On the Feasibility of Exact Unitary Transformations for Many-body Hamiltonians

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Exact unitary transformations play a central role in the analysis and simulation of many-body quantum systems, yet the conditions under which they can be carried out exactly and efficiently remain incompletely understood. We show that exact transformations arise whenever the adjoint action of a unitary's generator defines a linear map within a finite-dimensional operator space. In this regime, there exists a finite-degree polynomial that annihilates the adjoint map, rendering the Baker-Campbell-Hausdorff (BCH) expansion finite. We identify the role of Lie algebras and their modules in producing finite BCH expansions in all known cases. This perspective brings together previously disparate examples of exact transformations under a single unifying principle and clarifies how algebraic relations between generators and transformed operators determine the polynomial degree of the transformation. We illustrate this framework for previously known cases of efficient unitary transformations including unitary coupled-cluster and Pauli product generators. Using this framework, we propose a new class of fermionic generators that can be used for efficient transformations. The result establishes sufficient algebraic conditions for when exact unitary transformations are possible and provides new strategies for reducing their computational cost in quantum simulation and constructing feasible unitary transformations.

I. INTRODUCTION

Unitary transformations of a Hamiltonian,

$$\hat{H}' = \hat{U}\hat{H}\hat{U}^\dagger, \tag{1}$$

are central tools in quantum many-body theory and quantum algorithms. By systematically changing representation, they can simplify the structure of correlations and entanglement in the eigenstates of a Hamiltonian. In electronic structure theory, canonical transformations are used to approximately block-diagonalize Hamiltonians before truncating the Hilbert space, enabling downfolding approaches.[1] In variational quantum eigensolver (VQE) algorithms,[2] suitably chosen unitaries reduce circuit depth for ground- and excited-state preparation and enable efficient circuit cutting in distributed implementations.[3] In fault-tolerant settings, interaction-picture transformations are employed to reduce the cost of simulation algorithms.[4] Quantum-inspired classical techniques, such as iterative qubit coupled cluster (iQCC)[5] and Pauli propagation methods,[6] likewise rely on Hamiltonians transformed by simple unitaries in the Heisenberg picture.

Despite their ubiquity, it remains unclear under what conditions such transformations can be performed exactly and with polynomial computational cost. Evaluating the transformed Hamiltonian,

$$\hat{H}' = e^{i\theta\hat{G}}\hat{H}e^{-i\theta\hat{G}}, \tag{2}$$

typically involves an infinite Baker–Campbell–Hausdorff (BCH) expansion[7],

$$\hat{H}' = \sum_{j=0}^{\infty} \frac{\theta^j}{j!} \mathrm{ad}^j_{i\hat{G}}(\hat{H}), \tag{3}$$

where the j^{th}-order nested commutator of $i\hat{G}$ and $\hat{H}$ is

$$\mathrm{ad}^j_{i\hat{G}}(\hat{H}) = [i\hat{G}, \mathrm{ad}^{j-1}_{i\hat{G}}(\hat{H})], \qquad \mathrm{ad}^0_{i\hat{G}}(\hat{H}) = \hat{H}. \tag{4}$$

Direct computation of this series scales exponentially with the system size. Consequently, a central challenge is to identify situations where the series can be evaluated exactly using a few powers of the adjoint operation $(\mathrm{ad}_{i\hat{G}}(.))$.

A well-known simplification arises when the nested commutators close algebraically,

$$\mathrm{ad}^n_{i\hat{G}}(\hat{H}) = \sum_{j=0}^{n-1} c_j \, \mathrm{ad}^j_{i\hat{G}}(\hat{H}), \tag{5}$$

in which case the transformation requires only a finite number of terms. Many important examples of such algebraic closure are known, including fermionic orbital rotations,[8] Bogoliubov transformations for both fermions and bosons,[9] and Pauli-product unitaries.[5] Comprehensive treatments of these examples can be found in Ref. 10. Recent developments in quantum computing have extended this list to linear combinations of anti-commuting Pauli operators[11] and unitary coupled-cluster (UCC) generators.[12–14]

Although these examples demonstrate that algebraic closure can dramatically reduce computational cost, they

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are usually identified case by case. To date, no general algebraic condition has been established for when the BCH expansion can be expressed using a few terms due to the algebraic closure. Moreover, prior analyses have not clarified the mathematical structure underlying the operator relationships that make exact transformations possible.

In this work, we develop a unified algebraic framework that encompasses all known cases of finite BCH expansion and establishes the general condition for its termination. The central insight is to view the adjoint action $\mathrm{ad}_{i\hat{G}}(\cdot)$ as a linear map acting on a finite-dimensional operator space. The Cayley–Hamilton theorem then guarantees that this map satisfies a finite-degree characteristic polynomial, ensuring that any unitary transformation generated by such $\hat{G}$ is exactly representable by a polynomial of finite degree. This perspective unifies two key scenarios: when the generator $\hat{G}$ belongs to a finite-dimensional Lie algebra, and when it has a finite eigenspectrum. The framework further provides systematic guidance for exploiting additional algebraic properties of the transformed operator $\hat{H}$ to minimize the number of nested commutators required. Additionally, by enabling transformation under arbitrary generators of known small spectrum, the framework motivates construction of artificial generators with small spectrum and desired properties. As an example, we construct a class of generators with $\{\pm 1\}$ spectrum and are number preserving.

Finally, while our analysis naturally includes continuous families of transformations, we note that discrete unitary groups such as the Clifford group—which act as automorphisms of the Pauli group—are beyond the present scope. Optimization over such discrete structures involves qualitatively different considerations than the continuous settings addressed here.

II. THEORY

Before discussing algebraic closures for Hamiltonian transformations, it is useful to note a general property of any unitary transformation $\hat{U}$. When $\hat{U}$ is applied to an operator $\hat{H}$ that can be written as a polynomial of some operators $\{\hat{O}_i\}$,

$$\hat{H} = \mathrm{poly}(\{\hat{O}_i\}), \tag{6}$$

the transformed operator can be obtained by transforming each constituent operator individually:

$$\hat{U}\hat{H}\hat{U}^\dagger = \mathrm{poly}(\{\hat{U}\hat{O}_i\hat{U}^\dagger\}). \tag{7}$$

This observation shows that the transformation of a Hamiltonian reduces to understanding how the elementary operators $\hat{O}_i$ transform under conjugation.

A. Algebraic closure from the Cayley–Hamilton theorem

The algebraic closure condition in Eq. (5) follows from the existence of a finite-degree polynomial $p(\mathrm{ad}_{i\hat{G}}) = 0$. The operation $\mathrm{ad}_{i\hat{G}}(\hat{O}) = [i\hat{G}, \hat{O}]$ is a linear map, and when it is represented in a finite-dimensional linear space V, the Cayley–Hamilton theorem guarantees that this map is annihilated by its characteristic polynomial. Specifically, if $\mathbf{A}$ is the matrix representation of $\mathrm{ad}_{i\hat{G}}$ in some basis of V, then the characteristic polynomial

$$p_c(t) = \det(t\mathbf{1} - \mathbf{A}) \tag{8}$$

satisfies $p_c(\mathbf{A}) = 0$ and $\deg[p_c] = \dim(V) = d_V$. Consequently,

$$(\mathrm{ad}_{i\hat{G}})^{d_V} = p_{d_V-1}(\mathrm{ad}_{i\hat{G}}), \tag{9}$$

where p_{d_V-1} is a polynomial of degree $d_V - 1$. This relation directly yields the algebraic closure condition in Eq. (5) and ensures that the BCH series terminates.

To apply the Cayley–Hamilton theorem, one must represent $\mathrm{ad}_{i\hat{G}}$ as a linear operator in a finite-dimensional space V. In what follows, we discuss two situations where such a finite representation exists. In both cases, the transformed operator $\hat{O}$ is represented by a vector $\vec{O}$ in V as a linear combination of basis vectors $\{\vec{O}_i\}$, and $\mathrm{ad}_{i\hat{G}}$ acts as a linear transformation that maps $\vec{O}$ to another vector $\vec{O}'$ in the same basis.

B. Lie–algebraic representation

A particularly natural finite-dimensional representation of $\mathrm{ad}_{i\hat{G}}$ arises when the generator $\hat{G}$ belongs to a finite Lie algebra $\mathfrak{L}$ with generating elements $\{\hat{O}_i\}_{i=1}^N$. In this case,

$$\hat{G} = \sum_i c_i \hat{O}_i. \tag{10}$$

We also assume that the Hamiltonian $\hat{H}$ can be expressed as a polynomial of $\mathfrak{L}$ elements, $\hat{H} = \mathrm{poly}(\{\hat{O}_i\})$. Although the associative product of operators $\hat{O}_i$ does not belong to $\mathfrak{L}$—only their non-associative product defined by commutators,

$$[\hat{O}_i, \hat{O}_j] = \sum_k c_{ij}^{(k)} \hat{O}_k \in \mathfrak{L}, \tag{11}$$

does—the Hamiltonian is an element of the universal enveloping algebra (UEA) of $\mathfrak{L}$[15]. This poses no difficulty, since one only needs to transform each operator $\hat{O}_i \in \mathfrak{L}$ that enters $\hat{H}$.

The Lie algebra $\mathfrak{L}$ is itself a linear space, with elements represented as vectors $\vec{v} = \sum_i c_i \vec{O}_i$. The adjoint map $\mathrm{ad}_{i\hat{G}}$ acts linearly on $\mathfrak{L}$,

$$\mathrm{ad}_{i\hat{G}}(\vec{O}_i) = \sum_k A_{ik} \vec{O}_k, \tag{12}$$

where the constants A_{ik} define the matrix representation of $\mathrm{ad}_{i\hat{G}}$. The dimension of this representation is equal to the dimension of $\mathfrak{L}$, $\dim(\mathfrak{L}) = d_{\mathfrak{L}}$, providing an upper bound for the degree of the characteristic polynomial.

Further reduction of this degree is possible through known results from Lie algebra theory. For example, in an Abelian Lie algebra all elements commute, implying $\mathrm{ad}_{i\hat{G}} = 0$, and the transformation is trivial, $\hat{H}' = \hat{H}$. More generally, Lie algebras fall into three categories: (1) semisimple, (2) nilpotent, and (3) solvable.[15, 16] In semisimple algebras, one can choose a basis of eigenvectors $\{\vec{O}'_i\}$ for $\mathrm{ad}_{i\hat{G}}$,

$$\mathrm{ad}_{i\hat{G}}(\vec{O}'_i) = o_i \vec{O}'_i, \tag{13}$$

where o_i are either zero (commuting elements) or complex numbers (raising/lowering operators). In this representation, transforming $\hat{H}$ becomes straightforward if it is expressed as a polynomial of $\hat{O}'_i$. In nilpotent algebras, the degree of the characteristic polynomial cannot exceed the nilpotent class n_c of the algebra, defined by the condition

$$(\mathrm{ad}_{i\hat{G}})^{n_c}(\vec{O}_i) = 0, \qquad \forall\, \hat{G}, \hat{O}_i \in \mathfrak{L}. \tag{14}$$

For instance, in an Abelian algebra, $n_c = 1$.

Without delving further into algebra classification, we can show that transforming $\hat{H} = \mathrm{poly}(\{\hat{O}_i\})$ by $\hat{U} = e^{i\theta\hat{G}}$ always yields

$$\hat{H}' = \mathrm{poly}'(\{\hat{O}_i\}), \quad \deg[\mathrm{poly}(\cdot)] = \deg[\mathrm{poly}'(\cdot)]. \tag{15}$$

When $\hat{G} = \sum_i c_i \hat{O}_i$, conjugation by $\hat{U}$ defines an automorphism of $\mathfrak{L}$. Each basis element transforms linearly as

$$\hat{U}\hat{O}_\mu\hat{U}^\dagger = \sum_{\nu=1}^{d_{\mathfrak{L}}} [U]_{\nu\mu}\hat{O}_\nu, \tag{16}$$

where $[U]_{\nu\mu}$ are the matrix elements of $\exp[\mathrm{ad}_{i\theta\hat{G}}]$. To compute U, one can apply the BCH expansion from Eq. (3). Because the commutators close within the Lie algebra, the series can be resummed to a closed form. A faithful matrix representation $\rho : \mathfrak{L} \to \mathfrak{gl}(N)$, which preserves commutation relations and has a trivial kernel, allows this resummation explicitly:

$$\begin{aligned}\rho(e^{i\theta\hat{G}}\hat{O}_\mu e^{-i\theta\hat{G}}) &= \rho(\hat{O}_\mu) + i\theta[\rho(\hat{G}), \rho(\hat{O}_\mu)] + \dots \\ &= e^{i\theta\rho(\hat{G})}\rho(\hat{O}_\mu)e^{-i\theta\rho(\hat{G})}.\end{aligned} \tag{17}$$

Consequently,

$$\rho(\hat{U})\rho(\hat{O}_\mu)\rho(\hat{U})^\dagger = \sum_{\nu=1}^{d_{\mathfrak{L}}} [U]_{\nu\mu}\rho(\hat{O}_\nu), \tag{18}$$

where $\rho(\hat{U}) := \exp[i\theta\rho(\hat{G})]$. Equating elements in Eq. (18) gives a system of N^2 linear equations of $\{U_{\nu\mu}\}_{\nu=1}^{d_{\mathfrak{L}}}$ for each $\mu = 1, \dots, d_{\mathfrak{L}}$. The faithfulness of ρ ensures that these systems have unique solutions.

