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Symmetry principles in quantum systems theory

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General dynamic properties such as controllability and simulability of spin systems, fermionic and bosonic systems are investigated in terms of symmetry. Symmetries may be due to the interaction topology or due to the structure and representation of the system and control Hamiltonians. In either case, they obviously entail constants of motion. Conversely, the absence of symmetry implies irreducibility and provides a convenient necessary condition for full controllability much easier to assess than the well-established Lie-algebra rank condition. We give a complete lattice of irreducible simple subalgebras of $\mathfrak{su}(2^n)$ for up to $n = 15$ qubits. It complements the symmetry condition by allowing for easy tests solving homogeneous linear equations to filter irreducible representations of other candidate algebras of classical type as well as of exceptional types. Moreover, here we give the first single necessary and sufficient symmetry condition for full controllability. The lattice of irreducible simple subalgebras given also determines mutual simulability of dynamic systems of spin or fermionic or bosonic nature. We illustrate how controlled quadratic fermionic (and bosonic) systems can be simulated by spin systems and in certain cases also vice versa. © *2011 American Institute of Physics*. [doi:10.1063/1.3657939]

I. INTRODUCTION

Experimental control over quantum dynamics of manageable systems is paramount to exploiting the great potential of quantum systems. Both in simulation and computation the complexity of a problem may reduce upon going from a classical to a quantum setting.[1–3] On the computational end, where quantum algorithms efficiently solving hidden subgroup problems[4] have established themselves, the demands for accuracy ("error-correction threshold") may seem daunting at the moment. In contrast, the quantum simulation end is by far less sensitive. Thus simulating quantum systems[5]—in particular at phase-transitions[6,7]—has recently shifted into focus.[8–12] In view of experimental progress in cold atoms in optical lattice potentials[13,14] as well as in trapped ions,[15,16] Kraus *et al.*[17] have explored whether target quantum systems can be universally simulated on translationally invariant lattices of bosonic, fermionic, and spin systems. In some respect, their work can also be seen as a follow-up on a study by Schirmer *et al.*[18] (see also recent work by Wang *et al.*[19]) specifically addressing controllability of systems with degenerate transition frequencies. Many experimental tasks are engineering problems that profit from quantum systems theory as a framework and optimal control algorithms for solving the actual problem.

As compared to an abstract point of view,[20] the flavor of quantum systems theory pursued here is meant to be very pragmatic: it takes the causal formulation of dynamic systems[21] and does not care about specifics of the quantum measurement problem beyond the basic notions[22] and some recent developments.[23] Yet it is for these reasons that quantum systems and control has quite generally been recognized as a key generic tool[24–26] needed for advances in experimentally exploiting quantum systems for simulation or computation and even more so in future quantum technology. It

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paves the way for constructively optimizing strategies for experimental implementations in realistic settings. Moreover, since such realistic quantum systems are mostly beyond analytical tractability, numerical methods are often indispensable. To this end, gradient flows can be implemented on the control amplitudes thus iterating an initial guess into an optimized pulse scheme.[27–29] This approach has proven useful in spin systems[30] as well as in solid-state systems.[31] Moreover, it has recently been generalized from closed systems to open ones,[32] which are known to be a challenge to control,[33] where the Markovian setting can also be used as embedding of explicitly non-Markovian subsystems.[34]

However, in closed systems, the numerical tools usually require the system is universal or fully operator controllable.[35,36] For a plethora of systems with symmetry constraints we have recently determined explicit dynamic system algebras[37] (as subalgebras of $\mathfrak{su}(N)$), and conversely, we have derived design rules for the experimenter as guidelines ensuring universality of quantum architecture. While extending earlier work on branching diagrams of simple subalgebras of $\mathfrak{su}(N)$,[38,39] here we focus on *complete necessary and sufficient conditions* for full controllability (mostly) confining ourselves to arguments easy to check by inspection or to decide by computationally cheap algorithms such as solving a system of homogeneous linear equations.

In view of applications, we illustrate our findings by a comprehensive set of worked examples on spin chains. Actually Ising-ZZ coupled n-spin-$\frac{1}{2}$ chains with mostly *collective controls* or Heisenberg-XX chains with *one single local control* suffice to get *exponential growth* of dynamic degrees of freedom (in the sense their respective dynamic system algebras are $\mathfrak{sp}(2^{n-1})$ or $\mathfrak{so}(2^n)$). Our work thus adds to the recent spin-chain literature (see, e.g., Refs. 19, and 40–48 and compare Refs. 49–51) and—on a more general scale—it is anticipated to have significant impact on quantum simulation as well as distributed quantum computing (see, e.g., Refs. 52–54).

II. OVERVIEW AND MAIN RESULTS

More precisely, the first main part develops, starting from the basic notions of controllability (Sec. III) in terms of coupling graphs (Sec. IV) and their symmetries (Sec. V), *a single necessary and sufficient symmetry condition for full controllability* (Sec. VII). To this end and in view of practical applications, Sec. VI gives branching diagrams of *all irreducible simple subalgebras of the unitary algebras* $\mathfrak{su}(N)$ with $N \leq 2^{15}$. Concomitantly, we provide a set of efficient computational *algorithms for assessing controllability* by merely solving systems of homogeneous linear equations.

The second part focuses on simulability (Sec. VIII) in terms of dynamic system algebras. A plethora of worked examples is discussed in Sec. IX including *four full series of qubit chains coupled by pair interactions* such that their dynamic system algebras for the first three cases are $\mathfrak{so}(2n+1)$, $\mathfrak{so}(2n+2)$, and $\mathfrak{sp}(2^{n-1})$, respectively. Most remarkably, for $n \geq 4$, the fourth series results in dynamic system algebras $\mathfrak{so}(2^n)$ if (n mod 4) $\in \{0, 1\}$ and $\mathfrak{sp}(2^{n-1})$ else. The findings also interrelate spin systems, fermionic systems (Sec. X), and bosonic systems (Sec. XI). The algebraic conditions for simulability given are sufficient to ensure the existence of solutions to the actual task of quantum simulation of closed systems formulated as an observed optimal control problem in the outlook (Sec. XII).

Preliminary material to Secs. III, V, VI, and VII (without Subsection VII D) was presented as conference papers.[55,56]

III. CONTROLLABILITY

Consider the controlled Schrödinger equation lifted to unitary maps (quantum gates)

$$\dot{U}(t) = -i\big(H_d + \sum_{j=1}^{m} u_j(t) H_j\big)\, U(t)\,. \tag{1}$$

Here the system Hamiltonian H_d denotes a non-switchable drift term and the control Hamiltonians H_j can be steered by (piece-wise constant) control amplitudes $u_j(t) \in \mathbb{R}$ taken to be unbounded henceforth. The equation of motion governs the evolution of a unitary map of an entire basis set of vectors representing pure states. Using the short-hand notations $H := H_d + \sum_{j=1}^m u_j(t)H_j$ and $\mathrm{ad}_H(\mathrm{vec}\, A) := [H, A]$, the Liouville equation $\dot\rho(t) = -i[H, \rho(t)]$ can be rewritten

$$\mathrm{vec}\,\dot\rho(t) = -i\ \mathrm{ad}_H\ \mathrm{vec}\,\rho(t). \tag{2}$$

Both equations of motion take the form of a standard *bilinear control system* (Σ) known in classical systems and control theory[57]

$$\dot X(t) = \big(A + \sum_{j=1}^m u_j(t)B_j\big)\ X(t) \tag{3}$$

with "state" $X(t) \in \mathbb{C}^N$, drift $A \in \mathfrak{gl}(N, \mathbb{C})$, controls $B_j \in \mathfrak{gl}(N, \mathbb{C})$, and control amplitudes $u_j \in \mathbb{R}$, where $\mathfrak{gl}(N, \mathbb{C})$ denotes the set of complex $N \times N$ matrices. Since all the control systems considered henceforth are bilinear, we often drop the specification bilinear for short. Now lifting the (bilinear) control system (Σ) to group manifolds[58,59] by $X(t) \in GL(N, \mathbb{C})$, i.e., the set of non-singular complex $N \times N$ matrices, under the action of a compact connected Lie group $\mathbf{K}$ with Lie algebra $\mathfrak{k}$ while keeping $A, B_j \in \mathfrak{gl}(N, \mathbb{C})$, the condition for full controllability turns into the *Lie algebra rank condition*[59–61]

$$\langle A, B_j \mid j = 1, 2, \ldots, m\rangle_{\mathrm{Lie}} = \mathfrak{k}, \tag{4}$$

where $\langle\cdot\rangle_{\mathrm{Lie}}$ denotes (the linear span over) the *Lie closure* obtained by repeatedly taking mutual commutator brackets. **Algorithm 1** gives an explicit method to compute the Lie closure, see also Ref. 62.

Algorithm 1: Determine system algebra via Lie closure.

Input: Hamiltonians $I := \{iH_d; iH_1, \ldots, iH_m\} \subseteq \mathfrak{su}(N)$
1. $B :=$ maximal linearly independent subset of I
2. num $:= \#B$
3. If num $= N^2 - 1$ then $O := B$ else $O := \{\ \}$
4. If num $= N^2 - 1$ or $\#B = 0$ then terminate
5. $C := [O, B] \cup [B, B]$, where $[S_1, S_2] = \{[s_1, s_2] \mid s_1 \in S_1, s_2 \in S_2\}$
6. $O := O \cup B$
7. $B :=$ max. linear independent extension of O with elements from C
8. num $:=$ num $+ \#B$; Go to 4

Output: basis O of the generated Lie algebra and its dimension num

The complexity is roughly $\mathcal{O}(N^6 N^2)$, as about N^2 times a rank-revealing *LU* (or *QR*) decomposition has to be performed in Liouville space (with dimension N^2). For n qubits, $N := 2^n$.

Transferring the classical result[61] to the quantum domain,[36,63,64] the bilinear system of Eq. (1) is *fully (operator) controllable* if and only if the drift and controls are a generating set of the special unitary algebra $\mathfrak{su}(N)$:

$$\langle iH_d, iH_j \mid j = 1, 2, \ldots, m\rangle_{\mathrm{Lie}} = \mathfrak{k} = \mathfrak{su}(N). \tag{5}$$

In fully controllable systems, to every initial state ρ_0 the *reachable set* is the entire unitary orbit $\mathcal{O}_{\mathrm{U}}(\rho_0) := \{U\rho_0 U^\dagger \mid U \in SU(N)\}$. 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. Thus reachable sets and isospectral sets coincide.

In contrast, in systems with restricted controllability the Hamiltonians generate but a proper subalgebra of the full unitary algebra

$$\langle iH_d, iH_j \mid j = 1, 2, \ldots, m\rangle_{\mathrm{Lie}} = \mathfrak{k} \subsetneq \mathfrak{su}(N). \tag{6}$$

Then the dynamic group $\mathbf{K} := \exp \mathfrak{k}$ is but a proper subgroup $\mathbf{K} \subsetneq SU(N)$ of the full unitary group. Therefore, the corresponding *reachable sets* take the form of subgroup orbits of initial states

$$\mathfrak{reach}(\rho_0) = \mathcal{O}_{\mathbf{K}}(\rho_0) := \{K\rho_0 K^\dagger \mid K \in \mathbf{K} \subsetneq SU(N)\}. \tag{7}$$

IV. NATURAL TENSOR-PRODUCT STRUCTURE AND COUPLING GRAPHS IN QUBIT SYSTEMS WITH PAIR INTERACTIONS

We start out with the case of qubit systems coupled by pair interactions. Yet quantum simulation of effective many-body interactions in multi-level systems requires more refined notions, see Appendixes A and B. Thus, we choose a line-of-thought allowing for the extensions needed later in a natural way while trying to keep the overhead minimal here. Finally, it should be stressed that the results in Secs. V and VII are valid in full generality of Appendixes A and B.

To fix the basic terminology, observe that the abstract *direct sum* of Lie algebras has a matrix representation as the *Kronecker sum*, e.g., $\mathfrak{su}(d_1) \,\widehat{\oplus}\, \mathfrak{su}(d_2) := \mathfrak{su}(d_1) \otimes \mathbb{1}_{d_2} + \mathbb{1}_{d_1} \otimes \mathfrak{su}(d_2)$ and that it generates a group isomorphic to the *Kronecker product* (i.e., tensor product) $\mathbf{G} = SU(d_1) \otimes SU(d_2)$. The abstract direct sum of two algebras $\mathfrak{h}_1$ and $\mathfrak{h}_2$ (each given in an irreducible representation) has itself an irreducible representation as a single Kronecker sum $\mathfrak{h}_1 \,\widehat{\oplus}\, \mathfrak{h}_2$ (Theorem 11.6.II of Ref. 65). Such an irreducible direct sum representation always exists for every semi-simple Lie algebra which is not simple.

Control systems consisting of n qubits are usually embedded in $\mathfrak{su}(N)$ with $N := 2^n$. Their natural intrinsic *tensor-product structure* takes the form of the n-fold Kronecker sum $\mathfrak{su}(2) \,\widehat{\oplus}\, \mathfrak{su}(2) \,\widehat{\oplus}\, \cdots \,\widehat{\oplus}\, \mathfrak{su}(2)$. An N^2-1 dimensional skew-Hermitian tensor basis with respect to this tensor-product structure can be given in terms of the Pauli matrices

$$\mathrm{I} := \mathbb{1}_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \mathrm{X} := \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \mathrm{Y} := \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \text{ and } \mathrm{Z} := \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{8}$$

by defining the elements $-\frac{i}{2}\mathrm{H}_1\mathrm{H}_2\cdots\mathrm{H}_n$, where $\mathrm{H}_1\mathrm{H}_2\cdot\cdot\cdot\mathrm{H}_n := \mathrm{H}_1\otimes\mathrm{H}_2\otimes\cdot\cdot\cdot\otimes\mathrm{H}_n$ and $\mathrm{H}_j \in \{\mathrm{I}, \mathrm{X}, \mathrm{Y}, \mathrm{Z}\}$. The element corresponding to $\mathrm{H}_1 = \mathrm{H}_2 = \cdots = \mathrm{H}_n = \mathrm{I}$ is not traceless and hence cannot occur in $\mathfrak{su}(2^n)$. In terms of this tensor basis, we write Hamiltonians as linear combinations ($c_k \in \mathbb{R}$)

$$H = \sum_{k=1}^{m} c_k \mathcal{H}_k \tag{9}$$

of elements $\mathcal{H}_k = -\frac{i}{2}(\mathcal{H}_{k,1} \otimes \mathcal{H}_{k,2} \otimes \cdots \otimes \mathcal{H}_{k,n})$ with $\mathcal{H}_{k,j} \in \{\mathrm{I}, \mathrm{X}, \mathrm{Y}, \mathrm{Z}\}$. Considering local controls and pairwise coupling interactions the orders of the constituents are confined, i.e.,

$$\mathrm{ord}(\mathcal{H}_k) := \#\{\ell \,:\, \mathcal{H}_{k,\ell} \neq \mathbb{1}_2\} \in \{1, 2\}.$$

Usually, the control Hamiltonians H_j are local, i.e., all terms in Eq. (9) (for $H = H_j$) are of order one, while the corresponding terms in Eq. (9) for the drift Hamiltonian $H_0\ (= H)$ are of order two comprising the non-switchable *pairwise* coupling terms.

Now, in a *coupling graph* the vertices representing the local subsystems are connected by edges, where each edge stands for a pairwise coupling term occurring in the drift Hamiltonian H_d. An example of a *connected* coupling graph is shown in Figure 1. — Connected coupling graphs are essential for full controllability as elucidated by the following theorem:

Theorem 1: *Consider a bilinear control system with pair interactions on* $\mathfrak{su}(2^n)$*, where all the local subsystems* $\mathfrak{su}(2)$ *are independently fully controllable so the dynamic algebra* $\mathfrak{k} \supseteq \mathfrak{su}(2) \,\widehat{\oplus}\, \mathfrak{su}(2) \,\widehat{\oplus}\, \cdots \,\widehat{\oplus}\, \mathfrak{su}(2)$*. Then the system is fully controllable, i.e.,* $\mathfrak{k} = \mathfrak{su}(2^n)$*, if and only if its coupling graph is connected. In particular,* $\mathfrak{k} = \mathfrak{su}(2^n)$ *is simple.*

Proof: A proof is given in Ref. 66 (see Theorem 2, Remark 5.1, and Theorem 4), see also Ref. 64. □

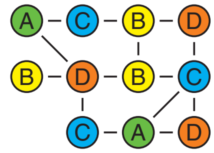


FIG. 1. (Color online) General coupling topology represented by a connected graph. The vertices denote the spin-$\frac{1}{2}$ qubits, while the edges represent pairwise couplings (e.g., of Heisenberg or Ising type). Qubits of the same color and letter are taken to be affected by joint local unitary operations (or none if the color is white), while qubits of different kind can be controlled independently. For a system to show an outer symmetry brought about by permutations within subsets of qubits of the same type, both the graph as well as the system plus all control Hamiltonians have to remain invariant.

V. SYMMETRY-CONSTRAINED CONTROLLABILITY

A Hamiltonian quantum system is said to have a symmetry expressed by the skew-Hermitian *symmetry operator* $s \in \mathfrak{su}(N)$, if

$$[s, H_\nu] = 0 \quad \text{for all} \quad \nu \in \{d; 1, 2, \ldots, m\}. \tag{10}$$

More precisely, we use the term *outer symmetry* if s generates a SWAP operation permuting a subset of qubits of the same type (cf. Fig. 1) such that the coupling graph and all Hamiltonians $\{H_\nu\}$ are left invariant. Now subsets of qubits are termed *indistinguishable* if and only if they can be interchanged by an outer symmetry, i.e., a SWAP operation that is a symmetry of the system; otherwise they are *distinguishable*. In contrast, an *inner symmetry* relates to elements s not generating a SWAP operation in the symmetric group of all qubit permutations.

In either case, a symmetry operator is an element of the *centralizer*

$$\{H_\nu\}' := \mathcal{Z}_{\mathfrak{su}(N)}(\{H_\nu\}) = \Big\{s \in \mathfrak{su}(N) \,|\, [s, H_\nu] = 0 \quad \forall \nu \in \{d; 1, 2, \ldots, m\}\Big\}, \tag{11}$$

recalling that the centralizer of a given subset $\mathfrak{m} \subseteq \mathfrak{su}(N)$ with respect to a Lie algebra $\mathfrak{su}(N)$ consists of all elements in $\mathfrak{su}(N)$ commuting with all elements in $\mathfrak{m}$. Jacobi's identity $[[a, b], s] + [[b, s], a] + [[s, a], b] = 0$ gives two useful facts: (1) an element s that commutes with the Hamiltonians $\{iH_\nu\}$ also commutes with their Lie closure $\mathfrak{k}$. For the dynamic Lie algebra $\mathfrak{k}$ we have

$$\mathfrak{k}' := \mathcal{Z}_{\mathfrak{su}(N)}(\mathfrak{k}) = \{s \in \mathfrak{su}(N) \mid [s, k] = 0 \quad \forall k \in \mathfrak{k}\}, \tag{12}$$

and hence $\{iH_\nu\}' \equiv \mathfrak{k}'$. Thus in practice it is (most) convenient to just evaluate the centralizer for a (minimal) generating set $\{iH_\nu\}$ of $\mathfrak{k}$ since the overall symmetry properties can be read from the local symmetries of the constituent Hamiltonians. Fact (2) means the centralizer $\mathfrak{k}'$ forms itself an invariant Lie subalgebra (or ideal) to $\mathfrak{su}(N)$ collecting *all symmetries*. In summary, we obtain the following straightforward, yet important result:

Theorem 2: *Lack of symmetry in the sense of a trivial centralizer is a necessary condition for full controllability.*

Proof: Any non-trivial element in the centralizer would generate a one-parameter subgroup in $\mathbf{K}' \subset SU(N)$ that is *not* in $\mathbf{K} = \exp \mathfrak{k}$. □

Algorithm 2: Determine centralizer (respectively commutant) to system algebra $\mathfrak{k}$.

Input: Hamiltonians $I := \{iH_d; iH_1, \ldots, iH_m\} \subseteq M$
1. For each $H \in I$ solve the homog. linear eqn. $\mathcal{S}_H := \{s \in M | (\mathbb{1} \otimes H - H^t \otimes \mathbb{1}) \operatorname{vec}(s) = 0\}$
2. $R := \bigcap_{H \in I} \mathcal{S}_H$
Output: R = either centralizer $\mathfrak{k}'$ [if $M = \mathfrak{su}(N)$] or commutant of $\mathfrak{k}$ [if $M = \mathfrak{gl}(N, \mathbb{C})$]

The complexity is roughly $\mathcal{O}((m+1)N^6)$, as in Liouville space $(m+1)N^2$ homogeneous linear equations have to be solved by *LU* decomposition (cf. p. 102 of Ref. 67). For n qubits, $N := 2^n$, we have $m \ll N$.

Throughout this paper, we consider finite-dimensional complex matrix representations of Lie algebras, a representation being a map from a given Lie algebra to the set of complex square matrices of appropriate (and finite) dimension. The matrix entries are given by complex polynomial (or equivalently holomorphic) functions. In the following, we will usually not consider the trivial representation, which maps any element to $1 \in \mathbb{C}$. One particular important example for a representation of a Lie algebra is the standard representation, which is the lowest-dimensional (non-trivial) representation (with some exceptions, see Appendix C) and which is typically used to define the corresponding Lie algebra in its matrix form. In analogy to the centralizer, one can define the *commutant* relative to a representation ϕ of dimension $\dim(\phi)$

$$\mathrm{comm}_\phi(\mathfrak{m}) := \left\{ g \in \mathfrak{gl}(\dim(\phi), \mathbb{C}) \,|\, [g, \phi(m)] = 0 \quad \forall m \in \mathfrak{m} \right\} \tag{13}$$

for a subset $\mathfrak{m} \subset \mathfrak{g}$ of a Lie algebra $\mathfrak{g}$. Now it is natural to ask how the notions of centralizer and commutant relate to irreducible representations.

Lemma 3: Let Φ denote the standard representation of $\mathfrak{su}(N)$. If $\mathfrak{k} \subseteq \mathfrak{su}(N)$, then the following statements are equivalent:

(1) The centralizer $\mathfrak{k}' = \mathcal{Z}_{\mathfrak{su}(N)}(\mathfrak{k})$ of $\mathfrak{k}$ in $\mathfrak{su}(N)$ is trivial, i.e., zero.
(2) The restriction of Φ from $\mathfrak{su}(N)$ to $\mathfrak{k}$ is irreducible.
(3) The commutant $\mathrm{comm}_\Phi(\mathfrak{k})$ of $\mathfrak{k}$ with respect to Φ is trivial, i.e., $= \{c \cdot \mathbb{1}_N \,|c \in \mathbb{C}\}$.

Proof: As $\mathfrak{su}(N)$ is compact, it follows that Φ and its restriction to $\mathfrak{k}$ are completely reducible in the sense of being a direct sum of irreducible representations (see Corollary 2.17 of Ref. 68). The representation Φ is even irreducible and faithful, i.e., injective. Hereafter, we will consider the complexification $\mathfrak{k}_\mathbb{C}$ of $\mathfrak{k}$ and $\mathfrak{su}(N)_\mathbb{C} = \mathfrak{sl}(N, \mathbb{C})$ as complexification of $\mathfrak{su}(N)$. The representation Φ has a unique extension $\Phi_\mathbb{C}$ to $\mathfrak{sl}(N, \mathbb{C})$, which is also irreducible and faithful. In addition, $\Phi_\mathbb{C}$ and its restriction to $\mathfrak{k}_\mathbb{C}$ are completely reducible. These facts can be deduced from Theorem 1, pp. 111–112 of Ref. 69 and Proposition 7.5 of Ref. 70.

Now it follows that (1) is equivalent to $\mathcal{Z}_{\mathfrak{sl}(N,\mathbb{C})}(\mathfrak{k}_\mathbb{C}) = \{0\}$. As $\Phi_\mathbb{C}$ is faithful, this holds if and only if $\mathrm{comm}_{\Phi_\mathbb{C}}(\mathfrak{k}_\mathbb{C})$ is trivial. Relying on the fact that $\Phi_\mathbb{C}$ is completely reducible, $\mathrm{comm}_{\Phi_\mathbb{C}}(\mathfrak{k}_\mathbb{C})$ is trivial if and only if the restriction of $\Phi_\mathbb{C}$ from $\mathfrak{sl}(N, \mathbb{C})$ to $\mathfrak{k}_\mathbb{C}$ is irreducible. Using Theorem 1, pp. 111–112 of Ref. 69, this is equivalent to (2). As Φ is completely reducible, (2) and (3) are equivalent. □

As a second consequence of a trivial centralizer the corresponding subalgebra $\mathfrak{k}$ of $\mathfrak{su}(N)$ has to be simple or semi-simple:

Lemma 4: Let $\mathfrak{k} \subseteq \mathfrak{su}(N)$ be a subalgebra to the Lie algebra $\mathfrak{su}(N)$. If its centralizer $\mathfrak{k}'$ in $\mathfrak{su}(N)$ is trivial, then $\mathfrak{k}$ is simple or semi-simple.

Proof: By compactness, $\mathfrak{k} = \mathfrak{z}_\mathfrak{k} \oplus \mathfrak{s}$ decomposes into its center $\mathfrak{z}_\mathfrak{k}$ and a semi-simple part $\mathfrak{s}$ (see, e.g., Corollary IV.4.25 of Ref. 70). As the center $\mathfrak{z}_\mathfrak{k} = \mathfrak{k}' \cap \mathfrak{k}$ is trivial, $\mathfrak{k}$ can only be *semi-simple* or *simple*. □

Note that the centralizer is "exponentially" easier to come by than the Lie closure in the sense of comparing the asymptotic complexity $\mathcal{O}(N^6 \cdot N^2)$ (with $N := 2^n$ for n qubits) of **Algorithm 1** for the Lie closure with the asymptotic complexity $\mathcal{O}((m{+}1)N^6)$ of **Algorithm 2** for the centralizer tabulated above, because $m \ll N$. — Therefore one would like to fill the gap between lack of symmetry as a necessary condition and sufficient conditions for full controllability in systems with a connected coupling topology. For pure-state controllability, this was analyzed in Ref. 66, for operator controllability the issue has been raised in Ref. 25, *inter alia* following the lines of Refs. 71 and 72, however, without a full answer. Further results in the case of pure-state controllability can be found in Ref. 39.

We have proven that the lack of symmetry is necessary for a control system to be fully controllable. Yet, in turn, a control system without symmetry need not be fully controllable, as the following elementary (and pathological) example shows:

Example 5: Assume we have a bilinear control system on two qubits, where the dynamic Lie algebra $\mathfrak{k} = \langle i\mathrm{XI}, i\mathrm{YI}, i\mathrm{ZI}, i\mathrm{IX}, i\mathrm{IY}, i\mathrm{IZ}\rangle_{\mathrm{Lie}} = \mathfrak{su}(2) \widehat{\oplus} \mathfrak{su}(2)$ is not simple. Although it has no symmetry and its centralizer $\mathfrak{k}'$ is in fact trivial, the system is not fully controllable: all pair terms like *i*ZZ cannot be generated, since its pathological "coupling graph" (Color online)

is clearly not connected.

Nevertheless, the somewhat trivial example is illuminating. While in the context of *C**-algebras, von Neumann's double-commutant theorem recovers the original algebra from the commutant of its commutant,[73,74] a similar theorem does not extend to Lie algebras.[75] Rather, if the dynamic algebra $\mathfrak{k} \subseteq \mathfrak{su}(N)$ has a trivial centralizer $\mathfrak{k}'$, then the double centralizer $\mathfrak{k}''$, i.e., the centralizer of the centralizer in $\mathfrak{su}(N)$, of all compact semi-simple and simple irreducible proper and improper subalgebras $\mathfrak{k}$ of $\mathfrak{su}(N)$ is given by $\mathfrak{su}(N)$ in line with Lemma 4. However, if one considers the associative matrix algebra (with identity) generated by the basis elements (including the identity matrix) of a Lie algebra via its standard representation, then von Neumann's double commutant theorem still holds, see Theorem (3.5.D) of Ref. 76. In the next step, we will thus add a criterion to single out the simple subalgebras.

Motivated by Example 5 one might conjecture that the dynamic algebra $\mathfrak{k}$ is simple if $\mathfrak{k}$ acts irreducibly and the coupling graph of the control system is connected. This is true for control systems in qubits with pairwise coupling interactions:

Theorem 6: *Consider a bilinear control system with pair interactions on* $\mathfrak{su}(2^n)$. *Assume that the tensor-product structure is given by* $\mathfrak{su}(2) \widehat{\oplus} \mathfrak{su}(2) \widehat{\oplus} \cdots \widehat{\oplus} \mathfrak{su}(2)$ *and that the centralizer* $\mathfrak{k}'$ *of the dynamic algebra* $\mathfrak{k}$ *is trivial. The dynamic algebra* $\mathfrak{k}$ *is simple if and only if the coupling graph of the control system is connected.*

Proof: See Corollary 43(2) in Appendix B. □

The general case beyond pair interactions (and qubit systems) is discussed in Appendix B. In the case of pair interactions, we say a control system is *connected* if its coupling graph is connected. This definition of a connected control system is a particular case of the general definition (see Appendix B) applicable to control systems which do not have a natural coupling graph.

