

Symmetry Principles in Quantum System Theory of Multi-Qubit Systems Made Simple

Thomas Schulte-Herbrüggen, Uwe Sander, and Robert Zeier

Abstract— Controllability and observability of multi-spin systems in architectures of various symmetries of coupling type and topology are investigated. We complement recent work [1] of explicitly determining the respective dynamic system Lie algebras and thereby also precise reachability sets under symmetry constraints. Here the focus is on the converse: under which conditions can the absence of symmetry be taken as an indicator of universality of the hardware architecture? More precisely, the absence of symmetry implies irreducibility and provides a convenient necessary condition for full controllability. Though much easier to assess than the well-established Lie-algebra rank condition, this is not sufficient unless in an n -qubit system with connected coupling topology the candidate dynamic simple Lie algebra can be identified uniquely as the full unitary algebra $\mathfrak{su}(2^n)$. — Here we discuss simple tests confined to solving homogeneous linear equations in order to filter irreducible unitary representations of other candidate algebras of classical type (orthogonal ones and unitary symplectic ones). Finally, we give an outlook under which conditions algebras of exceptional type can also be ruled out.

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 [2–4]. On the computational end, where quantum algorithms efficiently solving hidden subgroup problems [5] 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 [6]—in particular at phase-transitions [7]—has recently shifted into focus [8–11]. In view of experimental progress in cold atoms in optical lattice potentials [12, 13] as well as in trapped ions [14, 15], Kraus *et al.* have explored whether target quantum systems can be universally simulated on translationally invariant lattices of bosonic, fermionic, and spin systems [16]. Their work can also be seen as a follow-up on a study by Schirmer *et al.* [17] specifically addressing controllability of systems with degenerate transition frequencies.

Quite generally, quantum control has been recognised as a key generic tool [18–20] needed for advances in experimentally exploiting quantum systems for simulation or com-

putation (and even more so in future quantum technology). It paves the way for constructively optimising strategies for experimental implementation 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 optimised pulse scheme [21–23]. This approach has proven useful in spin systems [24] as well as in solid-state systems [25]. Moreover, it has recently been generalised from closed systems to open ones [26], where the Markovian setting can also be used as embedding of explicitly non-Markovian subsystems [27]. — However, in closed systems, all the numerical tools rely on the existence of perfect solutions, in other words, they require the system is universal or fully operator controllable [28].

II. CONTROLLABILITY

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

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

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

$$\text{vec } \dot{\rho}(t) = -i \text{ad}_{H_u} \text{vec } \rho(t) \quad . \quad (2)$$

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

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

with ‘state’ $X(t) \in \mathbb{C}^N$, drift $A \in \text{Mat}_N(\mathbb{C})$, controls $B_j \in \text{Mat}_N(\mathbb{C})$, and control amplitudes $u_j \in \mathbb{R}$. Now lifting the bilinear control system (Σ) to group manifolds [29, 30] by $X(t) \in GL(N, \mathbb{C})$ under the action of some compact connected Lie group \mathbf{K} with Lie algebra \mathfrak{k} (while keeping $A, B_j \in \text{Mat}_N(\mathbb{C})$), the condition for full controllability turns into the *Lie algebra rank condition* [30–32]

$$\langle A, B_j \mid j = 1, 2, \dots, m \rangle_{\text{Lie}} = \mathfrak{k} \quad , \quad (4)$$

This work was supported in part by the EU programmes QAP, Q-ESSENCE, and COQUIT, by the Bavarian PhD programme of excellence QCCC, as well as by *Deutsche Forschungsgemeinschaft* (DFG) in the collaborative research centre SFB 631.

T. Schulte-Herbrüggen, U. Sander, and R. Zeier are with the Dept. of Chemistry, Technical University of Munich (TUM), 85747 Garching, Germany; for correspondence: tosh@ch.tum.de

Algorithm 1 [34]: Determine Lie closure for n -qubit system with given set of drift (or system) and control Hamiltonians

1. Start with the initial basis $B_\nu := \{H_d; H_1, \dots, H_m\}$.
 2. If $m + 1 = \dim \mathfrak{su}(2^n) \Rightarrow$ terminate.
 3. Perform all Lie brackets $K_i = [H_j, H_k]$.
 4. For each new K_i check linear independence from span B_ν . If nothing new found \Rightarrow terminate.
 5. Extend basis by all independent new $\{K_i\}$
 $B_{\nu+1} := \{\{K_i\}, H_i\}$. Go to (1).
-

Algorithm 1 is of complexity $\mathcal{O}(32^n) - \mathcal{O}(64^n)$ for n qubits (depending on sparsity for QR rank determination).

where $\langle \cdot \rangle_{\text{Lie}}$ denotes (the linear span over) the *Lie closure* obtained by repeatedly taking mutual commutator brackets. Transferring the classical result [32] to the quantum domain [33], the bilinear system of Eqn. (1) is *fully operator controllable* iff the drift and controls are a generating set of $\mathfrak{su}(N)$

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

In fully controllable systems to every initial state ρ_0 the *reachable set* is the entire unitary orbit $\mathcal{O}_U(\rho_0) := \{U\rho_0U^\dagger \mid U \in SU(N)\}$. 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.

