Proceedings of the 19th International Symposium on Mathematical Theory of Networks and Systems – MTNS 2010 • 5–9 July, 2010 • Budapest, Hungary

Symmetry in Quantum System Theory of Multi-Qubit Systems

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***Abstract*— Controllability and observability of multi-spin systems under various symmetry constraints are investigated complementing recent work [1]. Conversely, 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 $\mathfrak{su}(2^n)$. Based on a complete list of irreducible simple subalgebras of the $\mathfrak{su}(N)$ in question, easy tests solving homogeneous linear equations filter irreducible unitary representations of other candidate algebras of classical type as well as of exceptional types. — Finally, having identified the dynamic system algebra, many observability issues can be treated immediately.**

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], [3], [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], [9], [10], [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], [19], [20] needed for advances in experimentally exploiting quantum systems for simulation or computation and even more so in future quantum technology. It paves the way for constructively optimising strategies for experimental implemention 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], [22], [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], [29].

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II. CONTROLLABILITY

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

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

The system Hamiltonian H_d denotes a non-switchable drift term. The control Hamiltonians H_j can be steered by (piecewise 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 $\mathrm{ad}_H(\cdot) := [H, (\cdot)]$, the Liouville equation $\dot{\rho}(t) = -i[H_u, \rho(t)]$ can be rewritten

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

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

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

with 'state' $X(t) \in \mathbb{C}^N$, drift $A \in \mathrm{Mat}_N(\mathbb{C})$, controls $B_j \in \mathrm{Mat}_N(\mathbb{C})$, and control amplitudes $u_j \in \mathbb{R}$. Now lifting the bilinear control system (Σ) to group manifolds [30], [31] by $X(t) \in GL(N, \mathbb{C})$ under the action of a compact connected Lie group $\mathbf{K}$ with Lie algebra $\mathfrak{k}$ [while keeping $A, B_j \in \mathrm{Mat}_N(\mathbb{C})$], the condition for full controllability turns into the *Lie algebra rank condition* [32], [33], [31]

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

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 [34].

Transferring the classical result [33] to the quantum domain [35], [36], [29], the bilinear system of Eqn. (1) is

Algorithm 1: Determine system algebra via Lie closure

Input: Hamiltonians $I := \{iH_d; iH_1, \dots, iH_m\} \subseteq \mathfrak{su}(N)$

1. $B :=$ maximal linearly independent subset of I
2. $\mathrm{num} := \#B$
3. If $\mathrm{num} = N$ then $O := B$ else $O := \{\,\}$
4. If $\mathrm{num} = N$ or $\#B = 0$ then terminate
5. $C := [O, B] \cup [B, B]$, where $[S_1, S_2] = \{[s_1, s_2] \,|\, s_1 \in S_1, s_2 \in S_2\}$
6. $O := O \cup B$
7. $B :=$ max. linear independent extension of O with elements from C
8. $\mathrm{num} := \mathrm{num} + \#B$; Go to 4

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

The complexity is roughly $\mathcal{O}(N^6 \cdot N^2)$, as about N^2 times a rank-revealing QR decomposition has to be performed in Liouville space (whose dimension is N^2).

Algorithm 2: Determine centraliser to system algebra $\mathfrak{k}$

Input: Hamiltonians $I := \{iH_d; iH_1, \dots, iH_m\} \subseteq \mathfrak{su}(N)$

1. For each $H \in I$ solve the homogeneous linear eqn. $\mathcal{S}_H := \{s \in \mathfrak{su}(N) | (\mathbb{1} \otimes H - H^t \otimes \mathbb{1}) \operatorname{vec}(s) = 0\}$
2. $\mathfrak{k}' := \bigcap_{H \in I} \mathcal{S}_H$.

Output: centraliser $\mathfrak{k}'$

The complexity is roughly $\mathcal{O}(N^6)$, as in Liouville space N^2 equations have to be solved by LU decomposition.

fully operator controllable iff the drift and controls are a generating set of $\mathfrak{su}(N)$

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

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.

