QHack 2023 - Simulations of BeH_2

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1 Introduction

This report describes the results obtained by the team, The Entangled Cats, during QHack 2023 open hackathon. Our team's project focused on the Quantum Chemistry challenge, but we also submit it to the category of Hybrid Quantum-Classical Computing and Quantum Computing Today!

The Quantum Chemistry challenge this year focused on the molecule BeH_2 and had as objective to obtain a result as close as possible to the real ground state energy value. In our work we used the Variational Quantum Eigensolver (VQE) and managed to obtain a simulated value of -15.57 Ha, which presents a relative error of 0.19% and a real value, physically measured in a Quantum Computer, of -15.69 which presents a relative error of 0.61%.

2 The Molecule BeH_2

This molecule is a bit larger than the usual suspect for toy models, H_2. This in itself offers new challenges, but the molecule its still small enough so that we can simulate it effectivelly with classical computers and Noisy Intermediate-Scale Quantum Era (NISQ) quantum computers.

The first step is obviously to define said molecule. This can be done very easily using *qiskit.nature* drivers. To obtain the ground state, we consider a linear molecule with a bond length of 1.334 Å, in accordance to online references and literature, [3]. This produces a groundstate energy of ~ -15.60 Ha, again in accordance to literary references.

This molecule thus has 6 electrons in a 14 orbital space. However, not all of these electrons and orbitals are active and we can leverage a bit of chemistry knowledge. Indeed, by using the Freeze Core approximation on the Be atom and removing non active orbitals ($2p_y$ and $2p_z$) we are left with an 8 orbitals active space.

In order to further reduce the qubit requirement, for we would need a qubit per active orbital, we employed the Parity mapper available in qiskit, which maps fermionic operators to qubit operators, because this mapper has the advantage of allowing for a further 2 qubit reduction. This means that we can reduce our active orbitals to just 6 orbitals! This can be run on IBM-7 qubit quantum computer available for the teams that manage to achieve the power ups in the coding challenges (as was our case).

This mapper also has the obvious advantage of allowing for less noise in actual runs (for if we have less qubits, we have less operators and less gates and therefore less noise).

The results obtained throughout this competition validate this approximation. Therefore we worked in a 6 qubit space.

3 VQE and Ansatz

In order to apply VQE (whose description can be found in qiskit documentation here: [2]), an ansatz is necessary. The typical ansatz would be the UCCSD ansatz applied to the Hartree Fock state, which preserves the number of electrons and efficiently simulates the evolution of the wavefunction of the system, therefore simulating an evolution under the chemical reaction that provides BeH_2. This was also our starting point, having achieved a groundstate energy of -15.57 Ha in an ideal simulation, that presents a relative error of 0.19%. This simulation took 50 seconds.

However, this ansatz is far to large and complex to be run in a real Quantum Computer. Indeed, the number of CNOT gates applied (which by virtue of being 2 qubit gates are usually the main source of noise in the QPU) is 212 !!! Therefore a simpler ansazt is required.

With that in mind we tried applying a very simple ansatz composed of just parameterized single qubit rotations around the X gate and 3 single excitations between the occupied qubits in the Hartree Fock state and the unoccupied ones. This allows for a vast decrease in the number of CNOT required: just 6. At the same time, the ideal simulation is also much faster, we go from 50 seconds to only 11.89.

