Seeing the Future: Demonstrating the Advantage of Cartan Decomposition on H_2, HeH^+, and BeH_2 Molecules for complex Hamiltonian exponential using Pennylane SDK

Bakhao Dioum, Zachary Elgood, Abdullah Kazi, & Aakash Warke

I. Problem statement

Your goal will be to implement state-of-the-art ways to construct the complex exponential of the Hamiltonian, or invent a new original way to achieve this task.

GitHub repo: https://github.com/zachelgood/Boson-Buzzers-QHACK-2024

II. Introduction

Quantum circuits are a means of translating various algorithms to work on a quantum computer. These circuits are equivalent to unitary transformations under $SU(2^n)$ for n qubits. One particular unitary that plays a major role in simulating quantum systems on quantum computers is Hamiltonian evolution. In the case of the time-independent Hamiltonian, this involves utilizing the Unitary $U(t) = e^{-i\mathcal{H}t}$, which solves the time-independent Schrodinger equation. Due to the exponentially increasing complexity that arises from the increasing qubits, numerous techniques have been developed to reduce circuit length, resulting in reduced error and improved execution time.

Our project attempts to minimize error compared to the standard Trotter application by using a method known as Cartan Decomposition. Consider an arbitrary time-independent Hamiltonian that takes the form

$$\mathcal{H} = \sum_i H_i \sigma^i, \tag{1}$$

where H_i are real coefficients and σ^i are Pauli string operators consisting of the Pauli group $(I, X, Y, Z)^{\otimes n}$. The unitary of this Hamiltonian is obtained by factorization

$$U(t) = e^{-i\mathcal{H}t} = \prod_{\bar{\sigma}^i \in SU(2^n)} e^{i\kappa_i \bar{\sigma}^i}, \tag{2}$$

with angles κ_i for Pauli strings $\bar{\sigma}^i$ which form the basis of $SU(2^n)$.

By expanding our Hamiltonian in equation 1 in terms of the Pauli strings, we can find a closure of the set of Pauli terms. This forms a subalgebra of $SU(2^n)$, $\mathfrak{g}(\mathcal{H})$, allowing us to restrict the elements to this subalgebra.

To determine the parameters κ_i from 2, we will use the Cartan decomposition:

Definition 1. *A **Cartan decomposition** of a Lie Algebra $\mathfrak{g}$ is defined as the orthogonal decomposition $\mathfrak{g} = k \oplus m$ satisfying*

$$[k, k] \subset k, \qquad [m, m] \subset k, \qquad [k, m] = m, \tag{3}$$

*and denoted by $(\mathfrak{g}, l)$. A **Cartan subalgebra** denoted by $\mathfrak{h}$ refers to a maximal Abelian algebra within m.*

III. Methodology

In this project, we examine an alternative to the Trotter decomposition to estimate the time evolution of a time independent Hamiltonian. This is accomplished through the use of a method known as Cartan decomposition, a procedure by which we can decompose a Hamiltonian algebra into smaller subalgebras. To accomplish this, we shall follow the procedure implemented in [1], utilizing their Cartan Quantum Synthesizer (CQS) program[2]. See said paper for further details regarding the mathematics behind Cartan decomposition.

Three steps are required in order to utilize the Cartan decomposition.

1) We must construct our Hamiltonian algebra $\mathfrak{g}(\mathcal{H})$
2) We must find our Cartan decomposition such that $\mathcal{H} \in m$, as well as our associated subalgebra $\mathfrak{h}$. This can be decomposed to the form $U(t) = e^{-i\mathcal{H}t} = Ke^{-iht}K^\dagger$, for $K \in e^{ik}$ and $h \in \mathfrak{h}$.
3) Finally, we must determine our element K. K can be decomposed into $K = \prod_i e^{ia_i k_i}$, where k_i is an element of the Pauli string basis for k, which will be the basis of the implementation of the Cartan decomposition circuit. See figure 1 for an example of how this might be implemented.

We have used the Cartan decomposition in three different cases: applied to H_2 (our main case), HeH^+, and BeH_2 with two active orbitals. Details about the specific calculations we are doing, as well as their associated results, can be found in each Jupyter notebook.

IV. Results

To provide a brief sample of our results, we have below images showing the comparison of the error with respect to the exact Unitary for both the Cartan and the Trotter decomposition at similar depth 2,3, 4. We also provide a comparison with the error of the QPE of H_2 5. See their respective notebooks for further details. In addition, in the

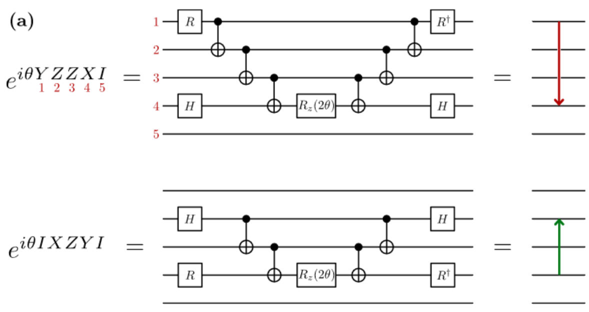

Fig. 1. An sample implementation of the Cartan circuit. Figure obtained from [1] on page 4.

