A Dynamic Systems Approach to Fermions and Their Relation to Spins

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Dynamic properties of fermionic systems, like controllability, reachability, and simulability, are investigated in a general Lie-theoretical frame for quantum systems theory. Observing the parity superselection rule, we treat the fully controllable and quasifree cases, as well as various translation-invariant and particle-number conserving cases. We determine the respective dynamic system Lie algebras to express reachable sets of pure (and mixed) states by explicit orbit manifolds.

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I. INTRODUCTION

Over the last decade, there has been a considerable experimental progress in achieving coherent control of ultra-cold gases including fermionic systems [1–6]. This is also of great interest in view of quantum simulation (e.g., [7]) of quantum phase transitions [8, 9], pairing phenomena [10], and in particular, for understanding phases in Hubbard models [11]. — Even earlier on, the simulation of fermionic systems on quantum computers had been in focus [12, 13]. For either case, there are interesting algebraic aspects going beyond the standard textbook approach [14], some of which can be found in [15–18]. Here we set out for a unified picture of quantum systems theory in a Lie-algebraic frame following the lines of [19] to pave the way for optimal-control methods to be applied to fermionic systems.

It is generally recognized that optimal control algorithms are key tools needed for further advances in experimentally exploiting these quantum systems for simulation as well as for computation [20–23]. In the implementation of these algorithms it is crucial to know beforehand to which extent the system can be controlled. The usual scenario (in coherent control) is that we are given a *drift Hamiltonian* and a set of *control Hamiltonians* with tunable strengths. The achievable operations will be characterized by the *system Lie algebra*, while the reachable sets of states are given by the respective *pure state orbits*. Dynamic Lie algebras and reachability questions have been intensively studied in the literature for qudit systems [19, 24–26]. However, in the case of fermions these questions have to be reconsidered mainly due to the presence of the *parity superselection rule*. Hence in a broader sense the present work on fermions can be envisaged also as a step towards quantum control theory for quantum simulation in the presence of superselection rules.

Apart from discussing the implications of the parity superselection rule in the theory of dynamic Lie algebras and of pure-state orbits, we will also treat the case when one imposes translation-invariance or particle-number conservation. Moreover, the experimentally relevant case of quasifree fermions (with and without translation invariance) is discussed in detail. Since we interrelate fermionic systems with the Lie-theoretical framework of quantum-dynamical systems, at times we will be somewhat more explicit and put known results into a new frame. The main results extend from general fermionic systems to the action of Hamiltonians with and without restrictions like quadratic interactions, translation invariance, reflection symmetry, or particle-number conservation.

The paper itself is structured as follows: In order to set a unified frame, we resume some basic concepts of Hamiltonian controllability of qudit systems in Sec. II, since for comparison these concepts will subsequently be translated to their fermionic counterparts, starting with the discussion of general fermionic systems in Sec. III.

Then the new results are presented in the following six sections: In Sec. IV we obtain the dynamic system algebra for *general fermionic systems* respecting the parity superselection rule (see Theorem 4 in Subsection IV A). An explicit example for a set of Hamiltonians that provides full controllability over the fermionic system is discussed in Subsection IV B. Some general results on the controllability of fermionic and spin systems, such as Theorem 51, are relegated to Appendix A. Following the same line, in Sec. V we wrap up some known results on *quasifree* fermionic systems in a general Lie-theoretic frame by streamlining the derivation for the respective system algebra in Proposition 9 of Sec. V. Corollary 16 provides a most general controllability condition of quasifree fermionic systems building on the tensor-square representation used in [19]. Furthermore, we develop methods for restricting the set of possible system algebras by analyzing their rank, see Theorem 13 as well as Appendices C and D. The structure and or-

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bits of *pure states* in quasifree fermionic systems are analyzed in Sec. VI leading to a complete characterization of pure-state controllability (Theorem 23). Sections VII and VIII are devoted to *translation-invariant systems*. For *spin chains* we give in Theorem 25 the first full characterization of the corresponding system algebras and strengthen in Theorem 27 earlier results on short-range interactions in [16]. The system algebras for *general translation-invariant fermionic chains* are given in Theorem 30 of Sec. VII C. We also identify translation-invariant fermionic Hamiltonians of bounded interaction length which cannot be generated from nearest-neighbor ones (see Theorem 33 of Sec. VII D). The particular case of *quadratic* interactions (see Sec. VIII A) is settled in Theorem 34. Corollary 35 considers systems which additionally carry a twisted reflection symmetry (or equivalently have no imaginary hopping terms) as discussed in [16]. Furthermore, we provide a *complete* classification of all pure quasifree state orbits in Theorem 39 of Sec. VIII B. This leads to Theorem 41 of Sec. VIII C presenting a bound on the scaling of the gap for a class of quadratic Hamiltonians which are translation-invariant. Section IX deals with *fermionic systems* conserving the *number of particles*. Their system algebras in the general case as well as in the quasifree case are derived in Proposition 42 and Proposition 43, respectively. Furthermore, a necessary and sufficient condition for quasifree pure-state controllability in the particle-number conserving setting is provided by Theorem 48.

In Sec. X, we summarize the main results as given in Theorem 4, Corollary 16, as well as in Theorems 23, 25, 27, 30, 33, 34, 39, 41, and 48. We conclude leaving a number of details and proofs to the Appendices in order to streamline the presentation.

II. BASIC QUANTUM SYSTEMS THEORY OF N-LEVEL SYSTEMS

As a starting point, consider the controlled Schrödinger (or Liouville) equation

$$\dot\rho(t) = -[iH_u, \rho(t)] := -(iH_u\rho(t) - \rho(t)iH_u) \qquad (1)$$

driven by the Hamiltonian $H_u := H_0 + \sum_{j=1}^m u_j(t)H_j$ and fulfilling the initial condition $\rho_0 := \rho(0)$. Here the *drift term* H_0 describes the evolution of the unperturbed system, while the *control terms* $\{H_j\}$ represent coherent manipulations from outside. Equation (1) defines a *bilinear control system* Σ [27], as it is linear both in the *density operator* $\rho(t)$ and in the *control amplitudes* $u_j(t) \in \mathbb{R}$.

For a N-level system, the natural representation as hermitian operators over $\mathbb{C}^N$ relates the Hamiltonians as generators of unitary time evolutions to the Lie algebra $\mathfrak{u}(N)$ of skew-hermitian operators that generate the unitary group $\mathrm{U}(N)$ of propagators. Let $L := \{iH_1, iH_2, \ldots, iH_m\}$ be a subset of Hamiltonians seen as Lie-algebra elements. Then the smallest subalgebra (with respect to the commutator $[A, B] := AB - BA$) of $\mathfrak{u}(N)$ containing L is called the *Lie closure* of L written as $\langle iH_1, iH_2, \ldots, iH_m\rangle_{\mathrm{Lie}}$. Moreover, for any element $iH \in \langle iH_1, \ldots, iH_m\rangle_{\mathrm{Lie}}$, there exist *control amplitudes* $u_j(t) \in \mathbb{R}$ with $j \in \{1, \ldots, m\}$ such that

$$\exp(-iH) = \mathcal{T}\int_{t=0}^{1} \exp\left[\sum_{j=1}^{m} -iu_j(t)H_j\right] \mathrm{d}t, \qquad (2)$$

where $\mathcal{T}$ denotes time-ordering.

Now taking the Lie closure over the system Hamiltonian and all control Hamiltonians of a bilinear control system (Σ) defines the *dynamic system Lie algebra* (or system algebra for short)

$$\mathfrak{g}_\Sigma := \langle iH_0, iH_j \,|\, j = 1, 2, \ldots, m\rangle_{\mathrm{Lie}}\,. \qquad (3)$$

It is the key to characterize the differential geometry of a dynamic system in terms of its complete set of Hamiltonian directions forming the tangent space to the time evolutions. For instance, the condition for *full controllability* of bilinear systems can readily be adopted from classical systems [28–31] to the quantum realm such as to take the form of

$$\langle iH_0, iH_j \,|\, j = 1, 2, \ldots, m\rangle_{\mathrm{Lie}} = \mathfrak{u}(N) \qquad (4)$$

saying that a N-level quantum system is fully controllable if and only if its system algebra is the full unitary algebra, which we will relax to $\mathfrak{su}(N)$ in a moment. This notion of controllability is also intuitive (recalling that the exponential map is surjective for compact connected Lie groups), as it requires that all Hamiltonian directions can be generated.

So in fully controllable closed systems, to every initial state ρ_0 the *reachable set* is the entire unitary orbit $\mathfrak{reach}_{\mathrm{full}}(\rho_0) := \{U\rho_0U^\dagger \mid U \in \mathrm{U}(N)\}$. With density operators being hermitian, this means any final state $\rho(t)$ can be reached from any initial state ρ_0 as long as both of them share the same spectrum of eigenvalues (including multiplicities). Thus the reachable set of ρ_0 equals the *isospectral set* of ρ_0.

Remark 1. Interestingly, this notion is stronger than the requirement that from any given (normalized) *pure* state one can reach any other (normalized) *pure* state, since it is well known [24–26] that for N being even, all rank-one projectors are already on the *unitary symplectic orbit*

$$\begin{aligned}\mathfrak{reach}(|\psi_0\rangle\langle\psi_0|) &= \{K|\psi_0\rangle\langle\psi_0|K^\dagger \,|\, K \in \mathrm{Sp}(N/2)\}\\ &= \{U|\psi_0\rangle\langle\psi_0|U^\dagger \,|\, U \in \mathrm{SU}(N)\}\end{aligned} \qquad (5)$$

and $\mathrm{Sp}(N/2)$ is a proper subgroup of $\mathrm{SU}(N)$.

In general, the *reachable set* to an initial state ρ_0 of a dynamic system (Σ) with *system algebra* $\mathfrak{g}_\Sigma$ is given by the orbit of the dynamic (sub)group $\mathbf{G}_\Sigma := \exp(\mathfrak{g}_\Sigma) \subseteq U(N)$ generated by the system algebra

$$\mathfrak{reach}_\Sigma(\rho_0) := \{G\rho_0G^\dagger \mid G \in \mathbf{G}_\Sigma = \exp(\mathfrak{g}_\Sigma)\}. \qquad (6)$$

Thus the system algebra $\mathfrak{g}_\Sigma$ can be envisaged as the *fingerprint* encoding all the dynamic properties of a dynamic system Σ. Via the respective reachable sets (see, e.g., [19]) it is easy to see that a coherently controlled dynamic system Σ_A *can simulate the dynamics of another system* Σ_B if and only if the system algebra $\mathfrak{g}_{\Sigma_A}$ of the simulating system Σ_A encompasses the system algebra $\mathfrak{g}_{\Sigma_B}$ of the simulated system Σ_B,

$$\mathfrak{g}_{\Sigma_A} \supseteq \mathfrak{g}_{\Sigma_B}. \tag{7}$$

In [19], we have analyzed the possibility of quantum simulation with respect to the dynamic degrees of freedom and have given a number of illustrating worked examples.

Next we describe dynamic symmetries of bilinear control systems whose Hamiltonians are given by $\mathfrak{m} := \{iH_\nu\} = \{iH_0, iH_1, \ldots, iH_m\}$. The *symmetry operators* s are collected in the *centralizer* of $\mathfrak{m}$ in $\mathfrak{u}(N)$:

$$\mathfrak{cent}(\mathfrak{m}) := \big\{s \in \mathfrak{u}(N) \,|\, [s, iH] = 0 \;\; \forall\, iH \in \mathfrak{m}\big\}. \tag{8}$$

More generally, let S' denote the *commutant* of a set S of matrices, i.e., the set of all complex matrices which commute simultaneously with all matrices in S. By Jacobi's identity $\big[[a,b],c\big]+\big[[b,c],a\big]+\big[[c,a],b\big] = 0$ one gets two properties of the centralizer pertinent for our context: First, an element s that commutes with all Hamiltonians $a, b \in \mathfrak{m}$ also commutes with their Lie closure $\mathfrak{g}_\Sigma := \langle \mathfrak{m} \rangle_{\rm Lie}$ (i.e. $\mathfrak{cent}(\mathfrak{m}) \equiv \mathfrak{cent}(\mathfrak{g}_\Sigma)$), as $[s,a] = 0$ and $[s,b] = 0$ imply $\big[s,[a,b]\big] = 0$. Second, for any $u \in \mathfrak{u}(N)$, $[s_1, u] = 0$ and $[s_2, u] = 0$ imply $\big[[s_1, s_2], u\big] = 0$, so the centralizer forms itself a Lie subalgebra to $\mathfrak{u}(N)$ consisting of all symmetry operators. By construction, $\mathfrak{cent}(\mathfrak{g}_\Sigma)$ is also a *normal subalgebra* or an *ideal* of $\mathfrak{u}(N)$ observing $[\mathfrak{cent}(\mathfrak{g}_\Sigma), \mathfrak{u}(N)] \subseteq \mathfrak{cent}(\mathfrak{g}_\Sigma)$.

Likewise one can describe the symmetries to a given set ρ_Σ of states by its centralizer

$$\begin{aligned}\mathfrak{cent}(\rho_\Sigma) &:= \{s \in \mathfrak{u}(N) \,|\, [s, \rho] = 0 \;\; \forall \rho \in \rho_\Sigma\} \\ &= \mathfrak{cent}(\langle \rho_\Sigma \rangle_\mathbb{R}),\end{aligned} \tag{9}$$

where $\langle\,\cdot\,\rangle_\mathbb{R}$ denotes the real span. Clearly, $\mathfrak{cent}(\rho_\Sigma) \subseteq \mathfrak{u}(N)$ generates the *stabilizer group* to the state space ρ_Σ of the control system (Σ).

Since in the absence of other symmetries the identity is the only and trivial symmetry of both any state space ρ_Σ as well as any set of Hamiltonians and their respective system algebra $\mathfrak{g}_\Sigma$, one has $\mathfrak{cent}(\mathfrak{g}_\Sigma) = \mathfrak{cent}(\rho_\Sigma) = \{i\,\lambda \mathbb{1}_N \,|\, \lambda \in \mathbb{R}\} =: \mathfrak{u}(1)$. So there is always a trivial stabilizer group $\mathrm{U}(1) := \{e^{i\phi}\mathbb{1}_N \,|\, \phi \in \mathbb{R}\}$. This explains why the time evolutions generated by two Hamiltonians H_1 and H_2 coincide for the set of all density operators if (and without other symmetries only if) $H_1 - H_2 = \lambda \mathbb{1}$. As is well known, by the same argument, in time evolutions

$$\rho(t) := U(t)\rho U^\dagger(t) = \mathrm{Ad}_{U(t)}(\rho_0) \tag{10}$$

following from Eq. (1), one may take $U(t) := \exp(-itH)$ equally well from $\mathrm{U}(N)$ or $\mathrm{SU}(N)$. Thus henceforth we will only consider special unitaries (of determinant $+1$) generated by traceless Hamiltonians $iH_\nu \in \mathfrak{su}(N)$, since for any Hamiltonian $\tilde{H}$ there exists an equivalent unique traceless Hamiltonian $H := \tilde{H} - \frac{1}{N}\,\mathrm{tr}(\tilde{H})\mathbb{1}_N$ generating a time evolution coinciding with the one of $\tilde{H}$ [32].

However, the above simple arguments are in fact much stronger, e.g., one readily gets the following statement:

Lemma 2. *Consider a bilinear control system with system algebra $\mathfrak{g}_\Sigma$ on a state space ρ_Σ. Let $iH_1 \in \mathfrak{g}_\Sigma$ and $iH_2 \in \mathfrak{u}(N)$ while assuming that $[H_1, \langle \rho_\Sigma \rangle_\mathbb{R}] \subseteq i\langle \rho_\Sigma \rangle_\mathbb{R}$ for all $iH_1 \in \mathfrak{g}_\Sigma$, i.e., operations generated by $\mathfrak{g}_\Sigma$ map the set $\langle \rho_\Sigma \rangle_\mathbb{R}$ into itself. Then the condition*

$$e^{-iH_1 t}\rho e^{iH_1 t} = e^{-i(H_1+H_2)t}\rho e^{i(H_1+H_2)t} \;\forall t \in \mathbb{R}, \rho \in \rho_\Sigma \tag{11}$$

is equivalent to $iH_2 \in \mathfrak{cent}(\rho_\Sigma)$.

Proof. Using the formula $e^{tA}Be^{-tA} = \exp[\mathrm{ad}_{tA}(B)] = \sum_{k=0}^\infty t^k/k!\,\mathrm{ad}_A^k(B)$ we show that Eq. (11) is equivalent to condition (a): $\mathrm{ad}^k_{H_1}(\rho) = \mathrm{ad}^k_{H_1+H_2}(\rho)$ for all non-negative integer k and all $\rho \in \langle \rho_\Sigma \rangle_\mathbb{R}$. Moreover, (a) implies condition (b): $(\mathrm{ad}_{H_2} \circ \mathrm{ad}^k_{H_1})(\rho) = 0$ for all non-negative integer k and all $\rho \in \langle \rho_\Sigma \rangle_\mathbb{R}$, as $[H_1, \mathrm{ad}^{k-1}_{H_1}(\rho)] = [H_1 + H_2, \mathrm{ad}^{k-1}_{H_1+H_2}(\rho)] = [H_1 + H_2, \mathrm{ad}^{k-1}_{H_1}(\rho)]$. Also, (a) follows from (b) due to $\mathrm{ad}^k_{H_1}(\rho) = [H_1 + H_2, \mathrm{ad}^{k-1}_{H_1}(\rho)] = [H_1 + H_2, [H_1 + H_2, \mathrm{ad}^{k-2}_{H_1}(\rho)]] = \cdots = \mathrm{ad}^k_{H_1+H_2}(\rho)$. Applying $[H_1, \langle \rho_\Sigma \rangle_\mathbb{R}] \subseteq i\langle \rho_\Sigma \rangle_\mathbb{R}$ to (b) completes the proof. $\square$

Therefore, let us consider a pair of Hamiltonians $iH_1, iH_3 \in \mathfrak{g}_\Sigma$ (fulfilling the conditions of Lemma 2) as *equivalent* on the state space ρ_Σ, if their difference $iH_2 := i(H_1 - H_3)$ falls into the centralizer $\mathfrak{cent}(\rho_\Sigma)$.

III. FERMIONIC QUANTUM SYSTEMS

In this section, we fix our notation by recalling basic notions for fermionic systems. In the first subsection, we discuss the Fock space and different operators acting on it as given by the creation and annihilation operators as well as the Majorana operators. We point out how the Lie algebra $\mathfrak{u}(2^d)$ of skew-hermitian matrices can be embedded as a real subspace in the set of the complex operators acting on the Fock space. In the second subsection, we focus on the parity superselection rule and how it structures a fermionic system.

A. The Fock Space and Majorana Monomials

The complex Hilbert space of a d-mode fermionic system with one-particle subspace $\mathbb{C}^d$ is the *Fock space*

$$\mathcal{F}(\mathbb{C}^d) := \bigoplus_{i=0}^{d} \left(\bigwedge^i \mathbb{C}^d \right) = \mathbb{C} \oplus \mathbb{C}^d \oplus \wedge^2\mathbb{C}^d \oplus \cdots \oplus (\wedge^d\mathbb{C}^d).$$

Given an orthonormal basis $\{e_i\}_{i=1}^d$ of $\mathbb{C}^d$, the *Fock vacuum* $\Omega := 1$ $(= 1 \oplus 0 \oplus \cdots \oplus 0)$ and the vectors of the form $e_{i_1} \wedge e_{i_2} \wedge \cdots \wedge e_{i_k}$ (with $i_1 < i_2 < \cdots < i_k$ and $1 \le k \le d$) form an orthonormal basis of $\mathcal{F}(\mathbb{C}^d)$. Note that $\mathcal{F}(\mathbb{C}^d)$ is a 2^d-dimensional Hilbert space isomorphic to $\otimes_{i=1}^d \mathbb{C}^2$ $(\cong \mathbb{C}^{2^d})$.

The fermionic *creation* and *annihilation operators*, $f_p^\dagger$ and f_p act on the Fock space in the following way: $f_p^\dagger \Omega = e_p$, $f_p\Omega = 0$, $f_p^\dagger e_q = e_p \wedge e_q$, and $f_p e_q = \delta_{pq}$; while in the general case of $1 \le \ell \le d$, their action is given by $f_p^\dagger(e_{q_1} \wedge e_{q_2} \wedge \cdots \wedge e_{q_\ell}) = (e_p \wedge e_{q_1} \wedge e_{q_2} \wedge \cdots \wedge e_{q_\ell})$ and $f_p(e_{q_1} \wedge e_{q_2} \wedge \cdots \wedge e_{q_\ell}) = \sum_{k=1}^n (-1)^k \delta_{pq_k}\, e_{q_1} \wedge \cdots \wedge e_{q_{(k-1)}} \wedge e_{q_{(k+1)}} \wedge \cdots \wedge e_{q_\ell}$. By their definition, these operators satisfy the fermionic *canonical anticommutation relations*

$$\{f_p^\dagger, f_q^\dagger\} = \{f_p, f_q\} = 0 \ \text{ and } \ \{f_p^\dagger, f_q\} = \delta_{pq}\mathbb{1},$$

where $\{A, B\} := AB + BA$ denotes the anticommutator. Moreover, every linear operator acting on $\mathcal{F}(\mathbb{C}^d)$ can be be written as a complex polynomial in the creation and annihilation operators.

Another set of polynomial generators acting on the Fock space is given by the $2d$ hermitian *Majorana operators* $m_{2p-1} := f_p + f_p^\dagger$ and $m_{2p} := i(f_p - f_p^\dagger)$, which satisfy the relations $(k, \ell \in \{1, \ldots, 2d\})$

$$\{m_k, m_\ell\} = 2\delta_{k\ell}\mathbb{1}.$$

A product $m_{q_1} m_{q_2} \cdots m_{q_k}$ of $k \ge 0$ Majorana operators is called a *Majorana monomial*. The ordered Majorana monomials with $q_1 < q_2 < \cdots < q_k$ form a linearly independent basis of the complex operators acting on $\mathcal{F}(\mathbb{C}^d)$. Each Majorana monomial acting on d-mode fermionic system can be identified with a complex operator acting on a chain of d qubits via the *Jordan-Wigner transformation* [33–36] which is induced by

$$m_{2p-1} \mapsto \underbrace{\mathrm{Z} \otimes \cdots \otimes \mathrm{Z}}_{p-1} \otimes \mathrm{X} \otimes \underbrace{\mathrm{I} \otimes \cdots \otimes \mathrm{I}}_{d-p}$$

and

$$m_{2p} \mapsto \underbrace{\mathrm{Z} \otimes \cdots \otimes \mathrm{Z}}_{p-1} \otimes \mathrm{Y} \otimes \underbrace{\mathrm{I} \otimes \cdots \otimes \mathrm{I}}_{d-p},$$

where the following notation for the Pauli matrices $\mathrm{X} := \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$, $\mathrm{Y} := \left(\begin{smallmatrix} 0 & -i \\ i & 0 \end{smallmatrix}\right)$, and $\mathrm{Z} := \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$ is used.

Now we highlight the real subspace contained in the set of complex operators acting on the Fock space $\mathcal{F}(\mathbb{C}^d)$ which consists of all skew-hermitian operators and which forms the real Lie algebra $\mathfrak{u}(2^d)$ closed under the commutator $[A, B] = AB - BA$ and real-linear combinations. More precisely, $\mathfrak{u}(2^d)$ is generated by all operators

$$L(M) := -\frac{1}{2} w(M) M\ , \tag{12}$$

where M denotes any ordered Majorana monomial and

$$w(M) := \begin{cases} i & \text{if } [\deg(M) \bmod 8] \in \{0, 1\}, \\ 1 & \text{if } [\deg(M) \bmod 8] \in \{2, 3\}, \\ -i & \text{if } [\deg(M) \bmod 8] \in \{4, 5\}, \\ -1 & \text{if } [\deg(M) \bmod 8] \in \{6, 7\}. \end{cases} \tag{13}$$

Similarly, one obtains a basis of $\mathfrak{su}(2^d)$ by excluding $-\frac{i}{2}\mathbb{1}$.

B. Parity Superselection Rule

An additional fundamental ingredient in describing fermionic systems is the *parity superselection rule*. Superselection rules were originally introduced by Wick, Wightman, and Wigner [37] (see also [38, 39]). These rules, in the finite-dimensional definition of Piron [40], describe the existence of non-trivial observables that commute with *all physical observables*. The existence of such a commuting observable in turn implies that a superposition of pure states from different blocks of a block-diagonal decomposition w.r.t. the eigenspaces of this observable are equivalent to an incoherent classical mixture.

The *parity superselection rule* identifies among the operators acting on $\mathcal{F}(\mathbb{C}^d)$ the *physical observables* $\mathbb{H}_F$ as those that do commute with the parity operator

$$P := i^d \prod_{k=1}^{2d} m_k\,, \tag{14}$$

where the adjoint action of P on a Majorana monomial is given as $P m_{k_1} m_{k_2} \cdots m_{k_\ell} P^{-1} = (-1)^\ell m_{k_1} m_{k_2} \cdots m_{k_\ell}$. These physical operators are also exactly the ones that can be written as a sum of products of an *even* number of Majorana operators (as P contains all Majorana operators whereof there exist an even number). They are therefore denoted as *even operators* for short. If the parity is the *only* non-trivial symmetry, we obtain $\mathbb{H}_F' = \langle \mathbb{1}, P \rangle$, where the bracket stands for the complex-linear span.

Now we will discuss why the set of all physical fermionic states ρ_F consists similarly of all density operators that commute with P, notably $\rho_F' = \langle \mathbb{1}, P \rangle$. As we will show, the parity superselection rule induces a decomposition into a direct sum of two *irreducible* state-space components exploiting $\mathbb{H}_F' \cap \rho_F' = \langle \mathbb{1}, P \rangle$. Recall that $P^2 = \mathbb{1}$ and the eigenspaces to the eigenvalues $+1$ and -1 are indeed of equal dimension, as there are exactly 2^{2d-1} even operators which map the vacuum state Ω into the $+1$ eigenspace of P. Note that $P e_{q_1} \wedge e_{q_2} \wedge \cdots \wedge e_{q_\ell} = (-1)^\ell e_{q_1} \wedge e_{q_2} \wedge \cdots \wedge e_{q_\ell}$. Thus the Fock space can be split up as a direct sum of two equal-dimensional eigenspaces of P, called the *positive* and *negative parity subspaces* (for clarity observe [41]):

$$\mathcal{F}(\mathbb{C}^d) = \left[\bigoplus_{i \text{ even}} \left(\bigwedge^i \mathbb{C}^d\right)\right] \bigoplus \left[\bigoplus_{i \text{ odd}} \left(\bigwedge^i \mathbb{C}^d\right)\right].$$

Now we may write $P^2 = \mathbb{1} = P_+ + P_-$ with the orthogonal projections $P_+ := \frac{1}{2}(\mathbb{1} + P)$ and $P_- := \frac{1}{2}(\mathbb{1} - P)$ projecting onto the respective subspaces. Any physical observable (i.e. even operator) A has a block-diagonal structure with respect to the above splitting, i.e. $A = P_+AP_+ + P_-AP_-$. This follows, as the requirement $[A, P] = \frac{1}{2}[A, P_+] = -\frac{1}{2}[A, P_-] = 0$ enforces $P_+AP_- = P_-AP_+ = 0$ for any operator $A = P_+AP_+ + P_+AP_- + P_-AP_+ + P_-AP_-$. We obtain

$$\begin{aligned}\mathrm{Tr}(\rho A) &= \mathrm{Tr}(\rho P_+AP_+ + \rho P_-AP_-)\\ &= \mathrm{Tr}[(P_+\rho P_+ + P_-\rho P_-)A]. \end{aligned} \tag{15}$$

Hence *physical* observables cannot distinguish between the density operator ρ and its block-diagonal projection to $P_+\rho P_+ + P_-\rho P_-$ (which is always an even density operator). In this sense, a physical linear combination (a formal superposition) of pure states from the positive and negative parity subspaces is equivalent to an incoherent classical mixture. Equation (15) also shows that without loss of generality we can restrict ourselves to even density operators and regard only those as physical.

Finally, we would like to recall three further aspects of the parity superselection rule. First, without the parity superselection rule, two noncommuting observables acting on two different and spatially-separated regions would exist which would allow for a violation of locality (e.g., by instantaneous signaling between the regions). Second, the parity superselection rule, of course, does not apply if one uses a spin system to simulate a fermionic system via the Jordan-Wigner transformation. This system respects locality, since the Majorana operators m_k are—in this case—localized on the *first* $[(k{+}1)\,\mathrm{div}\,2]$ spins; two noncommuting Majorana operators are therefore not acting on spatially-separated regions. Third, the parity superselection rule also affects the concept of entanglement as has been pointed out and studied in detail in [42, 43].

IV. FULLY CONTROLLABLE FERMIONIC SYSTEMS

Here we derive a general controllability result for fermions obeying the parity superselection rule. We illustrate that full controllability for a fermionic system can be achieved with quadratic Hamiltonians and a single fourth-order interaction term. For example, in a system with d modes, the complete fermionic dynamical algebra $\mathcal{L}_d \cong \mathfrak{su}(2^{d-1}) \oplus \mathfrak{su}(2^{d-1})$ (see Theorem 4) can be generated by a quartic interaction between the first two modes $ih_{\mathrm{int}} = i(2f_1^\dagger f_1 - \mathbb{1})(2f_2^\dagger f_2 - \mathbb{1}) = -im_1m_2m_3m_4$ combined with three quadratic Hamiltonians which are: the nearest-neighbor hopping term

$$\begin{aligned} ih_{\mathrm{h}} &= -2i\sum_{p=1}^{d-1} f_p^\dagger f_{p+1} + f_{p+1}^\dagger f_p\\ &= \sum_{p=1}^{d-1} -m_{2p-1}m_{2p+2} + m_{2p}m_{2p+1}, \end{aligned}$$

the on-site potential of the first site $ih_0 = i(2f_1^\dagger f_1 - \mathbb{1}) = m_1m_2$, and a pairing-hopping term between the first two modes $ih_{12} = i(f_1f_2 - f_1^\dagger f_2^\dagger) - i(f_1^\dagger f_2 - f_1f_2^\dagger) = m_2m_3$ (see Proposition 6). Finally, we provide a general discussion about when the commutant of a system algebra determines the algebra itself.

