




# On the Refinement of Cartan Decomposition: An Implicit Commutative Substructure in $\mathfrak{su}(2^n)$

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**Abstract.** The Cartan decomposition of a semisimple Lie algebra is pivotal in both theoretical exploration and practical application. It generalizes the classical spectral, polar, and singular value decompositions found in linear algebra. This paper explores an advanced refinement of the Cartan decomposition of  $\mathfrak{su}(2^n)$ , arising from the parameterization of a Hamiltonian for quantum simulation. Specifically, given an **AI**-type Cartan decomposition  $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$  of any Lie subalgebra  $\mathfrak{g}$  in  $\mathfrak{su}(2^n)$ , where  $\mathfrak{p} = \tilde{\mathfrak{p}} \oplus \mathfrak{h}$  and  $\mathfrak{h}$  is the maximal abelian subalgebra in  $\mathfrak{p}$ , it is revealed that both the subalgebra  $\mathfrak{k}$  and the corresponding  $\tilde{\mathfrak{p}}$  (which is generally not a subalgebra) can further be partitioned, respectively, as the direct sums of equal-dimensional commutative Lie subalgebras. With respect to the involution  $\theta(g) = -g^\top$ , any Lie subalgebra  $\mathfrak{g}$  in  $\mathfrak{su}(2^n)$  with nondegenerate Cartan decomposition can thus be fully decomposed as the orthogonal direct sum of  $\mathfrak{h}$  and pairs of commutative Lie subalgebras over  $\mathfrak{k}$  and  $\tilde{\mathfrak{p}}$ , all of which, except  $\mathfrak{h}$ , share the same dimension.

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## 1. Motivation

The theoretical results presented in this paper have immediate application to the ever critically important Hamiltonian simulation problem (HSP) [11, 18, 20, 24, 32]. To provide a comprehensive understanding, we will briefly outline

the motivation behind this work. Readers who are primarily interested in the theoretical aspects may proceed directly to the next section.

Given a Hermitian matrix  $\mathcal{H}$  in  $\mathbb{C}^{2^n \times 2^n}$ , the HSP concerns computing the time evolution of unitary matrices

$$U(t) = e^{-i\mathcal{H}t}, \quad (1)$$

by a quantum machine. The matrix  $\mathcal{H}$  typically represents the time-invariant Hamiltonian in a physical system and the  $U(t)$  represents how the wave function evolves in time according to the Schrödinger equation. If the physical system is composed of  $n$  spin- $\frac{1}{2}$  particles, the size is necessarily of  $2^n \times 2^n$ . When  $n$  is large, the conventional ways of using floating-point arithmetic to compute this matrix exponential, such as the widely used scaled and squared Padé approximation [34, 35], are no longer feasible on classical computers because the simulation of general Hamiltonians grows exponentially. It has thus been proposed, notably by Feynman, to use a quantum computer as a possible solution [20, 32].

The Hamiltonian  $i\mathcal{H}$  in its original numerical expression, however, cannot be directly implemented on quantum machines. To address this, various approximation techniques have been proposed for simulating the unitary evolution [2, 12, 14, 17, 22, 28, 33, 40, 42]. One promising method involves parameterizing a given unitary transformation over an  $n$ -qubit system using Pauli strings [13, 19, 22, 29, 30, 37]. The core mechanism behind the parameterization is the Cartan decomposition which we briefly review below. Some basic properties of Pauli strings will be reviewed in Section 2. For now, we merely point out that the individual Pauli strings are readily quantum implementable, but not the  $i\mathcal{H}$  in the linear combination form of Pauli strings. Additional manipulation is required, which motivates the current work to complete the analysis.

Given a real semisimple Lie algebra  $\mathfrak{g}$ , an isomorphism  $\theta : \mathfrak{g} \rightarrow \mathfrak{g}$  that preserves the Lie bracket structure is called an automorphism. An automorphism whose square is equal to the identity is referred to as an *involution*. Involutions come in various forms, each tailored to specific mathematical applications. For our application, we employ the mapping [15, 26, 31]

$$\theta_1(g) := -g^\top, \quad (2)$$

as the involution. Let the eigenspaces corresponding to the eigenvalues  $+1$  and  $-1$  of  $\theta_1$  be denoted as  $\mathfrak{k}$  and  $\mathfrak{p}$ , respectively. It thus leads to a vector space decomposition of  $\mathfrak{g}$  as the direct sum

$$\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}. \quad (3)$$

This decomposition is referred to as a *Cartan decomposition*<sup>1</sup>, characterized by the commutation relations:

$$[\mathfrak{k}, \mathfrak{k}] \subseteq \mathfrak{k}, [\mathfrak{k}, \mathfrak{p}] \subseteq \mathfrak{p}, \text{ and } [\mathfrak{p}, \mathfrak{p}] \subseteq \mathfrak{k}. \quad (4)$$

The term “AI-type Cartan decomposition” is most commonly associated with the classical Lie algebra  $\mathfrak{su}(N)$  itself. In this case, under the involution  $\theta_1$ , we find the familiar splitting that  $\mathfrak{k} = \mathfrak{so}(N)$  and  $\mathfrak{p}$  consists of all symmetric, purely imaginary  $N \times N$  matrices of trace 0. When extending the notion of an AI-type Cartan decomposition to a general subalgebra  $\mathfrak{g}$  of  $\mathfrak{su}(N)$ , the decomposition is naturally interpreted through the eigenspace structure induced by the restricted map  $\theta_1|_{\mathfrak{g}}$ . For this eigenspace decomposition to be well-defined, it is essential that  $\mathfrak{g}$  remains invariant under the transpose operation. This invariance may not hold in general, but is guaranteed if  $N = 2^n$  and the generators of  $\mathfrak{g}$  are chosen to be either symmetric or skew-symmetric matrices, which is a condition naturally satisfied by Pauli strings.

We say that the Cartan decomposition (3) is nondegenerate if both  $\mathfrak{k} \neq \{0\}$  and  $\mathfrak{p} \neq \{0\}$ . The pair  $(\mathfrak{k}, \mathfrak{p})$  is often referred to as a Cartan pair of  $\mathfrak{g}$ . Obviously,  $\mathfrak{k}$  is a Lie subalgebra by itself, whereas any subalgebra within  $\mathfrak{p}$  is necessarily commutative. A maximal subalgebras  $\mathfrak{h}$  contained in  $\mathfrak{p}$  is referred to as a *Cartan subalgebra*. Given a Cartan subalgebra  $\mathfrak{h} \subset \mathfrak{p}$ , let  $\tilde{\mathfrak{p}}$  denote its orthogonal complementary subspace in  $\mathfrak{p}$ . Thus, we may write the direct sum

$$\mathfrak{g} = \mathfrak{k} \oplus \tilde{\mathfrak{p}} \oplus \mathfrak{h}. \quad (5)$$

Corresponding to the Lie subalgebra  $\mathfrak{k}$  in a Cartan pair  $(\mathfrak{k}, \mathfrak{p})$ , let  $\mathfrak{K} = e^{\mathfrak{k}}$  denote the associated Lie subgroup. For a fixed group element  $K \in \mathfrak{K}$ , define the inner automorphism  $\text{Ad}_K : \mathfrak{g} \rightarrow \mathfrak{g}$  via the conjugation map

$$\text{Ad}_K(g) = KgK^{-1}. \quad (6)$$

The following theorem summarizes three main results in the general theory of Cartan decomposition [26, 31, 41].

**Theorem 1.** *Suppose that  $\mathfrak{g}$  is a semisimple Lie algebra with a nondegenerate Cartan decomposition (3). Then*

<sup>1</sup>In some references, e.g., [25, Page 185], [41, Page 202], and the Maple implementation [1], a Cartan decomposition is defined with additional constraints. It involves using the Cartan involution, which is an involutive automorphism on  $\mathfrak{g}$  such that the bilinear form  $B_{\theta}(\mathbf{x}, \mathbf{y}) := -B(\mathbf{x}, \theta(\mathbf{y}))$  is positive definite, where  $B(\mathbf{x}, \mathbf{y}) := \text{trace}(\text{ad}(\mathbf{x}) \circ \text{ad}(\mathbf{y}))$  denotes the Killing form on  $\mathfrak{g}$ . Additionally, it requires that the restricted Killing forms  $B|_{\mathfrak{k}}$  and  $B|_{\mathfrak{p}}$  are negative definite and positive definite, respectively. For a compact semisimple algebra such as  $\mathfrak{su}(N)$ , however, the identity map is the sole Cartan involution, resulting in a trivial Cartan decomposition. This triviality renders it useless for our applications. The decomposition (3), using (2) as the involution over  $\mathfrak{su}(N)$ , is referred to as the AI-type Cartan decomposition [25, Page 451].

1. Let  $\mathfrak{h}$  be a fixed Cartan subalgebra. Then the subset  $\mathfrak{p}$  can be split as the union

$$\mathfrak{p} = \bigcup_{K \in \mathfrak{K}} \text{Ad}_K(\mathfrak{h}), \quad (7)$$

2. If  $\widehat{\mathfrak{h}}$  is another Cartan subalgebra in  $\mathfrak{p}$ , then

$$\widehat{\mathfrak{h}} = \text{Ad}_K(\mathfrak{h}) \quad (8)$$

for some  $K \in \mathfrak{K}$ .