VI. IRREDUCIBLE SIMPLE SUBALGEBRAS OF $\mathfrak{su}(N)$

Starting from the knowledge that for a fully controllable system the dynamic algebra $\mathfrak{k}$ has to be simple and given in an irreducible representation (see, e.g., Appendix B), it is natural to ask for a classification of all these cases. Following the work of Killing, Élie Cartan[77] classified all simple (complex) Lie algebras (see, e.g., Ref. 78 and 79). The corresponding compact real forms[79,80] are the compact simple Lie algebras of classical type (assuming $\ell \in \mathbb{N} \setminus \{0\}$ henceforth):

$$\begin{aligned}
\mathfrak{a}_\ell &: \quad \mathfrak{su}(\ell+1),\\
\mathfrak{b}_\ell &: \quad \mathfrak{so}(2\ell+1),\\
\mathfrak{c}_\ell &: \quad \mathfrak{sp}(\ell) := \mathfrak{sp}(2\ell, \mathbb{C}) \cap \mathfrak{u}(2\ell, \mathbb{C}),\\
\mathfrak{d}_\ell &: \quad \mathfrak{so}(2\ell),
\end{aligned}$$

and of exceptional type $\mathfrak{e}_6$, $\mathfrak{e}_7$, $\mathfrak{e}_8$, $\mathfrak{f}_4$, $\mathfrak{g}_2$. Note also that for $\mathfrak{a}_\ell$ ($\ell \geq 1$), $\mathfrak{b}_\ell$ ($\ell \geq 2$), $\mathfrak{c}_\ell$ ($\ell \geq 3$), and $\mathfrak{d}_\ell$ ($\ell \geq 4$) the following isomorphisms (see, e.g., Theorem X.3.12 in Ref. 80) $\mathfrak{su}(2) \cong \mathfrak{so}(3) \cong \mathfrak{sp}(1)$, $\mathfrak{so}(5) \cong \mathfrak{sp}(2)$, and $\mathfrak{su}(4) \cong \mathfrak{so}(6)$ are no longer of concern. The same holds for the abelian case $\mathfrak{so}(2)$ as well as for the semi-simple one $\mathfrak{so}(4) \cong \mathfrak{su}(2) \widehat{\oplus} \mathfrak{su}(2)$.

Pro memoria: The classical, compact simple Lie algebras and some forms of their standard matrix representations may be given as follows:

Algebra	Definition and block forms ($U \in SU(N)$; $A, B, C \in \mathbb{C}^{\ell\times\ell}$; $u, v \in \mathbb{C}^\ell$)	Lie dimension
$\mathfrak{su}(N) := \{a \in \mathbb{C}^{N\times N} \mid a^\dagger = -a,\ \operatorname{tr} a = 0\}$		$N^2 - 1$
$\mathfrak{so}(N) := \{a = U\tilde{a}U^\dagger \in \mathbb{C}^{N\times N} \mid \tilde{a}^t = -\tilde{a},\ \operatorname{tr}\tilde{a} = 0, \tilde{a} \text{ real}\}$		$\frac{1}{2}N(N-1)$
$N = 2\ell$:	$a' = \begin{pmatrix} A & B \\ C & -A^t \end{pmatrix}$ where $A = -A^\dagger$ and $B = -B^t = -C^\dagger = \bar{C}$	
$N = 2\ell + 1$:	$a' = \begin{pmatrix} A & B & u \\ C & -A^t & v \\ -u^t & -v^t & 0 \end{pmatrix}$ with A, B, C as above and u, v real	
NB: The representations a' above need not be skew-symmetric themselves.		
$\mathfrak{sp}(N/2) := \{a = U\tilde{a}U^\dagger \in \mathbb{C}^{N\times N} \mid \tilde{a} = -\tilde{a}^\dagger, J\tilde{a} = -\tilde{a}^t J, \text{ and } J := \left(\begin{smallmatrix} 0 & -\mathbb{1}_\ell \\ \mathbb{1}_\ell & 0 \end{smallmatrix}\right)\}$		$\frac{1}{2}N(N+1)$
$N = 2\ell$:	$\tilde{a} = \begin{pmatrix} A & B \\ C & -A^t \end{pmatrix}$ where $A = -A^\dagger$ and $B = B^t = -C^\dagger = -\bar{C}$	

We remark that the list of *algebras* is indeed complete—note that in particular spin and pin *groups* are also generated by the algebras $\mathfrak{so}(N)$ and $\mathfrak{o}(N)$, respectively.[81] Therefore, Cartan's classification may be summarized as follows:

Corollary 7 (Candidate list)*: Consider a bilinear control system, where the drift and control Hamiltonians* $\{iH_\nu\}$ *generate the dynamic system Lie algebra* $\mathfrak{k} \subseteq \mathfrak{su}(N)$ *in an irreducible representation (*$\mathfrak{k}'$ *trivial) with the additional promise that* $\mathfrak{k}$ *is simple (e.g., due to a connected control system). Then, being a simple subalgebra of* $\mathfrak{su}(N)$*, the system algebra* $\mathfrak{k}$ *has to be one of the candidate compact simple Lie algebras:* $\mathfrak{su}(\ell+1)$*,* $\mathfrak{so}(2\ell+1)$*,* $\mathfrak{sp}(\ell)$*,* $\mathfrak{so}(2\ell)$*,* $\mathfrak{e}_6$*,* $\mathfrak{e}_7$*,* $\mathfrak{e}_8$*,* $\mathfrak{f}_4$*, or* $\mathfrak{g}_2$. □

For illustration of the Lie algebras of exceptional type, consider the dimensions of their standard representations (see, e.g., p. 218 of Ref. 79 or Refs. 82 and 83) $\mathfrak{e}_6 \subset \mathfrak{su}(27)$, $\mathfrak{e}_7 \subset \mathfrak{sp}(28)$, $\mathfrak{e}_8 \subset \mathfrak{so}(248)$, $\mathfrak{f}_4 \subset \mathfrak{so}(26)$, and $\mathfrak{g}_2 \subset \mathfrak{so}(7)$. As a final remark on exceptional Lie algebras suffice it to add that—with the single exception of $\mathfrak{g}_2$—they all fail to generate groups acting transitively on the sphere or on $\mathbb{R}^N \setminus \{0\}$. This has been shown in Refs. 57 and 84 building upon results of Ref. 85 to fill gaps in earlier work of Refs. 86 and 87.

Having listed all the candidates for proper simple subalgebras of $\mathfrak{su}(N)$, we now focus on the set of possible irreducible representations. To this end, in this chapter we describe the main results, while all the details shall be explained in Appendix C. The irreducible representations of simple (complex) Lie algebras were already determined by Élie Cartan.[88] This classification is equivalent for the compact simple Lie algebras (or the compact, simply connected, and simple Lie groups), see, e.g., Ref. 79. The irreducible simple subalgebras of $\mathfrak{su}(N)$ are found by enumerating for all simple Lie algebras all their irreducible representations of dimension N. The dimensions of the irreducible representations can be efficiently computed using computer algebra systems such as LiE[89] and MAGMA[90] via Weyl's dimension formula. Following the work of Dynkin[91,92] (see Appendix C 3 and Chap. 6, Sec. 3.2 of Ref. 93), one can determine the inclusion relations between irreducible simple subalgebras of $\mathfrak{su}(N)$. We obtained *all* the irreducible simple subalgebras of $\mathfrak{su}(N)$ for $N \leq 2^{15}$

TABLE I. The irreducible simple subalgebras of $\mathfrak{su}(N)$ for $N \leq 16$.

$\mathfrak{su}(N)$	Irreducible simple subalgebras
$\mathfrak{su}(2)$	$\mathfrak{su}(2)$
$\mathfrak{su}(3)$	$\mathfrak{su}(2) \leftarrow \mathfrak{su}(3)$
$\mathfrak{su}(4)$	$\mathfrak{su}(2) \leftarrow \mathfrak{sp}(2) \leftarrow \mathfrak{su}(4)$
$\mathfrak{su}(5)$	$\mathfrak{su}(2) \leftarrow \mathfrak{so}(5) \leftarrow \mathfrak{su}(5)$
$\mathfrak{su}(6)$	$\mathfrak{su}(2) \leftarrow \mathfrak{sp}(3) \leftarrow \mathfrak{su}(6)$; $\mathfrak{so}(6) \leftarrow \mathfrak{su}(6)$; $\mathfrak{su}(3) \leftarrow \mathfrak{su}(6)$
$\mathfrak{su}(7)$	$\mathfrak{su}(2) \leftarrow \mathfrak{g}_2 \leftarrow \mathfrak{so}(7) \leftarrow \mathfrak{su}(7)$
$\mathfrak{su}(8)$	$\mathfrak{su}(2) \leftarrow \mathfrak{sp}(4) \leftarrow \mathfrak{su}(8)$; $\mathfrak{su}(3) \leftarrow \mathfrak{so}(8) \leftarrow \mathfrak{su}(8)$; $\mathfrak{so}(7) \leftarrow \mathfrak{so}(8)$
$\mathfrak{su}(9)$	$\mathfrak{su}(2) \leftarrow \mathfrak{so}(9) \leftarrow \mathfrak{su}(9)$
$\mathfrak{su}(10)$	$\mathfrak{su}(2) \leftarrow \mathfrak{sp}(5) \leftarrow \mathfrak{su}(10)$; $\mathfrak{so}(5) \leftarrow \mathfrak{so}(10) \leftarrow \mathfrak{su}(10)$; $\mathfrak{su}(3) \leftarrow \mathfrak{su}(10)$; $\mathfrak{su}(4) \leftarrow \mathfrak{su}(10)$; $\mathfrak{su}(5) \leftarrow \mathfrak{su}(10)$
$\mathfrak{su}(11)$	$\mathfrak{su}(2) \leftarrow \mathfrak{so}(11) \leftarrow \mathfrak{su}(11)$
$\mathfrak{su}(12)$	$\mathfrak{su}(2) \leftarrow \mathfrak{sp}(6) \leftarrow \mathfrak{su}(12)$; $\mathfrak{so}(12) \leftarrow \mathfrak{su}(12)$
$\mathfrak{su}(13)$	$\mathfrak{su}(2) \leftarrow \mathfrak{so}(13) \leftarrow \mathfrak{su}(13)$
$\mathfrak{su}(14)$	$\mathfrak{su}(2) \leftarrow \mathfrak{sp}(7)$; $\mathfrak{sp}(3) \leftarrow \mathfrak{sp}(7)$; $\mathfrak{sp}(7) \leftarrow \mathfrak{su}(14)$; $\mathfrak{so}(5) \leftarrow \mathfrak{so}(14)$; $\mathfrak{sp}(3) \leftarrow \mathfrak{so}(14)$; $\mathfrak{g}_2 \leftarrow \mathfrak{so}(14)$; $\mathfrak{so}(14) \leftarrow \mathfrak{su}(14)$
$\mathfrak{su}(15)$	$\mathfrak{su}(2) \leftarrow \mathfrak{so}(15)$; $\mathfrak{so}(6) \leftarrow \mathfrak{so}(15)$; $\mathfrak{so}(15) \leftarrow \mathfrak{su}(15)$; $\mathfrak{su}(3) \leftarrow \mathfrak{su}(15)$; $\mathfrak{su}(5) \leftarrow \mathfrak{su}(15)$; $\mathfrak{su}(3) \leftarrow \mathfrak{su}(6) \leftarrow \mathfrak{su}(15)$
$\mathfrak{su}(16)$	$\mathfrak{su}(2) \leftarrow \mathfrak{sp}(8)$; $\mathfrak{sp}(2) \leftarrow \mathfrak{sp}(8)$; $\mathfrak{sp}(8) \leftarrow \mathfrak{su}(16)$; $\mathfrak{so}(9) \leftarrow \mathfrak{so}(16) \leftarrow \mathfrak{su}(16)$; $\mathfrak{so}(10) \leftarrow \mathfrak{su}(16)$

NB: $\mathfrak{so}(3) \cong \mathfrak{su}(2) \cong \mathfrak{sp}(1)$, $\mathfrak{so}(5) \cong \mathfrak{sp}(2)$, and $\mathfrak{so}(6) \cong \mathfrak{su}(4)$.

$= 32\,768$. This significantly extends previous work[38,39] for $N \leq 9$. The results for $N \leq 16$ are given in Table I, those for $N = 2^n$ and $1 \leq n \leq 15$ are relegated to Table II. A complete list with all the results for $N \leq 2^{15}$ is available as supplementary material in the online version of this article.[94]

Remark 8: With regard to Tables I and II, the occurrence of $\mathfrak{su}(2)$ as an *irreducible* simple subalgebra to any $\mathfrak{su}(N)$ with $N \geq 2$ is natural from the point of view of spin physics. We identify $\mathfrak{su}(N) = \mathfrak{su}(2j+1)$, where the (non-vanishing) half-integer and integer spin-quantum numbers may take the values $j \in \{\frac{1}{2}, 1, \frac{3}{2}, 2, \dots\}$. Now to any such j there is an irreducible spin-j representation of the three Pauli matrices generating $\mathfrak{su}(2)$. For instance, in $\mathfrak{su}(4)$ there is an irreducible spin-$\frac{3}{2}$ representation of $\mathfrak{su}(2)$ as a proper *irreducible* subalgebra $\mathfrak{su}(2) \subsetneq \mathfrak{su}(4)$. In contrast, the Gell-Mann basis to $\mathfrak{su}(2j+1)$ comprises a *reducible* representation of $\mathfrak{su}(2)$ as a subalgebra. Clearly, the two types of representations are *in*equivalent.

In the set of irreducible simple subalgebras of $\mathfrak{su}(N)$, the subalgebras $\mathfrak{sp}(N/2)$ with N even and $\mathfrak{so}(N)$ play a particularly important role. For $N \geq 5$, we discuss the irreducible simple subalgebras of $\mathfrak{su}(N)$ for N even and odd. If $N \geq 5$ is even, then $\mathfrak{su}(N)$ has both $\mathfrak{sp}(N/2)$ and $\mathfrak{so}(N)$ as irreducible simple subalgebras. In addition, $\mathfrak{su}(2) \subset \mathfrak{sp}(N/2)$ occurs as irreducible simple subalgebra. We consider two types of trivial cases. First, if $N \geq 5$ is even and if $\mathfrak{sp}(N/2)$, $\mathfrak{so}(N)$, and $\mathfrak{su}(2) \subset \mathfrak{sp}(N/2)$ are the only proper irreducible simple subalgebras, then we say the case is trivial. A trivial example is given by $\mathfrak{su}(12)$ in Table I. If $N \geq 5$ is odd, then $\mathfrak{so}(N)$ is an irreducible simple subalgebra of $\mathfrak{su}(N)$ but $\mathfrak{sp}(N/2)$ is not (as $N/2$ is not an integer). Moreover, $\mathfrak{su}(2) \subset \mathfrak{so}(N)$ occurs as irreducible simple subalgebra. Second, if $N \geq 5$ is odd and if $\mathfrak{so}(N)$ as well as $\mathfrak{su}(2) \subset \mathfrak{so}(N)$ are the only proper irreducible simple subalgebras, then we say the case is trivial. Examples of such trivial cases are given by $\mathfrak{su}(5)$, $\mathfrak{su}(9)$, $\mathfrak{su}(11)$, and $\mathfrak{su}(13)$ in Table I. The irreducible subalgebras $\mathfrak{sp}(N/2)$ and $\mathfrak{so}(N)$ correspond to the symmetric spaces SU(N)/Sp(N/2) and SU(N)/SO(N). These are two of three

TABLE II. The irreducible simple subalgebras of $\mathfrak{su}(2^n)$ for $1 \leq n \leq 15$.

n	Subalgebra diagram
1	$\mathfrak{su}(2)$
2	$\mathfrak{su}(2) \leftarrow \mathfrak{sp}(2) \leftarrow \mathfrak{su}(4)$
3	$\mathfrak{su}(2) \leftarrow \mathfrak{sp}(4) \leftarrow \mathfrak{su}(8)$; $\mathfrak{su}(3), \mathfrak{so}(7) \leftarrow \mathfrak{so}(8) \leftarrow \mathfrak{su}(8)$
4	$\mathfrak{su}(2), \mathfrak{sp}(2) \leftarrow \mathfrak{sp}(8) \leftarrow \mathfrak{su}(16)$; $\mathfrak{so}(9) \leftarrow \mathfrak{so}(16) \leftarrow \mathfrak{su}(16)$; $\mathfrak{so}(10) \leftarrow \mathfrak{su}(16)$
5	$\mathfrak{su}(2) \leftarrow \mathfrak{sp}(16) \leftarrow \mathfrak{su}(32)$; $\mathfrak{so}(11) \leftarrow \mathfrak{so}(12) \leftarrow \mathfrak{sp}(16)$; $\mathfrak{so}(32) \leftarrow \mathfrak{su}(32)$
6	$\mathfrak{su}(2), \mathfrak{so}(13), \mathfrak{sp}(2), \mathfrak{sp}(3) \leftarrow \mathfrak{sp}(32) \leftarrow \mathfrak{su}(64)$; $\mathfrak{su}(3), \mathfrak{so}(6), \mathfrak{g}_2 \leftarrow \mathfrak{so}(64) \leftarrow \mathfrak{su}(64)$; $\mathfrak{so}(14) \leftarrow \mathfrak{su}(64)$
7	$\mathfrak{su}(2) \leftarrow \mathfrak{sp}(64) \leftarrow \mathfrak{su}(128)$; $\mathfrak{so}(9), \mathfrak{so}(15) \leftarrow \mathfrak{so}(16) \leftarrow \mathfrak{so}(128) \leftarrow \mathfrak{su}(128)$
8	$\mathfrak{su}(2), \mathfrak{sp}(2) \leftarrow \mathfrak{sp}(128) \leftarrow \mathfrak{su}(256)$; $\mathfrak{so}(17) \leftarrow \mathfrak{so}(256) \leftarrow \mathfrak{su}(256)$; $\mathfrak{su}(4) \leftarrow \mathfrak{su}(256)$; $\mathfrak{so}(18) \leftarrow \mathfrak{su}(256)$
9	$\mathfrak{su}(2) \leftarrow \mathfrak{sp}(256) \leftarrow \mathfrak{su}(512)$; $\mathfrak{so}(19) \leftarrow \mathfrak{so}(20) \leftarrow \mathfrak{sp}(256)$; $\mathfrak{su}(3), \mathfrak{so}(7), \mathfrak{sp}(3) \leftarrow \mathfrak{so}(512) \leftarrow \mathfrak{su}(512)$
10	$\mathfrak{su}(2), \mathfrak{so}(21), \mathfrak{sp}(2) \leftarrow \mathfrak{sp}(512) \leftarrow \mathfrak{su}(1024)$; $\mathfrak{su}(5) \leftarrow \mathfrak{so}(1024) \leftarrow \mathfrak{su}(1024)$; $\mathfrak{so}(22) \leftarrow \mathfrak{su}(1024)$
11	$\mathfrak{su}(2) \leftarrow \mathfrak{sp}(1024) \leftarrow \mathfrak{su}(2048)$; $\mathfrak{so}(23) \leftarrow \mathfrak{so}(24) \leftarrow \mathfrak{so}(2048) \leftarrow \mathfrak{su}(2048)$
12	$\mathfrak{su}(2), \mathfrak{sp}(2) \leftarrow \mathfrak{sp}(2048) \leftarrow \mathfrak{su}(4096)$; $\mathfrak{su}(3), \mathfrak{so}(7), \mathfrak{so}(17), \mathfrak{so}(25), \mathfrak{sp}(4), \mathfrak{so}(6), \mathfrak{so}(8), \mathfrak{f}_4, \mathfrak{g}_2 \leftarrow \mathfrak{so}(4096) \leftarrow \mathfrak{su}(4096)$; $\mathfrak{so}(26) \leftarrow \mathfrak{su}(4096)$
13	$\mathfrak{su}(2) \leftarrow \mathfrak{sp}(4096) \leftarrow \mathfrak{su}(8192)$; $\mathfrak{so}(27) \leftarrow \mathfrak{so}(28) \leftarrow \mathfrak{sp}(4096)$; $\mathfrak{so}(8192) \leftarrow \mathfrak{su}(8192)$
14	$\mathfrak{su}(2), \mathfrak{so}(29), \mathfrak{sp}(2) \leftarrow \mathfrak{sp}(8192) \leftarrow \mathfrak{su}(16384)$; $\mathfrak{so}(16384) \leftarrow \mathfrak{su}(16384)$; $\mathfrak{su}(4) \leftarrow \mathfrak{su}(16384)$; $\mathfrak{so}(30) \leftarrow \mathfrak{su}(16384)$
15	$\mathfrak{su}(2), \mathfrak{su}(6) \leftarrow \mathfrak{sp}(16384) \leftarrow \mathfrak{su}(32768)$; $\mathfrak{su}(3), \mathfrak{sp}(3), \mathfrak{so}(8), \mathfrak{so}(32) \leftarrow \mathfrak{so}(32768) \leftarrow \mathfrak{su}(32768)$; $\mathfrak{so}(31) \leftarrow \mathfrak{so}(32)$

possible symmetric spaces[80] of SU(N), where the third type does not correspond to a semi-simple subalgebra of $\mathfrak{su}(N)$.

We call a representation ϕ of a subalgebra $\mathfrak{k}$ symplectic [orthogonal] if the subalgebra $\mathfrak{k}$ given in the representation ϕ is conjugate to a subalgebra of $\mathfrak{sp}(N/2)$ [$\mathfrak{so}(N)$]. If the representation is neither symplectic nor orthogonal, we term it unitary. In abuse of notation, we call also the subalgebra $\mathfrak{k}$ (with respect to some fixed but unspecified representation ϕ) symplectic, orthogonal, or unitary, if the respective representation ϕ is symplectic, orthogonal, or unitary. (We remark that this notation is motivated by the classification of representations and subalgebras as symplectic and orthogonal in Ref. 95 and in Chap. VIII, Sec. 7.5, Definition 2 of Ref. 79. Classifying representations and subalgebras as unitary appears to be non-standard notation. Unfortunately, the respective representations are also said to be of quaternionic, real, or complex type.) We emphasize that the classification of a subalgebra depends on the representations considered, see also Chap. IX, Appendix II.2, Proposition 3 of Ref. 79.

The property of a representation to be symplectic [respectively orthogonal] corresponds to the existence of an invariant (non-degenerate) skew-symmetric [respectively symmetric] bilinear form on the space of the representation. For irreducible representations in the compact case [e.g., for subgroups of SU(N)], this correspondence is an equivalence and a proof can be found in Sec. 3.11, Theorem H of Ref. 96. As an invariant (non-degenerate) bilinear form can either be skew-symmetric or symmetric, it follows that the same holds for the classification of (irreducible) symplectic, orthogonal, or unitary representations (Chap. IX, Sec. 7.2, Proposition 1 of Ref. 79):

Lemma 9: An irreducible representation $\phi(\mathfrak{k})$ can either be symplectic, or orthogonal, or unitary.

VII. FROM NECESSARY TO SUFFICIENT CONDITIONS FOR CONTROLLABILITY

While the ramification of *mathematically* admissible irreducible simple candidate subalgebras may seem daunting, in the following we will eliminate candidates by simple means. More precisely, we arrive at the following.

Corollary 10 (Task list)*: One way of showing full controllability amounts to excluding other candidates of irreducible simple subalgebras, which can be*

(1) symplectic, i.e., conjugate to a subalgebra of $\mathfrak{sp}(N/2)$,
(2) orthogonal, i.e., conjugate to a subalgebra of $\mathfrak{so}(N)$,
(3) or unitary in the remaining cases.

In particular, one has to exclude cases like the exceptional ones $\mathfrak{e}_6$, $\mathfrak{e}_7$, $\mathfrak{e}_8$, $\mathfrak{f}_4$, $\mathfrak{g}_2$. The unitary, irreducible simple subalgebras can occur in the cases $\mathfrak{su}(\ell+1) \subsetneq \mathfrak{su}(N)$ ($\ell \geq 2$), $\mathfrak{so}(4\ell+2)$, and $\mathfrak{e}_6$. □

In what follows, the plan is to make use of the fact that in Tables I and II, most of the irreducible subalgebras are symplectic or orthogonal. The symplectic and orthogonal ones (including their nested subalgebras!) will be excluded by merely solving simultaneous systems of linear homogeneous equations, which will also exclude the exceptional algebras $\mathfrak{e}_7$, $\mathfrak{e}_8$, $\mathfrak{f}_4$, and $\mathfrak{g}_2$, just leaving $\mathfrak{e}_6$. One may surmise that the observations up to $\mathfrak{su}(2^{15})$ may also hold in general: yet it remains to be proven that for systems of dimension 2^n, irreducible representations of $\mathfrak{e}_6$ cannot be an irreducible simple subalgebra of $\mathfrak{su}(2^n)$ without being a subalgebra to an intermediate orthogonal or symplectic algebra.

In principle, the task of identifying the dynamic Lie algebra can also be solved by algorithms[97,98] available in the computer algebra system MAGMA.[90] Yet, here we focus on exploiting algorithms that are more efficient, since they boil down to solving systems of homogeneous linear equations, which currently can—in general—be carried to matrix sizes of about $(6 \cdot 10^4) \times (6 \cdot 10^4)$ (and in extreme cases to $10^5 \times 10^5$).[99] So the algorithms presented here aim at the more specific task of distinguishing $\mathfrak{su}(N)$ from its proper irreducible simple subalgebras, a task our algorithms are more efficient in.

A. Symplectic and orthogonal subalgebras

In order to decide on conjugation to irreducible subalgebras which are symplectic and orthogonal, we need more detail. To this end, recalling the following lemma will prove useful to apply the lines of Ref. 100 in streamlined form leading to an explicit algorithm.

Lemma 11: (1) Every unitary symmetric matrix $S = S^t \in U(N, \mathbb{C})$ *is unitarily t-congruent to the identity, i.e.,* $S = T^t \mathbb{1} T$ *with T unitary.*

(2) Every unitary skew-symmetric matrix $S = -S^t \in U(N, \mathbb{C})$ *with N even is unitarily t-congruent to J, i.e.,* $S = T^t J T$ *with T unitary and*

$$J := \begin{pmatrix} 0 & -\mathbb{1}_{N/2} \\ \mathbb{1}_{N/2} & 0 \end{pmatrix}. \tag{14}$$

Proof: (1) Follows by singular-value decomposition and goes back to Hua (see Theorem 5 of Ref. 101). (2) Follows likewise from the same source (*ibid.*, Theorem 7). □

Lemma 12: Suppose $\mathfrak{k} \subset \mathfrak{su}(N)$ *is simple and J is defined as in Eq. (14). Then the element* $iH \in \mathfrak{k}$

(1) is unitarily conjugate to $i\widetilde{H} \in \mathfrak{so}(N)$*, where* $\widetilde{H}^t = -\widetilde{H}$*, if and only if there exists a symmetric unitary S (so* $S\bar{S} = +\mathbb{1}_N$*) satisfying* $SH + H^t S = 0$*;*

(2) is unitarily conjugate to $i\widetilde{H} \in \mathfrak{sp}(N/2)$ *(with N even), where* $J\widetilde{H} = -\widetilde{H}^t J$*, if and only if there is a skew-symmetric unitary S (so* $S\bar{S} = -\mathbb{1}_N$*) satisfying* $SH + H^t S = 0$.

Proof: First observe that whenever there is a unitary T such that $THT^\dagger =: \widetilde{H}$ with $L\widetilde{H} = -\widetilde{H}^t L$, this is equivalent to

$$LTHT^\dagger = -(THT^\dagger)^t L \Leftrightarrow LTH = -\bar{T}H^t T^t LT \Leftrightarrow (\underbrace{T^t L T}_{S})H = -H^t(\underbrace{T^t L T}_{S}).$$

Now it is easy to establish that the conditions are sufficient ("⇒"):

(1) Setting $L := \mathbb{1}_N$ and $S := T^t T$ gives $S\bar{S} = T^t T T^\dagger \bar{T} = +\mathbb{1}_N$. Thus $S = S^t$ is unitary, complex *symmetric* and satisfies $SH = -H^t S$.

(2) Setting $L := J$ and $S := T^t J T$ gives $S\bar{S} = T^t J T T^\dagger J \bar{T} = -\mathbb{1}_N$ by $J^2 = -\mathbb{1}_N$. Thus $S = -S^t$ is unitary, *skew-symmetric* and satisfies $SH = -H^t S$.