A. System Algebra

In the case of qubit systems mentioned in Sec. II, two Hamiltonians generate equivalent time evolutions if and only if they differ by a multiple of the identity. This condition can readily be modified for the fermionic case such as to match the parity-superselection rule as well.

Corollary 3. *Let H_1 and H_2 be two physical fermionic Hamiltonians, i.e., even hermitian operators acting on $\mathcal{F}(\mathbb{C}^d)$. Then by Lemma 2 the equality*

$$e^{-iH_1t}\rho e^{iH_1t} = e^{-iH_2t}\rho e^{iH_2t}$$

holds for all even (physical) density operators ρ_F with $\rho_F' = \langle \mathbb{1}, P\rangle$ in the sense that H_1 and H_2 generate the same time-evolution, if and only if $H_2 - H_1 = \lambda\mathbb{1} + \mu P = (\lambda + \mu)P_+ + (\lambda - \mu)P_-$ with $\lambda, \mu \in \mathbb{R}$.

This also implies that for any physical fermionic Hamiltonian H, there exists a unique Hamiltonian

$$\tilde{H} := H - \tfrac{\mathrm{tr}(P_+HP_+)}{\dim P_+}\, P_+ - \tfrac{\mathrm{tr}(P_-HP_-)}{\dim P_-}\, P_- \tag{16}$$

that is traceless on *both* the positive and the negative parity subspaces, i.e.,

$$\mathrm{tr}(P_+\tilde{H}P_+) = \mathrm{tr}(P_-\tilde{H}P_-) = 0\,, \tag{17}$$

and moreover, $\tilde{H}$ and H are equivalent and generate the same time evolution. If necessary, we can restrict ourselves to the set of Hamiltonians satisfying Eq. (17). These elements decompose as $H = H_+ \oplus H_-$, where H_+ and H_- are generic traceless hermitian operators each acting on a 2^{d-1}-dimensional Hilbert space. We explicitly define the linear space $\mathbb{F}_d$ of physical fermionic Hamiltonians as generated by the basis of all even Majorana monomials without the operators $\mathbb{1}$ and P, ensuring that $\mathbb{F}_d$ is traceless both on H_+ and H_-.—We summarize our exposition on fully controllable fermionic systems in the following result:

Theorem 4. *The Lie algebra corresponding to the physical fermionic (and hermitian) Hamiltonians* $\mathbb{F}_d$ *is*

$$\mathcal{L}_d := \mathfrak{su}(2^{d-1}) \oplus \mathfrak{su}(2^{d-1}). \tag{18}$$

The most general set of unitary transformations generated by $\mathcal{L}_d$ *is given as the block-diagonal decomposition* $\mathrm{SU}(2^{d-1}) \oplus \mathrm{SU}(2^{d-1})$. *Hence a set* $\{H_0, H_1, H_2, \ldots, H_m\}$ *of hermitian Hamiltonians defines a fully controllable fermionic system if and only if*

$$\langle iH_0, iH_1, \ldots, iH_m\rangle_{\mathrm{Lie}} = \mathfrak{su}(2^{d-1}) \oplus \mathfrak{su}(2^{d-1}) \, . \tag{19}$$

Remark 5. For Lie algebras, $\mathfrak{k}_1 + \mathfrak{k}_2$ will denote only an abstract direct sum without referring to any concrete realization. We reserve the notation $\mathfrak{k}_1 \oplus \mathfrak{k}_2$ to specify a direct sum of Lie algebras which is (up to a change of basis) represented in a block-diagonal form $\left(\begin{smallmatrix} \mathfrak{k}_1 & \\ & \mathfrak{k}_2 \end{smallmatrix}\right)$.

Proof. It follows from Sec. III that $\mathbb{F}_d$ commutes with P and that the matrix representation of $\mathbb{F}_d$ splits into two blocks of dimension 2^{d-1} corresponding to the $+$ and $-$ eigenspaces of P. As the center of $\mathbb{F}_d$ is given by $\mathbb{F}_d' \cap \mathbb{F}_d = \langle \mathbb{1}, P\rangle \cap \mathbb{F}_d = \{0\}$, the Lie algebra $\mathbb{F}_d$ is semisimple. As there are exactly $2^{2d-1} - 2$ linear-independent operators in $\mathbb{F}_d$, the system algebra could be $\mathfrak{su}(2^{d-1}) \oplus \mathfrak{su}(2^{d-1})$. And indeed, all other system algebras are ruled out as the subalgebras acting on each of the two matrix blocks would have a smaller Lie-algebra dimension than $\mathfrak{su}(2^{d-1})$. □

B. Examples and Discussion

We start out with an example realizing a fully controllable fermionic system by adding only one quartic operator to the set of quadratic Hamiltonians which will be discussed in Section V below (cf. Theorem 11):

Proposition 6. *Consider a fermionic quantum system with* $d > 2$ *modes. The system algebra* $\mathcal{L}_d = \mathfrak{su}(2^{d-1}) \oplus \mathfrak{su}(2^{d-1})$ *of a fully controllable fermionic system can be generated using the operators* $w_1 := L(v_1)$, $w_2 := L(v_2)$, $w_3 := L(v_3)$, *and* $w_4 := L(v_4)$ *with the map* L *as defined in Eqs.* (12) *and* (13), *where*

$$v_1 := \sum_{p=1}^{d-1} -m_{2p-1}m_{2p+2} + m_{2p}m_{2p+1}, \tag{20a}$$

$$v_2 := m_1m_2,\; v_3 := m_2m_3,\; v_4 := m_1m_2m_3m_4. \tag{20b}$$

Proof. It follows from the independent Theorem 11 (see Sec. V below) that w_1, w_2, and w_3 generate all quadratic Majorana monomials m_pm_q. Consider an even Majorana monomial $s_1 := L(\prod_{i\in\mathcal{I}} m_i)$ of degree $2d'$, where s_2 is defined using the ordered index set $\mathcal{I}$, and a quadratic operator $s_2 := L(m_pm_q)$ with $p \in \mathcal{I}$ and $q \notin \mathcal{I}$. We can change any index p of s_1 into q of using $L(\prod_{k\in(\mathcal{I}\setminus\{p\})\cup\{q\}} m_k) = \pm[s_1, s_2]$. Therefore, we get from w_4 and the quadratic operators all Majorana monomials of degree four.

Using the quartic Majorana monomials we can increase the degree of the monomials in steps of two: Consider the operators $s_3 := L(\prod_{i\in\mathcal{I}} m_i)$ and $s_4 := L(\prod_{j\in\mathcal{J}} m_j)$ which are defined using the ordered index sets $\mathcal{I}$ and $\mathcal{J}$ and have degrees $2d'' < 2(d-1)$ and 4, respectively. Assuming that $|\mathcal{I}\cap\mathcal{J}| = 1$, we can generate an operator $L(\prod_{k\in\mathcal{K}} m_k) = \pm[s_3, s_4]$ of degree $|\mathcal{K}| = 2(d''+1) < 2d$ where the corresponding ordered index set is given by $\mathcal{K} := (\mathcal{I}\cup\mathcal{J})\setminus(\mathcal{I}\cap\mathcal{J})$. By induction, we can now generate all even Majorana monomials except $L(\prod_{q=1}^{2d} m_q)$. Note that $L(\prod_{q=1}^{2d} m_q)$ cannot be obtained as $\mathcal{I}\cap\mathcal{J} \nsubseteq \mathcal{K}$ holds by construction. Thus, we get all elements of $\mathcal{L}_d$ (see Subsection IV A) and the proposition follows. □

The proof also implies that all the operators generated commute with $\prod_{q=1}^{2d} m_q = P/i^d$ [cf. Eq. (14)] (and the identity operator $\mathbb{1}$). In addition, all operators commuting simultaneously with all elements of $\mathcal{L}_d$ can be written as a complex-linear combination of $\mathbb{1}$ and P. We thus obtain a partial characterization of full controllability in fermionic systems:

Lemma 7. *Consider a fermionic quantum system with* $d \geq 2$ *modes. A necessary condition for full controllability of a given set of hermitian Hamiltonians* H_v *is that* $\{iH_v\}' = \langle \mathbb{1}, P\rangle$.

One can expect that the condition of Lemma 7 is not sufficient under any reasonable assumption by applying counterexamples from spin systems in [19]. These counterexamples could be lifted to fermionic systems by providing the explicit form of the embeddings from $\mathfrak{su}(2^{d-1})$ to the first and second component of the direct sum $\mathcal{L}_d = \mathfrak{su}(2^{d-1}) \oplus \mathfrak{su}(2^{d-1})$.

We guide the discussion in a different direction by emphasizing that the property $\{iH_v\}' = \langle \mathbb{1}, P\rangle$ does not determine the system algebra uniquely. We define the centralizer of a set $B \subseteq \mathfrak{su}(k)$ in $\mathfrak{su}(k)$ (e.g. $k = 2^d$) as

$$\mathfrak{cent}_{\mathfrak{su}(k)}(B) := \{g \in \mathfrak{su}(k) \,|\, [g, b] = 0 \text{ for all } b \in B\}.$$

We consider the algebras $\mathcal{L}_d = \mathfrak{su}(2^{d-1}) \oplus \mathfrak{su}(2^{d-1})$ and $\mathrm{s}[\mathfrak{u}(2^{d-1}) \oplus \mathfrak{u}(2^{d-1})]$, where the latter algebra is isomorphic to $\mathfrak{su}(2^{d-1}) + \mathfrak{su}(2^{d-1}) + \mathfrak{u}(1)$ and contains the additional (non-physical) generator $L(\prod_{q=1}^{2d} m_q)$. Note that $\mathfrak{cent}_{\mathfrak{su}(k)}(\mathcal{L}_d) = \mathfrak{cent}_{\mathfrak{su}(k)}(\mathrm{s}[\mathfrak{u}(2^{d-1}) \oplus \mathfrak{u}(2^{d-1})]) = L(\prod_{q=1}^{2d} m_q)$, i.e., the centralizers of both algebras are equal. However $\mathfrak{cent}_{\mathfrak{su}(k)}[L(\prod_{q=1}^{2d} m_q)] = \mathrm{s}[\mathfrak{u}(2^{d-1}) \oplus \mathfrak{u}(2^{d-1})] \neq \mathfrak{su}(2^{d-1}) \oplus \mathfrak{su}(2^{d-1})$. In particular, we have $\mathcal{L}_d \neq \mathfrak{cent}_{\mathfrak{su}(k)}(\mathfrak{cent}_{\mathfrak{su}(k)}(\mathcal{L}_d))$, and $\mathcal{L}_d$ does not fulfill the double-centralizer property. A more general incarnation of this effect in line with a discussion of double centralizers is given in Appendix A. It leads in the case of irreducible subalgebras to the following maximality result:

Corollary 8. *Let* $\mathfrak{g}$ *denote an irreducible subalgebra of* $\mathfrak{su}(k)$*, i.e.* $\mathfrak{cent}_{\mathfrak{su}(k)}(\mathfrak{g}) = \{0\}$*. Then one finds that* $\mathfrak{cent}_{\mathfrak{su}(k)}(\mathfrak{cent}_{\mathfrak{su}(k)}(\mathfrak{g})) = \mathfrak{g}$ *if and only if* $\mathfrak{g} = \mathfrak{su}(k)$*.*

To sum up, the symmetry properties of a Lie algebra $\mathfrak{g} \subseteq \mathfrak{su}(k)$, as given by its commutant w.r.t. a representation of $\mathfrak{g}$, do *not* determine the Lie algebra $\mathfrak{g}$ uniquely. Yet the commutant allows us to infer a *unique maximal Lie algebra* contained in $\mathfrak{su}(k)$, which is (up to an identity matrix) equal to the double commutant of $\mathfrak{g}$, but in general not to $\mathfrak{g}$ itself.

V. QUASIFREE FERMIONS

Here we present the dynamic system algebras for fermions with quadratic Hamiltonians. For illustration, also the relation to spin chains is worked out in detail. In this context, we show by free fermionic techniques that a Heisenberg-XX Hamiltonian of Eq. (24) combined with the one-site term $ih_0 = i\mathrm{Z} \otimes \mathrm{I} \otimes \cdots \otimes \mathrm{I} = m_1 m_2$ and the two-site interaction $ih_{12} = i\mathrm{X} \otimes \mathrm{X} \otimes \mathrm{I} \otimes \cdots \otimes \mathrm{I} = m_2 m_3$ gives rise to the system algebra $\mathfrak{so}(2d)$ (see Theorem 11), while the first two operators generate only the subalgebra $\mathfrak{u}(d)$ (see Theorem 13). Further results along this line are presented in Appendix C.

Finally, we arrive at a very useful general result: In order to decide if a set of operators generates the full quadratic algebra for d modes, we characterize quadratic operators by a real skew-symmetric matrix T whose entries are given via $-\frac{1}{2}\sum_{k,\ell}^{2d} T_{k\ell}\, m_k m_\ell$ (see Eq. (22)). Adapting our tensor-square criterion for full controllability from spin systems [19] to quasifree fermionic systems, a set of operators T_ν generates the full quadratic algebra $\mathfrak{so}(2d)$ if and only if the joint commutant of the operators $T_\nu \otimes \mathbb{1}_{2d} + \mathbb{1}_{2d} \otimes T_\nu$ has dimension three (see Corollary 16).

A. Quadratic Hamiltonians

A general quadratic Hamiltonian of a fermionic system can be written as (cf. [16, 44–47])

$$H = \sum_{p,q=1}^{d} A_{pq}(f_p^\dagger f_q - \delta_{pq}\tfrac{\mathbb{1}}{2}) + \frac{1}{2} B_{pq} f_p^\dagger f_q^\dagger - \frac{1}{2} B_{pq}^* f_p f_q, \tag{21}$$

where the coupling coefficients A_{pq} and B_{pq} are complex entries of the $d \times d$-matrices A and B, respectively. The canonical anticommutation relations and the hermiticity of H require that A is hermitian and B is (complex) skew-symmetric. The terms corresponding to the nonzero matrix entries of A and B are usually referred to as *hopping* and *pairing* terms, respectively. Related parameterizations for quadratic Hamiltonians are discussed in Appendix B.

In the Majorana monomial basis, the quadratic Hamiltonian H can be rewritten such that

$$-iH = \sum_{k,\ell=1}^{2d} T_{k\ell} \left[-\frac{1}{2} m_k m_\ell \right] \tag{22}$$

with

$$T = \frac{1}{2}\left[\mathfrak{Re}(A) \otimes \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} + \mathfrak{Re}(B) \otimes \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \right.$$
$$\left. + \mathfrak{Im}(A) \otimes \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} + \mathfrak{Im}(B) \otimes \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \right].$$

The properties of A and B directly imply that the matrix T is real and skew-symmetric. Using the formula

$$\begin{aligned}[m_p m_q, m_r m_s] &= -4(\delta_{ps}\delta_{qr}\mathbb{1} - \delta_{qs}\delta_{pr}\mathbb{1}) \\ &+2(\delta_{ps} m_q m_r - \delta_{pr} m_q m_s + \delta_{qr} m_p m_s - \delta_{qs} m_p m_r) \qquad (23a) \\ &= \delta_{ps}(m_q m_r - m_r m_q) - \delta_{pr}(m_q m_s - m_s m_q) \\ &+\delta_{qr}(m_p m_s - m_s m_p) - \delta_{qs}(m_p m_r - m_r m_p) \qquad (23b)\end{aligned}$$

one can easily verify that the space of quadratic Hamiltonians is closed under the commutator. To sum up, we have established the well-known Lie homomorphism from the system algebra generated by a set of quadratic Hamiltonians (whose control functions are given by the matrix entries of A and B) onto the system algebra $\mathfrak{so}(2d)$ represented by the entries of T (cf. pp. 183-184 of [36]):

Proposition 9. *The maximal system algebra for a system of quasifree fermions with* d *modes is given by* $\mathfrak{so}(2d)$*.*

Proof. Let the map h transform the Majorana monomial $-\frac{1}{2}(m_p m_q - m_q m_p)$ into the skew-symmetric matrix $e_{pq} - e_{qp}$ where e_{pq} has the matrix entries $[e_{pq}]_{uv} := \delta_{pu}\delta_{qv}$. We show that h is a Lie-homomorphism assuming $p \neq q$ and $r \neq s$ in the following, while the case of $p = q$ or $r = s$ holds trivially. Note that $\frac{1}{2}(m_p m_q - m_q m_p) = m_p m_q$. It follows from Eq. (23b) that $h([-\frac{1}{2}(m_p m_q - m_q m_p), -\frac{1}{2}(m_r m_s - m_s m_r)]) = [(e_{pq} - e_{qp}), (e_{rs} - e_{sr})] = [h(-\frac{1}{2}(m_p m_q - m_q m_p)), h(-\frac{1}{2}(m_r m_s - m_s m_r))]$. ∎

B. Examples and Explicit Realizations

We start by showing that the full system algebra $\mathfrak{so}(2d)$ of quasifree fermions can be generated using only three quadratic operators, namely $w_1 = L(v_1)$, $w_2 = L(v_2)$, and $w_3 = L(v_3)$ from Eq. (20) where $v_1 = \sum_{p=1}^{d-1} -m_{2p-1} m_{2p+2} + m_{2p} m_{2p+1}$, $v_2 = m_1 m_2$, and $v_3 = m_2 m_3$. The Jordan-Wigner transformation maps these generators respectively to the Heisenberg-XXterm

$$iH_{\mathsf{XX}} = -\frac{i}{2} \sum_{p=1}^{d-1} (\mathrm{X}_p \mathrm{X}_{p+1} + \mathrm{Y}_p \mathrm{Y}_{p+1}), \tag{24}$$

$-\frac{i}{2}\mathrm{Z}_1$, and $-\frac{i}{2}\mathrm{X}_1\mathrm{X}_2$, where operators as (e.g.) Z_1 are defined as $\mathrm{Z} \otimes \mathrm{I} \otimes \cdots \otimes \mathrm{I}$.

Lemma 10. *Consider a fermionic quantum system with $d \geq 2$ modes. The system algebras $\mathfrak{k}_1$ and $\mathfrak{k}_2$ generated by the set of Lie generators $\{w_1, w_2\}$ and $\{w_1, w_2, w_3\}$ contain the elements $L(a_p)$ with $a_p := m_{2p-1}m_{2p}$ for all $p \in \{1, \ldots, d\}$ as well as $L(b_p)$ with $b_p := -m_{2p-1}m_{2p+2} + m_{2p}m_{2p+1}$ and $L(c_p)$ with $c_p := m_{2p-1}m_{2p+1}+m_{2p}m_{2p+2}$ for all $p \in \{1, \ldots, d-1\}$.*

Note that the elements $L(a_p)$, $L(b_p)$, and $L(c_p)$ are mapped by the Jordan-Wigner transformation to the spin operators $-i\mathrm{Z}_p/2$, $-i(\mathrm{X}_p\mathrm{X}_{p+1} + \mathrm{Y}_p\mathrm{Y}_{p+1})/2$, and $-i(\mathrm{X}_p\mathrm{Y}_{p+1} - \mathrm{Y}_p\mathrm{X}_{p+1})/2$, respectively.

Proof. We compute the commutators $w_4 := -L(c_1) = [w_2, w_1]$, $w_5 := L(b_1) = [w_4, w_2]$, and $w_6 := L(a_2) = [w_5, w_4] - w_2$. We can now reduce the problem from d to $d-1$ by subtracting w_5 from w_1. The cases of $d \in \{2, 3, 4\}$ can be verified directly and the proof is completed by induction. □

This proof also yields an explicit realization for the algebra $\mathfrak{so}(2d)$ while providing a more direct line of reasoning as compared to our proof of Theorem 32 in [19].

Theorem 11. *Consider a fermionic quantum system with $d \geq 2$ modes. The system Lie algebra $\mathfrak{k}_2$ generated by $\{w_1, w_2, w_3\}$ is given by $\mathfrak{so}(2d)$.*

Proof. The cases of $d \in \{2, 3, 4\}$ can be verified directly. We build on Lemma 10 and remark that $\mathfrak{k}_2 \subseteq \mathfrak{so}(2d)$ as it is generated only by quadratic operators (see Proposition 9). We compute in the Jordan-Wigner picture $w_7 := -i(\mathrm{Y}_1\mathrm{Y}_2 - \mathrm{Y}_2\mathrm{Y}_3)/2 = [w_3, [w_3, w_1]]$, and $w_8 := -i\mathrm{X}_2\mathrm{X}_3/2 = L(b_2) - (w_5 - w_3 - w_7)$. This shows by induction that $\mathfrak{so}(2d) \supseteq \mathfrak{k}_2 \supsetneq \mathfrak{u}(1) + \mathfrak{so}(2d-2)$. As $\mathfrak{u}(1) + \mathfrak{so}(2d-2)$ is a maximal subalgebra of $\mathfrak{so}(2d)$ (see p. 219 of [48] or Sec. 8.4 of [49]), one obtains that $\mathfrak{k}_2 = \mathfrak{so}(2d)$. Alternatively, one can explicitly show that $\mathfrak{k}_2$ consists of all quadratic Majorana operators, which combined with Proposition 9 would also complete the proof. □

Note that the generators w_1, w_2, and w_3 can be described using the Hamiltonian of Eq. (21) while keeping the control functions given by the matrix entries A_{pq} and B_{pq} in the real range, see Appendix B for details. This also provides a simplified approach to Theorem 32 in [19], where only the real case was considered:

Corollary 12 (see Theorem 32 in [19])**.** *Consider a control system given by the Hamiltonian components of Eq. (21). The control functions are specified by the matrix entries A_{pq} and B_{pq} which are assumed to be real. The resulting system algebra is $\mathfrak{so}(2d)$.*

The relations between quasifree fermions and spin systems will be analyzed in Appendix C. — Next we treat the case of the algebra $\mathfrak{u}(d)$.

Theorem 13 (see Lem. 36 in [19])**.** *Consider a fermionic quantum system with $d \geq 2$ modes. The system Lie algebra $\mathfrak{k}_1$ generated by $\{w_1, w_2\}$ is given by $\mathfrak{u}(d)$.*

Here we just sketch ideas for the proof of Theorem 13 while leaving the full details to Appendix D. Our methods exploit the detailed structure of the appearing Majorana operators while being more explicit than in [19] and avoiding obstacles of the spin picture. Building on the notation of Lemma 10, we show that the elements $L(a_p)$ with $1 \leq p \leq d$ together with the elements $L(b_p^{(i)})$ with $b_p^{(i)} := -m_{2p-1}m_{2p+2i} + m_{2p}m_{2p+2i-1}$ and $L(c_p^{(i)})$ with $c_p^{(i)} := m_{2p-1}m_{2p+2i-1} + m_{2p}m_{2p+2i}$ where $p, i \geq 1$ and $p + i \leq d$ form a basis of $\mathfrak{k}_1$. One obtains that $\dim(\mathfrak{k}_1) = d + (d-1)d = d^2$. Furthermore, the elements $L(a_p)$ form a maximal abelian subalgebra and the rank of $\mathfrak{k}_1$ is equal to d [50]. We limit the possible cases further by showing that $\mathfrak{k}_1$ is a direct sum of a simple and a one-dimensional Lie algebra. A complete enumeration of all possible cases completes the proof.

Remark 14. A spin chain equivalent to the fermionic system in Theorem 13 was also considered in [51], where it was shown how to swap pairs of fermions using the given Hamiltonians. As a consequence of Theorem 13, the Lie algebra in the spin chain of [51] can be identified as $\mathfrak{u}(d)$. Clearly, its size grows only linearly with the number of modes d. However, the addition of controlled-Z gates, as discussed in [51], already allows for scalable quantum computation.

C. Tensor-Square Criterion

Consider a control system of quasifree fermions which is represented by matrices T_ν in the form of Eq. (22). For more than two modes (i.e. $d \geq 3$), we can efficiently decide if the system algebra is equal to $\mathfrak{so}(2d)$. Recall that the alternating square $\mathrm{Alt}^2(\phi)$ and the symmetric square $\mathrm{Sym}^2(\phi)$ of a representation ϕ are defined as restrictions to the alternating and symmetric subspace of the tensor square $\phi^{\otimes 2} = \phi \otimes \mathbb{1}_{\dim(\phi)} + \mathbb{1}_{\dim(\phi)} \otimes \phi$.

Theorem 15. *Assume that $\mathfrak{k}$ is a subalgebra of $\mathfrak{so}(2d)$ with $d \geq 3$ and denote by Φ the standard representation of $\mathfrak{so}(2d)$. Then, the following are equivalent:*
(1) $\mathfrak{k} = \mathfrak{so}(2d)$.
(2) The restriction of $\mathrm{Alt}^2\Phi$ to the subalgebra $\mathfrak{k}$ is irreducible and the restriction of $\mathrm{Sym}^2\Phi$ to $\mathfrak{k}$ splits into two irreducible components. Each irreducible component occurs only once.
(3) The commutant of all complex matrices commuting with the tensor square $(\Phi|_{\mathfrak{k}})^{\otimes 2}$ of $\mathfrak{k}$ has dimension three.

Proof. Assuming (1), condition (2) follows from the formulas for the alternating and symmetric square of $\mathfrak{so}(2d)$ with $d \geq 3$ given in its standard representation $\phi_{(1,0,\ldots,0)}$ [where $(1, 0, \ldots, 0)$ denotes the corresponding highest weight]: The alternating square is given as $\mathrm{Alt}^2\phi_{(1,0,0)} = \phi_{(0,1,1)}$ for $\mathfrak{so}(6)$ and $\mathrm{Alt}^2\phi_{(1,0,0,\ldots,0)} = \phi_{(0,1,0,\ldots,0)}$ for $\mathfrak{so}(2d)$ in the case of $d > 3$ (cf. Table 6 in [52] or Table X in [19]). The symmetric square $\mathrm{Sym}^2\phi_{(1,0,\ldots,0)} =$

$\phi_{(2,0,\ldots,0)} \oplus \phi_{(0,0,\ldots,0)}$ for $\mathfrak{so}(2d)$ and $d \geq 3$ can be computed using Example 19.21 of Ref. [53]. We verify the dimension of the commutant and show that (3) is a consequence of (2) by applying Proposition 50 which says that the dimension of the commutant of a representation ϕ is given by $\sum_i m_i^2$ where the m_i are the multiplicities of the irreducible components of ϕ. For the rest of the proof we assume that condition (3) holds. We remark that the representation $\Phi|_{\mathfrak{k}}$ is irreducible as otherwise the dimension of the commutant would be larger than three. Thus, we obtain that $\mathfrak{k}$ is semisimple. The dimension of the commutant allows only two possibilities: one of the restrictions $(\mathrm{Alt}^2\Phi)|_{\mathfrak{k}}$ or $(\mathrm{Sym}^2\Phi)|_{\mathfrak{k}}$ to the subalgebra $\mathfrak{k}$ has to be irreducible. We emphasize that $\mathfrak{k}$ is given in an orthogonal representation (i.e. a representation of real type) of even dimension, as $\mathfrak{k}$ is given in an irreducible representation obtained by restricting the standard representation of $\mathfrak{so}(2d)$. Therefore, we can use the list of all irreducible representations which are orthogonal or symplectic (i.e. of quaternionic type) and whose alternating or symmetric square is irreducible (Theorem 4.5 as well as Tables 7a and 7b of Ref. [52]): (a) for $\mathfrak{su}(2)$ the alternating square of the symplectic representation $\phi = (1)$ of dimension two, (b) for $\mathfrak{so}(3) \equiv \mathfrak{su}(2)$ the alternating square of the orthogonal representation $\phi = (2)$ of dimension three, (c) for $\mathfrak{so}(2\ell+1)$ with $\ell > 1$ the alternating square of the orthogonal representation $\phi = (1, 0, \ldots, 0)$ of dimension $2\ell + 1$, (d) for $\mathfrak{so}(2\ell)$ with $\ell \geq 3$ the alternating square of the orthogonal representation $\phi = (1, 0, \ldots, 0)$ of dimension 2ℓ, and (e) for $\mathfrak{sp}(\ell)$ with $\ell \geq 1$ the symmetric square of the symplectic representation $\phi = (1, 0, \ldots, 0)$ of dimension 2ℓ. Only possibility (d) fulfills all conditions which proves (1). □

Describing the matrices in the tensor square more explicitly along the lines of Ref. [19], we present a necessary and sufficient condition for full controllability in systems of quasifree fermions.

Corollary 16. *Consider a set of matrices $\{T_\nu \,|\, \nu \in \{0; 1, \ldots, m\}\}$ as given by Eq. (22) generating the system algebra $\mathfrak{k} \subseteq \mathfrak{so}(2d)$ with $d \geq 3$. We obtain $\mathfrak{k} = \mathfrak{so}(2d)$ if and only if the joint commutant of $\{T_\nu \otimes \mathbb{1}_{2d} + \mathbb{1}_{2d} \otimes T_\nu \,|\, \nu \in \{0; 1, \ldots, m\}\}$ has dimension three.* □

Along the lines of Eq. (22), one can apply Corollary 16 to the matrices T corresponding to the generators of $\mathfrak{so}(2d)$ of Theorem 11. For $d \geq 3$ one can verify that the commutant of the tensor square has dimension three. But for $d = 2$ one computes a dimension of four as $\mathfrak{so}(4) = \mathfrak{su}(2) + \mathfrak{su}(2)$ is not simple.

For illustration, note that two elements in the commutant are trivial, to wit the identity and the generator for the SWAP-operation between the two tensor copies. The third element does not yet occur in the unitary case described in [19]: it is the projector P_S onto the totally anti-symmetric state. To see this, recall that Ref. [54] implies that if the Hamiltonians $\{iH_\nu \,|\, \nu \in \{0; 1, \ldots, m\}\}$ generate a system algebra of orthogonal type, then there is an operator $S \in SL(N)$ satisfying

$$SH_\nu^t + H_\nu S = 0 \tag{25}$$

jointly for all $\nu \in \{0; 1, \ldots, m\}$ as in [19]. Using Kronecker products and writing $|S\rangle := \mathrm{vec}\,(S)$ [55], one sees that $|S\rangle$ is in the intersection of all the kernels of the tensor squares, so

$$\begin{aligned} &(H_\nu \otimes \mathbb{1} + \mathbb{1} \otimes H_\nu)|S\rangle = |0\rangle \\ \Leftrightarrow\ &(H_\nu \otimes \mathbb{1} + \mathbb{1} \otimes H_\nu)|S\rangle\langle S| = 0_N \\ \Leftrightarrow\ &|S\rangle\langle S|(H_\nu \otimes \mathbb{1} + \mathbb{1} \otimes H_\nu) = 0_N \end{aligned} \tag{26}$$

and thus $P_S := |S\rangle\langle S| \in (H_\nu \otimes \mathbb{1} + \mathbb{1} \otimes H_\nu)'$ holds jointly for all $\nu \in \{0; 1, \ldots, m\}$; 0_N denotes the zero matrix of degree N.