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

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

A. Symmetry Constrained Controllability

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

$$[s, H_\nu] = 0 \quad \text{for all } \nu \in \{d; 1, 2, \dots, m\} \quad . \quad (7)$$

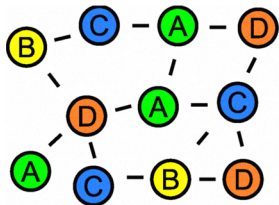


Fig. 1. General coupling topology represented by a connected graph. The vertices denote the spin- $\frac{1}{2}$ qubits, while the edges represent pairwise couplings of Heisenberg or Ising type. Qubits of the same colour and letter are taken to be affected by joint local unitary operations (or none), 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, see text.

Algorithm 2: Determine the centraliser to a given set of n -qubit drift and control Hamiltonians $\{iH_d; H_1, \dots, H_m\}$

1. For each Hamiltonian $H_\nu \in \{H_d; H_1, \dots, H_m\}$ determine all *solutions to the homogeneous linear eqn.*
 $\mathcal{S}_\nu := \{k \in \mathfrak{su}(N) \mid (\mathbf{1} \otimes H_\nu - H_\nu^\dagger \otimes \mathbf{1}) \text{vec}(k) = 0\}$
 2. The centraliser is the intersection of all sets of solutions
 $\mathfrak{k}' = \bigcap_\nu \mathcal{S}_\nu$.
-

The complexity of Algorithm 2 is $\mathcal{O}(4^n)$ for n qubits, as 4^n equations with real coefficients have to be solved.

More precisely, we use the term *outer symmetry* if s generates a SWAP operation permuting a subset of spin qubits of spins of the same type (cp. Fig. 1) such that the coupling graph and all Hamiltonians $\{H_\nu\}$ are left invariant. 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 centraliser

$$\{H_\nu\}' := \{s \in \mathfrak{su}(N) \mid [s, H_\nu] = 0 \forall \nu \in \{d; 1, 2, \dots, m\}\},$$

where the *centraliser* or *commutant* of a given subset $\mathfrak{m} \subseteq \mathfrak{g}$ with respect to a Lie algebra \mathfrak{g} consists of all elements in \mathfrak{g} that commute with all elements in \mathfrak{m} . Jacobi's identity $[[a, b], c] + [[b, c], a] + [[c, a], b] = 0$ 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

$$\mathfrak{k}' := \{s \in \mathfrak{su}(N) \mid [s, k] = 0 \forall k \in \mathfrak{k}\} \quad (8)$$

and hence $\{iH_\nu\}' \equiv \mathfrak{k}'$. Thus in practice it is (most) convenient to just evaluate the centraliser for a (minimal) generating set $\{iH_\nu\}$ of \mathfrak{k} . Fact (2) means the centraliser \mathfrak{k}' forms itself an invariant Lie subalgebra to $\mathfrak{su}(N)$ collecting *all symmetries*.

In summary, we note that lack of symmetry (i.e. a trivial centraliser) is a necessary condition for full controllability. Any non-trivial element would generate a one-parameter group $\mathbf{K}' \subset SU(N)$ that is not in $\mathbf{K} = \exp \mathfrak{k}$.

B. From Necessary to Sufficient Conditions for Controllability

Observe that the centraliser is exponentially easier to come by than the Lie closure: this is evident by comparing the complexity $\mathcal{O}(32^n)$ to $\mathcal{O}(64^n)$ of **Algorithm 1** for the Lie closure with the complexity $\mathcal{O}(4^n)$ of **Algorithm 2** for the centraliser tabulated above. The mere decision whether the centraliser is trivial is of complexity $\mathcal{O}(2^n)$. — 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 topology. For pure-state controllability, this was analysed in [35], for operator controllability the issue has been raised in [19],

inter alia following the lines of [36], however, without a full answer.

Lemma 2.1: Let $\mathfrak{k} \subseteq \mathfrak{su}(N)$ be a matrix Lie subalgebra to the compact simple Lie algebra of special unitaries $\mathfrak{su}(N)$. If its centraliser \mathfrak{k}' of \mathfrak{k} in $\mathfrak{su}(N)$ is trivial, then

- (1) \mathfrak{k} is given in an irreducible representation;
- (2) \mathfrak{k} is *simple or semi-simple*.