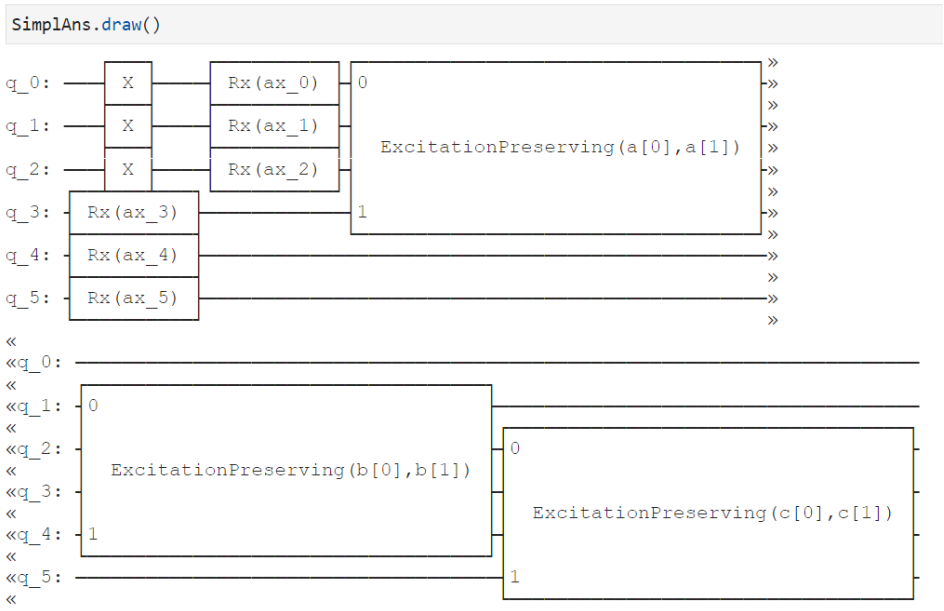

Figure 1: Simplified Ansatz

In the ideal simulation, the obtained result was -15.56 Ha, that presents a relative error of 0.23%.

Nonetheless, there is an even simpler ansatz, the Hartree Fock state itself. Indeed, when applying this state we obtain the previous result, a groundstate energy of -15.56 Ha with the obvious advantage of not using any CNOT gate and only needing 1 iteration (so the simulation only takes 0.1 seconds). All of these results can be found in the file AnsatzExperiment.ipynb .

It must be said, however, that using the Hartree Fock state as ansatz deviates a litle from the goal of the challenge - we are not using any algorithm, we are just preparing a state. Therefore, in addition to using this state for actual implementations in Quantum Computers, we also used the simplified ansatz to maintain the spirit of the competition.

As a final note, we used COBYLA as our classical optimizer, for this was the fastest one to converge in multiple simulations.

4 Executing on Quantum Computers

Given the team's good performance during the coding challenges (10^{th} place) we managed to obtain a power up that granted priority access to 2 7-qubit systems: ibm_nairobi and ibmq_jakarta. Therefore it was possible to run the VQE algorithm with all 3 anstaz in an actual Quantum Computer. Given that the waiting time in ibm_naioribi was significantly smaller than in ibmq_jakarta, this system was primarily used.

As a side note, given that we are trying to measure the expectation values of a 6-qubit Pauli operator in a 7-qubit system it is necessary to artificially extend our qubit Hamiltonian. This was performed by adding Identity operators in place of the qubit oh the system that we did not plan to use. In here we took advantage of the tomography of the system and chose to not use an extremal qubit whose CNOT error was bigger than the rest (often qubit 2 or 4, according to the system calibration).

In addition, we applied noise mitigation methods available in qiskit runtime primitives, namely a

linear Zero-Noise Extrapolation (optimization_level = 2) and Dynamical Decoupling (resilience_level = 3)..

For the UCCSD ansatz, we managed to perform 2 VQE runs, 1 on jakarta and one in nairobi. In the jakarta system, the obtained groundstate energy was of -13.06 Ha, which corresponds to a 16.3% relative error to the theoretical result. In the naiorobi system the obtained groundstate energy was of -13.14 Ha, which corresponds to a 15.75% of relative error. As expected, these results were significantly worse than the simulated ones. These results can be found in the files UCCSDJakarta.ipynb and UCCSDNairobi.ipynb respectively.

For the simplified Ansatz, we only managed to run the VQE in the nairobi system. We obtained a groundstate energy of $\mathbf{-14.99}$ Ha which corresponds to a relative error of $\mathbf{3.85}$ % . These results can be found in the file SimplAnsatz.ipynb. It is important to emphasize just how much better these results were when compared to the initial ansazt, we managed to decrease the relative error by a factor of ~ 4.

Simply preparing the Hartree Fock state, again in the nairobi systeam, we manage to obtain a groundstate energy value of $\mathbf{-15.23}$ Ha which corresponds to a relative error of $\mathbf{2.32}$ %. Which, as expected, was better than using VQE and the simplified ansatz. Additionally, given the simplicity of the preparation procedure we were also capable of going beyond ZNE and apply Probabilistic error cancellation (PEC), which was not possible using VQE due to computational requirements. In this case, the computed groundstate energy was of $\mathbf{-15.69}$ Ha, which corresponds to a relative error of just $\mathbf{0.61}$ %, by far our best result. These results can be found in the files HFZNE.ipynb and HFPEC.ipynb respectively.