VI. PURE-STATE CONTROLLABILITY FOR QUASIFREE SYSTEMS

In this section, we present a straightforward criterion for *pure-state controllability* of quasifree fermionic systems with d modes. A fermionic state is called quasifree if Majorana operators of odd degree map it to zero and even-degree ones map it to states which factorize into the Wick expansion form (see below). We obtain that quadratic Hamiltonians act transitively on pure quasifree states, i.e., every pure quasifree state can be transformed into any other pure quasifree state using only quadratic Hamiltonians (see Theorem 20).

In particular, an algebra isomorphic to $\mathfrak{u}(d)$ is left invariant by quadratic Hamiltonians and pure quasifree states can be related to an homogeneous space of type $\mathrm{SU}(2d)/\mathrm{U}(d)$. At first glance, this might suggest that for full pure-state controllability the system algebra has to be isomorphic to $\mathfrak{so}(2d)$. However, the central result of this section shows that this is in general not necessary: a quasifree fermionic system (with $d > 4$ or $d = 3$) is fully pure-state controllable iff its system algebra is isomorphic to $\mathfrak{so}(2d)$ or $\mathfrak{so}(2d-1)$, see Theorem 23.

A. Quasifree States

A fermionic state ρ on $\mathcal{F}(\mathbb{C}^d)$ is called *quasifree* or *Gaussian* if it vanishes on odd monomials of Majorana operators and factorizes on even monomials into the *Wick expansion form*

$$\mathrm{tr}(\rho m_{k_1} \ldots m_{k_{2d}}) = \sum_\pi \mathrm{sgn}(\pi) \prod_{p=1}^{d} \mathrm{tr}(\rho m_{k_{\pi(2p-1)}} m_{k_{\pi(2p)}}).$$

Here the sum runs over all pairings of $[1, \ldots, 2d]$, i.e., over all permutations π of $[1, \ldots, 2d]$ satisfying $\pi(2q-1) < \pi(2q)$ and $\pi(2q-1) < \pi(2q+1)$ for all q. The *covariance matrix* of ρ is defined as the $2d \times 2d$ skew-symmetric matrix with real entries

$$G^\rho_{pq} = i[\mathrm{Tr}(\rho \mathrm{m_p} \mathrm{m_q}) - \delta_{\mathrm{pq}}]. \tag{27}$$

Due to the Wick expansion property, a quasifree state is uniquely characterized by its covariance matrix. (General references for this section include [17, 56–59].) The following proposition resumes a known result on these covariance matrices (see, e.g., Lemma 2.1 and Theorem 2.3 in [57]), which will be useful in the later development:

Proposition 17. *The singular values of the covariance matrix of a $d-$mode fermionic state must lie between* 0 *and* 1*. Conversely, for any* $2d \times 2d$ *skew-symmetric matrix* G^ρ *with singular values between* 0 *and* 1 *there exist a quasifree state that has* G^ρ *as a covariance matrix.*

B. Orbits and Stabilizers of Quasifree States under the Action of Quadratic Hamiltonians

The action of the time-evolution unitaries generated by quadratic Hamiltonians on quasifree states can be described by the following proposition (see Lemma 2.6 in [57]):

Proposition 18. *Consider a quasifree state* ρ_a *corresponding to the (skew-symmetric) covariance matrix* G^a*. The quadratic Hamiltonian*

$$H = i \sum_{p,q=1}^{2d} T_{pq} \left(-\tfrac{1}{2} m_p m_q\right)$$

is defined using the skew-symmetric matrix T *and generates the time-evolution of* ρ_a*. The time-evolved state (at unit time),* $\rho_b = e^{-iH} \rho_a e^{iH}$ *is again a quasifree state with a (skew-symmetric) covariance matrix* $G^b = O_T G^a O_T^t$*, where* $O_T := e^{-iT} \in \mathrm{SO}(2d)$*.*

Any skew-symmetric matrix G can be brought into its canonical form

$$O_G G O_G^t = \begin{pmatrix} 0 & \nu_1 & & & & & & \\ -\nu_1 & 0 & & & & & & \\ & & 0 & \nu_2 & & & & \\ & & -\nu_2 & 0 & & & & \\ & & & & \ddots & & & \\ & & & & & & 0 & \nu_N \\ & & & & & & -\nu_N & 0 \end{pmatrix}$$

using a (not necessarily unique) element $O_G \in \mathrm{SO}(2d)$ where $\{\nu_i\}_{i=1}^d$ denotes the singular values of G. This means that a quasifree state can be reached from another one by the action of quadratic Hamiltonians if their covariance matrices share the same singular values (including multiplicities). Let us now recall another result related to the singular values of the covariance matrices of pure quasifree states (Theorem 6.2 in [57], and Lemma 1 in [59]):

Proposition 19. *A quasifree state* ρ *is pure iff the following (equivalent) conditions hold for its covariance matrix* G^ρ*:*
(a) The rows (and columns) of G^ρ *are real unit vectors which are pairwise orthogonal to each other.*
(b) The singular values of G^ρ *are all* 1*.*

Applying this result together with Proposition 18, we obtain the following theorem:

Theorem 20. *The set of quadratic Hamiltonians act transitively on pure quasifree states, and the corresponding stabilizer algebras are isomorphic to* $\mathfrak{u}(d)$*.*

Proof. We have already shown that the singular values of the covariance matrices (with multiplicities) form a separating set of invariants for the orbits generated by quadratic Hamiltonians over the set of quasifree states. This means, according to Proposition 19, that the pure quasifree states form a single orbit.

As the set of quadratic Hamiltonians generate a transitive action over the pure quasifree states, the corresponding stabilizer subalgebras are isomorphic to each other. Consider a quadratic Hamiltonian H with the coefficient matrices A and B as given in Eq. (21) and the Fock state ρ_Ω, which is the projection onto the Fock vacuum vector Ω. The state ρ_Ω is left invariant under the time evolution generated by H ($\rho_\Omega = e^{-iHt} \rho_\Omega e^{iHt}$) iff Ω is an eigenvector of H. We obtain that $H\Omega =$

$$\left[\sum_{p,q=1}^{d} A_{pq}(f_p^\dagger f_q - \delta_{pq}\tfrac{\mathbb{1}}{2}) + \frac{1}{2} B_{pq} f_p^\dagger f_q^\dagger - \frac{1}{2} B_{pq}^* f_p f_q\right] \Omega =$$
$$-\sum_{p=1}^{d} \frac{1}{2} A_{pp} \Omega + \sum_{p<q} B_{pq} f_p^\dagger f_q^\dagger \Omega.$$

By noting that Ω and $f_p^\dagger f_q^\dagger \Omega$ (with $p < q$) are linearly independent vectors, we can conclude that a quadratic Hamiltonian H leaves the Fock vacuum invariant iff $H = \sum_{p,q=1}^d A_{pq}(f_p^\dagger f_q - \delta_{pq}\frac{\mathbb{1}}{2})$. In Theorem 43 of Sec. IX we will show that these operators form a Lie algebra isomorphic to $\mathfrak{u}(d)$. $\square$

Corollary 21. *Theorem 20 identifies the space of pure quasifree states with the quotient space* $\mathrm{SO}(2d)/\mathrm{U}(d)$*.*

C. Conditions for Quasifree Pure-State Controllability

According to Theorem 20, a set of quasifree control Hamiltonians $\{H_1, \ldots, H_m\}$ allows for quasifree pure-state controllability, if the corresponding Hamiltonians generate the full quasifree system algebra, i.e. if $\langle iH_1, \ldots, iH_m \rangle_{\mathrm{Lie}} \cong \mathfrak{so}(2d)$. It is natural to ask whether this condition is also a necessary. Remarkably, it turns out that this is not the case, which is shown by the following proposition:

Lemma 22. *Consider a quasifree fermionic system with* $d > 1$ *modes. Let* K *be the subgroup of* $\mathrm{SO}(2d)$ *which is isomorphic to* $\mathrm{SO}(2d-1)$ *and stabilizes the first coordinate; the corresponding Lie algebra is denoted by* $\mathfrak{k}$*. Then*

(a) via its adjoint action the group K acts transitively on the set of all skew-symmetric covariance matrices of pure quasifree states (whose singular values are all 1);
(b) the quasifree system is pure-state controllable if its system algebra is conjugate under $\mathrm{SO}(2d)$ *to* $\mathfrak{k}$.

Proof. We prove the statement (a) by showing that all pure quasifree states can be transformed under K-conjugation to the same pure state. We employ an induction on d. The base case $d = 2$ can be directly verified. It follows from Proposition 19(b) that the skew-symmetric covariance matrix of a pure quasifree state can be written as

$$G^{\rho} = \begin{pmatrix} 0 & v_1^t \\ -v_1 & A_1 \end{pmatrix},$$

where v_1 denotes a normalized $(2d{-}1)$-dimensional vector and A_1 denotes a $(2d{-}1)\times(2d{-}1)$-dimensional skew-symmetric matrix. We consider the action of a general orthogonal transformation $1 \oplus O_1$ with $O_1 \in \mathrm{SO}(d-1)$:

$$\begin{pmatrix} 1 & \\ & O_1 \end{pmatrix} \begin{pmatrix} 0 & v_1^t \\ -v_1 & A_1 \end{pmatrix} \begin{pmatrix} 1 & \\ & O_1^t \end{pmatrix} = \begin{pmatrix} 0 & v_1^t O_1^t \\ -O_1 v_1 & O_1 A_1 O_1^t \end{pmatrix}.$$

Since any $(2d{-}1)$-dimensional vector v_1 with unit length can be transformed by an orthogonal transformation to $(1, 0, 0, \ldots, 0)$, we can choose O_1 such that $v_1^t O_1^t = (1, 0, 0, \ldots, 0)$. We have $(O_1 A_1 O_1^t)_{11} = 0$ as the transformed matrix is skew-symmetric. Again by Proposition 19(b) we obtain the transformed matrix as

$$\begin{pmatrix} 0 & 1 & & \\ -1 & 0 & & \\ & & 0 & v_2^t \\ & & -v_2 & A_2 \end{pmatrix},$$

where v_2 is a $2d-3$ dimensional unit real vector and A_2 is a $(2d-3)\times(2d-3)$ skew-symmetric matrix. Now the proof of (a) follows using the induction hypothesis. The statement (b) is a consequence of (a). □

We relate Lemma 22 to what is known about transitive actions on the coset space $\mathrm{SO}(2d)/\mathrm{U}(d)$. Only Lie groups isomorphic to $\mathrm{SO}(2d-1)$ and $\mathrm{SO}(2d)$ can act transitively (i.e. in a pure-state controllable manner) on the homogeneous space $\mathrm{SO}(2d)/\mathrm{U}(d)$ assuming $d \geq 3$. The case $d \geq 4$ is discussed in [60]. For $d = 3$ we have $\mathrm{SO}(6) \cong \mathrm{SU}(4)$ and $\mathrm{SU}(4)/\mathrm{U}(3) = \mathrm{CP}^3$ (where CP^3 denotes the complex projective space in four dimensions), and it is known that only subgroups of $\mathrm{SU}(4)$ isomorphic to $\mathrm{SU}(4)$ or $\mathrm{Sp}(2) \cong \mathrm{SO}(5)$ can act transitively on CP^3 (see p. 168 of [61] or p. 68 of [62]; refer also to [63]).

In most cases the $\mathfrak{so}(k-1)$-subalgebras of $\mathfrak{so}(k)$ are conjugate to each other. More precisely, Lemma 7 of [64] states that for $3 \leq k \notin \{4, 8\}$ all subalgebras of $\mathfrak{so}(k)$ whose dimension is equal to $(k{-}1)(k{-}2)/2$ are conjugate to each other under the action of the group $\mathrm{SO}(k)$. In particular, it follows in these cases that all subalgebras of $\mathfrak{so}(k)$ with dimension $(k-1)(k-2)/2$ are isomorphic to $\mathfrak{so}(k-1)$. Interestingly, the last statement holds also for $k \in \{4, 8\}$ (see Lemma 3 of [64]); however not all of these subalgebras of $\mathfrak{so}(k)$ are conjugate. We obtain the following theorem providing a necessary and sufficient condition for full quasifree pure-state controllability in the case of $d > 4$ or $d = 3$ modes:

Theorem 23. *A quasifree fermionic system with $d > 4$ or $d = 3$ modes is fully pure-state controllable iff its system algebra is isomorphic to $\mathfrak{so}(2d)$ or $\mathfrak{so}(2d-1)$.*

Proof. "$\Rightarrow$": Note that Theorem 20 identifies the space of pure quasifree states with the homogeneous space $\mathrm{SO}(2d)/\mathrm{U}(d)$. Assuming $d \geq 3$, we summarized above that a group acting transitively on this homogeneous space is isomorphic either to $\mathrm{SO}(2d)$ or $\mathrm{SO}(2d{-}1)$. Thus only the full quasifree system algebra $\mathfrak{so}(2d)$ or a system algebra isomorphic to $\mathfrak{so}(2d{-}1)$ can generate a transitive action on the space of pure quasifree states.
"$\Leftarrow$": As discussed, all $\mathfrak{so}(2d-1)$-subalgebras are conjugate to each other for $d > 4$ and $d = 3$. Lemma 22(b) then implies that any set of Hamiltonians generating a system algebra isomorphic to $\mathfrak{so}(2d{-}1)$ will allow for full quasifree pure-state controllability. □

Note that the cases $d = 2$ and $d = 4$ are well-known pathological exceptions. The algebra $\mathfrak{so}(4)$ breaks up into a direct sum of two $\mathfrak{so}(3)$-algebras which hence cannot be conjugate to each other. For $d = 4$, there are three classes of non-conjugate subalgebras of type $\mathfrak{so}(7)$ in $\mathfrak{so}(8)$ where two classes are given by irreducible embeddings and the third one is conjugate to the reducible standard embedding fixing the first coordinate [65].

On a more general level, Theorem 23 can be seen as a fermionic variant of the pure-state controllability criterion for spin systems [24–26]. We note here that the result for spin systems has been recently generalized from the transitivity over a set of one-dimensional projections (i.e. pure states) to the transitivity over a set of projections of arbitrary fixed rank (i.e., over Grassmannian spaces) [63]. We will use exactly this generalization in Section IX C in order to find a necessary and sufficient pure-state controllability condition for particle-conserving quasifree systems.

VII. TRANSLATION-INVARIANT SYSTEMS

We study system algebras generated by translation-invariant Hamiltonians of the type which arises approximately in experimental settings of, e.g., optical lattices. As the naturally occurring interactions are usually short-ranged, we pay particular attention to the case of Hamiltonians with restricted interaction length. For example, consider a d-site fermionic chain with Hamiltonians which are translation-invariant and are composed of nearest-neighbor (plus on-site) terms. All elements in its dynamic algebra can be written as linear combinations of

TABLE I. System algebras of translation-invariant fermionic systems with d modes for (a) nearest-neighbor interactions only and (b) arbitrary translation-invariant interactions

Case	d	System algebra
(a)	1	–
	2	$\sum_{i=1}^{2} \mathfrak{u}(1)$
	3	$\sum_{i=1}^{2} \mathfrak{su}(2) + \sum_{i=1}^{3} \mathfrak{u}(1)$
	4	$\sum_{i=1}^{5} \mathfrak{su}(2) + \sum_{i=1}^{4} \mathfrak{u}(1)$
	5	$\sum_{i=1}^{2} \mathfrak{su}(4) + \sum_{i=1}^{8} \mathfrak{su}(3) + \sum_{i=1}^{3} \mathfrak{u}(1)$
	6	$\sum_{i=1}^{4} \mathfrak{su}(6) + \sum_{i=1}^{8} \mathfrak{su}(5) + \sum_{i=1}^{3} \mathfrak{u}(1)$
(b)	1	–
	2	$\sum_{i=1}^{2} \mathfrak{u}(1)$
	3	$\sum_{i=1}^{2} \mathfrak{su}(2) + \sum_{i=1}^{4} \mathfrak{u}(1)$
	4	$\sum_{i=1}^{8} \mathfrak{su}(2) + \sum_{i=1}^{6} \mathfrak{u}(1)$
	5	$\sum_{i=1}^{2} \mathfrak{su}(4) + \sum_{i=1}^{8} \mathfrak{su}(3) + \sum_{i=1}^{8} \mathfrak{u}(1)$
	6	$\sum_{i=1}^{4} \mathfrak{su}(6) + \sum_{i=1}^{8} \mathfrak{su}(5) + \sum_{i=1}^{10} \mathfrak{u}(1)$

six types of terms: the chemical potential

$$h_0 := \sum_{n=1}^{d} \left(f_n^\dagger f_n - \tfrac{1}{2}\mathbb{1} \right), \tag{28}$$

the real and complex hopping Hamiltonians

$$h_{\rm rh} := \sum_{n=1}^{d} (f_n^\dagger f_{n+1} + f_{n+1}^\dagger f_n) \quad \text{and} \tag{29}$$

$$h_{\rm ch} := \sum_{n=1}^{d} i(f_n^\dagger f_{n+1} - f_{n+1}^\dagger f_n), \tag{30}$$

the real and complex pairing terms

$$h_{\rm rp} := \sum_{n=1}^{d} (f_n^\dagger f_{n+1}^\dagger + f_{n+1} f_n) \quad \text{and} \tag{31}$$

$$h_{\rm cp} := \sum_{n=1}^{d} i(f_n^\dagger f_{n+1}^\dagger - f_{n+1} f_n), \tag{32}$$

as well as a local density-density-type interaction

$$h_{\rm int} := \sum_{n=1}^{d} \left(f_n^\dagger f_n f_{n+1}^\dagger f_{n+1} - \tfrac{1}{4}\mathbb{1} \right). \tag{33}$$

The corresponding dynamic system algebras (given in Table I) were computed with the help of the computer algebra system MAGMA [66] for up to six modes while distinguishing nearest-neighbor interactions from arbitrary translation-invariant ones.

In this context, two sets of natural questions arise: (a) How does the dimension of these dynamic system algebras scale with the number of modes? (b) How do the system algebras generated by the nearest-neighbor terms differ from the general translation-invariant ones? Can one characterize those elements that are translation-invariant yet not generated by nearest-neighbor Hamiltonians? Are there, for example, next-nearest-neighbor interactions of this type? In this section, we will answer these questions partially. We determine the system algebra for general translation-invariant fermionic Hamiltonians, and conclude that its dimension scales exponentially with the the number of modes. We also provide translation-invariant fermionic Hamiltonians of bounded interaction length which cannot be generated by nearest-neighbor ones.

The structure of this section is the following: As the structure of system algebras for translation-invariant systems has only been studied sparsely even for simple scenarios of spin models, we start by examining this case first. In Secs. VII A and VII B, we determine the system algebras of all translation invariant spin-chain Hamiltonians with L qubits. In particular, we simplify and generalize results of [16] concerning finite-ranged interactions. Finally, we present the corresponding results for the fermionic case in Sec. VII C and VII D.

A. Translation-Invariant Spin Chains

Consider a chain of L qubits with Hilbert space $\otimes_{i=1}^{L}\mathbb{C}^2$. The *translation unitary* U_T is defined by its action on the canonical basis vectors as

$$U_T \, |n_1, n_2, \ldots, n_L\rangle = |n_L, n_1, \ldots, n_{L-1}\rangle \tag{34}$$

where $n_i \in \{0,1\}$. We will determine the translation-invariant system algebra which is defined as the maximal Lie algebra of skew-hermitian matrices commuting with the translation unitary U_T.

Lemma 24. *The translation unitary can be spectrally decomposed as* $U_T = \sum_{\ell=0}^{L-1} \exp(2\pi i \ell/L) P_\ell$*, and the rank* r_ℓ *of the spectral projection* P_ℓ *is given by the Fourier transform*

$$r_\ell := \frac{1}{L} \sum_{k=0}^{L-1} 2^{\gcd(L,k)} \exp(-2\pi i k \ell/L), \tag{35}$$

where $\gcd(L,k)$ *denotes the greatest common divisor of* L *and* k*.*

Proof. The eigenvalues of U_T are limited to $\exp(2\pi i\ell/L)$ with $\ell \in \{0,\ldots,L-1\}$ as the order of U_T is L, i.e. $U_T^L = \mathbb{1}$. Hence, the corresponding spectral decomposition is given by $U_T = \sum_{\ell=0}^{L-1} \exp(2\pi i\ell/L) P_\ell$. This induces a unitary representation D_T of the cyclic group $\mathbb{Z}_L$ which maps the k-th power of the generator $g \in \mathbb{Z}_L$ of degree L to $D_T(g^k) = U_T^k$. Note that D_T splits up into a direct sum $D_T \cong \oplus_{\ell \in \{0,\ldots,L-1\}} (D_\ell)^{\oplus \dim(P_\ell)}$ containing $\dim(P_\ell)$ copies of the one-dimensional representations satisfying

TABLE II. System algebras $\mathfrak{t}_M(L)$ of translation-invariant systems with $1 \leq L \leq 6$ spins and interaction lengths of less than M, where $\mathfrak{k}_a := \mathfrak{su}(4)+\sum_{i=1}^2 \mathfrak{su}(2)$, $\mathfrak{k}_b := \mathfrak{su}(6)+\mathfrak{su}(4)$, $\mathfrak{k}_c := \mathfrak{su}(8)+\sum_{i=1}^4 \mathfrak{su}(6)$, and $\mathfrak{k}_d := \mathfrak{su}(14)+\sum_{i=1}^2 \mathfrak{su}(11)+\mathfrak{su}(10)+\sum_{i=1}^2 \mathfrak{su}(9)$. Refer also to Theorem 25 for the structure of $\mathfrak{t}_L(L)$.

M	$L=1$	2	3	4	5	6
1	$\mathfrak{su}(2)$	$\mathfrak{su}(2)$	$\mathfrak{su}(2)$	$\mathfrak{su}(2)$	$\mathfrak{su}(2)$	$\mathfrak{su}(2)$
2	–	$\mathfrak{su}(3)+\mathfrak{u}(1)$	$\mathfrak{k}_a+\mathfrak{u}(1)$	$\mathfrak{k}_b+\sum_{i=1}^2 \mathfrak{su}(2)+\mathfrak{u}(1)$	$\mathfrak{k}_c+\mathfrak{u}(1)$	$\mathfrak{k}_d+\mathfrak{u}(1)$
3	–	–	$\mathfrak{k}_a+\sum_{i=1}^2 \mathfrak{u}(1)$	$\mathfrak{k}_b+\sum_{i=1}^2 \mathfrak{su}(3)+\sum_{i=1}^3 \mathfrak{u}(1)$	$\mathfrak{k}_c+\sum_{i=1}^2 \mathfrak{u}(1)$	$\mathfrak{k}_d+\sum_{i=1}^3 \mathfrak{u}(1)$
4	–	–	–	$\mathfrak{k}_b+\sum_{i=1}^2 \mathfrak{su}(3)+\sum_{i=1}^3 \mathfrak{u}(1)$	$\mathfrak{k}_c+\sum_{i=1}^4 \mathfrak{u}(1)$	$\mathfrak{k}_d+\sum_{i=1}^4 \mathfrak{u}(1)$
5	–	–	–	–	$\mathfrak{k}_c+\sum_{i=1}^4 \mathfrak{u}(1)$	$\mathfrak{k}_d+\sum_{i=1}^5 \mathfrak{u}(1)$
6	–	–	–	–	–	$\mathfrak{k}_d+\sum_{i=1}^5 \mathfrak{u}(1)$

$D_\ell(g^k) = \exp(2\pi i k\ell/L)$. Therefore, we determine the rank of a projection P_ℓ by computing the multiplicity of D_ℓ using the character scalar product

$$\begin{aligned} r_\ell &= \frac{1}{L}\sum_{k=0}^{L-1} \mathrm{tr}[D_T(g^k)]\ \mathrm{tr}[D_\ell(g^k)]^* \\ &= \frac{1}{L}\sum_{k=0}^{L-1} \mathrm{tr}[D_T(g^k)]\ \exp(-2\pi i k\ell/L). \end{aligned}$$

The trace of $D_T(g^k)$ is equal to the number of basis vectors left invariant since $D_T(g^k)$ is a permutation matrix in the canonical basis. From elementary combinatorial theory we know that a bit string $(n_1, n_2, \ldots, n_L)$ is left invariant under a cyclic shift by k positions if and only if it is of the form

$$(n_1, n_2, \ldots, n_{\gcd(L,k)}, \ldots, n_1, n_2, \ldots, n_{\gcd(L,k)})\,.$$

It follows that the number of U_T^k-invariant basis vectors and—hence—the trace of $D_T(g^k) = U_T^k$ is equal to $2^{\gcd(L,k)}$. Thus, the multiplicities of D_ℓ are given accordingly by $r_\ell = \frac{1}{L}\sum_{k=0}^{L-1} 2^{\gcd(L,k)} \exp(-2\pi i k\ell/L)$. □

Note that a Hamiltonian commutes with U_T iff it commutes with all spectral projections P_ℓ of U_T. Combining this fact with Theorem 51 we obtain a characterization of the system algebra for translation-invariant spin systems:

Theorem 25. *The translation-invariant Hamiltonians acting on a L-qubit system generate the system algebra* $\mathfrak{t}(L) := \mathfrak{s}[\oplus_{\ell=0}^{L-1} \mathfrak{u}(r_\ell)] \cong [\sum_{\ell=0}^{L-1} \mathfrak{su}(r_\ell)] + [\sum_{i=1}^{L-1} \mathfrak{u}(1)]$, *where the numbers r_ℓ are defined in Eq.* (35).

In complete analogy one can show that for a chain consisting of L systems with N levels, the system algebra is equal to $\mathfrak{s}[\oplus_{\ell=0}^{L-1} \mathfrak{u}(r_{N,\ell})]$, where $r_{N,\ell}$ denotes the Fourier transform of the function $N^{\gcd(L,k)}$.

B. Short-Ranged Spin-Chain Hamiltonians

In many physical scenarios, we may only have direct control over translation-invariant Hamiltonians of limited interaction range. We will investigate in this section how the limitations on the interaction range constrain the set of reachable operations. In particular, we provide upper bounds for the system algebras with finite interaction range.

Let us denote the Lie algebra corresponding to Hamiltonians of interaction length less than M by $\mathfrak{t}_M(L)$, or $\mathfrak{t}_M$ for short. In other words, $\mathfrak{t}_M(L)$ is the Lie subalgebra of $\mathfrak{t}(L)$ generated by the skew-hermitian operators

$$i\sum_{q=0}^{L-1} U_T^q \left[\left(\bigotimes_{p=1}^{M} Q_p\right) \otimes \mathbb{1}_2^{\otimes L-M}\right] U_T^{-q}$$

for all combinations of $Q_p \in \{\mathbb{1}_2, \mathrm{X}, \mathrm{Y}, \mathrm{Z}\}$ apart from the case when $Q_1 = \mathbb{1}_2$. In this way, $\mathfrak{t}_1(L)$ corresponds to the translation-invariant on-site Hamiltonians, while $\mathfrak{t}_2(L)$ is generated by the on-site terms and the nearest-neighbor interactions, and so on. Finally, we have $\mathfrak{t}_L(L) = \mathfrak{t}_L$.

We computed all the algebras $\mathfrak{t}_M(L)$ for $1 \leq L \leq 6$ and $1 \leq M \leq L$ using the computer algebra system MAGMA [66]. The results, shown in Table II, suggest that for certain restrictions on the interaction length (e.g., nearest-neighbor terms), there will be some translation-invariant interactions that cannot be generated. This is in accordance with the result of Kraus et al. [16]. Building partly on their work, we analyze the properties of the algebras $\mathfrak{t}_M(L)$ for general M and L values, and then compare our theorems with Table II.

We first mention a central proposition whose proof can be found in Appendix E:

Proposition 26. *Let $M < L$ denote a divisor of L. Given two elements $iH_M \in \mathfrak{t}_M$ and $iH_{M+1} \in \mathfrak{t}_{M+1}$, we obtain that*

$$\mathrm{tr}(U_T^{qM} H_M) = 0 \ \textit{and}\ \mathrm{tr}[(U_T^{qM} - U_T^{-qM})H_{M+1}] = 0$$

hold for any positive integer q.

Applying Proposition 26, we can present upper bounds for the system algebras with restricted interaction length.

Theorem 27. *Let $M < L$ denote a divisor of the number of spins L, and define $R := L/M$. We obtain:*

(a) The algebra $\mathfrak{t}_M$ *is isomorphic to a Lie subalgebra of* $[\sum_{\ell=0}^{L-1}\mathfrak{su}(r_\ell)]+[\sum_{i=1}^{L-R}\mathfrak{u}(1)]$ *and does not generate* $\mathfrak{t}_L$.
(b) The algebra $\mathfrak{t}_{M+1}$ *is isomorphic to a Lie subalgebra of* $[\sum_{\ell=0}^{L-1}\mathfrak{su}(r_\ell)]+[\sum_{i=1}^{L-1-\lfloor R/2\rfloor}\mathfrak{u}(1)]$ *and does not generate* $\mathfrak{t}_L$.
(c) In addition, $\mathfrak{t}_M \neq \mathfrak{t}_{M+1}$.