Proof. (1) Obvious. (2) By compactness, $\mathfrak{k} \subseteq \mathfrak{su}(N)$ decomposes into its centre and a semi-simple part $\mathfrak{k} = \mathfrak{z}_{\mathfrak{k}} \oplus \mathfrak{s}$ (see, e.g., [37] Corollary IV.4.25). As the centre $\mathfrak{z}_{\mathfrak{k}} = \mathfrak{k}' \cap \mathfrak{k}$ is trivial and \mathfrak{k} is traceless, \mathfrak{k} can only be semi-simple or simple. ■

Now observe that the abstract *direct sum* of Lie algebras has a matrix representation as the *Kronecker sum*, e.g., $\mathfrak{g} = \mathfrak{su}(N_1) \hat{\oplus} \mathfrak{su}(N_2) := \mathfrak{su}(N_1) \otimes \mathbf{1}_{N_2} + \mathbf{1}_{N_1} \otimes \mathfrak{su}(N_2)$ and generates a group isomorphic to the *tensor product* $\mathbf{G} = SU(N_1) \otimes SU(N_2)$. The abstract direct sum of two algebras \mathfrak{g} and \mathfrak{h} (each given in irreducible representation) has an irreducible representation as a single Kronecker sum $\mathfrak{g} \hat{\oplus} \mathfrak{h}$ ([38] Theorem 11.6.II). Such a sum representation always exists for every semi-simple Lie algebra.

Lemma 2.2: Given a controlled system of $n \geq 2$ qubits, where drift and control Hamiltonians $\{iH_\nu\}$ generate the Lie closure $\mathfrak{k} \subseteq \mathfrak{su}(N)$ in an irreducible representation, so \mathfrak{k}' is trivial. Set $N := 2^n$ here and henceforth. If in addition the drift Hamiltonian H_d corresponds to a topology of a *connected* coupling graph, and if H_d does not commute with all the control Hamiltonians H_j , then \mathfrak{k} is a *simple Lie algebra*.

Proof. For a drift Hamiltonian with a coupling topology of a graph that is *connected*, there exists no representation by a single Kronecker sum. Since every semi-simple Lie algebra allows for a representation as a Kronecker sum, the dynamic Lie algebra \mathfrak{k} can only be simple. ■

Corollary 2.1: Given a controlled system of $n \geq 2$ spin- $\frac{1}{2}$ qubits. Let its drift and control Hamiltonians $\{iH_\nu\}$ generate the Lie closure $\mathfrak{k} \subseteq \mathfrak{su}(N)$ in an irreducible representation (\mathfrak{k}' trivial) with the additional promise that \mathfrak{k} is simple.

Then (1) \mathfrak{k} has to be one of the candidate simple real compact Lie algebras of classical type

$$\begin{aligned} \mathfrak{a}_\ell (\ell \geq 1) &: \mathfrak{su}(\ell + 1, \mathbb{C}) \\ \mathfrak{b}_\ell (\ell \geq 2) &: \mathfrak{so}(2\ell + 1, \mathbb{R}) \\ \mathfrak{c}_\ell (\ell > 3) &: \mathfrak{usp}(\frac{\ell}{2}, \mathbb{C}) := \mathfrak{sp}(\ell, \mathbb{C}) \cap \mathfrak{u}(\ell, \mathbb{C}) \text{ with } \ell \text{ even} \\ \mathfrak{d}_\ell (\ell \geq 4) &: \mathfrak{so}(2\ell, \mathbb{R}), \end{aligned}$$

or of exceptional type $\mathfrak{g}_2; \mathfrak{f}_4; \mathfrak{e}_6, \mathfrak{e}_7, \mathfrak{e}_8$.

And (2) \mathfrak{k} has to occur as a simple subalgebra of $\mathfrak{su}(N)$.