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

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

III. 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

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

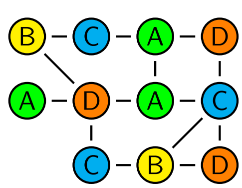


Fig. 1. General coupling topology represented by a connected graph. The vertices denote the spin-$\frac{1}{2}$ qubits, while the edges represent pairwise couplings of Heisenberg or Ising type. Qubits of the same colour and letter are taken to be affected by joint local unitary operations (or none), while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

A *symmetry operator* is an element of the centraliser

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

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

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

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 obtain the following straightforward, yet important result:

Theorem 1: Lack of symmetry in the sense of a trivial centraliser is a necessary condition for full controllability.

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

Lemma 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 $\mathfrak{k}$ is given in an irreducible representation and $\mathfrak{k}$ is *simple or semi-simple*.

Proof: The irreducibility is obvious. 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. ■

Note that the centraliser is 'exponentially' easier to come by than the Lie closure in the sense of comparing the complexity $\mathcal{O}(N^6 \cdot N^2)$ of **Algorithm 1** for the Lie closure with the complexity $\mathcal{O}(N^6)$ of **Algorithm 2** for the centraliser tabulated above. — 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 [38], for operator controllability the issue has been raised in [19], *inter alia* following the lines of [39], however, without a full answer.

Now observe that the abstract *direct sum* of Lie algebras has a matrix representation as the *Kronecker sum*, e.g., $\mathfrak{su}(N_1) \widehat{\oplus} \mathfrak{su}(N_2) := \mathfrak{su}(N_1) \otimes \mathbb{1}_{N_2} + \mathbb{1}_{N_1} \otimes \mathfrak{su}(N_2)$ and that it generates a group isomorphic to the *tensor product* $\mathbf{G} = SU(N_1) \otimes SU(N_2)$. The abstract direct sum of two algebras $\mathfrak{k}_1$ and $\mathfrak{k}_2$ (each given in irreducible representation) has an irreducible representation as a single Kronecker sum $\mathfrak{k}_1 \widehat{\oplus} \mathfrak{k}_2$ ([40] Theorem 11.6.II). Such a sum representation always exists for every semi-simple Lie algebra.

Lemma 2: Suppose a control system with drift and control Hamiltonians $\{iH_\nu\}$ generates the Lie closure $\mathfrak{k} \subseteq \mathfrak{su}(N)$ so that $\mathfrak{k}'$ is trivial. Then one finds:
(1) $\mathfrak{k}$ 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 dynamic system is not fully controllable.
(3) If the drift Hamiltoninan H_d corresponds to a topology of a *connected* coupling graph, then $\mathfrak{k}$ is a *simple Lie algebra.*

Proof: (1) immediately follows from $\mathfrak{k}'$ being trivial, while (2) is obvious, as $\mathfrak{su}(N)$ is simple. (3) For a drift Hamiltonian with a coupling topology of a graph that is *connected*, there exists no representation by a single Kronecker sum (rather a linear combination of Kronecker sums). Yet, since every semi-simple Lie algebra allows for a representation as a single Kronecker sum, the dynamic Lie algebra $\mathfrak{k}$ can only be simple. ■

IV. Irreducible Simple Subalgebras of $\mathfrak{su}(N)$

Starting from the knowledge that for a fully controllable system the system algebra $\mathfrak{k}$ has to be simple and given in an irreducible representation (see Section III), it is natural to ask for a classification of all these cases. Following the work of Killing, E. Cartan [41] classified all simple (complex) Lie algebras (see, e.g., [42], [43]). The corresponding compact real forms ([43], [44]) are the compact simple Lie algebras of classical type (assuming $\ell \in \mathbb{N} \setminus \{0\}$ henceforth):

