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PREPARING HAMILTONIANS FOR QUANTUM SIMULATION: A COMPUTATIONAL FRAMEWORK FOR CARTAN DECOMPOSITION VIA LAX DYNAMICS

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Abstract. Quantum algorithms usually are described via quantum circuits representable as unitary operators. Synthesizing the unitary operators described mathematically in terms of the unitary operators recognizable as quantum circuits is essential. One such a challenge lies in the Hamiltonian simulation problem, where the matrix exponential of a large-scale skew-Hermitian matrix is to be computed. Most current techniques are prone to approximation errors, whereas the parametrization of the underlying Hamiltonian via the Cartan decomposition is more promising. To prepare for such a simulation, this work proposes to tackle the Cartan decomposition by means of the Lax dynamics. The advantages include not only that it is numerically feasible with no matrices involved, but also that this approach offers a genuine unitary synthesis within the integration errors. This work contributes to the theoretic and algorithmic foundations in three aspects: exploiting the quaternary representation of Hamiltonian subalgebras; describing a common mechanism for deriving the Lax dynamics; and providing a mathematical theory of convergence.

1. Introduction

Quantum computing, with its potential capability of transmitting information massively, swiftly, concurrently, and securely, shows great promises to the next-generation quantum-enabled science and technology [1, 27, 52]. The range of applications is broad and far reaching, including communicating [4], sensing [29, 32], computing [55], machine learning and big data [35, 48, 65], and other societal grand challenges, just to name a few. The current development of hardware devices is still in its infancy, capable of handling only a few qubits. Even so, it is of great interest and vital importance to gain insight into how a quantum computation could be or should be conducted.

Among the wide range of research endeavors in the field, this paper focuses on one paradigmatic yet critically important problem—we want to synthesize the unitary transformation under a time-independent Hamiltonian operator $\mathcal{H}$ in time steps, i.e., compute the family of unitary matrices

$$U(t) = e^{-i\mathcal{H}t}, \tag{1.1}$$

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where $\mathcal{H}$ is represented as a fixed Hermitian matrix in $\mathbb{C}^{2^n \times 2^n}$. This problem is pivotal due to Feynman's conjecture, which posits that a quantum simulator composed of controllable spin-$\frac{1}{2}$ particles could replicate desired interactions, allowing us to predict physical quantities through appropriate measurements [20]. Lloyd's proof [44] further established that even small time-step evolutions of (1.1) enable efficient simulation of any many-body quantum Hamiltonian with few-particle interactions.

It is important to point out right away that traditional floating-point methods for computing the matrix exponential, such as the scaled and squared Padé approximation [49,50], are impractical on classical machines due to exponential scaling. These techniques are not implementable on quantum machines, either. Some innovative approaches are required to address this issue.

A host of approximation techniques have already been proposed in the literature for simulating the unitary evolution (1.1) on quantum machines. A partial list includes [5, 8, 9, 21, 23, 26, 33, 39, 44–46, 59, 62]. The ideas can roughly be classified into three categories. The first approach simulates the Hamiltonian dynamics with a truncated Taylor series where the terms are linear combinations of unitary operations together with a robust form of oblivious amplitude amplification [5]. The second approach, assuming that a qubit may only interact with qubits in its vicinity (the so-called lattice Hamiltonian), approximates the time-evolution unitary by a product of unitaries based on the Lieb–Robinson bounds and, hence, the performance is good only when the Hamiltonian is close to commuting [33]. These algorithms are reported to have been optimized in that the circuit depth scales almost linearly in the evolution time. However, these approaches are subject to inherent constraints and the approximation errors affect the simulation authenticity. The third approach involves explicitly parameterizing a unitary transformation, either over an n-qubit system using 1- and 2-qubit operations [22, 28, 42, 57] or through predefined quantum circuits of unitary operators [8, 46]. The former approach, for example, is based on the observation that elements of the special unitary group $\mathrm{SU}(2^n)$ can be determined by components generated from the so-called Cartan decomposition of the Lie algebra $\mathfrak{su}(2^n)$ [40, 41]. However, devising a constructive algorithm for such decomposition is challenging. The method in [57], for instance, is recursive and necessitates solving the zeros of a matrix polynomial derived from a truncated Baker-Campbell-Hausdorff (BCH) formula at each step. While the computational approach is promising, the need to truncate the BCH formula at higher orders to manage errors is concerning. Additionally, using the entire $\mathfrak{su}(2^n)$ basis typically results in exponential circuit depth for arbitrary unitaries, posing a significant limitation.

It is under such a background, we have outlined in an earlier paper [18] a different way to find the Cartan decomposition. The crux there is that, after applying the Cartan theory only to a necessary subalgebra of $\mathfrak{su}(2^n)$, a Lax dynamical system is constructed whose solution flow of the Lax dynamics can be tracked by any available numerical ODE techniques [38, 47, 58] to high precision. In this way, we will have prepared genuinely a given Hamiltonian with controlled precision for quantum simulation.

Our approach is motivated by our past experience with the Toda lattice [10, 11] for eigenvalue computation and the various isospectral flows for other applications [12, 13, 16]. The Cartan decomposition is not the spectral decomposition, but we see the similarity between the setting of the general Lax dynamics [15, 17] and

the Cartan decomposition. We therefore think that developing a computational framework for the unitary synthesis problem (1.1) in general is possible.

Building on our previous work [18], which highlighted the benefits, methodologies, and initial empirical evidence, this paper aims to provide rigorous mathematical justification for our computational framework. We establish the theoretical and algorithmic foundations from three perspectives: (i) Each Pauli string, traditionally represented as a matrix in $C^{2^n\times 2^n}$, is reinterpreted as a sequence of quaternary digits corresponding to unique integers. This allows us to generate Hamiltonian subalgebras efficiently without matrix multiplications. (ii) We reformulate the conventional Lax dynamics, which typically involves matrix evolution, to focus solely on the combination coefficients of Pauli strings, thereby eliminating matrix manipulations. (iii) We present a mathematical proof demonstrating that the Lax dynamical system converges to the desired Cartan decomposition, ensuring a reliable method for decomposing any given Hamiltonian $\mathcal{H}$ in preparation for unitary synthesis.

This paper is structured to provide a comprehensive understanding of the topic. Section 2 begins with a review of essential background information, including an effective mechanism for generating the necessary Lie subalgebra, a brief overview of the Cartan decomposition [40, 57], and the foundational model of Lax dynamics [15, 17]. In Section 3, we delve into the mechanism for constructing the Lax dynamics pertinent to the Cartan decomposition. To illustrate the construction and its convergence explicitly, we present a detailed example in Section 4. The dynamical system under consideration features a center manifold, whose stability is examined through its block structure in Section 5. Finally, Section 6 is dedicated to a thorough stability analysis, demonstrating that the dynamical system approach effectively achieves the Cartan decomposition.

2. Basics

In this section, we provide essential background information to support the development of our framework. While some of these materials have been previously discussed in [18], we restate key results here to ensure the presentation is self-contained and to facilitate easy reference to the notations used.

2.1. **Reducing dimension via encoded Pauli strings.**

To describe Hamiltonians in quantum simulation, we focus on the special unitary group $\mathrm{SU}(2^n)$ and its Lie algebra $\mathfrak{su}(2^n)$. The algebra $\mathfrak{su}(2^n)$ comprises skew-Hermitian matrices with zero trace and has a real dimension of 4^n-1. For quantum computation, a natural choice of the basis for $\mathfrak{su}(2^n)$ is the set $\imath\{X,Y,Z,I\}^{\otimes n}-\{\imath I^{\otimes n}\}$, where

$$X:=\begin{bmatrix}0&1\\1&0\end{bmatrix};\quad Y:=\begin{bmatrix}0&-\imath\\\imath&0\end{bmatrix};\quad Z:=\begin{bmatrix}1&0\\0&-1\end{bmatrix}, \tag{2.1}$$

are the Pauli matrices which are Hermitian, unitary, readily quantum observable describing the rotation of a spin-$\frac{1}{2}$ particle, I is the 2×2 identity matrix, and $^{\otimes n}$ denotes the n-th order tensor product. Replacing X,Y,Z,I by the Fraktur numerics $\mathfrak{1},\mathfrak{2},\mathfrak{3},\mathfrak{4}$, used both as an integer index and as a symbol, we identify every element in $\{X,Y,Z,I\}^{\otimes n}$ by a unique n-digit ID

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

which, when regarded as a quaternary sequence, can be translated into a unique ordinal number ℓ via

$$\ell := \sum_{j=1}^{n} 4^{j-1}(\mathfrak{d}_j - 1) + 1, \tag{2.2}$$

and vice versa. Other than an additional scalar multiplication by $\imath$, we may use the same conversion to encode the basis element B_ℓ of $\mathfrak{su}(2^n)$ by the single integer ℓ. In this way, we avoid forming the basis explicitly which, otherwise, would be $4^n - 1$ matrices in $\mathbb{C}^{2^n \times 2^n}$.

While any given Hamiltonian $\mathcal{H}$ can be expressed as a linear combination of Pauli strings, the trouble is that the matrix exponential of $-\imath\mathcal{H}$ in the summation form cannot easily be simulated on a quantum circuit. The primary obstacle is that both the Baker-Campbell-Hausdorff (BCH) formula and the Zassenhaus formula [60] result in expansions with infinitely many terms and products, making direct simulation impractical. This is where using the encoded Pauli strings for the dimension reduction becomes handy by using following lemma [2, 18].

Lemma 2.1. *Let B_ℓ, $\ell = 1, \ldots, 4^n$, denote elements in $\{X, Y, Z, I\}^{\otimes n}$ multiplied by $\imath$.*

1. *If the commutator $[B_i, B_j]$ of two distinct Pauli strings 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.*
2. *If $[B_i, B_j] = cB_k$, then $[B_j, B_k] = cB_i$ and $[B_k, B_i] = cB_j$.*
3. *The proportional constant c depends on the makeup of the Pauli strings.*

Lemma 2.1 suggests that for both the BCH and Zassenhaus applications to $\imath\mathcal{H}$, it is sufficient to consider the smallest Lie subalgebra $\mathfrak{g}(\imath\mathcal{H})$ within $\mathfrak{su}(2^n)$ that encompasses all terms in $\imath\mathcal{H}$. Only very recently the problem of generating $\mathfrak{g}(\imath\mathcal{H})$ for a given Hermitian matrix $\mathcal{H}$ is coined as the dynamical Lie algebra (DLA) [54]. For further details on DLA, refer to Appendix Section 8.1. Instead of classification up to isomorphisms, we need a practical way to generate the specific $\mathfrak{g}(\imath\mathcal{H})$ for any given $\mathcal{H}$. We now outline an efficient approach using Pauli string encoding, avoiding explicit commutator operations.

For clarity, the matrix multiplication is denoted by $*$ to distinguish it from the Kronecker product $\otimes$ whose longhand writing is suppressed. The Cayley table describing all possible matrix multiplications among $\{X, Y, Z, I\}$ is listed in Table 1.

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

$\downarrow * \rightarrow$	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

We carry out matrix-free commutator operations as follows. Suppose that the Pauli string B_i is expressed in terms of its n-digit ID as $B_i = \imath\mathfrak{d}_{i_n} \ldots \mathfrak{d}_{i_1}$, where

$\mathfrak{d}_{i_k} \in \{1, 2, 3, 4\}$ for $k = 1, \ldots, n$. Then the commutator $[B_i, B_j]$ is given by

$$\begin{aligned}[B_i, B_j] &= -((\mathfrak{d}_{i_n} \ldots \mathfrak{d}_{i_1}) * (\mathfrak{d}_{j_n} \ldots \mathfrak{d}_{j_1}) - (\mathfrak{d}_{j_n} \ldots \mathfrak{d}_{j_1}) * (\mathfrak{d}_{i_n} \ldots \mathfrak{d}_{i_1})) \\ &= -((\mathfrak{d}_{i_n} * \mathfrak{d}_{j_n}) \ldots (\mathfrak{d}_{i_1} * \mathfrak{d}_{j_1}) - (\mathfrak{d}_{j_n} * \mathfrak{d}_{i_n}) \ldots (\mathfrak{d}_{j_1} * \mathfrak{d}_{i_1})). \end{aligned} \tag{2.3}$$

Each matrix-to-matrix multiplication $\mathfrak{d}_{ik} * \mathfrak{d}_{jk}$, for $k = 1, \ldots, n$, can be referenced from Table 1. Notably, the products $\mathfrak{d}_{ik} * \mathfrak{d}_{jk}$ and $\mathfrak{d}_{jk} * \mathfrak{d}_{i_k}$ differ only by a sign, making the terms on the right side of (2.3) essentially identical. Consequently, $[B_i, B_j]$ is either zero or $-2(\mathfrak{d}_{in} * \mathfrak{d}_{jn}) \ldots (\mathfrak{d}_{i1} * \mathfrak{d}_{j1})$. This allows us to determine the n-digit ID of the bracket $[Bi, B_j]$ without performing any matrix or tensor multiplications. By simply retrieving or swapping indices, we can efficiently generate the subalgebra $\mathfrak{g}(\imath\mathcal{H})$ and verify membership through associated ordinal numbers. This method is particularly advantageous for handling large n and diverse compositions of $\mathcal{H}$.