Proof. (1) is obvious, since the classification (see, e.g., [39]) of the compact simple Lie algebras of classical and exceptional type is complete. In particular, observe that for multi-spin systems with $N \geq 4$ one has $\ell \geq 3$, so the isomorphisms (see, e.g., Thm. X.3.12 in [39]) $\mathfrak{a}_1 \sim \mathfrak{b}_1 \sim \mathfrak{c}_1$ and $\mathfrak{b}_2 \sim \mathfrak{c}_2$ or the isolated semi-simple case $\mathfrak{d}_2 \sim \mathfrak{a}_1 \hat{\oplus} \mathfrak{a}_1$ are of no concern. (2) follows, as \mathfrak{k} is by construction a subalgebra of $\mathfrak{su}(N)$. ■

The irreducible simple subalgebras of $\mathfrak{su}(N)$ were already determined by E. Cartan [40], which is now standard representation theory of connected compact Lie groups, see, e.g., [41]. The corresponding dimensions of the irreducible representations can then be efficiently computed using computer algebras systems such as LiE [42] and MAGMA [43] via Weyl's dimension formula. The irreducible simple subalgebras of $\mathfrak{su}(N)$ are found by enumerating for all simple Lie algebras all the irreducible representations of dimension N . Following the work of Dynkin [44], one can determine the maximal ones with respect to $\mathfrak{so}(N)$, $\mathfrak{usp}(N/2)$, and $\mathfrak{su}(N)$. The results are collected in Tab. I extending Refs. [45, 46] from $N \leq 9$ to $N \leq 16$.

While the ramification of *mathematically* admissible irreducible simple candidate subalgebras may seem daunting, in the following we will eliminate candidates by simple means. We make use of the fact that in Tab. I most of the irreducible subalgebras *directly attached* to the highest unitary algebra $\mathfrak{su}(N)$ are conjugate to orthogonal or symplectic subalgebras. Now the orthogonal and unitary symplectic ones (as well as all their nested subalgebras!) can be excluded by merely solving simultaneous systems of linear homogeneous equations. Many of the proper unitary subalgebras can be excluded by the promise that $\mathfrak{k} \subseteq \mathfrak{su}(N)$ represents a *physical* system of n distinguishable spins- $\frac{1}{2}$. Whether in higher dimensions 2^n , irreducible representations of exceptional Lie algebras (\mathfrak{e}_6) can directly link to $\mathfrak{su}(2^n)$ without being a subalgebra to an intermediate orthogonal or symplectic algebra remains to be treated separately.

Lemma 2.3 (Candidate Filter): Given a set of Hamiltonians $\{iH_\nu\}$ generating the Lie closure $\mathfrak{k} \subseteq \mathfrak{su}(2^n)$ with the promise that \mathfrak{k} is an irreducible representation of a simple Lie subalgebra to $\mathfrak{su}(2^n)$ for $n \geq 2$ distinguishable spins- $\frac{1}{2}$.

Then $\mathfrak{k} = \mathfrak{su}(2^n)$ may only hold, if the following four instances can be excluded:

- 1) all the $\{iH_\nu\}$ are jointly conjugate to a set $\{i\tilde{H}_\nu\}$, where each element is real and skew-symmetric $\tilde{H}_\nu^t = -\tilde{H}_\nu$;
- 2) all the $\{iH_\nu\}$ are jointly conjugate to a set $\{i\tilde{H}_\nu\}$, where each element is unitary and symplectic $J\tilde{H}_\nu = -\tilde{H}_\nu^t J$ with $J := \begin{pmatrix} 0 & -\mathbf{1}_{N/2} \\ \mathbf{1}_{N/2} & 0 \end{pmatrix}$;
- 3) the $\{iH_\nu\}$ generate a proper unitary subalgebra $\mathfrak{su}(N') \subsetneq \mathfrak{su}(N)$ with $N' < N$ that is compatible with an irreducible n spin- $\frac{1}{2}$ representation;
- 4) all the $\{iH_\nu\}$ are jointly conjugate to a set $\{i\tilde{H}_\nu\}$ generating one of the exceptional compact simple Lie algebras $\mathfrak{g}_2; \mathfrak{f}_4; \mathfrak{e}_6, \mathfrak{e}_7, \mathfrak{e}_8$.

Proof. Even for a single instance of N , there may be orthogonal, symplectic, lower-rank unitary or exceptional subalgebras. So (1) excludes the orthogonal subalgebras $\mathfrak{so}(N) \subset \mathfrak{su}(N)$, (2) excludes the unitary symplectic ones $\mathfrak{usp}(\frac{N}{2}) \subset \mathfrak{su}(N)$, (3) excludes cases like $\mathfrak{su}(N - k) \subset \mathfrak{su}(N)$, while finally (4) precludes exceptional ones.

