Gaussian state ρ, the set $\{\lambda_j\}$ and M are connected by the following lemma:

▶ **Lemma 6** (Bra05). *For any Gaussian state ρ with correlation matrix M, there exists some $R \in O(2n)$ such that the adjoint action of $O(2n)$ on M block-diagonalizes M into the following form:*

$$M = R \bigoplus_{j=1}^{n} \begin{pmatrix} 0 & \lambda_j \\ -\lambda_j & 0 \end{pmatrix} R^T, \tag{6}$$

where the λ_j are the same as in Definition 5. Thus, every real, anti-symmetric matrix M is the correlation matrix for some Gaussian state ρ.

4 Main approximation algorithm

In this section, we demonstrate our main technical ideas by proving an approximation ratio for k-sparse Hamiltonians with both 4-local and 2-local terms. We chose this specific case as it highlights all of our technical ideas, while also being the most physically interesting case. In Section 6 we show how these ideas generalize to the other cases described in Table 1.

▶ **Theorem 7.** *There is a classical polynomial time algorithm that, given as input the weights $\{H_\Gamma\}$ of some k-sparse and $4, 2$-local fermionic Hamiltonian H, returns a description of a quantum state ρ achieving energy*

$$Tr(H\rho) \geq \frac{1}{4k+1} \sum_\Gamma |H_\Gamma| \geq \frac{1}{4k+1} \lambda_{max}(H).$$

Proof. Define a graph $G = (V, E)$ with vertices corresponding to the nonzero terms in the Hamiltonian (i.e., $V = \mathcal{E}$). The graph G may contain vertices corresponding to 2-local or 4-local terms. We include an edge $(v_\Gamma, v_{\Gamma'}) \in E$ if and only if one of the following conditions is met:

(i) c^Γ and $c^{\Gamma'}$ share one or more Majorana operators (i.e., $\Gamma \cap \Gamma' \neq \emptyset$), or

(ii) Γ and Γ' are disjoint and $\Gamma \cup \Gamma' \in \mathcal{E}$.

If there are m nonzero terms in the Hamiltonian then the graph G has m vertices, and the degree of a vertex in the graph is at most $4k$. We can see the latter as follows. Fix some vertex v_Γ. By construction,

$$\deg(v_\Gamma) = |\{(\Gamma, \Gamma') \in \mathcal{E} \times \mathcal{E} \mid \Gamma \text{ and } \Gamma' \text{ satisfy (i) or (ii)}\}|. \tag{7}$$

We consider two cases:

- Γ is 4-local. Consider an edge $(v_\Gamma, v_{\Gamma'})$. As H contains no 6-local or 8-local terms, $\Gamma \cap \Gamma' \neq \emptyset$. As H is k sparse, there are at most $4k$ Γ' for which this can occur.
- Γ is 2-local. Let a equal the number of 4-local Hamiltonian terms overlapping with Γ, and let b equal the number of 2-local terms overlapping with Γ. We claim that the degree of v_Γ is at most $2a + b$.

  There are b 2-local Γ' satisfying (i) with Γ. Each 2-local Γ' satisfying (ii) results in a unique 4-local $\Gamma \cup \Gamma' \in \mathcal{E}$ overlapping with Γ, hence there at most a such Γ'. Finally, no 4-local Γ' may satisfy (ii), and there are a 4-local Γ' satisfying (i).

  Since Γ overlaps with at most $2k$ Γ', we have $a + b \leq 2k$ so that $2a + b \leq 4k$.

By Brooks' Theorem we can in polynomial time find a coloring of the vertices of G with at most $4k + 1$ colors. This means we can partition the vertices into at most $4k + 1$ independent sets, $\{S_1, ..., S_t\}$, with one of these sets having at least a $1/(4k+1)$ fraction of the sum of the absolute values of the weights:

$$\sum_\Gamma |H_\Gamma| = \sum_{S_i} \sum_{\Gamma \in S_i} |H_\Gamma| \leq (4k+1) \max_i \sum_{\Gamma \in S_i} |H_\Gamma|. \tag{8}$$