3. (KAK decomposition) For every group element  $X \in e^{\mathfrak{g}}$ , there exist group elements  $K_1, K_2 \in e^{\mathfrak{k}}$  and  $A \in e^{\mathfrak{h}}$  such that

$$X = K_1 A K_2. \quad (9)$$

Several observations are noteworthy. While all Cartan subalgebra are achievable via conjugations, note that the splitting (7) of  $\mathfrak{p}$  is not a direct sum of disjoint commutative subalgebras. We may also regard the KAK decomposition (9) of a general group element  $X$  as a generalization of its singular value decomposition (SVD).

When applying the Cartan theory to the HSP of an  $n$ -particle system, we focus on the Lie algebra  $\mathfrak{su}(2^n)$ . Indeed, since the theory holds in any semi-simple Lie algebra, it suffices to work within the subalgebra  $\mathfrak{g}(\mathcal{H})$ , defined as the closure involving all terms of a given Hermitian matrices  $\mathcal{H}$  under the commutator. Recently, there has been considerable research interest in classifying the dynamical Lie subalgebras  $\mathfrak{g}(\mathcal{H})$  associated with certain specified Hamiltonian systems [30, 43]. We are interested in generating  $\mathfrak{g}(V)$  for an arbitrary subset  $V \subset \mathfrak{su}(2^n)$ .

If  $\mathcal{H} \in \mathfrak{p}$ , then by (7) there exist  $\kappa \in \mathfrak{k}$  and  $\eta \in \mathfrak{h}$  such that

$$-\mathcal{H} = e^{\kappa} \eta e^{-\kappa}. \quad (10)$$

The relationship (10) resembles the classical spectral decomposition of the matrix  $-\mathcal{H}$ , except for the difference that  $\eta$  is not necessarily diagonal. It follows that the unitary synthesis can be realized from

$$e^{-\mathcal{H}t} = e^{\kappa} e^{\eta t} e^{-\kappa}. \quad (11)$$

In this way,  $\mathcal{H}$  has been parameterized by  $(\kappa, \eta)$  [29, 30, 37]. Observe that the commutativity of  $\mathfrak{h}$  ensures that the exponential  $e^{\eta t}$  on the right-hand side of (11) is readily implementable on quantum circuits. Since  $\mathfrak{k}$  is itself an algebra, we can repeat the process to break down the exponential  $e^{\kappa}$  in a similar way. If we can control the precision in computing  $\kappa \in \mathfrak{k}$  and  $\eta \in \mathfrak{h}$ , then the product on the right-hand side of (11) is a successful synthesis of  $e^{-\mathcal{H}t}$  for a quantum machine.

Identifying the decomposition (10), however, is as challenging as determining the spectral decomposition of  $-\mathcal{H}$ , which is precisely what is prohibited in the first place. Achieving the decomposition (10) without invoking spectral decomposition and, in fact, working with only the linear combination

coefficients of Pauli strings as variables, circumventing the involvement of any matrices of size  $2^n \times 2^n$  per se, represents a significant advancement in this area. That is exactly what we have proposed to do in an earlier paper [9] using the Lax dynamics to accomplish such a task. Without delving into great length, we synopsise that, if the variables  $\alpha := [\alpha_1, \dots, \alpha_r]^\top$ ,  $\beta := [\beta_1, \dots, \beta_s]^\top$  represents the linear combination coefficients of a flow  $x(t)$  in  $\mathfrak{g}(\mathcal{H})$  in terms of the basis of the Cartan decomposition, then the Lax dynamics appears in the form

$$\begin{cases} \dot{\alpha} = A(\beta)\alpha + f(\alpha), \\ \dot{\beta} = g(\alpha), \end{cases} \quad (12)$$

where  $f$  and  $g$  are homogeneous quadratic polynomials in  $\alpha$ , and  $A(\beta)$  is a matrix of size  $r \times r$  depending linearly in  $\beta$ . Here,  $\beta$  acts as a control variable, with  $g$  chosen to drive  $\alpha$  to zero. A more detailed description of the framework can be found in [10]. The solution of the Lax dynamics, traceable numerically by modern ODE techniques to high precision [27, 36, 38], is a generalization of earlier works on Toda lattice for the spectral decomposition [4–8].

In our exploration of the asymptotic behavior of the resulting Lax dynamics and its convergence to the desired decomposition (10), we uncover an interesting internal structure inherited in  $(\mathfrak{k}, \tilde{\mathfrak{p}})$ . This structure that the pair  $(\mathfrak{k}, \tilde{\mathfrak{p}})$  can be classified into pairs of orthogonal commutative subalgebras of equal dimensions is instrumental in characterizing the eigenvalues of  $A(\beta)$  which are crucial to our convergence analysis for the dynamics (12).

A well-known fact is that any subalgebra of  $\mathfrak{su}(N)$  is either abelian or a direct sum of compact simple Lie algebras and a center [16, 31]. It is remarkable that this commutative substructure, appearing as an orthogonal direct sum of commutative subalgebras, actually exists in the **AI**-type Cartan pair of any Lie subalgebra of  $\mathfrak{su}(2^n)$ . To the best of our knowledge, such a refined decomposition has not been previously documented in the literature. We thus think that a focused report on this structure in this paper might merit some attention.

Our theory below actually provides an algorithmic way to generate these hidden commutative subalgebras. The result can be interpreted as a matrix reordering for the commutator table of  $\mathfrak{g}$ , ensuring zero diagonal blocks due to commutativity.

This paper is organized as follows. Introduced in Section 2 is a mechanism that encodes each Pauli string into a unique integer, which can also be decoded to reveal the Pauli string's composition. This encoding not only orders Pauli strings systematically but also characterizes any subalgebra within  $\mathfrak{su}(2^n)$  by a subset of integers. Our main result is detailed in Section 3. We prove through a delicate argument that the basis of the subspace  $\tilde{\mathfrak{p}}$  can be partitioned into disjoint subsets, each spanning an abelian subalgebra. For each such subalgebra in  $\tilde{\mathfrak{p}}$ , there exists a corresponding abelian subalgebra in  $\mathfrak{k}$  of the same dimension, whose basis forms a disjoint partitioning of the basis of

†. In contrast to the splitting (7) for  $\mathfrak{p}$  where the Cartan subalgebras  $\text{Ad}_K(\mathfrak{h})$ ,  $K \in e^\mathfrak{k}$ , might overlap, we achieve an orthogonal direct sum of abelian subalgebras for  $\mathfrak{g}$ . Two examples are presented in Section 4 that should clearly illustrate this commutative structure.

## 2. Computing Dynamical Lie Subalgebras

Within the Lie algebra  $\mathfrak{su}(2^n)$ , we are particularly interested in the Cartan decomposition of its dynamical Lie subalgebra  $\mathfrak{g}(V)$ , abbreviated as  $\mathfrak{g}$  henceforth, under the involution (2). The focus of this paper is on the proof that the entire algebra  $\mathfrak{g}$  can be fully decomposed as the direct sum of commutative subalgebras. To achieve this goal, we choose the Pauli strings (multiplied by  $\imath$ ) as a special basis for  $\mathfrak{su}(2^n)$ .

The Pauli matrices,

$$X := \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}; \quad Y := \begin{bmatrix} 0 & -\imath \\ \imath & 0 \end{bmatrix}; \quad Z := \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad (13)$$

are Hermitian, unitary, and of trace zero. Together with the identity matrix  $I$ , an element in the set  $\{X, Y, Z, I\}^{\otimes n}$ , i.e., a tensor product of  $n$  matrices selected from the set  $\{X, Y, Z, I\}$ , is referred to as a Pauli string. Elements in  $\{X, Y, Z, I\}^{\otimes n}$  are mutually orthogonal with respect to the Frobenius inner product over  $\mathbb{C}^{2^n \times 2^n}$ , so they span all possible  $2^n \times 2^n$  Hermitian matrices. With a multiplication by the imaginary number  $\imath$  to the Pauli strings and by removing the element  $\imath I^{\otimes n}$  from the basis, we now have a mutually orthogonal basis for the Lie algebra  $\mathfrak{su}(2^n)$  which is of real dimension  $4^n - 1$ .

The Pauli matrices are the most fundamental single-qubit operators in a quantum system because, when exponentiated, they give rise to rotation matrices describing the gyration of a spin- $\frac{1}{2}$  particle around the coordinate axes [39]. The Pauli matrices satisfy the relationships

$$X * X = Y * Y = Z * Z = -\imath X * Y * Z = I, \quad (14)$$

where, for clarity, we have denoted the matrix multiplication by  $*$  to distinguish it from the Kronecker product  $\otimes$  whose writing is often suppressed. These are sufficient to establish other cyclic relationships such as  $X * Y = \imath Z = -Y * X$ ,  $Y * Z = \imath X = -Z * Y$ ,  $Z * X = \imath Y = -X * Z$ , and so on.

