Efficient ground state computation methodologies for BeH_2

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Abstract

In this project, we will compare the performance of different methodologies for finding the ground state of the molecule BeH_2. We use various methods, including orbital freezing, active space transformation, circuit cutting, and knitting [1] technique and Adaptive VQE. We also use error mitigation, including Twirled Readout Error extinction, Zero-Noise Extrapolation, and Probabilistic Error Cancellation integrated within qiskit runtime.

1 Introduction

We are trying to find the ground state of BeH_2, so it is worth knowing more about its physical chemistry. In the formation of BeH_2, the 2s orbital of beryllium and the 1s orbitals of both hydrogen atoms combine to form two molecular orbitals: a bonding molecular orbital and an antibonding molecular orbital. The molecule is linear, with a bond angle of 180 degrees, and the two hydrogen atoms occupy the antibonding molecular orbital. The task is to find the ground state energy of the molecule.

$$H|\Phi\rangle = E_G|\Phi\rangle \tag{1}$$

Knowing the ground state energy of a molecule can help predict its reactivity, chemical stability, and spectroscopic properties. With this motivation, we employ different VQE (variational quantum eigensolver) methods.

VQE stands for Variational Quantum Eigensolver [2], which is a quantum algorithm designed to estimate the ground state energy of a quantum system using quantum computers. The goal of VQE is to find the lowest energy state of a molecule, which is important for understanding its chemical properties and behavior. The algorithm starts with an initial guess for the wave function of the molecule and then uses a classical optimizer to adjust the parameters of the wave function to minimize the energy. The adjusted wave function is then sent to the quantum computer, which calculates the energy of the wave function. This process is repeated iteratively, with the classical optimizer updating the wave function parameters and the quantum computer calculating the energy until the energy converges to the ground state energy of the molecule.

We have the vanilla flavor VQE [3] method; then we explore the Tetris Adaptive VQE [4], and we finally worked with the Adaptive VQE [5, 6] method, which gave us the best results.

2 Circuit Knitting

Circuit knitting is a technique in quantum computing that involves combining multiple quantum circuits into a larger, more complex circuit. The idea behind circuit knitting is to use smaller, more specialized circuits as building blocks, which can be combined and stitched together to create larger, more powerful circuits for solving complex problems.

Overall, circuit knitting is a powerful technique in quantum computing that can help researchers tackle some of the most challenging problems in the field. It is a testament to the versatility and modularity of quantum circuits, and it has the potential to enable new breakthroughs in quantum technology.

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3 Entanglement Forging

Entanglement forging [1] [2] refers to a hypothetical process in which two parties can create a shared quantum state without actually having access to an entangled pair of qubits. This is accomplished through a combination of quantum operations and classical communication and would represent a significant breakthrough in the field of quantum information processing. The basic idea behind entanglement forging is to start with two separable qubits (i.e., qubits that are not entangled with each other) and then use a series of quantum gates and measurements to create a new state that is entangled.

Entanglement forging takes a generic circuit that operates on the combined system of the spin-up and spin-down halves and splits it into smaller circuits that only operate on one half at a time. In other words, the entanglement forging technique takes a circuit operating on $2N$ qubits and separates that circuit into two N-qubit halves.

4 Zero Noise Extrapolation

Zero noise extrapolation (ZNE) is a technique in quantum computing that can improve the accuracy of quantum algorithms by extrapolating the results of noisy quantum circuits to the limit of zero noise.

In a noisy quantum circuit, the presence of unwanted noise can cause errors in the computation, which can reduce the accuracy of the results. ZNE aims to mitigate this problem by extrapolating the noisy results to the limit of zero noise, where the true value of the computation can be obtained without any errors.

One advantage of the ZNE technique is that it can be applied to any quantum algorithm, regardless of its specific structure or purpose. Moreover, ZNE can be combined with other noise mitigation techniques, such as error correction and error suppression, to further improve the accuracy and reliability of quantum computations.

5 TREX (Twirled Readout and EXcitation

TREX (**T**wirled **R**eadout and **EX**citation) is an error mitigation technique in quantum computing that combines twirled readout with excitations to improve the accuracy of quantum measurements. The twirled readout is a technique that involves applying a random unitary transformation to the final state of a quantum circuit before measuring it. The idea behind this technique is to randomly rotate the state space in a way that cancels out certain types of noise, such as systematic errors in the measurement process.