Note that step (3) can sometimes be settled by the promise of spin- $\frac{1}{2}$ representations: e.g., in $\mathfrak{su}(4)$ there is an irreducible

TABLE I

IRREDUCIBLE SIMPLE SUBALGEBRAS OF $\mathfrak{su}(N)$ WITH $N \leq 16$

$N = 2$	$\mathfrak{su}(2)$
$N = 3$	$\mathfrak{su}(2) \subset \mathfrak{su}(3)$
$N = 4$	$\mathfrak{su}(2) \subset \mathfrak{usp}(\frac{4}{2}) \subset \mathfrak{su}(4)$
$N = 5$	$\mathfrak{su}(2) \subset \mathfrak{so}(5) \subset \mathfrak{su}(5)$
$N = 6$	$\mathfrak{su}(2) \subset \mathfrak{usp}(\frac{6}{2}) \subset \mathfrak{so}(6) \subset \mathfrak{su}(6)$ $\mathfrak{su}(3) \subset \mathfrak{su}(6)$
$N = 7$	$\mathfrak{su}(2) \subset \mathfrak{g}(2) \subset \mathfrak{so}(7) \subset \mathfrak{su}(7)$
$N = 8$	$\mathfrak{su}(2) \subset \mathfrak{usp}(\frac{8}{2}) \subset \mathfrak{so}(8) \subset \mathfrak{su}(8)$ $\{\mathfrak{su}(3), \mathfrak{so}(7)\} \subset \mathfrak{so}(8) \subset \mathfrak{su}(8)$
$N = 9$	$\mathfrak{su}(2) \subset \mathfrak{so}(9) \subset \mathfrak{su}(9)$
$N = 10$	$\mathfrak{su}(2) \subset \mathfrak{usp}(\frac{10}{2}) \subset \mathfrak{so}(10) \subset \mathfrak{su}(10)$ $\{\mathfrak{su}(3), \mathfrak{su}(4), \mathfrak{su}(5)\} \subset \mathfrak{su}(10)$
$N = 11$	$\mathfrak{su}(2) \subset \mathfrak{so}(11) \subset \mathfrak{su}(11)$
$N = 12$	$\mathfrak{su}(2) \subset \mathfrak{usp}(\frac{12}{2}) \subset \mathfrak{so}(12) \subset \mathfrak{su}(12)$
$N = 13$	$\mathfrak{su}(2) \subset \mathfrak{so}(13) \subset \mathfrak{su}(13)$
$N = 14$	$\{\mathfrak{su}(2), \mathfrak{usp}(\frac{6}{2})\} \subset \mathfrak{usp}(\frac{14}{2}) \subset \mathfrak{so}(14) \subset \mathfrak{su}(14)$ $\{\mathfrak{so}(5), \mathfrak{usp}(\frac{6}{2}), \mathfrak{g}(2)\} \subset \mathfrak{so}(14) \subset \mathfrak{su}(14)$
$N = 15$	$\{\mathfrak{su}(2), \mathfrak{su}(4)\} \subset \mathfrak{so}(15) \subset \mathfrak{su}(15)$ $\{\mathfrak{su}(3), \mathfrak{su}(5), \mathfrak{su}(6)\} \subset \mathfrak{su}(15)$ $\mathfrak{su}(3) \subset \mathfrak{su}(6)$
$N = 16$	$\{\mathfrak{su}(2), \mathfrak{so}(5)\} \subset \mathfrak{usp}(\frac{16}{2}) \subset \mathfrak{so}(16) \subset \mathfrak{su}(16)$ $\mathfrak{so}(9) \subset \mathfrak{so}(16) \subset \mathfrak{su}(16)$ $\mathfrak{so}(10) \subset \mathfrak{so}(16)$

spin- $\frac{3}{2}$ representation of $\mathfrak{su}(2)$ as a proper *irreducible* subalgebra $\mathfrak{su}(2)_{j=3/2} \subsetneq \mathfrak{su}(4)$. Yet a change in spin quantum number j and number of qubits n is ruled out by premiss. ■

The exceptional simple Lie algebras $\mathfrak{e}_\ell, \mathfrak{f}_\ell, \mathfrak{g}_\ell$ will need a more thorough treatment than here, given that in higher dimensions there is no complete list of irreducible representations of the exceptionals as compact simple subalgebras of $\mathfrak{su}(N)$ [45]. However, they can be generated using computer algebra systems as explained above. Considering the dimensions of their simplest representations [47] (see also [48])

$$\mathfrak{g}_2 \subset \mathfrak{so}_7; \mathfrak{f}_4 \subset \mathfrak{so}_{26}; \mathfrak{e}_6 \subset \mathfrak{sl}_{27}; \mathfrak{e}_7 \subset \mathfrak{sp}_{56}; \mathfrak{e}_8 \subset \mathfrak{so}_{248}$$

may help to exclude them from counting for irreducible n spin- $\frac{1}{2}$ representations of simple subalgebras to $\mathfrak{su}(2^n)$ in a follow-up study. Here, 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 [49] building upon more recent results in [50] to fill earlier work [51, 52].

