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Paulie: A Python package to study Lie algebraic properties of quantum systems

Konstantin Golovkin [1*], **Oxana Shaya** [2*¶], **Vincent Russo** [3], and **Mainak Roy** [4]

1 Independent Researcher, Russia **2** Institute for Information Processing, Leibniz University Hannover, Germany **3** Unitary Foundation, United States **4** Tata Institute of Fundamental Research, Mumbai, India

¶ Corresponding author * These authors contributed equally.

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Summary

The control of quantum systems lies at the heart of quantum computation and is studied via the dynamical Lie algebra (DLA), i.e. the Lie algebra that is generated by terms in the system's Hamiltonian. Tensor products of Pauli matrices (Pauli strings) form a basis of Hermitian operators and as such appear as generators in trotterized Hamiltonian simulation. Moreover, they naturally arise as effective control Hamiltonians in trapped-ion systems and also occur in measurement-based quantum computation. While a conceptually complete classification of systems that are generated by Pauli strings is known, this classification was not packaged as an explicit, scalable procedure, and therefore remained difficult to deploy in concrete design tasks. Within the Python package `paulie` we present an efficient algorithm for this classification that directly allows to study the controllability of Pauli string generated systems. We showcase the utility of our framework by numerically providing the optimal universal generator sets.

Statement of need

The dynamical Lie algebra (DLA) is generated via nested commutation of the interaction terms in the system's Hamiltonian. It constitutes the tangent space of the associated Lie group which captures the possible trajectories of the evolving quantum system. Therefore, the DLA is a pivotal tool to study the symmetries and dynamics of quantum systems and occurs in various fields within quantum information theory such as quantum control (Zeier & Schulte-Herbrüggen, 2011), simulation (Goh et al., 2025) and quantum machine learning Ragone et al. (2024).

Pauli strings form a basis for Hermitian operators and as such appear as generators in trotterized Hamiltonian simulation (Trotter, 1959). They also arise as native gate sets in trapped ion systems (Nam et al., 2020) and occur in measurement-based quantum computation (Raussendorf et al., 2003).

A recent line of work (Kökcü et al., 2024; Wiersema et al., 2024) culminated in a classification of DLAs generated by arbitrary sets of Pauli strings (Aguilar et al., 2024). While conceptually complete, this classification was not packaged as an explicit, scalable procedure, and therefore remained difficult to deploy in concrete design and compilation tasks. This work provides a bridge as we provide an efficient algorithm that takes any set of Pauli strings and outputs its DLA. This allows the direct study of controllability of quantum systems generated by Pauli strings. In addition equivalences of generating sets can be easily checked and transitions between algebras by changing the generator set studied. We demonstrate the utility of the framework by constructing universal generator sets with optimal generation rate.

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Preliminaries

A state of an isolated physical system is represented at a fixed time t by a vector $|\psi\rangle$ in a Hilbert space $\mathcal{H}$, that is, a complex vector space endowed with an inner product. The time evolution of the state is determined by the Schrödinger equation $i\frac{d}{dt}|\psi\rangle = H|\psi\rangle$, where we set $\hbar = 1$. H is the Hamiltonian that describes the observable corresponding to the total energy of the system. An observable is a Hermitian linear map acting on $\mathcal{H}$. The solution to this differential equation with initial state $|\psi_0\rangle$ and time-independent Hamiltonian H is $|\psi(t)\rangle = e^{-iHt}|\psi_0\rangle$. We specify a set of operators $\mathcal{G} = \{h_j\}_{j\in J}$ that describe the ways in which we can control the quantum system and that corresponds to the individual interaction terms of the Hamiltonian. The reachable states are then of the form

$$|\psi(t)\rangle = e^{-ih_{l_m}t_{l_m}} \dots e^{-ih_{l_1}t_{l_1}}|\psi_0\rangle \tag{1}$$

for some index set $\{l_i\}_{i=1}^m \subset J$. The associated matrix Lie algebra $\mathfrak{g}$, that is, a real subspace of complex matrices that is closed under the matrix commutator $i[h,g] = i(hg - gh)$, is dubbed dynamical Lie algebra (DLA). Hence, the elements of $\mathcal{G}$ span all elements in $\mathfrak{g}$ through nested commutators, $\mathfrak{g} = \text{span}_{\mathbb{R}}\langle\mathcal{G}\rangle_{Lie}$. In case the generator set $\mathcal{G}$ consists of tensor products of Pauli matrices (Paulistrings), $\mathfrak{g}$ is termed Pauli Lie algebra.

The classical compact simple Lie algebras are

$$\mathfrak{su}(d) = \{x \in \mathbb{C}^{d\times d} | x = -x^\dagger, \operatorname{tr} x = 0\} \tag{2}$$

$$\mathfrak{so}(d) = \{x \in \mathbb{R}^{d\times d} | x = -x^T\} \tag{3}$$

$$\mathfrak{sp}(2d) = \{x \in \mathfrak{su}(2d) | x = -\Omega x^T \Omega^T\} \tag{4}$$

where the symplectic form is denoted as

$$\Omega = \begin{pmatrix} 0 & \mathbb{I}_d \\ -\mathbb{I}_d & 0 \end{pmatrix}. \tag{5}$$

Considering a system out of n qubits, the Hilbert space is $\mathcal{H} = \mathbb{C}^{2^n}$. A generator set that spans all of $\mathfrak{su}(2^n)$ is called universal, and the system is fully controllable. To characterise spin chains, we employ the following graph

Definition 1 *The anticommutation graph has $\mathcal{G}$ as a node set and the edges are between the generators that anticommute $E = \{(p,q) | [p,q] \neq 0\}$.*

Classification algorithm

Optimal universal generator set

With the feature `get_optimal_su_2_n_generators` we find among all universal generator sets those that have optimal generation rate, i.e. the sets that generate $\mathfrak{su}(2^n)$ the fastest. In (Smith et al., 2025) it is derived that these are exactly generating sets with a fraction of anticommuting pairs of generators out of the total number of pairs to be approximately 0.706. Analytically this fraction maximizes a particular q-Pochhammer symbol. We can reframe the problem in terms of the anticommutation graph. Optimal universal generating sets have an anticommutation graph with approximately $\lfloor 0.706 \cdot \binom{n}{2} \rfloor$ edges. To search for such graphs, we start with the canonical graph of $\mathfrak{su}(2^n)$. We can obtain the canonical graph by the algorithm described in the previous section. The canonical graph is the anticommutation graph with minimal connectivity, hence we are guaranteed to be below the target anticommutation fraction. We iterate over the edge set of the canonical graph and perform a contraction such that the anticommutation fraction increases and become closer to the target value until we reach the target value. In the following example of usage we find the optimal universal Pauli string generator set in dimension four.

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```python
from paulie.application.get_optimal_su2_n import get_optimal_su_2_n_generators
from paulie.common.two_local_generators import G_LIE
from paulie.common.pauli_string_factory import get_pauli_string as p

n = 4  # dimension of the system
initial_generators = p(G_LIE["a12"], n=n) # some universal generator set
optimal_generators = get_optimal_su_2_n_generators(initial_generators)
print(f" {optimal_generators} fraction={optimal_generators.get_anticommutation_fraction(
```

which outputs:

```
XZYX,ZZXZ,IYYY,XZYY,IXZX,YYXY,YYYY,ZZIX,XXZY fraction=0.6944444444444444
```

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