$\mathfrak{L}$-module extension. The preceding discussion assumes that the transformed operator belongs to the same Lie algebra as the generator. More generally, one can consider the transformation of an operator $\hat{O}$ that lies in a linear space $\mathcal{A}$ closed under the adjoint action of $\mathfrak{L}$ elements:

$$\hat{O} = \sum_i c_i \hat{A}_i, \tag{19}$$

$$[\hat{O}_j, \hat{A}_i] = \sum_k a_{ji}^{(k)} \hat{A}_k. \tag{20}$$

The set $\{\hat{A}_i\}$ defines a basis of $\mathcal{A}$, and the coefficients $a_{ji}^{(k)}$ specify how $\mathfrak{L}$ acts on $\mathcal{A}$ under commutation. In this case, $\mathcal{A}$ is said to be an $\mathfrak{L}$-module. The adjoint action of $\hat{G} \in \mathfrak{L}$ on $\mathcal{A}$ can be written as

$$[\hat{G}, \hat{A}_i] = \sum_{j=1}^{N} [A]_{ij}\hat{A}_j, \tag{21}$$

where $\mathbf{A}$ is the matrix representation of $\mathrm{ad}_{i\hat{G}}$ on the module. Evaluating Eq. (21) for each $\hat{A}_i \in \mathcal{A}$ determines $\mathbf{A}$, and applying the BCH expansion yields

$$e^{i\theta\hat{G}}\hat{A}_i e^{-i\theta\hat{G}} = \sum_{j=1}^{N} [e^{i\theta\mathbf{A}}]_{ji}\hat{A}_j. \tag{22}$$

Thus, $[U]_{ji} = [e^{i\theta\mathbf{A}}]_{ji}$ in the notation of Eq. (16). The matrix exponential $e^{i\theta\mathbf{A}}$ defines the representation of the Lie group generated by $\mathfrak{L}$ on its module $\mathcal{A}$.

C. Eigen–subspace projector representation

More generally, when $\hat{G}$ is an arbitrary Hermitian operator with real spectrum,

$$\hat{G} = \sum_{i=1}^{L} g_i \hat{P}_i, \tag{23}$$

where $\{g_i\}_{i=1}^{L}$ are eigenvalues and $\{\hat{P}_i\}$ are orthogonal projectors onto the corresponding eigenspaces, $\sum_i \hat{P}_i = \mathbf{1}$ and $\hat{P}_i\hat{P}_j = \delta_{ij}\hat{P}_i$, the adjoint action admits a simple block structure:

$$\mathrm{ad}_{i\hat{G}}(\hat{O}) \;=\; \sum_{j,k=1}^{L} i(g_j - g_k)\, \hat{P}_j\hat{O}\hat{P}_k. \tag{24}$$

In this projector basis, the identity superoperator is

$$\mathcal{I}(\,\cdot\,) \;=\; \sum_{i,j=1}^{L} \hat{P}_i(\,\cdot\,)\hat{P}_j, \tag{25}$$

and the matrix representation of $\mathrm{ad}_{i\hat{G}}$ has eigenvalues $\{\, i(g_j - g_k)\,\}_{j,k=1}^{L}$ on the blocks $\hat{P}_j(\cdot)\hat{P}_k$. The representation space has dimension L^2, but the degree of the

characteristic (and minimal) polynomial of $\mathrm{ad}_{i\hat{G}}$ is governed only by the number of distinct differences $g_j - g_k$. Thus, in the worst case (all differences distinct) the upper bound for the degree is $L(L-1)$, and degeneracies or vanishing blocks reduce this degree.

$\mathfrak{L}$-module point of view. This construction can be viewed as an $\mathfrak{L}$-module, where $\mathfrak{L}$ is the Abelian Lie algebra generated by the projectors $\{\hat{P}_i\}$, $[\hat{P}_i, \hat{P}_j] = 0$. Consider the linear space $\mathcal{O}$ with basis elements

$$\hat{O}_{ij} := \hat{P}_i \hat{O} \hat{P}_j. \tag{26}$$

Any operator $\hat{O}' = \sum_{i,j} c_{ij} \hat{O}_{ij}$ remains in $\mathcal{O}$ under the adjoint action, since $\mathrm{ad}_{i\hat{G}}$ acts diagonally as in Eq. (24).

Unitary transformation via a finite polynomial in $ad_{i\hat{G}}$. We seek a finite polynomial representation of the conjugation,

$$e^{i\theta\hat{G}}\,\hat{O}\,e^{-i\theta\hat{G}} \;=\; \sum_{m=0}^{d} c_m(\theta)\,\big(\mathrm{ad}_{i\hat{G}}\big)^m(\hat{O}), \tag{27}$$

for suitable coefficients $\{c_m(\theta)\}_{m=0}^{d}$. Projecting Eq. (27) into the eigenspace blocks and using Eq. (24) gives

$$\sum_{j,k} e^{i\theta(g_j-g_k)}\,\hat{P}_j\hat{O}\hat{P}_k \;=\; \sum_{j,k}\sum_{m=0}^{d} c_m(\theta)\,\big(i(g_j-g_k)\big)^m \hat{P}_j\hat{O}\hat{P}_k. \tag{28}$$

Let $\|\hat{P}_j\hat{O}\hat{P}_k\| = 0$ denote a vanishing block. Because projectors onto distinct (j,k) pairs are orthogonal, the nonvanishing blocks are linearly independent. Equating coefficients on those blocks yields, for each nonvanishing block,

$$e^{i\theta\Delta_{jk}} \;=\; \sum_{m=0}^{d} c_m(\theta)\,(i(g_j-g_k))^m. \tag{29}$$

We define the set of relevant differences supported by $\hat{O}$,

$$S \;:=\; \big\{\, g_j - g_k \;:\; \|\hat{P}_j\hat{O}\hat{P}_k\| \neq 0 \,\big\}. \tag{30}$$

Collecting the equations in vector form with $\vec{e} \in \mathbb{C}^{|S|}$ and $\vec{c} \in \mathbb{C}^{d+1}$, where $\vec{e} = \{e^{i\theta\Delta}\}_{\Delta\in S}$ and $\vec{c} = \{c_m(\theta)\}_{m=0}^{d}$, we obtain

$$\vec{e} \;=\; W\,\vec{c}, \tag{31}$$

with the generalized Vandermonde matrix $W \in \mathbb{C}^{|S|\times(d+1)}$ defined by [17]

$$[W]_{\Delta,m} \;=\; (i\Delta)^m, \qquad \Delta \in S,\; m = 0,\ldots,d. \tag{32}$$

Choosing $d = |S| - 1$ makes W square; since the rows correspond to distinct $\Delta \in S$, W is invertible and the coefficients are uniquely determined by

$$\vec{c} \;=\; W^{-1}\,\vec{e}. \tag{33}$$

The invertibility of W and uniqueness of $\vec{c}$ implies that $\{\big(\mathrm{ad}_{i\hat{G}}\big)^j(\hat{O})\}_{j=0}^{|S|-1}$ are linearly independent operators. If $\hat{O}$ is Hermitian (and $\hat{G}$ is Hermitian), then $\mathrm{ad}_{i\hat{G}}(\hat{O}) = i[\hat{G},\hat{O}]$ is Hermitian, and so are $\big(\mathrm{ad}_{i\hat{G}}\big)^m(\hat{O})$ for all m. Therefore, the coefficients $\{c_m(\theta)\}$ are real (see Appendix A for an explicit proof).

Determining the nonzero blocks. The number of nested commutators and their coefficients depend on S in Eq. (30). To determine which projected blocks $\hat{P}_j\hat{O}\hat{P}_k$ are nonvanishing, one can construct polynomials in $\mathrm{ad}_{\hat{G}}$ that isolate the sum over blocks with a fixed eigenvalue difference Δ. Let $\mathcal{D}$ denote the set of all differences $\{g_j - g_k\}$. The Lagrange interpolation polynomial

$$\mathrm{Lag}_{\mathcal{D}}^{(\Delta)}(x) \;=\; \prod_{\substack{\delta\in\mathcal{D}\\ \delta\neq\Delta}} \frac{x-\delta}{\Delta-\delta} \tag{34}$$

satisfies $\mathrm{Lag}_{\mathcal{D}}^{(\Delta)}(\Delta) = 1$ and vanishes at every $\delta \in \mathcal{D}\backslash\{\Delta\}$. Using Eq. (24), applying $\mathrm{Lag}_{\mathcal{D}}^{(\Delta)}\big(\mathrm{ad}_{\hat{G}}\big)$ to $\hat{O}$ isolates the sum of blocks

$$\mathcal{B}_\Delta := \big\{\, \hat{P}_j\hat{O}\hat{P}_k \mid g_j - g_k = \Delta \,\big\}. \tag{35}$$

If $\big\|\mathrm{Lag}_{\mathcal{D}}^{(\Delta)}\big(\mathrm{ad}_{\hat{G}}\big)\,(\hat{O})\big\| \neq 0$, then at least one block in $\mathcal{B}_\Delta$ is nonvanishing. Repeating this test over all $\Delta \in \mathcal{D}$ yields

$$S \;=\; \big\{\, \Delta\in\mathcal{D} \;:\; \big\|\mathrm{Lag}_{\mathcal{D}}^{(\Delta)}\big(\mathrm{ad}_{\hat{G}}\big)\,(\hat{O})\big\| \neq 0 \,\big\}. \tag{36}$$

We illustrate this test for Pauli product generators in Section III B 1.

D. Block reduction due to additional algebraic structures

While the Lagrange-based projector method described above provides a systematic way to detect vanishing blocks $\hat{P}_i\hat{O}\hat{P}_j$, it can become cumbersome in practice, particularly when there is flexibility in the choice of operators to be transformed. For instance, if the Hamiltonian can be expressed as a polynomial in some operators, $\hat{H} = \mathrm{poly}(\{\hat{O}_i\})$, one could equally well apply a linear transformation of the operator basis, $\hat{O}'_i = \sum_j c_{ij}\hat{O}_j$, obtaining $\hat{H} = \mathrm{poly}(\{\hat{O}'_i\})$. The transformed set $\{\hat{O}'_i\}$ may have fewer nonvanishing projected blocks $\hat{P}_k\hat{O}'_i\hat{P}_j$, thus making the transformation under $\hat{U} = e^{i\theta\hat{G}}$ more efficient.

Exploiting additional algebraic relations such as commutation or anticommutation between $\hat{G}$ and $\hat{O}$ provides a direct route to identifying block sparsity without explicitly constructing the Lagrange projectors.

1. Lie algebras

If both $\hat{G}$ and $\hat{O}$ belong to the same Lie algebra $\mathfrak{L}$, then two different characteristic polynomials can be considered: (i) $p_{\mathfrak{L}}$, obtained from the Lie algebraic adjoint map

$\mathrm{ad}_{i\hat{G}}$ acting on $\mathfrak{L}$, and (ii) $p_{\Delta g}$, obtained from the eigendecomposition of $\hat{G}$ assuming all projected blocks are nonvanishing. These two polynomials need not coincide: $p_{\mathfrak{L}}$ reflects the algebraic structure of $\mathfrak{L}$, while $p_{\Delta g}$ captures the spectral properties of $\hat{G}$ as expressed through its eigenvalues and projectors $\hat{P}_i$. A lower polynomial degree in the $\mathfrak{L}$ Lie-algebraic representation,

$$\deg(p_{\mathfrak{L}}) < \deg(p_{\Delta g}),$$

implies that certain projected blocks $\hat{P}_i\hat{O}\hat{P}_j$ must vanish.

For semisimple Lie algebras, all generators can be chosen such that

$$[i\hat{G}, \hat{O}'_i] = o_i\hat{O}'_i, \tag{37}$$

where o_i are either zero or purely imaginary numbers. This yields two distinct cases:

- For $o_i = 0$, the operators commute with $\hat{G}$, and only diagonal blocks survive, $\hat{P}_j\hat{O}'_i\hat{P}_k = \delta_{jk}\,\hat{P}_j\hat{O}'_i$.
- For $o_i \neq 0$, the nonvanishing blocks satisfy $i(g_j - g_k) = o_i$. In this case, the degree of the characteristic polynomial of $\mathrm{ad}_{i\hat{G}}$ acting on $\hat{O}'_i$ is 1.

For non-semisimple Lie algebras, not all generators can be diagonalized in this manner, and the analysis of block structure must proceed case by case.

2. Anti-commutativity

Anti-commutativity between $\hat{G}$ and $\hat{O}$ likewise leads to systematic block reductions. Using the spectral decomposition of $\hat{G}$ in Eq. (23), the anti-commutator takes the form

$$[\hat{G}, \hat{O}]_+ = \sum_{i,j}(g_i + g_j)\,\hat{P}_i\hat{O}\hat{P}_j. \tag{38}$$

If $\hat{G}$ and $\hat{O}$ anticommute, i.e., $[\hat{G}, \hat{O}]_+ = 0$, then $\hat{P}_i\hat{O}\hat{P}_j = 0$ whenever $g_i + g_j \neq 0$. Consequently, the allowed eigenvalue differences $g_j - g_k$ over the nonvanishing projected blocks reduce to

$$S = \{\, 2g \mid g, -g \in \mathrm{eig}(\hat{G}),\ \|\hat{P}_g\hat{O}\hat{P}_{-g}\| \neq 0 \,\}. \tag{39}$$

Thus, in this case, $|S|$ is at most L, corresponding to the number of distinct eigenvalues of $\hat{G}$.

III. APPLICATIONS

To illustrate the theoretical framework developed above, we now examine two representative classes of unitary transformations for which the adjoint action $\mathrm{ad}_{i\hat{G}}$ operates within a finite-dimensional linear space. These examples demonstrate how the general conditions identified in Sec. II manifest in familiar physical contexts and lead to efficient, closed-form transformations.