2.2. **Unearthing commutativity via Cartan decomposition.** The notion of Cartan decomposition of a semisimple Lie algebra plays an important role in the theoretical study of structure and representation in the Lie theory [41, 61]. It turns out that the Cartan decomposition of the subalgebra $\mathfrak{g}(\imath\mathcal{H})$ also finds applications in the Hamiltonian simulation. See relevant discussions in [24, 28, 34, 40, 42, 57] and our introductory paper [18]. What is interesting is our innovative way to find the Cartan decomposition numerically by means of the Lax dynamics. The basic thrust is to recursively factorize the desired $e^{-\imath\mathcal{H}t}$ into the product of exponentials of commutative Pauli strings which are readily quantum implementable. Our idea is akin to the successive application of Givens rotations [22] or generalized polar decompositions [43, 51] used for matrix decomposition on classical computers. However, our focus on Pauli strings ensures quantum implementability with optimal depth. Additionally, we decompose one subalgebra at a time, effectively halving the dimension with each step, as explained in Section 8.2. Here, we highlight two crucial facts pertinent to our applications. For a comprehensive understanding, readers should refer to the foundational texts [36, 41, 61].

A Lie algebra automorphism $\theta : \mathfrak{g} \to \mathfrak{g}$ over a real semisimple Lie algebra $\mathfrak{g}$ is called an involution if its square is equal to the identity. The Cartan decomposition is a splitting of $\mathfrak{g}$ based on the eigenspaces of the underlying involution.

Theorem 2.2. *Given an involution θ on a semisimple Lie algebra $\mathfrak{g}$, let the eigenspaces corresponding to the eigenvalues $+1$ and -1 of θ be denoted as $\mathfrak{k}$ and $\mathfrak{p}$, respectively. Then $\mathfrak{g}$ can be decomposed as a direct sum*

$$\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}, \tag{2.4}$$

with the properties that

$$[\mathfrak{k}, \mathfrak{k}] \subseteq \mathfrak{k},\ [\mathfrak{k}, \mathfrak{p}] \subseteq \mathfrak{p},\ \textit{and}\ [\mathfrak{p}, \mathfrak{p}] \subseteq \mathfrak{k}. \tag{2.5}$$

Conversely, any decomposition of $\mathfrak{g}$ with properties (2.5) *defines an involution.*

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. Let $\mathfrak{h} \subset \mathfrak{p}$ be any of the maximal subalgebras contained in $\mathfrak{p}$ and denote

$$\mathfrak{p} = \widetilde{\mathfrak{p}} \oplus \mathfrak{h}. \tag{2.6}$$

The subalgebra $\mathfrak{h}$ is referred to as a *Cartan subalgebra*. There could be multiple Cartan subalgebras, but they are related by similarity transformations in the following sense.

Theorem 2.3. *Corresponding to the Lie subalgebra $\mathfrak{k}$ in a Cartan pair $(\mathfrak{k}, \mathfrak{p})$, let $\mathfrak{K} = e^{\mathfrak{k}}$ be the associated Lie subgroup. Corresponding to a group element $K \in \mathfrak{K}$, define the conjugation action $\mathrm{Ad}_K : \mathfrak{g} \to \mathfrak{g}$ via the map $\mathrm{Ad}_K(g) = KgK^{-1}$.*

(1) *Suppose that $\mathfrak{h}$ is a fixed Cartan subalgebra, then $\mathfrak{p} = \bigcup_{K \in \mathfrak{K}} \mathrm{Ad}_K(\mathfrak{h})$.*
(2) *If $\widehat{\mathfrak{h}}$ is another Cartan subalgebra in $\mathfrak{p}$, then $\widehat{\mathfrak{h}} = \mathrm{Ad}_K(\mathfrak{h})$ for some $K \in \mathfrak{K}$.*

In our context, the conjugation action will be a unitary similarity transformation, i.e., a rotation in $\mathbb{C}^{2^n \times 2^n}$. Suppose that $\imath\mathcal{H} \in \mathfrak{p}$. By Theorem 2.3, there exists $\kappa \in \mathfrak{k}$ and $\eta \in \mathfrak{h}$ such that

$$-\imath\mathcal{H} = e^{\kappa} \eta e^{-\kappa}, \tag{2.7}$$

which resembles the classical spectral decomposition of the matrix $-\imath\mathcal{H}$, where e^{κ} is unitary and η is unitarily similar to $-\imath\mathcal{H}$. However, (2.7) is not a spectral decomposition of $-\imath\mathcal{H}$ because η is not necessarily diagonal. It follows that the unitary synthesis can be realized from the factorization:

$$e^{-\imath\mathcal{H}t} = e^{\kappa} e^{\eta t} e^{-\kappa}. \tag{2.8}$$

Two key points merit attention. First, the commutativity of $\mathfrak{h}$ ensures that the exponential $e^{\eta t}$ on the right-hand side of (2.8) is a product of quantum-implementable matrix exponentials. Second, since $\mathfrak{k}$ is a subalgebra, the exponential e^{κ} can be similarly decomposed, though it remains time-independent. Refer to the concept of continued Cartan decomposition in [18]. By controlling the precision in computing $\kappa \in \mathfrak{k}$ and $\eta \in \mathfrak{h}$, the product on the right-hand side of (2.8) effectively synthesizes $e^{-\imath\mathcal{H}t}$. This results in $e^{-\imath\mathcal{H}t}$ being obtained through a time-independent unitary similarity transformation of $e^{\eta t}$, the sole time-dependent component composed of commutative matrix exponentials. Consequently, the depth of the associated quantum circuit remains independent of time.

2.3. **Tracking decomposition via Lax dynamics.** The challenge of finding the decomposition (2.7) is comparable to determining the spectral decomposition of $-\imath\mathcal{H}$, a task rendered impractical by the sheer size of $\mathcal{H}$. Our approach circumvents this obstacle by enabling the decomposition (2.7) without resorting to spectral methods and instead relying solely on scalar variables. This innovative method represents a significant advancement in the field. To achieve this, we leverage Lax dynamics and employ numerical ODE techniques to facilitate the calculation of the Cartan decomposition.

The Lax dynamics is a generalization of the so-called Toda lattice which has been shown to be the continuous realization of the QR algorithm for eigenvalue computation. A variety of such dynamical systems have been developed to imitate other types of matrix factorizations, including the polar decomposition and the singular value decomposition [10, 12, 14–16]. We now explain a new application to the Cartan decomposition with the distinctive advantage of being matrix-free.

The basic model of the Lax dynamics involves three differential systems. Let μ, $\nu : \mathfrak{gl}(N) \to \mathfrak{gl}(N)$ denote two linear operators on the general linear space $\mathfrak{gl}(N)$ of dimension N such that any element $X \in \mathfrak{gl}(N)$ can be expressed as

$$\mu(X) + \nu(X) = X. \tag{2.9}$$

The splitting of $\mathfrak{gl}(N)$ in (2.9) need not even be a direct sum. Different choices of μ and ν lead to different dynamics, including the so-called Toda lattice, the SVD

flow, and so on [14]. Let the dot $\dot{}$ denote the differential operator $\frac{d}{dt}$ with respect to the parameter t. Consider the initial value problem

$$\dot{X}(t) := [X(t), \mu(X(t))], \quad X(0) := X_0, \tag{2.10}$$

referred to as a general *Lax dynamical system*, and also the two associated systems:

$$\begin{cases} \dot{g}_1(t) := g_1(t)\mu(X(t)), & g_1(0) := I, \\ \dot{g}_2(t) := \nu(X(t))g_2(t), & g_2(0) := I, \end{cases} \tag{2.11}$$

referred to as the parameter dynamical systems. The following facts concerning the solution flows of the above dynamical systems have already established in [17].

Theorem 2.4. *For any t within the interval of existence, the solutions $X(t)$, $g_1(t)$, and $g_2(t)$ of the systems* (2.10) *and* (2.11)*, respectively, are related to each other by the following three properties:*

(1) *(Similarity Property)*

$$X(t) = g_1(t)^{-1} X_0 g_1(t) = g_2(t) X_0 g_2(t)^{-1}. \tag{2.12}$$

(2) *(Decomposition Property)*

$$e^{tX_0} = g_1(t) g_2(t). \tag{2.13}$$

(3) *(Reversal Property)*

$$e^{tX(t)} = g_2(t) g_1(t). \tag{2.14}$$

In view of these relationships and the similarity between (2.12) and (2.7), our idea is to obtain the decomposition (2.7) of a given $\xi \in \mathfrak{g}$, e.g., $-\imath\mathcal{H} \in \mathfrak{g}(\imath\mathcal{H})$, via the Lax dynamics in the form

$$\dot{x}(t) = [x(t), \mu(x(t))], \quad x(0) = \xi \in \mathfrak{g} \tag{2.15}$$

with a specially selected $\mu(x(t)) \in \mathfrak{k}$. To fix ideas, suppose further that the involution

$$\theta_1(g) := -g^\top \tag{2.16}$$

is used, where note that the transpose of $g \in \mathfrak{g}(\imath\mathcal{H})$ is taken. Then with regard to the Cartan decomposition

$$\mathfrak{g}(\imath\mathcal{H}) = \mathfrak{k} \otimes (\widetilde{\mathfrak{p}} \otimes \mathfrak{h}), \tag{2.17}$$

by Theorem 2.2, elements in $\mathfrak{k}$ are both skew-Hermitian and skew-symmetric and, hence, must be real-valued, while elements in $\mathfrak{p}$ are both skew-Hermitian and symmetric and, hence, its entries must be pure imaginary. It follows immediately that the parameter flow $g_1(t)$ defined by $\mu(x(t)) \in \mathfrak{k}$ according to (2.11) will remain unitary and that the Frobenius norm of $x(t)$ is preserved for all t. The question is how to choose $\mu(x(t)) \in \mathfrak{k}$ so that $x(t)$ has the desired limiting behavior.

3. Constructing Lax dynamics over $\mathfrak{g}(\imath\mathcal{H})$

By Theorem 2.3, it must be $\dim(\mathfrak{k}) = \dim(\widetilde{\mathfrak{p}})$. Accordingly, we may denote the basis in each subspace as

$$\widetilde{\mathfrak{p}} = \text{span}\{\widetilde{p}_1, \ldots \widetilde{p}_r\}; \quad \mathfrak{h} = \text{span}\{h_1, \ldots h_s\}; \quad \mathfrak{k} = \text{span}\{k_1, \ldots k_r\}, \tag{3.1}$$

respectively, and assume that these basis elements are made of B_ℓ's with suitable subsets of $\ell = 1, \ldots 4^n$. It is convenient to summarize the inclusion relationship between any two of the three subspaces $\mathfrak{k}$, $\widetilde{\mathfrak{p}}$ and $\mathfrak{h}$ under the Lie bracket operation in Table 2. Of particular importance is the fact that $[\mathfrak{h}, \mathfrak{k}] \subset \widetilde{\mathfrak{p}}$. In fact, by Lemma 2.1, it suffices to consider the transitions among the standard basis elements, i.e., $[h_\alpha, k_\beta] = \widetilde{p}_\gamma$ and so on.