It follows from Equation (8) that

$$\max_i \sum_{\Gamma \in S_i} |H_\Gamma| \geq \frac{1}{(4k+1)} \sum_\Gamma |H_\Gamma|.$$

Define $S_j = \arg\max_j \sum_{\Gamma \in S_j} |H_\Gamma|$, and consider the following state:

$$\rho = \frac{1}{2^n} \prod_{\Gamma \in S_j} (\mathbb{I} + \text{sign}(H_\Gamma) c^\Gamma). \tag{9}$$

We claim that ρ is a valid quantum state and obtains objective $\sum_{\Gamma \in S_j} |H_\Gamma|$. By definition, ρ is proportional to a projector on a stabilizer state with stabilizer generators given by c^Γ for $\Gamma \in S_j$: Observe that $[c^\Gamma, c^{\Gamma'}] = 0$ for all $\Gamma, \Gamma' \in S_j$ since S_j is an independent set. Hence, ρ is the product of commuting projectors and must be positive semidefinite.

To see that ρ obtains the desired objective, we first expand the product in Equation (9) as a sum and consider products of two or more terms, $\sigma = \prod_p c^{\Gamma_p}$ for $\Gamma_p \in S_j$. If any of the Γ_p are 4-local or $p \geq 3$, σ cannot be proportional to a term of H since the $\Gamma \in S_j$ are disjoint, and no cancellation in products of Majorona operators can occur. The remaining case is a product of two 2-local operators. For any such $\Gamma, \Gamma' \in S_j$, by (ii) and because S_j is an independent set, the product $c^\Gamma c^{\Gamma'}$ cannot be proportional to $c^{\Gamma''}$ for any $\Gamma'' \in \mathcal{E}$.

Hence we have

$$Tr(\mathbb{I}\rho) = 1,$$
$$Tr(c^\Gamma \rho) = \text{sign}(H_\Gamma) \quad \forall \Gamma \in S_j, \text{ and}$$
$$Tr(c^\Gamma \rho) = 0 \quad \forall \Gamma \in \mathcal{E} \setminus S_j.$$

This yields the desired claim that ρ is a normalized state for which

$$Tr(H\rho) = \sum_\Gamma H_\Gamma Tr(c^\Gamma \rho) = \sum_{\Gamma \in S_j} H_\Gamma Tr(c^\Gamma \rho) = \sum_{\Gamma \in S_j} |H_\Gamma| \geq \frac{1}{4k+1} \sum_\Gamma |H_\Gamma|. \qquad \blacktriangleleft$$

5   Conversion to a Gaussian state

The ρ constructed in Theorem 7 is, in fact, a mixture of Gaussian states. This is proven in the following lemma. This implies the existence of a Gaussian state with at least the same objective as ρ.

▶ **Lemma 8.** *The state ρ defined in Equation* (9) *is a mixture of Gaussian states.*

Proof. For each $\Gamma \in S_j$ let M_Γ be the perfect matching of the operators in Γ induced by the lexicographic ordering of Γ, and let M be a perfect matching of the Majorana operators in $\{c_1, ... c_{2n}\} \setminus \{c_i \mid \exists \Gamma \in S_j \text{ with } i \in \Gamma\}$ induced by the lexicographic ordering. Define the following Gaussian state:

$$\rho'(z) = \frac{1}{2^n} \prod_{\Gamma \in S_j} \prod_{gh \in M_\Gamma} (\mathbb{I} + z_{gh} \, ic_g c_h) \prod_{rs \in M} (\mathbb{I} + z_{rs} \, ic_r c_s), \tag{10}$$

where all $z_{gh}, z_{rs} \in \{\pm 1\}$.

Consider the state $\rho'' = \mathbb{E}_z[\rho'(z)]$ where for each Γ the set $\{z_{gh}\}_{gh \in M_\Gamma}$ is uniformly random distributed over $\{\pm 1\}^{|M_\Gamma|}$ subject to the constraint:

$$\text{sign}\left[\left(\prod_{gh \in M_\Gamma} z_{gh} \, ic_g c_h\right) c^\Gamma\right] = \text{sign}(H_\Gamma) \quad \forall \Gamma \in S_j, \tag{11}$$

where $\text{sign}(\pm\mathbb{I})$ is defined as ± 1. In other words, $\{z_{gh}\}_{gh \in M_\Gamma}$ is chosen as the uniform distribution over strings in $\{\pm 1\}^{|M_\Gamma|}$ which satisfy Equation (11). We will assume further that $\{z_{gh}\}_{gh \in M_\Gamma}$ is independent of all other $\{z_{gh}\}_{gh \in M_{\Gamma'}}$ and that each z_{rs} for $rs \in M$ is uniform and independent of all other random variables.