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

and of exceptional type $\mathfrak{e}_6$, $\mathfrak{e}_7$, $\mathfrak{e}_8$, $\mathfrak{f}_4$, $\mathfrak{g}_2$. Observe 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 isomorphisms (see, e.g., Thm. X.3.12 in [44]) $\mathfrak{su}(2) \cong \mathfrak{so}(3) \cong \mathfrak{sp}(1)$, $\mathfrak{so}(5) \cong \mathfrak{sp}(2)$, and $\mathfrak{su}(4) \cong \mathfrak{so}(6)$ are of no concern. The same holds for the abelian case $\mathfrak{so}(2)$ and the semi-simple one $\mathfrak{so}(4) \cong \mathfrak{su}(2) \widehat{\oplus} \mathfrak{su}(2)$. In summary, we thus obtain the following:

Corollary 1 (Candidate List): Consider a control system, where the 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, being a simple subalgebra of $\mathfrak{su}(N)$, $\mathfrak{k}$ 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, consider for the Lie algebras of exceptional type the dimensions of their standard representations [45] (see also [46]) $\mathfrak{e}_6 \subset \mathfrak{su}(27)$, $\mathfrak{e}_7 \subset \mathfrak{sp}(28)$, $\mathfrak{e}_8 \subset \mathfrak{so}(248)$, $\mathfrak{f}_4 \subset \mathfrak{so}(26)$, and $\mathfrak{g}_2 \subset \mathfrak{so}(7)$. Here, as a final remark 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 [47] building upon more recent results in [48] to fill earlier work [49], [50].

Having listed the candidates for subalgebras of $\mathfrak{su}(N)$, we now focus on the set of possible irreducible representations. To this end, here we describe the main results, while all the details shall be explained elsewhere [51]. The irreducible representations of simple (complex) Lie algebras were already determined by E. Cartan [52]. This classification is equivalent for the compact simple Lie algebras (or the compact connected simple Lie groups), see, e.g., [43]. 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 [53] and MAGMA [54] via Weyl's dimension formula. Following the work of Dynkin [55], one can determine the inclusion relations between irreducible simple subalgebras of $\mathfrak{su}(N)$. We obtained the irreducible simple subalgebras of $\mathfrak{su}(N)$ for $N \leq 2^{15} = 32768$. This significantly extends previous work [56], [57] for $N \leq 9$. The results for $N \leq 16$ are given in Tab. I, and the results for $N = 2^n$ and $5 \leq n \leq 15$ can be found in Tab. II.

In the set of irreducible simple subalgebras of $\mathfrak{su}(N)$, the subalgebras $\mathfrak{sp}(N/2)$ and $\mathfrak{so}(N)$ play a particularly important role. For $N \geq 5$, there are two cases: if N is even, then $\mathfrak{su}(N)$ has both $\mathfrak{sp}(N/2)$ and $\mathfrak{so}(N)$ as irreducible simple subalgebras; if N is odd, $\mathfrak{so}(N)$ is an irreducible simple subalgebra of $\mathfrak{su}(N)$ but $\mathfrak{sp}(N/2)$ is not. The irreducible subalgebras $\mathfrak{sp}(N/2)$ and $\mathfrak{so}(N)$ correspond to the symmetric spaces $\mathrm{SU}(N)/\mathrm{Sp}(N/2)$ and $\mathrm{SU}(N)/\mathrm{SO}(N)$. These are two of three possible symmetric spaces [44] of $\mathrm{SU}(N)$, 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 [resp. orthogonal] if the subalgebra $\mathfrak{k}$ given in the representation ϕ is conjugate to a subalgebra of $\mathfrak{sp}(N/2)$ [resp. $\mathfrak{so}(N)$]. If the representation is neither symplectic nor orthogonal, it is of complex type.[1]

In abuse of notation, we call also the subalgebra $\mathfrak{k}$ (w.r.t. some fixed but unspecified representation ϕ) symplectic, orthogonal, or complex, if the representation ϕ is, respectively, symplectic, orthogonal, or of complex type. We emphasise that the classification of a subalgebra depends on the representations considered. We obtain from Chapter IX, Section 7.1, Prop. 1 of [43] the following:

Lemma 3: A representation $\phi(\mathfrak{k})$ can either be symplectic, or orthogonal, or complex. ■

[1] One can find a similar notation for example in [58]. It is also used for finite groups. Unfortunately, the representations are also said to be, respectively, of quaternionic, real, or complex type. Versions of the terminology can be found in Ref. [43] in Chapter VIII, Section 7.6, Def. 2 and, respectively, in Chapter IX, Appendix II.2, Prop. 3.