A. Lie algebras and their modules

1. Orbital rotations

This example involves orbital rotations generated by the $\mathfrak{u}(N)$ Lie algebra, which exemplify the case where both the generator and the transformed operators belong to the same finite Lie algebra or its modules. In this setting, the transformation can be represented exactly through matrix exponentiation, and the transformed Hamiltonian remains within the same algebraic structure. In practice, such rotations are routinely used to localize molecular orbitals (e.g., Foster–Boys, Edmiston–Ruedenberg, Pipek–Mezey), which typically increases sparsity and spatial locality in $\hat{H}$ by concentrating one- and two-electron integral weight and shrinking the support of fermionic strings.[18–21] The same unitary can also be absorbed classically into the integrals prior to VQE, rather than compiled as a circuit, thereby reducing circuit depth and often the effective Hamiltonian 1-norm (and associated measurement cost) in chemistry VQE workflows.[22–24] These are precisely the adjoint actions our framework handles in closed form via finite-dimensional representations.

The second-quantized electronic Hamiltonian is given by

$$\hat{H} = \sum_{p,q=1}^{N} h_{pq}\,\hat{a}_p^\dagger\hat{a}_q + \sum_{p,q,r,s=1}^{N} g_{pqrs}\,\hat{a}_p^\dagger\hat{a}_q\hat{a}_r^\dagger\hat{a}_s, \tag{40}$$

where N is the number of spin orbitals and $\mathcal{C} := \{\hat{a}_p^\dagger\}_{p=1}^N$, $\mathcal{A} := \{\hat{a}_p\}_{p=1}^N$ denote the fermionic creation and annihilation operators, respectively. We consider unitary transformations of $\hat{H}$ generated by orbital rotations. Orbital rotations defined by a Hermitian matrix M take the form

$$\hat{V} = \exp\left[i\sum_{p,q=1}^{N}[M]_{pq}\,\hat{a}_p^\dagger\hat{a}_q\right]. \tag{41}$$

The excitation operators $\mathcal{E} := \{\hat{a}_p^\dagger\hat{a}_q\}_{p,q=1}^N$ satisfy the commutation relation

$$[\hat{a}_p^\dagger\hat{a}_q, \hat{a}_r^\dagger\hat{a}_s] = \delta_{qr}\,\hat{a}_p^\dagger\hat{a}_s - \delta_{ps}\,\hat{a}_r^\dagger\hat{a}_q, \tag{42}$$

and therefore generate a $\mathfrak{u}(N)$ Lie algebra. The creation and annihilation operators transform under the adjoint action of this algebra according to

$$[\hat{a}_p^\dagger\hat{a}_q, \hat{a}_r^\dagger] = \delta_{qr}\,\hat{a}_p^\dagger, \qquad [\hat{a}_p^\dagger\hat{a}_q, \hat{a}_r] = -\delta_{pr}\,\hat{a}_q, \tag{43}$$

implying that $\mathcal{C}$ and $\mathcal{A}$ are $\mathfrak{u}(N)$-modules. Since the Hamiltonian in Eq. (40) is a noncommuting polynomial in both $\mathcal{E}$ and $\mathcal{C} \cup \mathcal{A}$, the transformed Hamiltonian $\hat{H}' = \hat{V}\hat{H}\hat{V}^\dagger$ can be obtained by either of the two methods described in Sec. II B. We outline both below.

Matrix representation.— Consider the faithful (fundamental) representation of $\mathfrak{u}(N)$ defined by

$$[\rho(\hat{a}_p^\dagger\hat{a}_q)]_{ab} = \delta_{ap}\,\delta_{bq}, \tag{44}$$

where δ_{ap}, δ_{bq} are Kronecker delta functions. In this representation, $\rho(\hat{V}) = e^{iM}$. Solving Eq. (18) in this basis yields

$$\hat{V}\hat{a}_p^\dagger \hat{a}_q \hat{V}^\dagger = \sum_{r,s=1}^{N} [U]_{(rs)(pq)}\, \hat{a}_r^\dagger \hat{a}_s, \tag{45}$$

where the matrix elements of the adjoint action are

$$[U]_{(rs)(pq)} = [e^{iM}]_{rp}\, [e^{-iM}]_{qs}, \tag{46}$$

and (pq), (rs) denote compound indices. The transformed Hamiltonian $\hat{H}' = \hat{V}\hat{H}\hat{V}^\dagger$ retains the structure of Eq. (40), with renormalized coefficients given by tensor contractions:

$$h'_{pq} = \sum_{a,b=1}^{N} h_{ab}\, [U]_{(pq)(ab)}, \tag{47}$$

$$g'_{pqrs} = \sum_{a,b,c,d=1}^{N} g_{abcd}\, [U]_{(pq)(ab)} [U]_{(rs)(cd)}. \tag{48}$$

Commutator-based derivation.— Using Eq. (43), the commutators with the generator $\hat{G} = \sum_{p,q} [M]_{pq}\, \hat{a}_p^\dagger \hat{a}_q$ are

$$[\hat{G}, \hat{a}_p^\dagger] = \sum_{q=1}^{N} [M]_{qp}\, \hat{a}_q^\dagger, \qquad [\hat{G}, \hat{a}_p] = -\sum_{q=1}^{N} [M]_{pq}\, \hat{a}_q. \tag{49}$$

Using the BCH expansion, we find

$$\hat{V}\hat{a}_p^\dagger \hat{V}^\dagger = \sum_{q=1}^{N} [e^{iM}]_{qp}\, \hat{a}_q^\dagger, \qquad \hat{V}\hat{a}_p \hat{V}^\dagger = \sum_{q=1}^{N} [e^{-iM}]_{pq}\, \hat{a}_q. \tag{50}$$

The matrices $e^{\pm iM}$ constitute the defining representation of $U(N)$, and their products reproduce the adjoint transformation in Eq. (45), thus verifying consistency between the algebraic and spectral constructions.

2. Heisenberg Lie algebra

The Heisenberg algebra $\mathfrak{h}_N = \{\hat{x}_i, \hat{p}_i, \hat{I}\}_{i=1}^N$ provides a natural route for transforming bosonic Hamiltonians (polynomials in $\{\hat{x}_i, \hat{p}_i\}$) via displacement-type generators, in contrast to the orbital-rotation setting (Sec. III A 1) for fermions. Its defining relations

$$[\hat{x}_i, \hat{p}_j] = i\hbar\, \delta_{ij} \hat{I}, \qquad [\hat{x}_i, \hat{x}_j] = [\hat{p}_i, \hat{p}_j] = 0 \tag{51}$$

imply that $\hat{I}$ is central and all double commutators vanish. Hence $\mathfrak{h}_N$ is nilpotent of class 2, and the adjoint superoperator $\mathrm{ad}_{i\hat{G}}$ is nilpotent with index at most 2 on $\mathrm{span}\{\hat{x}_i, \hat{p}_i, \hat{I}\}$. Equivalently, the minimal (and characteristic) polynomial of $\mathrm{ad}_{i\hat{G}}$ has degree ≤ 2, so the BCH expansion truncates exactly after the first commutator—independently of the number of modes.

For a linear generator

$$\hat{G} = \sum_{i=1}^{N} \left(v_i \hat{p}_i - u_i \hat{x}_i\right) + z\hat{I}, \qquad u_i, v_i, z \in \mathbb{R}, \tag{52}$$

the adjoint actions are

$$\mathrm{ad}_{i\hat{G}}(\hat{x}_j) = \hbar v_j \hat{I}, \qquad \mathrm{ad}_{i\hat{G}}(\hat{p}_j) = \hbar u_j \hat{I}, \tag{53}$$

leading to the exact unitary transformations

$$e^{i\hat{G}} \hat{x}_j e^{-i\hat{G}} = \hat{x}_j + \hbar v_j \hat{I}, \tag{54}$$

$$e^{i\hat{G}} \hat{p}_j e^{-i\hat{G}} = \hat{p}_j + \hbar u_j \hat{I}. \tag{55}$$

Thus, elements of the Heisenberg group act as displacements on $(\hat{x}_j, \hat{p}_j)$, and conjugation by any such linear $\hat{G}$ evaluates in closed form with only single commutators. Practically, this yields clear computational savings for bosonic problems: the adjoint action is captured within a finite-dimensional representation, and transformed polynomial Hamiltonians are obtained exactly without growing commutator depth.

B. $\hat{G}$ eigensubspace decomposition

1. Single Pauli product

The generator for the unitary transformations used in a series of hybrid quantum-classical VQE[25, 26] and quantum inspired iQCC[5, 27] methods is the single Pauli product (string) $\hat{G} = \hat{\sigma}_1 \otimes \cdots \otimes \hat{\sigma}_N$, with $\hat{\sigma}_j \in \{\hat{e}, \hat{x}, \hat{y}, \hat{z}\}$. $\hat{G}$ squares to the identity operator,

$$\hat{G}^2 = \hat{I}, \tag{56}$$

and is involutory. Consequently, $\hat{G}$ has spectrum $\{\pm 1\}$, and it is compactly represented as $\hat{G} = \hat{P}_+ - \hat{P}_-$, where $\hat{P}_\pm$ are corresponding eigensubspace projectors.

For a generic $\hat{H}$, the projected blocks need not vanish; thus $S = \{0, \pm 2\}$ (recall S denotes the set of distinct eigenvalue differences on nonvanishing projected blocks). From Eq. (27), the transformed Hamiltonian can be written as

$$e^{i\theta\hat{G}} \hat{H} e^{-i\theta\hat{G}} = c_0\, \hat{H} + c_1\, [i\hat{G}, \hat{H}] + c_2\, [i\hat{G}, [i\hat{G}, \hat{H}]], \tag{57}$$

with coefficients obtained from Eq. (31) as

$$(c_0, c_1, c_2) = \left(1, \tfrac{1}{2}\sin 2\theta, \tfrac{1}{2}\sin^2\theta\right). \tag{58}$$

Using a suitable fermion–qubit mapping (e.g., Jordan–Wigner or Bravyi–Kitaev), the electronic Hamiltonian in Eq. (40) can be expressed as a sum of Pauli products,

$$\hat{H} = \sum_{\alpha=1}^{N_p} h_\alpha\, \hat{\sigma}^{(\alpha)}, \tag{59}$$

where N_p is the number of Pauli strings and $\hat{\sigma}^{(\alpha)} = \hat{\sigma}_1^{(\alpha)} \otimes \cdots \otimes \hat{\sigma}_N^{(\alpha)}$ with $\hat{\sigma}_j^{(\alpha)} \in \{\hat{e}, \hat{x}, \hat{y}, \hat{z}\}$. We transform each Pauli product in Eq. (59) individually. Since any two Pauli products either commute or anticommute, transforming terms individually requires fewer commutators.

When $\hat{G}$ and $\hat{\sigma}^{(\alpha)}$ commute, $S = \{0\}$, so $\hat{\sigma}^{(\alpha)\prime} = \hat{\sigma}^{(\alpha)}$. When they anticommute, we have

$$\hat{P}_+ \, \hat{\sigma}^{(\alpha)} \, \hat{P}_+ = \hat{P}_- \, \hat{\sigma}^{(\alpha)} \, \hat{P}_- = 0,$$

i.e., $\hat{\sigma}^{(\alpha)}$ is block off-diagonal in the eigenbasis of $\hat{G}$, and $S = \{\pm 2\}$, resulting in

$$\hat{\sigma}^{(\alpha)\prime} = c_0 \, \hat{\sigma}^{(\alpha)} + c_1 \, [i\hat{G}, \hat{\sigma}^{(\alpha)}], \tag{60}$$

with coefficients from Eq. (31) given by

$$(c_0, c_1) = \Big(\cos 2\theta, \tfrac{1}{2} \sin 2\theta\Big). \tag{61}$$

The above analysis can be carried out with Lagrange polynomials of $\mathrm{ad}_{\hat{G}}$. Since the eigenvalues of $\hat{G}$ are ± 1, $\mathcal{D} = \{-2, 0, 2\}$. Then

$$\mathrm{Lag}_{\mathcal{D}}^{(-2)}(\mathrm{ad}_{\hat{G}})(\hat{\sigma}^{(\alpha)}) = \tfrac{1}{8}\mathrm{ad}_{\hat{G}}^2(\hat{\sigma}^{(\alpha)}) - \tfrac{1}{4}\mathrm{ad}_{\hat{G}}(\hat{\sigma}^{(\alpha)}), \tag{62}$$

$$\mathrm{Lag}_{\mathcal{D}}^{(0)}(\mathrm{ad}_{\hat{G}})(\hat{\sigma}^{(\alpha)}) = -\tfrac{1}{4}\mathrm{ad}_{\hat{G}}^2(\hat{\sigma}^{(\alpha)}) + \hat{\sigma}^{(\alpha)}, \tag{63}$$

$$\mathrm{Lag}_{\mathcal{D}}^{(2)}(\mathrm{ad}_{\hat{G}})(\hat{\sigma}^{(\alpha)}) = \tfrac{1}{8}\mathrm{ad}_{\hat{G}}^2(\hat{\sigma}^{(\alpha)}) + \tfrac{1}{4}\mathrm{ad}_{\hat{G}}(\hat{\sigma}^{(\alpha)}). \tag{64}$$

When $\hat{\sigma}^{(\alpha)}$ commutes with $\hat{G}$ ($\mathrm{ad}_{\hat{G}}(\hat{\sigma}^{(\alpha)}) = 0$), Eqs. (62), (64) vanish while Eq. (63) does not, leading to $S = \{0\}$. When $\hat{\sigma}^{(\alpha)}$ anti-commutes with $\hat{G}$, we have $[\hat{G}, \hat{\sigma}^{(\alpha)}] = 2\hat{G}\hat{\sigma}^{(\alpha)}$ and Eqs. (62), (64) does not vanish while Eq. (63) vanishes due to Eq. (56). This yields $S = \{-2, 2\}$.