TREX has been shown to be effective in a variety of quantum computing applications, including quantum chemistry simulations, optimization problems, and machine learning tasks. It is a promising technique for overcoming the limitations of noisy, near-term quantum devices and enabling the development of more accurate and reliable quantum algorithms.

6 Approach

6.1 VQE

First, we do the usual hybrid VQE algorithm using single and double excitations UCCSD strategy. We use all such excitations to come up with the ground state energy calculation.

For this setup, we use 4 electrons in 6 orbitals inside the molecule. The pair of electrons in the 1s orbital(core) of Be atom is stable. Therefore, we don't include them in our active space. We use the sto-3g basis set and two-qubit reduction method using parity mapping to reduce the system size without affecting the calculation, due to symmetry. We first find the true ground state energy, which we will use throughout the file for reference, as the target. Note that this is calculated using NumpyEigenSolver.

[1] https://github.com/qiskit-community/prototype-entanglement-forging/blob/main/docs/3-explanatory_material/explanatory_material.md#picking-the-bitstrings

[2] https://research.ibm.com/blog/quantum-entanglement-forging

We then make a circuit and find the expected value of the hamiltonian using the ADAM optimizer. We calculate the

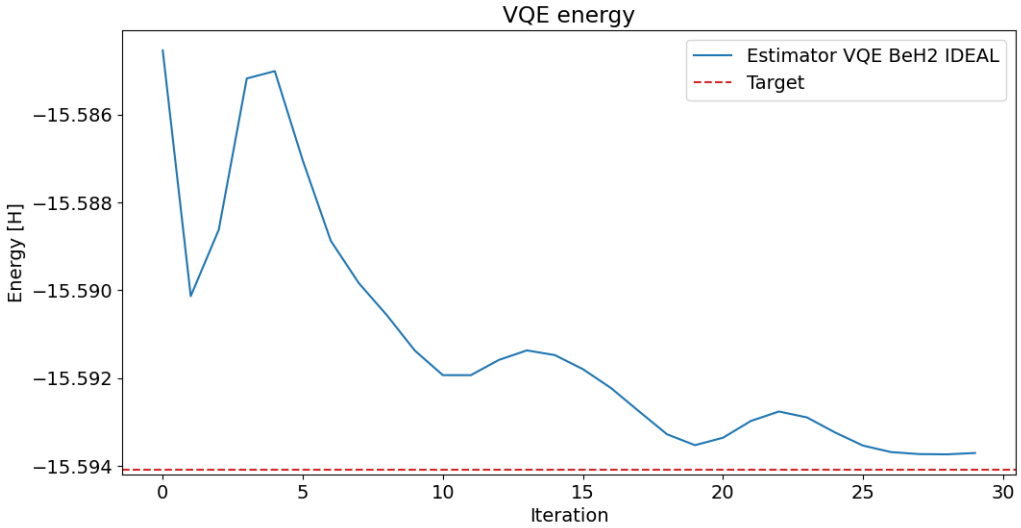

Figure 1: VQE

time taken for this method, along with the number of CNOT gates that are in the circuit. This number is calculated using the formula 13 × double_excitations + 2 × single_excitations. This is because of the number of CNOT gates used in the ansatz for the respective excitation schemes. Finally, we plot the graph of the GS Energy calculation over iterations.

6.2 Adapt VQE

In the previous calculation, we used all the single and double excitations. However, one can reduce their number by looking at the gradient w.r.t. parameters for those schemes. The idea is that if the parameters remain constant, then we can train the schemes where parameters need to change in order to reduce the time as well as the number of gates required.