TABLE I
IRREDUCIBLE SIMPLE SUBALGEBRAS OF $\mathfrak{su}(N)$ FOR $N \leq 16$

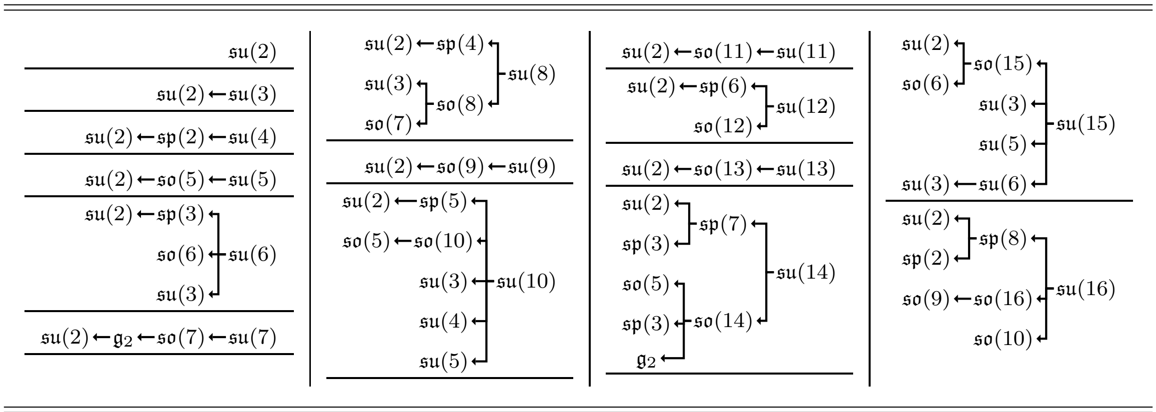
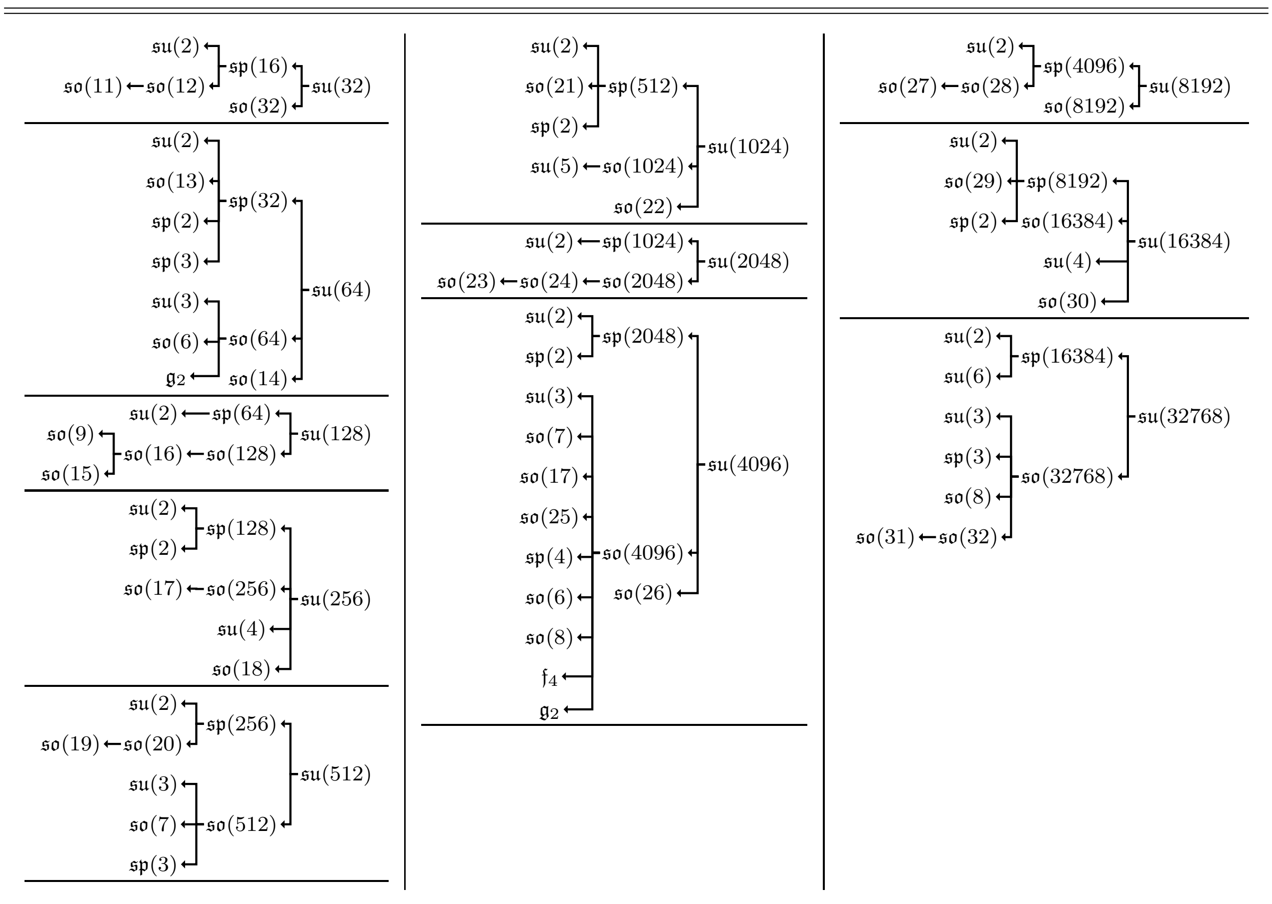