Moreover, the conditions are also necessary ("⇐") by Lemma 11, because with appropriate respective unitaries T

(1) for $L = \mathbb{1}_N$ any symmetric unitary matrix S can be written as $S = T^t T$;

(2) for $L = J$ any skew-symmetric unitary matrix S can be written as $S = T^t J T$. □

Now Lemma 12 can readily be applied to filter *irreducible* simple subalgebras along the lines of Lemma 3 of Ref. 100. In order to keep the presentation self-contained, we describe all the necessary details. Given a set of Hamiltonians $\{iH_\nu | \nu \in \{d; 1, \ldots, m\}\} = \{iH_d; iH_1, \ldots, iH_m\}$ generating the dynamic algebra $\mathfrak{k} \subseteq \mathfrak{su}(N)$ we introduce the linear solution spaces $\mathcal{S}_\nu := \{S \in \mathfrak{gl}(N, \mathbb{C}) | SH_\nu + H_\nu^t S = 0\}$ and, most importantly, their intersection

$$\mathcal{S} := \bigcap_{\nu \in \{d;1,\ldots,m\}} \mathcal{S}_\nu = \left\{S \in \mathfrak{gl}(N, \mathbb{C}) | SH_\nu + H_\nu^t S = 0 \text{ for all } \nu \in \{d; 1, \ldots, m\}\right\} \tag{15a}$$

$$= \left\{S \in \mathfrak{gl}(N, \mathbb{C}) | (H_\nu^t \otimes \mathbb{1}_N + \mathbb{1}_N \otimes H_\nu^t) \operatorname{vec}(S) = 0 \text{ for all } \nu \in \{d; 1, \ldots, m\}\right\}. \tag{15b}$$

We also consider the respective restrictions of $\mathcal{S}$ to the linear spaces of symmetric and skew-symmetric matrices

$$\mathcal{S}_{\text{sym}} := \mathcal{S} \cap \{S \in \mathfrak{gl}(N, \mathbb{C}) | S = +S^t\} = \mathcal{S} \cap \{S \in \mathfrak{gl}(N, \mathbb{C}) | (\mathbb{1}_N - K_{N,N}) \operatorname{vec}(S) = 0\}, \tag{16}$$

$$\mathcal{S}_{\text{skew}} := \mathcal{S} \cap \{S \in \mathfrak{gl}(N, \mathbb{C}) | S = -S^t\} = \mathcal{S} \cap \{S \in \mathfrak{gl}(N, \mathbb{C}) | (\mathbb{1}_N + K_{N,N}) \operatorname{vec}(S) = 0\}, \qquad (17)$$

where the $N^2 \times N^2$ permutation matrix $K_{N,N}$ is known as the *commutation matrix*.[102,103] Let e^a denote the vector such that $(e^a)_b = \delta_{a,b}$ with $a, b \in \{1, \ldots, N^2\}$. We define $K_{N,N}$ by the permutation $K_{N,N} \cdot e^a = e^{\pi(b)}$ where $\pi(N \cdot i + j + 1) = j \cdot N + i + 1$ and $i, j \in \{0, \ldots, N-1\}$. The commutation matrix operates on the vec-representation[102] of an $N \times N$ matrix A as the transposition operator in the sense $K_{N,N} \cdot \operatorname{vec}(A) = \operatorname{vec}(A^t)$. Finally, we summarize the properties of $\mathcal{S}$, $\mathcal{S}_{\text{sym}}$, and $\mathcal{S}_{\text{skew}}$ in all detail (which is more explicit than Ref. 100) by

Lemma 13: Assume that the commutant of a set of Hamiltonians $\{H_\nu | \nu \in \{d; 1, \ldots, m\}\}$ *is trivial. Using the definitions of* $\mathcal{S}$, $\mathcal{S}_{\text{sym}}$, *and* $\mathcal{S}_{\text{skew}}$ *in Eqs. (15)–(17) one obtains:*

(a) *Every non-zero element of* $\mathcal{S}$ *is non-singular.*
(b) $\dim(\mathcal{S}) \in \{0, 1\}$.
(c) *Every element of* $\mathcal{S}$ *is symmetric or skew-symmetric.*
(d) *If* $\dim(\mathcal{S}) = 1$, *then either* $\mathcal{S} = \mathcal{S}_{\text{sym}}$ *or* $\mathcal{S} = \mathcal{S}_{\text{skew}}$.
(e) *For all* $0 \neq S \in \mathcal{S}$, $SS^\dagger = S^\dagger S = \alpha \mathbb{1}_N$ *with* $0 < \alpha \in \mathbb{R}$ *and* $U := S/\sqrt{\alpha} \in \mathcal{S}$ *is unitary:*
(e1) *if S is symmetric, then* $\bar{S}S = S\bar{S} = +\alpha \mathbb{1}_N$ *and* $\bar{U}U = U\bar{U} = +\mathbb{1}_N$.
(e2) *if S is skew-symmetric, then* $\bar{S}S = S\bar{S} = -\alpha \mathbb{1}_N$ *and* $\bar{U}U = U\bar{U} = -\mathbb{1}_N$.
(f) $\dim(\mathcal{S}_{\text{sym}}) = 1 \Leftrightarrow \exists$ *symmetric unitary U s.t.* $UH_\nu + H_\nu^t U = 0$ *for all* ν
$\Leftrightarrow \exists$ *unitary U with* $\bar{U}U = U\bar{U} = +\mathbb{1}_N$ *s.t.* $UH_\nu + H_\nu^t U = 0$ *for all* ν.
(g) $\dim(\mathcal{S}_{\text{skew}}) = 1 \Leftrightarrow \exists$ *skew-symmetric unitary U s.t.* $UH_\nu + H_\nu^t U = 0$ *for all* ν
$\Leftrightarrow \exists$ *unitary U with* $\bar{U}U = U\bar{U} = -\mathbb{1}_N$ *s.t.* $UH_\nu + H_\nu^t U = 0$ *for all* ν.

Proof: In the sequel, let $S \in \mathcal{S}$. $SH_\nu = H_\nu^t S$ implies that S is an intertwining operator between two irreducible representations (given by iH_ν and iH_ν^t) of the Lie algebra $\mathfrak{k} \subseteq \mathfrak{su}(N)$ generated by $\{iH_\nu | \nu \in \{d; 1, \ldots, m\}\}$. By Schur's lemma we obtain that S is either zero or non-singular and (a) follows. Assuming that *two* non-zero and linear independent elements $S_1, S_2 \in \mathcal{S}$ existed, the equations $S_i H_\nu S_i^{-1} = H_\nu^t$ lead to $(S_2^{-1}S_1)H_\nu(S_2^{-1}S_1)^{-1} = H_\nu$. Again by Schur's lemma we get the contradiction $S_1 = cS_2$ with $c \in \mathbb{C}$ verifying (b). Statement (c) is trivially true for $S = 0$ and we prove it now for $S \neq 0$. We can write $S = P_{\text{sym}}(S) + P_{\text{skew}}(S)$ where $P_{\text{sym}}(S) := (S + S^t)/2$ and $P_{\text{skew}}(S) := (S - S^t)/2$ are the respective projections to the linear space of symmetric and skew-symmetric matrices. Assuming that both $P_{\text{sym}}(S)$ and $P_{\text{skew}}(S)$ are non-zero it follows that $[P_{\text{sym}}(S)H_\nu - H_\nu^t P_{\text{sym}}(S)] + [P_{\text{skew}}(S)H_\nu - H_\nu^t P_{\text{skew}}(S)] = 0$ and by transposition we get $-[P_{\text{sym}}(S)H_\nu - H_\nu^t P_{\text{sym}}(S)] + [P_{\text{skew}}(S)H_\nu - H_\nu^t P_{\text{skew}}(S)] = 0$. Thus, $P_{\text{sym}}(S)H_\nu = H_\nu^t P_{\text{sym}}(S)$ and $P_{\text{skew}}(S)H_\nu = H_\nu^t P_{\text{skew}}(S)$; moreover both $P_{\text{sym}}(S)$ and $P_{\text{skew}}(S)$ are (non-zero) elements in $\mathcal{S}$ and we obtain by (b) that $P_{\text{sym}}(S) = c\,P_{\text{skew}}(S)$ with $c \in \mathbb{C}$. Statement (c) follows by contradiction. Statement (d) is a consequence of the fact that if one non-zero element in $\mathcal{S}$ is symmetric (skew-symmetric) then all elements of $\mathcal{S}$ are symmetric (skew-symmetric). It follows from (c) that all elements in $\mathcal{S}$ are normal, $SS^\dagger = S^\dagger S$. For $S \neq 0$ the equations $SH_\nu = H_\nu^t S$ and $H_\nu S^\dagger = S^\dagger H_\nu^t$ hold and we obtain $H_\nu^t(SS^\dagger) = (SS^\dagger)H_\nu^t$. Schur's lemma implies that $SS^\dagger = \alpha \mathbb{1}_N$ with $\alpha \in \mathbb{R}$ as $SS^\dagger$ is Hermitian. As S is non-singular [see Statement (a)], $SS^\dagger$ is positive definite and has only strictly positive eigenvalues (see, e.g., p. 2f in Ref. 104). Thus $\alpha > 0$ and (e) follows. We prove (e1) and (e2): by applying the transposition to $SS^\dagger = \alpha \mathbb{1}_N$ we get $\bar{S}S = +\alpha \mathbb{1}_N$ for a symmetric S and $\bar{S}S = -\alpha \mathbb{1}_N$ for a skew-symmetric S. If $\dim(\mathcal{S}_{\text{sym}}) = 1$ it follows by (e) that a symmetric unitary U exists such that $UH_\nu + H_\nu^t U = 0$ for all ν which is equivalent to the existence of a unitary U with $\bar{U}U = U\bar{U} = +\mathbb{1}_N$ such that $UH_\nu + H_\nu^t U = 0$ for all ν. Assuming the existence of U we get a non-zero element of $\mathcal{S}_{\text{sym}}$. Statement (f) follows and Statement (g) is similar. □

Combining Lemma 12 and Lemma 13 gives the powerful **Algorithm 3**. It is important to note that this algorithm has a much lower complexity than verifying the necessary and sufficient condition given in Theorem 21 below, because it boils down to nothing else but computing the *dimensions* of the solution spaces for systems of homogeneous linear equations. Conjugation to the

Algorithm 3: Check conjugation to irreducible subalgebras of $\mathfrak{so}(N)$ or $\mathfrak{sp}(N/2)$.

Input: Hamiltonians $I := \{iH_\nu | \nu \in \{d; 1, \ldots, m\}\} = \{iH_d; iH_1, \ldots, iH_m\} \subseteq \mathfrak{su}(N)$ where the centralizer of I is trivial

1. compute $\mathcal{S} = \left\{S \in \mathfrak{gl}(N, \mathbb{C}) | (H_\nu^t \otimes \mathbb{1}_N + \mathbb{1}_N \otimes H_\nu^t)\,\mathrm{vec}(S) = 0 \text{ for all } \nu \in \{d; 1, \ldots, m\}\right\}$
2. compute $\mathcal{S}_{\mathrm{sym}} = \mathcal{S} \cap \{S \in \mathfrak{gl}(N, \mathbb{C}) | (\mathbb{1}_N - K_{N,N})\,\mathrm{vec}\,(S) = 0\}$
3. compute $\mathcal{S}_{\mathrm{skew}} = \mathcal{S} \cap \{S \in \mathfrak{gl}(N, \mathbb{C}) | (\mathbb{1}_N + K_{N,N})\,\mathrm{vec}\,(S) = 0\}$

Output: (a) $\dim(\mathcal{S}_{\mathrm{sym}}) = 1$ and $\dim(\mathcal{S}_{\mathrm{skew}}) = 0 \iff \mathfrak{k} \subseteq \mathfrak{so}(N)$
(b) $\dim(\mathcal{S}_{\mathrm{sym}}) = 0$ and $\dim(\mathcal{S}_{\mathrm{skew}}) = 1 \iff \mathfrak{k} \subseteq \mathfrak{sp}(N)$
(c) $\dim(\mathcal{S}_{\mathrm{sym}}) = 0$ and $\dim(\mathcal{S}_{\mathrm{skew}}) = 0 \iff \mathfrak{k} \not\subseteq \mathfrak{so}(N)$ and $\mathfrak{k} \not\subseteq \mathfrak{sp}(N/2)$

The complexity is roughly $\mathcal{O}((m+1)N^6)$, as in Liouville space $(m+1)N^2$ homogeneous linear equations have to be solved by *LU* decomposition (cf. p. 102 of Ref. 67). For n qubits, $N := 2^n$, we have $m \ll N$. (Refer to the main text for a definition of the commutation matrix $K_{N,N}$.)

symplectic algebras has also been treated in Ref. 87 by solving a system of linear equations, while Ref. 105 resorted to determining eigenvalues for discerning the unitary case (in the sense of Sec. VI) from conjugate symplectic or orthogonal subalgebras. The result for irreducible subalgebras can be summarized and extended as follows:

Theorem 14 (Candidate filter I): *Consider a set of Hamiltonians $\{iH_\nu\}$ generating the dynamic algebra $\mathfrak{k} \subseteq \mathfrak{su}(N)$ with the promise (by* ***Algorithm 2*** *and, e.g., due to a connected control system) that $\mathfrak{k} \subseteq \mathfrak{su}(N)$ is given in an irreducible representation and $\mathfrak{k}$ is simple. If in addition* ***Algorithm 3*** *has but a trivial set of solutions, then $\mathfrak{k}$ is neither conjugate to a simple subalgebra of $\mathfrak{sp}(N/2)$ nor of $\mathfrak{so}(N)$. In particular, $\mathfrak{k}$ is none of the following simple Lie algebras: $\mathfrak{e}_7$, $\mathfrak{e}_8$, $\mathfrak{f}_4$, or $\mathfrak{g}_2$.*

Proof: The cases $\mathfrak{so}(N)$ and $\mathfrak{sp}(N)$ are settled by combining Lemma 12 with Lemma 13. The cases $\mathfrak{e}_7$, $\mathfrak{e}_8$, $\mathfrak{f}_4$, and $\mathfrak{g}_2$ follow from the elaborate classification of Malcev[95] (see also, e.g., Refs. 38, 91, and 106 as well as Theorem 50 in Appendix C 3), as an irreducible representation of $\mathfrak{e}_8$, $\mathfrak{f}_4$, or $\mathfrak{g}_2$ is always conjugate to a subalgebra of $\mathfrak{so}(N)$, while an irreducible representation of $\mathfrak{e}_7$ is conjugate either to a subalgebra of $\mathfrak{so}(N)$ or of $\mathfrak{sp}(N/2)$. □

B. Unitary subalgebras

It also follows from Malcev[95] (again, see also Refs. 38, 91, and 106 as well as Theorem 50 in Appendix C 3) that only the subalgebras $\mathfrak{su}(\ell+1)$ $(\ell \geq 2)$, $\mathfrak{so}(4\ell+2)$, and $\mathfrak{e}_6$ can have unitary representations. These are in fact the only cases which might not be covered by Theorem 14. One can immediately deduce from the Tables I and II the following:

Corollary 15: The Lie algebras $\mathfrak{su}(2^n)$ do not possess (proper) unitary, irreducible simple subalgebras (in the sense of Sec. VI) if $n \in \{1, 2, 3, 5, 7, 9, 11, 13, 15\}$. In these cases ($n \neq 1$) and under the conditions of Theorem 14, ***Algorithm 3*** *provides a necessary and sufficient criterion for full controllability.*

We checked by explicit computations that $\mathfrak{e}_6$ does not occur as a unitary, irreducible simple subalgebra of $\mathfrak{su}(2^n)$ for $n \leq 100$ (i.e., for systems with up to 100 qubits) going well beyond the tabulated values in Table II. Together with Corollary 15 this motivates

Conjecture 16: (a) Theorem 14 already gives rise to a necessary and sufficient condition for full controllability in qubit systems with an odd number of qubits.

(b) The exceptional algebra $\mathfrak{e}_6$ does not occur as a unitary, irreducible simple subalgebra for qubit systems.

In general, however, Theorem 14 cannot lead to a necessary and sufficient condition—even if Conjecture 16(b) were true—as we present a counterexample of a control system whose dynamic algebra is a (proper) unitary subalgebra of $\mathfrak{su}(2^4)$. A series of similar examples (which are not necessarily counterexamples) are studied in Sec. IX (see Proposition 27). They will be interpreted in the context of fermionic systems in Sec. X (see Theorem 32 and Corollary 33).

Example 17: Consider a bilinear control system on $\mathfrak{su}(16)$ with four subsystems given by $\mathfrak{su}(2) \,\widehat{\oplus}\, \mathfrak{su}(2) \,\widehat{\oplus}\, \mathfrak{su}(2) \,\widehat{\oplus}\, \mathfrak{su}(2)$. The local dynamic algebra is given by

$$\langle i\text{XIII}, i\text{YIII}, i\text{ZIII}, i\text{IIIX}, i\text{IIIY}, i\text{IIIZ}\rangle_{\text{Lie}}.$$

In addition, we have a drift Hamiltonian $H_d = \text{XXII} + \text{YYII} + \text{IXXI} + \text{IYYI} + \text{IIXX} + \text{IIYY}$ (Heisenberg-XX interaction). The control system (Color online)

is connected and acts irreducibly. The dynamic algebra $\mathfrak{k} = \mathfrak{so}(10)$ is simple and a (proper) *unitary* subalgebra of $\mathfrak{su}(16)$.

C. System algebras comprising local actions $\mathfrak{su}(2)^{\oplus n}$

We now discuss the set of local unitary transformations $\text{SU}(2)^{\otimes n} \subseteq \text{SU}(2^n)$ and its Lie algebra $\mathfrak{su}(2)^{\oplus n} \subseteq \mathfrak{su}(2^n)$ where both are given in their respective standard representation, i.e., as n-fold Kronecker product and n-fold Kronecker sum (see Sec. IV)

$$\mathfrak{su}(2) \,\widehat{\oplus}\, \mathfrak{su}(2) \,\widehat{\oplus}\, \cdots \,\widehat{\oplus}\, \mathfrak{su}(2).$$

What is the classification of $\mathfrak{su}(2)^{\oplus n}$ with respect to symplectic, orthogonal, and unitary subalgebras? We obtain from Theorem 3 of Ref. 11 (see also Refs. 107 and 108):

Lemma 18: For the algebra $\mathfrak{su}(2)^{\oplus n}$ given in its (irreducible) standard representation there are two cases: (1) if n is odd, it is a symplectic subalgebra of $\mathfrak{su}(2^n)$ in the sense of being conjugate to a subalgebra of $\mathfrak{sp}(2^{n-1})$, and (2) if n is even, it is an orthogonal subalgebra in the sense of being conjugate to a subalgebra of $\mathfrak{so}(2^n)$.

Proof: Let ϕ denote an irreducible representation of a compact Lie group G. Then for the Frobenius-Schur indicator (Chap. IX, Appendix II.2, Proposition 4 of Ref. 79) one finds (in the sense of Sec. VI)

$$\int_G \text{Tr}[\phi^2(g)]\, dg = \begin{cases} -1 & \Leftrightarrow \quad \phi \text{ is a symplectic representation} \\ +1 & \Leftrightarrow \quad \phi \text{ is an orthogonal representation} \\ 0 & \Leftrightarrow \quad \phi \text{ is a unitary representation} \end{cases}$$

Let ψ denote the standard representation of the Lie group $\text{H} = \text{SU}(2)^{\otimes n}$. Reference 11 proves that $\int_H \text{Tr}[\psi^2(h)]\, dh = (-1)^n$. □

If the subsystems of a control system are independently fully controllable then it follows from Lemma 18 that some cases can be excluded:

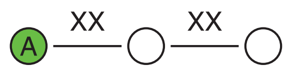
Lemma 19: Assume that the dynamic algebra $\mathfrak{k} \subseteq \mathfrak{su}(2^n)$ is irreducible and simple, and that the subsystems $\mathfrak{su}(2)$ are independently fully controllable, i.e., $\mathfrak{k} \supseteq \mathfrak{su}(2) \,\widehat{\oplus}\, \mathfrak{su}(2) \,\widehat{\oplus}\, \cdots \,\widehat{\oplus}\, \mathfrak{su}(2)$. If n is odd [respectively even] then $\mathfrak{k}$ is not an orthogonal [respectively symplectic] subalgebra.

Proof: We remark that $\mathfrak{h} = \mathfrak{su}(2) \,\widehat{\oplus}\, \mathfrak{su}(2) \,\widehat{\oplus}\, \cdots \,\widehat{\oplus}\, \mathfrak{su}(2)$ is given in an irreducible representation. It follows from the discussion prior to Lemma 9 that $\mathfrak{h}$ has an invariant (non-degenerate) skew-symmetric bilinear form and no invariant (non-degenerate) symmetric bilinear form if n is odd. Therefore, the dynamic algebra $\mathfrak{k}$ cannot have an invariant (non-degenerate) symmetric bilinear form and the lemma follows for odd n. The case of even n is similar. □

Unfortunately, we incorrectly gave more general results for dynamic algebras which contain a non-zero subset of the local operations in Theorems 3 and 4 of a conference paper.[56] But in light of

Examples 17 and 20 the more general results in Ref. 56 are not correct, as the non-zero subset is in general not given in an *irreducible* representation. Therefore, Lemma 19 is no longer true if the dynamic algebra contains only a non-zero (proper) subset of the local operations:

Example 20: Consider a bilinear control system on $\mathfrak{su}(8)$ with three subsystems given by $\mathfrak{su}(2) \,\widehat{\oplus}\, \mathfrak{su}(2) \,\widehat{\oplus}\, \mathfrak{su}(2)$. The local dynamic algebra is $\langle i\text{XII}, i\text{YII}, i\text{ZII}\rangle_{\text{Lie}}$. In addition, we have a drift Hamiltonian $H_d = \text{XXI} + \text{YYI} + \text{IXX} + \text{IYY}$. The control system (Color online)



is connected and acts irreducibly. The dynamic algebra $\mathfrak{k} = \mathfrak{so}(7)$ is simple and an orthogonal subalgebra. We emphasize that as a consequence of Lemma 19 this would have not been possible if $\mathfrak{k} \supseteq \mathfrak{su}(2) \,\widehat{\oplus}\, \mathfrak{su}(2) \,\widehat{\oplus}\, \mathfrak{su}(2)$.

D. A necessary and sufficient symmetry condition

In this subsection, we present a necessary and sufficient symmetry criterion for full controllability of control systems contained in $\mathfrak{su}(N)$. To this end, we introduce some additional notation: Assume that ϕ is a representation of a compact Lie algebra of dimension N. The tensor square $\phi^{\otimes 2} := \phi \otimes \mathbb{1}_N + \mathbb{1}_N \otimes \phi$ decomposes as $\phi^{\otimes 2} = \text{Alt}^2\phi \oplus \text{Sym}^2\phi$, where the alternating square $\text{Alt}^2\phi$ and the symmetric square $\text{Sym}^2\phi$ are the restrictions of $\phi^{\otimes 2}$ to the antisymmetric and the symmetric subspace, respectively. More details on this notation is given in Appendix D. We arrive at

Theorem 21: *Assume that $\mathfrak{k}$ is a subalgebra of $\mathfrak{su}(N)$ and denote by Φ the standard representation of $\mathfrak{su}(N)$. Then, the following are equivalent:*

(1) $\mathfrak{k} = \mathfrak{su}(N)$.
(2) The restrictions of $\text{Alt}^2\Phi$ *and* $\text{Sym}^2\Phi$ *to the subalgebra $\mathfrak{k}$ are both irreducible.*
(3) The commutant $\text{comm}_{\Phi^{\otimes 2}}(\mathfrak{k})$ *with respect to the tensor square $\Phi^{\otimes 2}$ has dimension two.*

Proof: (1) ⇒ (2) follows by Theorem 54 in Appendix D. We prove (2) ⇒ (1). As the restriction $(\text{Alt}^2\Phi)|_{\mathfrak{k}}$ of $\text{Alt}^2\Phi$ to $\mathfrak{k}$ is irreducible, we get that the restriction $\Phi|_{\mathfrak{k}}$ of Φ to $\mathfrak{k}$ is also irreducible. Otherwise, $\Phi|_{\mathfrak{k}} = \phi_1 \oplus \phi_2$ would be reducible and, as a consequence, $(\text{Alt}^2\Phi)|_{\mathfrak{k}} = \text{Alt}^2(\phi_1 \oplus \phi_2) = \text{Alt}^2\phi_1 \oplus (\phi_1 \otimes \phi_2) \oplus \text{Alt}^2\phi_2$ would also be reducible (which is impossible). Lemma 3 implies the centralizer $\mathfrak{k}'$ of $\mathfrak{k}$ in $\mathfrak{su}(N)$ is trivial, thus by Lemma 4 $\mathfrak{k}$ is semi-simple. Now (1) follows by Theorem 54 in Appendix D. Moreover Theorem 1.5 of Ref. 109 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. As we consider the representation $(\Phi^{\otimes 2})|_{\mathfrak{k}} = (\text{Alt}^2\Phi)|_{\mathfrak{k}} \oplus (\text{Sym}^2\Phi)|_{\mathfrak{k}}$, the equivalence of (2) and (3) readily follows. □

We now show that condition (3) of Theorem 21 can be easily tested using a set of Hamiltonians $\{iH_\nu\}$ generating the dynamic algebra $\mathfrak{k} \subseteq \mathfrak{su}(N)$. Therefore, we prove that the commutant of $\{(iH_\nu) \otimes \mathbb{1}_N + \mathbb{1}_N \otimes (iH_\nu)\}$ is equal to $\text{comm}_{\Phi^{\otimes 2}}(\mathfrak{k})$. Obviously, the latter commutant is contained in the former. Let $s \in \mathfrak{gl}(N^2, \mathbb{C})$ be an element of the former commutant. Then by Jacobi's identity $[[a, b], s] + [[b, s], a] + [[s, a], b] = 0$, s commutes with all commutators

$$
\begin{aligned}
&[(iH_\nu) \otimes \mathbb{1}_N + \mathbb{1}_N \otimes (iH_\nu), (iH_\mu) \otimes \mathbb{1}_N + \mathbb{1}_N \otimes (iH_\mu)] \\
&\quad = [iH_\nu, iH_\mu] \otimes \mathbb{1}_N + \mathbb{1}_N \otimes [iH_\nu, iH_\mu],
\end{aligned}
$$

and by induction, s is also contained in the latter commutant.

Together with Theorem 21, we thus obtain a *necessary and sufficient symmetry condition* for full controllability as a theoretical main result:

Corollary 22: Consider a set of Hamiltonians $\{iH_\nu \mid \nu \in \{d; 1, \ldots, m\}\}$ generating the dynamic algebra $\mathfrak{k} \subseteq \mathfrak{su}(N)$. The corresponding control system is fully controllable in the sense $\mathfrak{k} = \mathfrak{su}(N)$, *if and only if the joint commutant of* $\{(iH_\nu)\otimes\mathbb{1}_N+\mathbb{1}_N\otimes(iH_\nu)\,|\,\nu\in\{d;1,\ldots,m\}\}$ *has dimension two.* □

In spite of the beauty of simplicity of this result, from an algorithmic point of view the above symmetry condition is currently not appealing: In Corollary 22 one would have to compute the commutant of $N^2\times N^2$ matrices as compared to $N\times N$ matrices in the test for the lack of symmetry in **Algorithm 2** (cf. **Algorithm 3**). Thus, the complexity of testing for Corollary 22 would be the square of the complexity of **Algorithm 2** or **Algorithm 3**. Even in moderately sized examples one has to save computer memory by methods of sparse matrices due to the larger matrices. In larger examples, testing for Corollary 22 gets impractical. Yet compared with potential conditions involving even higher tensor powers, one should consider Corollary 22 as a fortunate incidence.

In order to characterize the commutant of Corollary 22 in more detail, recall that the $N^2\times N^2$ commutation matrix $K_{N,N}$ operates on the vec-representation of an $N\times N$ matrix A as the transposition operator: $K_{N,N}\cdot\mathrm{vec}(A)=\mathrm{vec}(A^t)$ (see Sec. VII A).

Lemma 23: The commutant of $\{(iH_\nu)\otimes\mathbb{1}_N+\mathbb{1}_N\otimes(iH_\nu)\,|\,\nu\in\{d;1,\ldots,m\}\}$ *always contains the elements* $\mathbb{1}_{N^2}$ *and* $K_{N,N}$.

Proof: As the identity matrix $\mathbb{1}_{N^2}$ always commutes, we have only to prove that $K_{N,N}$ is contained in the commutant. Sec. 3 of Ref. 103 says that $K_{N,N}(A\otimes B)=(B\otimes A)K_{N,N}$ for all $N\times N$ matrices A and B and thereby $K_{N,N}(A\otimes B+B\otimes A)=(A\otimes B+B\otimes A)K_{N,N}$. In particular one finds $K_{N,N}(A\otimes\mathbb{1}_N+\mathbb{1}_N\otimes A)=(A\otimes\mathbb{1}_N+\mathbb{1}_N\otimes A)K_{N,N}$ and the lemma is proven. □

The operator $K_{N,N}$ has two eigenspaces (see Sec. 4.2 of Ref. 103): The first one is given by the symmetric subspace (i.e., "bosons") and has the eigenvalue $+1$ with multiplicity $N(N+1)/2$. For even N, the permutation-symmetric subspace is equivalent to the Lie algebra $\mathfrak{sp}(N/2)$. The second one is given by the antisymmetric subspace (i.e., "fermions") and has the eigenvalue -1 with multiplicity $N(N-1)/2$. The permutation-antisymmetric subspace is equivalent to the Lie algebra $\mathfrak{so}(N)$.

The methods of this subsection thus shed new light on the symplectic and orthogonal subalgebras (see Subsection VII A). Proposition 3.5 of Ref. 110 (see also p. 446 of Ref. 111) says that an irreducible representation ϕ of a compact simple Lie algebra $\mathfrak{g}$ is either symplectic or orthogonal if and only if its tensor square $\phi^{\otimes 2}$ contains the trivial representation of $\mathfrak{g}$ exactly once. In particular, the irreducible representation ϕ is symplectic (respectively orthogonal) if the trivial representation occurs exactly once in $\mathrm{Alt}^2\phi$ (respectively $\mathrm{Sym}^2\phi$). A similar condition is given by Proposition 4.2 of Ref. 110: An irreducible representation ϕ of a compact simple Lie algebra $\mathfrak{g}$ is either symplectic or orthogonal if and only if its tensor square $\phi^{\otimes 2}$ contains the (irreducible) adjoint representation of $\mathfrak{g}$ at least once.

VIII. SIMULABILITY

Simulating quantum systems[1,5,112] is a promising mid-term perspective, because the accuracy demands are easier to come by than the "error-correction threshold" for actual quantum computing. Another practical advantage lies in the fact that sometimes the simulating systems allow for separating control parameters in the analogue that in the original (be it classical or quantum) cannot be tuned independently.

This section exploits that the dynamical algebra captures all the key properties of the dynamical system to be studied. More precisely, the question whether (and to which extent) one quantum system can simulate another one can be answered by analyzing the Lie-subalgebra structure of systems with a given dimension. Recently, Kraus *et al.* have explored whether target quantum systems can be universally simulated on translationally invariant lattices of bosonic, fermionic, and spin systems.[17] Based on the branching diagrams of simple subalgebras to $\mathfrak{su}(N)$, here we take a more general approach pursuing the question which type of quantum system can simulate a given one with least overhead in state-space dimension. In particular, we also allow for effective many-body interactions to be simulated by pair-interactions. To this end, the reader may wish to resort to the more general notion of tensor-product structures in Appendix A first.

In quantum simulation, one of the first natural questions to ask is whether and under which conditions a controlled quantum dynamical system Σ_a can simulate another (controlled or uncontrolled) dynamical system Σ_b given as bilinear control systems with $\mu = a, b$ on density matrices ρ_μ

$$\dot{\rho}_\mu(t) = -i\Big[\big(H_0^\mu + \sum_{j=1}^{m} u_j^\mu(t) H_j^\mu\big)\ ,\ \rho_\mu(t)\Big] \quad \text{with} \quad \rho_\mu(0) = \rho_{\mu o} \quad . \tag{18}$$

The dynamic Lie algebras $\mathfrak{k}_a$ and $\mathfrak{k}_b$ are given by the respective Lie closures as

$$\mathfrak{k}_\mu := \langle i H_0^\mu, i H_j^\mu \mid j = 1, 2, \dots, m\rangle_{\text{Lie}} \tag{19}$$

thus entailing the reachable sets take the form of $\mathbf{K}_\nu$-subgroup orbits as in Eq. (7)

$$\mathfrak{reach}(\rho_{ao}) := \{K_a \rho_{ao} K_a^\dagger \mid K_a \in \mathbf{K}_a := \exp \mathfrak{k}_a\}, \quad \text{and} \tag{20}$$

$$\mathfrak{reach}(\rho_{bo}) := \{K_b \rho_{bo} K_b^\dagger \mid K_b \in \mathbf{K}_b := \exp \mathfrak{k}_b\}\ . \tag{21}$$

An obvious requirement is that for any initial state ρ_{bo} of system Σ_b leading to the dynamics $\rho_b(t) \in \mathfrak{reach}(\rho_{bo})$ there is an initial state ρ_{ao} of system Σ_a such that under the dynamics of Σ_a one has

$$\rho_b(t) \in \mathfrak{reach}(\rho_{ao}) \quad \forall\, t \geq 0\ . \tag{22}$$

This requirement is obviously fulfilled by the following sufficient condition:

Proposition 24: A dynamic bilinear control system Σ_a with dynamical algebra $\mathfrak{k}_a$ can simulate another dynamic system Σ_b with dynamical algebra $\mathfrak{k}_b$ if $\mathfrak{k}_a \supseteq \mathfrak{k}_b$.