Let  $B_\ell$ ,  $\ell = 1, \dots, 4^n$ , denote elements in  $\{X, Y, Z, I\}^{\otimes n}$  multiplied by the imaginary number  $\imath$ . There are  $4^n$  Pauli strings. Each  $B_\ell$  is of size  $2^n \times 2^n$ . It is certainly desired to avoid forming such a large matrix explicitly, not to mention carrying out the Lie bracket formally. To effectively characterize a Lie subalgebra in term of its basis, we introduce the Fraktur numerals  $\mathfrak{1}, \mathfrak{2}, \mathfrak{3}, \mathfrak{4}$  to represent both the symbols of  $X, Y, Z, I$  and the digits in the quaternary numeral system (where 0 is replaced by 4). Every element in  $\{X, Y, Z, I\}^{\otimes n}$  has a unique  $n$ -digit ID

$$\mathfrak{d}_n \otimes \mathfrak{d}_{n-1} \otimes \dots \otimes \mathfrak{d}_1 \Rightarrow \mathfrak{d}_n \mathfrak{d}_{n-1} \dots \mathfrak{d}_1, \quad \mathfrak{d}_j \in \{\mathfrak{1}, \mathfrak{2}, \mathfrak{3}, \mathfrak{4}\},$$

which can be translated into a unique ordinal number  $\ell$  via

$$\ell := \sum_{j=1}^n 4^{j-1}(\mathfrak{d}_j - 1) + 1, \quad (15)$$

and vice versa.

This encoding offers the immediate advantage of representing a  $2^n \times 2^n$  Pauli string by a single integer, regardless of the potentially large value of  $n$ . It also provides a systematic way to order Pauli strings, which serves as an effective tool for characterizing any subalgebra in  $\mathfrak{su}(2^n)$  by a subset of integers. Apart from the additional scalar multiplication by  $\imath$ , the same conversion can be applied to encode  $B_\ell$  by the single integer  $\ell$ , and decode the integer  $\ell$  to reveal the content of  $B_\ell$ .

One of the advantages of employing the Pauli strings as the basis is their exchangeability under the Lie bracket [9].

**Lemma 2.** *If the commutator  $[B_i, B_j]$  of two distinct  $B_i, B_j$  is not zero, then  $[B_i, B_j] = cB_k$  for some  $k \neq i$  or  $j$ , and  $c$  is either 2 or -2. In this case, it is also true that  $[B_j, B_k] = cB_i$  and  $[B_k, B_i] = cB_j$ . The proportional constants  $c$ , known as the structure constants, depends on the makeup of the Pauli strings.*

Suppose that the Pauli string  $B_i$  is expressed in terms of its  $n$ -digit ID as  $B_i = \imath \mathfrak{d}_{i_n} \dots \mathfrak{d}_{i_1}$ , where  $\mathfrak{d}_{i_k} \in \{1, 2, 3, 4\}$  for  $k = 1, \dots, n$ . Then the commutator  $[B_i, B_j]$  is given by

$$\begin{aligned} [B_i, B_j] &= -((\mathfrak{d}_{i_n} \dots \mathfrak{d}_{i_1}) * (\mathfrak{d}_{j_n} \dots \mathfrak{d}_{j_1}) - (\mathfrak{d}_{j_n} \dots \mathfrak{d}_{j_1}) * (\mathfrak{d}_{i_n} \dots \mathfrak{d}_{i_1})) \\ &= -((\mathfrak{d}_{i_n} * \mathfrak{d}_{j_n}) \dots (\mathfrak{d}_{i_1} * \mathfrak{d}_{j_1}) - (\mathfrak{d}_{j_n} * \mathfrak{d}_{i_n}) \dots (\mathfrak{d}_{j_1} * \mathfrak{d}_{i_1})), \end{aligned} \quad (16)$$

By (14), each of the matrix-to-matrix multiplications  $\mathfrak{d}_{i_k} * \mathfrak{d}_{j_k}$ ,  $k = 1, \dots, n$ , can be looked up from Table 1.

Furthermore, since the products  $\mathfrak{d}_{i_k} * \mathfrak{d}_{j_k}$  and  $\mathfrak{d}_{j_k} * \mathfrak{d}_{i_k}$  differ by at most a negative sign, the two terms on the right side of (16) are essentially the same. We have either  $[B_i, B_j] = 0$  or  $[B_i, B_j] = -2(\mathfrak{d}_{i_n} * \mathfrak{d}_{j_n}) \dots (\mathfrak{d}_{i_1} * \mathfrak{d}_{j_1})$ . The  $n$ -digit ID of the bracket  $[B_i, B_j]$  is thus completely determined, without executing any matrix or tensor multiplications at all.

TABLE 1. Matrix-to-matrix multiplication table of  $\{X, Y, Z, I\}$

*	1	2	3	4
1	4	$\imath 3$	$-\imath 2$	1
2	$-\imath 3$	4	$\imath 1$	2
3	$\imath 2$	$-\imath 1$	4	3
4	1	2	3	4

The process described efficiently computes the Lie bracket with minimal index retrievals or swaps. Through encoding and decoding the associated ordinal numbers, this method is instrumental in generating the dynamical Lie subalgebra  $\mathfrak{g}(V)$ , the smallest subalgebra for arbitrary subset  $V \subset \mathfrak{g}(2^n)$ . No actual matrices are ever formed. This technique can also be employed to perform the **AI**-type Cartan decomposition effectively, as will be demonstrated in our examples. Our **Matlab** code is available to interested readers.

### 3. Commutative Substructure Within the Cartan Pair

Suppose that a Lie subalgebra  $\mathfrak{g}$  in  $\mathfrak{su}(2^n)$  is in hand. We now begin to discuss our major result concerning the additional structure within the pair  $(\mathfrak{k}, \tilde{\mathfrak{p}})$  associated with a given Cartan pair  $(\mathfrak{k}, \mathfrak{p})$  of  $\mathfrak{g}$ .

**Theorem 3.** *Suppose that a semisimple Lie algebra  $\mathfrak{g}$  has a nondegenerate Cartan decomposition (5). Then  $\dim(\mathfrak{k}) = \dim(\tilde{\mathfrak{p}})$ .*

*Proof.* The parameters needed to determine each of the matrix exponentials in the KAK decomposition (9) are precisely those in the associated subalgebras. We may thus count the numbers of parameters. On one hand, we observe from (5) that the dimension of the Lie algebra decomposes as  $\dim(\mathfrak{g}) = \dim(\mathfrak{k}) + \dim(\mathfrak{p}) + \dim(\mathfrak{h})$ . On the other hand, the alternative decomposition given by (9) yields  $\dim(\mathfrak{g}) = \dim(\mathfrak{k}) + \dim(\mathfrak{h}) + \dim(\tilde{\mathfrak{p}})$ . Comparing these two expressions, we deduce that  $\dim(\mathfrak{k}) = \dim(\tilde{\mathfrak{p}})$ .  $\square$

Denote the basis in each subspace as

$$\tilde{\mathfrak{p}} = \text{span}\{\tilde{p}_1, \dots, \tilde{p}_r\}; \quad \mathfrak{h} = \text{span}\{h_1, \dots, h_s\}; \quad \mathfrak{k} = \text{span}\{k_1, \dots, k_r\}, \quad (17)$$

respectively, where we may assume that these basis elements are in the form of  $B_\ell$  with suitable subsets of  $\ell = 1, \dots, 4^n$ . The inclusion relationship between any two of the three subspaces  $\mathfrak{k}$ ,  $\tilde{\mathfrak{p}}$  and  $\mathfrak{h}$  under the Lie bracket operation is listed in Table 2. Of particularly importance is the fact that [9]

$$[\mathfrak{h}, \mathfrak{k}] \subset \tilde{\mathfrak{p}}. \quad (18)$$

By Lemma 2, it suffices to characterize the relationships by considering only the transitions among the Pauli strings, that is,  $[h_\alpha, k_\beta] = c\tilde{p}_\gamma$  and so on.

TABLE 2. Inclusion of subsets  $\mathfrak{k}, \tilde{\mathfrak{p}}$  and  $\mathfrak{h}$  under Lie bracket

$[\cdot, \cdot]$	$\mathfrak{k}$	$\tilde{\mathfrak{p}}$	$\mathfrak{h}$
$\mathfrak{k}$	$\mathfrak{k}$	$\mathfrak{p}$	$\tilde{\mathfrak{p}}$
$\tilde{\mathfrak{p}}$	$\tilde{\mathfrak{p}}$	$\mathfrak{k}$	$\mathfrak{k}$
$\mathfrak{h}$	$\tilde{\mathfrak{p}}$	$\mathfrak{k}$	0



Introduce the index subsets

$$\mathfrak{H}_j := \{\ell | [h_j, k_\ell] \neq 0\}, \quad j = 1, \dots, s.$$

Based on (18), we may define the injective map  $\phi_j : \mathfrak{H}_j \rightarrow \{1, \dots, r\}$  such that  $\phi_j(\ell)$  is the unique integer satisfying the relationship

$$[h_j, k_\ell] = -c_{j\ell} \tilde{p}_{\phi_j(\ell)} \quad (19)$$

with the structure constant  $c_{j\ell} = \pm 2$ . By Lemma 2, it follows that

$$[\tilde{p}_{\phi_j(\ell)}, k_\ell] = c_{j\ell} h_j. \quad (20)$$

Building upon (19), we turn our attention to the dynamics in the entire commutator table  $[\mathfrak{h}, \mathfrak{k}]$ . In particular, we want to study on how clusters of  $\tilde{p}_i$ 's can be produced by using identical subsets of  $h_j$ 's and  $k_\ell$ 's in various combinations.