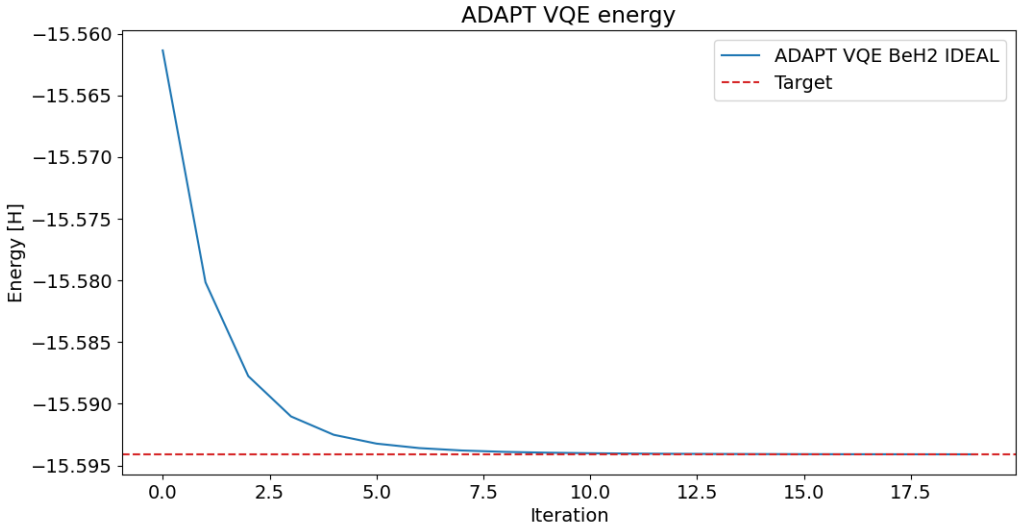

Figure 2: Adaptive VQE

The same is demonstrated using ADAPT_VQE, where we 'ADAPT' to non-vanishing gradients and using a similar ansatz with a restricted number of schemes, we get much faster and better results. This is basically due to the classical preprocessing of data. In the VQE algorithm, a parameterized quantum circuit is constructed to prepare a trial state, which is then measured to estimate the expectation value of the Hamiltonian of the system. This expectation value is used to calculate an estimate of the ground state energy of the system, and the parameters of the circuit are iteratively adjusted to minimize the energy.

The Adaptive VQE algorithm improves on this by dynamically adjusting the circuit during the optimization process based on the measurement outcomes obtained so far. This allows the algorithm to focus its resources on the most relevant parts of the quantum state space, leading to faster convergence and potentially better accuracy.

Adaptive VQE is particularly useful for problems where the Hamiltonian of the quantum system is not known in advance or where it is difficult to simulate classically. It is also a promising approach for implementing quantum machine learning algorithms.
The convergence can be seen after merely 10 iterations, and the time taken is less than a minute for optimization. The number of CNOT gates already reduce by a factor of 10.

6.3 Tetris VQE

The Tetris VQE algorithm aims to optimize the circuit depth and entangling structure of the parameterized quantum circuit used in the VQE algorithm, with the goal of reducing the total number of gate operations required to obtain an accurate estimate of the ground state energy of a quantum system. The algorithm achieves this by using a process similar to the game of Tetris, where circuit blocks are combined and rearranged to minimize the number of gates required.