5 Entanglement Forging

In the former section we presented measurement results that were only possible through the use of power-ups. However, if we did not have access to a 7-qubit Quantum Computer could we have simulated the molecule? Turns out the answer is yes - by using a new procedure called Entanglement Forging [4], [1] that allows us to represent expectation values of a 2n qubit wavefunction as sums of multiple expectation values of n-qubit states.

Indeed, in Entanglement forging we use a Schmidt decomposition of the 2n qubit system which allows for an accurate classical representation of the entanglement between them. This way, we can take our system after the freeze core approximation and orbital removing, which gives us an 8 qubit operator using any mapper (or a 6 qubit operator if we use the two-qubit reduction with the parity mapper) which can be run using entanglement forging on IBM's free to use 5-qubit system.

To apply this technique we need a new 4 qubit ansatz and 2 bitstrings. Taking inspiration on the simplified ansatz, we chose as our entanglement forging ansatz simply 2 PauliX gates, followed by Rx gates in the 4 qubits and 2 single Excitations. The 2 bit strings were simply (1,1,1,1) and (0,0,0,0), to represent 2 extreme cases of having all orbitals occupied or all empty.

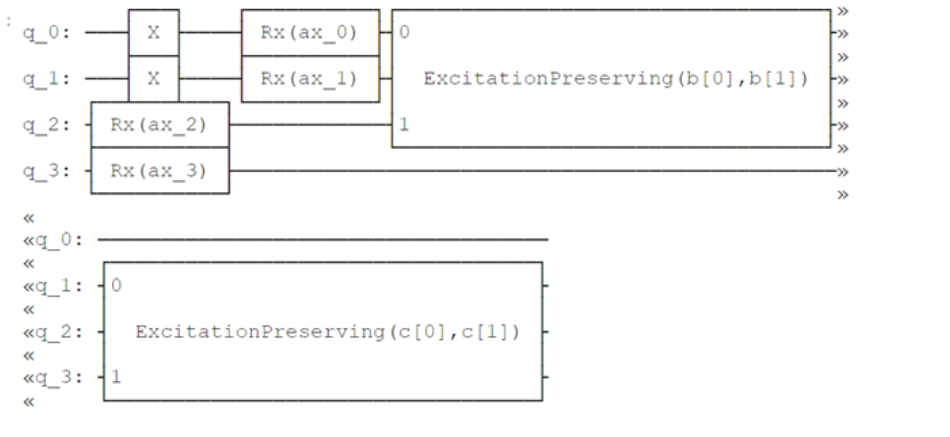

Figure 2: Entanglement Forging Ansatz

In file EntanglementForging.ipynb we show an ideal simulation and a noisy simulation of such a procedure, using the noise model extracted from ibmq_lima and (and again using linear ZNE and Dynamical Decoupling) and the statevector simulator. The results obtained were very promising: for the ideal simulation the obtained groundstate energy was -15.56 Ha, which corresponds to a 0.23% relative error to the analytical result, and for the noisy simulation the groundstate energy obtained was -15.05 Ha, showing only a 3.51% of error relative to the analytical result. Unfortunately since the power ups did not offer priority for this systems, we could not run the entanglement forging procedure on an actual Quantum Computer, where we would expect our results to worsen given that noisy simulations, although sufficient to give an image of the performance of an algorithm against noise, are frequently incapable of fully capturing the noise in a real system. Nevertheless, this shows just how powerful of a technique Entanglement Forging truly is.

6 Conclusion

In this project we explored mainly Quantum Chemistry using advanced Quantum-Hybrid Algorithms, namely VQE. We obtained very good results when compared with the theoretical ground-state energy of BeH_2, $\mathbf{-14.99}$ Ha using the simplified ansazt, which had a $\mathbf{3.85}$ % relative error, and $\mathbf{-15.69}$ using simply the Hartree Fock state preparation, which had an even smaller percentage of error of $\mathbf{0.61}$ %.

At the same time, we also explored new techniques concerning simulations, specifically entanglement forging that was only recently developed in the past year. We also demonstrated the power and promise of this technique, given that in simulations it achieved results very close to the theoretical ground-state with half of the qubit requirements.

To conclude, we are very satisfied with our results for this challenge and would like to thank Pennylane for the opportunity to participate in such a fun, exciting and rewarding event. As a final touch, the team also wanted to give a shout-out to qBraid, whose awesome environment helped during these stressful days of the open hackathon.

References

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