2. Mutually Anticommuting Pauli Products

A generalization of a single Pauli-product generator is the sum of mutually anticommuting Pauli products $\{\hat{A}_j\}$ [11]:

$$\hat{G} = \sum_j d_j \, \hat{A}_j, \qquad d_j \in \mathbb{R}, \tag{65}$$

with

$$\{\hat{A}_j, \hat{A}_k\} = 0 \ (j \neq k). \tag{66}$$

It follows that

$$\hat{G}^2 = \Big(\sum_j d_j^2\Big)\hat{I}, \tag{67}$$

so $\hat{G}$ is involutory when $\sum_j d_j^2 = 1$, and its spectrum is $\{\pm 1\}$. The eigensubspace-projector representation then coincides with the single Pauli-product case, $\hat{G} = \hat{P}_+ - \hat{P}_-$, and Eq. (57) holds exactly.

However, obtaining the single-commutator reduction of Eq. (60) is more restrictive: for a Pauli product $\hat{\sigma}^{(\alpha)}$ in $\hat{H}$ to commute (respectively, anticommute) with $\hat{G}$, it must commute (respectively, anticommute) with every $\hat{A}_j$. Consequently, not every Pauli product in $\hat{H}$ can be transformed with a single commutator with $\hat{G}$; in general, the quadratic term in Eq. (57) remains necessary.

3. Unitary Coupled Cluster Generators

A unitary coupled-cluster (UCC) generator is the sum of a fermionic excitation and its corresponding de-excitation. It has been widely used in VQE workflows[2, 12, 28] and quantum-inspired algorithms.[29, 30] To discuss algebraic properties of UCC generators, we introduce the notation

$$\hat{a}_A := \prod_{j \in A} \hat{a}_j, \qquad \hat{a}_A^\dagger := (\hat{a}_A)^\dagger, \tag{68}$$

for products of fermionic annihilation and creation operators over a subset A of spin-orbital indices (taken in increasing order to fix phases). Then a UCC generator has the form

$$\hat{G} = (-i)\big(\hat{T}_G - \hat{T}_G^\dagger\big), \tag{69}$$

where $\hat{T}_G = \hat{a}_A^\dagger \hat{a}_B$ is an excitation with $|A| = |B|$ and $A \cap B = \varnothing$. $\hat{G}$ has spectrum $\{0, \pm 1\}$.[12] Assuming no projected blocks vanish for a generic $\hat{H}$, the set of distinct eigenvalue differences on nonvanishing blocks is $S = \{0, \pm 1, \pm 2\}$. A polynomial of degree $|S| - 1 = 4$ (i.e., up to the fourth nested commutator) suffices:

$$\hat{H}' = \sum_{j=0}^{4} c_j \, \mathrm{ad}_{i\hat{G}}^j(\hat{H}) \tag{70}$$

with coefficients from Eq. (31):

$$c_0 = 1, \tag{71}$$

$$c_1 = \tfrac{4}{3}\sin\theta - \tfrac{1}{6}\sin 2\theta, \tag{72}$$

$$c_2 = \tfrac{5}{4} - \tfrac{4}{3}\cos\theta + \tfrac{1}{12}\cos 2\theta, \tag{73}$$

$$c_3 = \tfrac{1}{3}\sin\theta - \tfrac{1}{6}\sin 2\theta, \tag{74}$$

$$c_4 = \tfrac{1}{4} - \tfrac{1}{3}\cos\theta + \tfrac{1}{12}\cos 2\theta. \tag{75}$$

Motivated by the structure of the electronic Hamiltonian and the UCC generator, we consider fragments of the Hamiltonian of the form

$$\hat{H}_\alpha = \hat{T}_\alpha + \hat{T}_\alpha^\dagger, \tag{76}$$

where $\hat{T}_\alpha = \hat{a}_C^\dagger \hat{a}_D$ is a single fermionic string. Let $\hat{P}_\pm, \hat{P}_0$ denote the projectors onto the eigenspaces $\mathcal{V}_\pm, \mathcal{V}_0$, corresponding to eigenvalues $\pm 1, 0$ of $\hat{G}$, respectively. In Appendix C, we show that for any $\hat{T}_\alpha$, either the set $\{\hat{P}_\pm \hat{H}_\alpha \hat{P}_\pm, \ \hat{P}_\pm \hat{H}_\alpha \hat{P}_\mp\}$ or the set $\{\hat{P}_\pm \hat{H}_\alpha \hat{P}_0, \ \hat{P}_0 \hat{H}_\alpha \hat{P}_\pm\}$ is potentially nonvanishing, but not both simultaneously.

When the blocks $\{\hat{P}_\pm \hat{H}_\alpha \hat{P}_\pm, \ \hat{P}_\pm \hat{H}_\alpha \hat{P}_\mp, \ \hat{P}_0 \hat{H}_\alpha \hat{P}_0\}$ are nonvanishing, $S = \{0, \pm 2\}$ and the transformed fragment

is given by Eq. (57) with coefficients in Eq. (58). When the blocks $\{\hat{P}_\pm\hat{H}_\alpha\hat{P}_0,\ \hat{P}_0\hat{H}_\alpha\hat{P}_\mp,\ \hat{P}_0\hat{H}_\alpha\hat{P}_0\}$ are nonvanishing, $S=\{0,\pm1\}$ and the transformed fragment is again given by Eq. (57), but with coefficients from Eq. (31):

$$(c_0, c_1, c_2) = \big(1,\, \sin\theta,\, 1-\cos\theta\big). \tag{77}$$

This reduction in projected blocks thus far remain true for the transformation of a single (non Hermitian) Fermionic excitation operator $\hat{O}_\alpha = \hat{T}_\alpha$ and does not require number preservation ($|A| = |B|$). Hence our analysis agrees with findings of Ref. [14].

In addition, for the Hermitian fragments in Eq. (76), we identify two further cases in which a single commutator suffices. In one case, the blocks $\hat{P}_\pm\hat{H}_\alpha\hat{P}_\pm$, $\hat{P}_\pm\hat{H}_\alpha\hat{P}_\mp$, and $\hat{P}_0\hat{H}_\alpha\hat{P}_0$ vanish, leading to $S=\{\pm1\}$. The transformed fragment then has the form of Eq. (60), with coefficients from Eq. (31):

$$(c_0, c_1) = \big(\cos\theta,\, \sin\theta\big). \tag{78}$$

In the other case, the blocks $\hat{P}_\pm\hat{H}_\alpha\hat{P}_\pm$, $\hat{P}_0\hat{H}_\alpha\hat{P}_0$, $\hat{P}_\pm\hat{H}_\alpha\hat{P}_0$, and $\hat{P}_0\hat{H}_\alpha\hat{P}_\pm$ vanish. This yields $S=\{\pm2\}$ and a transformed fragment given by Eq. (60) with coefficients from Eq. (61). In both of these cases, $|S|=2$ and only a single nested commutator is required to represent $\hat{H}'_\alpha$.

The set of vanishing projected blocks depends on the spin-orbital indices present in $\hat{T}_\alpha$ and those shared with $\hat{T}_G$. To list and analyze all possibilities, we introduce the notation

$$\hat{T}_G = \tilde{T}_G\,\tilde{L}_G \tag{79}$$

$$\hat{T}_\alpha = \tilde{T}_\alpha\,\tilde{L}_\alpha \tag{80}$$

where $\tilde{T}_G, \tilde{T}_\alpha$ act on the shared spin-orbital indices $(A\cup B)\cap(C\cup D)$, while $\tilde{L}_G$ and $\tilde{L}_\alpha$ act on the disjoint sets $(A\cup B)\setminus(C\cup D)$ and $(C\cup D)\setminus(A\cup B)$, respectively. Conditions on $\{\tilde{T}_G, \tilde{L}_G, \tilde{T}_\alpha, \tilde{L}_\alpha\}$ that produce the various nonvanishing block structures described above are derived in Appendix C. The cases with examples are summarized in Table I, and Fig. 1 illustrates their projected-block patterns.

IV. NEW MANY-BODY TRANSFORMATIONS

The proposed framework not only encompasses all the known exact transformations but also enables us to create a new class of exact transformations. This new class is motivated by the desire to combine strengths of Pauli product based generators (lowest number of eigenvalues) with the electron number preserving character of the fermionic generators. Indeed, neither a single Pauli product nor a sum of mutually anticommuting Pauli products preserves the fermionic number symmetry of the transformed Hamiltonian. We introduce fermionic, electron number preserving, generators

$$\hat{G} = \hat{V}\hat{p}\hat{V}^\dagger, \tag{81}$$

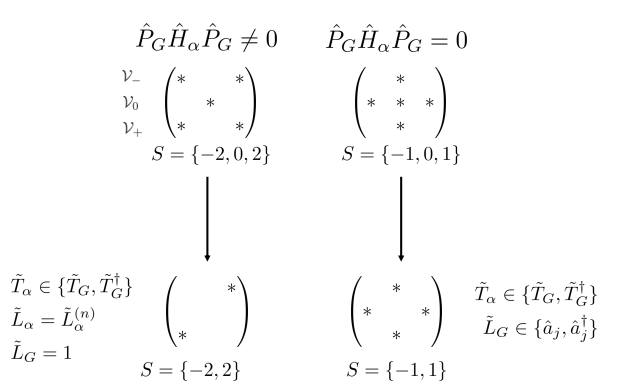

FIG. 1. Two patterns of nonvanishing projected blocks (depicted by $*$) of $\hat{H}_\alpha = \hat{T}_\alpha + \hat{T}_\alpha^\dagger$ in the eigenspaces $\{\mathcal{V}_-, \mathcal{V}_0, \mathcal{V}_+\}$ of $\hat{G} = (-i)(\hat{T}_G - \hat{T}_G^\dagger)$, depending on whether $\hat{P}_G\hat{H}_\alpha\hat{P}_G$ vanishes, where $\hat{P}_G := \hat{P}_+ + \hat{P}_-$. When the operators $\hat{T}_G := \tilde{T}_G\tilde{L}_G$ and $\hat{T}_\alpha := \tilde{T}_\alpha\tilde{L}_\alpha$ take the forms specified, additional projected blocks vanish. A superscript (n) denotes a product of occupation operators, $\{\hat{a}_p^\dagger\hat{a}_p\}_{p=1}^N$.

where $\hat{V}$ is an orbital rotation [Eq. (41)] and

$$\hat{p} = c_0 + \sum_p c_p\hat{n}_p + \sum_{pq} c_{pq}\hat{n}_p\hat{n}_q + \cdots \tag{82}$$

is a polynomial in the occupation operators $\hat{n}_p = \hat{a}_p^\dagger\hat{a}_p$ with only a few distinct eigenvalues. This form is motivated by the ease of constructing polynomials with a fixed number of eigenvalues from the simplest hermitian fermionic projectors, $\{\hat{n}_p\}$. The orbital rotations $\hat{V}$ do not alter either the eigenvalues determined by $\hat{p}$ or fermionic rank of $\hat{p}$. The form of $\hat{p}$ and $\hat{V}$ can be chosen to satisfy other desired properties, such as preservation of spin symmetries. Interestingly, a UCC generator cannot be expressed in the form of Eq. (81).[31]

There are several approaches for constructing operators $\hat{p}$ with the target eigenvalues $g_i \in \Lambda$. A simple approach is to construct orthogonal projectors $\hat{P}_i$ as products of $\{\hat{n}_p, 1-\hat{n}_p\}$. The generator is then constructed as a sum of projectors with the eigenvalues as coefficients. For example, to construct a fermionic rank 2 generator with four eigenvalues $\{g_{1-4}\}$, the projectors are constructed as $\{\hat{n}_1\hat{n}_2, \hat{n}_1(1-\hat{n}_2), (1-\hat{n}_1)\hat{n}_2, (1-\hat{n}_1)(1-\hat{n}_2)\}$ and the generator takes the form

$$\begin{aligned}\hat{p} =& g_1\hat{n}_1\hat{n}_2 + g_2\hat{n}_1(1-\hat{n}_2)\\ &+ g_3(1-\hat{n}_1)\hat{n}_2 + g_4(1-\hat{n}_1)(1-\hat{n}_2).\end{aligned} \tag{83}$$

When the number of distinct spin-orbital indices is greater than the desired fermionic rank of the generator, some of the constructed projectors are no longer orthogonal. In such cases, this method cannot be used.