Proof: Clearly $\mathfrak{k}_a \supseteq \mathfrak{k}_b$ implies $\mathbf{K}_a \supseteq \mathbf{K}_b$ and thus $\mathfrak{reach}(\rho_{ao}) \supseteq \mathfrak{reach}(\rho_{bo})$, which in turn ensures that Eq. (22) is fulfilled for any choice of initial states. □

In particular, if system Σ_b is uncontrolled it can be simulated if its drift Hamiltonian H_0^b can be simulated, i.e., provided $i H_0^b \in \mathfrak{k}_a$.

Two dynamic bilinear control systems Σ_a and Σ_b are said to be *dynamically equivalent* independent of the respective initial states $\rho_{\mu 0}$ if and only if they can mutually simulate one another, i.e., if $\mathfrak{k}_a \supseteq \mathfrak{k}_b$ and $\mathfrak{k}_b \supseteq \mathfrak{k}_a$ so $\mathfrak{k}_a = \mathfrak{k}_b$ (up to isomorphism).

Remark 25: It is important to note that in the *special case of pure states*, where by construction $\rho(t) = \rho^2(t)$, it suffices that, e.g., a system Σ_a has the dynamic Lie algebra $\mathfrak{k}_a = \mathfrak{sp}(N/2)$ in order to simulate system Σ_b with $\mathfrak{k}_b = \mathfrak{su}(N)$, because the unitary orbit of any pure state $\rho_0 = |\psi\rangle\langle\psi|$ coincides with its symplectic orbit for N even

$$\mathcal{O}_{\mathrm{SU}(N)}(|\psi\rangle\langle\psi|) = \mathcal{O}_{Sp(N/2)}(|\psi\rangle\langle\psi|) \quad \forall\, |\psi\rangle \in \mathcal{H}. \tag{23}$$

This is equivalent to a well-known result stating that for N even, a system is *pure-state controllable* as soon as its system algebra encapsulates the symplectic one.[36] Since we are interested in general results beyond pure states, the notion of full controllability maintained in this work is full operator controllability unless specified otherwise. Also for simulability we do not confine the state space to pure states henceforth.

Proposition 26: Consider two dynamic systems Σ_a and Σ_b whose respective dynamic Lie algebras $\mathfrak{k}_a$ and $\mathfrak{k}_b$ shall be irreducible over a given Hilbert space $\mathcal{H}$. Then Σ_a simulates Σ_b irreducibly and with least overhead in the very $\mathcal{H}$ given, if any interlacing system Σ_i with irreducible algebra $\mathfrak{k}_i$ fulfilling

$$\mathfrak{k}_a \supseteq \mathfrak{k}_i \supseteq \mathfrak{k}_b \tag{24}$$

enforces (up to isomorphism) $\mathfrak{k}_i = \mathfrak{k}_a$ or $\mathfrak{k}_i = \mathfrak{k}_b$ or trivially both. □

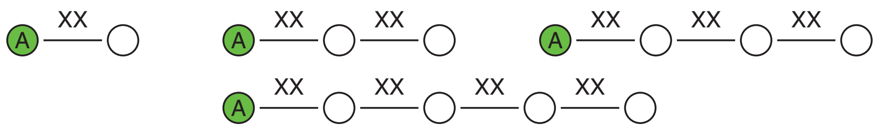


FIG. 2. (Color online) Heisenberg-XX spin chains with n spins-$\frac{1}{2}$ and odd-order orthogonal system algebras $\mathfrak{so}(2n+1)$ require one locally controllable qubit at the end. A full series can be constructed, the first examples being $\mathfrak{so}(5) \cong \mathfrak{sp}(4/2)$, $\mathfrak{so}(7)$, $\mathfrak{so}(9)$, and $\mathfrak{so}(11)$. For $n = 1$ one gets $\mathfrak{so}(3) \cong \mathfrak{su}(2)$.

Caveat: Note that the term "with least overhead" crucially depends on the Hilbert space *given a priori*: Thus there may be extreme realizations. For instance, in a fully controllable system of say 14 qubits with dynamic algebra $\mathfrak{su}(16\,384)$ there is an *irreducible* way to simulate a fully controllable $\mathfrak{su}(4)$-system of two qubits (or just a single spin-$\frac{3}{2}$ with control over all multipole moments) with "least overhead" in $\mathfrak{su}(2^{14})$, see the penultimate entry in Table II. Realizations of this type may not be very useful in practice, yet relate to the context of code spaces.

Here, we have dealt with quantum simulation of *unobserved control systems*. Now we illustrate the above findings by examples. Later, in Sec. XII, we will give an outlook on a weaker notion of quantum simulation of *observed control systems* with respect to expectation values by given sets of observables.

IX. WORKED EXAMPLES

A. Dynamic systems with orthogonal algebras

Take spin chains of n spins-$\frac{1}{2}$ with Heisenberg-XX (and XY) interactions and a *single* locally controllable qubit at one end. These instances serve as convenient topologies to simulate a full series of *odd-order* orthogonal algebras $\mathfrak{so}(2n+1)$ for n qubits. The first instances are shown in Fig. 2.

Proposition 27: Heisenberg-XX chains of n spin-$\frac{1}{2}$ qubits ($n \geq 1$) and a single locally controllable qubit at one end give rise to the dynamic system algebras $\mathfrak{so}(2n+1)$ as irreducible subalgebras embedded in $\mathfrak{su}(2^n)$.

Proof: In view of later applications, the proof is kept constructive. For better readability, let x, y, and z denote Pauli matrices.

First, as a foundation for induction, the case $n = 2$ can be settled by direct calculation to verify

$$i\langle x1,\, y1,\, (xx+yy)\rangle_{\text{Lie}} = i\{x1,\, y1,\, z1,\, xx,\, yy,\, xy,\, yx,\, zx,\, zy,\, 1z\} \overset{\text{rep}}{=} \mathfrak{so}(5)\,, \tag{25}$$

where the final identity can be corroborated by **Algorithm 3** as will be illustrated below in Eq. (26).

Second, for the induction from $(n-1)$ to n, where the drift Hamiltonian is extended by the final Heisenberg coupling between the qubit pair $(n-1), n$ to take the form $H_0 := \sum_{k=1}^{n-1} x_k x_{k+1} + y_k y_{k+1}$, observe that all the algebra elements for $n-1$ qubits re-occur. Upon twice commuting with $z1\cdots1$ arising at the controlled end, the first pair-coupling term $x_1x_2 + y_1y_2$ can be recovered: $\text{ad}^2_{i\,z_1}(i\sum_{k=1}^{n-1} x_k x_{k+1} + y_k y_{k+1}) = \text{ad}_{i\,z_1}(-i(y_1x_2 - x_1y_2)) = -i(x_1x_2 + y_1y_2)$ and then by virtue of Eq. (25) also $1z1\cdots1$ and thus recursively all the terms in the Lie closure at the stage $n-1$.

Third, once having embedded the $(n-1)$-qubit algebra into the n-qubit system, the induction boils down to including the coupling term $x_{n-1}x_n + y_{n-1}y_n$, which takes $1\cdots1z_{n-1}1$ to $1\cdots1z_n$. Writing braces $\left\{\begin{smallmatrix}x\\y\end{smallmatrix}\right\}$ whenever one has the choices $\{x, y\}$ one gets the complete list given in Table III.

Finally, counting terms gives a total of $2n + n + 4\sum_{k=1}^{n-1}(n-k) = 3n + 4\sum_{k=1}^{n-1} k = 3n + 2n(n-1) = 2n^2 + n = \dim\mathfrak{so}(2n+1) = n(2n+1)$ elements to span the basis of the Hamiltonians H_ν generating $\langle iH_\nu\rangle_{\text{Lie}} = \mathfrak{so}(2n+1)$. So for all n-spin-$\frac{1}{2}$ Heisenberg-XX chains controlled locally at one end we have obtained a constructive scheme to determine irreducible representations of their respective dynamic Lie algebras $\mathfrak{so}(2n+1)$ in terms of Pauli bases. □

TABLE III. Complete list of generators (Pauli basis) for $\mathfrak{so}(2n+1)$.

2 terms	$\left\{ {x \atop y} \right\} 1 \cdots 1$	
n terms	$z1 \cdots 1$	$1z1 \cdots 1$ etc
2 terms	$z \left\{ {x \atop y} \right\} 1 \cdots 1$	
$4(n-1)$ terms	$\left\{ {x \atop y} \right\} \left\{ {x \atop y} \right\} 1 \cdots 1$	$1 \left\{ {x \atop y} \right\} \left\{ {x \atop y} \right\} 1 \cdots 1$ etc
$\vdots$	$\vdots$	$\vdots$
2 terms	$zz \cdots z \left\{ {x \atop y} \right\}_k 1 \cdots 1$	
$4(n-k+1)$ terms	$\left\{ {x \atop y} \right\} z \cdots z \left\{ {x \atop y} \right\}_k 1 \cdots 1$	$1 \left\{ {x \atop y} \right\}_2 z \cdots z \left\{ {x \atop y} \right\}_{k+1} 1 \cdots 1$ etc
$\vdots$	$\vdots$	$\vdots$
2 terms	$zz \cdots z \left\{ {x \atop y} \right\}_n$	
4 terms	$\left\{ {x \atop y} \right\} z \cdots z \left\{ {x \atop y} \right\}_n$	

In contrast, n-spin-$\frac{1}{2}$ chains with Heisenberg-XX interactions and *two* independently controllable qubits, one at each end, provide a realization of a series of *even-oder* orthogonal algebras $\mathfrak{so}(2n+2)$ for n qubits, the first examples being shown in Fig. 3.

*Proposition 28: Heisenberg-*XX *chains of n spin-*$\frac{1}{2}$ *qubits (*$n \geq 2$*) and two individually locally controllable qubits, one at each end, give rise to the dynamic system algebras* $\mathfrak{so}(2n+2)$ *as irreducible subalgebras embedded in* $\mathfrak{su}(2^n)$*.*

Proof: The constructive proof follows in entire analogy to the one of Proposition 27: however, the local controls at the second end imply that the Lie closure comprises each term occurring in the above list also read from right to left thus duplicating the first line in each category from two terms to four terms. Since the second lines in each category already comprise the reverse terms, one obtains the complete list given in Table IV.

Finally, by the commutator $[(z \cdots z \left\{ {x \atop y} \right\}_k 1 \cdots 1), (1 \cdots 1 \left\{ {x \atop y} \right\}_{n-k'} z \cdots z)]$ with $k = n - k'$, the longitudinal spin-order term $z_1 z_2 \cdots z_n$ listed last arises. Counting terms, one arrives at a total of $4n + n + 1 + 4\sum_{j=1}^{n-1}(n-j) = 5n + 1 + 4\sum_{j=1}^{n-1} j = 5n + 1 + 2n(n-1) = 2n^2 + 3n + 1 = \dim \mathfrak{so}(2n+2)$ elements. Thus also for all n-spin-$\frac{1}{2}$ Heisenberg-XX chains individually controlled locally at the two ends we have provided a constructive scheme to determine irreducible representations of their respective dynamic Lie algebras $\mathfrak{so}(2n+2)$ in terms of Pauli bases. □

In both instances of Heisenberg-XX chains controlled locally at one end [Fig. 2 with $\mathfrak{so}(2n+1)$] or at two ends [Fig. 3 with $\mathfrak{so}(2n+2)$] there are convenient Cartan decompositions $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$: the $\mathfrak{k}$-parts consist of per-*anti*symmetric matrices, while the $\mathfrak{p}$-parts comprise the per-*symmetric* matrices, recalling that per-symmetry relates to reflection at the minor diagonal. In both of the above listings, the respective subalgebras $\mathfrak{k}$ to $\mathfrak{so}(2n+1)$ or $\mathfrak{so}(2n+2)$ encompass the Hamiltonians with *odd*

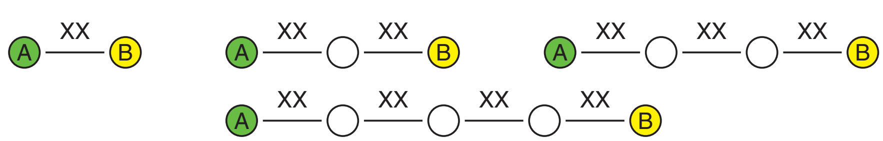


FIG. 3. (Color online) n-Spin-$\frac{1}{2}$ Heisenberg-XX chains with even-order orthogonal system algebras $\mathfrak{so}(2n+2)$ result by allowing just two locally controllable qubits at the ends. A full series can be constructed, the first examples of which are shown $\mathfrak{so}(6) \cong \mathfrak{su}(4)$, $\mathfrak{so}(8)$, $\mathfrak{so}(10)$, and $\mathfrak{so}(12)$. For $n = 2$ one gets $\mathfrak{so}(6) \cong \mathfrak{su}(4)$ as a fully controllable two-qubit system.

TABLE IV. Complete list of generators (Pauli basis) for $\mathfrak{so}(2n+2)$.

4 terms	$\{{x \atop y}\}1\cdots 1$	$1\cdots 1\{{x \atop y}\}$
n terms	$z1\cdots 1$	$1z1\cdots 1$ etc
4 terms	$z\{{x \atop y}\}1\cdots 1$	$1\cdots 1\{{x \atop y}\}z$
$4(n-1)$ terms	$\{{x \atop y}\}\{{x \atop y}\}1\cdots 1$	$1\{{x \atop y}\}\{{x \atop y}\}1\cdots 1$ etc
$\vdots$	$\vdots$	$\vdots$
4 terms	$z\cdots z\{{x \atop y}\}_k 1\cdots 1$	$1\cdots 1\{{x \atop y}\}_{n-k} z\cdots z$
$4(n-k+1)$ terms	$\{{x \atop y}\}z\cdots z\{{x \atop y}\}_k 1\cdots 1$	$1\{{x \atop y}\}_2 z\cdots z\{{x \atop y}\}_{k+1} 1\cdots 1$ etc
$\vdots$	$\vdots$	$\vdots$
4 terms	$z\cdots z\{{x \atop y}\}_n$	$\{{x \atop y}\}_1 z\cdots z$
4 terms	$\{{x \atop y}\}z\cdots z\{{x \atop y}\}_n$	
1 term	$zz\cdots zz$	

numbers of z-terms, while the respective subspaces $\mathfrak{p}$ contain the elements with *even* numbers of z-terms (including zero z-terms).

For illustration, in the first example, i.e., the two-qubit Heisenberg-XX chain of Fig. 2, a transformation matrix S simultaneously satisfying $SH_\nu + H_\nu^t S = 0$ for ν extending over drift and controls is—according to the computations in **Algorithm 3**—given by the unitary matrix [cf. Lemma 13(e)]

$$S_1 = \begin{pmatrix} 0 & 0 & 0 & +1 \\ 0 & 0 & +1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} \equiv J_2\ . \tag{26}$$

Here $S_1\bar{S}_1 = -\mathbb{1}$ reconfirms $\mathfrak{so}(5) \cong \mathfrak{sp}(4/2)$ [see Lemma 13(g)].

As a second example, for both of the three-qubit cases in Figs. 2 and 3 corresponding to $\mathfrak{so}(7)$ and $\mathfrak{so}(8)$, the computations in **Algorithm 3** provide the unitary matrix [cf. Lemma 13(e)]

$$S_2 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & +1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \tag{27}$$

where $S_2\bar{S}_2 = +\mathbb{1}$ shows the orthogonal type of the respective irreducible representations [see Lemma 13(f)].

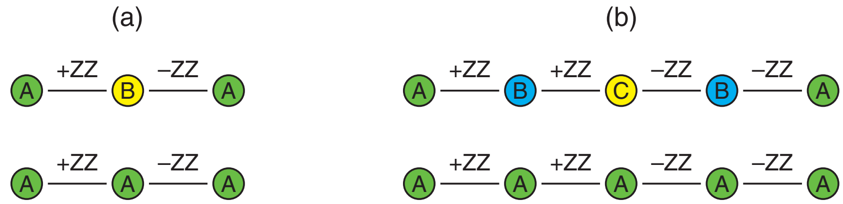


FIG. 4. (Color online) Quantum systems with dynamic Lie algebras $\mathfrak{sp}(4)$ [see (a)] and $\mathfrak{sp}(16)$ [see (b)] as examples of a series of Ising chains of $n = 2k + 1$ qubits with positive ZZ coupling terms on one branch and negative couplings on the other. They give rise to the dynamic algebras $\mathfrak{sp}(2^{n-1})$ irreducibly embedded in $\mathfrak{su}(2^n)$, respectively. The limiting case $k = 0$ gives $\mathfrak{sp}(1) \cong \mathfrak{su}(2)$ as a single fully controllable qubit.

B. Dynamic systems with symplectic algebras

Based on the smallest examples of qubit systems with Ising-ZZ interactions shown in Fig. 4, even on the basis of *collective controls* one may construct a full sequence of n-spin-$\frac{1}{2}$ chains with n odd, the dynamic system algebras of which are the symplectic ones $\mathfrak{sp}(2^{n-1})$. Note again that the bilinear control systems with symplectic system algebras are *pure-state controllable*,[36] whereas they fail to be fully operator controllable.

Proposition 29: Ising-ZZ chains of $n = 2k+1$ spin-$\frac{1}{2}$ qubits ($k \geq 1$) including k pairs of qubits which can be controlled simultaneously and one qubit in the middle of the chain which can be controlled independently as in the first row of Fig. 4 give rise to the dynamic system algebras $\mathfrak{sp}(2^{n-1}) = \mathfrak{sp}(2^{2k})$ as irreducible subalgebras embedded in $\mathfrak{su}(2^n) = \mathfrak{su}(2^{2k+1})$. We obtain the same dynamic algebras when all qubits can only be controlled simultaneously as in the second row of Fig. 4.

Proof: We focus on the dynamic algebra $\mathfrak{k}_k$ corresponding to the case when all $2k + 1$ qubits can only be controlled simultaneously as in the second row of Fig. 4. We denote by $\bar{\mathfrak{k}}_k$ the dynamic algebra corresponding to the first row of Fig. 4. We use the notation

$$\mathrm{X}_j := \underbrace{\mathrm{I}\cdots\mathrm{I}}_{j-1}\mathrm{X}\underbrace{\mathrm{I}\cdots\mathrm{I}}_{n-j}, \quad \mathrm{Y}_j := \underbrace{\mathrm{I}\cdots\mathrm{I}}_{j-1}\mathrm{Y}\underbrace{\mathrm{I}\cdots\mathrm{I}}_{n-j}, \quad \text{and} \quad \mathrm{Z}_j := \underbrace{\mathrm{I}\cdots\mathrm{I}}_{j-1}\mathrm{Z}\underbrace{\mathrm{I}\cdots\mathrm{I}}_{n-j} \tag{28}$$

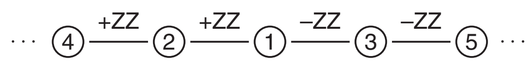
to denote the operators which act, respectively, as X, Y, and Z on the jth qubit and as the identity on all other qubits. We remark that the statements of the theorem can be directly verified for $k \in \{0, 1\}$. We organize the proof in steps: first we prove that $\mathfrak{k}_{k-1} \subseteq \mathfrak{k}_k$, second we prove that $\bar{\mathfrak{k}}_k = \mathfrak{k}_k$, later we show that $\mathfrak{k}_k$ is given in an irreducible (third step) and symplectic (fourth step) representation, and in the end we prove that $\mathfrak{k}_k$ is not a proper subalgebra of $\mathfrak{sp}(2^{n-1}) = \mathfrak{sp}(2^{2k})$. Recall, that $\mathfrak{k}_k$ is generated by the operators

$$f_1 = -\tfrac{i}{2}\sum_{j=1}^{2k+1}\mathrm{X}_j,\ \ f_2 = -\tfrac{i}{2}\sum_{j=1}^{2k+1}\mathrm{Y}_j,\ \ f_3 = -\tfrac{i}{2}\left(\sum_{j=1}^{k}\mathrm{Z}_j\mathrm{Z}_{j+1} - \sum_{j=k+1}^{2k}\mathrm{Z}_j\mathrm{Z}_{j+1}\right).$$

The corresponding algebra $\mathfrak{k}_{k-1}$ on $2k - 1$ qubits can be embedded into $2k + 1$ qubits using the operators

$$g_1 = -\tfrac{i}{2}\sum_{j=2}^{2k}\mathrm{X}_j,\ \ g_2 = -\tfrac{i}{2}\sum_{j=2}^{2k}\mathrm{Y}_j,\ \ g_3 = -\tfrac{i}{2}\left(\sum_{j=2}^{k}\mathrm{Z}_j\mathrm{Z}_{j+1} - \sum_{j=k+1}^{2k-1}\mathrm{Z}_j\mathrm{Z}_{j+1}\right).$$

We compute repeated commutators of f_3 with f_1. In the first two iterations, we get $f_4 = [f_3, f_1] = -\frac{i}{2}(\sum_{j=1}^{k}[\mathrm{Y}_j\mathrm{Z}_{j+1} + \mathrm{Z}_j\mathrm{Y}_{j+1}] - \sum_{j=k+1}^{2k}[\mathrm{Y}_j\mathrm{Z}_{j+1} + \mathrm{Z}_j\mathrm{Y}_{j+1}])$ and $f_5 = [f_3, f_4] = -\frac{i}{2}[-\mathrm{X}_1 - 2\sum_{j=2}^{2k}\mathrm{X}_j - \mathrm{X}_{2k+1} - 2(\sum_{j=2}^{k}\mathrm{Z}_{j-1}\mathrm{X}_j\mathrm{Z}_{j+1} - \mathrm{Z}_k\mathrm{X}_{k+1}\mathrm{Z}_{k+2} + \sum_{j=k+2}^{2k}\mathrm{Z}_{j-1}\mathrm{X}_j\mathrm{Z}_{j+1})]$. Repeating this process, we obtain the element $f_6 = [f_3, f_5] = -\frac{i}{2}[-\mathrm{Y}_1\mathrm{Z}_2 + \mathrm{Z}_{2k}\mathrm{Y}_{2k+1} - 4(\sum_{j=2}^{k}\mathrm{Y}_j\mathrm{Z}_{j+1} - \sum_{j=k+1}^{2k}\mathrm{Y}_j\mathrm{Z}_{j+1} + \sum_{j=1}^{k}\mathrm{Z}_j\mathrm{Y}_{j+1} - \sum_{j=k+1}^{2k-1}\mathrm{Z}_j\mathrm{Y}_{j+1})]$. Finally, we compute the next element $f_7 = [f_3, f_6] = -\frac{i}{2}(X_1 + 8\sum_{j=2}^{2k} X_j + X_{2k+1} + 8\sum_{j=2}^{k} Z_{j-1}X_jZ_{j+1} - 8Z_kX_{k+1}Z_{k+2} + 8\sum_{j=k+2}^{2k} Z_{j-1}X_jZ_{j+1})$. We obtain that $f_8 = -(4f_5 + f_7)/3 = -\frac{i}{2}(X_1 + X_{2k+1})$ and $g_1 = f_1 - f_8$. The proof for $f_9 = -\frac{i}{2}(Y_1 + Y_{2k+1})$ and $g_2 = f_2 - f_9$ is similar. We compute more commutators: First, we set $f_{10} = [f_3, g_1] = -\frac{i}{2}(\sum_{j=2}^{k}\left[Y_jZ_{j+1} + Z_jY_{j+1}\right] - \sum_{j=k+1}^{2k-1}\left[Y_jZ_{j+1} + Z_jY_{j+1}\right] + Z_1Y_2 - Y_{2k}Z_{2k+1})$. The other commutators are $f_{11} = [f_8, f_{10}] = -\frac{i}{2}(-Y_1Y_2 + Y_{2k}Y_{2k+1})$, $f_{12} = [f_1, f_{11}] = -\frac{i}{2}(-Z_1Y_2 - Y_1Z_2 + Z_{2k}Y_{2k+1} + Y_{2k}Z_{2k+1})$, and $f_{13} = [f_1, f_{12}] = -\frac{i}{2}(2Y_1Y_2 - 2Z_1Z_2 - 2Y_{2k}Y_{2k+1} + 2Z_{2k}Z_{2k+1})$. It follows that $f_{14} = -\frac{1}{2}f_{13} - f_{11} = -\frac{i}{2}(Z_1Z_2 - Z_{2k}Z_{2k+1})$ and $g_3 = f_3 - f_{14}$. We obtain $\mathfrak{k}_{k-1} \subseteq \mathfrak{k}_k$ completing the first step of the proof. Relying on the form of f_8 and f_9 we can prove by induction that $\bar{\mathfrak{k}}_k = \mathfrak{k}_k$ (second step). Assuming by induction that $\mathfrak{k}_{k-1}$ is irreducibly embedded on $2k - 1$ qubits, we obtain that the centralizer of $\mathfrak{k}_{k-1}$ (embedded on $2k + 1$ qubits) is given by all operators O which operate only on the two outer qubits. But the generators f_1, f_2, and f_3 of $\mathfrak{k}_k$ do not simultaneously commute with operators O. Therefore, $\mathfrak{k}_k$ is irreducibly embedded on $2k + 1$ qubits (third step). We switch to a new basis by reordering the qubits according to the numbers in the figure:



In this basis, we can provide a unitary matrix

$$S := \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \otimes M^{\otimes k} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}^{\otimes k},$$

which satisfies $SH + H^tS = 0$ for all elements iH of $\mathfrak{k}_k$. In particular, we have $S\bar{S} = -\mathbb{1}_{2^n}$. This can be readily verified on the generators for $k \in \{0, 1\}$. Using our commutator computations we obtain that $\mathfrak{k}_k = \langle f_1, f_2, f_3\rangle_{\mathrm{Lie}}$ is equal to $\langle g_1, g_2, g_3, f_8, f_9, f_{14}\rangle_{\mathrm{Lie}}$. Thus we can prove $SH + H^tS = 0$ by induction on k: Assuming the equation holds for g_1,g_2, and g_3 (i.e., for $k - 1$), we need to prove that it also holds for f_8,f_9, and f_{14} which are, respectively, given in the new basis by $-\frac{i}{2}(X_{2k} + X_{2k+1})$, $-\frac{i}{2}(Y_{2k} + Y_{2k+1})$, and $-\frac{i}{2}(Z_{2k-2}Z_{2k} - Z_{2k-1}Z_{2k+1})$. But this can be directly checked on the four outer qubits using $S_2 = M \otimes M$. As $\mathfrak{k}_k$ is given in an irreducible representation, the matrix S is unique up to a scalar factor. This shows that $\mathfrak{k}_k$ is given in a symplectic representation and that $\mathfrak{k}_k \subseteq \mathfrak{sp}(2^{2k})$ (fourth step). Staying in our new basis, we prove that $\mathfrak{k}_k$ contains the elements $P_j := -\frac{i}{2}(X_jZ_{j+1} - Z_jX_{j+1})$ and $Q_j := -\frac{i}{2}(X_jY_{j+1} - Y_jX_{j+1})$ for all even $j \in \{2, \ldots, 2k\}$ by induction on j. This can be readily verified for $j = 2$ considering $\mathfrak{k}_1 \subseteq \mathfrak{k}_k$. Assuming that $\mathfrak{k}_k$ contains the elements P_{j-2} and Q_{j-2} for $j \leq k$, we show that it also contains the elements P_j and Q_j. Recall that $\mathfrak{k}_k$ contains the elements f_8, f_9, and f_{14}. In addition, the elements $v_1 = -\frac{i}{2}(X_{2k-2} + X_{2k-1})$ and $v_2 = -\frac{i}{2}(Y_{2k-2} + Y_{2k-1})$ are contained in $\mathfrak{k}_k$. But one can directly check on the four outer qubits that P_j and Q_j are contained in the algebra $\mathfrak{m} = \langle f_8, f_9, f_{14}, P_{j-2}, Q_{j-2}, v_1, v_2\rangle_{\mathrm{Lie}} = \mathfrak{so}(2^4)$. Assuming that $\mathfrak{k}_j = \mathfrak{sp}(2^{2j})$ holds for $j < k$, it follows that $\mathfrak{sp}(2^{2k-4}) \otimes \mathfrak{so}(2^4) \subseteq \mathfrak{k}_k \subseteq \mathfrak{sp}(2^{2k})$. As $\mathfrak{sp}(2^{2k-4}) \otimes \mathfrak{so}(2^4)$ is a maximal subalgebra of $\mathfrak{sp}(2^{2k})$ (see Theorem 1.4 of Ref. 91) and $f_3 \in \mathfrak{k}_k$ is not of product form, we obtain by induction that $\mathfrak{k} = \mathfrak{sp}(2^{2k})$. □

Note the Cartan decomposition in the antisymmetric Ising chains of Fig. 4 can be taken with respect to the joint permutation of the qubits in the two branches with positive and negative ZZ couplings: the $\mathfrak{k}$-part consists of all terms with *odd* numbers of Pauli operators deviating from the identity, while the $\mathfrak{p}$-part collects the ones with *even* numbers.