### 3.1. Basic Tools

For each  $i = 1, \dots, r$ , define the index-ordered set

$$\mathfrak{L}_i := \uplus \{\ell | \phi_j(\ell) = i, \text{ for some } 1 \leq j \leq s\} \quad (21)$$

where  $\uplus$  is meant to indicate that elements  $\ell$  are arranged in the ascending order. Correspondingly, let

$$\mathfrak{J}_i := \uplus \{j | \phi_j^{-1}(i) \neq \emptyset\}, \quad (22)$$

be the index subset ordered according to that in  $\mathfrak{L}_i$ . The ordering will be used later, when specifying the position of that particular element matters; otherwise,  $\mathfrak{J}_i$  and  $\mathfrak{L}_i$  can simply represent subsets of integers without ambiguity. For a fixed  $i$ , consider the collection of all the pairs  $(j_\tau, \ell_\tau)$ ,  $j_\tau \in \mathfrak{J}_i$  and  $\ell_\tau \in \mathfrak{L}_i$ , ordered by  $\tau$ . By definition,  $\phi_{j_\tau}(\ell_\tau) = i$  for all  $\tau$ .

It is helpful to recognize that the index-ordered sets  $\mathfrak{L}_i$  and  $\mathfrak{J}_i$  correspond to the column and row indices where the specified  $\tilde{p}_i$  occurs in the  $[\mathfrak{h}, \mathfrak{k}]$  table. Analyzing the underlying structure involves significant mathematical manipulation. Two key lemmas are essential tools frequently employed in this analysis. The first lemma is a reformulation of the Jacobi identity, adapted here in an associative format for our needs. The second lemma facilitates the rearrangement of indices to another element within the  $[\mathfrak{h}, \mathfrak{k}]$  table.

**Lemma 4** (*Associative property*). *Given any three elements  $\Gamma, \Delta$  and  $\Theta$  in a Lie algebra, the identity*

$$[[\Gamma, \Delta], \Theta] = [\Gamma, [\Delta, \Theta]] - [\Delta, [\Gamma, \Theta]] \quad (23)$$

*always holds.*

Recall that the notations  $\mathfrak{J}_i$  and  $\mathfrak{L}_i$  denote ordered index sets. To clarify their association with  $\tilde{p}_i$ , we label their elements with superscripts such as  $j_\mu^{(i)}$ ,  $\ell_\eta^{(i)}$ , where the subscripts  $\mu$  and  $\eta$  refer to their ordinal numbers within

TABLE 3. Crossover relationships guaranteed by Lemma 5

...	$\widetilde{p}_a$	...	$\widetilde{p}_b$	...	$\widetilde{p}_\gamma$	...	$\widetilde{p}_i$	
$\vdots$	...	$\vdots$	...	$\vdots$	...	$\vdots$	$\vdots$	
$h_{j_\zeta}$	...	$h_{j_\nu}$	...	$h_{j_\mu}$	...	$h_{j_\eta}$	$k_{\ell_\eta}$	
$\vdots$	...	$\vdots$	...	$\vdots$	...	$\vdots$	$\vdots$	
$h_{j_\eta}$	...	$h_{j_\mu}$	...	$h_{j_\nu}$	...	$h_{j_\zeta}$	$k_{\ell_\zeta}$	
$\vdots$	...	$\vdots$	...	$\vdots$	...	$\vdots$	$\vdots$	

the respective ordered sets. By definition, when  $(j_\mu^{(i)}, \ell_\mu^{(i)})$  is paired together, it holds that

$$[h_{j_\mu^{(i)}}, k_{\ell_\mu^{(i)}}] = -c_{j_\mu^{(i)} \ell_\mu^{(i)}} \widetilde{p}_i, \quad (24)$$

with  $c_{j_\mu^{(i)} \ell_\mu^{(i)}} = \pm 2$  for all  $j_\mu^{(i)} \in \mathfrak{J}_i$  and  $\ell_\mu^{(i)} \in \mathfrak{L}_i$ . When  $i$  is fixed and there is no cause of ambiguity, we may omit the superscript  $(i)$  for simplicity.

**Lemma 5** (*Crossover property*). *For a fixed  $1 \leq i \leq r$ , suppose that indices  $j_\mu, j_\nu \in \mathfrak{J}_i$  and  $\ell_\eta, \ell_\zeta \in \mathfrak{L}_i$ , are such that  $\widetilde{p}_{\phi_{j_\mu}(\ell_\eta)} = \widetilde{p}_{\phi_{j_\nu}(\ell_\zeta)} = \widetilde{p}_\gamma$  for some  $\gamma$ . Then the identity*

$$[h_{j_\mu}, k_{\ell_\zeta}] = \pm [h_{j_\nu}, k_{\ell_\eta}] \quad (25)$$

holds. In particular,

$$[h_{j_\eta}, k_{\ell_\zeta}] = \pm [h_{j_\zeta}, k_{\ell_\eta}] \quad (26)$$

always holds for any  $\eta$  and  $\zeta$ .

*Proof.* By definitions and Lemma 4, we observe that

$$\begin{aligned} [h_{j_\mu}, k_{\ell_\zeta}] &= -\frac{1}{c_{j_\nu \ell_\zeta}} [h_{j_\mu}, [\widetilde{p}_\gamma, h_{j_\nu}]] = -\frac{1}{c_{j_\nu \ell_\zeta}} \{[h_{j_\nu}, [\widetilde{p}_\gamma, h_{j_\mu}]] - [\widetilde{p}_\gamma, [h_{j_\nu}, h_{j_\mu}]]\} \\ &= \frac{c_{j_\mu \ell_\eta}}{c_{j_\nu \ell_\zeta}} [h_{j_\nu}, k_{\ell_\eta}], \end{aligned} \quad (27)$$

where we have used the fact that  $\mathfrak{h}$  is commutative. Note that the ratio  $\frac{c_{j_\mu \ell_\eta}}{c_{j_\nu \ell_\zeta}}$  is either 1 or -1. The identity (26) follows from taking the special case  $\mu = \eta$  and  $\nu = \zeta$ .  $\square$

The identities in Lemma 5, particularly the relationship (27), can be conveniently expressed as in Table 3, which reads as the bracket product of  $h_j$  with the rightmost  $k_\ell$  in the same row results in a scalar multiplication  $\pm 2$  of the particular  $\widetilde{p}_{\phi_j(\ell)}$  directly above that  $h_j$ . The boxed quantities represent the conditions stipulated in the lemma.

### 3.2. Structure Analysis

Assuming that the Cartan decomposition of a subalgebra  $\mathfrak{g}$  has been established, we now delve into its substructure for further insights. The proof of this theory is complex, which may partly explain the previous challenges in understanding this substructure. For clarity, we derive a series of results that collectively delineate the intrinsic structures within the pair  $(\mathfrak{k}, \tilde{\mathfrak{p}})$ . Our aim is to reach the summary at the end of this section, which encapsulates the essence of this commutative substructure. The two worked-out examples given in Section 4 also help demonstrate this substructure.

To begin, we analyze the arrangement of zero elements within the  $[\mathfrak{h}, \mathfrak{k}]$  table by examining its rows.

**Lemma 6.** *There exists  $h_\sigma \in \mathfrak{h}$  such that  $[h_\sigma, k_{\ell_\eta}] = 0$  for some  $\ell_\eta \in \mathfrak{L}_i$  if and only if  $[\tilde{p}_i, h_\sigma] = 0$ . In this case,  $[h_\sigma, k_{\ell_\zeta}] = 0$  for all  $\ell_\zeta \in \mathfrak{L}_i$ .*

*Proof.* Observe first that

$$\begin{aligned} [\tilde{p}_i, h_\sigma] &= -\frac{1}{c_{j_\eta k_\eta}} [[h_{j_\eta}, k_{\ell_\eta}], h_\sigma] = -\frac{1}{c_{j_\eta k_\eta}} \{[h_{j_\eta}, [k_{\ell_\eta}, h_\sigma]] - [k_{\ell_\eta}, [h_{j_\eta}, h_\sigma]]\} \\ &= -\frac{1}{c_{j_\eta k_\eta}} [h_{j_\eta}, [k_{\ell_\eta}, h_\sigma]], \end{aligned}$$

where the second term in the second equation is zero due to the commutative nature of  $\mathfrak{h}$ . The identity can go in either direction, so the first claim is proved. Observe next that

$$[h_\sigma, k_{\ell_\zeta}] = -\frac{1}{c_{j_\zeta k_\zeta}} [h_\sigma, [\tilde{p}_i, h_{j_\zeta}]] = -\frac{1}{c_{j_\zeta k_\zeta}} \{[h_{j_\zeta}, [\tilde{p}_i, h_\sigma]] - [\tilde{p}_i, [h_{j_\zeta}, h_\sigma]]\} = 0.$$

The second claim follows.  $\square$

The implication of Lemma 6 is worth noting.