Alternatively, one can solve for coefficients $\{c_{p\cdots q}\}$ in $\hat{p}$ that satisfy the characteristic equation $p_\Lambda(\hat{p}) = \hat{0}$. Here p_Λ is the characteristic polynomial of the generator, and

Constraints	Vanishing blocks	S	$\hat{T}_G$	$\hat{T}_\alpha$
$\tilde{T}_\alpha \in \{\tilde{T}_G, \tilde{T}_G^\dagger\}$, $\tilde{L}_G = \tilde{L}_G^{(n)}$	$\hat{P}_\pm \hat{H}_\alpha \hat{P}_0$, $\hat{P}_0 \hat{H}_\alpha \hat{P}_\pm$	$\{-2, 0, 2\}$	$\hat{a}_2^\dagger \hat{a}_1^\dagger \hat{a}_2 \hat{a}_0$	$\hat{a}_3^\dagger \hat{a}_1^\dagger \hat{a}_4 \hat{a}_0$
$\tilde{T}_\alpha \in \{\tilde{T}_G \tilde{T}_G^\dagger, \tilde{T}_G^\dagger \tilde{T}_G\}$			$\hat{a}_3^\dagger \hat{a}_2^\dagger \hat{a}_1 \hat{a}_0$	$\hat{a}_1^\dagger \hat{a}_1$
$\tilde{T}_\alpha \in \{\tilde{T}_G, \tilde{T}_G^\dagger\}$, $\tilde{L}_G = 1$, $\tilde{L}_\alpha = \tilde{L}_\alpha^{(n)}$	$\hat{P}_\pm \hat{H}_\alpha \hat{P}_\pm$, $\hat{P}_0 \hat{H}_\alpha \hat{P}_0$, $\hat{P}_\pm \hat{H}_\alpha \hat{P}_0$, $\hat{P}_0 \hat{H}_\alpha \hat{P}_\pm$	$\{-2, 2\}$	$\hat{a}_3^\dagger \hat{a}_2^\dagger \hat{a}_1 \hat{a}_0$	$\hat{a}_3^\dagger \hat{a}_2^\dagger \hat{a}_1 \hat{a}_0$
$\tilde{T}_\alpha \in \{\tilde{T}_G, \tilde{T}_G^\dagger\}$, $\tilde{L}_G \in \{\hat{a}_j, \hat{a}_j^\dagger\}$, $j \notin C \cup D$	$\hat{P}_\pm \hat{H}_\alpha \hat{P}_\pm$, $\hat{P}_\pm \hat{H}_\alpha \hat{P}_\mp$, $\hat{P}_0 \hat{H}_\alpha \hat{P}_0$	$\{-1, 1\}$	$\hat{a}_3^\dagger \hat{a}_2^\dagger \hat{a}_1 \hat{a}_0$	$\hat{a}_4^\dagger \hat{a}_2^\dagger \hat{a}_1 \hat{a}_0$
$\hat{P}_G \hat{H}_\alpha \hat{P}_G = 0$ and not above-listed cases	$\hat{P}_\pm \hat{H}_\alpha \hat{P}_\pm$, $\hat{P}_\pm \hat{H}_\alpha \hat{P}_\mp$	$\{-1, 0, 1\}$	$\hat{a}_3^\dagger \hat{a}_2^\dagger \hat{a}_1 \hat{a}_0$	$\hat{a}_3^\dagger \hat{a}_2^\dagger \hat{a}_2 \hat{a}_0$

TABLE I. Examples of $\{\hat{T}_G, \hat{T}_\alpha\}$ pairs resulting in different vanishing block structures and eigenvalue-difference sets S, with the notation introduced in Eqs. (79) and (80). A superscript (n) denotes a product of occupation operators, $\{\hat{a}_p^\dagger \hat{a}_p\}_{p=1}^N$.

is defined as

$$p_\Lambda(x) = \prod_i (x - g_i). \tag{84}$$

The constraint $p_\Lambda(\hat{p}) = \hat{0}$ yields a system of nonlinear equations in the coefficients, which can be solved analytically. Since non-trivial $\hat{p}$ can satisfy factors $p_{\Lambda'}(\hat{p}) = \hat{0}$ for $\Lambda' \subset \Lambda, |\Lambda'| \geq 2$, such solutions do not exhibit the spectrum Λ and must be discarded.

A. Fermionic reflections

To construct up to two-electron generators (fermionic rank 2) with eigenvalues of ± 1, the only operators $\hat{p}$ (up to index relabeling and a global phase of ± 1) are

$$\begin{aligned}
\hat{p}_1 &= 1 - 2\hat{n}_p \\
\hat{p}_2 &= 1 - 2\hat{n}_p \hat{n}_q \\
\hat{p}_3 &= 1 - 2\hat{n}_p + 2\hat{n}_p \hat{n}_q \\
\hat{p}_4 &= 1 - 2\hat{n}_p - 2\hat{n}_q + 2\hat{n}_p \hat{n}_q \\
\hat{p}_5 &= 1 - 2\hat{n}_p - 2\hat{n}_q + 4\hat{n}_p \hat{n}_q \\
\hat{p}_6 &= 1 - 2\hat{n}_p - 2\hat{n}_q \hat{n}_r + 2\hat{n}_p \hat{n}_r \\
\hat{p}_7 &= 1 - 2\hat{n}_p - 2\hat{n}_q \hat{n}_r + 2\hat{n}_p \hat{n}_r + 2\hat{n}_p \hat{n}_q \\
\hat{p}_8 &= 1 - 2\hat{n}_p - 2\hat{n}_q + 2\hat{n}_p \hat{n}_r + 2\hat{n}_p \hat{n}_q \\
\hat{p}_9 &= 1 - 2\hat{n}_p - 2\hat{n}_q - 2\hat{n}_r + 2\hat{n}_q \hat{n}_r \\
&\quad + 2\hat{n}_p \hat{n}_r + 2\hat{n}_p \hat{n}_q \\
\hat{p}_{10} &= 1 - 2\hat{n}_p - 2\hat{n}_q - 2\hat{n}_r \hat{n}_s + 2\hat{n}_p \hat{n}_r \\
&\quad + 2\hat{n}_q \hat{n}_s + 2\hat{n}_p \hat{n}_q.
\end{aligned} \tag{85}$$

These solutions are obtained by imposing $(c_0 + \sum_p c_p \hat{n}_p + \sum_{pq} c_{pq} \hat{n}_p \hat{n}_q)^2 - \hat{1} = 0$ and solving exhaustively for non-trivial values of $c_0, \{c_p\}, \{c_{pq}\}$. We find that $c_0 = 1$, $c_p \in \{0, -2\}$ and $c_{pq} \in \{0, \pm 2, 4\}$, and that there are no solutions involving 5 distinct spin-orbital indices. Thus, no solutions exist with more than four distinct spin-orbital indices. The 10 polynomials form disjoint classes of generators because orbital rotations cannot map one of these polynomials to another (see Appendix D for a proof). Since the constructed generators are reflective ($\hat{G}^2 = \hat{1}$), we refer to these generators as fermionic reflections.

By selecting the polynomial $\hat{p}$ and matrix M defining the unitary rotations, one can optimize the generator for a specific cost function defined on the transformed Hamiltonian. One such cost function is the electronic energy of a product state

$$E(\theta, M; j) = \langle \mathrm{HF} | \, e^{i\theta \hat{G}} \hat{H} e^{-i\theta \hat{G}} \, | \mathrm{HF} \rangle \tag{86}$$

where $\hat{G} = \hat{V} \hat{p}_j \hat{V}^\dagger$. For each j, the matrix M can be optimized classically, using the exact transformation, to determine the generator that yields the largest energy lowering. To minimize the number of terms in the transformed Hamiltonian, M can instead be optimized to reduce the ℓ_0-norm of the coefficients of the transformed Hamiltonian. In practice, this can be approximated by minimizing the computationally less demanding ℓ_1-norm.

V. CONCLUSIONS

We have shown that an exact transformation of many-body operators, such as Hamiltonians, can be achieved when the adjoint action of the generator of the transforming unitary defines a linear map in a finite-dimensional space. According to the Cayley–Hamilton theorem, a finite-degree characteristic polynomial exists that annihilates the adjoint map. This observation enables one to represent the otherwise infinite Baker–Campbell–Hausdorff series for the transformed operator as a finite-degree polynomial, computable with polynomial effort on a classical computer.

We have analyzed two cases in which the adjoint map of the generator can be represented as a linear operator in a finite-dimensional space: (1) when the generator belongs to one of the known finite-dimensional Lie algebras that acts on the space of the transformed operator, and (2) when the generator has a finite number of distinct eigenvalues. In the latter case, the degree of the characteristic polynomial can be reduced by accounting for properties of the transformed operator arising from its commutation and anticommutation relations with the generator. The second case thus subsumes the first and provides a more general framework. Additionally, the second case can also be seen as the generator being the element of a finite abelian Lie algebra of eigen-subspace projectors.

When transforming complex operators such as many-body Hamiltonians, one can express them as polynomials

in operators whose algebraic relations with the generator simplify the transformation. Particularly efficient transformations arise when both the generator and the operator belong to the same Lie algebra.

Ensuring that the adjoint generator action has finite degree under either of the two conditions is sufficient, as all additional reductions stemming from more specific algebraic structures are recovered automatically through normal ordering of the resulting transformed operators. Consequently, while identifying specific operator fragments is not required to obtain the final result, such analysis explains why, for the same generator, some transformed expressions are more compact than others. For example, in the case of unitary coupled-cluster (UCC) generators, we identify fragments requiring only a single commutator, thereby extending prior results.

The framework introduced here opens several promising directions. A natural extension involves finite-spectrum generators of chemical relevance, such as spherical tensor operators that preserve spin and spatial symmetries. Automated procedures to identify fragments that require fewer nested commutators could further improve the computational efficiency of the exact transformation. Another avenue is to search for new generators that preserve molecular symmetries while having small spectra, thereby providing a useful class of optimizable unitaries for efficient quantum simulation. As an illustration, we construct a class of optimizable, number-conserving generators whose spectra are identical to those of Pauli products.

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CODE AVAILABLITY

Python scripts to determine the block structures, obtain nested commutator coefficients, and test examples listed in Table I can be found at https://github.com/Praveen91299/UnitaryTransforms.git.

Appendix A: Coefficients of nested commutators are real valued

For a Hermitian $\hat{H}$, $||\hat{P}_l\hat{H}\hat{P}_r|| \neq 0$ iff $||\hat{P}_r\hat{H}\hat{P}_l|| \neq 0$ and we have $-\Delta \in S$ iff $\Delta \in S$. Then both Δ and $-\Delta$ define constraint equations through Eq. (29). Adding and subtracting these constraints, we obtain an alternative system of equations

$$\frac{e^{i\theta\Delta} + e^{-i\theta\Delta}}{2} = \sum_{m=0}^{\lfloor(|S|-1)/2\rfloor} (-1)^m c_{2m}(\theta)\Delta^{2m} \tag{A1}$$

$$\frac{e^{i\theta\Delta} - e^{-i\theta\Delta}}{2i} = \sum_{m=0}^{\lfloor|S|/2\rfloor-1} (-1)^m c_{2m+1}(\theta)\Delta^{2m+1} \tag{A2}$$

for $\Delta \in \bar{S}$ from the set of non-negative unique eigenvalue differences

$$\bar{S} := \{|x| \mid x \in S\}. \tag{A3}$$

Equations (A1) can be re-expressed as

$$\vec{e}^{(0)} = W^{(0)}\vec{c}^{(0)} \tag{A4}$$

where $e^{(0)}_\Delta = \cos(\theta\Delta)$, $c^{(0)}_m = c_{2m}(\theta)$ and $[W^{(0)}]_{\Delta m} = (-1)^m\Delta^{2m}$ is the $|\bar{S}| \times |\bar{S}|$ dimensional generalized Vandermonde matrix defined by $\Delta \in \bar{S}$ and $m = 0, \ldots, |\bar{S}| - 1$.[17] Since Eq. (A2) vanishes for $\Delta = 0$, we re-express the equation as

$$\vec{e}^{(1)} = W^{(1)}\vec{c}^{(1)} \tag{A5}$$

where $e^{(1)}_\Delta = \sin(\theta\Delta)$, $c^{(1)}_m = c_{2m+1}(\theta)$, and $[W^{(1)}]_{\Delta m} = (-1)^m\Delta^{2m+1}$ is the $|\bar{S} \setminus \{0\}| \times |\bar{S} \setminus \{0\}|$ dimensional generalized Vandermonde matrix defined by $\Delta \in \bar{S} \setminus \{0\}$ and $m = 0, \ldots, |\bar{S} \setminus \{0\}| - 1$.

The matrices $W^{(0)}, W^{(1)}$ are real, square and invertible, thus yielding unique real solutions for $\vec{c}^{(0)}, \vec{c}^{(1)}$ and equivalently for $\vec{c}$. Since we have solved a system equations that are equivalent to the original system of equations in Eq. (29), the solution must be identical.

Appendix B: Projectors onto the eigenspaces of unitary coupled-cluster generators

Consider the UCC generator $\hat{G}$ defined in Eq. (69). $\hat{G}$ has spectrum $\{0, \pm 1\}$, and projectors onto its eigenspaces can be constructed using methods discussed in Ref. 32. Here we present an alternative approach based on enumerating the eigenstates of $\hat{G}$, which also reveals useful algebraic identities of the involved operators.

Consider a Slater determinant $|\phi_j\rangle$ in a basis of N spin-orbitals. If

$$\hat{T}_G |\phi_j\rangle = |\psi_j\rangle \neq 0, \tag{B1}$$

then $|\psi_j\rangle$ is a Slater determinant distinct from $|\phi_j\rangle$, and the states

$$|\psi^\pm_j\rangle = \frac{1}{\sqrt{2}} \left(|\phi_j\rangle \mp i\ |\psi_j\rangle\right) \tag{B2}$$

are eigenstates of $\hat{G}$ with eigenvalues ± 1, respectively. Suppose there are k such pairs $\{|\psi^\pm_j\rangle\}_{j=1}^k$. From Eq. (B1),

$$\sum_{j=1}^{k} |\psi_j\rangle \langle\phi_j| = \hat{T}_G, \tag{B3}$$

and consequently,

$$\sum_{j=1}^{k} |\phi_j\rangle \langle\psi_j| = \hat{T}_G^\dagger, \tag{B4}$$

$$\sum_{j=1}^{k} |\phi_j\rangle \langle\phi_j| = \hat{T}_G^\dagger \hat{T}_G, \tag{B5}$$

$$\sum_{j=1}^{k} |\psi_j\rangle \langle\psi_j| = \hat{T}_G \hat{T}_G^\dagger. \tag{B6}$$

From Eqs. (B3)–(B6), we have the identities

$$\hat{T}_G^2 = (\hat{T}_G^\dagger)^2 = 0, \tag{B7}$$

$$\hat{T}_G \hat{T}_G^\dagger \hat{T}_G = \hat{T}_G, \tag{B8}$$

$$\hat{T}_G^\dagger \hat{T}_G \hat{T}_G^\dagger = \hat{T}_G^\dagger. \tag{B9}$$

(These reflect nilpotency and partial-isometry properties of the ladder operators.)