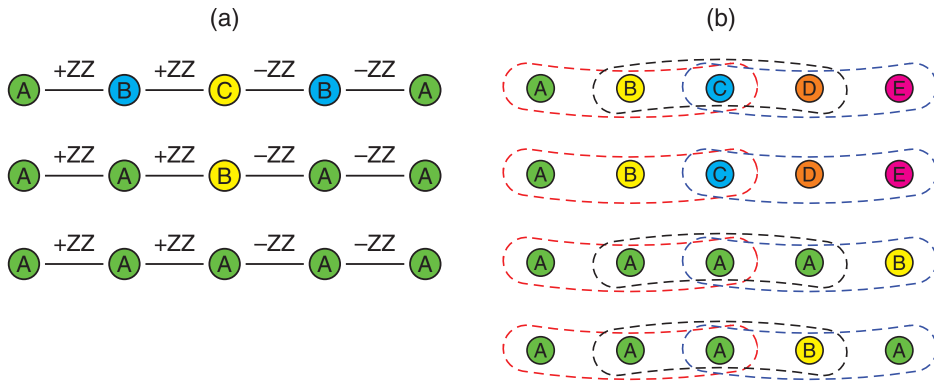


FIG. 5. (Color online) Quantum systems with dynamic Lie algebra $\mathfrak{sp}(16)$. (a) Examples with pairwise Ising-ZZ couplings and (b) examples with three-body ZZZ-interactions.

As a third example, consider the first Ising chain in Fig. 4 corresponding to $\mathfrak{sp}(8/2)$. Here the computations in **Algorithm 3** provide a unitary matrix [cf. Lemma 13(e)]

$$S_3 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & +1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & +1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & +1 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ +1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \tag{29}$$

with $S_3\bar{S}_3 = -\mathbb{1}$ underscoring the irreducible representation is symplectic [see Lemma 13(g)].

Moreover, since all the dynamic systems in Figures 5(a) and 5(b) share the same system algebra $\mathfrak{sp}(16)$, any two can mutually simulate each other by Proposition 24. So remarkably enough, the spin chains in Fig. 5(a) can simulate the effective three-qubit ZZZ-interactions shown in Fig. 5(b). In particular, note the lowest instance in Fig. 5(a): even only the *collective local controls* on all the qubits suffice to generate the three-body interactions with full local control shown at the top of Fig. 5(b). In turn, it may be astonishing at first sight that the system on top of Fig. 5(b) does not provide more dynamic degrees of freedom than the collective system at the bottom of Fig. 5(a), where the simulating power roots in the opposite signs of the couplings.

C. Dynamic systems with alternating orthogonal and symplectic algebras

Based on the smallest examples of Heisenberg-XX chains with one single local control on the second qubit as shown in Fig. 6, one may construct a full sequence of n-spin-$\frac{1}{2}$ chains, whose dynamic system algebras are orthogonal or symplectic depending on the value of $n \not\in \{1, 3\}$. Again, observe symplectic system algebras ensure *pure-state controllability*[36] without full operator controllability.

Quite remarkably, full local control on a single qubit suffices to get a dynamic algebra, where the number of dynamic degrees of freedom scales exponentially with the number of qubits, a finding

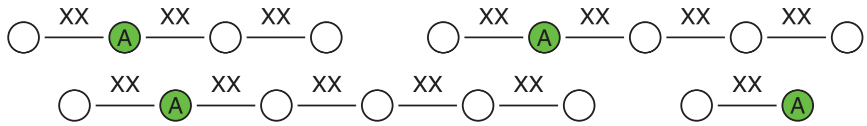


FIG. 6. (Color online) n-Spin-$\frac{1}{2}$ Heisenberg-XX chains with $n \notin \{1, 3\}$ and only *one locally controllable qubit at the second position* have orthogonal system algebras $\mathfrak{so}(2^n)$ if (n mod 4) $\in \{0, 1\}$ and symplectic system algebras $\mathfrak{sp}(2^{n-1})$ otherwise. A full series can be constructed for $n > 3$, and the examples shown for $n \in \{4, 5, 6, 2\}$ correspond to $\mathfrak{so}(16)$, $\mathfrak{so}(32)$, $\mathfrak{sp}(32)$, $\mathfrak{so}(5) \cong \mathfrak{sp}(4/2)$. In the single case of $n = 3$, central symmetry arises, which makes the respective algebra *reducible*.

described only for full isotropic Heisenberg-XXX coupling up to now.[41] More precisely, one arrives at the following:

*Proposition 30: Heisenberg-*XX *chains of $n \notin \{1, 3\}$ spin-$\frac{1}{2}$ qubits with only one locally controllable qubit at the second position give rise to the dynamic algebras*

$$\mathfrak{k}_n = \begin{cases} \mathfrak{so}(2^n) & \text{if } (n \bmod 4) \in \{0, 1\}, \\ \mathfrak{sp}(2^{n-1}) & \text{if } (n \bmod 4) \in \{2, 3\}, \end{cases}$$

which are irreducibly embedded in $\mathfrak{su}(2^n)$.

Proof: In the notation of Eq. (28) the generators of the dynamic algebra $\mathfrak{k}_n$ can be written as $f_1 = -\frac{i}{2}X_2$, $f_2 = -\frac{i}{2}Y_2$, and $f_3 = -\frac{i}{2}(\sum_{j=1}^{n-1} X_j X_{j+1} + Y_j Y_{j+1})$. We remark that the statements of the theorem can be directly verified for $n \in \{2, 4, 5\}$. Assuming $n \geq 6$ from now on, we complete the proof by induction. We organize the proof in steps: first we prove that $\mathfrak{k}_n \supsetneq \mathfrak{k}_2 \,\widehat{\oplus}\, \mathfrak{k}_{n-2}$, second we show that $\mathfrak{k}_n$ is given in an irreducible representation, and in the end we prove that $\mathfrak{k}_n$ is equal to $\mathfrak{so}(2^n)$ or $\mathfrak{sp}(2^{n-1})$. By computing sums of commutators we identify certain elements of $\mathfrak{k}_n$. The first elements are $f_4 := [f_1, [f_3, f_1]] + [f_2, [f_3, f_2]] = -\frac{i}{2}(X_1X_2 + Y_1Y_2 + X_2X_3 + Y_2Y_3)$, $f_5 := [[f_2, f_1], [f_1, [f_2, f_4]]] = -\frac{i}{2}(X_1X_2 + X_2X_3)$, and $f_6 := [[f_1, f_2], [f_2, [f_1, f_4]]] = -\frac{i}{2}(Y_1Y_2 + Y_2Y_3)$. Next we compute the elements $f_7 := [f_4, [f_3, f_4]] + [f_2, [f_6, [f_2, [f_3, f_4]]]] + [f_1, [f_5, [f_1, [f_3, f_4]]]] = -\frac{i}{2}(X_3X_4 + Y_3Y_4)$ and $f_8 := [[f_2, f_1], [[f_1, f_2], [f_3, [f_4, f_3]]]] - f_7 + [f_6, [f_7, f_3]] + [f_5, [f_7, f_3]] + [f_2, [f_6, [f_2, [f_3, f_4]]]] + [f_1, [f_5, [f_1, [f_3, f_4]]]] = -\frac{i}{2}(X_2X_3 + Y_2Y_3)$ leading to the elements $f_9 := f_4 - f_8 = -\frac{i}{2}(X_1X_2 + Y_1Y_2)$, $f_{10} := f_3 - f_4 = -\frac{i}{2}(\sum_{j=3}^{n-1} X_j X_{j+1} + Y_j Y_{j+1})$, and $f_{11} := f_4 + f_7 = -\frac{i}{2}(X_1X_2 + Y_1Y_2 + X_2X_3 + Y_2Y_3 + X_3X_4 + Y_3Y_4)$. By explicit computations on the first four qubits one can show that the elements $f_{12} = -\frac{i}{2}X_4$ and $f_{13} = -\frac{i}{2}Y_4$ are contained in $\mathfrak{k}_4 = \langle f_1, f_2, f_{11}\rangle_{\text{Lie}} \subseteq \mathfrak{k}_n$. We obtain that $\mathfrak{k}_2 = \langle f_1, f_2, f_9\rangle_{\text{Lie}} \subseteq \mathfrak{k}_n$ and $\mathfrak{k}_{n-2} = \langle f_{12}, f_{13}, f_{10}\rangle_{\text{Lie}} \subseteq \mathfrak{k}_n$. Therefore, $\mathfrak{k}_n = \langle f_1, f_2, f_9, f_{12}, f_{13}, f_{10}, f_8\rangle_{\text{Lie}} \supsetneq \mathfrak{k}_2 \,\widehat{\oplus}\, \mathfrak{k}_{n-2}$. This completes the first step of the proof. By induction $\mathfrak{k}_2$ and $\mathfrak{k}_{n-2}$ are given in an irreducible representation. Therefore, this holds also for $\mathfrak{k}_2 \,\widehat{\oplus}\, \mathfrak{k}_{n-2}$ and $\mathfrak{k}_n$, which completes the second step of the proof. Using the unitary matrices

$$S_2 := \begin{pmatrix} 0 & 0 & 0 & +1 \\ 0 & 0 & -1 & 0 \\ 0 & +1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} \quad \text{and} \quad S_3 := \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 & 0 & +1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

we define the unitary matrices $S_{2k} = (S_2)^{\otimes k}$ and $S_{2k+1} = (S_2)^{\otimes(k-1)} \otimes S_3$. We obtain that $S_{2k}\bar{S}_{2k} = (-1)^k \mathbb{1}_{2^{2k}}$ and $S_{2k+1}\bar{S}_{2k+1} = (-1)^k \mathbb{1}_{2^{2k+1}}$. Relying on direct computations in the case of $j \in \{2, 4,$

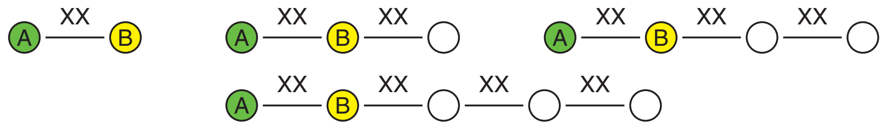


FIG. 7. (Color online) n-Spin-$\frac{1}{2}$ Heisenberg-XX chains with $n \geq 2$ (where the first two qubits can be independently, locally controlled) have fully controllable system algebras $\mathfrak{su}(2^n)$. A full series can be constructed: the first examples shown correspond to the algebras $\mathfrak{so}(6) \cong \mathfrak{su}(4)$, $\mathfrak{su}(8)$, $\mathfrak{su}(16)$, and $\mathfrak{su}(32)$.

5}, one can verify that $S_jH + H^tS_j = 0$ holds for all elements iH of $\mathfrak{k}_j$. Assuming by induction that $S_jH + H^tS_j = 0$ holds for all elements iH of $\mathfrak{k}_j$ where $j \in \{2, n-2\}$, we show that $S_nH + H^tS_n = 0$ holds also for all elements iH of the algebra $\mathfrak{k}_n = \langle f_1, f_2, f_9, f_{12}, f_{13}, f_{10}, f_8\rangle_{\text{Lie}} \supsetneq \mathfrak{k}_2 \mathbin{\widehat{\oplus}} \mathfrak{k}_{n-2}$ by directly verifying $S_4 f_8 + f_8^t S_4 = 0$ on the first four qubits. In summary, we proved that $\mathfrak{k}_2 \mathbin{\widehat{\oplus}} \mathfrak{k}_{n-2} \subsetneq \mathfrak{k}_n \subseteq \mathfrak{so}(2^n)$ or $\mathfrak{sp}(2^{n-1})$ depending on the value of n. But Theorem 1.4 of Ref. 91 says that $\mathfrak{k}_2 \mathbin{\widehat{\oplus}} \mathfrak{k}_{n-2}$ is a maximal subalgebra of $\mathfrak{so}(2^n)$ or $\mathfrak{sp}(2^{n-1})$. Thus, $\mathfrak{k}_n$ is equal to $\mathfrak{so}(2^n)$ if $(n \bmod 4) \in \{0, 1\}$ and equal to $\mathfrak{sp}(2^{n-1})$ otherwise. This completes the last step of the proof. □

D. Dynamic systems with unitary algebras

We close the series of worked examples by considering n-spin-$\frac{1}{2}$ Heisenberg-XX chains with $n \geq 2$, where the first two qubits can be independently, locally controlled (see Fig. 7). This case was recently studied in Refs. 46, 47, and 113. We show that these systems are fully controllable for arbitrary $n \geq 2$.

Corollary 31: Assume that the first two qubits of a Heisenberg-XX chain of n spin-$\frac{1}{2}$ qubits with $n \geq 2$ can be independently, locally controlled. Then, the dynamic algebra is $\mathfrak{k}_n = \mathfrak{su}(2^n)$.

Proof: The theorem can be directly verified for $n \in \{2, 3, 4, 5\}$. Building on the proof of Proposition 30, we prove the theorem for $n \geq 6$ by induction. We first show that $\mathfrak{k}_n \supsetneq \mathfrak{k}_2 \mathbin{\widehat{\oplus}} \mathfrak{k}_{n-2}$. From the proof of Proposition 30 it is only left to show that the elements X_3 and Y_3 can be generated. But this can be directly verified by computations on the first four qubits. Thus we proved that $\mathfrak{su}(2^n) \supseteq \mathfrak{k}_n \supsetneq \mathfrak{su}(2^2) \mathbin{\widehat{\oplus}} \mathfrak{su}(2^{n-2})$. Theorem 1.3 of Ref. 91 says that $\mathfrak{su}(2^2) \mathbin{\widehat{\oplus}} \mathfrak{su}(2^{n-2})$ is a maximal subalgebra of $\mathfrak{su}(2^n)$. The theorem follows immediately. □

X. FERMIONIC QUANTUM SYSTEMS

Fermionic d-level systems with any kind of quadratic (pair-interaction) Hamiltonians give rise to dynamic system Lie algebras limited to subalgebras like $\mathfrak{so}(2d)$ or $\mathfrak{so}(2d+1)$. By making use of the Jordan-Wigner transformation, which links the number of levels d with the number of qubits n, we show how these systems can be simulated by n-spin-$\frac{1}{2}$ chains with partial local control. For keeping the relation to mathematical literature, references are more extensive in this section.

A. Quadratic Hamiltonians

To fix notations, consider the fermionic creation and annihilation operators $f_p^\dagger$ and f_p which operate on a finite-dimensional quantum system of d levels and satisfy the anticommutation relations (with $1 \leq p, q \leq d$ and $\{a, b\}_+ := ab + ba$ and the Kronecker function $\delta_{p,q}$)

$$\{f_p^\dagger, f_q\}_+ = \delta_{p,q} \quad \text{and} \quad \{f_p^\dagger, f_q^\dagger\}_+ = 0 = \{f_p, f_q\}_+ \quad . \tag{30}$$

For the pth level of the system, $f_p^\dagger$ and f_p change the occupation numbers n_p labeling the respective states $|n_p\rangle$ such as to give $f_p^\dagger|0\rangle = |1\rangle = \binom{1}{0}$ and $f_p|1\rangle = |0\rangle = \binom{0}{1}$, where by the Pauli principle $n_p \in \{0, 1\}$, $(f_p^\dagger)^2 \equiv 0$, and $(f_p)^2 \equiv 0$. Now the properties of the usual *quadratic Hamiltonians* (see, e.g., Refs. 17 and 114–117)

$$H := \sum_{p,q=1}^{d} A_{pq} f_p f_q + B_{pq} f_p f_q^\dagger + C_{pq} f_p^\dagger f_q + D_{pq} f_p^\dagger f_q^\dagger \tag{31}$$

can be discussed in terms of their pair-interaction coupling coefficients A_{pq}, B_{pq}, C_{pq}, and D_{pq} seen as (possibly complex) entries of the $d \times d$-matrices A, B, C, and D. Hermiticity of H requires $A = D^\dagger$, $B = B^\dagger$, and $C = C^\dagger$, while in addition, the commutator relations of Eq. (30) imply

$$H = \sum_{p,q=1}^{d} -A_{pq} f_q f_p - D_{pq} f_q^\dagger f_p^\dagger \quad + \sum_{p,q=1,\, p\neq q}^{d} -B_{pq} f_q^\dagger f_p - C_{pq} f_q f_p^\dagger$$
$$+ \sum_{p=1}^{d} B_{pp}(1 - f_p^\dagger f_p) + C_{pp}(1 - f_p f_p^\dagger)\,,$$

which upon identification with Eq. (31) enforces $A = -A^t$, $B = -C^t$, and $D = -D^t$. Finally, keeping a widely used custom (see, e.g., p. 452 of Ref. 114 or p. 173 of Ref. 115) we also assume the entries of A, B, C, and D are real. Summing up, A is real skew-symmetric following $A = \bar{A} = -A^t = -D$ and B is real symmetric with $B = \bar{B} = B^t = -C$. So H of Eq. (31) can be given in "symmetrized" form (see, e.g., p. 2 of Ref. 118) as

$$H = \sum_{p,q=1}^{d} (-B_{pq})\big[f_p^\dagger f_q - f_p f_q^\dagger\big] + (-A_{pq})\big[f_p^\dagger f_q^\dagger - f_p f_q\big]\,. \tag{32}$$

B. Jordan-Wigner transformation

For simplicity, first recall the map from the non-compact, (real) special linear algebra $\mathfrak{sl}(2,\mathbb{R})$ to the compact, special unitary algebra $\mathfrak{su}(2)$. The generators of $\mathfrak{sl}(2,\mathbb{R})$ are given by $\mathrm{E} = \left(\begin{smallmatrix}0&1\\0&0\end{smallmatrix}\right) = \frac{1}{2}(\mathrm{X} + i\mathrm{Y})$, $\mathrm{H} = \left(\begin{smallmatrix}1&0\\0&-1\end{smallmatrix}\right) = \mathrm{Z}$, and $\mathrm{F} = \left(\begin{smallmatrix}0&0\\1&0\end{smallmatrix}\right) = \frac{1}{2}(\mathrm{X} - i\mathrm{Y})$ and the generators of $\mathfrak{su}(2)$ can be chosen as $i\mathrm{X}$, $i\mathrm{Z}$, and $i\mathrm{Y}$ where $\mathrm{X} = \left(\begin{smallmatrix}0&1\\1&0\end{smallmatrix}\right) = \mathrm{F} + \mathrm{E}$, $\mathrm{Z} = \left(\begin{smallmatrix}1&0\\0&-1\end{smallmatrix}\right) = \mathrm{H}$, and $\mathrm{Y} = \left(\begin{smallmatrix}0&-i\\i&0\end{smallmatrix}\right) = i(\mathrm{F} - \mathrm{E})$. Obviously, this also defines a map between the Lie algebras (see, e.g., p. 127 of Ref. 68 or Chap. IX, Sec. 3.6 of Ref. 79) readily serving as a prototype for maps between *non-compact* normal real forms and *compact* real forms of Lie algebras (cf. Ref. 80).

Likewise, the Jordan-Wigner transformation[119] maps the fermionic operators (for $1 \le p \le d$)

$$f_p^\dagger = \tfrac{1}{2}(c_p + i c_{p+d}) \quad \text{and} \quad f_p = \tfrac{1}{2}(c_p - i c_{p+d}) \quad \text{to the operators} \tag{33}$$

$$c_p := f_p + f_p^\dagger \quad \text{and} \quad c_{p+d} := i(f_p - f_p^\dagger)\,. \tag{34}$$

Now c_p and c_{p+d} can be given explicitly as d-qubit operators

$$c_p = \underbrace{\mathrm{Z}\cdots\mathrm{Z}}_{p-1}\mathrm{X}\underbrace{\mathrm{I}\cdots\mathrm{I}}_{d-p} \quad \text{and} \quad c_{p+d} = \underbrace{\mathrm{Z}\cdots\mathrm{Z}}_{p-1}\mathrm{Y}\underbrace{\mathrm{I}\cdots\mathrm{I}}_{d-p}\,. \tag{35}$$

We refer to Chap. VIII, Sec. 3 of Ref. 120, Sec. 9.6 of Ref. 121, or Sec. 44 of Ref. 122, where more information on this construction can be found and where connections to Clifford algebras are discussed. In the context of Clifford algebras this construction is sometimes named after Brauer and Weyl[123] (see, e.g., p. 183 of Ref. 124).

C. Quadratic Hamiltonians in qubit form

Now one can readily apply the Jordan-Wigner transformation to fermionic quadratic Hamiltonians. Assuming that the number of levels is d, the Hamiltonian of Eq. (32) is mapped to (see, e.g., Theorem VI.I of Ref. 118)

$$H = -\sum_{p=1}^{d} B_{pp} \underbrace{\mathrm{I}\cdots\mathrm{I}}_{p-1}\mathrm{Z}\underbrace{\mathrm{I}\cdots\mathrm{I}}_{d-p} \tag{36a}$$

$$+ \sum_{p,q=1,\,p>q}^{d} B_{pq}\Big(\underbrace{\mathrm{I}\cdots\mathrm{I}}_{q-1}\mathrm{X}\underbrace{\mathrm{Z}\cdots\mathrm{Z}}_{p-q-1}\mathrm{X}\underbrace{\mathrm{I}\cdots\mathrm{I}}_{d-p}+\underbrace{\mathrm{I}\cdots\mathrm{I}}_{q-1}\mathrm{Y}\underbrace{\mathrm{Z}\cdots\mathrm{Z}}_{p-q-1}\mathrm{Y}\underbrace{\mathrm{I}\cdots\mathrm{I}}_{d-p}\Big) \tag{36b}$$

$$- \sum_{p,q=1,\,p>q}^{d} A_{pq}\Big(\underbrace{\mathrm{I}\cdots\mathrm{I}}_{q-1}\mathrm{X}\underbrace{\mathrm{Z}\cdots\mathrm{Z}}_{p-q-1}\mathrm{X}\underbrace{\mathrm{I}\cdots\mathrm{I}}_{d-p}-\underbrace{\mathrm{I}\cdots\mathrm{I}}_{q-1}\mathrm{Y}\underbrace{\mathrm{Z}\cdots\mathrm{Z}}_{p-q-1}\mathrm{Y}\underbrace{\mathrm{I}\cdots\mathrm{I}}_{d-p}\Big). \tag{36c}$$

We obtain the dynamic algebra of a general fermionic Hamiltonian containing quadratic terms:

Theorem 32: *Let the entries of the real antisymmetric matrix A and the real symmetric matrix B denote the control functions of the Hamiltonian given in Eq. (36). We assume $d \geq 2$. The dynamic algebra $\mathfrak{so}(2d)$ of the corresponding control system is embedded in $\mathfrak{su}(2^d)$. The centralizer of the dynamic algebra is one-dimensional and is given by the d-qubit operator $-\frac{i}{2}\mathrm{Z}\cdots\mathrm{Z}$. The embedding of $\mathfrak{so}(2d)$ into $\mathfrak{su}(2^d)$ splits into two irreducible representations of equal dimension.*

Proof: Let $\mathfrak{k}_d$ denote the dynamic algebra of the control system. Both of the generators $-\frac{i}{2}\mathrm{I}\cdots\mathrm{IXZ}\cdots\mathrm{ZXI}\cdots\mathrm{I}$ and $-\frac{i}{2}\mathrm{I}\cdots\mathrm{IYZ}\cdots\mathrm{ZYI}\cdots\mathrm{I}$ arise from linear combinations of Eqs. (36b) and (36c), and computing commutators with the generators $-\frac{i}{2}\mathrm{I}\cdots\mathrm{IZI}\cdots\mathrm{I}$ from Eq. (36a) reveals the generators $-\frac{i}{2}\mathrm{I}\cdots\mathrm{IXZ}\cdots\mathrm{ZYI}\cdots\mathrm{I}$ and $-\frac{i}{2}\mathrm{I}\cdots\mathrm{IYZ}\cdots\mathrm{ZXI}\cdots\mathrm{I}$. By comparing with the (independent) proof of Theorem 34 it follows that $\mathfrak{k}_d$ is a subalgebra of $\mathfrak{so}(2d+1)$. The statements of the theorem can be directly verified for $d \in \{2, 3, 4, 5\}$. We assume by induction that the $(d-1)$-qubit operator $a = -\frac{i}{2}\mathrm{Z}\cdots\mathrm{Z}$ is the only element in the centralizer of $\mathfrak{k}_{d-1}$. Considering a as an d-qubit operator operating on the first $d-1$ qubits we obtain that the centralizer of $\mathfrak{k}_d$ can only contain linear combinations of elements from the set $-\frac{i}{2}\{\mathrm{I}\cdots\mathrm{IX}, \mathrm{I}\cdots\mathrm{IY}, \mathrm{I}\cdots\mathrm{IZ}, \mathrm{Z}\cdots\mathrm{ZI}, \mathrm{Z}\cdots\mathrm{ZX}, \mathrm{Z}\cdots\mathrm{ZY}, \mathrm{Z}\cdots\mathrm{ZZ}\}$. The second statement of the theorem follows from the fact that only the last element in the set commutes with all generators. We obtain from the structure of the generators that $\mathfrak{so}(2d-4) \oplus \mathfrak{so}(4) \subsetneq \mathfrak{k}_d$. We remark that $\mathfrak{so}(2d-4) \oplus \mathfrak{so}(4)$ is a maximal subalgebra of $\mathfrak{so}(2d)$ and that $\mathfrak{so}(2d)$ is a maximal subalgebra of $\mathfrak{so}(2d+1)$ (see, e.g., p. 219 of Ref. 125 or Table 12 on p. 150 of Ref. 126). Therefore, $\mathfrak{k}_d$ is equal to $\mathfrak{so}(2d)$ or $\mathfrak{so}(2d+1)$. But $\mathfrak{k}_d \neq \mathfrak{so}(2d+1)$ as the corresponding embedding would be irreducible, and the first statement of the theorem follows. We already showed that the centralizer is one-dimensional which is equivalent to the fact that the commutant is two-dimensional. Theorem 1.5 of Ref. 109 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. Thus, the embedding of $\mathfrak{so}(2d)$ into $\mathfrak{su}(2^d)$ splits into two irreducible representations. The third statement of the theorem follows now by proving that the simultaneous eigenvalues of the Hamiltonians corresponding to all generators are given by ± 1 occurring each with multiplicity 2^{d-1}. This can be directly verified for $d \in \{2, 3, 4, 5\}$. Assuming the statement by induction for all $\mathfrak{k}_{d'}$ with $d' < d$ we obtain the simultaneous eigenvalues of Hamiltonians corresponding to the algebras $\mathfrak{k}_{d-2}$ and $\mathfrak{k}_2$ acting on the first $d-2$ qubits and the last two qubits, respectively. As the eigenvalues of a tensor product of two matrices are given by the product of the eigenvalues of each matrix, we can prove the statement by induction. □

The first statement of Theorem 32 is related to the fact that the canonical transformations of fermionic systems are given by orthogonal transformations $\mathfrak{o}(2d)$ (see, e.g., p. 118 of Ref. 115 and p. 39 of Ref. 116). In more mathematical literature, the first statement of Theorem 32 can be found in Sec. 9.6 of Ref. 121, pp. 182–186 of Ref. 122, pp. 499–501 of Ref. 127, and pp. 180–186 of Ref. 124. Recently, this came again into focus.[17,117] The dynamic algebra $\mathfrak{so}(2d)$ was also discussed as symmetry of Hamiltonians in Refs. 128 and 129.

The polynomial growth (in d) of the algebra in Theorem 32 to the dynamic system of Eqs. (36) was identified as the reason why efficient classical simulation of quadratic, fermionic quantum systems is possible (cf., e.g., pp. 9–10 of Ref. 130, pp. 5–6 of Ref. 131, and pp. 3 of Ref. 132). Setting $n := d - 1$ in Proposition 28 we obtain

*Corollary 33: Heisenberg-*XX *chains of $d-1$ spin-$\frac{1}{2}$ qubits ($d \geq 3$) and two individually locally controllable qubits, one at each end, have the dynamic algebra $\mathfrak{so}(2d)$ and can thus simulate a general fermionic quadratic Hamiltonian on d levels and vice versa.*

By the second and third statement of Theorem 32, the embedding of $\mathfrak{so}(2d)$ into $\mathfrak{su}(2^d)$ splits into two irreducible representations of equal dimension, and thus $\mathfrak{so}(2d)$ acts simultaneously on both components. Therefore, this embedding is—besides a doubling of the dimension—equivalent to the embedding of $\mathfrak{so}(2d)$ into $\mathfrak{su}[2^{(d-1)}]$ via Proposition 28 as readily verifiable by resorting to the Pauli basis for $\mathfrak{so}(2d)$ given there. Referring to Table II, we further remark that the embedding of $\mathfrak{so}(2d)$ into $\mathfrak{su}[2^{(d-1)}]$ can arise (in the sense of Sec. VI) from a symplectic representation (for $d = 4k + 2$), an orthogonal one (for $d = 4k$), or a unitary one (for d odd).