**Corollary 7.** *If  $h_\sigma \in \mathfrak{h}$  is such that  $[h_\sigma, k_{\ell_\eta}] \neq 0$  for some  $\ell_\eta \in \mathfrak{L}_i$ , then it must be that  $\sigma \in \mathfrak{J}_i$ , and that  $[h_\sigma, k_{\ell_\zeta}]$  is a nontrivial element in  $\tilde{\mathfrak{p}}$  for every  $\ell_\zeta \in \mathfrak{L}_i$ .*

Choose an arbitrary index  $j_\tau \in \mathfrak{J}_i$ . By definition, we already have  $[h_{j_\tau}, k_{\ell_\tau}] = -c_{j_\tau \ell_\tau} \tilde{p}_i \neq 0$ . It follows that  $[h_{j_\tau}, k_{\ell_\zeta}] \neq 0$  for any  $\ell_\zeta \in \mathfrak{L}_i$ . For each fixed  $1 \leq i \leq r$ , define the sets

$$\mathfrak{p}_i := \{\tilde{p}_{\phi_{j_\tau}(\ell_\zeta)} | j_\tau \in \mathfrak{J}_i, \ell_\zeta \in \mathfrak{L}_i\}, \quad (28)$$

$$\mathfrak{k}_i := \{k_{\ell_\zeta} | \ell_\zeta \in \mathfrak{L}_i\}. \quad (29)$$

We now explore the structure within  $\mathfrak{p}_i$  and  $\mathfrak{k}_i$ . Our analysis aims to achieve three key objectives: first, to show that each  $\mathfrak{p}_i$  or  $\mathfrak{k}_i$ ,  $1 \leq i \leq r$ , spans a commutative subalgebra under the Lie bracket; second, to identify and describe any overlaps among these sets; and finally, to elucidate how they collectively decompose  $\mathfrak{k}$  and  $\tilde{\mathfrak{p}}$ .

**Theorem 8.** For a fixed  $1 \leq i \leq r$ , the subspace spanned by  $\mathfrak{k}_i$  is a commutative subalgebra of  $\mathfrak{k}$ .

*Proof.* If  $\mathfrak{k}_i$  contains only one basis element, then it is trivially true. Suppose  $\ell_\eta \neq \ell_\zeta$  are two distinct elements in  $\mathfrak{L}_i$ . Then there exist  $h_{j_\eta}$  and  $h_{j_\zeta}$  such that

$$[h_{j_\eta}, k_{\ell_\eta}] = -c_{j_\eta \ell_\eta} \tilde{p}_i, \quad [h_{j_\zeta}, k_{\ell_\zeta}] = -c_{j_\zeta \ell_\zeta} \tilde{p}_i.$$

On the one hand, observe that we have

$$\begin{aligned} [k_{\ell_\eta}, k_{\ell_\zeta}] &= -\frac{1}{c_{j_\eta \ell_\eta}} [[\tilde{p}_i, h_{j_\eta}], k_{\ell_\zeta}] = -\frac{1}{c_{j_\eta \ell_\eta}} \{[\tilde{p}_i, [h_{j_\eta}, k_{\ell_\zeta}]] - [h_{j_\eta}, [\tilde{p}_i, k_{\ell_\zeta}]]\} \\ &= -\frac{1}{c_{j_\eta \ell_\eta}} [\tilde{p}_i, [h_{j_\eta}, k_{\ell_\zeta}]]. \end{aligned}$$

If  $[h_{j_\eta}, k_{\ell_\zeta}] = 0$ , then we are done; otherwise, by the notation defined in (19) we may write that

$$[h_{j_\eta}, k_{\ell_\zeta}] = -c_{j_\eta \ell_\zeta} \tilde{p}_{\phi_{j_\eta}(\ell_\zeta)},$$

and thus

$$[k_{\ell_\eta}, k_{\ell_\zeta}] = \frac{c_{j_\eta \ell_\zeta}}{c_{j_\eta \ell_\eta}} [\tilde{p}_i, \tilde{p}_{\phi_{j_\eta}(\ell_\zeta)}].$$

On the other hand, by using the same argument for (25), observe that

$$[h_{j_\zeta}, k_{\ell_\eta}] = \frac{c_{j_\zeta \ell_\zeta}}{c_{j_\eta \ell_\eta}} [h_{j_\eta}, k_{\ell_\zeta}] = -\frac{c_{j_\zeta \ell_\zeta} c_{j_\eta \ell_\zeta}}{c_{j_\eta \ell_\eta}} \tilde{p}_{\phi_{j_\eta}(\ell_\zeta)}.$$

It follows that we also have

$$\begin{aligned} [k_{\ell_\eta}, k_{\ell_\zeta}] &= -\frac{1}{c_{j_\zeta \ell_\zeta}} [[h_{j_\zeta}, \tilde{p}_i], k_{\ell_\eta}] = -\frac{1}{c_{j_\zeta \ell_\zeta}} \{[h_{j_\zeta}, [\tilde{p}_i, k_{\ell_\eta}]] - [\tilde{p}_i, [h_{j_\zeta}, k_{\ell_\eta}]]\} \\ &= \frac{1}{c_{j_\zeta \ell_\zeta}} [\tilde{p}_i, [h_{j_\zeta}, k_{\ell_\eta}]] = -\frac{c_{j_\eta \ell_\zeta}}{c_{j_\eta \ell_\eta}} [\tilde{p}_i, \tilde{p}_{\phi_{j_\eta}(\ell_\zeta)}]. \end{aligned}$$

Regardless of the values of the coefficients, we find that these two equivalent expressions of  $[k_{\ell_\eta}, k_{\ell_\zeta}]$  have opposite signs. This is possible only if  $[k_{\ell_\eta}, k_{\ell_\zeta}] = 0$ .  $\square$

**Lemma 9.** For a fixed  $1 \leq i \leq r$ , if  $\tilde{p}_\gamma \in \mathfrak{p}_i$ , then  $[\tilde{p}_i, \tilde{p}_\gamma] = 0$ .

*Proof.* Assume that  $\gamma = \phi_{j_\mu}(\ell_\eta)$ . That is, there exist indices  $j_\mu, j_\eta \in \mathfrak{J}_i$  and  $\ell_\mu, \ell_\eta \in \mathfrak{L}_i$  such that

$$[h_{j_\mu}, k_{\ell_\eta}] = -c_{j_\mu \ell_\eta} \tilde{p}_\gamma, \quad [h_{j_\mu}, k_{\ell_\mu}] = -c_{j_\mu \ell_\mu} \tilde{p}_i, \quad [h_{j_\eta}, k_{\ell_\eta}] = -c_{j_\eta \ell_\eta} \tilde{p}_i.$$

It follows that

$$[\tilde{p}_\gamma, h_{j_\eta}] = -\frac{1}{c_{j_\mu \ell_\eta}} [[h_{j_\mu}, k_{\ell_\eta}], h_{j_\eta}] = -\frac{c_{j_\eta \ell_\eta}}{c_{j_\mu \ell_\eta}} [h_{j_\mu}, \tilde{p}_i] = -\frac{c_{j_\eta \ell_\eta} c_{j_\mu \ell_\mu}}{c_{j_\mu \ell_\eta}} k_{\ell_\mu}, \quad (30)$$

where the coefficient for  $k_{\ell_\mu}$  in the last equation can actually be abbreviated as  $c_{j_\eta \ell_\mu}$ . In other words, we see that  $\gamma = \phi_{j_\eta}(\ell_\mu)$ . Therefore,

$$\begin{aligned} [\tilde{p}_i, \tilde{p}_\gamma] &= -\frac{1}{c_{j_\eta \ell_\eta}} [[h_{j_\eta}, k_{\ell_\eta}], \tilde{p}_\gamma] = -\frac{1}{c_{j_\eta \ell_\eta}} \{[h_{j_\eta}, [k_{\ell_\eta}, \tilde{p}_\gamma]] - [k_{\ell_\eta}, [h_{j_\eta}, \tilde{p}_\gamma]]\} \\ &= \frac{c_{j_\mu \ell_\eta}}{c_{j_\eta \ell_\eta}} [h_{j_\eta}, h_{j_\mu}] + \frac{1}{c_{j_\eta \ell_\eta}} [k_{\ell_\eta}, [h_{j_\eta}, \tilde{p}_\gamma]] = -\frac{c_{j_\eta \ell_\mu}}{c_{j_\eta \ell_\eta}} [k_{\ell_\eta}, k_{\ell_\mu}] = 0, \end{aligned}$$

where the last equality follows from Lemma 8.  $\square$

**Theorem 10.** *For each  $\tilde{p}_\gamma \in \mathfrak{p}_i$ ,  $\mathfrak{L}_\gamma = \mathfrak{L}_i$  setwise. Since these sets are ordered, they are identically ordered.*