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

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

If we break down $x(t)$ in terms of its components in each subspace,

$$x(t) = x_{\widetilde{\mathfrak{p}}}(t) + x_{\mathfrak{h}}(t) + x_{\mathfrak{k}}(t),$$

then

$$\dot{x} = [x_{\widetilde{\mathfrak{p}}} + x_{\mathfrak{h}} + x_{\mathfrak{k}}, \mu(x)] = \underbrace{[x_{\widetilde{\mathfrak{p}}}, \mu(x)]}_{\in \mathfrak{p}} + \underbrace{[x_{\mathfrak{h}}, \mu(x)]}_{\in \widetilde{\mathfrak{p}}} + \underbrace{[x_{\mathfrak{k}}, \mu(x)]}_{\in \mathfrak{k}}.$$

Note that $\dot{x}_{\mathfrak{k}} = [x_{\mathfrak{k}}, \mu(x)] \in \mathfrak{k}$, so the flow $x_{\mathfrak{k}}(t)$ is separated from other components and stays in the subalgebra $\mathfrak{k}$ itself. Note also that the vector field $[x_{\widetilde{\mathfrak{p}}}, \mu(x)] \in \mathfrak{p}$ contains both $\mathfrak{h}$ and $\widetilde{\mathfrak{p}}$ components. We want to select

$$\mu(x(t)) = \sum_{\ell=1}^{r} z_\ell(t) k_\ell, \tag{3.2}$$

so that the component of $x(t)$ in the $\widetilde{\mathfrak{p}}$ direction is gradually annihilated. More specifically, our goal is to see that $x_{\widetilde{\mathfrak{p}}}(t) \to 0$ and that $x(t) \longrightarrow \kappa \in \mathfrak{k} \oplus \mathfrak{h}$ as $t \to \infty$.

It suffices also to consider the case that the initial value $\xi \in \mathfrak{p}$. Then $\mathbf{x}(t) \in \mathfrak{p}$ for all t. Upon expansions in terms of the basis, we have two ways to convey the derivative of $\dot{x}(t)$ in the Lax dynamics:

(3.3)

$$\dot{x}(t) = [x(t), \mu(x(t))] = \begin{cases} \sum_{i=1}^{r} \dot{\alpha}_i(t) \widetilde{p}_i + \sum_{j=1}^{s} \dot{\beta}_j(t) h_j, \\ \underbrace{\sum_{\ell=1}^{r} \sum_{i=1}^{r} \alpha_i(t) z_\ell(t) [\widetilde{p}_i, k_\ell]}_{\in \widetilde{\mathfrak{p}} \oplus \mathfrak{h}} + \underbrace{\sum_{j=1}^{s} \sum_{\ell=1}^{r} \beta_j(t) z_\ell(t) [h_j, k_\ell]}_{\in \widetilde{\mathfrak{p}}}. \end{cases}$$

Instead of working with matrices which are large-scale, we can define the Lax dynamics through the combination coefficients which are scalars.

We first characterize the vector field for $\dot{x}_{\mathfrak{h}}$. Introduce the index subsets

$$\begin{cases} \mathfrak{H}_j & := \{\ell | [h_j, k_\ell] \neq 0\}, \\ \mathfrak{K}_j & := \bigcup_{k=j+1}^{s} \mathfrak{H}_k, \end{cases} \quad j = 1, \ldots, s, \tag{3.4}$$

with $\mathfrak{H}_{s+1} = \emptyset$. Define the injective map $\phi_j : \mathfrak{H}_j \to \{1, \ldots, r\}$ such that $\phi_j(\ell)$ is the unique integer satisfying the relationship

$$[h_j, k_\ell] = -c_{j\ell} \widetilde{p}_{\phi_j(\ell)} \tag{3.5}$$

with $c_{j\ell} = \pm 2$. Therefore,

$$[\widetilde{p}_{\phi_j(\ell)}, k_\ell] = c_{j\ell} h_j. \tag{3.6}$$

These collections of indices in $\phi_j(\mathfrak{H}_j)$ help define the flow $\mu(x(t))$ segment by segment. We outline the idea as follows.

Rewrite

$$\sum_{\ell=1}^{r} \sum_{i=1}^{r} \alpha_i(t) z_\ell(t) [\widetilde{p}_i, k_\ell] = \sum_{j=1}^{s} \sum_{\ell \in \mathfrak{H}_j} \alpha_{\phi_j(\ell)} z_\ell c_{j\ell} h_j + \text{terms in } \widetilde{\mathfrak{p}}. \tag{3.7}$$

Therefore,

$$\dot{\beta}_j = \sum_{\ell \in \mathfrak{H}_j} \alpha_{\phi_j(\ell)} z_\ell c_{j\ell}, \quad j = 1, \ldots, s. \tag{3.8}$$

Reorder the basis, if necessary, assume the basis element h_s is such that $\mathfrak{H}_s$ has the largest cardinality. As the first step, define

$$z_\ell(t) := \frac{c_{s\ell}}{4} \alpha_{\phi_s(\ell)}(t), \quad \ell \in \mathfrak{H}_s. \tag{3.9}$$

Then

$$\dot{\beta}_s(t) = \sum_{\ell \in \mathfrak{H}_s} \alpha^2_{\phi_s(\ell)}(t). \tag{3.10}$$

Given that the right-hand side of (3.10) is a sum of squares, $\beta_s(t)$ is nondecreasing. By Theorem 2.4, $x(t)$ preserves its norm, ensuring that all combination coefficients $\alpha_i(t)$ and $\beta_j(t)$ remain bounded, as does the derivative $\dot{\beta}_s(t)$. Intuitively, $\beta_s(t)$ approaches an upper limit, with $\dot{\beta}_s(t) \to 0$ as $t \to \infty$. Consequently,

$$\alpha_{\phi s(\ell)}(t) \to 0, \quad \text{for all } \ell \in \mathfrak{H}_s.$$

Thus, a segment of components of $x(t)$ in the direction of $\widetilde{\mathfrak{p}}$ diminishes to zero. We will confirm this through rigorous stability analysis in Section 6.

We then continue to define the coefficients z_ℓ of $\mu(x(t))$ by segments in the order $j = s-1, \ldots, 1$. Note that the set $\mathfrak{K}_j$ contains all indices ℓ that have been implicated previously up to the jth segment. Rewrite (3.8) as

$$\dot{\beta}_j(t) = \sum_{\ell' \in \mathfrak{K}_j \bigcap \mathfrak{H}_j} \alpha_{\phi_j(\ell')}(t) z_{\ell'}(t) c_{j\ell'} + \sum_{\ell \in \mathfrak{H}_j - \mathfrak{K}_j} \alpha_{\phi_j(\ell)}(t) z_\ell(t) c_{j\ell}. \tag{3.11}$$

Elements $z_{\ell'}(t)$ involved in the first summation of (3.11) have already been defined. If $\mathfrak{H}_j - \mathfrak{K}_j \neq \emptyset$, then similar to (3.9) define

$$z_\ell(t) := \frac{c_{j\ell}}{4} \alpha_{\phi_j(\ell)}(t), \quad \ell \in \mathfrak{H}_j - \mathfrak{K}_j. \tag{3.12}$$

After finitely many segments, we will end up with $\mathfrak{H}_j - \mathfrak{K}_j = \emptyset$, implying that z_ℓ has been defined for all $\ell = 1, \ldots, r$.

Thus far, z_ℓ is defined segment by segment, so it refers to locally specified j and ℓ. When all z_ℓ are defined, it is convenient to re-enumerate the related $c_{j\ell}$ and $\alpha_{\phi_j(\ell)}$ as a one-parameter sequence

$$z_\ell(t) = \frac{c_{\psi(\ell)}}{4}\alpha_{\psi(\ell)}(t), \quad \ell = 1, \dots r, \tag{3.13}$$

where the map $\psi(\ell)$ is meant to indicate the explicit dependence on ℓ, although there is a segment number j involved implicitly in the process of constructing z_ℓ.

Our strategy has been defining the vector fields for $\dot{\beta}_j$, $j = 1, \dots, s$, by matching coefficients of h_j in (3.3). We choose z_ℓ to create perfect square terms in the vector field when possible. Once all z_ℓ, $\ell = 1, \dots, r$, are specified, we also compare coefficients associated with $\widetilde{p}_i$ to define the vector fields for $\dot{\alpha}_i$, $i = 1, \dots, r$. A close examination of (3.3) should manifest that the differential system for the variables $\boldsymbol{\alpha} := [\alpha_1, \dots, \alpha_r]^\top$, $\boldsymbol{\beta} := [\beta_1, \dots, \beta_s]^\top$ is of the form

$$\begin{cases} \dot{\boldsymbol{\alpha}} &= A(\boldsymbol{\beta})\boldsymbol{\alpha} + f(\boldsymbol{\alpha}), \\ \dot{\boldsymbol{\beta}} &= g(\boldsymbol{\alpha}), \end{cases} \tag{3.14}$$

where f and g are homogeneous quadratic polynomials in $\boldsymbol{\alpha}$, and $A(\boldsymbol{\beta})$ is a matrix of size $r \times r$ depending linearly in $\boldsymbol{\beta}$. We will analyze the stability of the system (3.14) and argue that every $\alpha_i(t)$, $i = 1, \dots, r$, will converge to zero, which then implies that $x(t) \longrightarrow \eta \in \mathfrak{h}$ as $t \to \infty$.

4. An example

Consider the case that $\imath\mathcal{H} \in \text{span}\{1, 4, 6, 7, 11, 12, 13\} \in \mathfrak{su}(2^3)$, with $n = 3$ and $\{X, Y, Z, I\}^{\otimes 3}$ forming 64 Pauli strings. The following discussion illustrates the construction of the Lax dynamics. We will also use it to demonstrate the structure of $A(\boldsymbol{\beta})$ and the resulting stability.

The subalgebra

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

is of dimension 30 only. Using θ_1 in (2.16), we find that

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

There are actually five Cartan subalgebras within $\mathfrak{p}$, spanned by the bases

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

respectively, whereas each of which can be reached by some suitable conjugations of others. Suppose we choose

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

to form the Lax dynamics. Thus, $r = 12$ and $s = 6$.

Now we specify the construction of z_ℓ, $\ell = 1, \dots, 12$. For demonstration purpose, we list the commutator table between $\mathfrak{h}$ and $\mathfrak{k}$ below:

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

by which we can conveniently identify the indices in $\mathfrak{H}_j$ and the signs of constants $c_{j\ell}$ needed for forming β_j. However, we stress that this information is readily accessible without creating these subsets physically. For instance, the column numbers of nonzero entries in the last row of $[\mathfrak{h}, \mathfrak{k}]$ are precisely the indices in $\mathfrak{H}_6 = \{1, 3, 5, 6, 7, 9, 11, 12\}$, and the negation of the signs of these entries multiplied by 2 give rise to $c_{s\ell}$, while the indices $\phi_s(\ell)$ are from the corresponding ordinal numbers in $\widetilde{p}$. In this way, the information needed for (3.9) is completely determined. The entire process can be automated.

Following our strategy, we begin defining z_ℓ for $\ell \in \mathfrak{H}_6$ according to (3.9), which gives rise to

$$\begin{cases} z_1 := \frac{\alpha_1}{2}; & z_3 := -\frac{\alpha_2}{2}; & z_5 := \frac{\alpha_4}{2}; & z_6 := \frac{\alpha_6}{2}; \\ z_7 := \frac{\alpha_7}{2}; & z_9 := -\frac{\alpha_8}{2}; & z_{11} := \frac{\alpha_{10}}{2}; & z_{12} := \frac{\alpha_{12}}{2}. \end{cases}$$

We then find that $\mathfrak{H}_5 - \mathfrak{H}_6 = \{2, 4, 8, 10\}$ from which we define the remaining z_ℓ according to (3.12) and obtain

$$\left\{ z_2 := \frac{\alpha_3}{2}; \quad z_4 := \frac{\alpha_5}{2}; \quad z_8 := \frac{\alpha_9}{2}; \quad z_{10} := \frac{\alpha_{11}}{2}. \right.$$

By now, all coefficients z_ℓ needed to characterize $\mu(x(t))$ in (3.2) are specified. Note also that in this example, the map ψ in (3.13) has values $\psi(1) = 1, \psi(2) = 3, \psi(3) = 2, \psi(5) = 4$, and so on. In fact, in this example we can use any two distinct rows of $[\mathfrak{h}, \mathfrak{k}]$ to completely define z_ℓ, $\ell = 1, \dots, 12$. Different row selections yield different sets of z_ℓ's. In each case, the indices of $\alpha_{\phi_j(\ell)}$ needed for defining z_ℓ are from the corresponding ordinal numbers in the basis of $\widetilde{\mathfrak{p}}$.