Proof. (a) Since M is a divisor of L, the equation

$$\begin{aligned} U_T^{qM} &= \sum_{\ell=0}^{L-1}\exp(2\pi i qM\ell/L)P_\ell = \sum_{\ell=0}^{L-1}\exp(2\pi i q\ell/R)P_\ell \\ &= \sum_{\ell'=0}^{R-1}\exp(2\pi i q\ell'/R)\left(\sum_{p=0}^{M-1}P_{pR+\ell'}\right) \end{aligned}$$

holds for any integer q. One can invert the equation as

$$\left(\sum_{p=0}^{M-1}P_{pR+\ell'}\right) = \frac{1}{R}\sum_{q=0}^{R-1}\exp(-2\pi i q\ell'/R)\,U_T^{qM}.$$

If $ih \in \mathfrak{t}_M$, we obtain by applying Proposition 26 that

$$\mathrm{tr}\left(ih\sum_{p=0}^{M-1}P_{pR+\ell'}\right) = 0 \tag{36}$$

holds for $\ell' \in \{0,1,\ldots,R-1\}$. It follows that $\mathfrak{t}_M$ is a subalgebra of the Lie algebra $\mathfrak{f}$ which consists of all skew-hermitian matrices satisfying the condition in Eq. (36). Note that $\mathfrak{f}$ is isomorphic to $\oplus_{\ell'=0}^{R-1}(\mathfrak{s}[\oplus_{p=0}^{M-1}u(r_{pR+\ell'})]) \cong [\sum_{\ell=0}^{L-1}\mathfrak{su}(r_\ell)]+[\sum_{i=1}^{L-R}\mathfrak{u}(1)]$, and part (a) follows.
(b) For elements $ig \in \mathfrak{t}_{M+1}$, Proposition 26 and Eq. (36) imply that

$$\mathrm{tr}\left[ig\sum_{p=0}^{M-1}\left(P_{pR+\ell'}-P_{pR+L-\ell'}\right)\right] = 0. \tag{37}$$

The maximal Lie algebra consisting of skew-hermitian matrices which satisfy the condition in Eq. (37) is isomorphic to $[\sum_{\ell=0}^{L-1}\mathfrak{su}(r_\ell)]+[\sum_{i=1}^{L-1-\lfloor R/2\rfloor}\mathfrak{u}(1)]$.
(c) Let

$$ih = i\sum_{q'=0}^{L-1}U_T^{q'}\left[X\otimes \mathbb{1}_2^{\otimes M-1}\otimes X\otimes \mathbb{1}_2^{\otimes L-M-1}\right]U_T^{-q'}.$$

Obviously, $ih \in \mathfrak{t}_{M+1}$ holds. Using the formula for $F(1,M{+}1)$, we obtain that $\mathrm{tr}(U_T^{qM}ih) = i2L$ holds for every integer q. Hence, $ih \notin \mathfrak{t}_M$. ∎

In particular, this theorem implies that the algebra $\mathfrak{t}(L) = \mathfrak{t}_L(L)$ of all translation-invariant Hamiltonians cannot be generated from the subclass of nearest-neighbor Hamiltonians, cp. also [16]. More precisely, one finds:

Corollary 28. *If* L *is even,* $\mathfrak{t}_2(L)$ *is isomorphic to a Lie subalgebra of* $[\sum_{\ell=0}^{L-1}\mathfrak{su}(r_\ell)]+[\sum_{i=1}^{L/2}\mathfrak{u}(1)]$. *For odd* $L \geq 3$, $\mathfrak{t}_2(L)$ *is isomorphic to a Lie subalgebra of* $[\sum_{\ell=0}^{L-1}\mathfrak{su}(r_\ell)]+[\sum_{i=1}^{(L-3)/2}\mathfrak{u}(1)]$.

Let us now compare our upper bounds with the results of Table II. Theorem 27 restricts the possibilities for the M-local algebras $\mathfrak{t}_M(L)$ only by some central elements $\mathfrak{u}(1)$ when compared to the corresponding full translation-invariant algebra $\mathfrak{t}(L)$. One can indeed identify in Table II some missing $\mathfrak{u}(1)$-parts for $L \in \{3,\ldots,6\}$. In general, the dimensions of the M-local algebras $\mathfrak{t}_M(L)$ can be even smaller than predicted by the upper bounds of Theorem 27 as can be seen in Table II for $L = 4$. Theorem 27 and Table II suggest that the prime decomposition of the chain length L will have strong implications on the dimension of $\mathfrak{t}_M(L)$.

C. Translation-Invariant Fermionic Systems

To determine the system algebra generated by all translation-invariant Hamiltonians of a fermionic chain, we can follow similar lines as in Sec. VII A. Here, however, we additionally have to consider the parity superselection rule. We define the fermionic translation-invariant system algebra as the maximal Lie subalgebra of $\mathfrak{su}(2^{d-1})\oplus\mathfrak{su}(2^{d-1})$ [see Theorem (4)] which contains only skew-hermitian matrices commuting with the fermionic translation unitary $\mathcal{U}$, which is defined below such that it commutes with the parity operator P (see Eq. (14)). The standard orthonormal basis in the Fock space for a chain of d fermionic modes is given by

$$|n_1,n_2,\ldots n_d\rangle := (f_1^\dagger)^{n_1}(f_2^\dagger)^{n_2}\cdots(f_d^\dagger)^{n_d}\,|0\rangle \tag{38}$$

with $n_i \in \{0,1\}$. Note that for the purpose of unambiguously defining this basis, we order the operators $(f_i^\dagger)^{n_i}$ in Eq. (38) with respect to their site index i. The fermionic translation unitary $\mathcal{U}$ is defined by its action

$$\begin{aligned} \mathcal{U}\,|n_1,n_2,\ldots n_d\rangle &= \mathcal{U}\,(f_1^\dagger)^{n_1}(f_2^\dagger)^{n_2}\cdots(f_d^\dagger)^{n_d}\,|0\rangle \\ &= (f_2^\dagger)^{n_1}\cdots(f_d^\dagger)^{n_{d-1}}(f_1^\dagger)^{n_d}\,|0\rangle \\ &= (-1)^{n_d(n_1+n_2+\ldots+n_{d-1})}(f_1^\dagger)^{n_d}(f_2^\dagger)^{n_1}\cdots(f_d^\dagger)^{n_{d-1}}\,|0\rangle \\ &= (-1)^{n_d(n_1+n_2+\ldots+n_{d-1})}\,|n_d,n_1,\ldots,n_{d-1}\rangle \end{aligned} \tag{39}$$

on the standard basis. The adjoint action of $\mathcal{U}$ on the creation operators $f_\ell^\dagger$ is then given by

$$\mathcal{U}\,f_\ell^\dagger\,\mathcal{U}^\dagger = f_{(\ell+1 \bmod d)}^\dagger.$$

The superselection rule for fermions splits the spectral decomposition of the translation unitary into two blocks corresponding to the positive and negative parity subspace. The translation unitary $\mathcal{U}$ commutes with the parity operator P, and hence $\mathcal{U} = \mathcal{U}_+ + \mathcal{U}_-$ is block-diagonal in the eigenbasis of P where $\mathcal{U}_+ := P_+\mathcal{U}P_+$ and $\mathcal{U}_- := P_-\mathcal{U}P_-$. The following lemma gives the spectral decomposition of the operators $\mathcal{U}_\pm$:

Lemma 29. *The unitary operators* $\mathcal{U}_\pm$ *can be spectrally decomposed as* $\mathcal{U}_\pm = \sum_{\ell=0}^{d-1}e^{2\pi i\ell/d}P_\ell^\pm$, *where the rank*

$\hat{r}_\ell$ of the spectral projection $P_\ell^\pm$ is given by the Fourier transform

$$\hat{r}_\ell := \frac{1}{d}\sum_{k=0}^{d-1} h(d,k)\,\exp(-2\pi i k\ell/d) \tag{40}$$

of $h(d,k)$ where $\ell \in \{0,\ldots,d-1\}$ and

$$h(d,k) := \begin{cases} 0 & \text{if } d/\gcd(d,k) \text{ is even,} \\ 2^{\gcd(d,k)-1} & \text{if } d/\gcd(d,k) \text{ is odd.} \end{cases}$$

Proof. We determine the spectral decomposition of $\mathcal{U}_+$ and $\mathcal{U}_-$ along the lines of Lemma 24. Let $\mathcal{F}_+(\mathbb{C}^d)$ denote the subspace spanned by those basis vectors of Eq. (38) for which $\bar{n} = \sum_{i=1}^d n_i$ is even. Likewise, $\mathcal{F}_-(\mathbb{C}^d)$ corresponds to the case of odd $\bar{n}$. As $(\mathcal{U}_\pm)^d = \mathbb{1}_{\mathcal{F}_\pm(\mathbb{C}^d)}$, the eigenvalues of $\mathcal{U}_\pm$ are of the form $\exp(2\pi i\ell/d)$ with $\ell \in \{0,\ldots,d-1\}$. Hence, the spectral decomposition is given by $\mathcal{U}_\pm = \sum_{\ell=0}^{d-1}\exp(2\pi i\ell/d)P_\ell^\pm$. We define representations $\mathcal{D}_\pm$ of the cyclic group $\mathbb{Z}_d$ which map the k-th power of the generator $g \in \mathbb{Z}_d$ of degree d to $\mathcal{D}_\pm(g^k) := \mathcal{U}_\pm^k$. Note that $\mathcal{D}_\pm$ splits up into a direct sum $\mathcal{D}_\pm \cong \oplus_{\ell\in\{0,\ldots,L-1\}}(D_\ell)^{\oplus \dim(P_\ell)}$ containing $\dim(P_\ell^\pm)$ copies of the one-dimensional representations satisfying $D_\ell(g^k) = \exp(2\pi i k\ell/d)$. The rank $r_k^\pm$ of the projection $P_\ell^\pm$ is equal to the multiplicity of D_ℓ in the decomposition of the reducible representation $\mathcal{D}_\pm$. This multiplicity can be computed as the character scalar product

$$\begin{aligned} r_k^\pm &= \frac{1}{d}\sum_{k=0}^{d-1}\mathrm{tr}[\mathcal{D}_\pm(g^k)]\;\mathrm{tr}[D_\ell(g^k)]^* \\ &= \frac{1}{d}\sum_{k=0}^{d-1}\mathrm{tr}[\mathcal{D}_\pm(g^k)]\;\exp(-2\pi i\ell k/d). \end{aligned}$$

In the standard basis, all matrix entries of $\mathcal{D}_\pm(g^k) = \mathcal{U}_\pm^k$ are elements of the set $\{0,1,-1\}$. It follows by repeated applications of Eq. (39) that $\mathcal{U}^k$ maps the basis vectors $|n_1,n_2,\ldots,n_d\rangle$ to $s|n_{\pi(1)},n_{\pi(2)},\ldots,n_{\pi(d)}\rangle$ where π is a cyclic shift by k positions and the sign s is given by

$$s := (-1)^{\left(\sum_{i=1}^{d-k} n_i\right)\left(\sum_{j=d-k+1}^{d} n_j\right)}. \tag{41}$$

Recall from the proof of Lemma 24 that a bit string $(n_1,n_2,\ldots,n_N)$ is left invariant under a cyclic shift by k positions iff it is of the form

$$(n_1,n_2,\ldots,n_{\gcd(d,k)},\ldots,n_1,n_2,\ldots,n_{\gcd(d,k)}).$$

If $d/\gcd(d,k)$ is even, the sum $\bar{n} = \sum_{i=1}^d n_i$ is even for all of the $2^{\gcd(d,k)}$ bit strings invariant under a cyclic shift by k positions. It follows that all the diagonal entries of $\mathcal{U}_-^k$ are zero, while $\mathcal{U}_+^k$ has $2^{\gcd(d,k)}$ non-zero diagonal entries. The non-zero diagonal entries of $\mathcal{U}_+^k$ are given by the number s of Eq. (41). Note that s is $+1$ if $\sum_{j=1}^{d-k} n_j$ is even; and -1 otherwise. Hence the frequencies of $+1$ and -1 in the set of diagonal entries are equal. In summary, $\mathrm{tr}(\mathcal{U}_\pm^k) = 0$ if $d/\gcd(d,k)$ is even.

Assume now that $d/\gcd(d,k)$ is odd. The sum $\bar{n}$ is odd for half of the $2^{\gcd(d,k)}$ bit strings and even for the other half. Applying again Eq. (41), we obtain always a positive sign. Hence, both traces $\mathrm{tr}(\mathcal{U}_\pm^k)$ are equal to $2^{\gcd(d,k)-1}$. This completes the proof. ☐

Lemma 29 together with Theorem 51 implies the following characterization of the system algebra for a translation-invariant fermionic system:

Theorem 30. *Consider the translation-invariant Hamiltonians acting on a fermionic system with d modes. The corresponding system algebra $\mathfrak{t}^f$ is given by*

$$\begin{aligned} \mathfrak{t}^f &\cong \mathfrak{s}[\oplus_{\ell=0}^{d-1}\mathfrak{u}(\hat{r}_\ell)] \oplus \mathfrak{s}[\oplus_{\ell=0}^{d-1}\mathfrak{u}(\hat{r}_\ell)] \\ &\cong \left[\sum_{\ell=0}^{d-1}\mathfrak{su}(\hat{r}_\ell) + \mathfrak{su}(\hat{r}_\ell)\right] + \sum_{\ell=1}^{2d-2}\mathfrak{u}(1), \end{aligned}$$

where the numbers $\hat{r}_\ell$ are defined in Eq. (40).

Remark 31. Note that $\hat{r}_0 \geq \hat{r}_\ell$ holds for any ℓ and that $\sum_{\ell=0}^d \hat{r}_\ell = 2^{d-1}$. It follows that $\hat{r}_0 \geq (2^{d-1}-1)/d$ and hence that the dimension of the system algebra in Theorem 30 scales exponentially with d.

Remark 32. Assuming that the number of modes is given by a prime number p, we can explicitly determine the numbers $\hat{r}_\ell$ from Eq. (40). The corresponding system algebras are

$$\sum_{i=1}^{2}\mathfrak{su}(F_p+1) + \sum_{i=1}^{2p-2}\mathfrak{su}(F_p) + \sum_{i=1}^{2p-2}\mathfrak{u}(1), \tag{42}$$

where $F_p = (2^{p-1}-1)/p$ is guaranteed to be an integer by Fermat's little theorem.

D. Fermionic Nearest-Neighbor Hamiltonians

For spin systems (see Section VII B) we verified that the translation-invariant nearest-neighbor interactions together with the on-site elements will never generate all translation-invariant operators, i.e. $\mathfrak{t}_L \neq \mathfrak{t}_2$ (if the number of spins L is greater than two). This means that there exist certain translation-invariant elements which cannot be generated by nearest-neighbor interactions and on-site elements, but we could not identify the explicit form of these translation-invariant elements for general L. In particular, it would be interesting to know if $\mathfrak{t}_M \neq \mathfrak{t}_2$ holds for interaction lengths less than M $(2 < M < L)$, where M is independent of L.

In the case of fermionic systems, we can provide a result in this direction due to the restriction imposed by the parity superselection rule, which strongly limits the set of nearest-neighbor Hamiltonians. As we have discussed at the beginning of this section, the fermionic translation-invariant Hamiltonians of nearest-neighbor type are spanned by only six elements: h_0, h_{rh}, h_{ch}, h_{rp}, h_{cp}, and h_{int} as defined in Eqs. (28)–(33). We can show that there exist next-nearest-neighbor or third-neighbor interactions for odd $d \geq 5$ which cannot be generated by these six Hamiltonians, while for even $d \geq 6$ we provide a fourth-neighbor element.

Let $\mathfrak{t}^f_M$ denote the subalgebra of $\mathfrak{t}^f$ (see Theorem 30) which is generated by all elements of interaction length less than M. In particular, $\mathfrak{t}^f_2$ is generated by nearest-neighbor and on-site elements. The result of this subsection is summarized in the following theorem:

Theorem 33. *Let us consider the Hamiltonian*

$$h_{\mathrm{o}} := \sum_{n=1}^{d} i(f_n^\dagger f_{n+3} - f_{n+3}^\dagger f_n),$$

and fourth-neighbor Hamiltonian $h_{\mathrm{e}} :=$

$$\sum_{n=1}^{d}(f_n^\dagger f_n f_{n+1}^\dagger f_{n+1} f_{n+2}^\dagger f_{n+2} f_{n+3}^\dagger f_{n+3} f_{n+4}^\dagger f_{n+4} - \tfrac{1}{32}\mathbb{1}).$$

The generator $ih_{\mathrm{o}} \in \mathfrak{t}^f_4$ *is not contained in the system algebra* $\mathfrak{t}^f_2$ *generated by nearest-neighbor interactions and on-site elements if* $d \geq 5$ *is odd, while the element* $ih_{\mathrm{e}} \in \mathfrak{t}^f_5$ *is not contained in* $\mathfrak{t}^f_2$ *if* $d \geq 6$ *is even. Hence* $\mathfrak{t}^f_2 \neq \mathfrak{t}^f_5$ *(when* $d \geq 5$*).*

Note that the Hamiltonian h_{o} of Theorem 33 is a third-neighbor Hamiltonian for $d \geq 7$ and a next-nearest-neighbor Hamiltonian for $d = 5$. The proof of Theorem 33 is rather involved. The proof for even d is given in Appendix F, while Appendix G contains the proof for odd d.

VIII. QUASIFREE FERMIONIC SYSTEMS SATISFYING TRANSLATION-INVARIANCE

We continue the discussion of translation-invariant fermionic systems from Sec. VII by narrowing the scope to quadratic Hamiltonians. In Sec. VIII A, we derive the dynamic algebras for systems with and without (twisted) reflection symmetry. Both of these cases are summarized for quasifree fermionic systems in Table III: the system algebras were computed using the computer algebra system MAGMA [66] for cases with low number of modes, while the complete picture is provided by Theorem 34 and Corollary 35. Sec. VIII B yields a classification of the orbit structure of pure translation-invariant quasifree states. This allows us to present an application to many-body physics in Sec. VIII C, where we bound the scaling of the gap for a class of quadratic Hamiltonians.

A. Translation-Invariant Quadratic Hamiltonians

A quadratic Hamiltonian H is translation-invariant (i.e. $[H,\mathcal{U}] = 0$) iff the coefficient matrices A and B in Eq. (21) are cyclic (i.e. $A_{nm} - A_{n+1,m+1} = B_{nm} - B_{n+1,m+1} = 0$). To study such Hamiltonians, it is useful to rewrite them in terms of the Fourier-transformed annihilation and creation operators

$$\tilde{f}_k := \frac{1}{\sqrt{d}}\sum_{p=1}^{d} f_p e^{-2\pi i pk/d} \text{ and } \tilde{f}_k^\dagger := \frac{1}{\sqrt{d}}\sum_{p=1}^{d} f_p^\dagger e^{2\pi i pk/d}, \tag{43}$$

with $k \in \{0, 1, \ldots, d-1\}$, which satisfy again the canonical anticommutation relations

$$\{\tilde{f}_k^\dagger, \tilde{f}_{k'}^\dagger\} = \{\tilde{f}_k, \tilde{f}_{k'}\} = 0 \text{ and } \{\tilde{f}_k^\dagger, \tilde{f}_{k'}\} = \delta_{kk'}\mathbb{1}. \tag{44}$$

A Hamiltonian from Eq. (21) with cyclic A and B can now be rewritten as

$$H = \sum_{k=0}^{d-1} \tilde{A}_k(\tilde{f}_k^\dagger \tilde{f}_k - \tfrac{1}{2}) + \tfrac{1}{2}\tilde{B}_k \tilde{f}_k^\dagger \tilde{f}_{d-k}^\dagger - \tfrac{1}{2}\tilde{B}_k^* \tilde{f}_k \tilde{f}_{d-k} \tag{45}$$

applying the definitions $\tilde{A}_k := \sum_{p=1}^{d} A_{1p}\exp(-2\pi i pk/d)$ and $\tilde{B}_k := \sum_{p=1}^{d} B_{1p}\exp(-2\pi i pk/d)$, as well as the notation $\tilde{f}_d = \tilde{f}_0$. The hermiticity of A and the skew-symmetry of B translates into the properties $\tilde{A}_k = \tilde{A}_{d-k}^*$ and $\tilde{B}_k = -\tilde{B}_{d-k}$. This allows us to decompose the Hamiltonian into a four-part sum

$$\begin{aligned} H = &\sum_{k=1}^{\lfloor (d-1)/2\rfloor} \mathfrak{Im}(\tilde{A}_k)\, \ell_k^{\mathbb{1}} + \sum_{k=1}^{\lfloor (d-1)/2\rfloor} \mathfrak{Re}(\tilde{B}_k)\, \ell_k^{\mathrm{X}}/2 \\ &+ \sum_{k=1}^{\lfloor (d-1)/2\rfloor} \mathfrak{Im}(\tilde{B}_k)\, \ell_k^{\mathrm{Y}}/2 + \sum_{k=0}^{\lfloor d/2\rfloor} \mathfrak{Re}(\tilde{A}_k)\, \ell_k^{\mathrm{Z}}, \end{aligned} \tag{46}$$

where one has the following definitions

$$\begin{aligned} &\ell_k^{\mathbb{1}} := i(\tilde{f}_k^\dagger \tilde{f}_k - \tilde{f}_{d-k}^\dagger \tilde{f}_{d-k}),\ \ell_k^{\mathrm{X}} := (\tilde{f}_k^\dagger \tilde{f}_{d-k}^\dagger + \tilde{f}_{d-k}\tilde{f}_k), \\ &\ell_k^{\mathrm{Y}} := i(\tilde{f}_k^\dagger \tilde{f}_{d-k}^\dagger - \tilde{f}_{d-k}\tilde{f}_k),\ \ell_k^{\mathrm{Z}} := (\tilde{f}_k^\dagger \tilde{f}_k + \tilde{f}_{d-k}^\dagger \tilde{f}_{d-k} - \mathbb{1}) \end{aligned} \tag{47}$$

TABLE III. System algebras of quasifree fermionic systems with d modes satisfying translation-invariance.

d	general case (see Theorem 34)	(twisted) reflection symm. (see Eq. (50) and Cor. 35)
1	-	-
2	$\mathfrak{u}(1)+\mathfrak{u}(1)$	$\mathfrak{u}(1)+\mathfrak{u}(1)$
3	$\mathfrak{u}(2)+\mathfrak{u}(1)$	$\mathfrak{su}(2)+\mathfrak{u}(1)$
4	$\mathfrak{u}(2)+\mathfrak{u}(1)+\mathfrak{u}(1)$	$\mathfrak{su}(2)+\mathfrak{u}(1)+\mathfrak{u}(1)$
5	$\mathfrak{u}(2)+\mathfrak{u}(2)+\mathfrak{u}(1)$	$\mathfrak{su}(2)+\mathfrak{su}(2)+\mathfrak{u}(1)$
6	$\mathfrak{u}(2)+\mathfrak{u}(2)+\mathfrak{u}(1)+\mathfrak{u}(1)$	$\mathfrak{su}(2)+\mathfrak{su}(2)+\mathfrak{u}(1)+\mathfrak{u}(1)$
$\vdots$	$\vdots$	$\vdots$
$2n-1$	$\sum_{i=1}^{n-1}\mathfrak{u}(2)+\mathfrak{u}(1)$	$\sum_{i=1}^{n-1}\mathfrak{su}(2)+\mathfrak{u}(1)$
$2n$	$\sum_{i=1}^{n-1}\mathfrak{u}(2)+\mathfrak{u}(1)+\mathfrak{u}(1)$	$\sum_{i=1}^{n-1}\mathfrak{su}(2)+\mathfrak{u}(1)+\mathfrak{u}(1)$

with $k \in \{1, \ldots, \lfloor (d-1)/2 \rfloor\}$ as well as

$$\ell^{\mathrm{Z}}_{d/2} := (\tilde{f}^\dagger_{d/2}\tilde{f}_{d/2} - \mathbb{1}/2) \text{ for } d \text{ even},$$
$$\ell^{\mathrm{Z}}_{0} := (\tilde{f}^\dagger_{0}\tilde{f}_{0} - \mathbb{1}/2). \tag{48}$$

Note that the operators $\ell^{\mathrm{Z}}_{d/2}$ (for d even), ℓ^{Z}_0, ℓ^{Z}_k, $\ell^{\mathbb{1}}_k$, ℓ^{X}_k, and ℓ^{Y}_k are linearly independent and span the $(\lfloor d{-}1\rfloor{+}d)$-dimensional space of all translation-invariant quadratic Hamiltonians. For notational convenience we also introduce the dummy operators $\ell^{\mathrm{Q}}_{d/2} := 0$ (assuming d is even) and $\ell^{\mathrm{Q}}_0 := 0$ for $\mathrm{Q} \in \{\mathbb{1}, \mathrm{X}, \mathrm{Y}\}$.

With these stipulations, we can characterize the system algebra:

Theorem 34. *Let $\mathfrak{q}_d$ denote the system algebra on a fermionic system with d modes which corresponds to the set of Hamiltonians that are translation-invariant and quadratic. Then the Lie algebra $\mathfrak{q}_d$ is isomorphic to $[\sum_{i=1}^{(d-1)/2} \mathfrak{u}(2)] + \mathfrak{u}(1)$ for odd d and to $[\sum_{i=1}^{(d-2)/2} \mathfrak{u}(2)] + \mathfrak{u}(1) + \mathfrak{u}(1)$ for even d.*

Proof. If $d = 2m-1$ is odd, the generators $i\ell^{\mathbb{1}}_k$, $i\ell^{\mathrm{X}}_k$, $i\ell^{\mathrm{Y}}_k$, $i\ell^{\mathrm{Z}}_k$, and $i\ell^{\mathrm{Z}}_0$ can be partitioned into m pairwise-commuting sets, which each span linear subspaces as

$$L_0 := \langle i\ell^{\mathrm{Z}}_0\rangle_{\mathbb{R}} \text{ and } L_k := \langle i\ell^{\mathbb{1}}_k, i\ell^{\mathrm{X}}_k, i\ell^{\mathrm{Y}}_k, i\ell^{\mathrm{Z}}_k\rangle_{\mathbb{R}}$$

with $k \in \{1, \ldots, m{-}1\}$. The commutation properties $[L_k, L_{k'}] = 0$ (with $k \neq k'$) follow from Eq. (44). Moreover, L_0 is one-dimensional and forms a $\mathfrak{u}(1)$-algebra. Using Eq. (44), the relations $[\tilde{f}^\dagger_a\tilde{f}_a, \tilde{f}^\dagger_a\tilde{f}^\dagger_b] = ([\tilde{f}^\dagger_a\tilde{f}_a, \tilde{f}_a\tilde{f}_b])^\dagger = \tilde{f}^\dagger_a\tilde{f}^\dagger_b$ and $[\tilde{f}^\dagger_a\tilde{f}^\dagger_b, \tilde{f}_b\tilde{f}_a] = \tilde{f}^\dagger_a\tilde{f}_a + \tilde{f}^\dagger_b\tilde{f}_b - \mathbb{1}$ can be deduced for $a \neq b$. Substituting k and $d-k$ into a and b in the previous formula, one can verify directly that the correspondence

$$i\ell^{\mathbb{1}}_k \mapsto i\mathbb{1},\ i\ell^{\mathrm{X}}_k \mapsto i\mathrm{X},\ i\ell^{\mathrm{Y}}_k \mapsto i\mathrm{Y},\ i\ell^{\mathrm{Z}}_k \mapsto i\mathrm{Z}$$

provides an explicit Lie isomorphism between L_k and $\mathfrak{u}(2)$. If $d = 2m$ is even, the system algebra consists of the above-described generators supplemented with the element $i\ell^{\mathrm{Z}}_{d/2}$. This additional element commutes with all the other generators and—therefore—provides an additional $\mathfrak{u}(1)$. □

The isomorphism between L_k and $\mathfrak{u}(2)$ as given in the proof leads to a compact formula for the time evolution (in the Heisenberg picture) of the elements of L_k. Since the operators ℓ^{X}_k, ℓ^{Y}_k, ℓ^{Z}_k, and $\ell^{\mathbb{1}}_k$ (with $k \in \{1, \ldots, \lfloor (d-1)/2 \rfloor\}$) satisfy the same commutation relations as the Pauli matrices X, Y, Z, and $\mathbb{1}$, their time-evolution generated by the Hamiltonian H in Eq. (46) can be straightforwardly related to a qubit time-evolution

$$e^{iHt} i\left(a_{\mathbb{1}}\ell^{\mathbb{1}}_k + a_{\mathrm{X}}\ell^{\mathrm{X}}_k + a_{\mathrm{Y}}\ell^{\mathrm{Y}}_k + a_{\mathrm{Z}}\ell^{\mathrm{Z}}_k\right) e^{-iHt} =$$
$$ia_{\mathbb{1}}\ell^{\mathbb{1}}_k + \sum_{\mathrm{Q}\in\{\mathrm{X},\mathrm{Y},\mathrm{Z}\}} ia_{\mathrm{Q}}\, \ell^{\mathrm{Q}}_k \operatorname{tr}(e^{iH_s}\mathrm{Q}\, e^{-iH_s}\mathrm{Q}), \tag{49}$$

where $H_s = \mathfrak{Re}(\tilde{A}_k)\mathrm{Z} + \mathfrak{Re}(\tilde{B}_k)\mathrm{X}/2 + \mathfrak{Im}(\tilde{B}_k)\mathrm{Y}/2$.