*Proof.* Assume  $\gamma = \phi_{j_\mu}(\ell_\eta)$ . By (30), we also have  $\gamma = \phi_{j_\eta}(\ell_\mu)$ , implying that  $\ell_\mu \in \mathfrak{L}_i \cup \mathfrak{L}_\gamma$ . To prove  $\mathfrak{L}_\gamma = \mathfrak{L}_i$  setwise, it suffices to prove the inclusion in one direction. Consider the scenario where  $\ell_\zeta \in \mathfrak{L}_i$  and  $\ell_\zeta \neq \ell_\eta$  nor  $\ell_\mu$ . There exists  $j_\zeta \in \mathfrak{J}_i$  such that

$$[h_{j_\zeta}, k_{\ell_\zeta}] = -c_{j_\zeta \ell_\zeta} \tilde{p}_i.$$

By the crossover relationship guaranteed by Lemma 5, we can further the relationships to

$$[h_{j_\mu}, k_{\ell_\zeta}] = \pm [h_{j_\eta}, k_{\ell_\mu}]$$

which, by (18), is associated with an element, say,  $\tilde{p}_a$ , in  $\mathfrak{p}_i$ . Similarly, we have the relationship

$$[h_{j_\eta}, k_{\ell_\zeta}] = \pm [h_{j_\zeta}, k_{\ell_\eta}]$$

which is associated with another element, say,  $\tilde{p}_b$ , in  $\mathfrak{p}_i$ . Thus, Table 4 reflects these relationships, where the value at the first three diagonal locations denoted by the question mark ? must be identical up to a  $\pm$  sign in order to satisfy the crossover relationship. It remains to determine the class to which this value belongs.

Observe that

$$\begin{aligned} \tilde{p}_a &= \frac{1}{c_{j_\zeta \ell_\mu} c_{j_\eta \ell_\mu}} [h_{j_\zeta}, [\tilde{p}_\gamma, h_{j_\eta}]] = \frac{1}{c_{j_\zeta \ell_\mu} c_{j_\eta \ell_\mu}} [h_{j_\eta}, [\tilde{p}_\gamma, h_{j_\zeta}]] \\ &= -\frac{c_{j_\zeta \delta}}{c_{j_\zeta \ell_\mu} c_{j_\eta \ell_\mu}} [h_{j_\eta}, k_\delta], \end{aligned} \quad (31)$$

where, by the fact that  $[\mathfrak{p}, \mathfrak{h}] \subset \mathfrak{k}$ , we have assumed that there exists  $\delta$  such that

$$[\tilde{p}_\gamma, h_{j_\zeta}] = -c_{j_\zeta \delta} k_\delta.$$

By now, together with the crossover relationships with others, we see that the last row of Table 4 holds. It remains to identify the set to which  $k_\delta$  belongs to.

Because  $\tilde{p}_a \in \mathfrak{p}_i$ , whereas we also know  $\tilde{p}_a$  can be expressed as (31) with  $h_{j_\eta} \in \mathfrak{J}_i$ , we conclude  $k_\delta \in \mathfrak{k}_i$ . Therefore, the value for all locations marked

TABLE 4. Relationships established in Theorem 10

...	$\tilde{p}_a$	...	$\tilde{p}_b$	...	$\tilde{p}_\gamma$	...	$\tilde{p}_i$
		...	$\vdots$	...	$\vdots$	...	$\vdots$
	?	...	$h_{j_\zeta}$	...	$h_{j_\mu}$	...	$h_{j_\eta}$
		...	$\vdots$	...	$\vdots$	...	$\vdots$
	$h_{j_\zeta}$	...	?	...	$h_{j_\eta}$	...	$h_{j_\mu}$
		...	$\vdots$	...	$\vdots$	...	$\vdots$
	$h_{j_\mu}$	...	$h_{j_\eta}$	...	?	...	$h_{j_\zeta}$
		...	$\vdots$	...	$\vdots$	...	$\vdots$
	$h_{j_\eta}$	...	$h_{j_\mu}$	...	$h_{j_\zeta}$	...	?
		...	$\vdots$	...	$\vdots$	...	$\vdots$

by ? must correspond to an element  $h_\sigma \in \mathfrak{h}$ , which implies that  $\sigma \in \mathfrak{J}_i$  and, hence,  $\ell_\zeta \in \mathfrak{L}_\gamma$ .  $\square$

**Theorem 11.** For each  $\tilde{p}_\gamma \in \mathfrak{p}_i$ ,  $\mathfrak{J}_\gamma = \mathfrak{J}_i$  setwise, but elements are in different order.

*Proof.* Since  $\mathfrak{L}_i$  and  $\mathfrak{L}_\gamma$  are ordered, we do not need to distinguish  $k_{\ell^{(\gamma)}}$  from  $k_{\ell^{(i)}}$ . For each  $\ell_\eta \in \mathfrak{L}_i$ , there exist  $j_\eta^{(\gamma)} \in \mathfrak{J}_\gamma$  and  $j_\eta \in \mathfrak{J}_i$  such that

$$[h_{j_\eta^{(\gamma)}}, k_{\ell_\eta}] = -c_{j_\eta^{(\gamma)}\ell_\eta} \tilde{p}_\gamma \quad \text{and} \quad [h_{j_\eta}, k_{\ell_\eta}] = -c_{j_\eta\ell_\eta} \tilde{p}_i,$$

respectively. Note  $j_\eta^{(\gamma)}$  refers to the ordered index corresponding to  $\ell_\eta$  in  $\mathfrak{L}_\gamma$ . Observe that

$$\begin{aligned} [\tilde{p}_i, h_{j_\eta^{(\gamma)}}] &= -\frac{1}{c_{j_\eta^{(\gamma)}\ell_\eta}} [\tilde{p}_i, [k_{\ell_\eta}, \tilde{p}_\gamma]] = -\frac{1}{c_{j_\eta^{(\gamma)}\ell_\eta}} \{[\tilde{p}_\gamma, [k_{\ell_\eta}, \tilde{p}_i]] - [k_{\ell_\eta}, [\tilde{p}_\gamma, \tilde{p}_i]]\} \\ &= \frac{c_{j_\eta\ell_\eta}}{c_{j_\eta^{(\gamma)}\ell_\eta}} [\tilde{p}_\gamma, h_{j_\eta}]. \end{aligned}$$

Because  $[\mathfrak{p}, \mathfrak{h}] \subset \mathfrak{k}$ , the two brackets above either both equate to zero or result in an element in the form of  $\pm 2k_\beta$  for some  $1 \leq \beta \leq r$ . In the latter case, by the way we pair the indices in  $\mathfrak{J}_i$  and  $\mathfrak{L}_i$ , it must be the case that  $\beta = j_\eta^{(\gamma)} \in \mathfrak{L}_i$ . It follows that  $j_\eta^{(\gamma)} \in \mathfrak{J}_i$  and  $j_\eta \in \mathfrak{J}_\gamma$  simultaneously. Repeating this argument for every  $\ell_\eta \in \mathfrak{L}_i$ , or equivalently for every  $j_\eta^{(\gamma)} \in \mathfrak{J}_\gamma$ , we conclude that  $\mathfrak{J}_\gamma = \mathfrak{J}_i$ .  $\square$

Theorems 10 and 11 are instructive in that all elements in  $\mathfrak{p}_i$  share the same column indices as those in  $\mathfrak{L}_i$  and the same row indices as those in  $\mathfrak{J}_i$ . However, while the column indices are ordered and fixed, the row indices

are from some reordering of those in  $\mathfrak{J}_i$ . By now, we should have enough information about the structure of  $\mathfrak{p}_i$ .

**Theorem 12.** *For a fixed  $1 \leq i \leq r$  and any  $\tilde{p}_\gamma \in \mathfrak{p}_i$ ,*

1.  $\mathfrak{p}_i = \mathfrak{p}_\gamma$ .
2. If  $|S|$  denotes the cardinality of a finite set  $S$ , then  $|\mathfrak{p}_i| = |\mathfrak{L}_i| = |\mathfrak{J}_i|$ .
3. The subspace spanned by  $\mathfrak{p}_i$  forms a commutative subalgebra of  $\tilde{\mathfrak{p}}$ .

*Proof.* We know by Theorems 10 and 11 that  $\mathfrak{L}_i = \mathfrak{L}_\gamma$  and  $\mathfrak{J}_i = \mathfrak{J}_\gamma$  setwise. By the definition (28), it must be  $\mathfrak{p}_i = \mathfrak{p}_\gamma$ . Also, by the definition (29),  $\mathfrak{k}_i = \mathfrak{k}_\gamma$  in a fixed order. In the proof of Theorem 10, we have shown that for each  $\ell_\zeta \in \mathfrak{L}_i$ ,  $\gamma = \phi_{j_\tau}(\ell_\zeta)$  holds only for a specific  $j_\tau \in \mathfrak{J}_i$ . Indeed, in Table 4 we also see that for each fixed  $j_\tau \in \mathfrak{J}_i$ , there is one and only one  $\ell_\zeta \in \mathfrak{L}_i$  such that  $\gamma = \phi_{j_\tau}(\ell_\zeta)$ . This injective relationship proves  $|\mathfrak{p}_i| = |\mathfrak{L}_i| = |\mathfrak{J}_i|$ .