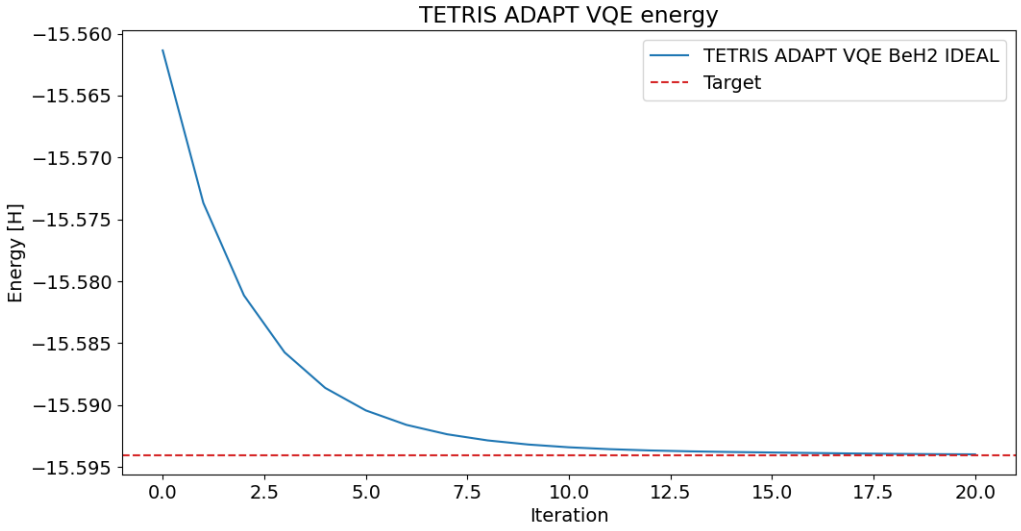

Figure 3: Tetris Adaptive VQE

Tetris VQE can be used for a variety of quantum chemistry applications, such as calculating the ground state energy of small molecules. By reducing the number of gate operations required, Tetris VQE has the potential to significantly reduce the computational resources needed for these types of calculations on near-term quantum computers.

Overall, Tetris VQE is an example of a new wave of algorithmic techniques that are emerging to make better use of the limited resources of current quantum computers and to pave the way for large-scale, fault-tolerant quantum computing in the future.

7 Results

We finally present and contrast the different VQE methods we used and various error correction and mitigation techniques we used. The GS energy values for the BeH_2using different molecules were found to converge to the expected value of -15.5943 hartrees:

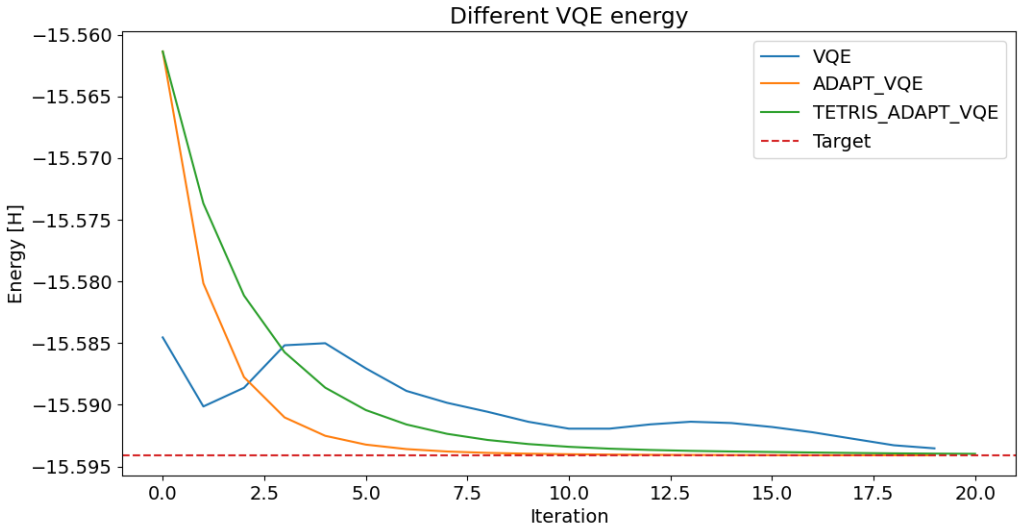

Figure 4: Using Different VQE

Here, the Adapt VQE method gives the best results, but we need to analyze the case on a noisy simulator as well, and this is what we provide.
Here, we also provide what GS values we get employing ZNE. The results show that the qiskit runtime error mitigation works quite well.