TABLE II
IRREDUCIBLE SIMPLE SUBALGEBRAS OF $\mathfrak{su}(2^n)$ FOR $5 \leq n \leq 15$



V. 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 2 (Task List): One can show full controllability by excluding 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 complex [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 complex, irreducible simple subalgebras can be excluded by treating the cases $\mathfrak{su}(\ell+1) \subsetneq \mathfrak{su}(N)$ ($\ell \geq 2$), $\mathfrak{so}(4\ell+2)$, and $\mathfrak{e}_6$ (see Section V-B). ■

In what follows, the plan is to make use of the fact that in Tab. I 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 $\mathfrak{e}_6$. It appears for systems of dimension 2^n that irreducible representations of $\mathfrak{e}_6$ can only link to $\mathfrak{su}(2^n)$ without being a subalgebra to an intermediate orthogonal or symplectic algebra. All complex, irreducible simple subalgebras shall be excluded by the promise that $\mathfrak{k} \subseteq \mathfrak{su}(2^n)$ represents a *physical* system of n spin-$\frac{1}{2}$ qubits containing at least one addressable qubit.

A. Symplectic and Orthogonal Subalgebras

In order to decide conjugation to irreducible subalgebras which are symplectic and orthogonal, recalling the following Lemma will prove useful to apply the lines of [59] in streamlined form.

Lemma 4: (1) Every unitary symmetric matrix $S = S^t \in \mathrm{Mat}_N$ is unitarily t-congruent to the identity, i.e. $S = T^t \mathbb{1} T$ with T unitary.

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

$$J := \begin{pmatrix} 0 & -\mathbb{1}_{N/2} \\ \mathbb{1}_{N/2} & 0 \end{pmatrix}. \tag{9}$$

Proof: (1) Follows by singular-value decomposition and goes back to Hua [60] (*ibid.*, Thm. 5). (2) Follows likewise from the same source ([60], Thm. 7). ■

Lemma 5: Suppose $\mathfrak{k} \subset \mathfrak{su}(N)$ is simple and J is defined as in Eqn. (9). 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 $SH + H^tS = 0$;

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

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

$$\begin{aligned} & LTHT^\dagger &=& -(THT^\dagger)^tL \\ \Leftrightarrow\quad & LTH &=& -\bar{T}H^tT^tLT \\ \Leftrightarrow\quad & (T^tLT)H &=& -H^t(T^tLT). \end{aligned}$$

The condition is sufficient ("⇒"):

(1) If $L = \mathbb{1}_N$ and $S = T^tT$ then $S\bar{S} = T^tTT^\dagger\bar{T} = +\mathbb{1}_N$. Thus $S = S^t$ is unitary, complex *symmetric* and satifies $SH = -H^tS$.