Suppose that  $\tilde{p}_a, \tilde{p}_b \in \mathfrak{p}_i$ . We may choose  $\ell_\eta, \ell_\zeta \in \mathfrak{L}_i$  such that

$$\phi_{j_1}(\ell_\eta) = a, \quad \phi_{j_1}(\ell_\zeta) = b,$$

respectively. By the crossover relationship, we also know

$$\tilde{p}_a = -\frac{1}{c_{j_\eta \ell_1}}[h_{j_\eta}, k_{\ell_1}].$$

By the one-to-oneness, we also know that corresponding to  $j_\eta$ , there exist  $\ell_\mu \in \mathfrak{L}_i$  such that

$$\tilde{p}_b = -\frac{1}{c_{j_\eta \ell_\mu}}[h_{j_\eta}, k_{\ell_\mu}].$$

Therefore,

$$\begin{aligned} [\tilde{p}_a, \tilde{p}_b] &= -\frac{1}{c_{j_\eta \ell_1}}[[h_{j_\eta}, k_{\ell_1}], \tilde{p}_b] = -\frac{1}{c_{j_\eta \ell_1}}\{[h_{j_\eta}, [k_{\ell_1}, \tilde{p}_b]] - [k_{\ell_1}, [h_{j_\eta}, \tilde{p}_b]]\} \\ &= -\frac{1}{c_{j_\eta \ell_1}}\{-c_{j_1 \ell_\zeta}[h_{j_\eta}, h_{j_\zeta}] + \frac{1}{c_{j_\eta \ell_\mu}}[k_{\ell_1}, k_{\ell_\mu}]\} = 0 \end{aligned}$$

because both  $\mathfrak{h}$  and  $\mathfrak{k}_i$  are commutative. The third statement is proved.  $\square$

The theory developed above can be summarized as follows:

1. The  $[\mathfrak{h}, \mathfrak{k}]$  table consists of elements of  $\tilde{\mathfrak{p}}$  and 0 only.
2. Corresponding to each  $\tilde{p}_i \in \tilde{\mathfrak{p}}$ ,  $1 \leq i \leq r$ , the indices corresponding to the columns and rows of  $\tilde{p}_i$  in the  $[\mathfrak{h}, \mathfrak{k}]$  table define the sets  $\mathfrak{L}_i$  and  $\mathfrak{J}_i$ , respectively. These sets, in turn, give rise to the sets  $\mathfrak{p}_i$  and  $\mathfrak{k}_i$ .
3. For all  $\tilde{p}_\gamma \in \mathfrak{p}_i$ ,  $\mathfrak{J}_\gamma = \mathfrak{J}_i$  setwise, but with different ordering. Meanwhile,  $\mathfrak{L}_\gamma = \mathfrak{L}_i$  in the same ordering.
4. The collection of these  $\mathfrak{p}_i$ 's classifies the basis  $\tilde{\mathfrak{p}}$  into disjoint subsets, each spans a commutative subalgebras in  $\tilde{\mathfrak{p}}$ .
5. Likewise, the sets  $\mathfrak{k}_i$  divide the basis of the subalgebra  $\mathfrak{k}$  into disjoint subsets, each spans a commutative subalgebras in  $\mathfrak{k}$ .
6. There are as many subalgebras  $\mathfrak{k}_i$  in  $\mathfrak{k}$  as there are subalgebras  $\mathfrak{p}_i$  in  $\tilde{\mathfrak{p}}$ .

## 4. Examples

The proof presented above for the existence of an innate commutative substructure seems complicated due to its intricate interplay of crossover relationships. To substantiate our theory, we provide two randomly generated examples to demonstrate this refined decomposition within a given Cartan decomposition. We first present a low dimensional problem so that all details can be seen. We then employ graphical representations to elucidate the commutativity of the  $[\mathfrak{h}, \mathfrak{k}]$  table for a high dimensional problem.

### 4.1. Case $n = 3$

Consider the example  $n = 3$ . The set  $\{X, Y, Z, I\}^{\otimes 3}$  comprises 64 distinct Pauli strings, which, by (15), are represented by integers ranging from 1 to 64. For instance, the Pauli string  $X \otimes Y \otimes Z$  corresponds to the integer 34. Upon multiplying the Pauli strings by  $\iota$ , the Lie algebra  $\mathfrak{su}(2^3)$  is spanned by basis  $\{B_1, \dots, B_{63}\}$ , where each basis element is also associated with an integer.

We randomly select a subset of integers  $\{1, 4, 6, 7, 11, 12, 13\}$ , where each integer identifies a certain basis element. Consider the vector space

$$V = \text{span}\{1, 4, 6, 7, 11, 12, 13\}.$$

Applying the technique from Section 2, we find that

$$\begin{aligned} \mathfrak{g}(V) = \text{span}\{ & 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, \\ & 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63\}, \end{aligned}$$

which has a dimension of 30. Using  $\theta_1$ , the Cartan pair  $(\mathfrak{k}, \mathfrak{p})$  is determined as follows:

$$\begin{aligned} \mathfrak{k} &= \text{span}\{2, 5, 7, 8, 10, 14, 50, 53, 55, 56, 58, 62\}, \\ \mathfrak{p} &= \text{span}\{1, 3, 4, 6, 9, 11, 12, 13, 15, 49, 51, 52, 54, 57, 59, 60, 61, 63\}, \end{aligned}$$

with dimensions 12 and 18, respectively. Within  $\mathfrak{p}$  there are five Cartan subalgebras spanned by the bases

$$\begin{aligned} &\{1, 4, 13, 49, 52, 61\}, \{3, 4, 15, 51, 52, 63\}, \{3, 6, 9, 51, 54, 57\}, \\ &\{1, 6, 11, 49, 54, 59\}, \{11, 12, 15, 59, 60, 63\}, \end{aligned}$$

respectively. Note that these Cartan subalgebras overlap, yet each can be reached through suitable conjugations of the others. Suppose we choose

$$\begin{aligned} \mathfrak{h} &= \text{span}\{1, 4, 13, 49, 52, 61\}, \\ \widetilde{\mathfrak{p}} &= \text{span}\{3, 6, 9, 11, 12, 15, 51, 54, 57, 59, 60, 63\}. \end{aligned}$$

Then  $r = 12$  and  $s = 6$ .

So that the readers can verify the subsequent calculations independently, we provide the complete commutator table entries between  $\mathfrak{h}$  and  $\mathfrak{k}$  as



$$[\mathfrak{h}, \mathfrak{k}] = \begin{bmatrix} -63 & -60 & 0 & -57 & 0 & -51 & -15 & -12 & 0 & -9 & 0 & -3 \\ 0 & -57 & -59 & -60 & 54 & 0 & 0 & -9 & -11 & -12 & 6 & 0 \\ -51 & 0 & 54 & 0 & -59 & -63 & -3 & 0 & 6 & 0 & -11 & -15 \\ -15 & -12 & 0 & -9 & 0 & -3 & -63 & -60 & 0 & -57 & 0 & -51 \\ 0 & -9 & -11 & -12 & 6 & 0 & 0 & -57 & -59 & -60 & 54 & 0 \\ -3 & 0 & 6 & 0 & -11 & -15 & -51 & 0 & 54 & 0 & -59 & -63 \end{bmatrix},$$

which reads, for example, that the  $(1, 2)$  entry is  $[B_1, B_6] = -2B_{60}$ . Here, the constant factor of 2, consistent throughout the table as per Lemma 2, is implied, while the sign is explicitly noted. We stress that these commutator multiplications can be quickly obtained by our techniques outlined in Section 2 without the need to explicitly construct these Pauli strings.