The *twisted reflection symmetry* plays an important role in translation-invariant quasifree fermionic systems. It is defined by the unitary

$$\mathcal{R}|n_1, n_2, \ldots n_d\rangle = i^{(\sum_{\ell=1}^d n_\ell)^2}|n_d, n_{d-1}, \ldots n_1\rangle. \tag{50}$$

whose adjoint action on creation operators and their Fourier transforms are specified as

$$\mathcal{R}\, f^\dagger_\ell\, \mathcal{R}^\dagger = i f^\dagger_{(d-\ell+1 \bmod d)},\ \mathcal{R}\, \tilde{f}^\dagger_k\, \mathcal{R}^\dagger = \tilde{f}^\dagger_{(-k \bmod d)}. \tag{51}$$

A given translation-invariant quasifree Hamiltonian is $\mathcal{R}$-symmetric (i.e. $[\mathcal{R}, H] = 0$) iff the coefficient matrix is restricted to be real. In our language, these Hamiltonians are exactly the ones for which $\mathfrak{Im}(\tilde{A}_k) = 0$, i.e., the corresponding generators are spanned by the operators $i\ell^{\mathrm{Z}}_{d/2}$ (for d even), $i\ell^{\mathrm{Z}}_0$, $i\ell^{\mathrm{Z}}_k$, $i\ell^{\mathrm{X}}_k$, and $i\ell^{\mathrm{Y}}_k$. From the proof of Theorem 34 one can immediately deduce the corresponding system algebra:

Corollary 35. *Consider a fermionic system with d modes and the set of quadratic Hamiltonians which are translation-invariant and $\mathcal{R}$-symmetric. The corresponding system algebra $\mathfrak{q}^{\mathcal{R}}_d$ is isomorphic to $[\sum_{i=1}^{(d-1)/2} \mathfrak{su}(2)] + \mathfrak{u}(1)$ for odd d and to $[\sum_{i=1}^{(d-2)/2} \mathfrak{su}(2)] + \mathfrak{u}(1) + \mathfrak{u}(1)$ for even d.*

Given the system algebras $\mathfrak{q}_d$ and $\mathfrak{q}^{\mathcal{R}}_d$, we investigate the subalgebras generated by short-range Hamiltonians. It will be useful to introduce for $p \in \{1, \ldots, \lfloor (d-1)/2 \rfloor\}$ the Hamiltonians

$$h^{\mathbb{1}}_p := \frac{1}{2}\sum_{\ell=1}^{d} i(f^\dagger_\ell f_{\ell+p} - f^\dagger_{\ell+p} f_\ell) = \sum_{k=0}^{\lfloor (d-1)/2 \rfloor} \sin(\tfrac{2\pi k p}{d})\, \ell^{\mathbb{1}}_k, \tag{52a}$$

$$h^{\mathrm{X}}_p := \frac{1}{2}\sum_{\ell=1}^{d} i(f^\dagger_\ell f^\dagger_{\ell+p} - f_{\ell+p} f_\ell) = \sum_{k=0}^{\lfloor (d-1)/2 \rfloor} \sin(\tfrac{2\pi k p}{d})\, \ell^{\mathrm{X}}_k, \tag{52b}$$

$$h^{\mathrm{Y}}_p := \frac{1}{2}\sum_{\ell=1}^{d} (f^\dagger_\ell f^\dagger_{\ell+p} + f_{\ell+p} f_\ell) = \sum_{k=0}^{\lfloor (d-1)/2 \rfloor} \sin(\tfrac{2\pi k p}{d})\, \ell^{\mathrm{Y}}_k, \tag{52c}$$

$$h^{\mathrm{Z}}_p := \frac{1}{2}\sum_{\ell=1}^{d} (f^\dagger_\ell f_{\ell+p} + f^\dagger_{\ell+p} f_\ell) = \sum_{k=0}^{\lfloor d/2 \rfloor} \cos(\tfrac{2\pi k p}{d})\, \ell^{\mathrm{Z}}_k, \tag{52d}$$

as well as the additional ones ($h^{\mathrm{Z}}_{d/2}$ only for even d)

$$h^{\mathrm{Z}}_0 := \frac{1}{2}\sum_{\ell=1}^{d} (f^\dagger_\ell f_\ell + f^\dagger_\ell f_\ell - \mathbb{1}) = \sum_{k=0}^{\lfloor d/2 \rfloor} \ell^{\mathrm{Z}}_k, \tag{52e}$$

$$h^{\mathrm{Z}}_{d/2} := \frac{1}{2}\sum_{\ell=1}^{d} (f^\dagger_\ell f_{\ell+p} + f^\dagger_{\ell+p} f_\ell) = \sum_{k=0}^{d/2} (-1)^k\, \ell^{\mathrm{Z}}_k. \tag{52f}$$

In these definition we used cyclic indices, e.g. $f_{d+a} = f_a$. The operators $h^{\mathrm{Z}}_{d/2}$ (for d even), h^{Z}_0, h^{Z}_p, $h^{\mathbb{1}}_p$, h^{X}_p, and h^{Y}_p span $\mathfrak{q}_d$ linearly. Using the identities above, the commutation relations of the ℓ^{Q}_k operators, and some trigonometric identities, we obtain

$$[ih^{\mathbb{1}}_a, ih^{\mathrm{Z}}_b] = [ih^{\mathbb{1}}_a, ih^{\mathrm{X}}_b] = [ih^{\mathbb{1}}_a, ih^{\mathrm{Y}}_b] = 0, \tag{53a}$$

$$[ih^{\mathrm{X}}_a, ih^{\mathrm{Y}}_b] = -\tfrac{i}{2}(h^{\mathrm{Z}}_{(a+b) \bmod \lfloor d/2\rfloor} - h^{\mathrm{Z}}_{(a-b) \bmod \lfloor d/2\rfloor}), \tag{53b}$$

$$[ih^{\mathrm{Y}}_a, ih^{\mathrm{Z}}_b] = -\tfrac{i}{2}(\mathrm{sgn}(d-a-b)\, h^{\mathrm{X}}_{(a+b) \bmod \lfloor d/2\rfloor} - \mathrm{sgn}(a-b)\, h^{\mathrm{X}}_{(a-b) \bmod \lfloor d/2\rfloor}), \tag{53c}$$

$$[ih^{\mathrm{Z}}_a, ih^{\mathrm{X}}_b] = -\tfrac{i}{2}(\mathrm{sgn}(d-a-b)\, h^{\mathrm{Y}}_{(a+b) \bmod \lfloor d/2\rfloor} - \mathrm{sgn}(a-b)\, h^{\mathrm{Y}}_{(a-b) \bmod \lfloor d/2\rfloor}) \tag{53d}$$

for $a, b \in \{0, \ldots, \lfloor d/2\rfloor\}$. In [16] it was shown that already the nearest-neighbor Hamiltonians of $\mathfrak{q}^{\mathcal{R}}_d$ generate the whole $\mathfrak{q}^{\mathcal{R}}_d$. Now we are in the position to provide a more systematic proof of their result:

Lemma 36. *The system algebra $\mathfrak{q}^{\mathcal{R}}_d$ can be generated using the one-site-local operator ih^{Z}_0 and a nearest-neighbor element $i(\alpha_1 h^{\mathrm{Z}}_1 + \alpha_2 h^{\mathrm{X}}_1 + \alpha_3 h^{\mathrm{Y}}_1)$ with $\alpha_i \in \mathbb{R}$ assuming that $\alpha_2 \neq 0$ or $\alpha_3 \neq 0$ for odd d and additionally requiring $\alpha_1 \neq 0$ for even d.*

Proof. (1) From Eq. (53) we know that ih^{Z}_0, ih^{Z}_1, ih^{X}_1, and ih^{Y}_1 would generate the whole $\mathfrak{q}^{\mathcal{R}}_d$. (2) Suppose that $\alpha_1 \neq 0$ and $\alpha_2^2 + \alpha_3^2 \neq 0$. From $2[ih^{\mathrm{Z}}_0, i(\alpha_1 h^{\mathrm{Z}}_1 + \alpha_2 h^{\mathrm{X}}_1 + \alpha_3 h^{\mathrm{Y}}_1)] = \alpha_2 ih^{\mathrm{Y}}_1 - \alpha_3 ih^{\mathrm{X}}_1$ and $2[ih^{\mathrm{Z}}_0, \alpha_2 ih^{\mathrm{Y}}_1 - \alpha_3 ih^{\mathrm{X}}_1] = -\alpha_2 ih^{\mathrm{X}}_1 - \alpha_3 ih^{\mathrm{Y}}_1$ it follows that one can generate ih^{Z}_0, ih^{Z}_1, ih^{X}_1, and ih^{Y}_1. Hence according to observation (1), the whole $\mathfrak{q}^{\mathcal{R}}_d$ is generated. (3) Suppose now that $\alpha_1 = 0$, d is odd, and $\alpha_2^2 + \alpha_3^2 \neq 0$. From $2[ih^{\mathrm{Z}}_0, i(\alpha_2 h^{\mathrm{X}}_1 + \alpha_3 h^{\mathrm{Y}}_1)] = \alpha_2 ih^{\mathrm{Y}}_1 - \alpha_3 ih^{\mathrm{X}}_1$ one can generate ih^{Z}_0, ih^{X}_1, and ih^{Y}_1. From Eq. (53) it follows that these generators in turn generate all $ih^{\mathrm{Z}}_{2p \bmod d}$. Since d is odd, ih^{Z}_1 is also generated. Hence we obtain ih^{Z}_0, ih^{Z}_1, ih^{X}_1, and ih^{Y}_1, and according to (1), the algebra $\mathfrak{q}^{\mathcal{R}}_d$ is generated. □

For the more general $\mathfrak{q}_d$, we obtain a slightly larger system algebra when we do *not* assume $\mathcal{R}$-symmetry:

Proposition 37. *The elements of $\mathfrak{q}_d$ with interaction length less than M (where $2 \leq M \leq \lceil d/2\rceil$ and $d \geq 3$) generate a system algebra which is isomorphic to $[\sum_{i=1}^{(d-1)/2} \mathfrak{su}(2)] + \sum_{i=1}^{M} \mathfrak{u}(1)$ for odd d and to $[\sum_{i=1}^{(d-2)/2} \mathfrak{su}(2)] + \sum_{i=1}^{M+1} \mathfrak{u}(1)$ for even d.*

Proof. From Lemma 36 we know that the operators h^{Q}_a with $\mathrm{Q} \in \{\mathrm{X}, \mathrm{Y}, \mathrm{Z}\}$ already generate $\mathfrak{q}^{\mathcal{R}}_d$ which is isomorphic to $[\sum_{i=1}^{(d-1)/2} \mathfrak{su}(2)] + \mathfrak{u}(1)$ for odd d and to $[\sum_{i=1}^{(d-2)/2} \mathfrak{su}(2)] + \mathfrak{u}(1) + \mathfrak{u}(1)$ for even d. We have $M-1$ additional operators $h^{\mathbb{1}}_q$ with $q \in \{1, \ldots, M-1\}$ which are linearly independent and commuting. These generate the other parts corresponding $\sum_{i=1}^{M-1} \mathfrak{u}(1)$. □

We illustrate Lemma 36 and Proposition 37 with a fermionic ring of $d = 6$ modes. Suppose that the drift Hamiltonian of this system is the nearest-neighbor hopping Hamiltonian $ih^{\mathrm{Z}}_1 = \frac{i}{2}\sum_{\ell=1}^{6}(f_\ell f^\dagger_{\ell+1} + f^\dagger_{\ell+1} f_\ell)$, and that one can additionally control the on-site potential $ih^{\mathrm{Z}}_0 = \frac{i}{2}\sum_{\ell=1}^{6}(f^\dagger_\ell f_\ell - \frac{1}{2}\mathbb{1})$, the pairing strength $ih^{\mathrm{Y}}_1 = \frac{i}{2}\sum_{\ell=1}^{6}(f^\dagger_\ell f^\dagger_{\ell+1} + f_{\ell+1} f_\ell)$, and the magnetic flux $ih^{\mathbb{1}}_1 = -\frac{1}{2}\sum_{\ell=1}^{6}(f^\dagger_\ell f_{\ell+1} - f^\dagger_{\ell+1} f_\ell)$ in the ring. Lemma 36 implies that the first three Hamiltonians generate the Lie algebra $\mathfrak{q}^{\mathcal{R}}_6$ of all Hamiltonians which are simultaneously $\mathcal{R}$-invariant, translation-invariant, and quadratic. The magnetic flux term $ih^{\mathbb{1}}_1$ commutes with all elements of $\mathfrak{q}^{\mathcal{R}}_6$ and contributes only an additional $\mathfrak{u}(1)$ to the system algebra. Thus, the system algebra generated by all nearest-neighbor quadratic Hamiltoinans that are translation-invariant is given by $\mathfrak{q}^{\mathcal{R}}_6 + \mathfrak{u}(1) \cong \mathfrak{su}(2) + \mathfrak{su}(2) + \mathfrak{u}(1) + \mathfrak{u}(1) + \mathfrak{u}(1)$. In order to achieve full controllability for a translation-invariant and quasifree fermionic system (which corresponds to the Lie algebra $\mathfrak{q}_6 \cong \mathfrak{su}(2) + \mathfrak{su}(2) + \mathfrak{u}(1) + \mathfrak{u}(1) + \mathfrak{u}(1) + \mathfrak{u}(1)$), one has to add a next-nearest neighbor Hamiltonian as $ih^{\mathbb{1}}_2 = -\frac{1}{2}\sum_{\ell=1}^{6}(f^\dagger_\ell f_{\ell+2} - f^\dagger_{\ell+2} f_\ell)$.

B. Orbits of Pure Translation-Invariant Quasifree States

We characterize now the orbits of pure translation-invariant quasifree states under the action of translation-invariant quadratic Hamiltonians. Since the operators $\ell^{\mathbb{1}}_k = i(\tilde{f}^\dagger_k \tilde{f}_k - \tilde{f}^\dagger_{d-k} \tilde{f}_{d-k})$ commute with all the other translation-invariant quadratic Hamiltonians (as discussed in Sec. VIII A), their expectation values stay invariant under the considered time evolutions. At the end of the section, we show that these invariant expectation values even form a separating set of invariants for the orbits of pure translation-invariant quasifree states.

Let us recall that a quasifree state is fully characterized by its Majorana covariance matrix, defined in Eq. (27). The translation unitary $\mathcal{U}$ acts on the Majorana operators by conjugation as $\mathcal{U}\, m_p \mathcal{U}^\dagger = m_{(p+2 \bmod 2d)}$. It follows that a quasifree state ρ is translation-invariant (i.e. $[\rho, \mathcal{U}] = 0$) iff its covariance matrix G_{pq} is doubly-cyclic, i.e. $G_{pq} = G_{(p+2 \bmod 2d),(q+2 \bmod 2d)}$. The double-cyclicity of G implies that it can be expressed as a block-Fourier transform of a block-diagonal matrix, i.e.

$$\tilde{G} = U_F\, G\, U_F^\dagger\,, \tag{54}$$

where $U_F := \left(\begin{smallmatrix}1 & 0\\ 0 & 1\end{smallmatrix}\right) \otimes W$ with $W_{pq} := \exp(2\pi i/d)^{q-p}$ and $\tilde{G} = \oplus_{k=0}^{d-1} i\tilde{g}(k)$ with $\tilde{g}(k)$ being 2×2-matrices. The matrices $\tilde{g}(k)$ can be calculated by the inverse block-Fourier transform

$$\tilde{g}(k) = -i \sum_{\ell=1}^{d} e^{2\pi k \ell i/d} \begin{pmatrix} G_{1,2\ell-1} & G_{1,2\ell} \\ G_{2,2\ell-1} & G_{2,2\ell} \end{pmatrix}. \tag{55}$$

The fact that G is skew-symmetric and real implies

$$\tilde{g}(d-k) = -\tilde{g}^T(k). \tag{56}$$

Moreover, due to Eq. (54) the set of eigenvalues of all the matrices $\tilde{g}(k)$ equals the one of $-iG$ (including multiplicities). Combining these observations with Proposition 17 and Proposition 19, we obtain the following characterization of pure translation-invariant quasifree states:

Lemma 38. *A set of 2×2 matrices $\tilde{g}(k)$ (with $k \in \{0,\ldots,d-1\}$) defines a covariance matrix of a pure quasifree state through Eq. (54) iff they satisfy Eq. (56) and their eigenvalues are in the set $\{1,-1\}$.*

The entries of $\tilde{g}(k)$ and the expectation values of the ℓ_k operators defined in Eq. (47) can be related by

$$i\tilde{g}(k) = \mathbb{1}_2\langle \ell_k^{\mathbb{1}}\rangle + \mathrm{X}\langle \ell_k^{\mathrm{X}}\rangle + \mathrm{Y}\langle \ell_k^{\mathrm{Y}}\rangle + \mathrm{Z}\langle \ell_k^{\mathrm{Z}}\rangle \tag{57}$$

using Eq. (55) and the definitions for $\ell_k^{\mathbb{1}}$, ℓ_k^{X}, ℓ_k^{Y}, and ℓ_k^{Z}. Now we can prove the main theorem of this subsection:

Theorem 39. *Two pure quasifree states ρ_1 and ρ_2 can be connected through the action of a translation-invariant quadratic Hamiltonian if and only if $\mathrm{tr}(\rho_1\ell_k^{\mathbb{1}}) = \mathrm{tr}(\rho_2\ell_k^{\mathbb{1}})$ holds for all $\ell_k^{\mathbb{1}}$ with $k \in \{0,\ldots,\lfloor (d-1)/2\rfloor\}$.*

Proof. First, we consider the 'if'-case: Let H be a translation-invariant quadratic Hamiltonians for which $\rho_1 = e^{-iHt}\rho_2 e^{iHt}$ holds. Since the operators $\ell_k^{\mathbb{1}}$ commute with any translation-invariant Hamiltonian, we have that $\mathrm{tr}(\rho_1\ell_k^{\mathbb{1}}) = \mathrm{tr}(e^{-iHt}\rho_2 e^{iHt}\ell_k^{\mathbb{1}}) = \mathrm{tr}(\rho_2 e^{iHt}\ell_k^{\mathbb{1}} e^{-iHt}) = \mathrm{tr}(\rho_2\ell_k^{\mathbb{1}})$. Second, we treat the 'only if'-case: Let $\tilde{g}_1(k)$ and $\tilde{g}_2(k)$ denote the Fourier-transformed Majorana two-point functions (defined as in Eq. (55)) of ρ_1 and ρ_2, respectively. The action of a translation-invariant Hamiltonian, $\rho_a \mapsto e^{-iH}\rho_a e^{iH}$ is represented by the map

$$\tilde{g}_a(k) \mapsto U(k)\,\tilde{g}_a(k)\,U(k)^\dagger \tag{58}$$

where $U(k)$ is given by $\exp[-i\mathfrak{Re}(\tilde{A}_k)\mathrm{Z} - i\mathfrak{Re}(\tilde{B}_k)\mathrm{X}/2 - i\mathfrak{Im}(\tilde{B}_k)\mathrm{Y}/2]$. Using Eq. (57), we obtain $\mathrm{tr}(\rho_a\ell_k^{\mathbb{1}}) = i\,\mathrm{tr}[g_a(k)]$ for $a\in\{1,2\}$. These expectation values have to be in the set $\{-2,0,2\}$, since the eigenvalues of $\tilde{g}_1(k)$ and $\tilde{g}_2(k)$ are in the set $\{-1,1\}$. Then, it follows from $\mathrm{tr}(\rho_1\ell_k^{\mathbb{1}}) = \mathrm{tr}(\rho_2\ell_k^{\mathbb{1}})$ that the expectation values of $\tilde{g}_1(k)$ and $\tilde{g}_2(k)$ coincide. Thus, we obtain from Eq. (58) that ρ_1 and ρ_2 can be transformed into each other. ∎

Finally, we turn to the $\mathcal{R}$-symmetric setting, as introduced in Sec. VIII A, and determine the orbit structure of quasifree pure states which are translation-invariant and $\mathcal{R}$-symmetric under the action of operators in $\mathfrak{q}_d^{\mathcal{R}}$.

Proposition 40. *The unitaries generated by the Lie algebra $\mathfrak{q}_d^{\mathcal{R}}$ act transitively on the set of quasifree pure states which are translation-invariant and $\mathcal{R}$-symmetric.*

Proof. Since $\mathcal{R}\ell_k^{\mathbb{1}}\mathcal{R}^{-1} = -\ell_k^{\mathbb{1}}$, the expectation value of these operators in $\mathcal{R}$-symmetric states must vanish as $\mathrm{tr}(\rho\ell_k^{\mathbb{1}}) = -\mathrm{tr}(\rho\mathcal{R}\ell_k^{\mathbb{1}}\mathcal{R}^{-1}) = -\mathrm{tr}(\mathcal{R}^{-1}\rho\mathcal{R}\ell_k^{\mathbb{1}}) = -\mathrm{tr}(\rho\ell_k^{\mathbb{1}})$. Moreover, by Theorem 39 we know that two pure translation-invariant states are on the same $\mathfrak{q}_d$-orbit iff the expectation values of the $\ell_k^{\mathbb{1}}$ operators coincide for all $k\in\{0,\ldots,\lfloor (d-1)/2\rfloor\}$. Hence the translation-invariant $\mathcal{R}-$symmetric states lie on the same $\mathfrak{q}_d$-orbit. As Eq. (58) implies that the $\mathfrak{q}_d$-orbits are equivalent to $\mathfrak{q}_d^{\mathcal{R}}$-orbits, we have proved the proposition. ∎

C. An Application to Many-Body Physics

In many-body physics, one of the important characteristics of quantum criticality is the *closing of the gap*. This means that the energy difference between the ground state and the first excited state goes to zero in the thermodynamic limit, when the number of spins or fermionic modes goes to infinity. Quasifree fermionic models can display both gapped and gapless behavior. Using the techniques developed in the previous subsections, we will prove that the gap always disappears (i.e. closes) for translation-invariant quasifree models if the coefficient matrix A of Eq. (21) is purely imaginary while B is an arbitrary, complex skew-symmetric matrix.

To formalize this statement, let us consider a set a_r of fixed (finite) real numbers with $r\in\{1,\ldots,M-1\}$ and a set b_r of fixed complex numbers (of finite modulus) with $r\in\{1,\ldots,M-1\}$. With these stipulations, we define for any $d\geq 2M$ the cyclic $d\times d$ matrices A_d and B_d (or A and B for short) by specifying their entries

$$A_{pq} := \begin{cases} ia_{q-p} & \text{if } q-p\in\{1,\ldots,M-1\},\\ -ia_{p-q} & \text{if } p-q\in\{1,\ldots,M-1\},\\ 0 & \text{otherwise,}\end{cases} \tag{59}$$

and

$$B_{pq} := \begin{cases} b_{q-p} & \text{if } q-p\in\{1,\ldots,M-1\},\\ -b_{p-q} & \text{if } p-q\in\{1,\ldots,M-1\},\\ 0 & \text{otherwise.}\end{cases} \tag{60}$$

By applying these definitions to Eq. (21) we obtain:

Theorem 41. *Given the positive integers d and M with $d\geq 2M$, consider the corresponding translation-invariant quasifree Hamiltonian*

$$H_d = \sum_{p,q=1}^{d} A_{pq}(f_p^\dagger f_q - \delta_{pq}\tfrac{\mathbb{1}}{2}) + \tfrac{1}{2}B_{pq}f_p^\dagger f_q^\dagger - \tfrac{1}{2}B_{pq}^* f_p f_q,$$

where A and B are defined in Eqs. (59) and (60). Assume that H_d has a unique ground state. Then the gap Δ_d of H_d is bounded by $\Delta_d \leq \frac{8\pi(M-1)}{d}\sum_{p=1}^{M-1}(|a_p|+|b_p|)$, i.e. the gap closes algebraically in the thermodynamic limit of d going to infinity.

Proof. Since H_d is translation-invariant and its coefficient matrix is imaginary, it can be decomposed in terms of the operators ℓ_k^{Q} with $\mathrm{Q} \in \{\mathbb{1}, \mathrm{X}, \mathrm{Y}\}$ and $k \in \{1, \ldots, \lfloor (d-1)/2 \rfloor\}$ as

$$H_d = \sum_{k=1}^{\lfloor (d-1)/2 \rfloor} \tilde{a}_k \ell_k^{\mathbb{1}} + \tfrac{1}{2} \tilde{b}_k^X \ell_k^{\mathrm{X}} + \tfrac{1}{2} \tilde{b}_k^Y \ell_k^{\mathrm{Y}},$$

using the definitions $\tilde{a}_k := -\sum_{p=1}^{M-1} a_p \sin(-2\pi pk/d)$, $\tilde{b}_k^X := -\mathfrak{Re}[\sum_{p=1}^{M-1} b_p \sin(-2\pi pk/d)]$, as well as $\tilde{b}_k^Y := -\mathfrak{Im}[\sum_{p=1}^{M-1} b_p \sin(-2\pi pk/d)]$. Let ρ_d be a pure quasifree state, and let $\tilde{g}_d(k)$ denote its Fourier-transformed Majorana two-point functions (see Eq. (55)). From Eq. (49) we know that ρ_d is an eigenstate of H_d iff $[\tilde{b}_k^X \mathrm{X} + \tilde{b}_k^Y \mathrm{Y}, \tilde{g}_d(k)] = 0$. The eigenvalue of H_d corresponding to this state is given by

$$\mathrm{tr}(\rho_d H_d) = \sum_{k=1}^{\lfloor (d-1)/2 \rfloor} \mathrm{tr}[i g_d(k)(\tilde{a}_k \mathbb{1}_2 + \tfrac{1}{2}\tilde{b}_k^X \mathrm{X} + \tfrac{1}{2}\tilde{b}_k^Y \mathrm{Y})]. \tag{61}$$

Let us emphasize that the proof builds on the fact that M is fixed and finite, while d goes to infinity in the thermodynamic limit. Among the eigenstates of H_d, consider the (unique) ground state ρ_{gs}^d, whose Fourier-transformed Majorana two-point functions (see Eq. (55)) will be denoted by $\tilde{g}_{gs}^d(k)$. From this ground state let us construct another quasifree state ρ_e^d which is defined through its Majorana two-point functions

$$\tilde{g}_e^d(1) := \begin{cases} \mathbb{1}_2 & \text{if } \tilde{g}_{gs}^d(1) \neq -\mathbb{1}_2, \\ -\mathbb{1}_2 & \text{otherwise,} \end{cases}$$

while for general $k \neq 1$ we assign $\tilde{g}_e^d(k) := \tilde{g}_{gs}^d(k)$.

The corresponding pure quasifree state ρ_e^d is an eigenstate of H_d, since according to Eq. (58) its Fourier-transformed Majorana two-point function stays invariant during the time-evolution generated by H_d. Using Eq. (61), we can calculate the difference between the energies corresponding to ρ_{gs}^d and ρ_e^d as

$$\begin{aligned}
\Delta_d &:= \mathrm{tr}[(\rho_e^d - \rho_{gs}^d) H_d] \\
&= \sum_{k=1}^{\lfloor (d-1)/2 \rfloor} \mathrm{tr}\left([\tilde{g}_e^d(k) - \tilde{g}_{gs}^d(k)](\tilde{a}_k \mathbb{1}_2 + \tfrac{1}{2}\tilde{b}_k^X \mathrm{X} + \tfrac{1}{2}\tilde{b}_k^Y \mathrm{Y})\right) \\
&= \mathrm{tr}\left([\tilde{g}_e^d(1) - \tilde{g}_{gs}^d(1)](\tilde{a}_1 \mathbb{1}_2 + \tfrac{1}{2}\tilde{b}_1^X \mathrm{X} + \tfrac{1}{2}\tilde{b}_1^Y \mathrm{Y})\right) \\
&\leq 2 \| [\tilde{g}_e^d(1) - \tilde{g}_{gs}^d(1)](\tilde{a}_1 \mathbb{1}_2 + \tfrac{1}{2}\tilde{b}_1^X \mathrm{X} + \tfrac{1}{2}\tilde{b}_1^Y \mathrm{Y}) \| \\
&\leq 4(|\tilde{a}_1| + \tfrac{1}{2}|\tilde{b}_1^X| + \tfrac{1}{2}|\tilde{b}_1^Y|) \\
&\leq 4 \left| \sum_{p=1}^{M-1} a_p \sin(2\pi p/d) \right| + 4 \left| \sum_{p=1}^{M-1} b_p \sin(2\pi p/d) \right| \\
&\leq \frac{8\pi(M-1)}{d} \sum_{p=1}^{M-1} (|a_p| + |b_p|)
\end{aligned}$$

This completes the proof of the theorem. □

IX. PARTICLE-NUMBER CONSERVING SYSTEMS

Finally, we treat fermionic systems whose particle-number is conserved. The corresponding system algebras are given both in the general case as well as in the quasifree case. Furthermore, a necessary and sufficient condition for quasifree pure-state controllability in this setting is provided.

A. The System Algebra of Particle-Number Conserving Hamiltonians

Let P_n denote the orthogonal projection from the Fock space $\mathcal{F}(\mathbb{C}^d) = \oplus_{n=0}^d \wedge^n \mathbb{C}^d$ onto the n-particle subspace $\wedge^n \mathbb{C}^d \subset \mathcal{F}(\mathbb{C}^d)$ of dimension $\binom{d}{n}$. The *particle-number operator* $\hat{n}$ of a fermionic system is defined as $\hat{n} := \sum_{n=0}^d n P_n$. Note that $\sum_{p=1}^d f_p^\dagger f_p \psi_n = n\psi_n$ holds for any $\psi_n \in \wedge^n \mathbb{C}^d$. Hence, the particle number operator can also be expressed as

$$\hat{n} = \sum_{p=1}^d f_p^\dagger f_p \, .$$

A fermionic Hamiltonian H is called particle-number conserving if it commutes with $\hat{n}$. Using the general Theorem 51 of Appendix A, one directly obtains the corresponding system algebra.