We claim that $\rho = \rho''$. Begin by using independence to push the expectation past the first and third products in Equation (10):

$$\rho'' = \frac{1}{2^n} \prod_{\Gamma \in S_j} \left(\mathbb{E}_z \Big[\prod_{gh \in M_\Gamma} (\mathbb{I} + z_{gh}\ ic_g c_h) \Big] \right) \prod_{rs \in M} \left(\mathbb{E}_z \Big[(\mathbb{I} + z_{rs}\ ic_r c_s) \Big] \right), \qquad (12)$$

We first focus on the final product. Observe that:

$$\prod_{rs \in M} \left(\mathbb{E}_z \Big[(\mathbb{I} + z_{rs}\ ic_r c_s) \Big] \right) = \mathbb{I} \qquad (13)$$

This follows from the independence of the $\{z_{rs} \mid rs \in M\}$ and because $\mathbb{E}_z[z_{rs}] = 0$ for all $rs \in M$. Hence:

$$\rho'' = \frac{1}{2^n} \prod_{\Gamma \in S_j} \left(\mathbb{E}_z \Big[\prod_{gh \in M_\Gamma} (\mathbb{I} + z_{gh}\ ic_g c_h) \Big] \right). \qquad (14)$$

For fixed $\Gamma \in S_j$, we claim that:

$$\mathbb{E}_z \Big[\prod_{gh \in M_\Gamma} (\mathbb{I} + z_{gh}\ ic_g c_h) \Big] = \mathbb{I} + \text{sign}(H_\Gamma) c^\Gamma. \qquad (15)$$

Lemma 8 follows immediately from Equation (15). For any strict subset $\Gamma' \subsetneq \Gamma$, define

$$M_{\Gamma' \cap \Gamma} := \{ gh \in M_\Gamma : g \in \Gamma', h \in \Gamma' \}.$$

We may then expand the left-hand side of Equation (15) as:

$$\mathbb{E}_z \Big[\prod_{gh \in M_\Gamma} (\mathbb{I} + z_{gh}\ ic_g c_h) \Big] = \mathbb{I} + \sum_{\Gamma' \subsetneq \Gamma} \mathbb{E}_z \Big[\prod_{gh \in M_{\Gamma' \cap \Gamma}} z_{gh}\ ic_g c_h \Big] + \mathbb{E}_z \Big[\prod_{gh \in M_\Gamma} z_{gh}\ ic_g c_h \Big] \qquad (16)$$

$$= \mathbb{I} + \text{sign}(H_\Gamma) c^\Gamma \qquad (17)$$

The final expectation in Equation (16) evaluates to $\text{sign}(H_\Gamma) c^\Gamma$ due to constraint 11. The sum of expectations in Equation (16) disappears as the marginal distribution of the z when restricted to a matching on a strict subset $\Gamma' \subsetneq \Gamma$ of size $|M_{\Gamma' \cap \Gamma}| = p$ is totally uniform over $\{\pm 1\}^p$. Therefore $\mathbb{E}_z[z_{gh}] = 0$ for any such matching. ◀

Although $\rho'(z)$ in Lemma 8 is a Gaussian state for any z, the state ρ'' is a mixture of Gaussian states by definition. However, we may derandomize the choice of z to obtain a Gaussian state. We only require pairwise independence of the elements of z, hence using standard derandomization approaches, we can obtain a Gaussian state $\rho'(z)$ in polynomial time such that $Tr(H\rho'(z)) \geq Tr(H\rho'')$.

6 Extensions

In this section, we demonstrate how our core approach in the proof of Theorem 7 leads to improved classical approximation algorithms for the ground state energies of various sparse, local Hamiltonians. Each case is dealt with as its own corollary to Theorem 7.