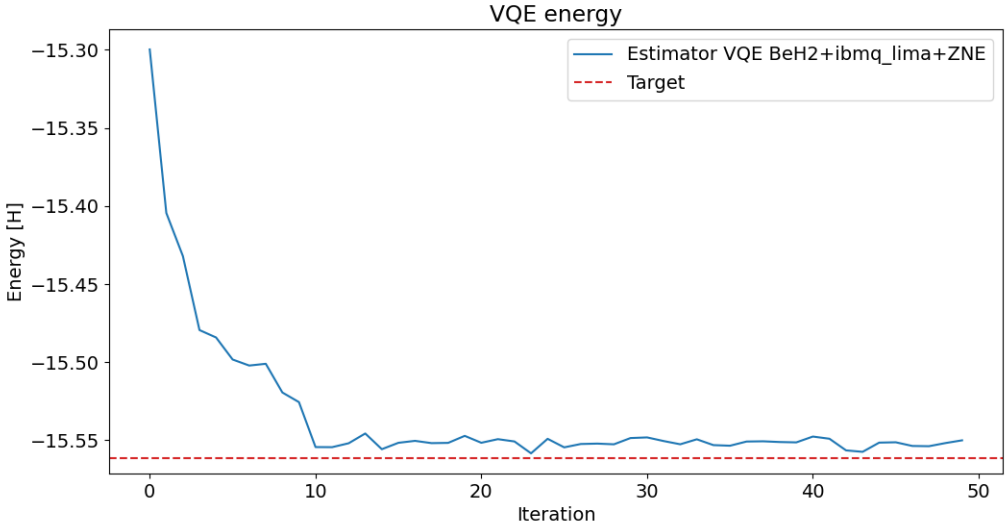

Figure 5: VQE using ZNE

Additionally, we have error-mitigated results from the real backend ibmq_lima using TREX and ZNE. While TREX results show monotonic convergence to the ground state, we show ZNE results.

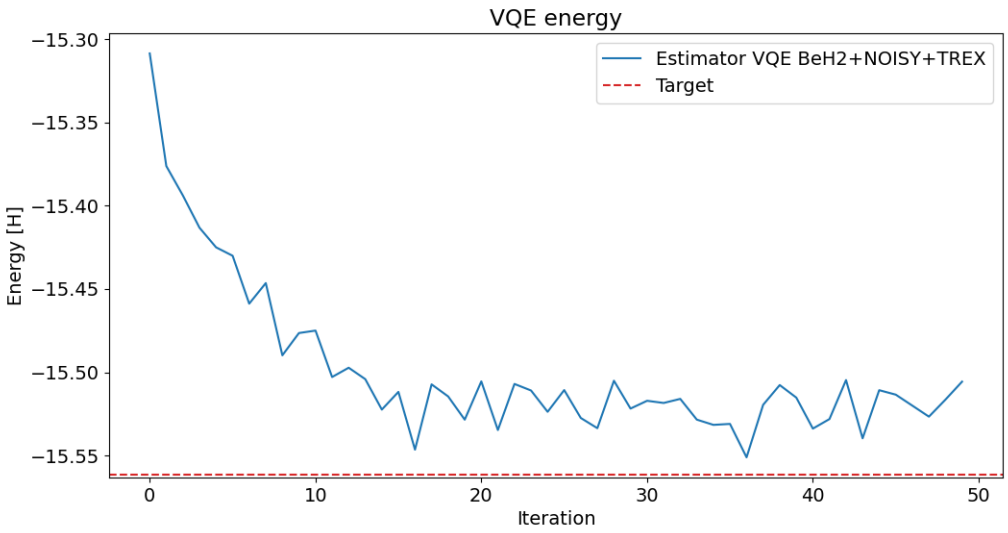

Figure 6: VQE on a noisy simulator

In conclusion, we provide different methodologies for ground state computation on noiseless and noisy backends (including the real backend). We see ADAPT VQE works best for the noiseless backend. For real quantum devices, we used error mitigation techniques of TREX and ZNE to realize that we get very close to the actual answer, which is incredible even after using a subsystem.

References

[1] Christophe Piveteau and David Sutter. Circuit knitting with classical communication, 2022.

[2] Abhinav Kandala, Antonio Mezzacapo, Kristan Temme, Maika Takita, Markus Brink, Jerry M. Chow, and Jay M. Gambetta. Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets. *Nature*, 549(7671):242–246, sep 2017.

[3] Dmitry A. Fedorov, Bo Peng, Niranjan Govind, and Yuri Alexeev. Vqe method: A short survey and recent developments, 2021.

[4] Panagiotis G. Anastasiou, Yanzhu Chen, Nicholas J. Mayhall, Edwin Barnes, and Sophia E. Economou. Tetris-adapt-vqe: An adaptive algorithm that yields shallower, denser circuit ansätze, 2022.

[5] Harper R. Grimsley, George S. Barron, Edwin Barnes, Sophia E. Economou, and Nicholas J. Mayhall. Adapt-vqe is insensitive to rough parameter landscapes and barren plateaus, 2022.

[6] César Feniou, Muhammad Hassan, Diata Traoré, Emmanuel Giner, Yvon Maday, and Jean-Philip Piquemal. Overlap-adapt-vqe: Practical quantum chemistry on quantum computers via overlap-guided compact ansätze, 2023.