Using Eqs. (B3)–(B6), the projectors onto the ± 1 eigenspaces are

$$\begin{aligned}\hat{P}_\pm &= \sum_{j=1}^{k} |\psi_j^\pm\rangle \langle\psi_j^\pm| \\ &= \frac{1}{2}\sum_{j=1}^{k} (|\phi_j\rangle \langle\phi_j| + |\psi_j\rangle \langle\psi_j| \pm i\, |\phi_j\rangle \langle\psi_j| \mp i\, |\psi_j\rangle \langle\phi_j|) \\ &= \frac{1}{2}\left(\hat{T}_G^\dagger \hat{T}_G + \hat{T}_G \hat{T}_G^\dagger \pm i\, \hat{T}_G^\dagger \mp i\, \hat{T}_G\right),\end{aligned} \tag{B10}$$

and the projector onto the null space is

$$\hat{P}_0 = \hat{I} - \hat{P}_+ - \hat{P}_-. \tag{B11}$$

Define the projector onto the nonzero eigenspaces of $\hat{G}$ as

$$\hat{P}_G := \hat{P}_+ + \hat{P}_- \tag{B12}$$

$$= \hat{T}_G \hat{T}_G^\dagger + \hat{T}_G^\dagger \hat{T}_G \;=\; \hat{G}\hat{G}^\dagger \;=\; \hat{G}^\dagger \hat{G}, \tag{B13}$$

where the second equality uses $\hat{G} = (-i)(\hat{T}_G - \hat{T}_G^\dagger)$ together with Eq. (B7). The operator $\hat{P}_G$ projects onto $\mathrm{span}\big(\{|\phi_j\rangle, |\psi_j\rangle\}_{j=1}^k\big)$ and is orthogonal to $\hat{P}_0$ (i.e., $\hat{P}_G \hat{P}_0 = 0$). Since the spectrum of $\hat{G}$ is $\{0, \pm 1\}$, we have the compact relations

$$\hat{P}_\pm = \frac{1}{2}\left(\hat{P}_G \pm \hat{G}\right), \tag{B14}$$

$$\hat{P}_0 = \hat{I} - \hat{P}_G. \tag{B15}$$

Appendix C: Nonzero projected blocks for unitary coupled-cluster generators

Consider the case in which $\hat{H}_\alpha := \hat{T}_\alpha + \hat{T}_\alpha^\dagger$ is the sum of a fermionic excitation $\hat{T}_\alpha = \hat{a}_C^\dagger \hat{a}_D$ and its Hermitian conjugate. We determine the set S of unique eigenvalue differences over nonzero projected blocks for all fermionic strings $\hat{T}_\alpha$. We use the notation introduced in Eqs. (79) and (80).

First, consider the commuting case $[\hat{H}_\alpha, \hat{G}] = 0$. Then $S = \{0\}$. This includes the case in which the excitations $\hat{T}_\alpha$ and $\hat{T}_G$ do not share spin-orbital indices ($\tilde{T}_G = \tilde{T}_\alpha = \hat{I}$).

When $\hat{T}_\alpha$ and $\hat{T}_G$ share indices, use Eq. (B13) and consider the block of $\hat{H}_\alpha$ on the ± 1 eigenspaces:

$$\begin{aligned}\hat{P}_G \hat{H}_\alpha \hat{P}_G = {} & \tilde{T}_G \tilde{T}_G^\dagger \tilde{T}_\alpha \tilde{T}_G \tilde{T}_G^\dagger \cdot \tilde{L}_G \tilde{L}_G^\dagger \tilde{L}_G \tilde{L}_G^\dagger \tilde{L}_\alpha \\ & + \tilde{T}_G \tilde{T}_G^\dagger \tilde{T}_\alpha \tilde{T}_G^\dagger \tilde{T}_G \cdot \tilde{L}_G \tilde{L}_G^\dagger \tilde{L}_G^\dagger \tilde{L}_G \tilde{L}_\alpha \\ & + \tilde{T}_G^\dagger \tilde{T}_G \tilde{T}_\alpha \tilde{T}_G \tilde{T}_G^\dagger \cdot \tilde{L}_G^\dagger \tilde{L}_G \tilde{L}_G \tilde{L}_G^\dagger \tilde{L}_\alpha \\ & + \tilde{T}_G^\dagger \tilde{T}_G \tilde{T}_\alpha \tilde{T}_G^\dagger \tilde{T}_G \cdot \tilde{L}_G^\dagger \tilde{L}_G \tilde{L}_G^\dagger \tilde{L}_G \tilde{L}_\alpha \\ & + \text{h.c.}\end{aligned} \tag{C1}$$

(Here, we separate the operator factors over shared and unshared spin-orbitals by "$\cdot$".) Since

$$\hat{P}_G \hat{H}_\alpha \hat{P}_G = \hat{P}_+ \hat{H}_\alpha \hat{P}_+ + \hat{P}_+ \hat{H}_\alpha \hat{P}_- + \hat{P}_- \hat{H}_\alpha \hat{P}_+ + \hat{P}_- \hat{H}_\alpha \hat{P}_-, \tag{C2}$$

if $\hat{P}_G \hat{H}_\alpha \hat{P}_G$ is zero, then all blocks in $\{\hat{P}_\pm \hat{H}_\alpha \hat{P}_\pm, \hat{P}_\pm \hat{H}_\alpha \hat{P}_\mp\}$ vanish. For $\hat{P}_G \hat{H}_\alpha \hat{P}_G$ to be nonzero, at least one product in Eq. (C1) must be nonzero, leading to the following cases:

$$\text{(i) } \tilde{T}_\alpha = \tilde{T}_G, \quad \tilde{L}_G = \tilde{L}_G^{(n)}, \tag{C3}$$

$$\text{(ii) } \tilde{T}_\alpha = \tilde{T}_G^\dagger, \quad \tilde{L}_G = \tilde{L}_G^{(n)}, \tag{C4}$$

$$\text{(iii) } \tilde{T}_\alpha = \tilde{T}_G \tilde{T}_G^\dagger, \tag{C5}$$

$$\text{(iv) } \tilde{T}_\alpha = \tilde{T}_G^\dagger \tilde{T}_G, \tag{C6}$$

$$\text{(v) } \tilde{T}_\alpha = \tilde{T}_\alpha^{(n)}, \quad \tilde{T}_G = \tilde{T}_G^{(n)}. \tag{C7}$$

Here a superscript (n) denotes a product of occupation operators $\hat{n}_p := \hat{a}_p^\dagger \hat{a}_p$ (including $\hat{I}$). Case (v) is trivial ($[\hat{H}_\alpha, \hat{G}] = 0$) and is not considered further. In cases (i)–(iv) we assume $\tilde{T}_G$ is not a pure number-operator product. In all four cases,

$$\begin{aligned}[\hat{P}_G, \hat{T}_\alpha] = {} & \tilde{T}_G \tilde{T}_G^\dagger \tilde{T}_\alpha \tilde{L}_G \tilde{L}_G^\dagger \tilde{L}_\alpha - \tilde{T}_\alpha \tilde{T}_G \tilde{T}_G^\dagger \tilde{L}_G \tilde{L}_G^\dagger \tilde{L}_\alpha \\ & + \tilde{T}_G^\dagger \tilde{T}_G \tilde{T}_\alpha \tilde{L}_G^\dagger \tilde{L}_G \tilde{L}_\alpha - \tilde{T}_\alpha \tilde{T}_G^\dagger \tilde{T}_G \tilde{L}_G^\dagger \tilde{L}_G \tilde{L}_\alpha \;=\; 0,\end{aligned} \tag{C8}$$

so $[\hat{P}_G, \hat{H}_\alpha] = 0$ and therefore

$$\hat{P}_G \hat{H}_\alpha \hat{P}_0 = \hat{H}_\alpha \hat{P}_G \hat{P}_0 = 0, \tag{C9}$$

$$\Rightarrow \quad \hat{P}_\pm \hat{H}_\alpha \hat{P}_0 = \hat{P}_0 \hat{H}_\alpha \hat{P}_\pm = 0. \tag{C10}$$

Thus either the set $\{\hat{P}_\pm \hat{H}_\alpha \hat{P}_\pm, \hat{P}_\pm \hat{H}_\alpha \hat{P}_\mp\}$ or the set $\{\hat{P}_\pm \hat{H}_\alpha \hat{P}_0, \hat{P}_0 \hat{H}_\alpha \hat{P}_\pm\}$ can be nonzero, but not both simultaneously. Consequently, $S = \{0, \pm 2\}$ or $S = \{0, \pm 1\}$, so that $|S| - 1 = 2$ nested commutators suffice to represent $\hat{H}'_\alpha$.

Note that cases (i)-(iv) also correspond to cases when $\hat{P}_G\hat{T}_\alpha\hat{P}_G$ is nonzero. From Eq. (C8), it follows that either the set $\{\hat{P}_\pm\hat{T}_\alpha\hat{P}_\pm, \hat{P}_\pm\hat{T}_\alpha\hat{P}_\mp\}$ or the set $\{\hat{P}_\pm\hat{T}_\alpha\hat{P}_0, \hat{P}_0\hat{T}_\alpha\hat{P}_\pm\}$ can be nonzero, but not both simultaneously. Consequently, $S = \{0, \pm 2\}$ or $S = \{0, \pm 1\}$ for a single Fermionic excitation.

When $\hat{\mathbf{P}}_\mathbf{G}\hat{\mathbf{H}}_\alpha\hat{\mathbf{P}}_\mathbf{G} \neq \mathbf{0}$. Using the partial-isometry identities $\tilde{T}_G\tilde{T}_G^\dagger\tilde{T}_G = \tilde{T}_G$ and $\tilde{T}_G^\dagger\tilde{T}_G\tilde{T}_G^\dagger = \tilde{T}_G^\dagger$ in cases (i) and (ii), we have

$$\begin{aligned}\hat{P}_0\hat{H}_\alpha\hat{P}_0 &= \hat{H}_\alpha(\hat{I} - \hat{P}_G)\\ &= \hat{H}_\alpha\big(\hat{I} - \tilde{L}_G^{(n)}\big)\end{aligned} \tag{C11}$$

Whereas in case (iii) we have

$$\hat{P}_0\hat{H}_\alpha\hat{P}_0 = \hat{H}_\alpha\big(\hat{I} - \tilde{L}_G\tilde{L}_G^\dagger\big), \tag{C12}$$

and in case (iv) we have

$$\hat{P}_0\hat{H}_\alpha\hat{P}_0 = \hat{H}_\alpha\big(\hat{I} - \tilde{L}_G^\dagger\tilde{L}_G\big). \tag{C13}$$

In all four cases, when $\tilde{L}_G = \hat{I}$, $\hat{P}_0\hat{H}_\alpha\hat{P}_0$ vanishes; otherwise it is nonzero.

The operator $\tilde{L}_\alpha$ remains unspecified; its form may allow further reductions in the number of nonzero projected blocks. If the off-diagonal blocks $\{\hat{P}_\pm\hat{H}_\alpha\hat{P}_\mp\}$ vanish, then $[\hat{H}_\alpha, \hat{G}] = 0$, which we do not consider further here. To test whether the diagonal blocks $\{\hat{P}_\pm\hat{H}_\alpha\hat{P}_\pm\}$ can vanish, we examine the anti-commutator $[\hat{H}_\alpha, \hat{G}]_+$ for cases (i)–(iv).

Case (i): $\tilde{T}_\alpha = \tilde{T}_G$ and $\tilde{L}_G = \tilde{L}_G^{(n)}$. $\tilde{T}_G$ is a product of an even number of fermionic operators (since $\tilde{L}_G = \tilde{L}_G^{(n)}$), and the operators $\tilde{T}_G, \tilde{L}_G^{(n)}$ and $\tilde{L}_\alpha$ do not share spin-orbital indices, so

$$[\tilde{T}_G, \tilde{L}_\alpha] = [\tilde{T}_G, \tilde{L}_G^{(n)}] = [\tilde{L}_G^{(n)}, \tilde{L}_\alpha] = 0. \tag{C14}$$

Then

$$\hat{H}_\alpha\hat{G} = i\big(\tilde{T}_G\tilde{T}_G^\dagger\tilde{L}_G^{(n)}\tilde{L}_\alpha - \tilde{T}_G^\dagger\tilde{T}_G\tilde{L}_G^{(n)}\tilde{L}_\alpha^\dagger\big), \tag{C15}$$

$$\Rightarrow \quad [\hat{H}_\alpha, \hat{G}]_+ = i\big(\tilde{T}_G^\dagger\tilde{T}_G + \tilde{T}_G\tilde{T}_G^\dagger\big)\,\tilde{L}_G^{(n)}\big(\tilde{L}_\alpha - \tilde{L}_\alpha^\dagger\big). \tag{C16}$$

When $\tilde{L}_\alpha = \tilde{L}_\alpha^{(n)}$ is a number-operator product, $\tilde{L}_\alpha^\dagger = \tilde{L}_\alpha$ and the anti-commutator in Eq. (C16) vanishes, implying the diagonal blocks $\{\hat{P}_\pm\hat{H}_\alpha\hat{P}_\pm\}$ vanish. Moreover, when $\tilde{L}_G = \hat{I}$, $\hat{P}_0\hat{H}_\alpha\hat{P}_0$ vanishes and $S = \{\pm 2\}$, so $|S| = 2$.