With this information in hand, the differential equations for the coefficients β_j can be derived. For instance, if the last two rows of $[\mathfrak{h}, \mathfrak{k}]$ are used so that z_ℓ's are defined as above, then we have the differential system:

$$\begin{cases} \dot{\beta}_1 &= 2(\alpha_1\alpha_{12} + \alpha_3\alpha_{11} + \alpha_5\alpha_9 + \alpha_6\alpha_7); \\ \dot{\beta}_2 &= 2(\alpha_3\alpha_9 - \alpha_2\alpha_{10} + \alpha_5\alpha_{11} - \alpha_4\alpha_8); \\ \dot{\beta}_3 &= 2(\alpha_1\alpha_7 + \alpha_2\alpha_8 + \alpha_4\alpha_{10} + \alpha_6\alpha_{12}); \\ \dot{\beta}_4 &= 2(\alpha_1\alpha_6 + \alpha_3\alpha_5 + \alpha_7\alpha_{12} + \alpha_9\alpha_{11}); \\ \dot{\beta}_5 &= \alpha_3^2 + \alpha_5^2 + \alpha_9^2 + \alpha_{11}^2 - 2(\alpha_2\alpha_4 + \alpha_8\alpha_{10}); \\ \dot{\beta}_6 &= \alpha_1^2 + \alpha_2^2 + \alpha_4^2 + \alpha_6^2 + \alpha_7^2 + \alpha_8^2 + \alpha_{10}^2 + \alpha_{12}^2, \end{cases}$$

which is in the form $\dot{\boldsymbol{\beta}} = g(\boldsymbol{\alpha})$, where g is a homogeneous quadratic polynomial system in $\boldsymbol{\alpha}$.

As is expected by design, observe that $\dot\beta_6(t) \ge 0$, which is exactly the reason of choosing $z_\ell(t)$ in the specified way. Since $\beta_6(t)$ is bounded above, it is expected that $\dot\beta_6(t) \to 0$ as $t \to \infty$, leading to $\alpha_i(t) \to 0$ for $i \in \mathfrak{H}_6$. This effect cascades to $\dot\beta_5(t)$, causing $\alpha_i(t) \to 0$ for $i \in \mathfrak{H}_5$, and spills further into other $\dot\beta_i(t)$. We shall argue through rigorous stability analysis in the next section that this expectation indeed is the case in general.

With the same set of z_ℓ's defined, we also match coefficients of $\widetilde{p}_i$ in (3.3) to retrieve information for $\dot\alpha_i$, $i = 1, \ldots, 12$, each of which will depend on a mixture of α_k and β_j. Again, the retrieval process can be accomplished by merely checking through proper indices. For this particular example, the details of the differential equations for α_k's are as follows:

$$\begin{cases}
\dot\alpha_1 &= \alpha_4\,\alpha_{11} - \alpha_5\,\alpha_8 - \alpha_2\,\alpha_{11} + \alpha_5\,\alpha_{10} - \alpha_1\,\beta_6 - \alpha_6\,\beta_4 - \alpha_7\,\beta_3 - \alpha_{12}\,\beta_1\\
\dot\alpha_2 &= \alpha_4\,\beta_5 - \alpha_5\,\alpha_7 - \alpha_3\,\alpha_{12} - \alpha_6\,\alpha_9 - \alpha_2\,\beta_6 - \alpha_1\,\alpha_{11} - \alpha_8\,\beta_3 + \alpha_{10}\,\beta_2\\
\dot\alpha_3 &= 2\,\alpha_4\,\alpha_{12} + 2\,\alpha_6\,\alpha_{10} - \alpha_3\,\beta_5 - \alpha_5\,\beta_4 - \alpha_9\,\beta_2 - \alpha_{11}\,\beta_1\\
\dot\alpha_4 &= \alpha_2\,\beta_5 - \alpha_5\,\alpha_7 - \alpha_3\,\alpha_{12} - \alpha_6\,\alpha_9 - \alpha_1\,\alpha_{11} - \alpha_4\,\beta_6 + \alpha_8\,\beta_2 - \alpha_{10}\,\beta_3\\
\dot\alpha_5 &= 2\,\alpha_1\,\alpha_8 + 2\,\alpha_2\,\alpha_7 - \alpha_3\,\beta_4 - \alpha_5\,\beta_5 - \alpha_9\,\beta_1 - \alpha_{11}\,\beta_2\\
\dot\alpha_6 &= \alpha_2\,\alpha_9 + \alpha_3\,\alpha_8 - \alpha_3\,\alpha_{10} - \alpha_4\,\alpha_9 - \alpha_1\,\beta_4 - \alpha_7\,\beta_1 - \alpha_6\,\beta_6 - \alpha_{12}\,\beta_3\\
\dot\alpha_7 &= \alpha_4\,\alpha_5 - \alpha_2\,\alpha_5 - \alpha_8\,\alpha_{11} + \alpha_{10}\,\alpha_{11} - \alpha_1\,\beta_3 - \alpha_6\,\beta_1 - \alpha_7\,\beta_6 - \alpha_{12}\,\beta_4\\
\dot\alpha_8 &= \alpha_4\,\beta_2 - \alpha_3\,\alpha_6 - \alpha_7\,\alpha_{11} - \alpha_9\,\alpha_{12} - \alpha_2\,\beta_3 - \alpha_1\,\alpha_5 - \alpha_8\,\beta_6 + \alpha_{10}\,\beta_5\\
\dot\alpha_9 &= 2\,\alpha_4\,\alpha_6 + 2\,\alpha_{10}\,\alpha_{12} - \alpha_3\,\beta_2 - \alpha_5\,\beta_1 - \alpha_9\,\beta_5 - \alpha_{11}\,\beta_4\\
\dot\alpha_{10} &= \alpha_2\,\beta_2 - \alpha_3\,\alpha_6 - \alpha_7\,\alpha_{11} - \alpha_9\,\alpha_{12} - \alpha_1\,\alpha_5 - \alpha_4\,\beta_3 + \alpha_8\,\beta_5 - \alpha_{10}\,\beta_6\\
\dot\alpha_{11} &= 2\,\alpha_1\,\alpha_2 + 2\,\alpha_7\,\alpha_8 - \alpha_3\,\beta_1 - \alpha_5\,\beta_2 - \alpha_9\,\beta_4 - \alpha_{11}\,\beta_5\\
\dot\alpha_{12} &= \alpha_2\,\alpha_3 - \alpha_3\,\alpha_4 + \alpha_8\,\alpha_9 - \alpha_9\,\alpha_{10} - \alpha_1\,\beta_1 - \alpha_6\,\beta_3 - \alpha_7\,\beta_4 - \alpha_{12}\,\beta_6,
\end{cases}$$

which is in the form $\dot{\boldsymbol{\alpha}} = A(\boldsymbol{\beta})\boldsymbol{\alpha} + f(\boldsymbol{\alpha})$, where f is a homogeneous quadratic polynomial system in $\boldsymbol{\alpha}$ and A is linear in $\boldsymbol{\beta}$. We will study the structure of $A(\boldsymbol{\beta})$ to to extract its spectral information.

Though it is not necessarily the most ideal environment, we have developed an experimental general-purpose code written in Matlab that implements the above-mentioned construction. From any given Hamiltonian $\mathcal{H}$, we can generate the Hamiltonian subalgebra $\mathfrak{g}(\imath\mathcal{H})$, the Cartan subalgebra $\mathfrak{h}$, all other essential information, and the differential system (3.14) automatically. This code is available to interested readers upon request.

5. Structure analysis

Thus far, we have explained how to construct a special Lax dynamics (2.15) with the hope of obtaining the factorization (2.7) numerically. Of practical importance is that the dynamics system is built entirely upon the combination coefficients $\boldsymbol{\alpha} := [\alpha_1, \ldots, \alpha_r]^\top$ and $\boldsymbol{\beta} := [\beta_1, \ldots, \beta_s]^\top$ of the fixed basis of $\mathfrak{g}(\imath\mathcal{H})$. We have completely avoided invoking matrices in $\mathbb{C}^{2^n \times 2^n}$. We have shown that $\boldsymbol{\alpha}(t)$ and $\boldsymbol{\beta}(t)$ are governed by the differential system (3.14). For our purpose, it remains to show that $\boldsymbol{\alpha}(t) \to 0$ as $t \to \infty$.

It is clear that the equilibrium points $\{(0,\boldsymbol{\beta})|\boldsymbol{\beta}$ arbitrary$\}$ form a subspace which is also a center manifold. In order to understand the stable or unstable manifold passing through these equilibrium points, we need information about the spectrum of $A(\boldsymbol{\beta})$. See the theory in [7]. In order to understand the spectrum of $A(\boldsymbol{\beta})$, we first study its structure.

5.1. **Symmetry of $A(\boldsymbol{\beta})$.** For each $i=1,\dots,r$, define the index-ordered set

$$\mathfrak{L}_i := \uplus\{\ell|\phi_j(\ell)=i, \text{ for some } 1\le j\le s\}, \tag{5.1}$$

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

$$\mathfrak{J}_i := \uplus\{j|\phi_j^{-1}(i)\neq\emptyset\} \tag{5.2}$$

be the index subset ordered according to that in $\mathfrak{L}_i$. The ordering will be used later, when specifying the position of that element is important; otherwise, without causing ambiguity, $\mathfrak{J}_i$ and $\mathfrak{L}_i$ are also used to denote subsets of mere integers.

Observe that the second summation in (3.3) can be expressed as

(5.3)

$$\sum_{j=1}^{s}\sum_{\ell=1}^{r}\beta_j z_\ell[h_j,k_\ell]=\sum_{j=1}^{s}\sum_{\ell\in\mathfrak{H}_j}\beta_j z_\ell(-c_{j\ell}\widetilde{p}_{\phi_j(\ell)})=-\sum_{i=1}^{r}\left(\sum_{j\in\mathfrak{J}_i}\beta_j z_{\phi_j^{-1}(i)}c_{j\phi_j^{-1}(i)}\right)\widetilde{p}_i,$$

where we have replaced ℓ by $z_{\phi_j^{-1}(i)}$ which, given by either (3.9) or (3.12), depends linearly on one particular element in the array $\boldsymbol{\alpha}$. In this way, the elements of $A(\boldsymbol{\beta})$ in (3.14) can easily be identified. That is, the $(i,\psi(\phi_j^{-1}(i)))$ entry of $A(\boldsymbol{\beta})$ is of value $-\beta_j\frac{c_{\psi(\phi_j^{-1}(i))}c_{j\phi_j^{-1}(i)}}{4}$. Depending on the values of $c_{\psi(\phi_j^{-1}(i))}$ and $c_{j\phi_j^{-1}(i)}$, the fraction is ±1.

The matrix $A(\boldsymbol{\beta})$ corresponding to the preceding section, for example, is given by

$$A(\boldsymbol{\beta})=\begin{bmatrix}
-\beta_6 & 0 & 0 & 0 & 0 & -\beta_4 & -\beta_3 & 0 & 0 & 0 & 0 & -\beta_1\\
0 & -\beta_6 & 0 & \beta_5 & 0 & 0 & 0 & -\beta_3 & 0 & \beta_2 & 0 & 0\\
0 & 0 & -\beta_5 & 0 & -\beta_4 & 0 & 0 & 0 & -\beta_2 & 0 & -\beta_1 & 0\\
0 & \beta_5 & 0 & -\beta_6 & 0 & 0 & 0 & \beta_2 & 0 & -\beta_3 & 0 & 0\\
0 & 0 & -\beta_4 & 0 & -\beta_5 & 0 & 0 & 0 & -\beta_1 & 0 & -\beta_2 & 0\\
-\beta_4 & 0 & 0 & 0 & 0 & -\beta_6 & -\beta_1 & 0 & 0 & 0 & 0 & -\beta_3\\
-\beta_3 & 0 & 0 & 0 & 0 & -\beta_1 & -\beta_6 & 0 & 0 & 0 & 0 & -\beta_4\\
0 & -\beta_3 & 0 & \beta_2 & 0 & 0 & 0 & -\beta_6 & 0 & \beta_5 & 0 & 0\\
0 & 0 & -\beta_2 & 0 & -\beta_1 & 0 & 0 & 0 & -\beta_5 & 0 & -\beta_4 & 0\\
0 & \beta_2 & 0 & -\beta_3 & 0 & 0 & 0 & \beta_5 & 0 & -\beta_6 & 0 & 0\\
0 & 0 & -\beta_1 & 0 & -\beta_2 & 0 & 0 & 0 & -\beta_4 & 0 & -\beta_5 & 0\\
-\beta_1 & 0 & 0 & 0 & 0 & -\beta_3 & -\beta_4 & 0 & 0 & 0 & 0 & -\beta_6
\end{bmatrix}.$$

This matrix exhibits some peculiar patterns, such as its symmetry and the recurrence of the same subsets of $\boldsymbol{\beta}$ in columns. We shall explore these patterns subsequently to help the stability analysis.

Theorem 5.1 asserts that this symmetry is in fact true in general and hence the eigenvalues of $A(\boldsymbol{\beta})$ are always real.