Check for Conjugation to Orthogonal or Symplectic Irreducible Subalgebras: Determine all *simultaneous* non-singular solutions S of $SH_\nu + H_\nu^t S = 0$ for all $\{H_\nu\}$. If the set of solutions is empty, then the $\{iH_\nu\}$ are neither conjugate to an orthogonal algebra nor a symplectic one. If S is a solution, then—invoking irreducibility of \mathfrak{k} —it follows from Schur's Lemma that $SS^t = \pm \mathbf{1}$, which is nicely explained in Lemma 3 of Ref. [53]. In case of a plus sign, the subalgebra \mathfrak{k} of $\mathfrak{su}(N)$ generated by the $\{iH_\nu\}$ is conjugate to a subalgebra of $\mathfrak{so}(N)$, while in case of a minus sign, \mathfrak{k} is conjugate to a subalgebra of $\mathfrak{usp}(\frac{N}{2})$. — Conjugation to the unitary symplectic algebras has also been treated in Ref. [52] by solving a system of linear equations, while Ref. [54] resorted to determining eigenvalues for discerning the unitary case from conjugate symplectic or orthogonal subalgebras.

III. 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, we have shown easy means (solving systems of linear equations) to determine the symmetry of the dynamic system algebra \mathfrak{k} merely in terms of its commutant or centraliser \mathfrak{k}' . If the system Hamiltonian corresponds to a connected coupling graph, the absence of any symmetry can be further exploited to decide universality (full controllability): it means the dynamic system algebra is irreducible. Now, conjugation to irreducible orthogonal or symplectic candidate subalgebras can again be decided on the basis of solving systems of linear equations only. The final identification task is between proper unitary subalgebras and irreducible exceptional algebras; it can often be made on the basis of physical properties (spin quantum numbers) or by dimensionality as to be exemplified in follow-up studies specifically addressing higher dimensions.

Here the symmetry identification was confined to solving systems of homogeneous linear equations in order to avoid the usual yet significantly more costly way of explicitly calculating Lie closures. — Since full controllability entails observability (while in the quantum domain the converse does not necessarily hold [19]), symmetry constraints immediately pertain to observability as discussed in detail in Ref. [1].

ACKNOWLEDGEMENTS

The 2009 workshops at the Kavli Institute in Santa Barbara and in Benasque allowed to include Peter Pemberton-Ross, Sonia Schirmer, and Alastair Kay into exchange with Daniel Burgarth over their related works [55–59].