Now we illustrate that a controlled spin chain can simulate a quadratic fermionic system, while the converse does not hold. To this end, consider the case where the general quadratic ("physical") Hamiltonian is supplemented by the ("unphysical") linear terms $\sum_{p=1}^{d} j_p f_p^\dagger + k_p f_p$ with $j_p, k_p \in \mathbb{C}$. Hermiticity implies $j_p = \bar{k}_p$. Assume again that the coefficients j_p and k_p are real, i.e., $j_p = \bar{j}_p$ and $k_p = \bar{k}_p$ to obtain $j_p = \bar{j}_p = k_p$. Thus the linear terms can be written as $\sum_{p=1}^{d} j_p(f_p^\dagger + f_p)$; they are mapped via the Jordan-Wigner transformation to the operators

$$H_2 = \sum_{p=1}^{d} j_p \underbrace{\mathrm{Z}\cdots\mathrm{Z}}_{p-1}\mathrm{X}\underbrace{\mathrm{I}\cdots\mathrm{I}}_{d-p} . \tag{37}$$

As will be shown next, this determines the dynamic algebra of a fictitious Hamiltonian system containing quadratic *and* linear terms (see also the Pauli basis for $\mathfrak{so}(2d+1)$ given in the proof to Proposition 27):

Theorem 34: *Let $j_p \in \mathbb{R}$ ($1 \leq p \leq d$) and the entries of the real antisymmetric matrix A and the real symmetric matrix B denote the control functions in the Hamiltonian $H + H_2$, where H and H_2 are given by Eqs. (36) and (37), respectively. The dynamic algebra $\mathfrak{so}(2d+1)$ of the corresponding control system is irreducibly embedded in $\mathfrak{su}(2^d)$.*

Proof: Computing commutators of generators $-\frac{i}{2}\mathrm{Z}\cdots\mathrm{ZXI}\cdots\mathrm{I}$ from Eq. (37) with generators $-\frac{i}{2}\mathrm{I}\cdots\mathrm{IZI}\cdots\mathrm{I}$ from Eq. (36a), we obtain the additional generators $-\frac{i}{2}\mathrm{Z}\cdots\mathrm{ZYI}\cdots\mathrm{I}$. Furthermore, the generators $-\frac{i}{2}\mathrm{I}\cdots\mathrm{IXZ}\cdots\mathrm{ZXI}\cdots\mathrm{I}$ and $-\frac{i}{2}\mathrm{I}\cdots\mathrm{IYZ}\cdots\mathrm{ZYI}\cdots\mathrm{I}$ arise from linear combinations of Eqs. (36b) and (36c) and computing commutators with generators $-\frac{i}{2}\mathrm{I}\cdots\mathrm{IZI}\cdots\mathrm{I}$ from Eq. (36a) reveals the additional generators $-\frac{i}{2}\mathrm{I}\cdots\mathrm{IXZ}\cdots\mathrm{ZYI}\cdots\mathrm{I}$ and $-\frac{i}{2}\mathrm{I}\cdots\mathrm{IYZ}\cdots\mathrm{ZXI}\cdots\mathrm{I}$. Now the theorem follows by comparing all the generators with the table in the proof of Proposition 27. □

Moreover, setting $n := d$ in Proposition 27 we get

*Corollary 35: Heisenberg-*XX *chains of d spin-$\frac{1}{2}$ qubits ($d \geq 1$) and a single locally controllable qubit at one end have the dynamic algebra $\mathfrak{so}(2d+1)$ and can simulate a general fermionic quadratic Hamiltonian on d levels with its dynamic algebra $\mathfrak{so}(2d)$, but obviously not vice versa (as is also illustrated by the unphysical linear terms above).*

D. Discussion

We analyze three further cases of fermionic Hamiltonians. First, consider quadratic Hamiltonians (without linear terms) which are particle-number preserving, i.e., $A = 0$ in Eq. (36). Assuming the elements of B are control functions, we obtain $\mathfrak{u}(d)$ as dynamic algebra (cf. p. 501 of Ref. 127). Second, the diagonal normal form (see, e.g., Appendix A of Ref. 114, Sec. III.8 of Ref. 115, Sec. 3.3 of Ref. 116, and Theorem II.1 of Ref. 118) for the Hamiltonian H of Eq. (32)

$$\sum_{p=1}^{d} E_p \left(f_p^\dagger f_p - \tfrac{1}{2}\right) = \sum_{p=1}^{d} \frac{E_p}{2} \left(f_p^\dagger f_p - f_p f_p^\dagger\right) \tag{38}$$

(with E_p positive and real) is mapped by the Jordan-Wigner transformation to the d-qubit operator

$$\sum_{p=1}^{d} \frac{E_p}{2} \underbrace{\mathrm{I}\cdots\mathrm{I}}_{p-1}\mathrm{Z}\underbrace{\mathrm{I}\cdots\mathrm{I}}_{d-p}. \tag{39}$$

Considering E_p ($1 \leq p \leq d$) as controls, we get a d-dimensional abelian Lie algebra as dynamic algebra. Third, if we allow for fermionic operators of arbitrary order (less than or equal to d), we get $\mathfrak{su}(2^d)$ as dynamic algebra.

In summary, the sequence of dynamic Lie algebras

$$\mathfrak{su}(2^d) \supseteq \mathfrak{so}(2d+1) \supset \mathfrak{so}(2d) \supseteq \mathfrak{u}(d) \tag{40}$$

plays a prominent role for fermionic quantum systems as pointed out in Chap. 22 of Ref. 133 and Sec. IV of Ref. 134. This sequence of Lie algebras is also widely studied in particle physics.[135,136]

E. Spinless Hubbard model with periodic boundary conditions

First, specify a spinless version of the Hubbard model (see p. 20 in Ref. 137 or p. 61 in Ref. 138) with periodic boundary conditions where $d + 1 = 1$ due to the periodicity, $d \geq 2$, and $t, u \in \mathbb{R}$:

$$H = -t \sum_{p=1}^{d} (f_p^\dagger f_{p+1} - f_p f_{p+1}^\dagger) \tag{41a}$$

$$+u \sum_{p=1}^{d} (f_p^\dagger f_p - \tfrac{1}{2})\,. \tag{41b}$$

Equation (41a) resembles a spinless tight-binding model (see p. 437 in Ref. 137 or p. 59 in Ref. 138) and equals the quadratic Hamiltonian of Eq. (32) with $A = 0$ and

$$B = -\frac{1}{2} \begin{pmatrix} 0 & 1 & & & & & & 1 \\ 1 & 0 & 1 & & & & & \\ & 1 & 0 & \cdot & & & & \\ & & \cdot & \cdot & \cdot & & & \\ & & & \cdot & \cdot & \cdot & & \\ & & & & \cdot & 0 & 1 & \\ & & & & & 1 & 0 & 1 \\ 1 & & & & & & 1 & 0 \end{pmatrix}.$$

The Jordan-Wigner transform of the Hamiltonian H of Eq. (41) takes the form

$$H = \frac{t}{2}\Big[\Big(\sum_{p=1}^{d-1} \underbrace{\mathrm{I}\cdots\mathrm{I}}_{p-1}\mathrm{YY}\underbrace{\mathrm{I}\cdots\mathrm{I}}_{d-1-p} + \underbrace{\mathrm{I}\cdots\mathrm{I}}_{p-1}\mathrm{XX}\underbrace{\mathrm{I}\cdots\mathrm{I}}_{d-1-p}\Big) + \Big(\mathrm{X}\underbrace{\mathrm{Z}\cdots\mathrm{Z}}_{d-2}\mathrm{X} + \mathrm{Y}\underbrace{\mathrm{Z}\cdots\mathrm{Z}}_{d-2}\mathrm{Y}\Big)\Big] \tag{42a}$$

$$+\,u \sum_{p=1}^{d} \underbrace{\mathrm{I}\cdots\mathrm{I}}_{p-1}\mathrm{Z}\underbrace{\mathrm{I}\cdots\mathrm{I}}_{d-p}\;. \tag{42b}$$

Extending Eq. (41b) to $\sum_{p=1}^{d} u_p(f_p^\dagger f_p - \frac{1}{2})$ such that it contains site-dependent control functions $u_p \in \mathbb{R}$, we obtain (by building on Appendix B of Ref. 117)

Lemma 36: The dynamic control system corresponding to the Hamiltonian

$$H = -t\sum_{p=1}^{d}(f_p^\dagger f_{p+1} - f_p f_{p+1}^\dagger) + \sum_{p=1}^{d} u_p(f_p^\dagger f_p - \tfrac{1}{2}) \tag{43}$$

has $\mathfrak{u}(d)$ *as dynamic Lie algebra assuming that* $u_p \in \mathbb{R}$ *are controls and* $d \geq 2$.

Proof: Let $\mathfrak{k}_d$ denote the dynamic algebra of the control system. We obtain from Eq. (42a) one generator a_1 and from Eq. (42b) the generators $(0 \leq p \leq d)$

$$\mathrm{z}_p := -\tfrac{i}{2}\mathrm{Z}_p = -\tfrac{i}{2}\underbrace{\mathrm{I}\cdots\mathrm{I}}_{p-1}\mathrm{Z}\underbrace{\mathrm{I}\cdots\mathrm{I}}_{d-p}.$$

One can verify on the generators that the d-qubit operators $-\frac{i}{2}\mathrm{Z}\cdots\mathrm{Z}$ and $-\frac{i}{2}\sum_{p=1}^{d}\mathrm{Z}_p$ are both elements of the centralizer of $\mathfrak{k}_d$. By comparison with Theorem 32 we obtain that $\mathfrak{k}_d \subseteq \mathfrak{so}(2d)$. As the centralizer in Theorem 32 is one-dimensional and the centralizer of $\mathfrak{k}_d$ is at least two-dimensional, it follows that $\mathfrak{k}_d \subsetneq \mathfrak{so}(2d)$. We remark that $\mathfrak{u}(d)$ is a maximal subalgebra of $\mathfrak{so}(2d)$ and that $\mathfrak{su}(q) \oplus \mathfrak{u}(d-q)$ is a maximal subalgebra of $\mathfrak{su}(d)$ (see, e.g., p. 219 of Ref. 125). In particular, $\mathfrak{u}(q) \oplus \mathfrak{u}(d-q)$ is a maximal subalgebra of $\mathfrak{u}(d)$. The theorem can be directly verified for $d \in \{2, 3, 4, 5\}$. We assume by induction that the theorem is true for all $\mathfrak{k}_{d'}$ with $d' < d$. The theorem follows by induction if we show that $\mathfrak{k}_d \supsetneq \mathfrak{u}(q) \oplus \mathfrak{u}(d-q)$ holds for any q. We compute the commutators $a_2 := [\mathrm{z}_1, [\mathrm{z}_2, a_1]] = -\frac{i}{2}(\mathrm{X}_1\mathrm{X}_2 + \mathrm{Y}_1\mathrm{Y}_2)$ and $a_3 := [\mathrm{z}_3, [\mathrm{z}_2, a_1]] = -\frac{i}{2}(\mathrm{X}_2\mathrm{X}_3 + \mathrm{Y}_2\mathrm{Y}_3)$ [using again the notation of Eq. (28)]. For $3 \leq j \leq d-1$ we have $g_j := [\mathrm{z}_{j+1}, [\mathrm{z}_j, a_1]] = -\frac{i}{2}(\mathrm{X}_j\mathrm{X}_{j+1} + \mathrm{Y}_j\mathrm{Y}_{j+1})$ and by linear combinations we obtain the d-qubit operator $a_4 := -\frac{i}{2}(\mathrm{XZ}\cdots\mathrm{ZX} + \mathrm{YZ}\cdots\mathrm{ZY})$. We further compute the commutators $a_5 := [\mathrm{z}_2, [a_2, a_4]] = -\frac{i}{2}(\mathrm{IXZZ}\cdots\mathrm{ZX} + \mathrm{IYZZ}\cdots\mathrm{ZY})$ and $a_6 := [\mathrm{z}_3, [a_3, a_5]] = -\frac{i}{2}(\mathrm{IIXZ}\cdots\mathrm{ZX} + \mathrm{IIYZ}\cdots\mathrm{ZY})$. Using the elements g_j and a_6 we can build the element $a_6 - \frac{i}{2}(\sum_{j=3}^{d-1}\mathrm{X}_j\mathrm{X}_{j+1} + \mathrm{Y}_j\mathrm{Y}_{j+1})$ which together with a_2 and the elements z_j generates $\mathfrak{u}(2) \oplus \mathfrak{u}(d-2)$. As a_3 is not contained in $\mathfrak{u}(2) \oplus \mathfrak{u}(d-2)$ we proved that $\mathfrak{k}_d \supsetneq \mathfrak{u}(2) \oplus \mathfrak{u}(d-2)$. □

F. Note on the Hubbard model with periodic boundary conditions and spin

Including the spin $\sigma = \pm$ in the Hubbard model gives

$$H = -t\left[\sum_{\sigma=\pm}\sum_{p=1}^{d}(f_{p,\sigma}^\dagger f_{p+1,\sigma} - f_{p,\sigma} f_{p+1,\sigma}^\dagger)\right] \tag{44a}$$

$$+\sum_{p=1}^{d} u_p(f_{p,+}^\dagger f_{p,+} - \tfrac{1}{2})(f_{p,-}^\dagger f_{p,-} - \tfrac{1}{2}), \tag{44b}$$

where the anticommutation relations of Eq. (30) still hold among operators with *equal spin values*, while operators with *different spin values* anticommute. The spin degrees of freedom just split each of the original levels p into two sub-levels. Thus the image of the Hamiltonian form Eq. (44) under the Jordan-Wigner transformation operates on a space of squared dimension as compared to the case without spin and the dynamic algebra is embedded in $\mathfrak{su}(2^{2d})$. The drift Hamiltonian of Eq. (44a) is mapped to $A_0 \otimes \mathbb{1} + \mathbb{1} \otimes A_0$ with

$$A_0 := \Big(\sum_{p=1}^{d-1}\underbrace{\mathrm{I}\cdots\mathrm{I}}_{p-1}\mathrm{YY}\underbrace{\mathrm{I}\cdots\mathrm{I}}_{d-1-p} + \underbrace{\mathrm{I}\cdots\mathrm{I}}_{p-1}\mathrm{XX}\underbrace{\mathrm{I}\cdots\mathrm{I}}_{d-1-p}\Big) + \Big(\mathrm{X}\underbrace{\mathrm{Z}\cdots\mathrm{Z}}_{d-2}\mathrm{X} + \mathrm{Y}\underbrace{\mathrm{Z}\cdots\mathrm{Z}}_{d-2}\mathrm{Y}\Big).$$

The control Hamiltonians of Eq. (44b) are mapped to $A_p \otimes A_p$ where

$$A_p := \underbrace{\mathrm{I}\cdots\mathrm{I}}_{p-1}\mathrm{Z}\underbrace{\mathrm{I}\cdots\mathrm{I}}_{d-p}.$$

TABLE V. (Color online) Summarizing overview on simulating quantum systems.

System type of n spins-$\frac{1}{2}$	Levels[a]	Order of coupling: Fermionic	Order of coupling: Bosonic[b]	System algebra
	n	quadratic (i.e., 2)	...	$\mathfrak{so}(2n+1)$
	$n+1$	quadratic (i.e., 2)	...	$\mathfrak{so}(2n+2)$
				
for (n mod 4) $\in \{0, 1\}$	n	up to n	...	$\mathfrak{so}(2^n)$
for (n mod 4) $\in \{2, 3\}$	n	...	up to n	$\mathfrak{sp}(2^{n-1})$
	n	up to n	up to n	$\mathfrak{su}(2^n)$

[a]In second quantization, the number of levels for the fermionic or bosonic system usually arises as a map from the number of qubits in the spin system. For fermions, the mapping is given by the Jordan-Wigner transformation.
[b]Here Bosonic is to be understood as the compact real form of the dynamic algebra for a bosonic system as in Section XI.

For $d = 2$, direct computation using the computer algebra system MAGMA[90] gives the system Lie algebra $\mathfrak{su}(2) \oplus \mathfrak{su}(2) \oplus \mathfrak{u}(1)$ embedded in $\mathfrak{su}(2^4)$. The general case appears more intricate and goes beyond the scope of this work.

XI. BOSONIC QUANTUM SYSTEMS

Finally, we comment on the bosonic case. As opposed to the Pauli principle in the fermionic case, in bosons the occupation number n_p is not bounded and—even for a finite number d of levels—the dynamic algebra of Hamiltonians of arbitrary order need not be finite unless the particle number is also bounded. Yet, the dynamic algebra for *quadratic (pair-interaction) Hamiltonians* is given by the real symplectic algebra $\mathfrak{sp}(2d, \mathbb{R})$ (see, e.g., p. 36 of Ref. 116, p. 186 of Ref. 122, or p. 501 of Ref. 127). We have not yet found an appropriate spin system that would be dynamically equivalent to the compact real form $\mathfrak{sp}(d)$ of a quadratic bosonic system with algebra $\mathfrak{sp}(2d, \mathbb{R})$. However, in Secs. IX B–IX C, we have already presented spin systems with dynamic algebras $\mathfrak{sp}(2^{n-1})$ which are actually *more powerful than required* and contain the compact real form $\mathfrak{sp}(d)$ of a quadratic bosonic system with algebra $\mathfrak{sp}(2d, \mathbb{R})$. For further analysis of the bosonic case, the Holstein-Primakoff transformation may be of help (see, e.g., p. 78 of Ref. 138). Finally, the results of mutually simulating quantum systems are summarized in Table V.

XII. OUTLOOK: QUANTUM SIMULATION AS AN OBSERVED OPTIMAL-CONTROL PROBLEM

Clearly, in view of experimental settings, one may take a more specific point of view by comparing the *time course* of two *observed bilinear control systems* (Σ_μ), $\mu = a, b$ with respect to (i) a set of Hermitian (and mutually orthogonal) observables $C_\nu^{(a)}$ and $C_{\nu'}^{(b)}$ with $\nu, \nu' \in \mathcal{I} \subseteq \{1, 2, \ldots, N^2-1\}$, (ii) the initial states ρ_0^μ, (iii) a given time interval $[0, T]$, and (iv) admissible controls $u_j^\mu(t) \in \mathcal{U}^\mu \subseteq \mathbb{R}$

$$\dot{\rho}^\mu(t) = -i\Big[\Big(H_0^\mu + \sum_{j=1}^m u_j^\mu(t) H_j^\mu\Big)\,,\ \rho^\mu(t)\Big] \quad \text{with} \quad \rho^\mu(0) = \rho_0^\mu \tag{45}$$

$$\langle C\rangle_\nu^\mu(t) = \operatorname{tr}\{(C_\nu^\mu)^\dagger \rho^\mu(t)\} \quad \text{with} \quad \{C_\nu^\mu\},\ \nu \in \mathcal{I}\,. \tag{46}$$

Now the comparison resorts to the expectation values $\langle C\rangle^\mu(t)$ via states $\rho^\mu(t)$, drifts H_0^μ, controls H_j^μ, and control amplitudes $u_j^\mu(t)$. Note that $\{C_\nu^{(a)}\}$ and $\{C_{\nu'}^{(b)}\}$ need not coincide, but if Σ_a shall simulate Σ_b it is convenient to require $|\{C_\nu^{(a)}\}| \geq |\{C_{\nu'}^{(b)}\}|$ so that (by invoking the above orthogonality of the observables with respect to the Hilbert-Schmidt scalar product) one can ensure: rank $\operatorname{span}_{\mathbb{R}} \{C_\nu^{(a)}\} \geq$ rank $\operatorname{span}_{\mathbb{R}} \{C_{\nu'}^{(b)}\}$.

Now for simultaneous measurement, it is useful to pick several observables C^μ_ν as long as they are compatible (mutually commute), or, more generally, as long as they are mutually non-disturbing in the sense of the recent findings in Ref. 23. Simultaneous expectation values are conveniently collected in the observation vectors

$$[\langle \mathsf{C}\rangle^\mu(t)] := [\langle C\rangle^\mu_1(t), \langle C\rangle^\mu_2(t), ...]^t \quad \text{with} \quad \mu = a, b\ . \tag{47}$$

Likewise, we define the respective dynamic system algebras of Σ_a and Σ_b as

$$\mathfrak{k}_\mu := \langle iH^\mu_0, iH^\mu_j \,|\, j = 1, 2, \ldots, m_\mu\rangle_{\text{Lie}} \quad \text{with} \quad \mu = a, b\ . \tag{48}$$

Clearly, $\mathfrak{k}_a \supseteq \mathfrak{k}_b$ implies Σ_a can simulate Σ_b. However, if Σ_a comes with a larger set of observables $\{C^{(a)}_\nu\}$, the above condition is still sufficient, but it is no longer necessary. This is analogous to the fact that in *quantum systems* controllability implies observability, whereas the converse need not hold[25] (for details see Ref. 37). In *classical systems*, however, controllability and observability are dual to one another (see, e.g., Ref. 139), since no observables accounting for the quantum-specific measurement process are involved. Now the notion of *weak simulation*, for which simulability can be seen as a strong condition, comes naturally:

Proposition 37: A dynamic system Σ_a can weakly simulate another dynamic system Σ_b in time interval $[0, T]$ *and with respect to the two sets of observables $\{C^a_\nu\}$ and $\{C^b_\nu\}$, if there exists a pair of initial conditions ρ^a_0 and ρ^b_0 (reachable form the respective equilibrium states) and two sets of admissible control vectors $u^a_j(t)$ and $u^b_j(t')$ such that $M[\langle \mathsf{C}\rangle^a(t)] = [\langle \mathsf{C}\rangle^b(t')]$ for all $t \in [0, T]$ and $t' \in [\tau(0), \tau(T)]$, where $\tau(t)$ is a bijective function of t for all $t \in [0, T]$ and M is a map $M : \mathbb{R}^n \to \mathbb{R}^m$, $[\langle \mathsf{C}\rangle^a(t)] \mapsto [\langle \mathsf{C}\rangle^b(t)]$ with $n \geq m$.*

As will be described elsewhere, the previous proposition motivates to view simulability as a generic precondition to formulate weak quantum simulation as an optimal-control task: minimize $||M[\langle \mathsf{C}\rangle^a(t)] - [\langle \mathsf{C}\rangle^b(t')]||^2_2$ subject to the differential equations of motion given in Eq. (45).

XIII. CONCLUSION

Often the presence or absence of symmetries in quantum hardware architectures can already be assessed by inspection. Given the system Hamiltonian as well as the control Hamiltonians, (i) we have provided a single necessary and sufficient symmetry condition ensuring full controllability, and (ii) in view of practical applications we have shown easy means (solving systems of homogeneous linear equations) to determine the symmetry of the dynamic system algebra $\mathfrak{k}$ merely in terms of its commutant or centralizer $\mathfrak{k}'$. If the system Hamiltonian corresponds to a connected coupling graph, the absence of any symmetry can be further exploited to decide full controllability: it means the dynamic system algebra is irreducible and *simple*. Now conjugation to (irreducible) simple orthogonal or symplectic candidate subalgebras can again be decided solely on the basis of solving systems of homogeneous linear equations. The final identification task can now be settled because here we have given a *complete* list of irreducible simple subalgebras of $\mathfrak{su}(N)$ compatible with the physical constituents as a dynamic pseudo-spin system. This avoids the usual and significantly more costly way of explicitly calculating Lie closures. We have significantly extended the list of irreducible simple subalgebras of $\mathfrak{su}(N)$ up to dimension $N = 2^{15}$; we anticipate this will spur further insight into them, in particular wherever the subalgebra is not also contained in an intermediate orthogonal or symplectic subalgebra.

We have thus made precise and easily accessible the following four conditions ensuring full controllability of a dynamic qubit system in terms of its system algebra $\mathfrak{k} \subseteq \mathfrak{su}(N)$:

(1) the system must not show a symmetry ($\mathfrak{k}$ must have a trivial centralizer $\mathfrak{k}'$),
(2) the coupling graph of the control system must be connected,
(3) the system algebra $\mathfrak{k}$ must not be given in a symplectic or an orthogonal representation, and finally

(4) if $\mathfrak{k}$ is given in a unitary representation (in the sense of Sec. VI), it must not be on the list of proper unitary, irreducible simple subalgebras of $\mathfrak{su}(N)$, in particular, $\mathfrak{k} \neq \mathfrak{e}_6$.

The structural achievements culminate in the single necessary and sufficient symmetry condition for full controllability given by Theorem 21.

The system algebra completely determines the possible dynamics of controlled Hamiltonian systems. Therefore, the lattice of irreducible simple subalgebras to $\mathfrak{su}(N)$ given here also provides an easy means to assess not only the somewhat easier cases of *mutual simulability* but also the more intricate cases of *simulability with least overhead* of dynamic systems of spin or fermionic or bosonic nature. In a number of examples (see also Table V), we have illustrated how controlled quadratic fermion and boson systems can be simulated by spin chains and in certain cases also vice versa.

Finally, since full controllability entails observability (while in the quantum domain the converse does not necessarily hold), symmetry constraints immediately pertain to observability as discussed in more detail in Ref. 37.

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APPENDIX A: TENSOR-PRODUCT STRUCTURE IN QUDIT SYSTEMS WITH MANY-BODY INTERACTIONS

For quantum simulation, we generalize the discussion such as to embrace *qudit* systems with (effective) many-body interactions. Treating them as control systems embedded in $\mathfrak{su}(N)$, now $\mathfrak{su}(d_1) \mathbin{\widehat{\oplus}} \mathfrak{su}(d_2) \mathbin{\widehat{\oplus}} \cdots \mathbin{\widehat{\oplus}} \mathfrak{su}(d_n)$ is a *tensor-product structure* of $\mathfrak{su}(N)$, where $\prod_{j=1}^{n} d_j = N$ and $d_j \geq 2$. We consider the subalgebras $\mathfrak{su}(d_j)$ as subsystems of the tensor-product structure. We say that the tensor-product structure $\mathfrak{h}_1 \mathbin{\widehat{\oplus}} \mathfrak{h}_2 \mathbin{\widehat{\oplus}} \cdots \mathbin{\widehat{\oplus}} \mathfrak{h}_n$ is a refinement of the tensor-product structure $\mathfrak{su}(d_1) \mathbin{\widehat{\oplus}} \mathfrak{su}(d_2) \mathbin{\widehat{\oplus}} \cdots \mathbin{\widehat{\oplus}} \mathfrak{su}(d_n)$ if $\mathfrak{h}_j$ is either equal to $\mathfrak{su}(d_j)$ or equal to $\mathfrak{su}(c_{j,1}) \mathbin{\widehat{\oplus}} \mathfrak{su}(c_{j,2}) \mathbin{\widehat{\oplus}} \cdots \mathbin{\widehat{\oplus}} \mathfrak{su}(c_{j,m_j})$, where $\prod_{k=1}^{m_j} c_{j,k} = d_j$ and $m_j \geq 2$. We call $\mathfrak{h}_1 \mathbin{\widehat{\oplus}} \mathfrak{h}_2 \mathbin{\widehat{\oplus}} \cdots \mathbin{\widehat{\oplus}} \mathfrak{h}_n$ a proper refinement if there is one j such that $\mathfrak{h}_j \neq \mathfrak{su}(d_j)$. For a given quantum system in $\mathfrak{su}(N)$, there exists a common refinement $\mathfrak{su}(p_1) \mathbin{\widehat{\oplus}} \mathfrak{su}(p_2) \mathbin{\widehat{\oplus}} \cdots \mathbin{\widehat{\oplus}} \mathfrak{su}(p_n)$ of all tensor-product structures, where $\prod_{j=1}^{n} p_j$ is the factorization of N into prime numbers. The common refinement is unique up to permutations of subsystems.

Now with respect to tensor-product structure $\mathfrak{su}(d_1) \mathbin{\widehat{\oplus}} \mathfrak{su}(d_2) \mathbin{\widehat{\oplus}} \cdots \mathbin{\widehat{\oplus}} \mathfrak{su}(d_n)$, again we write Hamiltonians as a linear combination ($c_k \in \mathbb{R}$)

$$H = \sum_{k=1}^{m} c_k \mathcal{H}_k \tag{A1}$$

of elements $\mathcal{H}_k = -\frac{i}{2}(\mathcal{H}_{k,1} \otimes \mathcal{H}_{k,2} \otimes \cdots \otimes \mathcal{H}_{k,n})$ forming a *tensor basis* of $\mathfrak{su}(N)$. The elements $\mathcal{H}_{k,\ell} \in \mathcal{B}_\ell \cup \{\mathbb{1}_{d_\ell}\}$ are chosen relative to bases

$$\left\{-i\mathrm{A} \mid \mathrm{A} \in \mathcal{B}_\ell := \{\mathrm{B}_{\ell,1}, \mathrm{B}_{\ell,2}, \ldots, \mathrm{B}_{\ell,(d_\ell)^2-1}\}\right\}$$

of $\mathfrak{su}(d_\ell)$. In addition, we assume that the order

$$\mathrm{ord}(\mathcal{H}_k) := \#\{\ell \,:\, \mathcal{H}_{k,\ell} \neq \mathbb{1}_{d_\ell}\} \geq 1.$$

Recall that the Hamiltonian H has a *coupling graph* if the Hamiltonian's order $\mathrm{ord}(H) = \mathrm{ord}(\sum_{k=1}^{m} c_k \mathcal{H}_k) := \max(\{\mathrm{ord}(\mathcal{H}_k) \mid k = 1, \ldots, m\})$ is equal to 2, which is the case in pairwise coupling interactions. The vertices j are given by the subsystems $\mathfrak{su}(d_j)$ and we get an edge between the nodes k_1 and k_2 with $k_1 \neq k_2$ if there exists a $\mathcal{H}_k$ in Eq. (A1) such that $\{k_1, k_2\} = \{j : \mathcal{H}_{k,j} \neq \mathbb{1}_{d_j}\}$. If all control Hamiltonians are local, i.e., are contained in $\mathfrak{su}(d_1) \widehat{\oplus} \mathfrak{su}(d_2) \widehat{\oplus} \cdots \widehat{\oplus} \mathfrak{su}(d_n)$, then we say that the coupling graph of the drift Hamiltonian H_d is the coupling graph of the control system.