Theorem 5.1. *Given a fixed $1\le i\le r$, then for any $j\in\mathfrak{J}_i$ it is true that*

$$\mathfrak{J}_{\psi(\phi_j^{-1}(i))}=\mathfrak{J}_i. \tag{5.4}$$

It follows that

$$\psi(\phi_j^{-1}(\psi(\phi_j^{-1}(i))))=i, \quad \text{for all } j\in\mathfrak{J}_i. \tag{5.5}$$

The entries of $A(\boldsymbol{\beta})$ at $(i, \psi(\phi_j^{-1}(i)))$ and $(\psi(\phi_j^{-1}(i)), i)$ are the same, i.e., $A(\boldsymbol{\beta})$ is symmetric.

Proof. : Suppose $i \in \phi_s(\mathfrak{H}_s)$. Denote $\ell = \phi_s^{-1}(i)$. Then $\ell \in \mathfrak{H}_s$ and $s \in \mathfrak{J}_i$. By definition (3.9), $\psi(\ell) = \phi_s(\ell)$. Therefore, $\psi(\phi_s^{-1}(i)) = i$. If there exists an element $j \in \mathfrak{J}_i$ which is distinct from s, denote $w = \phi_j^{-1}(i)$. Then $w \in \mathfrak{H}_j$, but $w \notin \mathfrak{H}_s$. Without loss of generality, assume that $w \in \mathfrak{H}_j - \mathfrak{K}_j$. By definition (3.12), $\psi(w) = \phi_j(w)$. We still have $\psi(\phi_j^{-1}(i)) = i$.

Suppose $i \in \phi_{s-1}(\mathfrak{H}_{s-1} - \mathfrak{K}_{s-1})$. Denote $\ell = \phi_{s-1}^{-1}(i)$. Then $\ell \in \mathfrak{H}_{s-1} - \mathfrak{K}_{s-1}$ and $s - 1 \in \mathfrak{J}_i$. By definition (3.12), $\psi(\ell) = \phi_{s-1}(\ell)$. Therefore, $\psi(\phi_{s-1}^{-1}(i)) = i$. Repeatedly applying the same argument, (5.4) is proved. □

A close examination shows that, without referring to the differential system for $\boldsymbol{\alpha}(t)$, we can generate elements of $A(\boldsymbol{\beta})$ directly as follows:

Theorem 5.2. *Let Ψ denote the permutation matrix represented by the integer array $[\psi(1), \ldots, \psi(r)]$. Then the q-th column (and row) of the matrix $\Psi^\top A(\boldsymbol{\beta})\Psi$ can be characterized as follows:*

1. *Nonzero entries occur only at the positions specified by indices in $\mathfrak{L}_{\psi(q)}$.*
2. *The values of the nonzero entries are $\pm\beta_{\mathfrak{J}_{\psi(q)}}$.*
3. *If the (p, q) entry of $\Psi^\top A(\boldsymbol{\beta})\Psi$ is not zero, then its sign is $-\mathrm{sgn}(c_{\psi(q)}c_{jq})$ where j is such that $\phi_j(q) = \psi^{-1}(p)$.*

Proof. Note first that the representation of Ψ means the action $\psi(i) \to i$, i.e., the $\psi(i)$-th entry is swapped to the i-th entry, which is in fact the inverse map of ψ. We have already argued that, by (5.3), the nonzero entries of $A(\boldsymbol{\beta})$ occurs at positions $(i, \psi(\phi_j^{-1}(i)))$ and $(\psi(\phi_j^{-1}(i)), i)$, $i = 1, \ldots, r$, $j \in \mathfrak{J}_i$, with values $\pm\beta_j$ where the sign is determined by that of the product $c_{\psi(\phi_j^{-1}(i))}c_{j\phi_j^{-1}(i)}$. After the permutation, these elements are relocated to the positions $(\psi^{-1}(i), \phi_j^{-1}(i))$ and $(\phi_j^{-1}(i), \psi^{-1}(i))$. Denote $q := \psi^{-1}(i)$. Then $\phi_j^{-1}(i) = \phi_j^{-1}(\psi(q)) \in \mathfrak{L}_{\psi(q)}$.

The above argument can also be interpreted as, for a fixed q, the j value that makes $\phi_j^{-1}(\psi(q)) \neq \emptyset$ are those in $\mathfrak{J}_{\psi(q)}$ by the definition (5.2). □

5.2. **An example continued.** A demonstration of applying the above theorem to our preceding example should help to see better the structure of $A(\boldsymbol{\beta})$. The permutation resulted from (3.13) is represented by

$$\Psi = [1, 3, 2, 5, 4, 6, 7, 9, 8, 11, 10, 12].$$

Thus, we find that

$$\Psi^\top A(\boldsymbol{\beta})\Psi = \begin{bmatrix}
-\beta_6 & 0 & 0 & 0 & 0 & -\beta_4 & -\beta_3 & 0 & 0 & 0 & 0 & -\beta_1 \\
0 & -\beta_5 & 0 & -\beta_4 & 0 & 0 & 0 & -\beta_2 & 0 & -\beta_1 & 0 & 0 \\
0 & 0 & -\beta_6 & 0 & \beta_5 & 0 & 0 & 0 & -\beta_3 & 0 & \beta_2 & 0 \\
0 & -\beta_4 & 0 & -\beta_5 & 0 & 0 & 0 & -\beta_1 & 0 & -\beta_2 & 0 & 0 \\
0 & 0 & \beta_5 & 0 & -\beta_6 & 0 & 0 & 0 & \beta_2 & 0 & -\beta_3 & 0 \\
-\beta_4 & 0 & 0 & 0 & 0 & -\beta_6 & -\beta_1 & 0 & 0 & 0 & 0 & -\beta_3 \\
-\beta_3 & 0 & 0 & 0 & 0 & -\beta_1 & -\beta_6 & 0 & 0 & 0 & 0 & -\beta_4 \\
0 & -\beta_2 & 0 & -\beta_1 & 0 & 0 & 0 & -\beta_5 & 0 & -\beta_4 & 0 & 0 \\
0 & 0 & -\beta_3 & 0 & \beta_2 & 0 & 0 & 0 & -\beta_6 & 0 & \beta_5 & 0 \\
0 & -\beta_1 & 0 & -\beta_2 & 0 & 0 & 0 & -\beta_4 & 0 & -\beta_5 & 0 & 0 \\
0 & 0 & \beta_2 & 0 & -\beta_3 & 0 & 0 & 0 & \beta_5 & 0 & -\beta_6 & 0 \\
-\beta_1 & 0 & 0 & 0 & 0 & -\beta_3 & -\beta_4 & 0 & 0 & 0 & 0 & -\beta_6
\end{bmatrix}.$$

Theorem 5.2 can be interpreted as that the row indices (and column indices as well, by symmetry) of nontrivial entries in $\Psi^\top A(\boldsymbol{\beta})\Psi$ per column are recorded as

columns of the matrix

$$\mathfrak{L}_\psi := [\mathfrak{L}_{\psi(1)}, \dots \mathfrak{L}_{\psi(12)}] = \begin{bmatrix} 1 & 2 & 3 & 2 & 3 & 1 & 1 & 2 & 3 & 2 & 3 & 1 \\ 6 & 4 & 5 & 4 & 5 & 6 & 6 & 4 & 5 & 4 & 5 & 6 \\ 7 & 8 & 9 & 8 & 9 & 7 & 7 & 8 & 9 & 8 & 9 & 7 \\ 12 & 10 & 11 & 10 & 11 & 12 & 12 & 10 & 11 & 10 & 11 & 12 \end{bmatrix},$$

while the indices of the corresponding $\boldsymbol{\beta}$ variables in each corresponding column are given by the matrix

$$\mathfrak{J}_\psi := [\mathfrak{J}_{\psi(1)}, \dots \mathfrak{J}_{\psi(12)}] = \begin{bmatrix} 6 & 5 & 6 & 4 & 5 & 4 & 3 & 2 & 3 & 1 & 2 & 1 \\ 4 & 4 & 5 & 5 & 6 & 6 & 1 & 1 & 2 & 2 & 3 & 3 \\ 3 & 2 & 3 & 1 & 2 & 1 & 6 & 5 & 6 & 4 & 5 & 4 \\ 1 & 1 & 2 & 2 & 3 & 3 & 4 & 4 & 5 & 5 & 6 & 6 \end{bmatrix}.$$

Note that $\mathfrak{L}_\psi$ has identical columns and that the entries from the corresponding columns in $\mathfrak{J}_\psi$ form the same subsets of indices. We shall explain why and where these clusters occur in the next section. For now, if we introduce by merely inspection the permutation matrix $P := [1, 6, 7, 12, 2, 4, 8, 10, 3, 5, 9, 11]$, then the diagonal block structure shows up:

$$P^\top \Psi^\top A(\boldsymbol{\beta}) \Psi P = \begin{bmatrix} -\beta_6 & -\beta_4 & -\beta_3 & -\beta_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\beta_4 & -\beta_6 & -\beta_1 & -\beta_3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\beta_3 & -\beta_1 & -\beta_6 & -\beta_4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\beta_1 & -\beta_3 & -\beta_4 & -\beta_6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\beta_5 & -\beta_4 & -\beta_2 & -\beta_1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\beta_4 & -\beta_5 & -\beta_1 & -\beta_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\beta_2 & -\beta_1 & -\beta_5 & -\beta_4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\beta_1 & -\beta_2 & -\beta_4 & -\beta_5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\beta_6 & \beta_5 & -\beta_3 & \beta_2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \beta_5 & -\beta_6 & \beta_2 & -\beta_3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\beta_3 & \beta_2 & -\beta_6 & \beta_5 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \beta_2 & -\beta_3 & \beta_5 & -\beta_6 \end{bmatrix}. \tag{5.6}$$

It is further noticed that, regardless of the values of $\boldsymbol{\beta}$, each diagonal block of $P^\top \Psi^\top A(\boldsymbol{\beta}) \Psi P$ has the same set of eigenvectors. Indeed, the columns of the Hadamard matrix of order 4:

$$H_4 = \begin{bmatrix} 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

are the eigenvectors. The question is what $\boldsymbol{\beta}$ will produce negative eigenvalues so as to make an equilibrium point $(0, \boldsymbol{\beta})$ asymptotically stable or, more fundamentally, whether such a point exists at all.

To answer this question, let $\Lambda = \operatorname{diag}(\lambda_1, \dots, \lambda_4)$ denote the diagonal matrix with desired eigenvalues. We consider the inverse eigenvalue problem of reconstructing the blocks of $P^\top \Psi^\top A(\boldsymbol{\beta}) \Psi P$ from Λ. That is, from

$$H_4 \Lambda H_4^{-1} = \frac{1}{4} \begin{bmatrix} \lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 & \lambda_1 + \lambda_2 - \lambda_3 - \lambda_4 & \lambda_1 - \lambda_2 + \lambda_3 - \lambda_4 & \lambda_1 - \lambda_2 - \lambda_3 + \lambda_4 \\ \lambda_1 + \lambda_2 - \lambda_3 - \lambda_4 & \lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 & \lambda_1 - \lambda_2 - \lambda_3 + \lambda_4 & \lambda_1 - \lambda_2 + \lambda_3 - \lambda_4 \\ \lambda_1 - \lambda_2 + \lambda_3 - \lambda_4 & \lambda_1 - \lambda_2 - \lambda_3 + \lambda_4 & \lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 & \lambda_1 + \lambda_2 - \lambda_3 - \lambda_4 \\ \lambda_1 - \lambda_2 - \lambda_3 + \lambda_4 & \lambda_1 - \lambda_2 + \lambda_3 - \lambda_4 & \lambda_1 + \lambda_2 - \lambda_3 - \lambda_4 & \lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 \end{bmatrix}, \tag{5.7}$$

we want to match (5.7) with the blocks of (5.6). It quickly becomes clear that, by the way the block is structured, it suffices to solve the equation

$$\tilde{H}_4 \boldsymbol{\lambda} := \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \\ \lambda_4 \end{bmatrix} = 4\mathbf{b} \tag{5.8}$$

by matching $\mathbf{b}$ with the first column of the corresponding blocks. We do so independently for each block. We also have $\mathbf{b} = \frac{1}{4} \tilde{H}_4^{-1} \boldsymbol{\lambda}$ with any specified $\{\lambda_1, \dots, \lambda_4\}$. It is now obvious that there are infinitely many choices of $\mathbf{b}$ such that the resulting eigenvalues of $A(\boldsymbol{\beta})$ are all negative, and vice versa. We thus conclude that the center manifold does contain a feasible region of $\boldsymbol{\beta}$ at which $A(\boldsymbol{\beta})$ has negative eigenvalues, that is, when the flow $\boldsymbol{\alpha}(t), \boldsymbol{\beta}(t)$ defined in Section 2.3 is close enough

to this region, it will be attracted to an asymptotically stable equilibrium on the center manifold.