Proposition 42. *The system algebra of particle-number conserving fermionic interactions with d modes is*

$$\mathfrak{s}\left(\bigoplus_{n \text{ even}} \mathfrak{u}\left[\tbinom{d}{n}\right] \right) \oplus \mathfrak{s}\left(\bigoplus_{n \text{ odd}} \mathfrak{u}\left[\tbinom{d}{n}\right] \right).$$

B. Quadratic Hamiltonians

A quadratic Hamiltonian H is particle-number conserving iff its coefficient matrix B of Eq. (21) is zero, i.e., iff $H = \sum_{p,q=1}^d A_{pq}(f_p^\dagger f_q - \delta_{pq} \frac{\mathbb{1}}{2})$ where A denotes any hermitian matrix. The corresponding system algebra is given by the following proposition:

Proposition 43. *The system algebra of the particle-number conserving quadratic d-mode Hamiltonians is isomorphic to $\mathfrak{u}(d)$.*

Proof. Let ι denote the $\mathbb{R}$-linear mapping from the d-mode Hamiltonians which are quadratic and particle-number conserving to the $d \times d$ skew-hermitian matrices. We define ι using $\iota(i(f_p^\dagger f_q + f_q^\dagger f_p - \frac{\mathbb{1}}{2})) = i(e_{pq} + e_{qp})$ and $\iota(f_p^\dagger f_q - f_q^\dagger f_p) = e_{pq} - e_{qp}$, where e_{pq} denotes a matrix with entries $[e_{pq}]_{uv} := \delta_{pu}\delta_{qv}$. Note that the canonical anticommutation relations imply that $[f_p^\dagger f_q, f_r^\dagger f_s] =$

$$\delta_{ps} f_q f_r^\dagger + \delta_{qr} f_p^\dagger f_s - \delta_{ps}\delta_{qr}\mathbb{1} - \delta_{ps}\delta_{qr}\delta_{pq}(f_q f_r^\dagger + f_p^\dagger f_s - \tfrac{\mathbb{1}}{2}).$$

Thus, ι is a homomorphism since

$$\begin{aligned}
&\iota([\kappa_\pm(f_p^\dagger f_q \pm f_q^\dagger f_p - \delta_{pq}\tfrac{\mathbb{1}}{2}), \kappa_\pm(f_r^\dagger f_s \pm f_r^\dagger f_s - \delta_{rs}\tfrac{\mathbb{1}}{2})]) \\
&= \kappa_\pm^2 \iota([\delta_{qr}(f_p^\dagger f_s \mp f_s^\dagger f_p) \pm \delta_{pr}(f_q^\dagger f_s \mp f_s^\dagger f_q), \\
&\qquad \delta_{ps}(f_q^\dagger f_r \mp f_r^\dagger f_q) \pm \delta_{qs}(f_p^\dagger f_r \mp f_r^\dagger f_p)]) \\
&= [\kappa_\pm(e_{pq} \pm e_{qp}), \kappa_\pm(e_{rs} \pm e_{sr})] \\
&= [\iota(\kappa_\pm(f_p^\dagger f_q \pm f_q^\dagger f_p - \delta_{pq}\tfrac{\mathbb{1}}{2})), \iota(\kappa_\pm(f_r^\dagger f_s \pm f_r^\dagger f_s - \delta_{rs}\tfrac{\mathbb{1}}{2}))],
\end{aligned}$$

where $\kappa_+ = i$ and $\kappa_- = 1$. The map ι is even an isomorphism as its kernel is trivial. The proposition follows as the Lie algebra $\mathfrak{u}(d)$ is isomorphic to the Lie algebra of $d \times d$ skew-hermitian matrices. □

Remark 44. Obviously, the ι map from the previous proof establishes an isomorphism $ih^{(k)} \mapsto i \sum_{p,q=1}^d A_{pq}^{(k)}(f_p^\dagger f_q - \delta_{pq}\frac{\mathbb{1}}{2})$ from $\langle ih^{(1)}, \ldots, ih^{(\ell)} \rangle_{\mathrm{Lie}}$ to $\langle iA^{(1)}, \ldots, iA^{(\ell)} \rangle_{\mathrm{Lie}}$ for any set $\{A^{(1)}, \ldots, A^{(\ell)}\}$ of $d \times d$ Hermitian matrices.

C. Quasifree Pure-State Controllability in the Particle-Number Conserving Setting

We presented in Section VI C a necessary and sufficient condition for quasifree pure-state controllability. Here, we provide an analogous result in the particle-number conserving setting using a Lie-theoretic result of Ref. [63].

A quasifree state ρ_F is called particle-number conserving if $[\rho_F, P_n] = 0$ holds for all $n \in \{0, \ldots, d\}$. As discussed in Section VI A, quasifree states are uniquely characterized by the expectation values of the $m_x m_y$ operators. We obtain in the number-conserving case that $\mathrm{tr}(\rho_F\, f_q f_p) = 0$ as the condition $[\rho_F, P_n] = 0$ implies $\sum_{n=0}^d P_n \rho_F P_n = \rho_F$ as well as $\mathrm{tr}(\rho_F f_p f_q) = \sum_{n=0}^d \mathrm{tr}(P_n \rho_F P_n f_p f_q) = \sum_{n=0}^d \mathrm{tr}(\rho_F P_n f_p f_q P_n) = 0$. Similarly, one can prove $\mathrm{tr}(\rho_F\, f_p^\dagger f_q^\dagger) = 0$. It follows that ρ_F is uniquely determined by the $d \times d$ Hermitian matrix $M_{p,q} = \mathrm{tr}(\rho_F\, f_p^\dagger f_q)$. In the literature, this matrix is usually called the *one-particle density matrix* of ρ_F [67]. Let us shortly summarize three well-known statements about one-particle density matrices of quasifree states (see [12, 57]):

Proposition 45. *Consider a particle-number conserving quasifree state ρ_F of a fermionic system, and let M denote its one-particle density matrix. The following statements hold: (a) The eigenvalues of M lie between* 0 *and* 1. *(b) ρ_F is pure iff M is a projection. (c) If ρ_F is pure, then $\mathrm{tr}(M) = n$ is an integer, and ρ_F is supported on the n-particle subspace $\wedge^n \mathbb{C}^d$ of the Fock space, i.e.*

$$P_k \rho_F P_k = \begin{cases} \rho_F & \text{if } k = n, \\ 0 & \text{if } k \neq n. \end{cases} \tag{62}$$

The dynamics of particle-number conserving quasifree fermions can also be represented using the one-particle density matrices (see [12, 57]):

Proposition 46. *Consider a particle-number conserving quasifree state ρ_a corresponding to the one-particle density matrix M_a. Assume that the quadratic Hamiltonian*

$$H = \sum_{p,q=1}^d A_{pq}(f_p^\dagger f_q - \delta_{pq}\tfrac{\mathbb{1}}{2}),$$

which is defined by the Hermitian matrix A, generates the time-evolution of ρ_a. The time-evolved state (at unit time), $\rho_b = e^{-iH}\rho_a e^{iH}$ is again a number-conserving quasifree state with a one-particle density matrix $M_b = U_A M_a U_A^\dagger$, where $U_A = e^{-iA} \in \mathrm{U}(d)$.

A particle-number conserving pure quasifree state ρ_F with $\mathrm{tr}(M) = n$ is sometimes called an *n-particle pure quasifree state*, since according to Proposition 45 its state is supported on the n-particle subspace $\wedge^n \mathbb{C}^d$. We will denote the set of such quasifree pure states by $\mathcal{QF}_n$. A system of number-conserving quadratic Hamiltonians $\mathcal{S} = \{ih_1, \ldots, ih_\ell\}$ is said to provide quasifree pure-state controllability for a fixed particle number n if there exists an $iH \in \langle \mathcal{S} \rangle_{\mathrm{Lie}}$ for any $\rho_a, \rho_b \in \mathcal{QF}_n$ such that $\rho_b = e^{-iH}\rho_a e^{iH}$. To find a necessary and sufficient conditions for this type of controllability, let us invoke a Theorem 4.1 of Ref. [63]:

Theorem 47. *Consider the Lie algebra s_Σ generated by the traceless $d \times d$ skew-Hermitian matrices $iB_1, \ldots, iB_\ell$ and let $\mathfrak{P}(d, n)$ denote the set of all projections acting on $\mathbb{C}^d$ whose rank n lies between* 1 *and* $d-1$. *The Lie group corresponding to s_Σ acts naturally via the adjoint action on $\mathfrak{P}(d, n)$. This action is transitive if and only if either (a) s_Σ is isomorphic to $\mathfrak{su}(d)$ or (b) d is even, $n \in \{1, d-1\}$, and s_Σ is isomorphic to $\mathfrak{sp}(d/2)$.*

The theorem implies the following necessary and sufficient condition:

Theorem 48. *Consider the set $\mathcal{S} = \{ih_1, \ldots, ih_\ell\}$ corresponding to number-conserving quadratic Hamiltonians of a fermionic system with $d \geq 2$ modes. The set $\mathcal{S}$ generates a particle-number conserving system giving rise to full quasifree pure-state controllability on the n-particle subspace with $1 \leq n \leq d-1$, iff either (a) d is odd and $\langle \mathcal{S} \rangle_{\mathrm{Lie}}$ is isomorphic to $\mathfrak{u}(d)$ or $\mathfrak{su}(d)$ or (b) d is even, $n \in \{1, d-1\}$ and $\langle \mathcal{S} \rangle_{\mathrm{Lie}}$ is isomorphic to $\mathfrak{u}(d)$, $\mathfrak{su}(d)$, $\mathfrak{u}(1) + \mathfrak{sp}(d/2)$, or $\mathfrak{sp}(d/2)$.*

Proof. We consider the set $\mathcal{A} = \{iA^{(1)}, iA^{(2)}, \ldots, iA^{(\ell)}\}$ of skew-Hermitian matrices which correspond to the generators in $\mathcal{S}$, i.e. $ih_k = i\sum_{p,q=1}^d A_{pq}^{(k)}(f_p^\dagger f_q - \delta_{pq}\mathbb{1}/2)$. We apply Remark 44 and obtain that $\langle \mathcal{S} \rangle_{\mathrm{Lie}}$ is isomorphic to $\langle \mathcal{A} \rangle_{\mathrm{Lie}}$. We combine this result with Propositions 45 and 46: There exists an $ih_{ab} \in \langle \mathcal{S} \rangle_{\mathrm{Lie}}$ for each pair $\rho_a, \rho_b \in \mathcal{QF}_n$ such that $e^{-ih_{ab}}\rho_a e^{ih_{ab}} = \rho_b$, iff there exists an $iA_{ab} \in \langle \mathcal{A} \rangle_{\mathrm{Lie}}$ for each pair $M_a, M_b \in \mathfrak{P}(d, n)$ such that $e^{-iA_{ab}} M_a e^{iA_{ab}} = M_b$. Thus we have to find necessary and sufficient conditions under which $\langle \mathcal{A} \rangle_{\mathrm{Lie}}$ generates a transitive action on $\mathfrak{P}(d, n)$

for a given d and n. For any skew-Hermitian iA and $M \in \mathfrak{P}(d,n)$, we have that $\exp(-iA)M\exp(iA) = \exp[-i(A-\mathrm{tr}(A)\mathbb{1}/d)]M\exp[i(A-\mathrm{tr}(A)\mathbb{1}/d)]$. Hence we can infer that $\langle\mathcal{A}\rangle_{\mathrm{Lie}}$ generates a transitive action iff the system algebra generated by the set $\mathcal{A}' := \{i(A^{(1)} - \mathrm{tr}(A^{(1)})\mathbb{1}/d), \ldots, i(A^{(\ell)} - \mathrm{tr}(A^{(\ell)})\mathbb{1}/d)\}$ also gives rise to a transitive action. Since $\mathcal{A}'$ contains only traceless skew-Hermitian operators, we know from Theorem 47 that it can act transitively on $\mathfrak{P}(d,n)$ if and only if either $\langle\mathcal{A}'\rangle_{\mathrm{Lie}}$ is isomorphic to $\mathfrak{su}(d)$, or d is even, $n \in \{1, d-1\}$, and $\langle\mathcal{A}'\rangle_{\mathrm{Lie}}$ is isomorphic to $\mathfrak{sp}(d/2)$.

On the other hand, if $\langle\mathcal{A}'\rangle_{\mathrm{Lie}} = \mathfrak{su}(d)$ or $\langle\mathcal{A}'\rangle_{\mathrm{Lie}} = \mathfrak{sp}(d/2)$ then $\langle\mathcal{A}'\rangle_{\mathrm{Lie}}$ is a simple irreducible Lie subalgebra of $\mathfrak{su}(d)$. It follows that $\langle\mathcal{A}\rangle_{\mathrm{Lie}}$ is either isomorphic to $\langle\mathcal{A}'\rangle_{\mathrm{Lie}}$ if $\mathrm{tr}(A^{(k)}) = 0$ for all $k \in \{1,\ldots,\ell\}$ or to $\mathfrak{u}(1) + \langle\mathcal{A}'\rangle_{\mathrm{Lie}}$ if there exists a k such that $\mathrm{tr}(A^{(k)}) \neq 0$. This proves the theorem. □

X. CONCLUSION

We have put dynamic systems theory of coherently controlled fermions into a Lie-algebraic frame in order to answer problems of controllability, reachability, and simulability in a unified picture. As summarized in Tab. IV, to this end we have determined the dynamic system Lie algebras in a comprehensive number of cases, illustrated by examples, with and without confinement to quadratic interactions (quasifree particles) as well as with and without symmetries such as translation invariance, twisted reflection symmetry, or particle-number conservation. Once having established the system algebras, the group orbits of a given (pure or mixed) initial quantum state determine the respective reachable sets of all states a system can be driven into by coherent control. In this respect, different types of pure-state reachability and its relation to coset spaces has been treated with particular attention.

There are illuminating analogies and differences between spin and fermionic systems. For quasifree systems, this was discussed in Sec. V and in Appendix C, while the translation-invariant case is addressed in Sec. VII. In particular, translation-invariant Hamiltonians which cannot be generated from nearest-neighbor ones appear both for spin systems (Sec. VII B) and for fermionic systems (Sec. VII D). Moreover, for fermionic systems some of these Hamiltonians have bounded interaction length. It is an open question if the same also holds for spin systems.

On a general scale, the system algebras determined serve as a dynamic fingerprint. Their application to quantum simulation has been elucidated in a plethora of paradigmatic settings. Hence we anticipate the comprehensive findings presented here will find a broad scope of use.

TABLE IV. System algebras for d-mode fermionic systems

Symmetries[a]	System algebra	Details
general systems:	$\mathfrak{su}(2^{d-1}) \oplus \mathfrak{su}(2^{d-1})$	Thm. 4
{T}	$\mathfrak{s}[\oplus_{\ell=0}^{d-1}\mathfrak{u}(\hat{r}_\ell)] \oplus \mathfrak{s}[\oplus_{\ell=0}^{d-1}\mathfrak{u}(\hat{r}_\ell)]$	Thm. 30
{N}	$\mathfrak{s}\left(\oplus_{n\text{ even}}\mathfrak{u}[\binom{d}{n}]\right) \oplus \mathfrak{s}\left(\oplus_{n\text{ odd}}\mathfrak{u}[\binom{d}{n}]\right)$	Prop. 42
quasifree systems:	$\mathfrak{so}(2d)$[b]	Prop. 9
{T}, d odd	$[\sum_{i=1}^{(d-1)/2}\mathfrak{u}(2)] + \mathfrak{u}(1)$	Thm. 34
{T}, d even	$[\sum_{i=1}^{(d-2)/2}\mathfrak{u}(2)] + \mathfrak{u}(1) + \mathfrak{u}(1)$	Thm. 34
{T, R}, d odd	$[\sum_{i=1}^{(d-1)/2}\mathfrak{su}(2)] + \mathfrak{u}(1)$	Cor. 35
{T, R}, d even	$[\sum_{i=1}^{(d-2)/2}\mathfrak{su}(2)] + \mathfrak{u}(1) + \mathfrak{u}(1)$	Cor. 35
{N}	$\mathfrak{u}(d)$	Prop. 43

[a] besides parity superselection rule P: T = translation-invariance, R = twisted reflection symmetry, N = particle-no. conservation

[b] the orthogonal algebra is represented as direct sum of two equal copies given as irreducible blocks of dimension 2^{d-1}; the system algebra $\mathfrak{so}(2d)$ itself was determined already, e.g., in Ref. [36].

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Appendix A: Discussion of Double Centralizers

Motivated by Sec. IV B, in this appendix we discuss how the form of the double centralizer of a Lie algebra $\mathfrak{g} \subset \mathfrak{su}(k)$ limits the possibilities for $\mathfrak{g}$:

Proposition 49. *Let $\mathfrak{g}$ denote a subalgebra of $\mathfrak{su}(k)$. There exists a set $A \subset \mathfrak{su}(k)$ such that $\mathfrak{g} = \mathfrak{cent}_{\mathfrak{su}(k)}(A)$, if and only if $\mathfrak{cent}_{\mathfrak{su}(k)}(\mathfrak{cent}_{\mathfrak{su}(k)}(\mathfrak{g})) = \mathfrak{g}$.*

Proof. First, let us assume the existence of the set A. As $\mathfrak{cent}_{\mathfrak{su}(k)}(\mathfrak{cent}_{\mathfrak{su}(k)}(\mathfrak{cent}_{\mathfrak{su}(k)}(A))) = \mathfrak{cent}_{\mathfrak{su}(k)}(A)$ holds for any set A, which can also be inferred from [68, Proposition 6.1.3.1(iii)], we obtain $\mathfrak{cent}_{\mathfrak{su}(k)}(\mathfrak{cent}_{\mathfrak{su}(k)}(\mathfrak{g})) = \mathfrak{g}$. Second, we assume that $\mathfrak{cent}_{\mathfrak{su}(k)}(\mathfrak{cent}_{\mathfrak{su}(k)}(\mathfrak{g})) = \mathfrak{g}$ holds. We choose $A := \mathfrak{cent}_{\mathfrak{su}(k)}(\mathfrak{g})$ and verify its existence. □

To further analyze the influence of symmetry properties on the system algebra, we recall some elementary representation theory (see, e.g., Theorem 1.5 of [69]):

Proposition 50. *Consider a completely reducible complex matrix representation $\Phi(g)$ of a group G, where k is* *the degree of* Φ. *Let* $\mathfrak{comm}(\Phi) = \Phi'$ *denote the commutant algebra of all complex* $k \times k$*-matrices simultaneously commuting with* $\Phi(g)$ *for* $g \in G$. *Then,* $\Phi(g)$ *is equivalent to*

$$\bigoplus_{j=1}^{w} \left[\mathbb{1}_{e_j} \otimes \phi_j(g)\right],$$

where ϕ_j *denote for* $j \in \{1, \ldots, w\}$ *distinct inequivalent irreducible complex matrix representations of* G *with degree* k_j, *occurring with multiplicity* e_j *in* Φ. *In particular,*
(a) $\dim \mathfrak{comm}(\Phi) = \sum_{j=1}^{w} e_j^2$,
(b) $\dim \mathfrak{center}(\mathfrak{comm}(\Phi)) = w$,
(c) $k = \sum_{j=1}^{w} k_j e_j$.

Obviously, the same is true for representations of a compact Lie group or its Lie algebra. Given a subalgebra $\mathfrak{g}$ of $\mathfrak{su}(k)$ (or respectively of $\mathfrak{u}(k)$) and a representation Φ of $\mathfrak{g}$ with degree k, we discuss the easiest case of Proposition 50 where $w = 1$ and $e_1 = 1$. Hence, Φ is irreducible and $\mathfrak{g}$ is an irreducible subalgebra of $\mathfrak{su}(k)$ (or respectively of $\mathfrak{u}(k)$). But $\mathfrak{g}$ is not necessarily equal to $\mathfrak{su}(k)$ (or respectively to $\mathfrak{u}(k)$). Irreducible simple subalgebras of $\mathfrak{su}(k)$ were studied extensively in this regard in Ref. [19]. Note that the irreducible subalgebras of $\mathfrak{u}(k)$ are of the form $\mathfrak{g}$ or $\mathfrak{g}+\mathfrak{u}(1)$ where $\mathfrak{g}$ denotes any irreducible subalgebra of $\mathfrak{su}(k)$ (cf. pp. 27–28 and p. 321 of [49]). — A slight generalization is given by the case of an abelian commutant algebra, i.e. $\dim \mathfrak{comm}(\Phi) = \dim \mathfrak{center}(\mathfrak{comm}(\Phi))$ and $e_j = 1$ for all $j \in \{1, \ldots, w\}$. One may thus apply the spectral theorem (see, e.g., [70–72]) simultaneously to all the elements of the commutant algebra:

Theorem 51. *Consider a Lie algebra* $\mathfrak{g} \subseteq \mathfrak{su}(k)$ *and its representation* Φ *of degree* k. *Assume that the corresponding commutant algebra* $\mathcal{C} = \mathfrak{comm}(\Phi)$ *is abelian. One obtains that* $\mathfrak{g}$ *is a subalgebra of* $\mathfrak{s}[\oplus_{j=1}^{\dim \mathcal{C}} \mathfrak{u}(k_j)]$ *and it is equivalent to* $\mathfrak{s}[\oplus_{j=1}^{\dim \mathcal{C}} \mathfrak{g}_j]$, *where* $k = \sum_{j=1}^{\dim \mathcal{C}} k_j$ *and* $\mathfrak{g}_j$ *are irreducible subalgebras of* $\mathfrak{u}(k_j)$. *Furthermore, one finds* $k_j = \dim(P_j)$, *where* P_j *are the orthogonal projection operators given by the joint spectral decomposition of* $\mathcal{C}$ *with* $\sum_{j=1}^{\dim \mathcal{C}} P_j = \mathbb{1}_k$ *and* $P_i P_j = 0$ *for* $i \neq j$. *If* $\mathfrak{g}$ *is the maximal Lie algebra with these properties, then* $\mathfrak{g} = \mathfrak{s}[\oplus_{j=1}^{\dim \mathcal{C}} \mathfrak{u}(k_j)]$.

Using Proposition 50 one can directly characterize a maximal Lie algebra $\mathfrak{g}$ contained in $\mathfrak{su}(k)$ which is defined by all its symmetries including cases where the commutant to $\mathfrak{g}$ is not necessarily abelian. Observe the notation of Remark 5 and the one of Proposition 50.

Theorem 52. *Consider a Lie algebra* $\mathfrak{g} \subseteq \mathfrak{su}(k)$ *and its representation* Φ *of degree* k. *Let* $\mathcal{C} = \mathfrak{comm}(\Phi)$ *denote the commutant of* $\mathfrak{g}$. *If* $\mathfrak{g}$ *is the maximal Lie algebra with these properties, then* $\mathfrak{g} = \mathfrak{s}[\sum_{j=1}^{\omega} \mathfrak{u}(k_j)]$ *where* $\omega = \dim[\mathfrak{center}(\mathcal{C})]$ *and* $\sum_{j=1}^{\omega} k_j \leq k$.

Proof. Using Proposition 50 (and its notation) one obtains that $\mathfrak{g}$ is equivalent to $\oplus_{j=1}^{w} \left[\mathbb{1}_{e_j} \otimes \phi_j(g)\right]$. Therefore, $\mathfrak{g}$ is a subalgebra of $\mathfrak{s}[\sum_{j=1}^{\omega} \mathfrak{u}(k_j)]$ with $\sum_{j=1}^{\omega} k_j \leq k$. The maximality of $\mathfrak{g}$ completes the proof.

In a dual approach, one could start from a set S of symmetries of $\mathfrak{g}$. Due to the maximality of $\mathfrak{g}$, the set S has to comprise *all symmetries of* $\mathfrak{g}$. Next, one can apply Proposition 50 to the subalgebra of $\mathfrak{su}(k)$ generated by the linear span intersected with $\mathfrak{su}(k)$, i.e. $\langle S \rangle \cap \mathfrak{su}(k)$. The theorem then follows directly using Schur's lemma and the maximality of $\mathfrak{g}$. $\square$

The reader familiar with the double-commutant theorem in algebraic quantum mechanics will wonder about the different power of symmetries for characterizing algebras of observables on the one hand and Lie algebras on the other: a von-Neumann algebra $\mathcal{A}$ is entirely determined by its commutant $\mathcal{A}'$, since $\mathcal{A}'' = \mathcal{A}$ [73, 74]. In this sense, there is a duality between the algebra $\mathcal{A}$ and its commutant $\mathcal{A}'$ encapsulating all *symmetries*. On the other hand, consider the illustrative case of an irreducible Lie subalgebra $\mathfrak{g}$ of $\mathfrak{su}(k)$ [75], where the centralizer $\mathfrak{cent}_{\mathfrak{su}(k)}(\mathfrak{g})$ is trivial, i.e. zero. This centralizer is shared with *all* irreducible Lie subalgebras of $\mathfrak{su}(k)$. So in turn, the double centralizer in $\mathfrak{su}(k)$ to all these subalgebras is $\mathfrak{su}(k)$ itself. We thus obtain the following corollary to Proposition 49 and Theorem 51, where the double centralizer gives a maximality criterion ensuring that an irreducible subalgebra $\mathfrak{g}$ of $\mathfrak{su}(k)$ is in fact fulfilling $\mathfrak{g} = \mathfrak{su}(k)$ [76]:

Corollary 8. *Let* $\mathfrak{g}$ *denote an irreducible subalgebra of* $\mathfrak{su}(k)$, *i.e.* $\mathfrak{cent}_{\mathfrak{su}(k)}(\mathfrak{g}) = \{0\}$. *Then one finds that* $\mathfrak{cent}_{\mathfrak{su}(k)}(\mathfrak{cent}_{\mathfrak{su}(k)}(\mathfrak{g})) = \mathfrak{g}$ *if and only if* $\mathfrak{g} = \mathfrak{su}(k)$

Note that Corollary 8 can be readily generalized: Let $\mathfrak{g}, \mathfrak{h}$ denote two irreducible subalgebras of $\mathfrak{su}(k)$ with $\mathfrak{g} \subseteq \mathfrak{h} \subseteq \mathfrak{su}(k)$ so that $\mathfrak{cent}_{\mathfrak{h}}(\mathfrak{g}) = \{0\} = \mathfrak{cent}_{\mathfrak{h}}(\mathfrak{h})$. Then one finds $\mathfrak{cent}_{\mathfrak{h}}(\mathfrak{cent}_{\mathfrak{h}}(\mathfrak{g})) = \mathfrak{g}$ if and only if $\mathfrak{g} = \mathfrak{h}$.

Summarizing the general case, the symmetry properties of a Lie algebra $\mathfrak{g} \subseteq \mathfrak{su}(k)$, as given by its commutant w.r.t. a representation of $\mathfrak{g}$, do *not* determine the Lie algebra $\mathfrak{g}$ uniquely. Yet the commutant allows us to infer a *unique maximal Lie algebra* contained in $\mathfrak{su}(k)$, which is (up to an identity matrix) equal to the double commutant of $\mathfrak{g}$, but in general not to $\mathfrak{g}$ itself. Although all representations of compact Lie algebras, such as $\mathfrak{su}(k)$ and its semisimple subalgebras, are completely reducible, the situation for Lie algebras also differs from the case of *associative algebras*: here complete reducibility of a representation implies the double-commutant theorem (see Theorem (3.5.D) of [77] or Theorem 4.1.13 of [78]), whereas the double-commutant theorem does not apply to Lie algebras as discussed above.

Appendix B: Parameterizations of Quadratic Hamiltonians

In this appendix, we discuss various parameterizations of quadratic Hamiltonians related to the one of Eq. (21)

in Sec. V. We start with the parametrization

$$H := \sum_{p,q=1}^{d} C_{pq} f_p f_q + D_{pq} f_p f_q^\dagger + E_{pq} f_p^\dagger f_q + F_{pq} f_p^\dagger f_q^\dagger$$

by complex $d \times d$-matrices C, D, E, and F. Hermiticity of H requires $C = F^\dagger$, $D = D^\dagger$, and $E = E^\dagger$, while the (anti-)commutator relations enforce $C = -C^t$, $D = -E^t$, and $F = -F^t$. Setting $A := 2E$ and $B := -2C^*$, we recover the notation of Eq. (21) and obtain

$$\begin{aligned} H &= \frac{1}{2} \sum_{p,q=1}^{d} -B_{pq}^* f_p f_q - A_{pq}^* f_p f_q^\dagger + A_{pq} f_p^\dagger f_q + B_{pq} f_p^\dagger f_q^\dagger \\ &= \frac{1}{2} \sum_{p,q=1}^{d} -B_{pq}^* f_p f_q + 2A_{pq}(f_p^\dagger f_q - \delta_{pq} \tfrac{\mathbb{1}}{2}) + B_{pq} f_p^\dagger f_q^\dagger \\ &= \frac{1}{2} \sum_{p,q=1}^{d} \mathfrak{Re}(B_{pq}) \left(f_p^\dagger f_q^\dagger - f_p f_q\right) + \mathfrak{Re}(A_{pq}) \left(f_p^\dagger f_q - f_p f_q^\dagger\right) \\ &\quad + \mathfrak{Im}(B_{pq})\, i \left(f_p^\dagger f_q^\dagger + f_p f_q\right) + \mathfrak{Im}(A_{pq})\, i \left(f_p^\dagger f_q + f_p f_q^\dagger\right). \end{aligned}$$

Note $\mathfrak{Re}(A) = \mathfrak{Re}(A)^t$, $\mathfrak{Im}(A) = -\mathfrak{Im}(A)^t$, $\mathfrak{Re}(B) = -\mathfrak{Re}(B)^t$, and $\mathfrak{Im}(B) = -\mathfrak{Im}(B)^t$ which is a consequence of $A = A^\dagger$ and $B = -B^t$. We rewrite the Hamiltonian using Majorana operators such that

$$-iH = -\frac{1}{2} \left[\sum_{p=1}^{d} -\mathfrak{Re}(A_{pp})\, m_{2p-1} m_{2p} + \sum_{p,q=1;p>q}^{d} V_{pq} \right],$$

where

$$\begin{aligned} V_{pq} = &- \mathfrak{Re}(B_{pq})\, (m_{2p-1} m_{2q} - m_{2q-1} m_{2p}) \\ &- \mathfrak{Re}(A_{pq})\, (m_{2p-1} m_{2q} + m_{2q-1} m_{2p}) \\ &- \mathfrak{Im}(B_{pq})\, (m_{2p-1} m_{2q-1} - m_{2p} m_{2q}) \\ &- \mathfrak{Im}(A_{pq})\, (m_{2p-1} m_{2q-1} + m_{2p} m_{2q}). \end{aligned}$$

By applying the Jordan-Wigner transformation we obtain the Hamiltonian for the corresponding spin system (for better readability, the tensor-product symbol is omitted, e.g., $\mathrm{IXY} := \mathrm{I} \otimes \mathrm{X} \otimes \mathrm{Y}$):

$$-iH = -\frac{i}{2} \Big[\sum_{p=1}^{d} -\mathfrak{Re}(A_{pp}) \underbrace{\mathrm{I} \cdot\cdot \mathrm{I}}_{p-1} \mathrm{Z} \underbrace{\mathrm{I} \cdot\cdot \mathrm{I}}_{d-p} + \sum_{p,q=1;p>q}^{d} W_{pq} \Big]$$

with $W_{pq} =$

$$\begin{aligned} &+ \mathfrak{Re}(B_{pq}) \big(\underbrace{\mathrm{I} \cdot\cdot \mathrm{I}}_{q-1} \mathrm{X} \underbrace{\mathrm{Z} \cdot\cdot \mathrm{Z}}_{p-q-1} \mathrm{X} \underbrace{\mathrm{I} \cdot\cdot \mathrm{I}}_{d-p} - \underbrace{\mathrm{I} \cdot\cdot \mathrm{I}}_{q-1} \mathrm{Y} \underbrace{\mathrm{Z} \cdot\cdot \mathrm{Z}}_{p-q-1} \mathrm{Y} \underbrace{\mathrm{I} \cdot\cdot \mathrm{I}}_{d-p} \big) \\ &+ \mathfrak{Re}(A_{pq}) \big(\underbrace{\mathrm{I} \cdot\cdot \mathrm{I}}_{q-1} \mathrm{X} \underbrace{\mathrm{Z} \cdot\cdot \mathrm{Z}}_{p-q-1} \mathrm{X} \underbrace{\mathrm{I} \cdot\cdot \mathrm{I}}_{d-p} + \underbrace{\mathrm{I} \cdot\cdot \mathrm{I}}_{q-1} \mathrm{Y} \underbrace{\mathrm{Z} \cdot\cdot \mathrm{Z}}_{p-q-1} \mathrm{Y} \underbrace{\mathrm{I} \cdot\cdot \mathrm{I}}_{d-p} \big) \\ &- \mathfrak{Im}(B_{pq}) \big(\underbrace{\mathrm{I} \cdot\cdot \mathrm{I}}_{q-1} \mathrm{Y} \underbrace{\mathrm{Z} \cdot\cdot \mathrm{Z}}_{p-q-1} \mathrm{X} \underbrace{\mathrm{I} \cdot\cdot \mathrm{I}}_{d-p} + \underbrace{\mathrm{I} \cdot\cdot \mathrm{I}}_{q-1} \mathrm{X} \underbrace{\mathrm{Z} \cdot\cdot \mathrm{Z}}_{p-q-1} \mathrm{Y} \underbrace{\mathrm{I} \cdot\cdot \mathrm{I}}_{d-p} \big) \\ &+ \mathfrak{Im}(A_{pq}) \big(\underbrace{\mathrm{I} \cdot\cdot \mathrm{I}}_{q-1} \mathrm{Y} \underbrace{\mathrm{Z} \cdot\cdot \mathrm{Z}}_{p-q-1} \mathrm{X} \underbrace{\mathrm{I} \cdot\cdot \mathrm{I}}_{d-p} - \underbrace{\mathrm{I} \cdot\cdot \mathrm{I}}_{q-1} \mathrm{X} \underbrace{\mathrm{Z} \cdot\cdot \mathrm{Z}}_{p-q-1} \mathrm{Y} \underbrace{\mathrm{I} \cdot\cdot \mathrm{I}}_{d-p} \big). \end{aligned}$$

Appendix C: Applications of Quasifree Fermions to Spin Systems

Here we take new fermionic approaches to exhaustively prove and improve some results of Ref. [19], where some proofs were still sketchy—thereby also filling a desideratum voiced in [79].