Case (ii): $\tilde{T}_\alpha = \tilde{T}_G^\dagger$ and $\tilde{L}_G = \tilde{L}_G^{(n)}$. Then

$$\hat{H}_\alpha\hat{G} = i\big(\tilde{T}_G^\dagger\tilde{T}_G\tilde{L}_G^{(n)}\tilde{L}_\alpha^\dagger - \tilde{T}_G\tilde{T}_G^\dagger\tilde{L}_G^{(n)}\tilde{L}_\alpha\big), \tag{C17}$$

$$\Rightarrow \quad [\hat{H}_\alpha, \hat{G}]_+ = i\big(\tilde{T}_G^\dagger\tilde{T}_G + \tilde{T}_G\tilde{T}_G^\dagger\big)\,\tilde{L}_G^{(n)}\big(\tilde{L}_\alpha^\dagger - \tilde{L}_\alpha\big), \tag{C18}$$

which is analogous to case (i), yielding $S = \{\pm 2\}$ for $\tilde{L}_\alpha = \tilde{L}_\alpha^{(n)}$ and $\tilde{L}_G^{(n)} = \hat{I}$.

Case (iii): $\tilde{T}_\alpha = \tilde{T}_G\tilde{T}_G^\dagger$. Then

$$\hat{H}_\alpha\hat{G} = -i\big(\tilde{L}_\alpha + \tilde{L}_\alpha^\dagger\big)\,\tilde{T}_G\tilde{L}_G, \tag{C19}$$

$$\Rightarrow \quad [\hat{H}_\alpha, \hat{G}]_+ = -i\big(\tilde{L}_\alpha + \tilde{L}_\alpha^\dagger\big)\,\big(\tilde{T}_G\tilde{L}_G - \tilde{L}_G^\dagger\tilde{T}_G^\dagger\big). \tag{C20}$$

Since $[\hat{H}_\alpha, \hat{G}]_+$ cannot vanish for any choice of $\tilde{L}_\alpha$ in this case, at least one of the diagonal blocks $\{\hat{P}_\pm\hat{H}_\alpha\hat{P}_\pm\}$ is nonzero, and no further reduction of S is possible.

Case (iv): $\tilde{T}_\alpha = \tilde{T}_G^\dagger\tilde{T}_G$. Then

$$\hat{H}_\alpha\hat{G} = i\big(\tilde{L}_\alpha + \tilde{L}_\alpha^\dagger\big)\,\tilde{L}_G^\dagger\tilde{T}_G^\dagger, \tag{C21}$$

$$\Rightarrow \quad [\hat{H}_\alpha, \hat{G}]_+ = -i\big(\tilde{L}_\alpha + \tilde{L}_\alpha^\dagger\big)\,\big(\tilde{T}_G\tilde{L}_G - \tilde{L}_G^\dagger\tilde{T}_G^\dagger\big), \tag{C22}$$

which is analogous to case (iii) and likewise does not permit further reduction of S.

When $\hat{\mathbf{P}}_\mathbf{G}\hat{\mathbf{H}}_\alpha\hat{\mathbf{P}}_\mathbf{G} = \mathbf{0}$. The blocks $\{\hat{P}_0\hat{H}_\alpha\hat{P}_0, \hat{P}_\pm\hat{H}_\alpha\hat{P}_0, \hat{P}_0\hat{H}_\alpha\hat{P}_\pm\}$ can potentially be nonzero. Since $\hat{H}_\alpha$ is Hermitian, $\hat{P}_\pm\hat{H}_\alpha\hat{P}_0$ is nonzero iff $\hat{P}_0\hat{H}_\alpha\hat{P}_\pm$ is nonzero. Hence the only avenues for reducing S are: (i) all blocks in $\{\hat{P}_\pm\hat{H}_\alpha\hat{P}_0, \hat{P}_0\hat{H}_\alpha\hat{P}_\pm\}$ vanish (the commuting case $[\hat{H}_\alpha, \hat{G}] = 0$, not considered further), or (ii) $\hat{P}_0\hat{H}_\alpha\hat{P}_0$ vanishes. For the latter, we compute

$$\begin{aligned}\hat{P}_0\hat{H}_\alpha\hat{P}_0 = {}& \tilde{T}_\alpha\tilde{L}_\alpha\\ &- \tilde{T}_G^\dagger\tilde{T}_G\tilde{T}_\alpha\cdot\tilde{L}_G^\dagger\tilde{L}_G\tilde{L}_\alpha && \text{(C23)}\\ &- \tilde{T}_G\tilde{T}_G^\dagger\tilde{T}_\alpha\cdot\tilde{L}_G\tilde{L}_G^\dagger\tilde{L}_\alpha && \text{(C24)}\\ &- \tilde{L}_G^\dagger\tilde{L}_G\tilde{L}_\alpha^\dagger\cdot\tilde{T}_G^\dagger\tilde{T}_G\tilde{T}_\alpha^\dagger && \text{(C25)}\\ &- \tilde{L}_G\tilde{L}_G^\dagger\tilde{L}_\alpha^\dagger\cdot\tilde{T}_G\tilde{T}_G^\dagger\tilde{T}_\alpha^\dagger && \text{(C26)}\\ &+ \text{h.c.} && \text{(C27)}\end{aligned}$$

(Here, the first line collects the direct term; "$\cdot$" separates operator factors over shared and unshared spin-orbital indices.) If only one of the terms in Eqs. (C23)–(C26) is nonzero, then $\hat{P}_0\hat{H}_\alpha\hat{P}_0$ cannot vanish. For example, if Eq. (C23) is nonzero,

$$\hat{P}_0\hat{H}_\alpha\hat{P}_0 = \big(\hat{I} - \hat{T}_G^\dagger\hat{T}_G\big)\,\hat{T}_\alpha + \text{h.c.} \tag{C28}$$

is nonzero. The same reasoning applies if only Eq. (C24), (C25), or (C26) is nonzero.

Next, consider nonzero *pairs* among Eqs. (C23)–(C26). Nonzero (C23) and (C25) require $\tilde{T}_\alpha = \tilde{T}_G^\dagger\tilde{T}_G$ (case (iv)), which implies $\hat{P}_G\hat{H}_\alpha\hat{P}_G \neq 0$. Similarly, nonzero (C24) and (C26) require $\tilde{T}_\alpha = \tilde{T}_G\tilde{T}_G^\dagger$ (case (iii)). There is no nontrivial $\tilde{T}_\alpha$ for which both (C23) and (C24) are nonzero, and likewise (C25) and (C26) cannot both be nonzero.

When $\tilde{T}_\alpha = \tilde{T}_G$, Eqs. (C24) and (C25) can be nonzero, and

$$\hat{P}_0\hat{H}_\alpha\hat{P}_0 = \big(\tilde{T}_G\tilde{L}_\alpha + \tilde{L}_\alpha^\dagger\tilde{T}_G^\dagger\big)\big(\hat{I} - \tilde{L}_G^\dagger\tilde{L}_G - \tilde{L}_G\tilde{L}_G^\dagger\big). \tag{C29}$$

If $\tilde{L}_G^\dagger \tilde{L}_G + \tilde{L}_G \tilde{L}_G^\dagger = \hat{I}$, then $\hat{P}_0 \hat{H}_\alpha \hat{P}_0 = 0$. This occurs when $\tilde{L}_G \in \{\hat{a}_j^\dagger, \hat{a}_j\}$ is a single creation or annihilation operator on some spin-orbital index $j \notin C \cup D$. Similarly, when $\tilde{T}_\alpha = \tilde{T}_G^\dagger$, Eqs. (C23) and (C26) can be nonzero and

$$\hat{P}_0 \hat{H}_\alpha \hat{P}_0 = \big(\tilde{L}_\alpha^\dagger \tilde{T}_G + \tilde{T}_G^\dagger \tilde{L}_\alpha\big)\big(\hat{I} - \tilde{L}_G^\dagger \tilde{L}_G - \tilde{L}_G \tilde{L}_G^\dagger\big), \tag{C30}$$

which again vanishes when $\tilde{L}_G$ is a single creation or annihilation operator.

Because the nonzero pairs among Eqs. (C23)–(C26) are disjoint, there is no single choice of $\hat{T}_\alpha, \hat{T}_G$ for which three products are nonzero; having all four nonzero would require $\tilde{T}_\alpha = \tilde{T}_G = \tilde{T}_G^\dagger$, i.e., the trivial case (v).

Appendix D: Disjoint classes of fermionic involutory generators

Here, we show that the fermionic operators $\{\hat{p}_j\}_{j=1}^{10}$ in Eq. (85), defined as polynomials in $\{\hat{n}_p\}$, cannot be transformed into one another by orbital-rotation unitaries [Eq. (41)]. We first identify properties of these polynomials that remain invariant under orbital rotations. Polynomials with distinct values of these invariants cannot be related by orbital rotations. For the remaining cases with identical invariant values, we explicitly show that no orbital rotation can transform one polynomial into another.

We begin by noting that orbital rotations can be chosen to permute the indices defining a given polynomial. This allows us to group together polynomials that are related by index relabelling.

Lemma 1. *There always exists an orbital rotation $\hat{V}$ whose action on $p(\{n_p\})$ yields $p(\{n_{P(p)}\})$ for some permutation P of the indices.*

Proof. The orbital rotation

$$\hat{V} = \exp\Big[i\frac{\pi}{2}\big(\hat{a}_p^\dagger \hat{a}_q + \hat{a}_q^\dagger \hat{a}_p\big)\Big] \tag{D1}$$

swaps $\hat{n}_p$ and $\hat{n}_q$ while leaving $\hat{n}_r$ for $r \neq p, q$ unchanged. Since any permutation can be expressed as a product of swaps, we can always construct an orbital rotation that implements the desired permutation. □

The fermionic rank $r(\hat{O})$ of a normal-ordered fermionic string $\hat{O}$ consisting of an equal number of creation and annihilation operators is defined as the number of creation–annihilation pairs. When $\hat{O}$ is a sum of fermionic strings, we define its rank to be the maximum of the ranks of the individual strings. For instance, both $\hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l$ and $\hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l + \hat{a}_i^\dagger \hat{a}_j$ have rank 2.

Lemma 2. *The fermionic rank of normal-ordered operators is preserved under orbital rotations. Equivalently, if two normal-ordered fermionic operators $\hat{A}$ and $\hat{B}$ have different fermionic ranks, then no orbital rotation $\hat{V}$ satisfies $\hat{V}\hat{A}\hat{V}^\dagger = \hat{B}$.*

Proof. Let $\hat{A} = \hat{a}_{i_1}^\dagger \cdots \hat{a}_{i_N}^\dagger \hat{a}_{j_1} \cdots \hat{a}_{j_N}$ be a fermionic string of rank N. The transformed operator is of the form

$$\hat{V}\hat{A}\hat{V}^\dagger = \sum_{p_1,\ldots,p_N,\, q_1,\ldots,q_N} V_{p_1 i_1} \cdots V_{p_N i_N} V^*_{q_1 j_1} \cdots V^*_{q_N j_N} \hat{a}_{p_1}^\dagger \cdots \hat{a}_{p_N}^\dagger \hat{a}_{q_1} \cdots \hat{a}_{q_N}, \tag{D2}$$

where $V = \exp[iM]$ is the single-particle representation of the orbital rotation $\hat{V}$. Terms with $p_i = p_j$ or $q_i = q_j$ for some $i \neq j$ vanish, since $(\hat{a}_{p_i})^2 = (\hat{a}_{p_i}^\dagger)^2 = 0$. The surviving terms all contain distinct indices, $p_i \neq p_j$ and $q_i \neq q_j$ for all $i \neq j$. Normal ordering these terms only introduces an overall sign in $\{\pm 1\}$ and leaves the number of creation–annihilation pairs equal to N. There cannot be a reduction in rank under the transformation, since creation operators always precede annihilation operators in the normal-ordered fermionic strings. These arguments extend directly to operators that are sums of fermionic strings, by restricting attention to the highest-rank contributions in $\hat{A}$ and $\hat{B}$. □

Rank equivalence is therefore a necessary condition for two operators to be related by an orbital rotation. Consequently, if an orbital rotation acts on a linear combination of normal-ordered fermionic operators with multiple ranks, it must map the contribution at each rank to a contribution of the same rank.

Lemma 3. *Let $\hat{A} = \sum_k \hat{A}_k$ and $\hat{B} = \sum_k \hat{B}_k$ be sums of normal-ordered fermionic operators with $r(\hat{A}_k) = r(\hat{B}_k) = k$. If an orbital rotation $\hat{V}$ satisfies $\hat{V}\hat{A}\hat{V}^\dagger = \hat{B}$, then $\hat{V}\hat{A}_k\hat{V}^\dagger = \hat{B}_k$ for all k, and $\mathrm{Tr}(\hat{A}_k) = \mathrm{Tr}(\hat{B}_k)$.*

Proof. By Lemma 2, $\hat{V}\hat{A}_k\hat{V}^\dagger$ has rank k. Since operators of different rank cannot coincide, the result follows. □

Normal ordering of arbitrary fermionic strings may produce sums of strings of multiple ranks. In contrast, products of $\{\hat{n}_p\}$ remain single strings under normal ordering. This allows us to extend Lemma 3 to polynomials in $\{\hat{n}_p\}$.