REFERENCES

- [1] U. Sander and T. Schulte-Herbrüggen, "Symmetry in Quantum System Theory of Multi-Qubit Systems: Rules for Quantum Architecture Design," 2009, e-print: <http://arXiv.org/pdf/0904.4654>.
- [2] R. P. Feynman, "Simulating Physics with Computers," *Int. J. Theo. Phys.*, vol. 21, pp. 467–488, 1982.
- [3] —, *Feynman Lectures on Computation*. Perseus Books, Reading, MA., 1996.
- [4] A. Y. Kitaev, A. H. Shen, and M. N. Vyalyi, *Classical and Quantum Computation*. American Mathematical Society, Providence, 2002.
- [5] M. Ettinger, P. Høyer, and E. Knill, "The Quantum Query Complexity of the Hidden Subgroup Problem is Polynomial," *Inf. Process. Lett.*, vol. 91, pp. 43–48, 2004.
- [6] S. Lloyd, "Universal Quantum Simulators," *Science*, vol. 273, pp. 1073–1078, 1996.
- [7] S. Sachdev, *Quantum Phase Transitions*. Cambridge University Press, Cambridge, 1999.
- [8] C. Bennett, I. Cirac, M. Leifer, D. Leung, N. Linden, S. Popescu, and G. Vidal, "Optimal Simulation of Two-Qubit Hamiltonians Using General Local Operations," *Phys. Rev. A*, vol. 66, p. 012305, 2002.
- [9] J. Dodd, M. Nielsen, M. Bremner, and R. Thew, "Universal Quantum Computation and Simulation Using Any Entangling Hamiltonian and Local Unitaries," *Phys. Rev. A*, vol. 65, p. 040301(R), 2002.
- [10] E. Jané, G. Vidal, W. Dür, P. Zoller, and J. Cirac, "Simulation of quantum dynamics with quantum optical systems," *Quant. Inf. Computation*, vol. 3, pp. 15–37, 2003.
- [11] D. Porras and J. Cirac, "Effective quantum spin systems with trapped ions," *Phys. Rev. Lett.*, vol. 92, p. 207901, 2004.
- [12] M. Greiner, O. Mandel, T. Esslinger, T. W. Hänsch, and I. Bloch, "Quantum Phase Transition from a Superfluid to a Mott Insulator in a Gas of Ultracold Atoms," *Nature (London)*, vol. 415, pp. 39–44, 2002.
- [13] I. Bloch, J. Dalibard, and W. Zwerger, "Many-Body Physics with Ultracold Gases," *Rev. Mod. Phys.*, vol. 80, pp. 885–964, 2008.
- [14] D. Leibfried, R. Blatt, C. Munroe, and D. Wineland, "Quantum Dynamics of Single Trapped Ions," *Rev. Mod. Phys.*, vol. 75, pp. 281–324, 2003.
- [15] R. Blatt and D. Wineland, "Entangled States of Trapped Atomic Ions," *Nature (London)*, vol. 453, pp. 1008–1015, 2008.
- [16] C. V. Kraus, M. M. Wolf, and J. I. Cirac, "Quantum Simulations under Translational Symmetry," *Phys. Rev. A*, vol. 75, p. 022303, 2007.
- [17] S. G. Schirmer, I. H. C. Pullen, and A. I. Solomon, "Identification of Dynamical Lie Algebras for Finite-Level Quantum Control Systems," *J. Phys. A*, vol. 35, pp. 2327–2340, 2002.
- [18] J. Dowling and G. Milburn, "Quantum Technology: The Second Quantum Revolution," *Phil. Trans. R. Soc. Lond. A*, vol. 361, pp. 1655–1674, 2003.
- [19] D. D'Alessandro, *Introduction to Quantum Control and Dynamics*. Chapman & Hall/CRC, Boca Raton, 2008.
- [20] H. M. Wiseman and G. J. Milburn, *Quantum Measurement and Control*. Cambridge University Press, Cambridge, 2009.
- [21] A. Peirce, M. Dahleh, and H. Rabitz, "Optimal Control of Quantum Mechanical Systems: Existence, Numerical Approximations and Applications," *Phys. Rev. A*, vol. 37, pp. 4950–4962, 1987.
- [22] V. F. Krotov, *Global Methods in Optimal Control*. Marcel Dekker, New York, 1996.
- [23] N. Khaneja, T. Reiss, C. Kehlet, T. Schulte-Herbrüggen, and S. J. Glaser, "Optimal Control of Coupled Spin Dynamics: Design of NMR Pulse Sequences by Gradient Ascent Algorithms," *J. Magn. Reson.*, vol. 172, pp. 296–305, 2005.
- [24] T. Schulte-Herbrüggen, A. K. Spörl, N. Khaneja, and S. J. Glaser, "Optimal Control-Based Efficient Synthesis of Building Blocks of Quantum Algorithms: A Perspective from Network Complexity towards Time Complexity," *Phys. Rev. A*, vol. 72, p. 042331, 2005.
- [25] A. K. Spörl, T. Schulte-Herbrüggen, S. J. Glaser, V. Bergholm, M. J. Storz, J. Ferber, and F. K. Wilhelm, "Optimal Control of Coupled Josephson Qubits," *Phys. Rev. A*, vol. 75, p. 012302, 2007.
- [26] T. Schulte-Herbrüggen, A. Spörl, N. Khaneja, and S. J. Glaser, "Optimal Control for Generating Quantum Gates in Open Dissipative Systems," 2006, e-print: <http://arXiv.org/pdf/quant-ph/0609037>.
- [27] P. Rebentrost, I. Serban, T. Schulte-Herbrüggen, and F. Wilhelm, "Optimal Control of a Qubit Coupled to a Non-Markovian Environment," *Phys. Rev. Lett.*, vol. 102, p. 090401, 2009.