1. A Spin System with System Algebra $\mathfrak{so}(2n+1)$

Proposition 53 (see Proposition 27 in [19]). *Consider a Heisenberg-*XX *chain with the drift Hamiltonian*

$$H_d = \mathrm{XX} \cdot\cdot \mathrm{II} + \mathrm{YY} \cdot\cdot \mathrm{II} + \cdots + \mathrm{II} \cdot\cdot \mathrm{XX} + \mathrm{II} \cdot\cdot \mathrm{YY}$$

on n spin-$\frac{1}{2}$ qubits with $n \geq 2$. Assume that one end qubit is individually locally controllable. The system algebra is given as the subalgebra $\mathfrak{so}(2n+1)$ which is irreducibly embedded in $\mathfrak{su}(2^n)$.

Proof. We use the fermionic picture where the number of modes d equals the number of spins n. The generators are given by $w_1 = L(v_1)$ with $v_1 = \sum_{p=1}^{d-1} -m_{2p-1} m_{2p+2} + m_{2p} m_{2p+1}$, $L(m_1)$, and $L(m_2)$. Obviously, the element $w_2 = L(v_2)$ with $v_2 = m_1 m_2$ can also be generated. One can verify that exactly all Majorana operators of degree one or two can be obtained: One line of reasoning uses Lemma 10 together with the commutation relations $[L(m_{2p-1}), (b_p)] = L(m_{2p+2})$ and $[L(m_{2p}), L(b_p)] = -L(m_{2p+1})$ to show that all degree-one operators can be generated. This immediately gives all quadratic operators as well, while operators of higher degree are not attainable. Therefore, the dimension of the system algebra is $2d^2 + d$. Note that the operators $L(m_{2p-1} m_{2p})$ form a maximal abelian subalgebra $\mathfrak{a}$ which proves that the system algebra has rank d. In the spin picture, we can directly verify that $\mathfrak{a} = \langle -i\mathrm{Z}_1/2, \ldots, -i\mathrm{Z}_n/2 \rangle_{\mathrm{Lie}}$ by computing the centralizer $\mathfrak{c}_{\mathfrak{a}} := \langle -\frac{i}{2} \prod_{j \in S} \mathrm{Z}_j \,|\, \{\} \neq S \subset \{1, \ldots, n\} \rangle_{\mathrm{Lie}}$ of $\mathfrak{a}$ in $\mathfrak{su}(2^n)$. Let us compute the centralizer $\mathfrak{c}_{\mathfrak{b}}$ of $\mathfrak{b} = \langle m_{2p} m_{2p+1}, -m_{2p-1} m_{2p+2} \,|\, p \in \{1, \ldots, d-1\} \rangle_{\mathrm{Lie}}$ in $\mathfrak{su}(2^n)$. Note that the generators of $\mathfrak{b}$ are given in the spin picture by $-i\mathrm{X}_p \mathrm{X}_{p+1}/2$ and $-i\mathrm{Y}_p \mathrm{Y}_{p+1}/2$. One can readily show by induction that $\mathfrak{c}_{\mathfrak{b}} = \langle -\frac{i}{2} \prod_{j=1}^{n} \mathrm{X}_j, -\frac{i}{2} \prod_{j=1}^{n} \mathrm{Y}_j, -\frac{i}{2} \prod_{j=1}^{n} \mathrm{Z}_j \rangle_{\mathrm{Lie}}$. It follows that the centralizer $\mathfrak{c}$ of the full system algebra in $\mathfrak{su}(2^n)$ has to be contained in $\mathfrak{c}_{\mathfrak{a}} \cap \mathfrak{c}_{\mathfrak{b}} = \langle -\frac{i}{2} \prod_{j=1}^{n} \mathrm{Z}_j \rangle_{\mathrm{Lie}}$. One can now easily prove that the centralizer of the full system algebra in $\mathfrak{su}(2^n)$ is trivial and that the system algebra is irreducibly embedded in $\mathfrak{su}(2^d)$. As the coupling graph of the spin system is connected, we conclude with Theorem 6 of [19] that the system algebra is simple. Listing all simple (and compact) Lie algebras with the correct dimension and rank, we obtain (a) $\mathfrak{so}(2d+1)$ for $d \geq 1$, (b) $\mathfrak{sp}(d)$ for $d \geq 1$, (c) $\mathfrak{su}(2) \cong \mathfrak{so}(3)$ for $d = 1$, and (d) $\mathfrak{e}_6$ for $d = 6$. As the system algebra contains also all quadratic operators, it has a subalgebra $\mathfrak{so}(2d)$ which is of maximal rank. This rules out the cases (b) and (d) (see p. 219 of [48] or Sec. 8.4 of [49]) for $d \neq 2$. But the case (b) agrees with (a) for $d = 2$. For $d = 1$, the cases (a) and (c) coincide. This completes the proof. $\square$

Note that with our fermionic approach one can readily determine the dimension and rank of the system algebra. Likewise, we establish that all fermionic operators act irreducibly from which we can infer that the system algebra is simple. The rest of the proof follows by an exhaustive enumeration.—In more general terms, as in Theorem 34 and Corollary 35 of [19], we connect a spin system with a fictitious fermionic system:

Corollary 54. *Consider a fictitious fermionic system with d modes which consists of all linear and quadratic operators and whose generators can, e.g., be chosen as all Majorana operators of type $L(m_{2p-1})$ combined with the Hamiltonian from Eq. (21) where the control functions A_{pq} and B_{pq} can be assumed to be real. This fictitious fermionic system and the spin system of Proposition 53 with $n = d$ spins can simulate each other. In particular, both can simulate a general quasifree fermionic system with d modes and system algebra $\mathfrak{so}(2d)$ as presented in Proposition 9 and Theorem 11.*

2. A Spin System with System Algebra $\mathfrak{so}(2n+2)$

Proposition 55 (see Proposition 28 in [19])**.** *Consider a Heisenberg-XX chain with the drift Hamiltonian*

$$H_d = \mathrm{XX}\cdot\cdot\mathrm{II} + \mathrm{YY}\cdot\cdot\mathrm{II} + \cdots + \mathrm{II}\cdot\cdot\mathrm{XX} + \mathrm{II}\cdot\cdot\mathrm{YY}$$

on n spin-$\frac{1}{2}$ qubits with $n \geq 2$. Assume that each of the two end qubits is individually locally controllable. The system algebra is given as the subalgebra $\mathfrak{so}(2n+2)$ which is irreducibly embedded in $\mathfrak{su}(2^n)$.

Proof. We switch to a fermionic picture where the number of modes d equals the number of spins n. The generators are $w_1 = L(v_1)$ with $v_1 = \sum_{p=1}^{d-1} -m_{2p-1}m_{2p+2} + m_{2p}m_{2p+1}$, $L(m_1)$, $L(m_2)$, $L(m_{2d-1}\prod_{p=1}^{d-1} m_{2p-1}m_{2p})$, and $L(m_{2d}\prod_{p=1}^{d-1} m_{2p-1}m_{2p})$. One can verify by explicit computations that exactly all Majorana operators of degree one, two, $2d-1$, and $2d$ can be generated. Therefore, the dimension of the system algebra is $2d^2+3d+1$. Using a similar argument as in the proof of Proposition 53, we conclude that the operators $L(m_{2p-1}m_{2p})$ together with the operator $L(\prod_{p=1}^{d} m_{2p-1}m_p)$ form a maximal abelian subalgebra which proves that the system algebra has rank $d+1$. One can also show that the system algebra is irreducibly embedded in $\mathfrak{su}(2^d)$. As the coupling graph of the spin system is connected, we conclude with Theorem 6 of [19] that the system algebra is simple. The proof is completed by listing all simple (and compact) Lie algebras with the correct dimension and rank. We obtain (a) $\mathfrak{so}(2d+2)$ for $d \geq 1$ and (b) $\mathfrak{su}(4) \cong \mathfrak{so}(6)$ for $d = 2$. $\square$

Principle Remark: Now we have established a setting that allows for exploiting the powerful general results of [64] on the structure of orthogonal groups that provide a second avenue to Proposition 53 assuming we have already established Proposition 55: Lemmata 3 and 4 of [64] show that for $k \geq 3$ any subalgebra of $\mathfrak{so}(k)$ with dimension $(k-1)(k-2)/2$ is isomorphic to $\mathfrak{so}(k-1)$; moreover $\mathfrak{so}(k-1)$ is a maximal subalgebra of $\mathfrak{so}(k)$. Thus, by proving that the system algebra has dimension $2d^2 + d$ with $d \geq 1$, it can be identified as the subalgebra $\mathfrak{so}(2d+1)$ of $\mathfrak{so}(2d+2)$. We emphasize that this particular proof technique should be widely applicable in quantum systems theory.

Relying on the proof of Proposition 55 and building on Theorem 32 as well as Corollary 34 of [19], we obtain connections between a spin system, a quasifree fermionic system, and a fictitious fermionic system:

Corollary 56. *The following control systems all have the system algebra $\mathfrak{so}(2k+2)$ and can simulate each other:*
(a) the spin system of Proposition 55 with k spins,
(b) the quasifree fermionic system with $k+1$ modes as presented in Proposition 9 and Theorem 11, and
(c) a fictitious fermionic system with k modes which contains all Majorana operators of degree one, two, $2k-1$, and $2k$, and whose generating Hamiltonian can be chosen from Eq. (21) where the control functions A_{pq} and B_{pq} can be assumed to be real.

Appendix D: Proof of Theorem 13

The cases of $d \in \{2, 3, 4\}$ can be verified directly and we assume in the following that $d \geq 5$ holds. We build on Lemma 10 and obtain a basis of $\mathfrak{k}_1$ consisting of $L(a_p)$ with $1 \leq p \leq d$ as well as $L(b_p^{(i)})$ with

$$b_p^{(i)} := -m_{2p-1}m_{2p+2i} + m_{2p}m_{2p+2i-1}$$

and $L(c_p^{(i)})$ with

$$c_p^{(i)} := m_{2p-1}m_{2p+2i-1} + m_{2p}m_{2p+2i}$$

where $p, i \geq 1$ and $p + i \leq d$. One can systematically enlarge the index (i) starting from the elements $L(b_p^{(1)}) = L(b_p) \in \mathfrak{k}_1$ and $L(c_p^{(1)}) = (c_p) \in \mathfrak{k}_1$ and generate all $L(b_p^{(i)})$ and $L(c_p^{(i)})$ by combining the commutator relations $[L(c_p), L(b_{p+1}^{(i)})] = -L(b_p^{(i+1)})$ and $[L(c_{p+i}), L(b_p^{(i)})] = L(b_p^{(i+1)})$ with the commutator relations $[L(a_p), L(b_p^{(i)})] = -L(c_p^{(i)})$ and $[L(a_p), L(c_p^{(i)})] = L(b_p^{(i)})$. It is straightforward to check that no further elements are generated by commutators starting from the elements $L(a_p)$, $L(b_p^{(i)})$, and $L(c_p^{(i)})$. We obtain that $\dim(\mathfrak{k}_1) = d + (d-1)d = d^2$. Furthermore, the elements $L(a_p)$ form a maximal abelian subalgebra of $\mathfrak{k}_1$ and the rank of $\mathfrak{k}_1$ is d. It follows that $\mathfrak{k}_1$ is a subalgebra of maximal rank in $\mathfrak{so}(2d)$.

We now show that the center of $\mathfrak{k}_1$ is one-dimensional and is generated by $L(c)$ with $c := \sum_{p=1}^{d} a_p$. Combining the commutator relations $[L(a_{p+i}), L(b_p^{(i)})] = L(c_p^{(i)})$ and $[L(a_{p+i}), L(c_p^{(i)})] = -L(b_p^{(i)})$ with the ones for $L(a_p)$ mentioned above, we conclude that $[L(a_p{+}a_{p+i}), L(b_p^{(i)})] = [L(a_p{+}a_{p+i}), L(c_p^{(i)})] = 0$. In addition, we obtain $[L(a_j), L(b_p^{(i)})] = [L(a_j), L(c_p^{(i)})] = 0$ if $p \neq j \neq p+i$. It follows that $[L(c), L(b_p^{(i)})] = [L(c), L(c_p^{(i)})] = 0$ and that $L(c)$ commutes with all elements of $\mathfrak{k}_1$. We rule out the existence of further elements in the center by explicitly computing the semisimple part $\mathfrak{s} := [\mathfrak{k}_1, \mathfrak{k}_1]$ of $\mathfrak{k}_1$. By applying $[L(b_p^{(i)}), L(c_p^{(i)})]/2 = L(a_{p+i} - a_p)$ combined with previously mentioned commutator relations, we can fix a basis of $\mathfrak{s}$ consisting of the elements $L(b_p^{(i)})$, $L(c_p^{(i)})$, and $L(a_p - a_{p+1})$ where $1 \leq p \leq d-1$ and $1 \leq i \leq d-p$.

We proceed to prove in the following that $\mathfrak{s}$ is actually simple by showing that $\mathfrak{s}$ is not abelian (which obviously holds) and that any non-zero ideal $\mathfrak{i}$ of $\mathfrak{s}$ is equal to $\mathfrak{s}$. Starting from $(\mathrm{ad}^2(L(a_q)))\, L(b_p^{(i)}) = -L(b_p^{(i)})$ and $(\mathrm{ad}^2(L(a_q)))\, L(c_p^{(i)}) = -L(c_p^{(i)})$ for $q = p$ or $q = p+i$, we deduce that $\mathrm{ad}^2(L(a_q)) + \mathrm{ad}^4(L(a_q)) = 0$. Likewise, $y_p^{(i)} := [\mathrm{ad}^2(L(a_p{-}a_{p+i})) + \mathrm{ad}^4(L(a_p{-}a_{p+i}))]/12$ annihilates all basis elements of $\mathfrak{s}$ except for $L(b_p^{(i)})$ and $L(c_p^{(i)})$ which are left invariant. Using the definition $x_p^{(i)} := [\mathrm{ad}^2(L(b_p^{(i)})) - \mathrm{ad}^2(L(c_p^{(i)}))]/4$ and verifying $x_p^{(i)}\, L(a_p) = x_p^{(i)}\, L(a_{p+i}) = 0$, we can infer that $x_p^{(i)}\, L(a_q{-}a_{q+j}) = 0$ holds for all valid q and j. Furthermore, we have $x_p^{(i)}\, L(b_q^{(j)}) = x_p^{(i)}\, L(c_q^{(j)}) = 0$ for all valid q and j unless when both $q = p$ and $j = i$ hold. We obtain $x_p^{(i)}\, L(b_p^{(i)}) = L(b_p^{(i)})$ and $x_p^{(i)}\, L(c_p^{(i)}) = -L(c_p^{(i)})$ in this exceptional case. As $\mathfrak{s}$ is semisimple, $\mathfrak{i}$ cannot be abelian and has to contain an element which is supported on some $L(b_p^{(i)})$ or $L(c_p^{(i)})$. Relying on the ideal property $[\mathfrak{s}, \mathfrak{i}] \subseteq \mathfrak{i}$ and the operators $x_p^{(i)}$ and $y_p^{(i)}$, we conclude that $L(b_p^{(i)}) \in \mathfrak{i}$ or $L(c_p^{(i)}) \in \mathfrak{i}$. Obviously, the conditions $L(b_p^{(i)}) \in \mathfrak{i}$, $L(c_p^{(i)}) \in \mathfrak{i}$, and $L(a_p{-}a_{p+i}) \in \mathfrak{i}$ are equivalent. By applying previously mentioned commutator relations, we can verify that $L(b_q^{(j)}) \in \mathfrak{i}$ holds for all $q \leq p$ and $q+j \geq p+i$. In particular, $L(b_1^{d-1}) \in \mathfrak{i}$. Using the commutator relations $[L(c_p), L(b_p^{(i)})] = L(b_{p+1}^{(i-1)})$ and $[L(c_{p+i-1}), L(b_p^{(i)})] = -L(b_p^{(i-1)})$ where $i > 1$, we can reach the conclusion that $L(b_q^{(j)}) \in \mathfrak{i}$ for all valid q and j. Thus, we have shown that $\mathfrak{i} = \mathfrak{s}$ and $\mathfrak{s}$ has to be simple.

We summarize that $\mathfrak{k}_1$ has dimension d^2, has rank d, and is a subalgebra of maximal rank in $\mathfrak{so}(2d)$. In addition, it is a direct sum of a simple subalgebra and a one-dimensional abelian subalgebra. We list all compact, simple Lie algebras $\mathfrak{s}$ of rank $k := d-1 \geq 4$: $\mathfrak{su}(k{+}1)$ has dimension $k^2{+}2k$, $\mathfrak{so}(2k{+}1)$ has dimension $2k^2{+}k$, $\mathfrak{sp}(k)$ has dimension $2k^2 + k$, $\mathfrak{so}(2k)$ has dimension $2k^2 - k$, as well as the exceptional ones. Note that the exceptional cases $\mathfrak{g}_2$, $\mathfrak{f}_4$, $\mathfrak{e}_6$, $\mathfrak{e}_7$, and $\mathfrak{e}_8$ are ruled out by their respective ranks 2, 4, 6, 7, and 8 as well as dimensions 14, 52, 78, 133, and 248. We obtain $\mathfrak{s} \cong \mathfrak{su}(d)$ and $\mathfrak{k}_1 \cong \mathfrak{u}(d)$.

Appendix E: Proof of Proposition 26

Here, a proof for the Proposition 26 of Section VII B is provided. We start in Subsection E 1 by generalizing a key observation of Ref. [16] (where the particular case of Proposition 57 when K divides L was already considered). This generalization is then applied in Subsection E 2 where the details for the proof of Proposition 26 are given.

1. Generalizing a Key Observation of Ref. [16]

Proposition 57. *The trace of the product of U_T^{-K} with a tensor product of Pauli operators $Q_i \in \{\mathbb{1}_2, \mathrm{X}, \mathrm{Y}, \mathrm{Z}\}$ can be computed as*

$$\mathrm{tr}\left[U_T^{-K}\left(\bigotimes_{i=1}^{L} Q_i\right)\right] = \prod_{p=1}^{c} \mathrm{tr}\left[\prod_{q=0}^{L/c-1} Q_{(qK+p) \bmod L}\right], \tag{E1}$$

where $c := \gcd(K, L)$.

Proof. To simplify our calculations, let us introduce the notation $v(\ell) = (K+\ell) \bmod L$, note that $(v \circ v)(\ell) = v(v(\ell)) = (2K+\ell) \bmod L$, or more generally $v^{\circ p}(\ell) = (pK+\ell) \bmod L$. We can now write the action of U_T^{-K} on an arbitrary standard basis vector as

$$U_T^{-K}\,|n_1, \ldots, n_\ell, \ldots, n_L\rangle = |n_{v(1)}, \ldots, n_{v(\ell)}, \ldots, n_{v(L)}\rangle.$$

Without loss of generality we can confine the discussion to the case where $K \leq L$. We complete the proof, by evaluating the trace in Eq. (E1) as

$$\begin{aligned}
&\mathrm{tr}\left[U_T^{-K}\left(\bigotimes_{i=1}^{L} Q_i\right)\right] = \mathrm{tr}\left[\left(\bigotimes_{i=1}^{L} Q_i\right) U_T^{-K}\right] \\
&= \sum_{\underline{n} \in \{0,1\}^L} \langle n_1, \ldots, n_L| \left(\bigotimes_{i=1}^{L} Q_i\right) U_T^{-K} |n_1, \ldots, n_L\rangle \\
&= \sum_{\underline{n} \in \{0,1\}^L} \langle n_1, \ldots, n_L| \left(\bigotimes_{i=1}^{L} Q_i\right) |n_{v(1)}, \ldots, n_{v(L)}\rangle \\
&= \sum_{\underline{n} \in \{0,1\}^L} \prod_{\ell=1}^{L} \langle n_\ell | Q_\ell | n_{v(\ell)}\rangle
\end{aligned}$$

which can be further simplified to

$$\begin{aligned}
&\sum_{\underline{n} \in \{0,1\}^L} \prod_{\ell=1}^{L} \langle n_\ell | Q_\ell | n_{(K+\ell) \bmod L}\rangle \\
&= \sum_{\underline{n} \in \{0,1\}^L} \prod_{p=1}^{c} \prod_{q=1}^{L/c-1} \langle n_{v^{\circ q}(p)} | Q_p | n_{v^{\circ (q+1)}(p)}\rangle \\
&= \prod_{p=1}^{c} \mathrm{tr}\left[\prod_{q=0}^{L/c-1} Q_{[(qL/c+p) \bmod L]}\right]. \qquad \square
\end{aligned}$$

2. Details of the Proof of Proposition 26

The Lie algebras $\mathfrak{t}_M$ and $\mathfrak{t}_{M+1}$ are generated by elements of the form of

$$i\sum_{q'=0}^{L-1} U_T^{q'}\left[\left(\bigotimes_{p=1}^{M} Q_p\right)\otimes \mathbb{1}_2^{\otimes L-M}\right]U_T^{-q'} \text{ and}$$
$$i\sum_{q'=0}^{L-1} U_T^{q'}\left[\left(\bigotimes_{p=1}^{M+1} Q_p\right)\otimes \mathbb{1}_2^{\otimes L-M-1}\right]U_T^{-q'},$$

respectively. Here, we consider all combinations of $Q_p \in \{\mathbb{1}_2, \mathrm{X}, \mathrm{Y}, \mathrm{Z}\}$ apart from the case when $Q_1 = \mathbb{1}_2$. We introduce the notation $F(a, W) :=$

$$\begin{aligned}
&\operatorname{tr}\left(U_T^{aqM} i\sum_{q'=0}^{L-1} U_T^{q'}\left[\left(\bigotimes_{p=1}^{W} Q_p\right)\otimes \mathbb{1}_2^{\otimes L-W}\right]U_T^{-q'}\right)\\
&=\operatorname{tr}\left(i\sum_{q'=0}^{L-1} U_T^{q'}U_T^{aqM}\left[\left(\bigotimes_{p=1}^{W} Q_p\right)\otimes \mathbb{1}_2^{\otimes L-W}\right]U_T^{-q'}\right)\\
&=i\sum_{q'=0}^{L-1}\operatorname{tr}\left(U_T^{q'}U_T^{aqM}\left[\left(\bigotimes_{p=1}^{W} Q_p\right)\otimes \mathbb{1}_2^{\otimes L-W}\right]U_T^{-q'}\right)\\
&=i\sum_{q'=0}^{L-1}\operatorname{tr}\left(U_T^{aqM}\left(\bigotimes_{p=1}^{W} Q_p\right)\otimes \mathbb{1}_2^{\otimes L-W}\right),
\end{aligned}$$

where $a \in \{1, -1\}$ and $W \in \{M, M+1\}$. Using Proposition 57, we compute the formulas

$$F(1, M) = iL\prod_{p=1}^{M}\operatorname{tr}[Q_p] = 0,$$
$$F(1, M+1) = iL\operatorname{tr}[Q_1 Q_{M+1}]\prod_{p=2}^{M}\operatorname{tr}[Q_p],$$
$$F(-1, M+1) = iL\operatorname{tr}[Q_{M+1} Q_1]\prod_{p=2}^{M}\operatorname{tr}[Q_p].$$

It follows that the respective statements in the proposition hold for the generators of $\mathfrak{t}_M$ and $\mathfrak{t}_{M+1}$. Now we prove this consequence also for any element in $\mathfrak{t}_M$ (or $\mathfrak{t}_{M+1}$). First, let us note that the elements generated must be contained in $[\mathfrak{t}_M, \mathfrak{t}_M]$ (or $[\mathfrak{t}_{M+1}, \mathfrak{t}_{M+1}]$). Second, since all elements in $\mathfrak{t}_{M+1}$ (and hence in $\mathfrak{t}_M$) commute with U_T^{qM}, we have that $\operatorname{tr}(U_T^{qM} ih) = 0$ holds for any element $ih \in [\mathfrak{t}_{M+1}, \mathfrak{t}_{M+1}]$, as

$$\begin{aligned}
&\operatorname{tr}([ih^1_{M+1}, ih^2_{M+1}]U_T^{qM})\\
&=\operatorname{tr}(ih^1_{M+1}\, ih^2_{M+1}\, U_T^{qM}) - \operatorname{tr}(ih^2_{M+1}\, ih^1_{M+1}\, U_T^{qM})\\
&=\operatorname{tr}(ih^1_{M+1}\, ih^2_{M+1}\, U_T^{qM}) - \operatorname{tr}(ih^2_{M+1}\, U_T^{qM}\, ih^1_{M+1})\\
&=\operatorname{tr}(ih^1_{M+1}\, ih^2_{M+1}\, U_T^{qM}) - \operatorname{tr}(ih^1_{M+1}\, ih^2_{M+1}\, U_T^{qM}) = 0.
\end{aligned}$$

Thus Proposition 26 follows.

Appendix F: Proof of Theorem 33 for d Even

Let us introduce the notation $\mathcal{N}_2$, which corresponds to the linear space spanned by the nearest-neighbor (and on-site) operators. Note that $\mathcal{N}_2$ forms only a linear space and is in general not equal to the Lie algebra $\mathfrak{t}_2^f$ generated by its elements. We first prove a fermionic generalization of Lemma 26.