(2) If $L = J$ and $S = T^tJT$ then $S\bar{S} = T^tJTT^\dagger J\bar{T} = -\mathbb{1}_N$ by $J^2 = -\mathbb{1}_N$. Thus $S = -S^t$ is unitary, *skew-symmetric* and satifies $SH = -H^tS$.

The condition is necessary ("⇐") by Lemma 4, because with appropriate respective unitaries T

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

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

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

Input: Hamiltonians $I := \{iH_d; iH_1, \ldots, iH_m\} \subseteq \mathfrak{su}(N)$

1. For each Hamiltonian $H \in I$ determine all non-singular solutions to the homogeneous linear equation $\mathcal{S}_H := \{S \in SL(N) | SH + H^tS = 0\}$
2. $\mathcal{S} := \bigcap_{H\in I} \mathcal{S}_H$

Output:
- (a) $\exists S \in \mathcal{S}$ s.t. $S\bar{S} = +\mathbb{1} \Leftrightarrow \mathfrak{k} \subseteq \mathfrak{so}(N)$
- (b) $\exists S \in \mathcal{S}$ s.t. $S\bar{S} = -\mathbb{1} \Leftrightarrow \mathfrak{k} \subseteq \mathfrak{sp}(N/2)$
- (c) $\nexists S \in \mathcal{S} \Rightarrow \mathfrak{k} \not\subseteq \mathfrak{so}(N)$ and $\mathfrak{k} \not\subseteq \mathfrak{sp}(N/2)$

The cases (a) and (b) are mutually exclusive.

The complexity is roughly $\mathcal{O}(N^6)$, as in Liouville space N^2 equations have to be solved by LU decomposition.

In the context of filtering simple subalgebras, Lemma 5 can be turned into the powerful **Algorithm 3**. It boils down to checking a system of homogenous linear equations for solutions S satisfying $SH_\nu = -H_\nu^tS$ for *all* $iH_\nu \in \mathfrak{k}$ *simultaneously*: if S is a solution with $S\bar{S} = +\mathbb{1}$, 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 $S\bar{S} = -\mathbb{1}$, $\mathfrak{k}$ is conjugate to a subalgebra of $\mathfrak{sp}(N/2)$.

Remark 1: By irreducibility of $\mathfrak{k}$, those subgroups generated by $\mathfrak{k} \subset \mathfrak{su}(2^n)$ with a unitary representation equivalent to its complex conjugate are limited to orthogonal and symplectic ones: it follows from Schur's Lemma that $S\bar{S} = \pm\mathbb{1}$ are in fact *the only types of solutions* for $SH = -H^tS$ with $iH \in \mathfrak{k}$, as nicely explained in Lem. 3 of Ref. [59].

Conjugation to the symplectic algebras has also been treated in Ref. [50] by solving a system of linear equations, while Ref. [61] resorted to determining eigenvalues for discerning the unitary case from conjugate symplectic or orthogonal subalgebras.