▶ **Corollary 9** (Strictly q-local Hamiltonians.). *Let H be a k-sparse, strictly q-local fermionic Hamiltonian. There exists a classical polynomial time algorithm that, given $\{H_\Gamma\}$ as input, outputs a description of a quantum state ρ achieving energy*

$$Tr(H\rho) \geq \frac{1}{qk+1} \sum_\Gamma |H_\Gamma| \geq \frac{\lambda_{max}(H)}{qk+1}. \qquad (18)$$

Proof. In this case we only need to include edges in G between v_Γ and $v_{\Gamma'}$ precisely when condition (i) holds, since (ii) is vacuous. Consequently we may omit the second case below Equation (7) and simply bound the degree as qk. We then effectively replace "4" with q in the remaining proof. ◀

▶ **Corollary 10** (Hamiltonians with bounded locality.). *Let H be a k-sparse, q-local fermionic Hamiltonian. There exists a classical polynomial time algorithm that, given $\{H_\Gamma\}$ as input, outputs a description of a quantum state ρ achieving energy*

$$Tr(H\rho) \geq \frac{1}{Cqk^2} \sum_\Gamma |H_\Gamma| \geq \frac{\lambda_{max}(H)}{Cqk^2}, \tag{19}$$

for some constant $C \in \mathbb{R}$.

Proof. In this case we need an appropriate generalization of condition (ii) from Theorem 7. Let us start by defining G using only the condition (i); the maximum possible degree in G is qk. The purpose of (ii) in the proof is to ensure that for Γ, Γ' in the independent set S_j, $c^\Gamma c^{\Gamma'}$ cannot be proportional to $c^{\Gamma''}$ for any $\Gamma'' \in \mathcal{E}$. Note that if this happens, then Γ'' must contain both Γ and Γ'. Thus it would suffice for our independent set S_j in G to satisfy the additional property that no $v_\Gamma, v_{\Gamma'} \in S_j$ could have a common neighbor $v_{\Gamma''} \in V$ with $\Gamma, \Gamma' \subset \Gamma''$. We could satisfy this by adding an edge in G between all pairs v_Γ and $v_{\Gamma'}$ with such a common neighbor. By k-sparsity, the vertex v_Γ has at most k neighbors $v_{\Gamma''}$ in G with $\Gamma \subset \Gamma''$. Since any such $v_{\Gamma''}$ has degree at most qk, the degree of v_Γ increases by at most $k(qk-1)$, and maximum degree in the resulting graph G' is $O(qk^2)$. Applying Brooks' Theorem in G' produces the desired approximation. ◀

▶ **Corollary 11** (Qubit Hamiltonians). *Consider a k-sparse, q-local qubit Hamiltonian H defined analogously to the fermionic Hamiltonian in Definition 2. Given the appropriate assumptions on the locality of H, there exists a classical polynomial time algorithm that, given as inputs the weights $\{H_\Gamma\}$, outputs a description of a quantum state ρ achieving energy at least:*

Hamiltonian	Energy
strictly q-local	$1/(qk+1)$
k-sparse, 2-local	$1/(2k+1)$
k-sparse, q-local	$1/\mathcal{O}(qk^2)$

Proof. For qubit Hamiltonians, condition (i) in Theorem 7 is modified to cover any pair of local terms which involve the same qubit, while condition (ii) is modified to be "Γ and Γ' do not involve the same qubit." Our results for k-sparse and: (i) strictly q-local, (ii) 2-local, and (iii) q-local qubit Hamiltonians follow from this modification and considering Corollary 9, Theorem 7, and Corollary 10 respectively. ◀

7   Optimality of our strictly q-local result

For k-sparse H where all terms are q-local, since $\|H\| \geq \lambda_{\max}(H)$, our results show that

$$\|H\| \geq \lambda_{\max}(H) \geq \frac{m}{qk+1},$$

where we recall $m = \sum_\Gamma |H_\Gamma|$ and $\| \cdot \|$ denotes the operator norm. We give an explicit family of fermionic 2-local n-sparse Hamiltonians $\{H_n\}_{n=1}^\infty$ demonstrating this bound is asymptotically tight (i.e., cannot be improved for all q and k, up to constant factors).