5.3. **Block structure in general.** The above structure, that there are identical columns $\mathfrak{L}_i$ which can be grouped together, is true in general. We now explain why these grouping arises. Since $A(\boldsymbol{\beta})$ is completely determined by (5.3), the discussion is focused on the $[\mathfrak{h}, \mathfrak{k}]$ table, especially on how a cluster of $\widetilde{p}_i$'s can be produced by using the same subsets of h_j's and k_ℓ's in different combinations. The analysis relies on our recent result that the Cartan pair $(\mathfrak{k}, \widetilde{\mathfrak{p}})$ of any subalgebra in $\mathfrak{su}(2^n)$ can be partitioned in pairs as direct sums of commutative subalgebras [19]. To maintain focus on the stability analysis of Lax dynamics, we summarize known results about these clusters, with detailed proofs available in [19].

First, we identify the distribution of zero elements in the $[\mathfrak{h}, \mathfrak{k}]$ table.

Lemma 5.3. *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 $[\widetilde{p}_i, h_\sigma] = 0$. In this case, $[h_\sigma, k_{\ell_\zeta}] = 0$ for all $\ell_\zeta \in \mathfrak{L}_i$. Conversely, 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 $[h_\sigma, k_{\ell_\zeta}]$ is a nontrivial element in $\widetilde{\mathfrak{p}}$ for every $\ell_\zeta \in \mathfrak{L}_i$.*

Then, we collect the nonzero elements in $[\mathfrak{h}, \mathfrak{k}]$ table to groups. Choose an arbitrary index $j_\tau \in \mathfrak{J}_i$. By definition, we already have $[h_{j_\tau}, k_{\ell_\tau}] = -c_{j_\tau \ell_\tau} \widetilde{p}_i \neq 0$. By the above lemma, 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

$$\mathfrak{p}_i := \{\widetilde{p}_{\phi_{j_\tau}(\ell_\zeta)} | j_\tau \in \mathfrak{J}_i, \ell_\zeta \in \mathfrak{L}_i\}, \tag{5.9}$$

$$\mathfrak{k}_i := \{k_{\ell_\zeta} | \ell_\zeta \in \mathfrak{L}_i\}. \tag{5.10}$$

Theorem 5.4 lists properties within $\mathfrak{p}_i$ and $\mathfrak{k}_i$ which eventually characterize the intrinsic commutative substructures within the Cartan pair $(\mathfrak{k}, \widetilde{\mathfrak{p}})$.

Theorem 5.4. *For a fixed $1 \leq i \leq r$,*

1. *The subspace spanned by $\mathfrak{k}_i$ is a commutative subalgebra of $\mathfrak{k}$.*
2. *The subspace spanned by $\mathfrak{p}_i$ forms a commutative subalgebra of $\widetilde{p}$.*
3. *The three subsets $\mathfrak{p}_i$, $\mathfrak{L}_i$ and $\mathfrak{J}_i$ have the same cardinality.*
4. *For each $\widetilde{p}_\gamma \in \mathfrak{p}_i$,*
   (a) *$\mathfrak{L}_\gamma = \mathfrak{L}_i$ in identical ordering.*
   (b) *$\mathfrak{J}_\gamma = \mathfrak{J}_i$ only setwise.*
   (c) *$\mathfrak{p}_\gamma = \mathfrak{p}_i$.*

Accordingly, we find that, in addition to the fact that $\mathfrak{h}$ is already a maximal commutative subalgebra in $\mathfrak{p}$, the collection of these $\mathfrak{p}_i$'s defined in (5.9) classifies $\widetilde{\mathfrak{p}}$ into disjoint commutative subalgebras. Likewise, the sets $\mathfrak{k}_i$ defined in (5.10) divide the subalgebra $\mathfrak{k}$ into disjoint commutative subalgebras. Furthermore, there are as many subalgebras $\mathfrak{k}_i$ in $\mathfrak{k}$ as there are subalgebras $\mathfrak{p}_i$ in $\widetilde{\mathfrak{p}}$. This partition holds for the Cartan decomposition of any subalgebra $\mathfrak{g}$ in $\mathfrak{su}(2^n)$. In particular, we have

$$\mathfrak{g}(\imath\mathcal{H}) = \underbrace{\bigoplus_i \text{span}(\mathfrak{k}_i)}_{\mathfrak{k}} \underbrace{\bigoplus_i \text{span}(\mathfrak{p}_i)}_{\widetilde{\mathfrak{p}}} \oplus \mathfrak{h}. \tag{5.11}$$

Such a structure and regrouping has been seen in the expressions of $\mathfrak{L}_\psi$ and $\mathfrak{J}_\psi$ in Section 5.2.

For a given $\widetilde{p}_i$, enumerate elements in $\mathfrak{J}_i$ and $\mathfrak{L}_i$ with superscripts such as $j_\mu^{(i)}$, $\ell_\eta^{(i)}$, respectively, where the subscripts $_\mu$ and $_\eta$ refer to their ordinal numbers in the respective ordered sets. By definition, when $(j_\mu^{(i)}, \ell_\mu^{(i)})$ is paired together, it is universally true that

$$[h_{j_\mu^{(i)}}, k_{\ell_\mu^{(i)}}] = -c_{j_\mu^{(i)}\ell_\mu^{(i)}}\widetilde{p}_i, \tag{5.12}$$

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 sometime suppress the writing of the superscript $^{(i)}$. Based on these, we can write (5.3) as

$$\sum_{j=1}^{s}\sum_{\ell=1}^{r}\beta_j(t)z_\ell(t)[h_j, k_\ell] = -\sum_i \sum_{\widetilde{p}_\gamma \in \mathfrak{p}_i}\left(\sum_{j_\mu^{(\gamma)} \in \mathfrak{J}_\gamma} \beta_{j_\mu^{(\gamma)}} z_{\ell_\mu^{(\gamma)}} c_{j_\mu^{(\gamma)}\ell_\mu^{(\gamma)}}\right)\widetilde{p}_\gamma, \tag{5.13}$$

where the first summation on the right-hand side for i is to run over all possible disjoint subsets $\mathfrak{p}_i$ and then, for each $\widetilde{p}_\gamma \in \mathfrak{p}_i$, $\ell_\mu^{(\gamma)} \in \mathfrak{L}_\gamma$ is automatically associated with $j_\mu^{(\gamma)} \in \mathfrak{J}_\gamma$. Since $\mathfrak{L}_\gamma = \mathfrak{L}_i$, the subset $\{z_{\ell_\mu^{(\gamma)}}\}$, and the corresponding subset $\{\alpha_{\psi(\ell_\mu^{(\gamma)})}\}$, is the same for all $\widetilde{p}_\gamma \in \mathfrak{p}_i$. Therefore, we may rewrite the first part of (3.14) as

$$\mathfrak{P}\dot{\boldsymbol{\alpha}} = (\mathfrak{P}A(\boldsymbol{\beta})\mathfrak{P}^\top)(\mathfrak{P}\boldsymbol{\alpha}) + \mathfrak{P}f(\boldsymbol{\alpha}), \tag{5.14}$$

where $\mathfrak{P}$ is the permutation arranging entries of the vector $\mathfrak{P}\boldsymbol{\alpha}$ in such a way that, for each disjoint $\mathfrak{L}_i$, all $\boldsymbol{\alpha}_{\psi(\mathfrak{L}_i)}$ are grouped together. In other words, for each $\widetilde{p}_\gamma \in \mathfrak{p}_i$, it is the collection of all $\beta_{j_\mu^{(\gamma)}}$ with proper signs, $j_\mu^{(\gamma)} \in \mathfrak{J}_\gamma$, that constitutes one row of the block. Since $\mathfrak{J}_\gamma = \mathfrak{J}_i$ setwise, rows in this block are made of the same set of elements, but in different order. The block structure in (5.6) is thus explained with that special $\mathfrak{P} = (\Psi P)^\top$. Because $\mathfrak{P}A(\boldsymbol{\beta})\mathfrak{P}^\top$ remains symmetric, we happen to have also proved the following results.

Theorem 5.5. *With regard to the set* $\mathfrak{p}_i$*,*

1. *Each block is necessarily a square matrix and is symmetric.*
2. $\mathfrak{p}_i = \{\widetilde{p}_\gamma | \gamma \in \psi(\mathfrak{L}_i)\}$.

6. Stability analysis

In the above, we have employed our earlier work [19] that the pair $(\mathfrak{k}, \widetilde{\mathfrak{p}})$ can be decomposed into disjoint commutative subalgebras to explain why the matrix $A(\boldsymbol{\beta})$ can be organized into a block diagonal form through proper permutations. Thus, the mechanism described in Section 4 can be applied to the general case, and the procedure can be automated. Based on (5.13), the subscripts for elements of $\boldsymbol{\beta}$ in the diagonal blocks of $\mathfrak{P}A(\boldsymbol{\beta})\mathfrak{P}^\top$ are precisely those of the various $\mathfrak{J}_\gamma$, where γ is such that $\widetilde{p}_\gamma \in \mathfrak{p}_i$.

Although the block sizes of $\mathfrak{P}A(\boldsymbol{\beta})\mathfrak{P}^\top$ are not necessarily the same, we have observed in our experiments consistently that there is an interesting symmetry such as that manifested in (5.6) within each block. That is, the diagonal blocks of $\mathfrak{P}A(\boldsymbol{\beta})\mathfrak{P}^\top$ are super-centrosymmetric in that they consist of centrosymmetric sub-blocks each of which is nested with centrosymmetric sub-blocks, and this trend

continues until the core is reduced to a singleton. The structure of the diagonal blocks of $\mathfrak{P}A(\boldsymbol{\beta})\mathfrak{P}^\top$ may be more precisely described as having the form

$$I \otimes \Xi + X \otimes \Upsilon = \begin{bmatrix} \Xi & \Upsilon \\ \Upsilon & \Xi \end{bmatrix} \tag{6.1}$$

with I being the 2×2 identity matrix and X the first Pauli matrix, where the blocks Ξ and Υ themselves are also of the same form but are generated from some one-half size smaller centrosymmetric matrices which are themselves of the same form, and this trend repeats.

To characterize the block structure, it suffices to consider the collective arrangement of elements in the $[\mathfrak{h}, \mathfrak{k}]$ table. By our theory above, it is the structure of $\mathfrak{J}_\gamma$, $\gamma \in \mathfrak{p}_i$, that matters. Starting with $\mathcal{H}_1$ consisting of one arbitrary term of $\mathcal{H}$, we gradually add one additional term at a time to form $\mathcal{H}_{k-1} \subset \mathcal{H}_k$ until all terms of $\mathcal{H}$ are exhausted. We then generate the chain

$$\mathfrak{g}(\imath\mathcal{H}_1) \subseteq \mathfrak{g}(\imath\mathcal{H}_2) \ldots \subseteq \mathfrak{g}(\imath\mathcal{H}). \tag{6.2}$$

In this way, we progressively expand the $[\mathfrak{h}, \mathfrak{k}]$ table and its subsets $\mathfrak{L}i$, $\mathfrak{J}i$, and $\widetilde{p}i$. To track changes relative to a fixed $\widetilde{p}i$, we use the superscript $^{[k]}$, such as in $\mathfrak{p}i^{[k]}$ and $\mathfrak{J}i^{[k]}$, indicating quantities related to $\mathfrak{g}(\imath\mathcal{H}_k)$. The crossover relationship [19] facilitates constructing the table from a simple singleton.

Lemma 6.1. *For a fixed $1 \le i \le r$, 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 γ. Then the identity*

$$[h_{j_\mu}, k_{\ell_\zeta}] = \pm[h_{j_\nu}, k_{\ell_\eta}] \tag{6.3}$$

holds. Indeed, the subspace

$$\operatorname{span}\{k_{\ell_\eta}, k_{\ell_\zeta}\} \oplus \operatorname{span}\{\widetilde{p}_\gamma, \widetilde{p}_{\phi_{j_\mu}(\ell_\zeta)}\} \oplus \operatorname{span}\{h_{j_\mu}, h_{j_\nu}\} \tag{6.4}$$

stands alone as a subalgebra with its own Cartan decomposition.