The results can be summarised and extended as follows:

Theorem 2 (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 connectedness of the coupling graph) that $\mathfrak{k}$ is an irreducible representation of a simple Lie subalgebra to $\mathfrak{su}(N)$. If in addition **Algorithm 3** has but an empty 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 Lemma 5. The cases $\mathfrak{e}_7$, $\mathfrak{e}_8$, $\mathfrak{f}_4$, and $\mathfrak{g}_2$ follow from the elaborate classification of Malcev [58] (see, e.g., [55], [62],

[56]), as a representation of $\mathfrak{e}_8$, $\mathfrak{f}_4$, or $\mathfrak{g}_2$ is always conjugate to a subalgebra of $\mathfrak{so}(N)$, while a representation of $\mathfrak{e}_7$ is conjugate either to a subalgebra of $\mathfrak{so}(N)$ or of $\mathfrak{sp}(N/2)$. ■

B. Complex Subalgebras

It also follows from Malcev [58] that only the subalgebras $\mathfrak{su}(\ell+1)$ ($\ell \geq 2$), $\mathfrak{so}(4\ell+2)$, and $\mathfrak{e}_6$ can have representations of complex type. One can immediately deduce from the Tables I and II the following

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

We checked by explicit computations that $\mathfrak{e}_6$ does not occur as a complex, irreducible simple subalgebra of $\mathfrak{su}(2^n)$ for $n \leq 100$, i.e. for qubit systems with up to 100 qubits. Thus one might conjecture that $\mathfrak{e}_6$ does not occur as a complex, irreducible simple subalgebra for qubit systems in general.

C. System Algebras Comprising Local Actions $\mathfrak{su}(2)^{\oplus n}$

We now discuss the set of local unitary transformations $\mathrm{SU}(2)^{\otimes n} \subseteq \mathrm{SU}(2^n)$ 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 $\mathfrak{su}(2) \,\widehat{\oplus}\, \mathfrak{su}(2) \,\widehat{\oplus} \cdots \widehat{\oplus}\, \mathfrak{su}(2)$ (see Section III). What is the classification of $\mathfrak{su}(2)^{\oplus n}$ w.r.t. symplectic, orthogonal, and complex subalgebras? The answer to this question leads to a convenient necessary and sufficient criterion for full controllability. We obtain from Thm. 3 of Ref. [63] (see also [64], [65]):

Lemma 6: The algebra $\mathfrak{su}(2)^{\oplus n}$ (given in its standard representation) is a symplectic subalgebra of $\mathfrak{su}(2^n)$ [i.e. is conjugate to a subalgebra of $\mathfrak{sp}(2^{n-1})$] if n is odd, and an orthogonal subalgebra [i.e. is conjugate to a subalgebra of $\mathfrak{so}(2^n)$] if n is even. ■

As a consequence, a proper subalgebra $\mathfrak{k} \subsetneq \mathfrak{su}(2^n)$ that contains $\mathfrak{su}(2)^{\oplus n}$ (or one of its non-trivial subalgebras) cannot be complex. In particular, $\mathfrak{k}$ is symplectic (resp. orthogonal) if n is odd (resp. even).

Theorem 3: Consider a set of Hamiltonians $\{iH_\nu\}$ generating the dynamic algebra $\mathfrak{k} \subseteq \mathfrak{su}(2^n)$ for $n \geq 2$ with the promise (by **Algorithm 2** and connectedness of the coupling graph) that $\mathfrak{k}$ is an irreducible representation of a simple Lie subalgebra to $\mathfrak{su}(2^n)$. In addition, assume that $\mathfrak{k}$ contains a non-trivial subalgebra of $\mathfrak{su}(2)^{\oplus n}$, where $\mathfrak{su}(2)^{\oplus n}$ is given in its standard representation. If n is odd [resp. even], the control system is fully controllable if and only if $\mathfrak{k}$ is not conjugate to a subalgebra of $\mathfrak{sp}(N/2)$ [resp. $\mathfrak{so}(N)$]. This can be decided using **Algorithm 3**. ■

The above theorem states as a condition *that* $\mathfrak{k}$ *contains a subalgebra of* $\mathfrak{su}(2)^{\oplus n}$. An important case when this condition applies is the following: Assume we have a dynamic system of n spin-$\frac{1}{2}$ qubits. The Lie algebra $\mathfrak{su}(2)^{\oplus n}$ generates the set of local unitary transformations $\mathrm{SU}(2)^{\otimes n}$ and it describes a physical system where each spin-$\frac{1}{2}$ can be addressed independently (without the coupling). But even if not all qubits can be addressed independently (see Fig. 1), the dynamical algebra has to contain a subalgebra of $\mathfrak{su}(2)^{\oplus n}$. The same holds even in case when some (but not all) of the spins cannot be addressed at all.