- [28] V. Ramakrishna and H. Rabitz, "Relation between Quantum Computing and Quantum Controllability," *Phys. Rev. A*, vol. 54, pp. 1715–1716, 1995.
- [29] R. W. Brockett, "System Theory on Group Manifolds and Coset Spaces," *SIAM J. Control*, vol. 10, pp. 265–284, 1972.
- [30] V. Jurdjevic, *Geometric Control Theory*. Cambridge University Press, Cambridge, 1997.
- [31] H. Sussmann and V. Jurdjevic, "Controllability of Nonlinear Systems," *J. Diff. Equat.*, vol. 12, pp. 95–116, 1972.
- [32] V. Jurdjevic and H. Sussmann, "Control Systems on Lie Groups," *J. Diff. Equat.*, vol. 12, pp. 313–329, 1972.
- [33] V. Ramakrishna, M. Salapaka, M. Daleh, H. Rabitz, and A. Peirce, "Controllability of Molecular Systems," *Phys. Rev. A*, vol. 51, pp. 960–966, 1995.
- [34] S. G. Schirmer, H. Fu, and A. I. Solomon, "Complete Controllability of Quantum Systems," *Phys. Rev. A*, vol. 63, p. 063410, 2001.
- [35] F. Albertini and D. D'Alessandro, "The Lie Algebra Structure and Controllability of Spin Systems," *Lin. Alg. Appl.*, vol. 350, pp. 213–235, 2002.
- [36] G. Turinici and H. Rabitz, "Wavefunction Controllability for Finite-Dimensional Bilinear Quantum Systems," *J. Phys. A*, vol. 36, pp. 2565–2576, 2003.
- [37] A. W. Knap, *Lie Groups beyond an Introduction*, 2nd ed. Birkhäuser, Boston, 2002.
- [38] J. F. Cornwell, *Group Theory in Physics*. Academic Press, London, 1984, vol. 2.
- [39] S. Helgason, *Differential Geometry, Lie Groups, and Symmetric Spaces*. Academic Press, New York, 1978.
- [40] E. Cartan, "Les groupes projectifs qui ne laissent invariante aucune multiplicité plane," *Bull. Soc. Math.*, vol. 41, pp. 53–96, 1913.
- [41] N. Bourbaki, *Elements of Mathematics, Lie Groups and Lie Algebras, Chapters 7–9*. Springer, Berlin, 2008.
- [42] "LiE—A Computer Algebra Package for Lie Group Computations," 2000. [Online]. Available: <http://www.mathlabo.univ-poitiers.fr/~maavl/LiE/>
- [43] W. Bosma, J. J. Cannon, and C. Playoust, "The MAGMA Algebra System I: The User Language," *J. Symbolic Comput.*, vol. 24, pp. 235–265, 1997.
- [44] E. B. Dynkin, "Maximal Subgroups of the Classical Groups," *Amer. Math. Soc. Transl. Ser. 2*, vol. 6, pp. 245–378, 1957.
- [45] W. G. McKay and J. Patera, *Tables of Dimensions, Indices, and Branching Rules for Representations of Simple Lie Algebras*. Marcel Dekker, New York, 1981.
- [46] T. Polack, H. Suchowski, and D. J. Tannor, "Uncontrollable Quantum Systems," *Phys. Rev. A*, vol. 79, p. 053403, 2009.
- [47] A. N. Minchenko, "The Semisimple Subalgebras of Exceptional Lie Algebras," *Trans. Moscow Math. Soc.*, vol. 2006, pp. 225–259, 2006.
- [48] J. C. Baez, "The Octonions," *Bull. Amer. Math. Soc.*, vol. 39, pp. 145–205, 2001.
- [49] G. Dirr and U. Helmke, "Lie Theory for Quantum Control," *GAMM-Mitteilungen*, vol. 31, pp. 59–93, 2008.
- [50] L. Kramer, "Two-Transitive Lie Groups," *J. Reine Angew. Math.*, vol. 563, pp. 83–113, 2003.
- [51] R. W. Brockett, "Lie Theory and Control Systems Defined on Spheres," *SIAM J. Appl. Math.*, vol. 25, pp. 213–225, 1973.
- [52] W. M. Boothby and E. N. Wilson, "Determination of the Transitivity of Bilinear Systems," *SIAM J. Control Optim.*, vol. 17, pp. 212–221, 1979.
- [53] M. Obata, "On Subgroups of the Orthogonal Group," *Trans. Amer. Math. Soc.*, vol. 87, pp. 347–358, 1958.
- [54] S. G. Schirmer, A. I. Solomon, and J. V. Leahy, "Criteria for Reachability of Quantum States," *J. Phys. A*, vol. 35, pp. 8551–8562, 2002.
- [55] S. G. Schirmer, I. C. H. Pullen, and P. J. Pemberton-Ross, "Global Controllability with a Single Local Actuator," *Phys. Rev. A*, vol. 78, p. 030501, 2008.
- [56] A. Kay, "A Review of Perfect State Transfer and its Application as a Constructive Tool," 2009, e-print: <http://arXiv.org/pdf/0903.4274>.
- [57] D. Burgarth, K. Maruyama, S. Montangero, T. Calarco, F. Noi, and M. Plenio, "Scalable Quantum Computation via Local Control of Only Two Qubits," 2009, e-print: <http://arXiv.org/pdf/0905.3373>.
- [58] A. Kay and P. Pemberton-Ross, "Computation on Spin Chains with Limited Access," 2009, e-print: <http://arXiv.org/pdf/0905.4070>.
- [59] S. G. Schirmer and P. J. Pemberton-Ross, "Fast, High-Fidelity Information Transmission through Spin-Chain Quantum Wires," 2009, e-print: <http://arXiv.org/pdf/0907.1887>.