Lemma 4. *Fermionic rank is preserved under orbital rotations of homogeneous polynomials in $\{\hat{n}_p\}$. Furthermore, suppose $\hat{V}\hat{A}\hat{V}^\dagger = \hat{B}$ for $\hat{A} = \sum_k \hat{A}_k$ and $\hat{B} = \sum_k \hat{B}_k$, where $\hat{A}_k$ and $\hat{B}_k$ are homogeneous polynomials in $\{\hat{n}_p\}$ of rank k. Then $\hat{V}\hat{A}_k\hat{V}^\dagger = \hat{B}_k$ for all k, and $\mathrm{Tr}(\hat{A}_k) = \mathrm{Tr}(\hat{B}_k)$.*

Proof. Each $\hat{n}_p = \hat{a}_p^\dagger \hat{a}_p$ is already normal-ordered, and products of $\{\hat{n}_p\}$ contain no repeated indices in our construction. Normal ordering such a product yields a single fermionic string of fixed length. By Lemma 2, orbital rotations preserve the fermionic rank of this string, and the statement follows. □

Thus, the trace of a polynomial in $\{\hat{n}_p\}$, as well as the traces of its individual homogeneous components, are invariant under orbital rotations. The ten reflection polynomials $\hat{p}_i$ can therefore be separated based on their

Class	Fermionic rank(s)	Trace	Fixed-rank trace
$\hat{p}_1$	$\{0,1\}$	0	(16, -16, 0)
$\hat{p}_2$	$\{0,2\}$	8	(16, 0, -8)
$\hat{p}_3$	$\{0,1,2\}$	8	(16, -16, 8)
$\hat{p}_4$	$\{0,1,2\}$	-8	(16, -32, 8)
$\hat{p}_5$	$\{0,1,2\}$	0	(16, -32, 16)
$\hat{p}_6$	$\{0,1,2\}$	0	(16, -16, 0)
$\hat{p}_7$	$\{0,1,2\}$	8	(16, -16, 8)
$\hat{p}_8$	$\{0,1,2\}$	0	(16, -32, 16)
$\hat{p}_9$	$\{0,1,2\}$	-8	(16, -48, 24)
$\hat{p}_{10}$	$\{0,1,2\}$	0	(16, -32, 16)

TABLE II. Traces of the quadratic fermionic reflection polynomials over the four-mode Fock space $\mathcal{F} = \bigoplus_{j=0}^{4} \mathcal{F}_j$. The column "Fixed-rank trace" lists the traces of the homogeneous components of ranks 0, 1, and 2.

traces and on the traces of their homogeneous components (listed in Table II). To define the trace, we must specify the underlying Fock space. By Lemma 1, it is sufficient to work in a four-mode Fock space with indices $(p, q, r, s) = (0, 1, 2, 3)$.

It is immediate that $\hat{p}_1$ and $\hat{p}_2$ cannot be converted into any other class, because they lack homogeneous components of both ranks 1 and 2. From the traces, it remains to explicitly show that the following classes are disjoint:

1. $\hat{p}_3$ and $\hat{p}_7$,

2. $\hat{p}_5$, $\hat{p}_8$, and $\hat{p}_{10}$.

Case 1: $\hat{p}_3$ and $\hat{p}_7$.
Here $\hat{p}_3 = 1 - 2\hat{n}_p + 2\hat{n}_p\hat{n}_q$ and $\hat{p}_7 = 1 - 2\hat{n}_p - 2\hat{n}_q\hat{n}_r + 2\hat{n}_p\hat{n}_r + 2\hat{n}_p\hat{n}_q$. If $\hat{V}\hat{p}_3\hat{V}^\dagger = \hat{p}_7$, then by Lemma 4,

$$\hat{V}\hat{n}_p\hat{n}_q\hat{V}^\dagger = -\hat{n}_q\hat{n}_r + \hat{n}_p\hat{n}_r + \hat{n}_p\hat{n}_q. \tag{D3}$$

The left-hand side is a projector because $\hat{n}_p\hat{n}_q$ is idempotent. The right-hand side is not idempotent, so no such orbital rotation $\hat{V}$ can exist.

Case 2: $\hat{p}_5$, $\hat{p}_8$, and $\hat{p}_{10}$.

Case 2(a): $\hat{p}_5$ and $\hat{p}_8$.
The same type of argument as in Case 1 applies. Assuming $\hat{V}\hat{p}_5\hat{V}^\dagger = \hat{p}_8$ and using Lemma 4 leads to a rank-2 projector on the left-hand side being mapped to a non-idempotent operator on the right-hand side, which is impossible.

Case 2(b): $\hat{p}_5$ and $\hat{p}_{10}$.
Again, the same argument as in Case 1 shows that an orbital rotation mapping $\hat{p}_5$ to $\hat{p}_{10}$ cannot exist.

Case 2(c): $\hat{p}_8$ and $\hat{p}_{10}$.
Suppose there exists an orbital rotation $\hat{V}$ such that $\hat{V}\hat{p}_8\hat{V}^\dagger = \hat{p}_{10}$. Then, by Lemma 4, the rank-2 parts must satisfy

$$\hat{V}\big(\hat{n}_p\hat{n}_r + \hat{n}_p\hat{n}_q\big)\hat{V}^\dagger = -\hat{n}_r\hat{n}_s + \hat{n}_p\hat{n}_r + \hat{n}_q\hat{n}_s + \hat{n}_p\hat{n}_q. \tag{D4}$$

Squaring Eq. (D4), we obtain

$$\begin{aligned}&\hat{V}\big(\hat{n}_p\hat{n}_r + \hat{n}_p\hat{n}_q + 2\hat{n}_p\hat{n}_q\hat{n}_r\big)\hat{V}^\dagger = \\ &\hat{n}_r\hat{n}_s + \hat{n}_p\hat{n}_r + \hat{n}_q\hat{n}_s + \hat{n}_p\hat{n}_q - 2\hat{n}_p\hat{n}_r\hat{n}_s - 2\hat{n}_q\hat{n}_r\hat{n}_s \\ &\quad + 2\hat{n}_p\hat{n}_q\hat{n}_r + 2\hat{n}_p\hat{n}_q\hat{n}_s.\end{aligned} \tag{D5}$$

By Lemma 4, the rank-2 parts of Eq. (D5) must individually transform into one another,

$$\hat{V}(\hat{n}_p\hat{n}_r + \hat{n}_p\hat{n}_q)\hat{V}^\dagger = \hat{n}_r\hat{n}_s + \hat{n}_p\hat{n}_r + \hat{n}_q\hat{n}_s + \hat{n}_p\hat{n}_q. \tag{D6}$$

Since $\hat{V}$ is unitary, we require

$$\mathrm{Tr}(\hat{n}_p\hat{n}_r + \hat{n}_p\hat{n}_q) = \mathrm{Tr}(\hat{n}_r\hat{n}_s + \hat{n}_p\hat{n}_r + \hat{n}_q\hat{n}_s + \hat{n}_p\hat{n}_q) \tag{D7}$$

$$\Rightarrow \mathrm{Tr}(\hat{n}_r\hat{n}_s + \hat{n}_q\hat{n}_s) = 0, \tag{D8}$$

which is false for distinct indices p, q, r, s. Therefore, no such orbital rotation exists.

[1] S. R. White, Numerical Canonical Transformation Approach to Quantum Many-body Problems, The Journal of Chemical Physics **117**, 7472 (2002).

[2] A. Peruzzo, J. McClean, P. Shadbolt, M.-H. Yung, X.-Q. Zhou, P. J. Love, A. Aspuru-Guzik, and J. L. O'Brien, A Variational Eigenvalue Solver on a Photonic Quantum Processor, Nature Communications **5**, 4213 (2014).

[3] P. Schleich, J. Boen, L. Cincio, A. Anand, J. S. Kottmann, S. Tretiak, P. A. Dub, and A. Aspuru-Guzik, Partitioning Quantum Chemistry Simulations with Clifford Circuits, Journal of Chemical Theory and Computation **19**, 4952 (2023).

[4] I. Loaiza, A. M. Khah, N. Wiebe, and A. F. Izmaylov, Reducing molecular electronic hamiltonian simulation cost for linear combination of unitaries approaches, Quantum Science and Technology **8**, 035019 (2023).

[5] I. G. Ryabinkin, R. A. Lang, S. N. Genin, and A. F. Izmaylov, Iterative Qubit Coupled Cluster Approach with Efficient Screening of Generators, Journal of Chemical Theory and Computation **16**, 1055 (2020).

[6] M. S. Rudolph, T. Jones, Y. Teng, A. Angrisani, and Z. Holmes, Pauli Propagation: A Computational Framework for Simulating Quantum Systems, arXiv preprint arXiv:2505.21606 (2025).

[7] Formally, the series used here corresponds to the Campbell identity, which is a special case of the more general Baker–Campbell–Hausdorff relation. We retain the conventional term 'BCH expansion,' as it is standard in physics and quantum chemistry.

[8] T. Helgaker, P. Jørgensen, and J. Olsen, *Molecular Electronic-Structure Theory* (John Wiley & Sons, Chichester, 2000).

[9] N. N. Bogoliubov and N. N. B. Jr., *Introduction to Quantum Statistical Mechanics* (World Scientific, Singapore,

2010).
[10] M. Wagner, *Unitary Transformations in Solid State Physics* (North-Holland Publishing Company, Amsterdam, 1986).
[11] R. A. Lang, I. G. Ryabinkin, and A. F. Izmaylov, Unitary Transformation of the Electronic Hamiltonian with an Exact Quadratic Truncation of the Baker-Campbell-Hausdorff Expansion, Journal of Chemical Theory and Computation **17**, 66 (2021).
[12] J. S. Kottmann, A. Anand, and A. Aspuru-Guzik, A Feasible Approach for Automatically Differentiable Unitary Coupled-Cluster on Quantum Computers, Chemical Science **12**, 3497 (2021).
[13] A. F. Izmaylov, R. A. Lang, and T.-C. Yen, Analytic Gradients in Variational Quantum Algorithms: Algebraic Extensions of the Parameter-Shift Rule to General Unitary Transformations, Physical Review A **104**, 062443 (2021).
[14] F. A. Evangelista and I. Magoulas, Exact Closed-form Unitary Transformations of Fermionic Operators, Physical Review A **111**, 042825 (2025).
[15] A. O. Barut and R. Ráczka, *Theory of Group Representations and Applications*, 2nd ed. (World Scientific, Singapore, 1986) pp. xix+717.
[16] R. Gilmore, *Lie Groups, Physics, and Geometry: An Introduction for Physicists, Engineers and Chemists* (Cambridge University Press, Cambridge, 2008).
[17] F. Gantmacher and A. M. S. Staff, *The Theory of Matrices, Volume 2* (American Mathematical Society, New York, 2025).
[18] S. F. Boys, Construction of Some Molecular Orbitals to Be Approximately Invariant for Changes from One Molecule to Another, Reviews of Modern Physics **32**, 296 (1960).
[19] C. Edmiston and K. Ruedenberg, Localized Atomic and Molecular Orbitals, Reviews of Modern Physics **35**, 457 (1963).
[20] J. Pipek and P. G. Mezey, A Fast Intrinsic Localization Procedure Applicable for *ab initio* and Semiempirical Linear Combination of Atomic Orbital Wave Functions, The Journal of Chemical Physics **90**, 4916 (1989).
[21] S. Lehtola and H. Jónsson, Pipek–Mezey Orbital Localization Using Various Partial Charge Estimates, Journal of Chemical Theory and Computation **10**, 642 (2014).
[22] E. Koridon, S. Yalouz, B. Senjean, F. Buda, T. E. O'Brien, and L. Visscher, Orbital Transformations to Reduce the 1-Norm of the Electronic Structure Hamiltonian for Quantum Computing Applications, Physical Review Research **3**, 033127 (2021).
[23] J. F. Gonthier, M. D. Radin, C. Buda, E. J. Doskocil, C. M. Abuan, and J. Romero, Measurements as a Roadblock to Near-Term Practical Quantum Advantage in Chemistry: Resource Analysis, Physical Review Research **4**, 033154 (2022).
[24] K. N. Okada, K. Osaki, K. Mitarai, and K. Fujii, Classically Optimized Variational Quantum Eigensolver with Applications to Topological Phases, Physical Review Research **5**, 043217 (2023).
[25] I. G. Ryabinkin, T.-C. Yen, S. N. Genin, and A. F. Izmaylov, Qubit Coupled Cluster Method: A Systematic Approach to Quantum Chemistry on a Quantum Computer, Journal of Chemical Theory and Computation **14**, 6317 (2018).
[26] H. L. Tang, V. O. Shkolnikov, G. S. Barron, H. R. Grimsley, N. J. Mayhall, E. Barnes, and S. E. Economou, Qubit-ADAPT-VQE: An Adaptive Algorithm for Constructing Hardware-Efficient Ansätze on a Quantum Processor, PRX Quantum **2**, 020310 (2021).
[27] I. G. Ryabinkin, A. F. Izmaylov, and S. N. Genin, A posteriori Corrections to the Iterative Qubit Coupled Cluster Method to Minimize the Use of Quantum Resources in Large-scale Calculations, Quantum Science and Technology **6**, 024012 (2021).
[28] N. P. Bauman, E. J. Bylaska, S. Krishnamoorthy, G. H. Low, N. Wiebe, C. E. Granade, M. Roetteler, M. Troyer, and K. Kowalski, Downfolding of Many-body Hamiltonians Using Active-space Models: Extension of the Subsystem Embedding Sub-algebras Approach to Unitary Coupled Cluster Formalisms, The Journal of Chemical Physics **151**, 014107 (2019).
[29] J. Chen, H.-P. Cheng, and J. K. Freericks, Quantum-Inspired Algorithm for the Factorized Form of Unitary Coupled Cluster Theory, Journal of Chemical Theory and Computation **17**, 841 (2021).
[30] J. W. Mullinax and N. M. Tubman, Large-scale Sparse Wave Function Circuit Simulator for Applications with the Variational Quantum Eigensolver, The Journal of Chemical Physics **162**, 074114 (2025).
[31] A UCC generator is a linear combination of commuting Pauli products (under any fermion-qubit mapping). Hence, it can be diagonalized by a Clifford unitary rather than by an orbital rotation.
[32] A. F. Izmaylov, On Construction of Projection Operators, The Journal of Physical Chemistry A **123**, 3429 (2019).