We already know, by (5.12), that $\phi_{j_\eta}(\ell_\eta) = \phi_{j_\zeta}(\ell_\zeta) = i$ for arbitrary η and ζ. Thus, a special case of (6.3) is that

$$[h_{j_\eta}, k_{\ell_\zeta}] = \pm[h_{j_\zeta}, k_{\ell_\eta}] \tag{6.5}$$

always holds, which implies the following fact.

Corollary 6.2. *Except for possible singletons, every column in the block must be paired with one and only one other column. No block of $\mathfrak{P}A(\boldsymbol{\beta})\mathfrak{P}^\top$ can be of odd size.*

Consider the scenario that in $\mathfrak{g}(\imath\mathcal{H}_k)$ we have obtained $\mathfrak{L}_i$ consisting of four indices $\{\ell_1, \ldots, \ell_4\}$ and that the corresponding $\mathfrak{J}_i$ containing indices of $\{j_1, \ldots j_4\}$. (For simplicity, the superscript $^{[k]}$ is not used.) By the definition, the pair $(\mathfrak{L}_i, \mathfrak{J}_i)$ implies that $[h_{j_\mu}, k_{\ell_\mu}] = -c_{j_\mu \ell_\mu} \widetilde{p}_i$ and $\phi_{j_\mu}(\ell_\mu) = i$ for $\mu = 1, \ldots, 4$, and that the elements in $\mathfrak{L}_i$ are ordered. Define $\mathfrak{p}_i$ in the order that

$$\widetilde{\mathrm{p}}_{\phi_{j_\mu}(\ell_1)} := -\frac{1}{c_{j_\mu \ell_1}}[h_{j_\mu}, k_{\ell_1}], \quad \mu = 1, \ldots, 4. \tag{6.6}$$

Since $\mathfrak{L}_i$ and $\mathfrak{L}_{\phi_{j_\mu}(\ell_1)}$ share at least one common index ℓ_1, by Theorem 5.4, it must be that $\widetilde{\mathrm{p}}_{\phi_{j_\mu}(\ell_1)} \in \mathfrak{p}_i$ and that they share the same $\mathfrak{J}_i$ setwise. The exact ordering of the elements $\{j_1, \ldots j_4\}$ for $\widetilde{p}_{\phi_{j_\mu}(\ell_1)}$ determines the structure of the block associated with $(\mathfrak{L}_i, \mathfrak{J}_i, \mathfrak{p}_i)$.

Based on (6.6), we can now apply Lemma 6.1 to establish the relationships in Table 3, which reads as h_μ taking the bracket product with the rightmost k_η in the same row gives rise to a scalar multiplication ± 2 of the particular $\widetilde{p}_\nu$ above that h_μ. The indices of h_μ in the lower-left 4×4 matrix in Table 3 correspond to those of β_j in the block associated with $(\mathfrak{L}_i, \mathfrak{J}_i)$. Note that they are of the form (6.1) with $\Xi = \begin{bmatrix} h_{j_1} & h_{j_2} \\ h_{j_2} & h_{j_1} \end{bmatrix}$ and $\Upsilon = \begin{bmatrix} h_{j_3} & h_{j_4} \\ h_{j_4} & h_{j_3} \end{bmatrix}$ which themselves are centrosymmetric.

TABLE 3. Centrosymmetry when $|\mathfrak{L}_i| = 4$

$\widetilde{p}_i$	$\widetilde{p}_{\phi_{j_2}(\ell_1)}$	$\widetilde{p}_{\phi_{j_3}(\ell_1)}$	$\widetilde{p}_{\phi_{j_4}(\ell_1)}$	
h_{j_1}	h_{j_2}	h_{j_3}	h_{j_4}	k_{ℓ_1}
h_{j_2}	h_{j_1}	h_{j_4}	h_{j_3}	k_{ℓ_2}
h_{j_3}	h_{j_4}	h_{j_1}	h_{j_2}	k_{ℓ_3}
h_{j_4}	h_{j_3}	h_{j_2}	h_{j_1}	k_{ℓ_4}

Note that any $\widetilde{p}_\gamma \in \mathfrak{p}_i$ could represent $\widetilde{p}_i$ and generate the corresponding block $\mathfrak{T}_\gamma$, situated between $\mathfrak{J}_\gamma$ and $\mathfrak{L}_\gamma$. Since $\mathfrak{L}_\gamma$ is identical to $\mathfrak{L}_i$, even in order, $\mathfrak{T}_\gamma$ is merely a column rearrangement of the block in Table 3. Given the symmetry of each block in $\mathfrak{P}A(\boldsymbol{\beta})\mathfrak{P}^\top$, this column permutation necessitates other permutations. The arrangement of elements in a general $\mathfrak{T}_\gamma$ must be special, and the super-centrosymmetric structure meets that criterium. Note that embedded in Table 3 are several 6-dimensional subalgebras of the form (6.4).

We now interpret Table 3 backward by assuming that the upper left corner in Table 3 is formed from the subalgebra

$$\mathfrak{g}(\imath\mathcal{H}_{k-1}) = \underbrace{\operatorname{span}\{k_{\ell_1}, k_{\ell_2}\}}_{\mathfrak{k}_i^{[k-1]}} \oplus \underbrace{\operatorname{span}\{\widetilde{p}_i, \widetilde{p}_{\phi_{j_2}(\ell_1)}\}}_{\mathfrak{p}_i^{[k-1]}} \oplus \operatorname{span}\{h_{j_1}, h_{j_2}\}.$$

Suppose that a new element $\widetilde{p}_s \in \mathfrak{g}(\imath\mathcal{H}_k)$, together with its companion $\widetilde{p}_t \in \mathfrak{g}(\imath\mathcal{H}_k)$ guaranteed according to Corollary 6.2 and the existing $\mathfrak{p}_i^{[k-1]}$, constitute a new $\mathfrak{p}_i^{[k]}$. Since $\mathfrak{k}_i^{[k-1]} \subseteq \mathfrak{k}_i^{[k]} = \mathfrak{k}_s^{[k]}$, there must be two indices, say, $j_3, j_4 \in \mathfrak{J}_i^{[k]}$, such that $[h_{j_3}, k_{\ell_1}] = c_{j_3\ell_1}\widetilde{p}_s$ and $[h_{j_4}, k_{\ell_2}] = c_{j_4\ell_1}\widetilde{p}_s$. Using 6.1, we find that the upper right corner in Table 3 is formed. By symmetry, we have the lower left corner in Table 3, which forces the existence of $k_{\ell_3}, k_{\ell_4} \in \mathfrak{k}_i^{[k]}$. By the crossover relationship, we establish the entire Table 3.

Suppose that the current subalgebra $\mathfrak{g}(\imath\mathcal{H}_k)$ is further extended to $\mathfrak{g}(\imath\mathcal{H}_{k+1})$. Then either $\mathfrak{p}_i^{[k]} = \mathfrak{p}_i^{[k+1]}$ and the associated block remains intact, or that $\mathfrak{p}_i^{[k+1]}$ contains at least two new elements, say, $\widetilde{p}_s$ and its companion $\widetilde{p}_t$, from the newly expanded $\widetilde{\mathfrak{p}}^{[k+1]}$. By the same argument above, since $\mathfrak{k}_i^{[k]} \subseteq \mathfrak{k}_i^{[k+1]} = \mathfrak{k}_s^{[k+1]} = \mathfrak{k}_t^{[k+1]}$, there exists indices, say, $j_{\tau_1}, \ldots, j_{\tau_4} \in \mathfrak{J}_i^{[k+1]}$, such that the relationships in Table 4 hold. The blank spots must be filled with the crossover relationships. In particular, $\widetilde{p}_s$ and $\widetilde{p}_t$ must induce two additional elements, marked by $*$, in $\mathfrak{p}_i^{[k+1]}$. Together with the symmetry and the crossover relationships with the existing block in Table 3, we conclude that the block corresponding to $\mathfrak{g}(\imath\mathcal{H}_{k+1})$ is of size 8×8 and maintains the structure (6.1). The argument can now be generalized to every subalgebra in the chain (6.2), which proves that all diagonal blocks in the ultimate $\mathfrak{P}A(\boldsymbol{\beta})\mathfrak{P}^\top$ are of the structure (6.1) and are of sizes powers of 2.

TABLE 4. A possible expansion from $\mathfrak{p}_i^{[k]}$ to $\mathfrak{p}_i^{[k+1]}$

$\widetilde{p}_i$	$\widetilde{p}_{\phi_{j_2}(\ell_1)}$	$\widetilde{p}_{\phi_{j_3}(\ell_1)}$	$\widetilde{p}_{\phi_{j_4}(\ell_1)}$	$\widetilde{p}_s$	$\widetilde{p}_t$	*	*	
h_{j_1}	h_{j_2}	h_{j_3}	h_{j_4}	h_{τ_1}	h_{τ_2}			k_{ℓ_1}
h_{j_2}	h_{j_1}	h_{j_4}	h_{j_3}	h_{τ_2}	h_{τ_1}			k_{ℓ_2}
h_{j_3}	h_{j_4}	h_{j_1}	h_{j_2}	h_{τ_3}	h_{τ_4}			k_{ℓ_3}
h_{j_4}	h_{j_3}	h_{j_2}	h_{j_1}	h_{τ_4}	h_{τ_3}			k_{ℓ_4}

Theorem 6.3. *The eigenvectors of a super-centrosymmetric matrix in the sense of* (6.1) *with sizes powers of* 2 *are independent of the entries and form a Hadamard matrix.*

Proof. It is easy to check the assertion for 2×2 and 4×4 super-centrosymmetric matrices. Suppose that Ξ and Υ are two super-centrosymmetric matrices with spectral decompositions

$$\Xi H = H\Lambda,$$
$$\Upsilon H = H\Sigma,$$

where Λ and Σ are diagonal matrices of eigenvalues, and H is a Hadamard matrix independent of the entries of the super-centrosymmetric matrix. Then

$$(I \otimes \Xi + X \otimes \Upsilon) \begin{bmatrix} H & H \\ -H & H \end{bmatrix} = \begin{bmatrix} H & H \\ -H & H \end{bmatrix} \begin{bmatrix} \Lambda - \Sigma & 0 \\ 0 & \lambda + \Sigma \end{bmatrix}$$

is the spectral decomposition of the super-centrosymmetric matrix $I \otimes \Xi + X \otimes \Upsilon$, whereas the matrix $\begin{bmatrix} H & H \\ -H & H \end{bmatrix}$ remains to be a Hadamard matrix. □

Theorem 6.4. *The dynamical system* (3.14) *defined according to* (3.3) *with the special choice* (3.13) *converges.*

Proof. Because of Theorem 6.3, we can solve an inverse eigenvalue problem in a way similar to (5.8) to ensure values of $\boldsymbol{\beta}$ so that $\mathfrak{P}A(\boldsymbol{\beta})\mathfrak{P}^\top$ has negative eigenvalues. Therefore, the dynamical system (3.14) does have an asymptotically stable submanifold. Since we already know, by the choices of (3.3), that $\boldsymbol{\alpha}(t)$ converges to zero, the flow $(\boldsymbol{\alpha}(t), \boldsymbol{\beta}(t))$ is attracted to the center manifold and the asymptotically stable manifold indeed. □

By now, we have a matrix-free method to generate the subalgebra $\mathfrak{g}(\imath\mathcal{H})$ which is cost effective. We have a matrix-free mechanism to characterize the Lax dynamical system which involves only scalars. We have convergence analysis which guarantees that $\imath\mathcal{H}$ can be properly decomposed into quantum implementable unitary operators. The mathematics behind the three main components of the computational framework is firmly established.

7. CONCLUSION

To simulate the unitary matrix $e^{-\imath\mathcal{H}t}$ of a Hermitian matrix $\mathcal{H} \in \mathbb{C}^{2^n \times 2^n}$ on a quantum machine, we aim to compute the Cartan decomposition of $-\imath\mathcal{H}$. This decomposition provides a precise quantum-implementable parametrization but is as challenging as the traditional spectral decomposition on a classical machine. By generalizing the Toda lattice concept, we introduce a Lax dynamical system to

address the Cartan decomposition. A key advantage of our method is that it only requires working with integers and real-valued coefficients, avoiding the formation of large complex matrices, thus significantly reducing computational costs. The main contribution of this paper is proving the convergence of the proposed Lax dynamical system, establishing a solid mathematical foundation for our novel approach to Hamiltonian simulation.