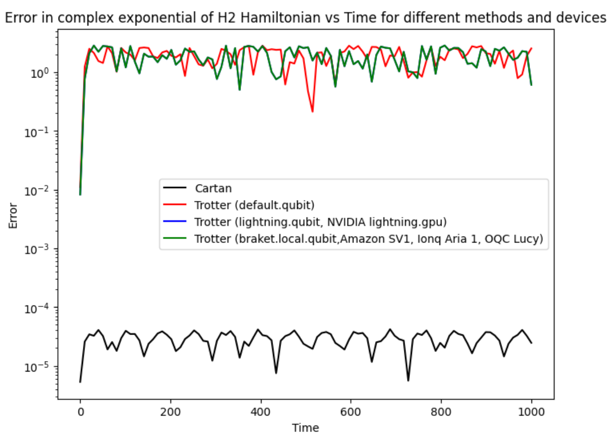

Fig. 2. Error for the H_2 Molecule

particular case of H_2 using Quantum Phase Estimation (QPE), we will obtain the molecular energy of H_2 from the time evolution of the Hamiltonian on the Pennylane and Nvidia "lightning" devices. By using the Cartan decomposition, the error in our molecular energy (an error of approximately 0.8%) is greatly reduced compared to Trotterization (an error of approximately 11%).

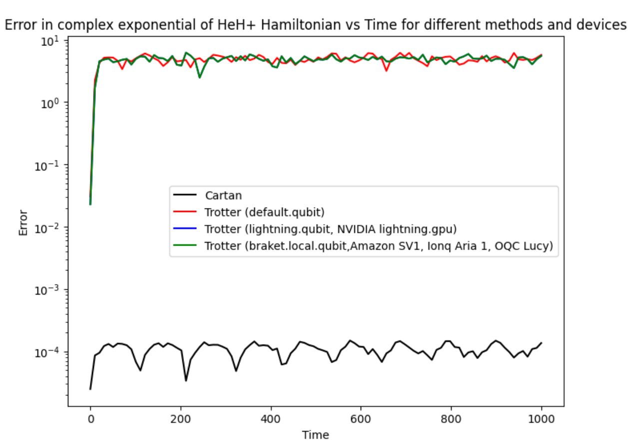

Fig. 3. Error for the HeH^+ Molecule

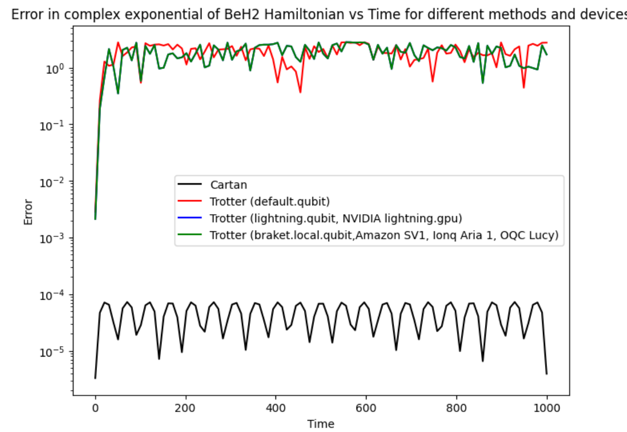

Fig. 4. Error for the $BeH2$ Molecule

Comparison table from Quantum Phase Estimation results

	Target	From exact Unitary	From Cartan decomposition	From Trotterisation decomposition
Energy (Hartree)	3.11383	3.14159	3.14159	2.74889
Relative Error (%)	-	0.89150	0.89150	11.71993

Fig. 5. Table showing the error associated with the Quantum Phase Estimation (QPE)

V. Conclusion

In this project, we have illustrated that through use of Cartan decomposition, we can produce a significantly smaller error with respect to the exact Unitary compared to the error associated with the Trotter decomposition. This implies that theoretically, we could lower the depth of the Cartan decomposition even further if we were content with a higher error.

VI. Acknowledgement

We would like to thank NVIDIA and Amazon for providing us with use of a Nvidia GPU and access to Amazon Web Service respectively due to our placement in the QHACK 2024 coding competition and our preliminary submission. Have you ever used the Braket Hybrid Jobs feature? If so, what made you choose it?

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YES

AWS What your project does. In this project, we have illustrated that through use of Cartan decomposition, we can produce a significantly smaller error with respect to the exact Unitary compared to the error associated with the Trotter decomposition. This implies that theoretically, we could lower the depth of the Cartan decomposition even further if we were content with a higher error. Why it is interesting. We have used the Cartan decomposition in three different cases: applied to H2, HeH+, and BeH2 with two active orbitals. Details about the specific calculations we are doing, as well as their associated results, can be found in each Jupyter notebook.

How you use CUDA Quantum and NVIDIA GPUs. We have used Nvidia lightning GPU Performance results, numerical / scientific analysis. performance, results are in the notebooks

REFERENCES

[1] Efekan Kökcü, Thomas Steckmann, Yan Wang, J.K. Freericks, Eugene F. Dumitrescu, and Alexander F. Kemper. Fixed depth hamiltonian simulation via cartan decomposition. *Physical Review Letters*, 129(7), August 2022.

[2] Kemperlab. Kemperlab/cartan-quantum-synthesizer: Quantum computing – unitary synthesis based on cartan decomposition. https://github.com/kemperlab/cartan-quantum-synthesizer.