Lemma 58. *Consider a fermionic system for which the number $d \geq 6$ of modes is even. For any $ih \in \mathcal{N}_2$ the condition $\operatorname{tr}(ih\,\mathcal{U}^{-2}) = 0$ holds if $d \bmod 4 = 2$, while $\operatorname{tr}(ih\,\mathcal{U}^{-4}) = 0$ holds if $d \bmod 4 = 0$.*

Proof. By definition, any element $ih \in \mathcal{N}_2$ can be written as $ih = \sum_{n=0}^{d-1}\mathcal{U}^n\, ih_{12}\,\mathcal{U}^{-n}$, where ih_{12} is a traceless skew-Hermitian operator acting only on the first two modes of the fermionic system. Therefore, ih_{12} is a linear combination of the elements $i\, m_1 m_2 m_3 m_4$ and $m_a m_b$ where $a, b \in \{1, 2, 3, 4\}$ and $a \neq b$. We obtain that $\operatorname{tr}(ih\,\mathcal{U}^{-b}) = \operatorname{tr}[\sum_{n=0}^{d-1}(\mathcal{U}^n\, ih_{12}\,\mathcal{U}^{-n})\mathcal{U}^{-b}] = \sum_{n=0}^{d-1}\operatorname{tr}(\mathcal{U}^n\, ih_{12}\,\mathcal{U}^{-n}\,\mathcal{U}^{-b}) = d\operatorname{tr}(ih_{12}\,\mathcal{U}^{-b})$. If $d \bmod 4 = 2$, we write out explicitly $\operatorname{tr}(ih\,\mathcal{U}^{-b})/d$ for $b = 2$ by applying Eq. (39):

$$\begin{aligned}
&\operatorname{tr}(ih\,\mathcal{U}^{-2})/d = \operatorname{tr}(ih_{12}\,\mathcal{U}^{-2})\\
&= \sum_{\underline{n}\in\{0,1\}^d}\langle n_1,\ldots,n_d|ih_{12}\,\mathcal{U}^{-2}|n_1,\ldots,n_d\rangle\\
&= \sum_{\underline{n}\in\{0,1\}^d}\kappa(\underline{n})\,\langle n_1,\ldots,n_d|ih_{12}|n_3,\ldots,n_d,n_1,n_2\rangle,
\end{aligned}$$

where

$$\kappa(\underline{n}) = (-1)^{(n_1+n_2)(n_3+n_4+\cdots+n_d)}. \tag{F1}$$

In the sum given above, the basis vectors are orthogonal and thus most of the terms are zero. The only terms with non-zero contributions can occur in the cases of $n_1 = n_{2\ell-1}$ and $n_2 = n_{2\ell}$ with $\ell \in \{1, \ldots, d/2\}$. In particular, we have $\kappa(n_1, n_2, n_1, n_2, \ldots, n_1, n_2) = 1$ as $d/2$ is an odd number if $d \bmod 4 = 2$. Hence we obtain that

$$\begin{aligned}
&\operatorname{tr}(ih\,\mathcal{U}^{-2})/d = \operatorname{tr}(ih_{12}\,\mathcal{U}^{-2})\\
&= \sum_{n_1,n_2\in\{0,1\}}\langle n_1,n_2,n_1,n_2,\ldots|ih_{12}|n_1,n_2,n_1,n_2,\ldots\rangle\\
&= \sum_{n_1,n_2\in\{0,1\}}\langle n_1,n_2|ih_{12}|n_1,n_2\rangle = \operatorname{tr}(ih_{12}) = 0.
\end{aligned}$$

If $d \bmod 4 = 0$, we can explicitly write out the trace:

$$\begin{aligned}
&\operatorname{tr}(ih\,\mathcal{U}^{-4})/d = \operatorname{tr}(ih_{12}\,\mathcal{U}^{-4}) =\\
&= \sum_{\underline{n}\in\{0,1\}^d}\langle n_1,\ldots,n_d|ih_{12}\,\mathcal{U}^{-4}|n_1,\ldots,n_d\rangle\\
&= \sum_{\underline{n}\in\{0,1\}^d}\lambda(\underline{n})\,\langle n_1,\ldots,n_d|ih_{12}|n_5,\ldots,n_d,n_1,\ldots,n_4\rangle,
\end{aligned}$$

where

$$\lambda(\underline{n}) = (-1)^{(n_1+n_2+n_3+n_4)(n_5+n_6+\cdots+n_d)}. \tag{F2}$$

The basis vectors in the sum are again orthogonal, and most of the terms are zero. The only terms that can give non-zero contributions are for the cases of $n_1 = n_{4\ell-3}$, $n_2 = n_{4\ell-2}$, $n_3 = n_{4\ell-1}$, and $n_4 = n_{4\ell}$ with $\ell \in \{1,\ldots,d/4\}$. It follows in these cases that

$$\begin{aligned}\lambda(\underline{n}) &= (-1)^{(n_1+n_2+n_3+n_4)(d/4-1)}\\ &= \begin{cases}1 & \text{if } d \bmod 8 = 4,\\ (-1)^{(n_1+n_2+n_3+n_4)} & \text{if } d \bmod 8 = 0.\end{cases}\end{aligned} \tag{F3}$$

The notation $\chi := n_1, n_2, n_3, n_4, n_1, n_2, n_3, n_4, \ldots, n_4$ is used, and we obtain

$$\begin{aligned}&\operatorname{tr}(ih\,\mathcal{U}^{-4})/d = \operatorname{tr}(ih_{12}\,\mathcal{U}^{-4})\\ &= \sum_{n_1,\ldots,n_4\in\{0,1\}} \lambda(\underline{n})\,\langle\chi|ih_{12}|\chi\rangle\\ &= \sum_{n_1,\ldots,n_4\in\{0,1\}} \lambda(\underline{n})\,\langle n_1,\ldots,n_4|ih_{12}|n_1,\ldots,n_4\rangle.\end{aligned} \tag{F4}$$

We apply Eq. (F3) and obtain that the Eq. (F4) is zero if $d \bmod 8 = 4$. We can also prove that Eq. (F4) is zero for $d \bmod 8 = 0$ as Eq. (F4) simplifies to

$$\begin{aligned}&\left[\sum_{n_1,n_2\in\{0,1\}} (-1)^{(n_1+n_2)}\langle n_1n_2|ih_{12}|n_1n_2\rangle\right]\\ &\times\left[\sum_{n_3,n_4\in\{0,1\}} (-1)^{(n_3+n_4)}\right] = 0.\end{aligned}$$

□

Lemma 59. *Consider a fermionic system for which the number $d \geq 6$ of modes is even. The properties $\operatorname{tr}(ih_\mathrm{e}\,\mathcal{U}^{-2}) \neq 0$ and $\operatorname{tr}(ih_\mathrm{e}\,\mathcal{U}^{-4}) \neq 0$ hold for the operator ih_e of Theorem 33.*

Proof. We proceed similarly as in the proof of Lemma 58. The operator ih_e can be written as $\sum_{n=0}^{d-1}\mathcal{U}^n\,ih_5\,\mathcal{U}^{-n}$, where $ih_5 := (f_1^\dagger f_1 f_2^\dagger f_2 f_3^\dagger f_3 f_4^\dagger f_4 f_5^\dagger f_5 - \mathbb{1}/32)$. Due to this particular structure of ih_5, we can simplify the trace $\operatorname{tr}(ih_\mathrm{e}\,\mathcal{U}^{-b}) = \operatorname{tr}[\sum_{n=0}^{d-1}(\mathcal{U}^n\,ih_5\,\mathcal{U}^{-n})\,\mathcal{U}^{-b}] = \sum_{n=0}^{d-1}\operatorname{tr}(\mathcal{U}^n\,ih_5\,\mathcal{U}^{-n}\,\mathcal{U}^{-b}) = d\,\operatorname{tr}(ih_5\,\mathcal{U}^{-b})$. Let us explicitly write out the trace for $b=2$ by applying Eq. (39):

$$\begin{aligned}&tr(ih_\mathrm{e}\,\mathcal{U}^{-2})/d = tr(ih_5\,\mathcal{U}^{-2}) =\\ &= \sum_{\underline{n}\in\{0,1\}^d} \langle n_1,\ldots,n_d|ih_5\,\mathcal{U}^{-2}|n_1,\ldots,n_d\rangle\\ &= \sum_{\underline{n}\in\{0,1\}^d} \kappa(\underline{n})\,\langle n_1,\ldots,n_d|ih_5|n_3,\ldots,n_d,n_1,n_2\rangle\\ &= \sum_{\underline{n}\in\{0,1\}^d} \theta(\underline{n})\,\langle n_1,\ldots,n_d|n_3,\ldots,n_d,n_1,n_2\rangle.\end{aligned}$$

where $\theta(\underline{n}) := (\delta_{n_3,1}\delta_{n_4,1}\delta_{n_5,1}\delta_{n_6,1}\delta_{n_7,1} - 1/32)\,\kappa(\underline{n})$ and $\kappa(\underline{n})$ was defined in Eq. (F1). Most of the terms in the sum are zero as the basis vectors are orthogonal. The only terms with non-zero contributions occur for $n_{2\ell-1} = n_1$ and $n_{2\ell} = n_2$ with $\ell \in \{1,\ldots,d/2\}$. If $d \bmod 4 = 2$, it follows that $\theta(\underline{n}) = 31/32$ for $n_1 = n_2 = 1$, and $\theta(\underline{n}) = -1/32$ otherwise. If $d \bmod 4 = 0$, we have $\theta(\underline{n}) = 31/32$ for $n_1 = n_2 = 1$, and $\theta(\underline{n}) = 1/32$ for $n_1 + n_2 = 1$, and $\theta(\underline{n}) = -1/32$ for $n_1 = n_2 = 0$. We obtain

$$\begin{aligned}&\operatorname{tr}(ih_\mathrm{e}\,\mathcal{U}^{-2})/d = \operatorname{tr}(ih_5\,\mathcal{U}^{-2})\\ &= \sum_{n_1,n_2\in\{0,1\}} \theta(\underline{n})\,\langle n_1,n_2,n_1,n_2,\ldots|n_1,n_2,n_1,n_2,\ldots\rangle\\ &= \begin{cases}7/8 & \text{if } d \bmod 4 = 2,\\ 1 & \text{if } d \bmod 4 = 0.\end{cases}\end{aligned}$$

Let us now consider the trace with $\mathcal{U}^{-4}$:

$$\begin{aligned}&\operatorname{tr}(ih_\mathrm{e}\,\mathcal{U}^{-4})/d = \operatorname{tr}(ih_5\,\mathcal{U}^{-4}) =\\ &= \sum_{\underline{n}\in\{0,1\}^d} \langle n_1,\ldots,n_d|ih_5\,\mathcal{U}^{-4}|n_1,\ldots,n_d\rangle\\ &= \sum_{\underline{n}\in\{0,1\}^d} \lambda(\underline{n})\,\langle n_1,\ldots,n_d|ih_5|n_5,\ldots,n_d,n_1,\ldots,n_4\rangle\\ &= \sum_{\underline{n}\in\{0,1\}^d} \mu(\underline{n})\,\langle n_1,\ldots,n_d|n_5,\ldots,n_d,n_1,\ldots,n_4\rangle\end{aligned}$$

where $\mu(\underline{n}) := (\delta_{n_5,1}\delta_{n_6,1}\delta_{n_7,1}\delta_{n_8,1}\delta_{n_9,1} - 1/32)\,\lambda(\underline{n})$ and $\lambda(\underline{n})$ was defined in Eq. (F2). Again, most of the terms in the sum are zero as the basis vectors are orthogonal. Provided that $d \bmod 4 = 2$, the only terms with non-zero contributions can occur in the case of $n_{2\ell-1} = n_1$ and $n_{2\ell} = n_2$ where $\ell \in \{1,\ldots,d/2\}$. In this case $\mu(\underline{n}) = 31/32$ for $n_1 = n_2 = 1$, and $\mu(\underline{n}) = -1/32$ otherwise. It follows that $\operatorname{tr}(ih_\mathrm{e}\,\mathcal{U}^{-4})/d =$

$$\sum_{n_1,n_2\in\{0,1\}} \mu(\underline{n})\,\langle n_1,n_2,n_1,n_2,\ldots|n_1,n_2,n_1,n_2,\ldots\rangle = \frac{7}{8}.$$

If $d \bmod 4 = 0$, terms with non-zero contributions can occur for $n_{4\ell-3} = n_1$, $n_{4\ell-2} = n_2$, $n_{4\ell-1} = n_3$, and $n_{4\ell} = n_4$ with $\ell \in \{1,\ldots,d/4\}$. For these cases we obtain from Eq. (F3) that

$$\begin{aligned}\mu(\underline{n}) &= (\delta_{n_5,1}\delta_{n_6,1}\delta_{n_7,1}\delta_{n_8,1}\delta_{n_9,1} - \tfrac{1}{32})\\ &\times\begin{cases}1 & \text{if } d \bmod 8 = 4,\\ (-1)^{(n_1+n_2+n_3+n_4)} & \text{if } d \bmod 8 = 0.\end{cases}\end{aligned}$$

Using $\chi = n_1, n_2, n_3, n_4, n_1, n_2, n_3, n_4, \ldots, n_4$ we can simplify the trace to

$$\begin{aligned}&\operatorname{tr}(ih_\mathrm{e}\,\mathcal{U}^{-4})/d = \operatorname{tr}(ih_5\,\mathcal{U}^{-4}) = \sum_{n_1,\ldots,n_4\in\{0,1\}} \mu(\underline{n})\,\langle\chi|\chi\rangle\\ &= \begin{cases}1/2 & \text{if } d \bmod 8 = 4,\\ 1 & \text{if } d \bmod 8 = 0.\end{cases}\end{aligned}$$

□

Now we can prove Theorem 33 for even d as summarized in the following proposition:

Proposition 60. *Consider a fermionic system for which the number $d \geq 6$ of modes is even. The fourth-neighbor element $ih_{\rm e} \in \mathfrak{t}_5^f$ of Theorem 33 is not contained in the system algebra $\mathfrak{t}_2^f$ of nearest-neighbor interactions.*

Proof. We introduce the operator

$$\mathcal{C}_d = \begin{cases} \mathcal{U}^{-2} & \text{if } d \bmod 4 = 2, \\ \mathcal{U}^{-4} & \text{if } d \bmod 4 = 0. \end{cases}$$

It follows from Lemma 58 that the equality $\mathrm{tr}(ih\,\mathcal{C}_d) = 0$ holds for any $ih \in \mathcal{N}_2$. Since $\mathcal{C}_d$ commutes with all elements of $\mathfrak{t}_2^f$ and $\mathfrak{t}_2^f = \mathrm{span}(\mathcal{N}_2, [\mathfrak{t}_2^f, \mathfrak{t}_2^f])$, we have

$$\begin{aligned}\mathrm{tr}(\mathcal{C}_d\,[ih_1, ih_2]) &= \mathrm{tr}(\mathcal{C}_d\,ih_1\,ih_2) - \mathrm{tr}(\mathcal{C}_d\,ih_2\,ih_1)\\ &= \mathrm{tr}(\mathcal{C}_d\,ih_1\,ih_2) - \mathrm{tr}(ih_1\,\mathcal{C}_d\,ih_2)\\ &= \mathrm{tr}(\mathcal{C}_d\,ih_1\,ih_2) - \mathrm{tr}(\mathcal{C}_d\,ih_1\,ih_2) = 0.\end{aligned}$$

This means that $\mathrm{tr}(\mathcal{C}_d\,ik) = 0$ for all $ik \in \mathfrak{t}_2^f$. On the other hand, we know from Lemma 59 that $\mathrm{tr}(ih_{\rm e}\,\mathcal{C}_d) \neq 0$. This means that $ih_{\rm e} \notin \mathfrak{t}_2^f$. □

Appendix G: Proof of Theorem 33 for d Odd

The proof of Theorem 33 for odd number of modes uses an expansion of the translation unitary $\mathcal{U}$ by the Fourier transformed Majorana operators, which are defined as

$$\widetilde{m}_{2k} := i(\tilde{f}_k - \tilde{f}_k^\dagger) \text{ and } \widetilde{m}_{2k+1} := \tilde{f}_k + \tilde{f}_k^\dagger\,. \tag{G1}$$

Note that the operators $\tilde{f}_k$ were defined in Eq. (43). The self-adjoint operators $\widetilde{m}_x$ satisfy again the Majorana anticommutation relations $\{\widetilde{m}_x, \widetilde{m}_y\} = 2\delta_{x,y}\mathbb{1}$. Moreover, the trace of any $\widetilde{m}_x$-monomial is zero, since it is a linear combination of Majorana monomials. The following lemma relates these operators to the translation unitary.

Lemma 61. *The translation unitary $\mathcal{U}$ can be written as*

$$\begin{aligned}\mathcal{U} &= (-i)^{d-1}\exp\left[-i\sum_{k=0}^{d-1}\tfrac{2\pi k}{d}(\tilde{f}_k^\dagger\tilde{f}_k - \tfrac{1}{2}\mathbb{1})\right] && \text{(G2)}\\ &= (-i)^{d-1}\exp\left[-\sum_{k=0}^{d-1}\tfrac{\pi k}{d}\,\widetilde{m}_{2k+1}\widetilde{m}_{2k}\right] && \text{(G3)}\\ &= (-i)^{d-1}\prod_{k=0}^{d-1}[\cos(\tfrac{\pi k}{d})\mathbb{1} - \sin(\tfrac{\pi k}{d})\,\widetilde{m}_{2k+1}\widetilde{m}_{2k}] && \text{(G4)}\end{aligned}$$

using the Fourier-transformed operators $\tilde{f}_k$ and $\tilde{f}_k^\dagger$ as well as $\widetilde{m}_{2k}$ and $\widetilde{m}_{2k+1}$.

Proof. Let us denote the right hand side of Eq. (G2) by

$$\mathcal{V} := (-i)^{d-1}\exp\left[-i\sum_{k=0}^{d-1}\tfrac{2\pi k}{d}(\tilde{f}_k^\dagger\tilde{f}_k - \tfrac{1}{2}\mathbb{1})\right].$$

Applying the identity $\widetilde{m}_{2k+1}\widetilde{m}_{2k} = i(2\tilde{f}_k^\dagger\tilde{f}_k - \mathbb{1})$, it follows that $\mathcal{V} = (-i)^{d-1}\exp(-\sum_{k=0}^{d-1}\pi k\,\widetilde{m}_{2k+1}\widetilde{m}_{2k}/d)$. Since the formula $[\widetilde{m}_{2k+1}\widetilde{m}_{2k}, \widetilde{m}_{2k'+1}\widetilde{m}_{2k'}] = 0$ holds for $k \neq k'$, we can split the exponential into the product $\mathcal{V} = (-i)^{d-1}\prod_{k=0}^{d-1}\exp(-\pi k\,\widetilde{m}_{2k+1}\widetilde{m}_{2k}/d)$. We employ $(\widetilde{m}_{2k+1}\widetilde{m}_{2k})^2 = -\mathbb{1}$ and obtain the formula

$$\begin{aligned}\exp(-\tfrac{\pi k}{d}\,\widetilde{m}_{2k+1}\widetilde{m}_{2k}) &= \sum_{n=0}^{\infty}\tfrac{(-\pi k)^n}{n!\,d^n}(\widetilde{m}_{2k+1}\widetilde{m}_{2k})^n\\ &= \sum_{n=0}^{\infty}\tfrac{(-1)^n(\pi k)^{2n}}{(2n)!\,d^{2n}}\mathbb{1} - \sum_{n=0}^{\infty}\tfrac{(-1)^n(\pi k)^{2n+1}}{(2n+1)!\,d^{2n+1}}\,\widetilde{m}_{2k+1}\widetilde{m}_{2k}\\ &= \cos(\tfrac{\pi k}{d})\mathbb{1} - \sin(\tfrac{\pi k}{d})\,\widetilde{m}_{2k+1}\widetilde{m}_{2k}.\end{aligned}$$

Thus, $\mathcal{V}$ is equal to the right hand side of Eq. (G4). Similarly, the adjoint of $\mathcal{V}$ can be written as

$$\begin{aligned}\mathcal{V}^\dagger &= i^{(d-1)}\prod_{k=0}^{d-1}\exp(\tfrac{\pi k}{d}\,\widetilde{m}_{2k+1}\widetilde{m}_{2k})\\ &= i^{(d-1)}\prod_{k=0}^{d-1}\left[\cos(\tfrac{\pi k}{d})\mathbb{1} + \sin(\tfrac{\pi k}{d})\,\widetilde{m}_{2k+1}\widetilde{m}_{2k}\right].\end{aligned}$$

The commutation relations of Eq. (44) imply the formula $\widetilde{m}_{2k+1}\widetilde{m}_{2k}\tilde{f}_k^\dagger = -\tilde{f}_k^\dagger\widetilde{m}_{2k+1}\widetilde{m}_{2k} = i\tilde{f}_k^\dagger$. It follows that

$$\begin{aligned}\mathcal{V}\tilde{f}_k^\dagger\mathcal{V}^\dagger &= [\cos(\tfrac{\pi k}{d})\mathbb{1} - \sin(\tfrac{\pi k}{d})\,\widetilde{m}_{2k+1}\widetilde{m}_{2k}]\\ &\quad\times\tilde{f}_k^\dagger[\cos(\tfrac{\pi k}{d})\mathbb{1} + \sin(\tfrac{\pi k}{d})\,\widetilde{m}_{2k+1}\widetilde{m}_{2k}]\\ &= e^{-2\pi ik/d}\tilde{f}_k^\dagger,\end{aligned}$$

which implies that

$$\begin{aligned}\mathcal{V}f_n^\dagger\mathcal{V}^\dagger &= \mathcal{V}\left(\frac{1}{\sqrt{d}}\sum_{k=1}^{d}\tilde{f}_k^\dagger e^{-2\pi ink/d}\right)\mathcal{V}^\dagger\\ &= \frac{1}{\sqrt{d}}\sum_{k=1}^{d}\tilde{f}_k^\dagger e^{-2\pi i(n+1)k/d} = f_{n+1}^\dagger.\end{aligned} \tag{G5}$$

Applying the formulas $\tilde{f}_k|0\rangle = 0$ and $[\tilde{f}_k^\dagger\tilde{f}_k, \tilde{f}_{k'}^\dagger\tilde{f}_{k'}] = 0$, we conclude that $\exp[-i\sum_{k=0}^{d-1}2\pi k\tilde{f}_k^\dagger\tilde{f}_k/d]|0\rangle = |0\rangle$. This allows to investigate how $\mathcal{V}$ acts on the Fock vacuum $|0\rangle$:

$$\begin{aligned}\mathcal{V}|0\rangle &= (-i)^{d-1}\exp\left[-i\sum_{k=0}^{d-1}\tfrac{2\pi k}{d}(\tilde{f}_k^\dagger\tilde{f}_k - \tfrac{1}{2}\mathbb{1})\right]|0\rangle\\ &= (-i)^{d-1}e^{i\sum_{k=0}^{d-1}\frac{\pi k}{d}}\exp\left[-i\sum_{k=0}^{d-1}\tfrac{2\pi k}{d}(\tilde{f}_k^\dagger\tilde{f}_k)\right]|0\rangle\\ &= (-i)^{d-1}e^{i\frac{\pi}{2}(d-1)}|0\rangle = |0\rangle.\end{aligned} \tag{G6}$$

It follows from Eqs. (G5) and (G6) that $\mathcal{V}$ satisfies Eq. (39) if we substitute $\mathcal{V}$ for $\mathcal{U}$. As Eq. (39) defines $\mathcal{U}$ uniquely, $\mathcal{U} = \mathcal{V}$ must hold. □

In the next step, we provide a polynomial of $\mathcal{U}$ which multiplied by any nearest-neighbor Hamiltonian gives an operator with zero trace (if the system is composed of an odd number of modes). One key observation is that the action of the twisted reflection operator on the translation unitary is

$$\mathcal{R}\,\mathcal{U}\,\mathcal{R}^{\dagger} = \mathcal{U}^{-1}\,, \tag{G7}$$

which follows directly form the definition of $\mathcal{R}$, see Eq. (51). Using this equation and Lemma 61, one can prove the following statement:

Lemma 62. *Consider a fermionic system for which the number $d \geq 5$ of modes is odd and introduce the operator*

$$\mathcal{C}'_d = (-1)^{\lfloor d/4 \rfloor}(\mathcal{U}^2 - \mathcal{U}^{-2}) - (-1)^d(\mathcal{U}^4 - \mathcal{U}^{-4}). \tag{G8}$$

The equality $\mathrm{tr}(ih\,\mathcal{C}'_d) = 0$ *holds for any* $ih \in \mathfrak{t}_2^f$.

Proof. We will first prove that $\mathrm{tr}(v\,\mathcal{C}'_d) = 0$ holds for all $v \in \mathcal{N}_2$, where $\mathcal{N}_2$ denotes the linear space spanned by the nearest-neighbor interactions (as in Appendix F). The equation $\mathcal{R}\,\mathcal{C}'_d\,\mathcal{R}^{\dagger} = -\mathcal{C}'_d$ follows from Eq. (G7). On the other hand, Eq. (51) implies that $\mathcal{R}\,ih\,\mathcal{R}^{\dagger} = ih$ holds for any $ih \in \{ih_0, ih_{\mathrm{rh}}, ih_{\mathrm{rp}}, ih_{\mathrm{cp}}, ih_{\mathrm{int}}\}$, hence $\mathrm{tr}(ih\,\mathcal{C}'_d) = \mathrm{tr}(\mathcal{R}\,ih\,\mathcal{R}^{-1}\mathcal{R}\,\mathcal{C}'_d\,\mathcal{R}^{-1}) = -\mathrm{tr}(ih\,\mathcal{C}'_d) = 0$.

In order to calculate $\mathrm{tr}(ih_{\mathrm{ch}}\,\mathcal{C}'_d)$, we first note that using Eq. (52a) the operator ih_{ch} can be written as

$$ih_{\mathrm{ch}} = -\sum_{k=0}^{d-1} \sin(\tfrac{2\pi k}{d})\,\widetilde{m}_{2k+1}\widetilde{m}_{2k}\,. \tag{G9}$$

Next, let us expand $\mathcal{U}^2$ using Lemma 61:

$$\begin{aligned}\mathcal{U}^2 &= \prod_{k=0}^{d-1}\left[\cos(\tfrac{2\pi k}{d})\mathbb{1} - \sin(\tfrac{2\pi k}{d})\,\widetilde{m}_{2k+1}\widetilde{m}_{2k}\right]\\ &= \lambda_1\mathbb{1} - \lambda_1\sum_{k=0}^{d-1}\tan(\tfrac{2\pi k}{d})\,\widetilde{m}_{2k+1}\widetilde{m}_{2k} + M_1,\end{aligned} \tag{G10}$$

where M_1 is a linear combination of Majorana monomials of degree greater than two and $\lambda_1 := \prod_{k=0}^{d-1}\cos\left(\frac{2\pi k}{d}\right)$. Similarly, let us expand $\mathcal{U}^4$:

$$\begin{aligned}\mathcal{U}^4 &= \prod_{k=0}^{d-1}\left[\cos(\tfrac{4\pi k}{d})\mathbb{1} - \sin(\tfrac{4\pi k}{d})\,\widetilde{m}_{2k+1}\widetilde{m}_{2k}\right]\\ &= \lambda_1\mathbb{1} - \lambda_1\sum_{k=0}^{d-1}\tan(\tfrac{4\pi k}{d})\,\widetilde{m}_{2k+1}\widetilde{m}_{2k} + M_2,\end{aligned}$$

where M_2 is a linear combination of Majorana monomials of degree greater than two. We employed that $\prod_{k=0}^{d-1}\cos(\frac{4\pi k}{d}) = \prod_{k=0}^{d-1}\cos(\frac{2\pi k}{d})$ holds for odd d.

We note that all monomials of Fourier-transformed Majorana operators have zero trace and determine the traces $\mathrm{tr}(\mathcal{U}^2\,ih_{\mathrm{ch}})$ and $\mathrm{tr}(\mathcal{U}^4\,ih_{\mathrm{ch}})$ by calculating the coefficient of $\mathbb{1}$ in $\mathcal{U}^2\,ih_{\mathrm{ch}}$ and $\mathcal{U}^4\,ih_{\mathrm{ch}}$:

$$\begin{aligned}\mathrm{tr}(\mathcal{U}^2\,ih_{\mathrm{ch}}) &= 2^d\lambda_1\sum_{k=0}^{d-1}\tan(\tfrac{2\pi k}{d})\sin(\tfrac{2\pi k}{d}) = (-1)^d 2^d d\lambda_1,\\ \mathrm{tr}(\mathcal{U}^4\,ih_{\mathrm{ch}}) &= 2^d\lambda_1\sum_{k=0}^{d-1}\tan(\tfrac{4\pi k}{d})\sin(\tfrac{2\pi k}{d})\\ &= (-1)^{\lfloor d/4\rfloor}2^d d\lambda_1.\end{aligned}$$

Note that $\mathrm{tr}(ih_{\mathrm{ch}}\,\mathcal{U}^{-\ell}) = \mathrm{tr}(\mathcal{R}\,ih_{\mathrm{ch}}\,\mathcal{R}^{\dagger}\mathcal{R}\,\mathcal{U}^{-\ell}\,\mathcal{R}^{\dagger}) = -\mathrm{tr}(ih_{\mathrm{ch}}\,\mathcal{U}^{\ell})$, which allows us to conclude

$$\mathrm{tr}(ih_{\mathrm{ch}}\,\mathcal{C}'_d) = 2(-1)^{\lfloor d/4\rfloor}\,\mathrm{tr}(ih_{\mathrm{ch}}\,\mathcal{U}^2) - 2(-1)^d\,\mathrm{tr}(ih_{\mathrm{ch}}\,\mathcal{U}^4).$$

This implies that $\mathrm{tr}(\mathcal{C}'_d\,ih_{\mathrm{ch}}) = 0$, and thus $\mathrm{tr}(v\,\mathcal{C}'_d) = 0$ holds for all $v \in \mathcal{N}_2$. As $\mathcal{C}'_d$ commutes with all elements of $\mathfrak{t}_2^f$, it also follows that $\mathrm{tr}(ih\,\mathcal{C}'_d) = 0$ for any $ih \in \mathfrak{t}_2^f$. □

After these preparations we can prove Theorem 33 for odd d as summarized in the following proposition:

Proposition 63. *Consider a fermionic system with $d \geq 5$ odd modes and the Hamiltonian h_{o} of Theorem 33. The generator $ih_{\mathrm{o}} \in \mathfrak{t}_4^f$ is not contained in the system algebra $\mathfrak{t}_2^f$ of nearest-neighbor interactions.*

Proof. Using Eq. (52a), ih_{o} can be written as

$$ih_{\mathrm{o}} = -\sum_{k=0}^{d-1}\sin(\tfrac{6\pi k}{d})\,\widetilde{m}_{2k+1}\widetilde{m}_{2k}. \tag{G11}$$

Observe that $\mathrm{tr}(ih_{\mathrm{o}}\,\mathcal{U}^{-\ell}) = \mathrm{tr}(\mathcal{R}\,ih_{\mathrm{o}}\,\mathcal{R}^{\dagger}\mathcal{R}\,\mathcal{U}^{-\ell}\,\mathcal{R}^{\dagger}) = -\mathrm{tr}(ih_{\mathrm{o}}\,\mathcal{U}^{\ell})$ and conclude that the formula $\mathrm{tr}(ih_{\mathrm{o}}\,\mathcal{C}'_d) = 2(-1)^{\lfloor d/4\rfloor}\,\mathrm{tr}(ih_{\mathrm{o}}\,\mathcal{U}^2) - 2(-1)^d\,\mathrm{tr}(ih_{\mathrm{o}}\,\mathcal{U}^4)$ holds. Now, the expansion of $\mathcal{U}$ given by Eq. (G10) allows us to calculate the trace of $ih_{\mathrm{o}}\,\mathcal{C}'_d$:

$$\begin{aligned}\mathrm{tr}(ih_{\mathrm{o}}\,\mathcal{C}'_d) &= 2^{d+1}(-1)^{\lfloor d/4\rfloor}\lambda_1\sum_{k=0}^{d-1}\tan(\tfrac{2\pi k}{d})\sin(\tfrac{6\pi k}{d})\\ &\quad - 2^{d+1}(-1)^d\lambda_1\sum_{k=0}^{d-1}\tan(\tfrac{4\pi k}{d})\sin(\tfrac{6\pi k}{d})\\ &= 2^{d+1}(-1)^{\lfloor d/4\rfloor}\lambda_1(-1)^{d-1}d\\ &\quad - 2^{d+1}(-1)^d\lambda_1(-1)^{\lfloor d/4\rfloor}d\\ &= 2^{d+2}(-1)^{\lfloor d/4\rfloor}(-1)^{d-1}d\lambda_1 \neq 0.\end{aligned}$$

On the other hand, we know from Lemma 62 that the equality $\mathrm{tr}(\mathcal{C}'_d\,ih) = 0$ holds for any $ih \in \mathfrak{t}_2^f$. Therefore, $ih_{\mathrm{o}} \notin \mathfrak{t}_2^f$. □

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