8. Appendix

Our focus has been on the algorithmic formulation and convergence analysis of our proposed method for Hamiltonian simulation. However, several critical questions remain. A comprehensive discussion of these issues would significantly extend this presentation and venture into areas beyond the author's current expertise. Here, we briefly highlight these problems and provide a limited list of potentially relevant references.

8.1. **Dynamical Lie algebra.** Given a subset $V \subset \mathfrak{su}(2^n)$, how to characterize the minimal subalgebra $\mathfrak{g}(V)$ spanned by all possible nested commutators of the elements in V? How large can the dimension of the subalgebra $\mathfrak{g}(V)$ be? For our application, we are interested in the case when V contains all terms in a given Hamiltonian $\imath\mathcal{H}$. Very recently such a task of generating $\mathfrak{g}(V)$ has been termed the dynamical Lie algebra (DLA) [54]. To our knowledge, furnishing an *a priori* estimate for the dimension of $\mathfrak{g}(\imath\mathcal{H})$ for a general $\mathcal{H}$ is still an open question. Recall that any subalgebra of $\mathfrak{su}(N)$ is either Abelian or a direct sum of compact simple Lie algebras and a center [25,41]. A notable achievement in the paper [66] is its 95-page supplementary material which, using trees to describe all possible irreducible simple subalgebras, lists a complete lattice of irreducible simple subalgebras of $\mathfrak{su}(N)$ for $2 \leq N \leq 2^{15}$. Given $\imath\mathcal{H} \in \mathfrak{su}(2^n)$ with $1 \leq n \leq 15$, we can theoretically break downthe subalgebra $\mathfrak{g}(\imath\mathcal{H})$ to identify its isomorphic irreducible components within the lattice. However, this process is challenging in practice [31,56].

For some specifically structure quantum models, it is possible to exploit the structure to give an analytic description of $\mathfrak{g}(\imath\mathcal{H})$. For instance, the Heisenberg model assumes that the n spin-$\frac{1}{2}$ particles interact with only the nearest neighbors. The corresponding Hamiltonian appears in the form

$$\mathcal{H} = -\frac{1}{2}\sum_{j=1}^{n-1}(J_X\sigma_j^X * \sigma_{j+1}^X + J_Y\sigma_j^Y * \sigma_{j+1}^Y + J_Z\sigma_j^Z * \sigma_{j+1}^Z) + \gamma\sum_{j=1}^{n}\sigma_j^Z, \tag{8.1}$$

where $\sigma_j^A := I^{\otimes(j-1)} \otimes A \otimes I^{\otimes(n-j)}$ and J_A is the coupling constant with A standing for any of the Pauli matrices X, Y, or Z, γ denotes a transverse interfering magnetic field, and $*$ denotes the matrix multiplication. In this case, it can be argued that $\dim(\mathfrak{g}(\imath\mathcal{H})) = 4^n - 4$, so there is not much gain in using $\mathfrak{g}(\imath\mathcal{H})$ for the Heisenberg model [42]. For the Ising model

$$\mathcal{H} = -\frac{1}{2}\sum_{j=1}^{n-1}J_Z\sigma_j^Z * \sigma_{j+1}^Z + \gamma\sum_{j=1}^{n}\sigma_j^X, \tag{8.2}$$

we find that $\dim(\mathfrak{g}(\imath\mathcal{H})) = n(2n-1)$, which is a significant reduction in the dimension. For the general translation-invariant 2-local spin chain Hamiltonians,

$$\mathcal{H} = \sum_{j=1}^{n-1} \sum_{\mathbf{a}\otimes\mathbf{b}\in\mathcal{A}} c_{j,\mathbf{a},\mathbf{b}} I^{\otimes(j-1)} \otimes \mathbf{a} \otimes \mathbf{b} \otimes I^{\otimes(n-j-1)}, \tag{8.3}$$

where $\mathcal{A} \subset \{I, X, Y, Z\}^{\otimes 2}$, whose elements are called the generator, characterizes a special 2-local lattice configuration of the system, it has been discovered that there are 17 unique dynamical Lie subalgebras, all classified in [64]. This case-by-case closed-form analysis is interesting. The classification such as these provides information on the dimension of $\mathfrak{g}(\imath\mathcal{H})$ for some special quantum models.

By introducing an anti-commutation graph for an arbitrarily given set of Pauli strings, and employing the notion of graph contractions, a recent work shows that every anti-commutation graph is reducible to one of a few canonical types [2]. It is claimed that one can then classify the Lie algebras generated by a minimal set of Pauli strings by only looking at their graph and the canonical representative it maps to. In this way, all Pauli Lie subalgebras can be classified. While the computation idea is outlined, the explicit algorithm is deferred. In contrast, our approach in Section 2.1 encodes Pauli strings to numerically generate $\mathfrak{g}(\imath\mathcal{H})$ for any general $\mathcal{H}$.

In all, the notion of DLA is crucial in quantum information theory. On the one hand, considerable research has been dedicated to classifying all possible subalgebras associted to a given lattice configuration of a quantum system or within a given ambient algebra, providing crucial insights into the growth of $\dim(\mathfrak{g}(\imath\mathcal{H}))$ case by case. On the other hand, equally important is the development of an efficient algorithm to generate $\mathfrak{g}(\imath\mathcal{H})$. The complexity analysis of such an algorithm remains an intriguing and unexplored area.

8.2. **Dimensions of $\mathfrak{k}$, $\widetilde{\mathfrak{p}}$ and $\mathfrak{h}$.** The main characteristic in the decomposition (2.7) is the retrieval of $\eta \in \mathfrak{h}$. In terms of the basis (3.1), we may say that we want to retrieve s commutative components out of $\imath\mathcal{H}$, where

$$\dim(\mathfrak{g}(\imath\mathcal{H})) = 2r + s, \tag{8.4}$$

and that once η is retrieved, it remains to treat $\kappa \in \mathfrak{k}$ which is of dimension r with another round of Cartan decomposition. There could be different choices of $\mathfrak{h}$ in (2.17). By Theorem 2.3, all choices are conjugate to each other and, thus, have the same dimension s (which is called the rank of the Lie algebra $\mathfrak{g}(\imath\mathcal{H})$). We do not think that the choice effects the overall Hamiltonian simulation procedure. We may repeat the decomposition process to produce

$$\begin{aligned} e^{-\imath\mathcal{H}t} &= e^{\kappa_0} e^{\eta_0 t} e^{-\kappa_0} \\ &= (e^{\kappa_1} e^{\eta_1} e^{-\kappa_1}) e^{\eta_0 t} (e^{\kappa_1} e^{-\eta_1} e^{-\kappa_1}) \\ &= ((e^{\kappa_2} e^{\eta_2} e^{-\kappa_2}) e^{\eta_1} (e^{\kappa_2} e^{-\eta_2} e^{-\kappa_2})) e^{\eta_0 t} ((e^{\kappa_2} e^{\eta_2} e^{-\kappa_2}) e^{-\eta_1} (e^{\kappa_2} e^{-\eta_2} e^{-\kappa_2})) = \dots \end{aligned} \tag{8.5}$$

until every exponent is made of commutative Pauli strings, whence $e^{-\imath\mathcal{H}t}$ is now quantum implementable. The total length of this chain, if implemented all together as is expressed, should indicate the depth needed for the associated quantum circuit. Since the only time-dependent component is $e^{\eta_0 t}$ which is made of commutative factors, the depth of the quantum circuit is independent of t. This feature effectively bypasses a limitation of existing techniques whose circuit complexity does depend

on the overall time of simulation. To quantify the actual quantum complexity should be an interesting question.

Another challenging question is to determine the rank s of a given subalgebra $\mathfrak{g}(\imath\mathcal{H})$. Based on numerous numerical experiments, we conjecture that s is a divisor of $\dim(\mathfrak{g}(\imath\mathcal{H}))$. For certain Lie algebras, their ranks are known. For instance, the general linear algebra $\mathfrak{ln}(N)$, consisting of all square matrices, has a real dimension of $2N^2$ and a rank of N. The algebra $\mathfrak{sl}(N)$, comprising all matrices with zero trace, has a real dimension of $2N^2-2$ and a rank of $N-1$. The algebra of all upper-triangular matrices has a real dimension of $N(N+1)$ and a rank of N. The algebra of upper-triangular matrices with zeros on the principal diagonal has a real dimension of $N(N-1)$ and a rank of $N(N-1)/2$. Lastly, the algebra of all diagonal matrices has a real dimension of $2N$ and a rank of N. These examples support our conjecture, though a general proof for $\mathfrak{g}(\imath\mathcal{H})$ remains elusive in the literature.

By the count (8.4), each application of the Cartan decomposition will effectively halve the dimension of the problem. We should have

$$\begin{aligned}\dim(\mathfrak{g}(\imath\mathcal{H})) &= r_0 + (r_0 + s_0)\\ &= (2r_1 + s_1) + (r_0 + s_0)\\ &= (2r_2 + s_2) + (r_1 + s_1) + (r_0 + s_0) = \dots,\end{aligned}$$

where s_j and r_j are the numbers of terms involved in η_j and κ_j, respectively. It is yet to be investigated to estimate the total complexity of the procedure, but the fact that $r_{j+1} < \frac{1}{2} r_j$ suggests that the reduction need not be too many steps.

8.3. **Polynomial integrators.** One key advantage of our approach is that it is matrix free. We work with the combination coefficients which are governed by the differential system (3.14). This raises the question of whether this dynamical system can be efficiently solved with an ODE solver on a classical computer, especially when considering circuit depth. In our numerical experiments we have used only some existent numerical ODE packages only to study the functionality of our method, but not its complexity. Since most state-of-the-art ODE packages employ a variety of tactics to vary step sizes and orders, it is hard to really pinpoint the complexity. For fixed-step explicit Runge-Kutta methods, it has been argued in [63] that the minimal number of arithmetic operations required to attain a given precision ϵ is between $O((\ln \frac{1}{\epsilon})^2)$ and $O((\ln \frac{1}{\epsilon})^3 \ln(\ln \frac{1}{\epsilon}))$. An improvement in the thesis [37] shows that the cost of solving initial value problems for ordinary differential equations is polynomial in the number of digits of accuracy.

We have pointed out that the vector field in (3.14) is made of polynomials. It is possible to develop special algorithms for this type of ODEs that has guaranteed accuracy [6, 53]. It has been shown, in terms of both algebraic complexity and bit complexity, these algorithms can compute the approximated solution in polynomial time in several quantities including the integration time, the accuracy of the output and the arc length. Thus far, we have not tried out this special algorithm.

8.4. **Using basis other than Pauli strings.** Thus far, we have been using the Pauli strings as the basis for $\mathfrak{su}(2^n)$ for reasons of their being Hermitian, unitary, mutually orthogonal, and readily quantum implementable as primitive gates. Their simple commutation relation, i.e., Lemma 2.1, is particularly useful. Still, it is possible to employ other basis to characterize the Hamiltonian $\mathcal{H}$. For instance, it is known that any complex matrix can be expressed as a linear combination of general

unitary operators (LCU). In spirit, using Pauli strings corresponds to merely the most primitive LCU. There has been interest of using more sophisticated unitary operators to gain more space and gate efficiency [8, 46]. For example, suppose that we can write

$$\mathcal{H} = \sum_{j=1}^{d} \alpha_j U_j, \tag{8.6}$$

where each U_j is provided as a quantum circuit composed of constant number, say $O(c)$, of primitive gates, and we choose that $\|\mathcal{H}\|_F \le \|\boldsymbol{\alpha}\|_1$. Define the ancilla state creation operator $|G\rangle$ by

$$|G\rangle := \sum_{j=1}^{d} \sqrt{\frac{\alpha_j}{\|\boldsymbol{\alpha}\|_1}}\, |j\rangle\,, \tag{8.7}$$

which obvious can be implemented with $O(d)$ primitive gates. Define also the selector oracle $\widehat{U}$ by

$$\widehat{U} := \sum_{j=1}^{d} |j\rangle\langle j| \otimes U_j, \tag{8.8}$$

which can be implemented with O(cd) primitive gates. Then it is easy to see that the given $\mathcal{H}$ can be encoded in the standard form

$$\mathcal{H} = \|\boldsymbol{\alpha}\|_1 (|G\rangle \otimes I)\widehat{U}(|G\rangle \otimes I). \tag{8.9}$$

Using controlled versions of the oracle $\widehat{U}$, it is possible to further improve the LCU approach by using quantum walks to perform quantum phase estimation with optimal query complexity. The technique, called qubitization, can essentially be viewed as an advanced version of phase kickback in reverse. See [46] for further discussions. This development is interesting, but is beyond the scope of this paper.

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