Theorem 4 (Candidate Filter II): Given a set of Hamiltonians $\{iH_\nu\}$ generating the dynamic algebra $\mathfrak{k} \subseteq \mathfrak{su}(2^n)$ ($n \geq 2$) now with the promises that

(1) $\mathfrak{k}$ is a simple subalgebra of $\mathfrak{su}(2^n)$ and is given in an irreducible representation,
(2) $\mathfrak{k}$ is neither conjugate to a simple subalgebra of $\mathfrak{so}(2^n)$ nor of $\mathfrak{sp}(2^{n-1})$, and
(3) the physical system contains n spin-$\frac{1}{2}$ qubits (and at least one qubit can be addressed).

Then the system is fully controllable in the sense $\mathfrak{k} = \mathfrak{su}(2^n)$.

Proof: By (1) and (2), one may exploit Theorem 2 to cut the admissible candidate dynamic subalgebras down to $\mathfrak{su}(2^n)$ or one of its *complex*, irreducible simple subalgebras. However, by assumption (3), it follows from Theorem 3 that $\mathfrak{k}$ cannot be complex with the only exception $\mathfrak{k} = \mathfrak{su}(2^n)$. ■

Remark 2: Part of the proof of Theorem 4 may become more obvious in terms of spin physics: the $\{iH_\nu\}$ cannot generate a proper subalgebra $\mathfrak{su}(N') \subsetneq \mathfrak{su}(N)$ with $N' < N$ that is compatible with an irreducible n spin-$\frac{1}{2}$ representation, because a change in spin quantum number j and number of qubits n is ruled out by premiss (3). This is also illustrated next.

Note some further observations with regard to Tables I and II: The occurence 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 $j = \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$. Now to any such j there is an irreducible spin-j representation of the three PAULI matrices generating $\mathfrak{su}(2)_j$. For instance, in $\mathfrak{su}(4)$ there is an irreducible spin-$\frac{3}{2}$ representation of $\mathfrak{su}(2)$ as a proper *irreducible* subalgebra $\mathfrak{su}(2)_{j=3/2} \subsetneq \mathfrak{su}(4)$. — In contrast, the GELL-MANN basis to $\mathfrak{su}(2j+1)$ comprises a *reducible* representation of $\mathfrak{su}(2)$ as a subalgebra.

VI. 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 and *simple*. Now, conjugation to simple orthogonal or symplectic candidate subalgebras can again be decided solely on the basis of solving systems of linear equations. The final identification task is settled by generating a *complete* list of irreducible simple subalgebras of $\mathfrak{su}(N)$ compatible with the physical constituents as a dynamic pseudo-spin system.

To sum up, based on the *complete* list of simple subalgebras of $\mathfrak{su}(N)$ one can assess dynamic system algebras solely by solving systems of homogeneous linear equations. This avoids the usual and significantly more costly way of explicitly calculating Lie closures. 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 $\mathfrak{k}$:

(1) the system must not show any symmetry (i.e. $\mathfrak{k}$ must have a trivial centraliser $\mathfrak{k}'$),
(2) the coupling graph to its Hamiltonians must be connected,
(3) the system algebra $\mathfrak{k}$ must not be of symplectic or orthogonal type, and finally
(4) the system algebra $\mathfrak{k}$ must allow for a semi-simple subalgebra of local action $\mathfrak{su}(2)^{\oplus n}$.

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 detail in Ref. [1].

VII. Acknowledgement

This work was supported in part by the EU programmes QAP, Q-ESSENCE, and COQUIT, by the Bavarian excellence network ENB via the International Doctorate Programme of Excellence *Quantum Computing, Control, and Communication* (QCCC) as well as by the *Deutsche Forschungsgemeinschaft* (DFG) in the collaborative research centre SFB 631.

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