We say a control system on $\mathfrak{su}(N)$ is *weakly connected*, if the dynamic algebra $\mathfrak{k}$ contains for each proper partition of its tensor-product structure in $(\mathcal{I}_1 \cup \mathcal{I}_2 = \{1, 2, \ldots, m\}, \mathcal{I}_1 \cap \mathcal{I}_2 = \{\})$

$$\mathfrak{h}_1 = \widehat{\bigoplus}_{j \in \mathcal{I}_1} \mathfrak{su}(d_j) \quad \text{and} \quad \mathfrak{h}_2 = \widehat{\bigoplus}_{j \in \mathcal{I}_2} \mathfrak{su}(d_j)$$

an element of $\mathfrak{su}(N) \setminus [\mathfrak{h}_1 \widehat{\oplus} \mathfrak{h}_2]$. For Hamiltonians H of $\mathrm{ord}(H) = 2$, this is equivalent to the fact that the coupling graph is connected. We will also use the stronger notion of a *directly connected* control system for which the dynamic algebra $\mathfrak{k}$ contains an element of $\mathfrak{su}(d_{j_1} d_{j_2}) \setminus [\mathfrak{su}(d_{j_1}) \widehat{\oplus} \mathfrak{su}(d_{j_2})]$ for each pair of subsystems $\mathfrak{su}(d_{j_1})$ and $\mathfrak{su}(d_{j_2})$ with $j_1 \neq j_2$. With these notions, Theorem 1 generalizes as follows:

Theorem 38: *Consider a bilinear control system on $\mathfrak{su}(\prod_{j=1}^{n} d_j)$, where $d_j \geq 2$. Assume that the subsystems $\mathfrak{su}(d_j)$ with $j \in \{1, \ldots, n\}$ are independently fully controllable so the dynamic algebra $\mathfrak{k} \supseteq \mathfrak{su}(d_1) \widehat{\oplus} \mathfrak{su}(d_2) \widehat{\oplus} \cdots \widehat{\oplus} \mathfrak{su}(d_n)$. The control system is fully controllable, i.e., $\mathfrak{k} = \mathfrak{su}(\prod_{j=1}^{n} d_j)$, if and only if the control system is directly connected. In particular, $\mathfrak{k} = \mathfrak{su}(\prod_{j=1}^{n} d_j)$ is simple.*

Proof: The "only if"-direction is obvious. We prove the "if"-direction. First, we assume that $n = 2$. As the subsystems are independently fully controllable, we obtain $\mathfrak{k} \supseteq \mathfrak{su}(d_1) \widehat{\oplus} \mathfrak{su}(d_2)$. The dynamic algebra $\mathfrak{k}$ contains an element of $\mathfrak{su}(d_1 d_2) \setminus [\mathfrak{su}(d_1) \widehat{\oplus} \mathfrak{su}(d_2)]$, as the control system is directly connected. It follows from Theorem 1.3 of Ref. 91 that $\mathfrak{su}(d_1) \widehat{\oplus} \mathfrak{su}(d_2)$ is a maximal subalgebra of $\mathfrak{su}(d_1 d_2)$. As $\mathfrak{k} \supsetneq \mathfrak{su}(d_1) \widehat{\oplus} \mathfrak{su}(d_2)$, this proves $\mathfrak{k} = \mathfrak{su}(d_1 d_2)$. The general case follows by induction on the number of subsystems. We remark that $\mathfrak{su}(\prod_{j=1}^{n} d_j)$ is simple so the last assertion follows. □

This complements results on the controllability of quantum circuits,[140] where the controllability of continuous and discrete sets of unitary transformations is considered. In particular, Theorems 4.1 and 4.2 of Ref. 141 (see also Ref. 142) rely also on the maximality of the subgroup of local operations on two qudits [i.e., on $\mathrm{SU}(d^2) \supset \mathrm{SU}(d) \otimes \mathrm{SU}(d)$]. Our controllability proof can be compared to proofs relying on Cartan decompositions (refer to Theorem 5 of Ref. 143 as well as Proposition 2.4 of Ref. 84). Unfortunately, one cannot substitute "directly connected" with "weakly connected" in Theorem 38:

Example 39: Consider a bilinear control system on $\mathfrak{su}(8)$ with the tensor-product structure $\mathfrak{su}(2) \widehat{\oplus} \mathfrak{su}(2) \widehat{\oplus} \mathfrak{su}(2)$. We assume that the subsystems are independently fully controllable, i.e.,

$$\mathfrak{k} \supseteq \langle i\mathrm{XII}, i\mathrm{YII}, i\mathrm{ZII}, i\mathrm{IXI}, i\mathrm{IYI}, i\mathrm{IZI}, i\mathrm{IIX}, i\mathrm{IIY}, i\mathrm{IIZ} \rangle_{\mathrm{Lie}}.$$

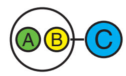
In addition, we have a drift Hamiltonian $H_d = \mathrm{ZZZ}$. The control system is weakly connected and $\mathfrak{k}$ acts irreducibly. The dynamic algebra is $\mathfrak{k} = \mathfrak{sp}(4) \neq \mathfrak{su}(8)$ and hence the system is not fully controllable.

APPENDIX B: CONNECTED CONTROL SYSTEMS IN QUDIT SYSTEMS WITH MANY-BODY INTERACTIONS

In this Appendix, we build on Sec. V and discuss a more general notion of *connected* control systems in qudit systems with many-body interactions which do not necessarily have a natural coupling graph. We freely use the notation of Appendix A.

Recall Example 5 of Sec. V. Motivated by this example one might conjecture that the dynamic algebra $\mathfrak{k}$ is simple if the control system is weakly connected and $\mathfrak{k}$ acts irreducibly. Unfortunately, this is not true.

Example 40: Assume that we have a bilinear control system on $\mathfrak{su}(8)$ with two subsystems corresponding to the tensor-product structure $\mathfrak{su}(4) \widehat{\oplus} \mathfrak{su}(2)$. On the first subsystem we pick $\mathfrak{h}_1 = \langle i\mathrm{XII}, i\mathrm{YII}, i\mathrm{ZII}, i\mathrm{IXI}, i\mathrm{IYI}, i\mathrm{IZI}\rangle_{\mathrm{Lie}}$ as the local dynamic Lie algebra. On the second subsystem we pick the local dynamic Lie algebra $\mathfrak{h}_2 = \langle i\mathrm{IIX}, i\mathrm{IIY}, i\mathrm{IIZ}\rangle_{\mathrm{Lie}}$. In addition, we have a drift Hamiltonian $H_d = \mathrm{IZZ}$. The control system is weakly connected and $\mathfrak{k}$ acts irreducibly. We obtain that the dynamic Lie algebra is $\mathfrak{k} = \mathfrak{su}(2) \widehat{\oplus} \mathfrak{su}(4)$. It is neither simple nor fully controllable. In particular, the dynamic Lie algebra does not respect our chosen tensor-product structure. The problem is that the control system (Color online)



is not weakly connected with respect to the tensor-product structures $\mathfrak{su}(2) \widehat{\oplus} \mathfrak{su}(4)$ and $\mathfrak{su}(2) \widehat{\oplus} \mathfrak{su}(2) \widehat{\oplus} \mathfrak{su}(2)$.

Generalizing Sec. V, we say that a control system is *connected*, if the dynamic algebra $\mathfrak{k}$ contains an element of $\mathfrak{su}(N) \setminus [\mathfrak{su}(e_1) \widehat{\oplus} \mathfrak{su}(e_2)]$ for each tensor-product structure $\mathfrak{su}(e_1) \widehat{\oplus} \mathfrak{su}(e_2)$ with $N = e_1 e_2$ and $e_1, e_2 \geq 2$. For control systems with pair interactions this definition is equivalent to the one given in Sec. V.

Lemma 41: The following are equivalent:

(1) The control system is connected.
(2) The control system is weakly connected with respect to the common unique refinement of its tensor-product structure.
(3) The control system is weakly connected with respect to any tensor-product structure. □

We now generalize Theorem 6 and prove that the dynamic algebra $\mathfrak{k}$ is simple if its centralizer is trivial and the corresponding control system is connected.

Theorem 42: *Assume that the dynamic algebra $\mathfrak{k}$ of a bilinear control system on $\mathfrak{su}(N)$ has a trivial centralizer $\mathfrak{k}'$. Then one finds:*

(1) The dynamic algebra $\mathfrak{k}$ is given in an irreducible representation.
(2) If $\mathfrak{k}$ is semi-simple but not simple, then $\mathfrak{k} \neq \mathfrak{su}(N)$ and the control system is not fully controllable.
(3) The dynamic algebra $\mathfrak{k}$ is simple if and only if the control system is connected.

Proof: (1) immediately follows from $\mathfrak{k}'$ being trivial and Lemma 3, while (2) is obvious, as $\mathfrak{su}(N)$ is simple. We now prove the "if"-part of (3). We obtain from Lemma 4 that $\mathfrak{k}$ is simple or semi-simple. In the following, we assume that $\mathfrak{k}$ is not simple. Thus, $\mathfrak{k}$ is an irreducible semi-simple (but not simple) subalgebra of $\mathfrak{su}(N)$. Using Theorem 2.1 of Ref. 91, it follows that $\mathfrak{k} = \mathfrak{k}_1 \widehat{\oplus} \mathfrak{k}_2 \widehat{\oplus} \cdots \widehat{\oplus} \mathfrak{k}_m$ and that the $\mathfrak{k}_j$ are irreducible simple subalgebras of some $\mathfrak{su}(d_j)$ such that $\mathfrak{k} \subseteq \mathfrak{su}(d_1) \widehat{\oplus} \mathfrak{su}(d_2) \widehat{\oplus} \cdots \widehat{\oplus} \mathfrak{su}(d_m)$, $\prod_{j=1}^{m} d_j = N$, and $m \geq 2$. In particular, we can choose two non-zero algebras

$$\mathfrak{h}_1 = \widehat{\oplus}_{j \in \mathcal{I}_1} \mathfrak{k}_j \quad \text{and} \quad \mathfrak{h}_2 = \widehat{\oplus}_{j \in \mathcal{I}_2} \mathfrak{k}_j,$$

where $\mathfrak{k} = \mathfrak{h}_1 \widehat{\oplus} \mathfrak{h}_2 \subseteq \mathfrak{su}(c_1) \widehat{\oplus} \mathfrak{su}(c_2)$, $\mathcal{I}_1 \cup \mathcal{I}_2 = \{1, 2, \ldots, m\}$, $\mathcal{I}_1 \cap \mathcal{I}_2 = \{\}$, and $c_1 c_2 = N$. As the control system is connected, the dynamic algebra $\mathfrak{k}$ contains an element of $\mathfrak{su}(N) \setminus [\mathfrak{su}(c_1) \widehat{\oplus} \mathfrak{su}(c_2)]$ for each tensor-product structure $\mathfrak{su}(c_1) \widehat{\oplus} \mathfrak{su}(c_2)$. This is a contradiction to $\mathfrak{k} \subseteq \mathfrak{su}(c_1) \widehat{\oplus} \mathfrak{su}(c_2)$ and the "if"-part of (3) follows. To prove the "only if"-part of (3) we assume that the control system is not connected. It immediately follows that the dynamic algebra has to be a (non-trivial) direct sum. Thus it cannot be simple, which proves the "only if"-part by contradiction. □

In important special cases more convenient conditions hold:

Corollary 43: Given a bilinear control system on $\mathfrak{su}(N)$*, where the centralizer* $\mathfrak{k}'$ *of the dynamic algebra* $\mathfrak{k}$ *is trivial. We obtain:*

(1) Assume that the subsystems of the tensor-product structure are independently fully controllable. The dynamic algebra $\mathfrak{k}$ *is simple if and only if the control system is weakly connected.*

(2) Assume that $\mathfrak{su}(p_1)\,\widehat{\oplus}\,\mathfrak{su}(p_2)\,\widehat{\oplus}\,\cdots\,\widehat{\oplus}\,\mathfrak{su}(p_n)$ *is the tensor-product structure of the control system, where* $\prod_{j=1}^{n} p_j$ *is a factorization of N into prime numbers. For example,* $p_j = 2$ *for all j. The following are equivalent:*
  - *(a) The dynamic algebra* $\mathfrak{k}$ *is simple.*
  - *(b) The control system is weakly connected.*
  - *(c) The control system is connected.*

Proof: We first prove (1). As the subsystems are independently fully controllable, any irreducible semi-simple (but not simple) dynamic algebra $\mathfrak{k} \supseteq \mathfrak{su}(d_1)\,\widehat{\oplus}\,\mathfrak{su}(d_2)\,\widehat{\oplus}\,\cdots\,\widehat{\oplus}\,\mathfrak{su}(d_m)$ has to be (irreducibly) contained in the algebra $\mathfrak{h} = \mathfrak{su}(d_1')\,\widehat{\oplus}\,\mathfrak{su}(d_2')\,\widehat{\oplus}\,\cdots\,\widehat{\oplus}\,\mathfrak{su}(d_m')$, where $\mathfrak{su}(d_1)\,\widehat{\oplus}\,\mathfrak{su}(d_2)\,\widehat{\oplus}\,\cdots\,\widehat{\oplus}\,\mathfrak{su}(d_m)$ is a refinement of the tensor-product structure $\mathfrak{h}$. All these cases are excluded as the control system is weakly connected, and (1) follows along the same lines as Theorem 42. As $\mathfrak{su}(p_1)\,\widehat{\oplus}\,\mathfrak{su}(p_2)\,\widehat{\oplus}\,\cdots\,\widehat{\oplus}\,\mathfrak{su}(p_n)$ is the common unique refinement of all tensor-product structures in the case of (2), the control system is weakly connected if and only if it is connected (by Lemma 41) and (2) follows by Theorem 42. □

APPENDIX C: COMPUTATIONAL TECHNIQUES FOR REPRESENTATION THEORY

For computationally exploiting Lie theory to list all irreducible representations of a given dimension N for all irreducible simple subalgebras of $\mathfrak{su}(N)$, a *self-consistent frame* is indispensable. It requires the highest weights and the dimensions of their respective representations to be linked to the classification by the standard Dynkin diagrams. Here we explicitly give all the details in such a consistent frame, since combining different literature sources runs the risk of arriving at erroneous results due to possibly inconsistent conventions.

In particular, this Appendix is meant to complement Sec. VI. It describes the methods we used to compute the irreducible simple subalgebras of $\mathfrak{su}(N)$ and their inclusion relations.

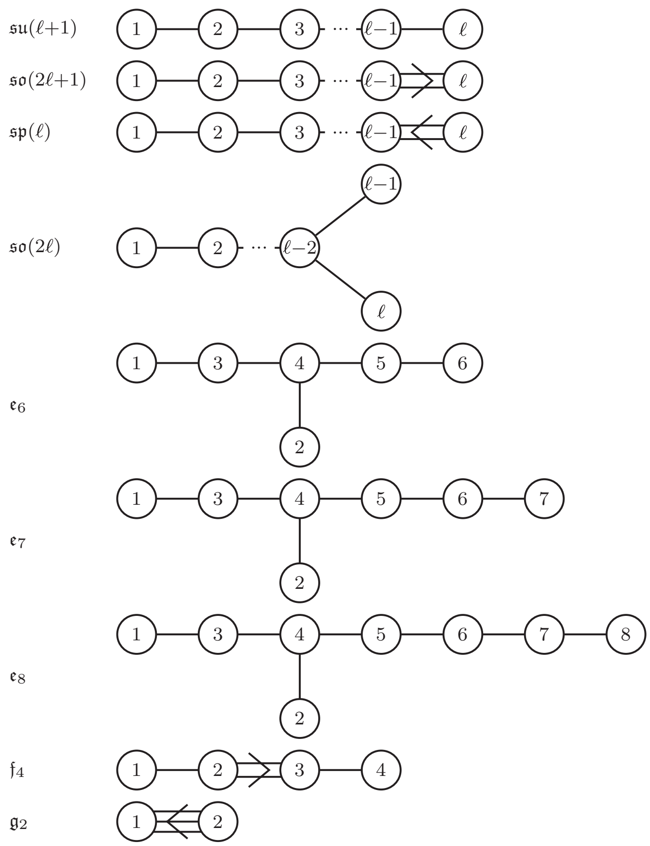
1. Highest weights and dimension formulas

The irreducible simple subalgebras of $\mathfrak{su}(N)$ are found by enumerating for all simple Lie algebras all their irreducible representations of dimension N. The irreducible representations can be enumerated using highest weights $(x_1, \ldots, x_\ell)$ which are (non-negative) integer vectors. The length ℓ of the highest weight is given by the rank (i.e., dimension of the maximal abelian subalgebra) of the considered Lie algebra. Details on the theory of highest weights can be found, e.g., in Chap. IX, Sec. 7 of Ref. 79.

Different orderings for the coefficients x_i of the highest weights are used in the literature. We use the so-called Bourbaki ordering which is detailed in Table VI by numbering the nodes of the Dynkin diagrams (see Chap. VI, Sec. 4.2, Theorem 3 of Ref. 78) for the compact simple Lie algebras. In Table VII, we present the highest weights and dimensions for the standard representation of each compact simple Lie algebra. We put highest weights together if they differ only with respect to an outer automorphism, i.e., an permutation which leaves the Dynkin diagram invariant. Note that the standard representation is the lowest-dimensional (non-trivial) representation [with the exception of $\mathfrak{so}(3)$, $\mathfrak{so}(5)$, and $\mathfrak{so}(6)$] and is typically used to introduce the corresponding Lie algebra in matrix form.

We already remarked in Sec. VI that the dimensions of irreducible representations can be efficiently computed using computer algebra systems such as LiE[89] and MAGMA[90] via Weyl's dimension formula. Now we present explicit formulas for the dimensions, which allowed us to

TABLE VI. The compact simple[a] Lie algebras and their Dynkin diagrams.



[a] $\mathfrak{so}(2\ell)$ is only simple for $\ell \geq 3$.

speed up the computation of the dimensions considerably. While for $\mathfrak{su}(\ell+1)$, $\mathfrak{so}(2\ell+1)$, and $\mathfrak{sp}(\ell)$ these formulas can readily be found on pp. 340–341 of Ref. 75, we had to correct the one for $\mathfrak{so}(2\ell)$, since we could not find a reference with the proper formula either.

Lemma 44 (Classical Lie algebras)*: Given the highest weight* $(x_1, \ldots, x_\ell)$ *the dimensions of the corresponding irreducible representations are:*

1. $\mathfrak{su}(\ell+1):\ \dim = \prod_{1\leq i<j\leq \ell+1}\left\{1+\frac{x_i+\cdots+x_{j-1}}{j-i}\right\}$.
2. $\mathfrak{so}(2\ell+1):\ \dim = \prod_{1\leq i<j\leq \ell}\left\{1+\frac{x_i+\cdots+x_{j-1}+2(x_j+\cdots+x_{\ell-1})+x_\ell}{2\ell+1-i-j}\right\}$ $\times \prod_{1\leq i<j\leq \ell}\left\{1+\frac{x_i+\cdots+x_{j-1}}{j-i}\right\} \times \prod_{1\leq i\leq \ell}\left\{1+\frac{2(x_i+\cdots+x_{\ell-1})+x_\ell}{2\ell+1-2i}\right\}$.
3. $\mathfrak{sp}(\ell):\ \dim = \prod_{1\leq i<j\leq \ell}\left\{1+\frac{x_i+\cdots+x_{j-1}}{j-i}\right\} \times \prod_{1\leq i\leq \ell}\left\{1+\frac{x_i+\cdots+x_\ell}{\ell+1-i}\right\}$ $\times \prod_{1\leq i<j\leq \ell}\left\{1+\frac{x_i+\cdots+x_{j-1}+2(x_j+\cdots+x_\ell)}{2\ell+2-i-j}\right\}$.
4. $\mathfrak{so}(2\ell):\ \dim = \prod_{1\leq i<j\leq \ell}\left\{1+\frac{x_i+\cdots+x_{j-1}}{j-i}\right\} \times \prod_{1\leq i\leq \ell-1}\left\{1+\frac{x_i+\cdots+x_{\ell-2}+x_\ell}{\ell-i}\right\}$ $\times \prod_{1\leq i<j\leq \ell-1}\left\{1+\frac{x_i+\cdots+x_{j-1}+2(x_j+\cdots+x_{\ell-2})+x_{\ell-1}+x_\ell}{2\ell-i-j}\right\}$.

□

Here we present the dimension formulas for the exceptional Lie algebras only for $\mathfrak{g}_2$ (cf. Ref. 144, pp. 257–258) and $\mathfrak{f}_4$, omitting the even longer and more complicated ones for $\mathfrak{e}_6$, $\mathfrak{e}_7$, and

$\mathfrak{e}_8$. We remark that these formulas are—in principle—well known but are usually not given in the literature due to their complexity.

Lemma 45 ($\mathfrak{g}_2$ and $\mathfrak{f}_4$): Given the highest weight $(x_1, \ldots, x_\ell)$ the dimensions of the corresponding irreducible representations are:

1. $\mathfrak{g}_2:\ \dim = (1+x_2)(1+x_1)\left(1+\frac{x_1+x_2}{2}\right)\left(1+\frac{x_1+2x_2}{3}\right)\left(1+\frac{x_1+3x_2}{4}\right)\left(1+\frac{2x_1+3x_2}{5}\right).$
2. $\mathfrak{f}_4:\ \dim = (1+x_4)(1+x_3)(1+x_2)(1+x_1)\left(1+\frac{x_3+x_4}{2}\right)\left(1+\frac{x_2+x_3}{2}\right)\left(1+\frac{x_1+x_2}{2}\right)$
$\times\left(1+\frac{x_2+x_3+x_4}{3}\right)\left(1+\frac{2x_2+x_3}{3}\right)\left(1+\frac{x_1+x_2+x_3}{3}\right)\left(1+\frac{2x_2+x_3+x_4}{4}\right)\left(1+\frac{x_1+x_2+x_3+x_4}{4}\right)$
$\times\left(1+\frac{x_1+2x_2+x_3}{4}\right)\left(1+\frac{2x_2+2x_3+x_4}{5}\right)\left(1+\frac{x_1+2x_2+x_3+x_4}{5}\right)\left(1+\frac{2x_1+2x_2+x_3}{5}\right)$
$\times\left(1+\frac{x_1+2x_2+2x_3+x_4}{6}\right)\left(1+\frac{2x_1+2x_2+x_3+x_4}{6}\right)\left(1+\frac{x_1+3x_2+2x_3+x_4}{7}\right)$
$\times\left(1+\frac{2x_1+2x_2+2x_3+x_4}{7}\right)\left(1+\frac{2x_1+3x_2+2x_3+x_4}{8}\right)\left(1+\frac{2x_1+4x_2+2x_3+x_4}{9}\right)$
$\times\left(1+\frac{2x_1+4x_2+3x_3+x_4}{10}\right)\left(1+\frac{2x_1+4x_2+3x_3+2x_4}{11}\right).$

Proof: Computational explicit dimension formulas for the exceptional Lie algebras were obtained using the computer algebra system MAGMA[90] via Weyl's dimension formula. □

We emphasize that in order to compute the dimensions efficiently, one has to use the dimension formulas in the given factorized form. That is, one has to evaluate each factor and multiply the results. The alternative of evaluating the multiplied formula is considerably less efficient.

2. Enumerating representations

The aim of determining the irreducible simple subalgebras of $\mathfrak{su}(N)$ for a given N is reached by enumerating for all simple Lie algebras all their irreducible representations of dimension N. Therefore, we have to enumerate for all simple Lie algebras all highest weights $(x_1, \ldots, x_\ell)$ corresponding to irreducible representations of dimension N. In doing so, how can one reduce the combined search space of Lie algebras and highest weights?

To this end, recall that the standard representation is the lowest-dimensional (non-trivial) representation [with the exception of $\mathfrak{so}(3)$, $\mathfrak{so}(5)$, and $\mathfrak{so}(6)$]. It follows from the dimension formulas for the standard representations in Table VII that only a finite number of Lie algebras have irreducible representations of dimension equal (or less than or equal) to a given N. Thus we have to search only through a finite set of Lie algebras. In addition, we have to consider merely one instance of isomorphic Lie algebras [$\mathfrak{su}(2) \cong \mathfrak{so}(3) \cong \mathfrak{sp}(1)$, $\mathfrak{so}(5) \cong \mathfrak{sp}(2)$, and $\mathfrak{su}(4) \cong \mathfrak{so}(6)$] and can neglect $\mathfrak{so}(2)$ and $\mathfrak{so}(4)$ as they are not simple. It follows from Chap. IX, Sec. 8.5, Corollary 2 of Ref. 79

TABLE VII. The compact simple Lie algebras and their standard representations.

Algebra	Highest weight(s)[a]	dim[b]	Algebra	Highest weight(s)[a]	dim[b]
$\mathfrak{su}(\ell+1)$	(1, 0, ..., 0),(0, ..., 0, 1)	$\ell+1$	$\mathfrak{so}(8)$	(1, 0, 0, 0),(0, 0, 1, 0),(0, 0, 0, 1)	8
$\mathfrak{so}(3)$	(2)	3	$\mathfrak{so}(2\ell)$[e]	(1, 0, ..., 0)	2ℓ
$\mathfrak{so}(2\ell+1)$[c]	(1, 0, ..., 0)	$2\ell+1$	$\mathfrak{e}_6$	(1, 0, 0, 0, 0, 0),(0, 0, 0, 0, 0, 1)	27
$\mathfrak{sp}(\ell)$	(1, 0, ..., 0)	2ℓ	$\mathfrak{e}_7$	(0, 0, 0, 0, 0, 0, 1)	56
$\mathfrak{so}(2)$[d]	(1)	2	$\mathfrak{e}_8$	(0, 0, 0, 0, 0, 0, 0, 1)	248
$\mathfrak{so}(4)$[d]	(1, 1)	4	$\mathfrak{f}_4$	(0, 0, 0, 1)	26
$\mathfrak{so}(6)$	(1, 0, 0)	6	$\mathfrak{g}_2$	(1, 0)	7

[a]Variable vectors have length ℓ.
[b]Dimension of the standard representation.
[c]$\ell \geq 2$.
[d]Not simple.
[e]$\ell \geq 5$.

that for a Lie algebras the set of irreducible representations of dimension less than or equal to N is finite. We obtain:

Lemma 46: Each Lie algebra can only have a finite number of irreducible representations of dimension equal (or less than or equal) to a given N. Furthermore, only a finite number of Lie algebras have any irreducible representations of dimension equal (or less than or equal) to a given N.

It follows from Lemma 46 that the search space for the highest weights is finite. Using the following lemma, one can obtain stopping criteria for the search for the highest weights with dimension equal (or less than or equal) to a given N.

Lemma 47: For a given Lie algebra, let $\dim[x]$ *denote the dimension of an irreducible representation with the highest weight* $x = (x_1, \ldots, x_\ell)$.

1. *The dimension is strictly monotonic increasing in each entry* x_i *of the highest weight:* $\dim[(x_1, \ldots, x_i + 1, \ldots, x_\ell)] > \dim[(x_1, \ldots, x_i, \ldots, x_\ell)]$.
2. *Let* e^i *denote the vector such that* $(e^i)_j = \delta_{i,j}$. *If* $\sum x_i > 1$, *then*

$$\dim[x] \geq \min[\{\max[\dim(e^i), \dim(e^j)]\}_{i \neq j} \cup \{\dim(2e^i)\}_{1 \leq i \leq \ell}].$$

Proof: See, e.g., Corollary 5.2 and Corollary 5.4 of Ref. 145. □

Let us fix a Lie algebra. We start our search for the highest weights of dimension less than or equal to N with all vectors $x = (x_1, \ldots, x_\ell)$ such that $\sum x_i = 1$. In each step, we compute the dimension corresponding to the highest weight $x = (x_1, \ldots, x_\ell)$. If $\dim[x] \leq N$, we include x into the list of highest weights with dimension $\dim[x]$ and we branch our search to all $\tilde{x} = (x_1, \ldots, x_i + 1, \ldots, x_\ell)$. If $\dim[x] > N$, we prune this branch in our search tree (Part 1 of Lemma 47). We have to search through all Lie algebras such that the lowest-dimensional (non-trivial) irreducible representation is less than or equal to N. One can further reduce the search space with respect to potential Lie algebras by using knowledge on the second-lowest-dimensional (non-trivial) irreducible representations:

Theorem 48: *For a given Lie algebra, let* $y = (y_1, \ldots, y_\ell)$ *denote the highest weight of the second-lowest-dimensional (non-trivial) irreducible representation.*

1. *For* $\mathfrak{su}(\ell+1)$ *and* $\ell \geq 3$, *we obtain* $y = (0, 1, 0, \ldots, 0)$ *or* $y = (0, \ldots, 0, 1, 0)$. *In addition,* $\dim[y] = \ell(\ell+1)/2$.
2. *For* $\mathfrak{so}(2\ell+1)$ *and* $\ell \geq 7$, *we obtain* $y = (0, 1, 0, \ldots, 0)$ *and* $\dim[y] = (2\ell+1)\ell$.
3. *For* $\mathfrak{sp}(\ell)$ *and* $\ell \geq 4$, *we obtain* $y = (0, 1, 0, \ldots, 0)$ *and* $\dim[y] = 2\ell^2 - \ell - 1$.
4. *For* $\mathfrak{so}(2\ell)$ *and* $\ell \geq 8$, *we obtain* $y = (0, 1, 0, \ldots, 0)$ *and* $\dim[y] = 2\ell^2 - \ell$.

Proof: Again, let e^i denote the vector such that $(e^i)_j = \delta_{i,j}$. We apply Lemma 47 in each of the following cases:

1. $\mathfrak{su}(\ell+1)$: Recall that $\dim[e^r] = \binom{\ell+1}{r}$ for $1 \leq r \leq \ell$. It follows $\dim[e^2] = \ell(\ell+1)/2$ for $\ell \geq 3$. One can deduce from Lemma 44 that $\dim[2e^1] = (\ell+1)(\ell+2)/2$ and that $\dim[(1, 0, \ldots, 0, 1)] = \ell(\ell+2)$ for $\ell \geq 2$. Now, we obtain that $\dim[e^2] < \dim[2e^1] < \dim[(1, 0, \ldots, 0, 1)]$ for $\ell \geq 3$. The first part follows.
2. $\mathfrak{so}(2\ell+1)$: Recall that $\dim[e^\ell] = 2^\ell$ and $\dim[e^r] = \binom{2\ell+1}{r}$ for $1 \leq r \leq \ell - 1$ (see, e.g., p. 340 of Ref. 75). It follows that $\dim[e^2] = (2\ell+1)\ell$ for $\ell \geq 3$. We obtain that $\dim[e^2] < \dim[e^\ell]$ for $\ell \geq 7$. One can deduce from Lemma 44 that $\dim[2e^1] = \ell(2\ell+3) > \dim[e^2]$ for $\ell \geq 3$. The second part follows.
3. $\mathfrak{sp}(\ell)$: Recall that $\dim[e^1] = 2\ell$ and $\dim[e^r] = \binom{2\ell}{r} - \binom{2\ell}{r-2}$ for $2 \leq r \leq \ell$ (see, e.g., p. 341 of Ref. 75). It follows that $\dim[e^2] = 2\ell^2 - \ell - 1$. We obtain that $\dim[e^r] = \frac{2\ell+2-2r}{2\ell+2}\binom{2\ell+2}{r}$. One can deduce that $\dim[e^3] = \frac{4}{3}\ell^3 - 2\ell^2 - \frac{4}{3}\ell > \dim[e^2]$ for $\ell \geq 4$. If $r \geq 4$, it follows that $\dim[e^r] - \dim[e^2] = \frac{2\ell+2-2r}{2\ell+2}\binom{2\ell+2}{r} - 2\ell^2 + \ell + 1 \geq \frac{1}{\ell+1}\binom{2\ell+2}{4} - 2\ell^2 + \ell + 1$

$= \frac{2}{3}\ell^3 - 2\ell^2 + \frac{5}{6}\ell + 1 > 0$ for $\ell \geq 4$. One can obtain from Lemma 44 that $\dim[2e^1] = 2\ell^2 + \ell > \dim[e^2]$. The third part follows.