Each H_n is expressed as a sum of monomials in $2n$ Majorana operators $\{c_1, c_2, ..., c_{2n}\}$ satisfying the usual canonical anti-commutation relations. For each n, partition $[2n]$ evenly into $A = \{1, ..., n\}$ and $B = \{n+1, ..., 2n\}$. Then:

$$H_n := \sum_{a \in A, b \in B} i c_a c_b = i \left(\sum_{a \in A} c_a \right) \left(\sum_{b \in B} c_b \right).$$

The eigenvalues of H_n are easy to determine, define $R \in O(2n)$ as some orthogonal matrix satisfying:

$$R_{a,1} = 1/\sqrt{n} \quad \forall a \in A \text{ and } R_{b,2} = 1/\sqrt{n} \quad \forall b \in B.$$

Note that this is well defined since the first two columns are orthonormal. We can then define a new set of Majorana operators (also satisfying the canonical anti-commutation relations) by:

$$\tilde{c}_i = \sum_{i=1}^{2n} R_{j,i} c_j.$$

In particular, we have

$$\tilde{c}_1 = \frac{1}{\sqrt{n}} \sum_{a \in A} c_a \text{ and } \tilde{c}_2 = \frac{1}{\sqrt{n}} \sum_{b \in B} c_b,$$

so

$$H = n i \tilde{c}_1 \tilde{c}_2.$$

Since $i \tilde{c}_1 \tilde{c}_2$ is Hermitian and satisfies $(i \tilde{c}_1 \tilde{c}_2)^2 = \mathbb{I}$, it has eigenvalues in $\{\pm 1\}$. Thus the eigenvalues of H_n are $\{\pm n\}$. Note that H_n is n-sparse, $m = n^2$, and $\|H_n\| = \lambda_{\max}(H_n)$ so that

$$\|H_n\| = \lambda_{\max}(H_n) = n = \Theta\left(\frac{n^2}{2n+1} \right) = \Theta\left(\frac{m}{qk+1} \right).$$

References

1   Sergey Bravyi. Lagrangian representation for fermionic linear optics. *Quantum Information & Computation.*, 5(3):216–238, 2005. `doi:10.5555/2011637.2011640`.

2   Sergey Bravyi, David Gosset, Robert Koenig, and Kristan Temme. Approximation algorithms for quantum many-body problems. *Journal of Mathematical Physics*, 60, 2019. `doi:10.1063/1.5085428`.

3   Aram W. Harrow and Ashley Montanaro. Extremal eigenvalues of local Hamiltonians. *Quantum*, 1:6, 2017. `doi:10.22331/q-2017-04-25-6`.

4   Matthew B. Hastings and Ryan O'Donnell. Optimizing strongly interacting fermionic hamiltonians. In *Proceedings of the 54th Annual ACM SIGACT Symposium on Theory of Computing*, STOC 2022, pages 776–789, New York, NY, USA, 2022. Association for Computing Machinery. `doi:10.1145/3519935.3519960`.

5   Yaroslav Herasymenko, Maarten Stroeks, Jonas Helsen, and Barbara Terhal. Optimizing sparse fermionic hamiltonians, 2022. `arXiv:2211.16518`.

6   John Hubbard. Electron correlations in narrow energy bands. *Proceedings of the Royal Society R. Society A*, 276:238–257, 1963. `doi:10.1098/rspa.1963.0204`.

7   Julia Kempe, Alexei Kitaev, and Oded Regev. The complexity of the local hamiltonian problem. In Kamal Lodaya and Meena Mahajan, editors, *FSTTCS 2004: Foundations of Software Technology and Theoretical Computer Science*, pages 372–383, Berlin, Heidelberg, 2005. Springer Berlin Heidelberg. `doi:10.1007/978-3-540-30538-5_31`.

8   Alexei Yu Kitaev, Alexander Shen, Mikhail N Vyalyi, and Mikhail N Vyalyi. *Classical and quantum computation*. Number 47 in Graduate Studies in Mathematics. American Mathematical Society, 2002. `doi:10.1090/gsm/047`.