The subspace  $\tilde{\mathfrak{p}}$  itself is not an algebra. However, by our theory it is the direct sum of three four-dimensional subspaces

$$\tilde{\mathfrak{p}} = \text{span}\{3, 15, 51, 63\} \oplus \text{span}\{6, 11, 54, 59\} \oplus \text{span}\{9, 12, 57, 60\},$$

each of which is a commutative subalgebra. The set of basis  $\{3, 15, 51, 63\}$ , for instance, is identified by ordinal indices  $\mathfrak{L}_1 = \{1, 6, 7, 12\}$  in  $\tilde{\mathfrak{p}}$  which are also column numbers in the  $[\mathfrak{h}, \mathfrak{k}]$  table above. Our theory ensures that  $\mathfrak{p}_1 = \mathfrak{p}_6 = \mathfrak{p}_7 = \mathfrak{p}_{12} = \{\tilde{p}_1, \tilde{p}_6, \tilde{p}_7, \tilde{p}_{12}\}$ . Correspondingly, our theory asserts that the subspace  $\mathfrak{k}$  is the direct sum of three four-dimensional subspaces

$$\mathfrak{k} = \text{span}\{2, 14, 50, 62\} \oplus \text{span}\{7, 10, 55, 58\} \oplus \text{span}\{5, 8, 53, 56\},$$

each of which is a commutative subalgebra. The basis of  $\mathfrak{k}_1 = \{2, 14, 50, 62\}$ , for example, is enumerated as  $\{k_1, k_6, k_7, k_{12}\}$  and so on. Furthermore, we can pair up the bases of these subalgebras as  $(\mathfrak{k}_i, \mathfrak{p}_i)$ ,  $i = 1, 2, 3$ , where the  $[\mathfrak{k}_i, \mathfrak{p}_i]$  table (see Table 4) is such that

$$\begin{aligned} [\mathfrak{k}_1, \mathfrak{p}_1] &= \begin{bmatrix} -61 & -49 & -13 & -1 \\ -49 & -61 & -1 & -13 \\ -13 & -1 & -61 & -49 \\ -1 & -13 & -49 & -61 \end{bmatrix}, \quad [\mathfrak{k}_2, \mathfrak{p}_2] = \begin{bmatrix} 61 & -52 & 13 & -4 \\ 52 & -61 & 4 & -13 \\ 13 & -4 & 61 & -52 \\ 4 & -13 & 52 & -61 \end{bmatrix}, \\ [\mathfrak{k}_3, \mathfrak{p}_3] &= \begin{bmatrix} -52 & -49 & -4 & -1 \\ -49 & -52 & -1 & -4 \\ -4 & -1 & -52 & -49 \\ -1 & -4 & -49 & -52 \end{bmatrix}. \end{aligned}$$

Note that in each of these commutator tables, the entries within each column form identical subsets of  $\mathfrak{h}$ , differing at most by their signs. Note also that these entries must be meticulously ordered to reflect the specific crossover relationships inherent in the structure.

In short, for this particular example, we find that

$$\mathfrak{g}(V) = \underbrace{\text{span}(\mathfrak{k}_1) \oplus \text{span}(\mathfrak{k}_2) \oplus \text{span}(\mathfrak{k}_3)}_{\mathfrak{k}} \oplus \underbrace{\text{span}(\mathfrak{p}_1) \oplus \text{span}(\mathfrak{p}_2) \oplus \text{span}(\mathfrak{p}_3)}_{\tilde{\mathfrak{p}}} \oplus \mathfrak{h}, \quad (32)$$

where each of the seven subspaces on the right side is commutative.

#### 4.2. Case $n = 12$

Consider the case where  $n = 12$  and the Hamiltonian  $\imath\mathcal{H}$  in a linear combination with the space

$$\imath\mathcal{H} \in \text{span}\{1, 4, 5, 6, 7, 11, 12, 15, 22, 50, 51\}.$$

The algebra  $\mathfrak{su}(2^{12})$  has real dimension  $4^{12} - 1 = 16777215$ . Each basis element  $B_\ell$  in this Lie algebra is of size  $2^{12} \times 2^{12} = 4096 \times 4096$ . Constructing the full commutator table for all  $[B_i, B_j]$  would result in an immense matrix of size  $(4^{12} - 1) \times (4^{12} - 1)$ . However, by utilizing our techniques described in Section 2, each  $B_\ell$  is represented by a 12-digit ID which is further converted via (15) into a unique ordinal number  $\ell$ . We can efficiently determine the basis of the subalgebra  $\mathfrak{g}(\imath\mathcal{H})$  and, indeed,  $\dim(\mathfrak{g}(\imath\mathcal{H})) = 126$ . This method significantly reduces the computational effort compared to traditional unitary synthesis techniques for  $e^{-\imath\mathcal{H}}$ .

Instead of enumerating the elements in the commutator table for  $\mathfrak{g}(\imath\mathcal{H})$ , we present a visual representation in Figure 1 to represent the  $126 \times 126$  commutator table, where each dot signifies a nonzero entry. There are 8064 such entries, yet no discernible patterns emerge at this stage.

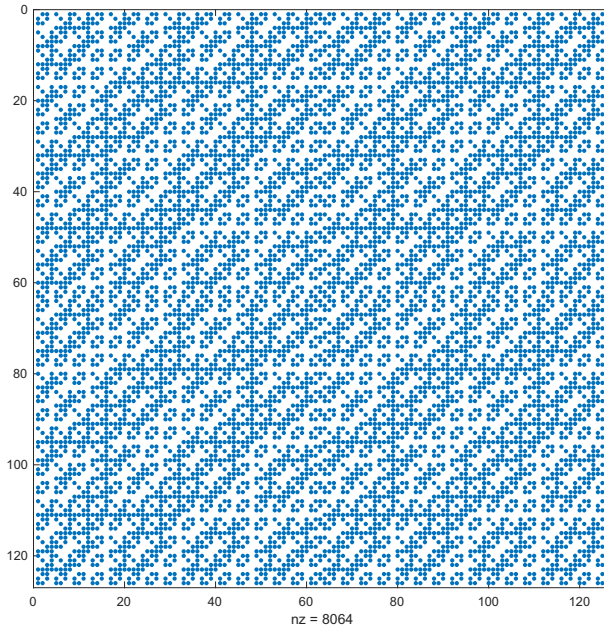


FIGURE 1. Nonzero Lie brackets among elements of  $\mathfrak{g}(\imath\mathcal{H})$ , if not ordered by commutative subalgebras

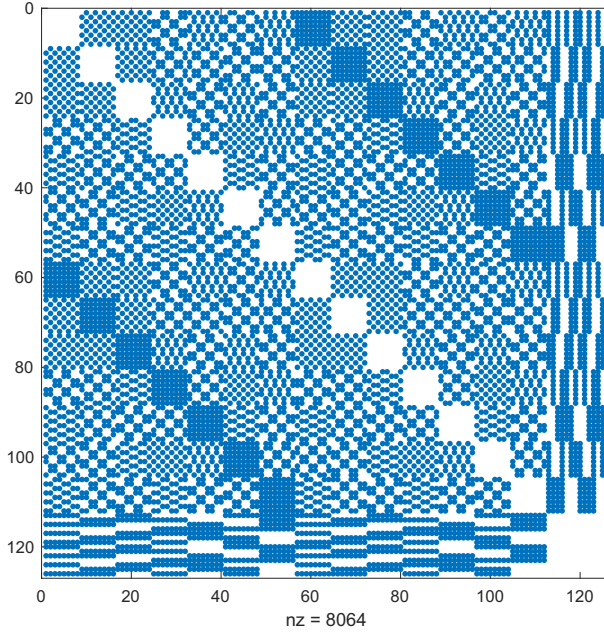


FIGURE 2. Nonzero Lie brackets among elements of  $\mathfrak{g}(\mathcal{H})$  after reordering by commutative subalgebras

The **AI**-type Cartan decomposition of  $\mathfrak{g}(\mathcal{H})$  is found to have  $\dim(\mathfrak{k}) = \dim(\tilde{\mathfrak{p}}) = 56$  and  $\dim(\mathfrak{h}) = 14$ . Using our theory<sup>2</sup>, it is further discovered that the Pauli basis elements in  $\tilde{\mathfrak{p}}$  (and  $\mathfrak{k}$ ) can be categorized into 7 disjoint groups, each of which spans an 8-dimensional commutative subalgebra. By reorganizing the basis elements of  $\mathfrak{g}(\mathcal{H})$  akin to the arrangement in (32), we have:

$$\mathfrak{g}(\mathcal{H}) = \underbrace{\bigoplus_{i=1}^7 \text{span}(\mathfrak{k}_i)}_{\mathfrak{k}} \underbrace{\bigoplus_{i=1}^7 \text{span}(\mathfrak{p}_i)}_{\tilde{\mathfrak{p}}} \oplus \mathfrak{h}, \quad (33)$$

where each of these 15 subalgebras are commutative among themselves. The commutator table under this ordering of Pauli strings is represented in Figure 2. This table contains exactly the same entries as those in Figure 1, yet the 15 zero blocks along the main diagonal clearly manifest the commutative subalgebras established by our theory. This matrix representation may appear as a result of graph reordering, but it is fundamentally a consequence of identifying the commutative subalgebras.

<sup>2</sup>We have developed an algorithm in **Matlab** to automate the process. The software can be provided to interested readers.

## 5. Conclusion

The theory developed in this note applies to the **AI**-type Cartan decomposition of any subalgebra of  $\mathfrak{su}(2^n)$ . The key finding is that this decomposition can be further divided into an orthogonal direct sum of abelian subalgebras. This algebraic insight into the commutative substructure within any Cartan pair should be of mathematical interest in its own right. In practical terms, such partitioning is crucial for examining the limiting behavior of Lax dynamics, which is detailed in a separate study and is instrumental for addressing the Hamiltonian simulation problem in quantum simulation.

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## Declarations

**Competing Interests** The author has no relevant financial or non-financial interests to disclose.

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