4. $\mathfrak{so}(2\ell)$: Recall that $\dim[e^{\ell-1}] = \dim[e^\ell] = 2^{\ell-1}$ and $\dim[e^r] = \binom{2\ell}{r}$ for $1 \leq r \leq \ell - 2$ (see, e.g., p. 341 of Ref. 75). It follows that $\dim[e^2] = 2\ell^2 - \ell$ for $\ell \geq 4$. We obtain that $\dim[e^2] < \dim[e^\ell]$ for $\ell \geq 8$. One can deduce from Lemma 44 that $\dim[2e^1] = 2\ell^2 + \ell - 1 > \dim[e^2]$ for $\ell \geq 4$. The fourth part follows. □

Now one obtains bounds on ℓ such that the dimension of the second-lowest-dimensional (non-trivial) irreducible representation is greater than N:

Corollary 49: For a given Lie algebra, let $y = (y_1, \ldots, y_\ell)$ denote the highest weight of the second-lowest-dimensional (non-trivial) irreducible representation.

1. *For $\mathfrak{su}(\ell+1)$ and $\ell \geq 3$, we obtain:* $\dim[y] > N \Leftrightarrow \ell > \sqrt{1/4 + 2N} - 1/2$.
2. *For $\mathfrak{so}(2\ell+1)$ and $\ell \geq 7$, we obtain:* $\dim[y] > N \Leftrightarrow \ell > (\sqrt{1 + 8N} - 1)/4$.
3. *For $\mathfrak{sp}(\ell)$ and $\ell \geq 4$, we obtain:* $\dim[y] > N \Leftrightarrow \ell > (\sqrt{9 + 8N} + 1)/4$.
4. *For $\mathfrak{so}(2\ell)$ and $\ell \geq 8$, we obtain:* $\dim[y] > N \Leftrightarrow \ell > (\sqrt{1 + 8N} + 1)/4$.

Now we explain how to use Corollary 49 in order to reduce the search space. Consider $\mathfrak{su}(k+1)$ and $k \geq 3$. If $N \geq k + 1$ but $k > \sqrt{1/4 + 2N} - 1/2$ then the standard representation of $\mathfrak{su}(k+1)$ occurs with dimension less than or equal to N. But no other (non-trivial) irreducible representation of $\mathfrak{su}(k+1)$ has dimension less than or equal to N. We include the highest weight of the standard representation in the list corresponding to the dimension $k + 1$. But we do not have to search for other irreducible representations. The search space is reduced from a size linear in N to a square-root in N.

TABLE VIII. Irreducible simple subalgebras not maximal in $\mathfrak{su}(\dim)$, $\mathfrak{sp}(\dim/2)$, or $\mathfrak{so}(\dim)$.

Subalgebra	Type	Highest weight(s)	Algebra	Highest weight(s)	dim
$\mathfrak{su}(\ell+1)$[a]	u	$(1, 0, 1, 0, \ldots, 0), (0, \ldots, 0, 1, 0, 1)$	$\mathfrak{su}[\ell(\ell+1)/2]$	$(0, 1, 0, \ldots, 0), (0, \ldots, 0, 1, 0)$	$3\binom{\ell+2}{4}$
$\mathfrak{su}(\ell+1)$[b]	u	$(2, 1, 0, \ldots, 0), (0, \ldots, 0, 1, 2)$	$\mathfrak{su}[\ell(\ell+3)/2+1]$	$(0, 1, 0, \ldots, 0), (0, \ldots, 0, 1, 0)$	$3\binom{\ell+3}{4}$
$\mathfrak{su}(2)$	o	(6)	$\mathfrak{g}_2$	$(1, 0)$	7
$\mathfrak{su}(6)$	o	$(0, 1, 0, 1, 0)$	$\mathfrak{sp}(10)$	$(0, 1, 0, \ldots, 0)$	189
$\mathfrak{so}(4k+3)$[c]	s/o[d]	$(0, \ldots, 0, m)$	$\mathfrak{so}(4k+4)$	$(0, \ldots, 0, m, 0), (0, \ldots, 0, 0, m)$	[e]
$\mathfrak{so}(9)$	o	$(1, 0, 0, 1)$	$\mathfrak{so}(16)$	$(0, \ldots, 0, 1, 0), (0, \ldots, 0, 0, 1)$	128
$\mathfrak{sp}(3)$	o	$(0, 2, 0)$	$\mathfrak{sp}(7)$	$(0, 1, 0, 0, 0, 0, 0)$	90
$\mathfrak{sp}(3)$	s	$(0, 2, 1)$	$\mathfrak{sp}(7)$	$(0, 0, 1, 0, 0, 0, 0)$	350
$\mathfrak{so}(10)$	u	$(0, 1, 0, 1, 0), (0, 1, 0, 0, 1)$	$\mathfrak{su}(16)$	$(0, 0, 1, 0, \ldots, 0), (0, \ldots, 0, 1, 0, 0)$	560
$\mathfrak{so}(12)$	o	$(0, 0, 0, 1, 0, 0)$	$\mathfrak{sp}(16)$	$(0, 1, 0, 0, \ldots, 0)$	495
$\mathfrak{so}(12)$	s	$(0, 0, 1, 0, 1, 0), (0, 0, 1, 0, 0, 1)$	$\mathfrak{sp}(16)$	$(0, 0, 1, 0, \ldots, 0)$	4928
$\mathfrak{e}_6$	u	$(0, 0, 1, 0, 0, 0), (0, 0, 0, 0, 1, 0)$	$\mathfrak{su}(27)$	$(0, 1, 0, 0, 0, \ldots, 0)$	351
$\mathfrak{e}_6$	u	$(0, 1, 1, 0, 0, 0), (0, 1, 0, 0, 1, 0)$	$\mathfrak{su}(27)$	$(0, 0, 0, 1, 0, \ldots, 0)$	17550
$\mathfrak{e}_7$	o	$(0, 0, 0, 0, 0, 1, 0)$	$\mathfrak{sp}(28)$	$(0, 1, 0, \ldots, 0)$	1539
$\mathfrak{e}_7$	s	$(0, 0, 0, 0, 1, 0, 0)$	$\mathfrak{sp}(28)$	$(0, 0, 1, 0, \ldots, 0)$	27664
$\mathfrak{e}_7$	o	$(0, 0, 0, 1, 0, 0, 0)$	$\mathfrak{sp}(28)$	$(0, 0, 0, 1, 0, \ldots, 0)$	365750
$\mathfrak{e}_7$	s	$(0, 1, 1, 0, 0, 0, 0)$	$\mathfrak{sp}(28)$	$(0, 0, 0, 0, 1, 0, \ldots, 0)$	3792096
$\mathfrak{g}_2$[f]	o	$(m, 0)$	$\mathfrak{so}(7)$	$(m, 0, 0)$	$\frac{2m+5}{5}\binom{m+4}{4}$

[a] $\ell \geq 4$.
[b] $\ell \geq 3$.
[c] $k \geq 1$, $m \geq 1$; but not $k = m = 1$ (corrected) as $\mathfrak{so}(7) \subset \mathfrak{so}(8) \subset \mathfrak{su}(8)$.
[d] If $(k+1)m$ is odd then s else o.
[e] $\prod_{s=1}^{2k+1} \left[\binom{m+2s-1}{m} / \binom{m+s-1}{m} \right]$ (corrected).
[f] $m \geq 2$.

3. Inclusion relations

Once having obtained all irreducible simple subalgebras of $\mathfrak{su}(N)$, one can determine their inclusion relations following the work of Dynkin[91] (see, e.g., Chap. 6, Sec. 3.2 of Ref. 93). Related literature can be found in Ref. 146. For example, Refs. 147 and 148 generalize the work of Dynkin[91] to classical and exceptional Lie algebras over prime fields. References 82, 149, and 150 contain most recent findings. It follows from Theorem 1.5 in Ref. 91 that almost all irreducible simple subalgebras (of dimension dim) are maximal in $\mathfrak{su}(\dim)$, $\mathfrak{sp}(\dim/2)$, or $\mathfrak{so}(\dim)$. Relying on Table I of Ref. 91, the exceptions are listed in Table VIII, which contains irreducible simple subalgebras of $\mathfrak{su}(\dim)$ including the algebra in which the subalgebra is maximal. In addition, the highest weights of the corresponding representations as well as the type of the subalgebra (s for symplectic, o for orthogonal, and u for unitary) are given. For reference, we give the Malcev classification[95] (see also, e.g., Refs. 38, 91, and 106) of symplectic, orthogonal, and unitary representations:

Theorem 50 (Malcev)**:** *Let $x = (x_1, \ldots, x_\ell)$ denote the highest weight corresponding to an irreducible representation ϕ of a Lie algebra $\mathfrak{k}$ and* div *denotes integer division (e.g., $(5 \operatorname{div} 2) = 2$). As ϕ is irreducible, the different cases of symplectic, orthogonal, and unitary representations (in the sense of Sec. VI) are mutually exclusive:*

1. $\mathfrak{k} = \mathfrak{su}(\ell + 1)$*:*
   - *(a) ϕ is symplectic if x is symmetric, $(\ell \bmod 4) = 1$, and $x_{((\ell-1) \operatorname{div} 2)+1}$ is odd.*
   - *(b) ϕ is orthogonal if x is symmetric as well as either (i) $(\ell \bmod 4) = 1$ and $x_{((\ell-1) \operatorname{div} 2)+1}$ is even or (ii) $(\ell \bmod 4) \neq 1$.*
   - *(c) ϕ is unitary if x is not symmetric.*
2. $\mathfrak{k} = \mathfrak{so}(2\ell + 1)$ *for* $\ell \geq 2$*:*
   - *(a) ϕ is symplectic if $(\ell \bmod 4) \in \{1, 2\}$ and x_ℓ is odd.*
   - *(b) ϕ is orthogonal if either $(\ell \bmod 4) \in \{0, 3\}$ or x_ℓ is even.*
3. $\mathfrak{k} = \mathfrak{sp}(\ell)$ *for $\ell \geq 2$: ϕ is symplectic if $\sum_{1 \leq 2j+1 \leq \ell} x_{2j+1}$ is odd ($j \in \mathbb{N} \cup \{0\}$). Otherwise, ϕ is orthogonal.*
4. $\mathfrak{k} = \mathfrak{so}(2\ell)$ *for* $\ell \geq 3$*:*
   - *(a) ϕ is symplectic if $(\ell \bmod 4) = 2$ and $x_{\ell-1} + x_\ell$ is odd.*
   - *(b) ϕ is orthogonal if either (i) $(\ell \bmod 4) = 2$ and $x_{\ell-1} + x_\ell$ is even, (ii) $(\ell \bmod 4) = 0$, or (iii) ℓ is odd and $x_{\ell-1} = x_\ell$.*
   - *(c) ϕ is unitary if ℓ is odd and $x_{\ell-1} \neq x_\ell$.*
5. *$\mathfrak{k} = \mathfrak{g}_2$, $\mathfrak{k} = \mathfrak{f}_4$, or $\mathfrak{k} = \mathfrak{e}_8$: ϕ is always orthogonal.*
6. *$\mathfrak{k} = \mathfrak{e}_6$: ϕ is orthogonal if $x_1 = x_6$ and $x_3 = x_5$. Otherwise, ϕ is unitary.*
7. *$\mathfrak{k} = \mathfrak{e}_7$: ϕ is symplectic if $x_2 + x_5 + x_7$ is odd. Otherwise, ϕ is orthogonal.*

Results for dimension $\dim \leq 16$ can be found in Table IX, where the irreducible simple subalgebras of $\mathfrak{su}(\dim)$ are given again with their type (s for symplectic, o for orthogonal, and u for unitary) plus the highest weight of the corresponding irreducible representation. This information is essential for deriving Table I.

4. Examples

Using two concrete examples, we illustrate how the methods of this Appendix can be combined and applied to finding irreducible simple subalgebras:

Example 51: We use the methods of Appendix C 2 in the case of dimension $N = 7$ and compute the irreducible simple subalgebras of $\mathfrak{su}(7)$, where the corresponding irreducible representations are specified by highest weights. (The definition of the highest weight is discussed in Appendix C 1.) We find the following irreducible simple subalgebras (see Table IX): $\mathfrak{su}(7)$ with the highest weights $(1, 0, 0, 0, 0, 0)$ and $(0, 0, 0, 0, 0, 1)$ (where the two irreducible representations of $\mathfrak{su}(7)$ are related by an outer automorphism), $\mathfrak{so}(7)$ with $(1, 0, 0)$, $\mathfrak{g}_2$ with $(1, 0)$, as well as $\mathfrak{su}(2)$ with (6). We conclude from Theorem 50 that the given irreducible representations of $\mathfrak{su}(7)$ are unitary (in the sense of

TABLE IX. Highest weights of the irreducible representations up to dimension 16.

dim	Algebra	Type	Highest weight(s)	dim	Algebra	Type	Highest weight(s)
2	$\mathfrak{su}(2)$	s	(1)	11	$\mathfrak{su}(11)$	u	(1, 0, . . . , 0), (0, . . . , 0, 1)
3	$\mathfrak{su}(3)$	u	(1, 0), (0, 1)		$\mathfrak{so}(11)$	o	(1, 0, 0, 0, 0)
	$\mathfrak{su}(2)$	o	(2)		$\mathfrak{su}(2)$	o	(10)
4	$\mathfrak{su}(4)$	u	(1, 0, 0), (0, 0, 1)	12	$\mathfrak{su}(12)$	u	(1, 0, . . . , 0), (0, . . . , 0, 1)
	$\mathfrak{sp}(2)$	s	(1, 0)		$\mathfrak{sp}(6)$	s	(1, 0, 0, 0, 0, 0)
	$\mathfrak{su}(2)$	s	(3)		$\mathfrak{su}(2)$	s	(11)
5	$\mathfrak{su}(5)$	u	(1, 0, 0, 0), (0, 0, 0, 1)		$\mathfrak{so}(12)$	o	(1, 0, 0, 0, 0, 0)
	$\mathfrak{so}(5)$	o	(1, 0)	13	$\mathfrak{su}(13)$	u	(1, 0, . . . , 0), (0, . . . , 0, 1)
	$\mathfrak{su}(2)$	o	(4)		$\mathfrak{so}(13)$	o	(1, 0, 0, 0, 0, 0)
6	$\mathfrak{su}(6)$	u	(1, 0, 0, 0, 0), (0, 0, 0, 0, 1)		$\mathfrak{su}(2)$	o	(12)
	$\mathfrak{sp}(3)$	s	(1, 0, 0)	14	$\mathfrak{su}(14)$	u	(1, 0, . . . , 0), (0, . . . , 0, 1)
	$\mathfrak{su}(2)$	s	(5)		$\mathfrak{sp}(7)$	s	(1, 0, 0, 0, 0, 0, 0)
	$\mathfrak{so}(6)$	o	(1, 0, 0)		$\mathfrak{su}(2)$	s	(13)
	$\mathfrak{su}(3)$	u	(2, 0), (0, 2)		$\mathfrak{sp}(3)$	s	(0, 0, 1)
7	$\mathfrak{su}(7)$	u	(1, 0, 0, 0, 0, 0), (0, 0, 0, 0, 0, 1)		$\mathfrak{so}(14)$	o	(1, 0, 0, 0, 0, 0, 0)
	$\mathfrak{so}(7)$	o	(1, 0, 0)		$\mathfrak{so}(5)$	o	(2, 0)
	$\mathfrak{g}_2$	o	(1, 0)		$\mathfrak{sp}(3)$	o	(0, 1, 0)
	$\mathfrak{su}(2)$	o	(6)		$\mathfrak{g}_2$	o	(0, 1)
8	$\mathfrak{su}(8)$	u	(1, 0, 0, 0, 0, 0, 0), (0, 0, 0, 0, 0, 0, 1)	15	$\mathfrak{su}(15)$	u	(1, 0, . . . , 0), (0, . . . , 0, 1)
	$\mathfrak{sp}(4)$	s	(1, 0, 0, 0)		$\mathfrak{so}(15)$	o	(1, 0, 0, 0, 0, 0, 0)
	$\mathfrak{su}(2)$	s	(7)		$\mathfrak{su}(2)$	o	(14)
	$\mathfrak{so}(8)$	o	(1, 0, 0, 0), (0, 0, 1, 0), (0, 0, 0, 1)		$\mathfrak{so}(6)$	o	(0, 1, 1)
	$\mathfrak{su}(3)$	o	(1, 1)		$\mathfrak{su}(3)$	u	(4, 0), (0, 4)
	$\mathfrak{so}(7)$	o	(0, 0, 1)		$\mathfrak{su}(5)$	u	(2, 0, 0, 0), (0, 0, 0, 2)
9	$\mathfrak{su}(9)$	u	(1, 0, 0, 0, 0, 0, 0, 0), (0, 0, 0, 0, 0, 0, 0, 1)		$\mathfrak{su}(6)$	u	(0, 1, 0, 0, 0), (0, 0, 0, 1, 0)
	$\mathfrak{so}(9)$	o	(1, 0, 0, 0)		$\mathfrak{su}(3)$	u	(2, 1), (1, 2)
	$\mathfrak{su}(2)$	o	(8)	16	$\mathfrak{su}(16)$	u	(1, 0, . . . , 0), (0, . . . , 0, 1)
10	$\mathfrak{su}(10)$	u	(1, 0, 0, 0, 0, 0, 0, 0, 0), (0, 0, 0, 0, 0, 0, 0, 0, 1)		$\mathfrak{sp}(8)$	s	(1, 0, 0, 0, 0, 0, 0, 0)
	$\mathfrak{sp}(5)$	s	(1, 0, 0, 0, 0)		$\mathfrak{su}(2)$	s	(15)
	$\mathfrak{su}(2)$	s	(9)		$\mathfrak{sp}(2)$	s	(1, 1)
	$\mathfrak{so}(10)$	o	(1, 0, 0, 0, 0)		$\mathfrak{so}(16)$	o	(1, 0, 0, 0, 0, 0, 0, 0)
	$\mathfrak{so}(5)$	o	(0, 2)		$\mathfrak{so}(9)$	o	(0, 0, 0, 1)
	$\mathfrak{su}(3)$	u	(3, 0), (0, 3)		$\mathfrak{so}(10)$	u	(0, 0, 0, 1, 0), (0, 0, 0, 0, 1)
	$\mathfrak{su}(4)$	u	(2, 0, 0), (0, 0, 2)				
	$\mathfrak{su}(5)$	u	(0, 1, 0, 0), (0, 0, 1, 0)				

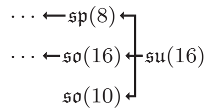
Sec. VI) and that all the other ones are orthogonal (see Table IX). It follows that $\mathfrak{so}(7)$ is directly embedded in $\mathfrak{su}(7)$:

$$\cdots \leftarrow \mathfrak{so}(7) \leftarrow \mathfrak{su}(7)$$

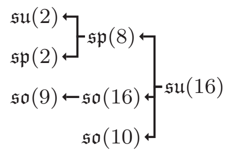
The algebras $\mathfrak{g}_2$ and $\mathfrak{su}(2)$ are embedded in $\mathfrak{so}(7)$, but we still have to determine the inclusion relations. All algebras not listed with the corresponding highest weight in Table VIII are *directly contained* either in $\mathfrak{su}(N)$, $\mathfrak{sp}(N/2)$ [for N even], or in $\mathfrak{so}(N)$ depending on whether the irreducible representation is unitary, symplectic, or orthogonal. We find the algebra $\mathfrak{su}(2)$ with the highest weight (6) in the third row of Table VIII. Thus the algebra $\mathfrak{su}(2)$ is contained in $\mathfrak{so}(7)$ but only indirectly so—via $\mathfrak{g}_2$:

$$\mathfrak{su}(2) \leftarrow \mathfrak{g}_2 \leftarrow \mathfrak{so}(7) \leftarrow \mathfrak{su}(7)$$

Example 52: Consider the case of $N = 16$. First, we obtain all the irreducible simple subalgebras of $\mathfrak{su}(16)$ (see Table IX): $\mathfrak{su}(16)$ with highest weights (1, 0, . . . , 0) and (0, . . . , 0, 1) as well as $\mathfrak{so}(10)$ with (0, 0, 0, 1, 0). The cases of irreducible symplectic representations are $\mathfrak{sp}(8)$ with highest weight (1, 0, 0, 0, 0, 0, 0, 0), $\mathfrak{su}(2)$ with (15), and $\mathfrak{sp}(2)$ with (1, 1). The irreducible orthogonal representations are given by $\mathfrak{so}(16)$ with highest weight (1, 0, 0, 0, 0, 0, 0, 0) and $\mathfrak{so}(9)$ with highest weight (0, 0, 0, 1). We immediately conclude that the algebras $\mathfrak{sp}(8)$, $\mathfrak{so}(16)$, and $\mathfrak{so}(10)$ are directly embedded in $\mathfrak{su}(16)$:



It follows that all the other cases are *directly contained* either in $\mathfrak{sp}(8)$ or $\mathfrak{so}(16)$ as they are not listed in Table VIII:



APPENDIX D: ALTERNATING AND SYMMETRIC SQUARES OF REPRESENTATIONS

In this Appendix, we enumerate for all compact semi-simple Lie algebras those representations whose alternating and symmetric squares are both irreducible. We obtain that only the standard representation of $\mathfrak{su}(\ell+1)$ with $\ell \geq 0$ has this property. This result is used in Sec. VII D. We freely use the notation of Appendix C.

Assume that ϕ is a representation of a compact semi-simple Lie algebra $\mathfrak{g}$ on a finite-dimensional vector space V with basis $\{v_1, \ldots, v_k\}$. The representation ϕ is given as a map from $\mathfrak{g}$ to the set of complex $k \times k$ matrices $\mathfrak{gl}(k, \mathbb{C})$. Starting from the representation ϕ we construct its tensor square $\phi^{\otimes 2} = \phi \otimes \mathbb{1}_k + \mathbb{1}_k \otimes \phi$ which acts on the k^2-dimensional vector space $V \otimes V$ with basis $\{v_{i_1} \otimes v_{i_2} \,|\, i_1, i_2 \in \{1, \ldots, k\}\}$. This action is defined on the basis by ($g \in \mathfrak{g}$)

$$\phi^{\otimes 2}(g)[v_{i_1} \otimes v_{i_2}] := [\phi(g)v_{i_1}] \otimes v_{i_2} + v_{i_1} \otimes [\phi(g)v_{i_2}],$$

and it can be extended to the full vector space $V \otimes V$ by linearity. Now we can define for ϕ its alternating square $\mathrm{Alt}^2\phi := \phi^{\otimes 2}|_{\mathrm{Alt}^2 V}$ by restricting $\phi^{\otimes 2}$ to the $k(k-1)/2$-dimensional subspace $\mathrm{Alt}^2 V \subset V \otimes V$ with basis

$$\{v_{i_1} \otimes v_{i_2} - v_{i_2} \otimes v_{i_1} \,|\, i_1, i_2 \in \{1, \ldots, k\} \text{ and } i_1 \neq i_2\}.$$

It is clear that $\mathrm{Alt}^2\phi$ is well defined as ($g \in \mathfrak{g}$)

$$(\mathrm{Alt}^2\phi)(g)[v_{i_1} \otimes v_{i_2} - v_{i_2} \otimes v_{i_1}] = \big([\phi(g)v_{i_1}] \otimes v_{i_2} - v_{i_2} \otimes [\phi(g)v_{i_1}]\big) + \big(v_{i_1} \otimes [\phi(g)v_{i_2}] - [\phi(g)v_{i_2}] \otimes v_{i_1}\big)$$

is contained in $\mathrm{Alt}^2 V$. Similarly, one defines the symmetric square $\mathrm{Sym}^2\phi := \phi^{\otimes 2}|_{\mathrm{Sym}^2 V}$ as the restriction to the $k(k+1)/2$-dimensional subspace $\mathrm{Sym}^2 V \subset V \otimes V$ with basis $\{v_{i_1} \otimes v_{i_2} + v_{i_2} \otimes v_{i_1} \,|\, i_1, i_2 \in \{1, \ldots, k\}\}$. We obtain that the tensor square $\phi^{\otimes 2} = \mathrm{Alt}^2\phi \oplus \mathrm{Sym}^2\phi$ decomposes in a direct sum, exactly as the tensor product $V \otimes V = \mathrm{Alt}^2 V \oplus \mathrm{Sym}^2 V$. Dynkin[91] classified the cases when $\mathrm{Alt}^2\phi$ is irreducible, so that our final theorem builds upon the following:

Theorem 53 (Dynkin)*: Assume ϕ is a (finite-dimensional) representation of a compact semi-simple Lie algebra $\mathfrak{g}$. The representation $\mathrm{Alt}^2\phi$ is irreducible if and only if ϕ is irreducible and the pair $(\mathfrak{g}, \phi)$ is (up to an outer automorphism of $\mathfrak{g}$) given in Table X.*

Proof: If $\phi = \phi_1 \oplus \phi_2$ is not irreducible then neither is $\mathrm{Alt}^2(\phi_1 \oplus \phi_2) = \mathrm{Alt}^2\phi_1 \oplus (\phi_1 \otimes \phi_2) \oplus \mathrm{Alt}^2\phi_2$ irreducible. The theorem follows from Theorem 4.7 and Table VI of Ref. 91. □

Theorem 54: *Assume ϕ is a (finite-dimensional) representation of a compact semi-simple Lie algebra $\mathfrak{g}$. The representations $\mathrm{Alt}^2\phi$ and $\mathrm{Sym}^2\phi$ are both irreducible if and only if $\mathfrak{g} = \mathfrak{su}(\ell+1)$ with $\ell \geq 1$ and ϕ is (up to an outer automorphism of $\mathfrak{g}$) the standard representation [i.e., its highest weight is $(1, 0, \ldots, 0)$].*

TABLE X. Irreducible representations whose alternating square is also irreducible (Dynkin).

Case	$\mathfrak{g}$	ℓ	ϕ	dim(ϕ)	$\mathrm{Alt}^2\phi$	dim($\mathrm{Alt}^2\phi$)
(1a)	$\mathfrak{so}(2\ell+1)$	$\ell > 2$	$(1, 0, \dots, 0)$	$2\ell+1$	$(0, 1, 0, \dots, 0)$	$(2\ell+1)\ell$
(1b)	$\mathfrak{so}(5)$	–	$(1, 0)$	5	$(0, 2)$	10
(2a)	$\mathfrak{so}(2\ell)$	$\ell > 3$	$(1, 0, \dots, 0)$	2ℓ	$(0, 1, 0, \dots, 0)$	$(2\ell-1)\ell$
(2b)	$\mathfrak{so}(6)$	–	$(1, 0, 0)$	6	$(0, 1, 1)$	15
(3)	$\mathfrak{su}(\ell+1)$	$\ell \geq 3$	$(0, 1, 0, \dots, 0)$	$\frac{\ell(\ell+1)}{2}$	$(1, 0, 1, 0, \dots, 0)$	$3\binom{\ell+2}{4}$
(4)	$\mathfrak{su}(\ell+1)$	$\ell \geq 2$	$(2, 0, \dots, 0)$	$\frac{(\ell+1)(\ell+2)}{2}$	$(2, 1, 0, \dots, 0)$	$3\binom{\ell+3}{4}$
(5)	$\mathfrak{so}(10)$	–	$(0, 0, 0, 1, 0)$	16	$(0, 0, 1, 0, 0)$	120
(6)	$\mathfrak{e}_6$	–	$(1, 0, 0, 0, 0, 0)$	27	$(0, 0, 1, 0, 0, 0)$	351
(7)	$\mathfrak{su}(\ell+1)$	$\ell \geq 1$	$(1, 0, \dots, 0)$	$\ell+1$	$(0, 1, 0, \dots, 0)$	$\frac{\ell(\ell+1)}{2}$

Proof: We go through the cases of Theorem 53. Let us denote by ϕ_x the representation with highest weight x. In the cases (1a)-(2b), it follows from Example 19.21 of Ref. 111 that $\mathrm{Sym}^2\phi_{(1,0,\dots,0)} = \phi_{(2,0,\dots,0)} \oplus \phi_{(0,\dots,0)}$ decomposes. In the case of (3), we can use a Pieri-type formula (see Proposition 15.25(ii) of Ref. 111) to show that $\mathrm{Sym}^2\phi_{(0,1,0)} = \phi_{(0,0,0)} \oplus \phi_{(0,2,0)}$ and $\mathrm{Sym}^2\phi_{(0,1,0,\dots,0)} = \phi_{(0,0,0,1,0,\dots,0)} \oplus \phi_{(0,2,0,\dots,0)}$ decompose. In the case of (4), we can use again a Pieri-type formula (see Proposition 15.25(i) of Ref. 111) to show that $\mathrm{Sym}^2\phi_{(2,0,\dots,0)} = \phi_{(0,2,0,\dots,0)} \oplus \phi_{(4,0,\dots,0)}$ decomposes. In the cases (5) and (6), we explicitly compute the decomposition using computer algebra systems such as LiE[89] and MAGMA.[90] We get for (5) that $\mathrm{Sym}^2\phi_{(0,0,0,1,0)} = \phi_{(0,0,0,2,0)} \oplus \phi_{(1,0,0,0,0)}$ and for (6) that $\mathrm{Sym}^2\phi_{(1,0,0,0,0,0)} = \phi_{(0,0,0,0,0,1)} \oplus \phi_{(2,0,0,0,0,0)}$. In the case of (7), we use again a Pieri-type formula (see Proposition 15.25(i) of Ref. 111) to show that $(\phi_{(1,0,\dots,0)})^{\otimes 2} = \phi_{(2,0,\dots,0)} \oplus \phi_{(0,1,0,\dots,0)} = \mathrm{Sym}^2\phi_{(1,0,\dots,0)} \oplus \mathrm{Alt}^2\phi_{(1,0,\dots,0)}$. Therefore, case (7) is the only case for which both the alternating and symmetric square are irreducible. □

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