Bridging the gap

1 Introduction

As explained in the challenge description, the spectral gap of a Hermitian matrix (Hamiltonian) H is the difference between the two lowest eigenvalues. For our computations we assume the two lowest eigenvalues to be different. We denote the lowest eigenvalue (the ground state) as λ_0 and the second lowest eigenvalue as λ_1. The variational quantum eigensolver (VQE) uses the variational principle, which states that

$$\lambda_0 \leq \langle\psi|H|\psi\rangle \quad \text{for every quantum state } |\psi\rangle.$$

We express the quantum state $|\psi\rangle$ as $|\psi\rangle = U(\theta)|0\rangle$, where $U(\theta)$ is a parametrized unitary (the *ansatz*) that can be implemented on a quantum computer. The VQE aims at solving the optimization problem

$$\lambda_0 = \min_\theta \langle 0|U^\dagger(\theta)HU(\theta)|0\rangle.$$

In our project, we compute the ground state with the VQE. That is, we compute parameters θ_* such that $\langle 0|U^\dagger(\theta_*)HU(\theta_*)|0\rangle$ becomes minimal. The quantum state $|\psi_0\rangle = U(\theta_*)|0\rangle$ is the corresponding eigenvector of the ground state.

To compute the second lowest eigenvalue, we use the fact that for Hermitian matrices, eigenspaces of different eigenvalues are orthogonal. The variational principle ensures that

$$\lambda_1 \leq \langle\psi|H|\psi\rangle \quad \text{for every quantum state } |\psi\rangle \text{ in the orthogonal complement of } |\psi_0\rangle.$$

If we can ensure that the ansatz of the VQE generates only states that are in the orthogonal complement of the ground state eigenvector, we can approximate the second lowest eigenvalue. More precisely, the ansatz must act trivially on the ground state and it must map the orthogonal complement of the ground state to itself. If we then pick a state in the orthogonal complement as the initial state it is ensured that the ansatz generates only states in the orthogonal complement. [SN22] gives some examples for such ansätze. However, these ansätze are either adapted to specific problems or involve time-evolving a Hamiltonian. In our project, we provide an ansatz that is easy to implement but is also general enough to be applicable for different problems.

2 Generation of the orthogonal ansatz

2.1 Idea

Our idea is to adapt a general hardware-efficient ansatz such that this new ansatz fulfils the requirements explained above. We denote the ansatz as U and look at an example of 3 qubits to explain the idea. For now let's assume that the eigenvector of the ground state is $|000\rangle$. Fig. 1 shows our ansatz.

Let's assume that $U(\theta)$ maps the state $|00\rangle$ to $U(\theta)|00\rangle = a|00\rangle + b|01\rangle + c|10\rangle + d|11\rangle$ (where $a, b, c, d \in \mathbb{C}$). Then, after the first controlled U has been applied, the quantum state is

$$(U(\theta)|00\rangle)|1\rangle = a|001\rangle + b|011\rangle + c|101\rangle + d|111\rangle.$$

Applying the multi-controlled X gates gives us

$$a|001\rangle + b|010\rangle + c|100\rangle + d|110\rangle.$$

Now we apply the ansatz U again (but with different parameters θ', that is, $U(\theta') = e|00\rangle + f|01\rangle + g|10\rangle + h|11\rangle$ for $e, f, g, h \in \mathbb{C}$) and obtain

$$ae|001\rangle + af|011\rangle + ag|101\rangle + ah|111\rangle + b|010\rangle + c|100\rangle + d|110\rangle.$$

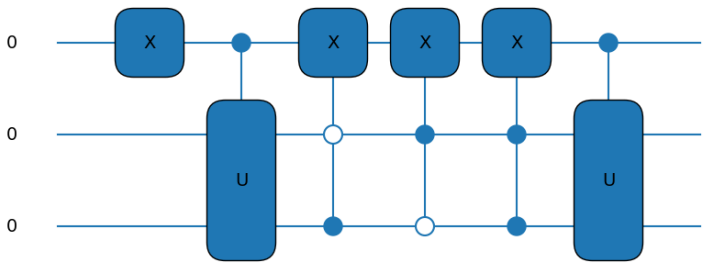

Figure 1: Ansatz to compute the first excited state of a Hamiltonian, if the eigenstate of the groundstate is equal to $|000\rangle$.

This state is orthogonal to $|000\rangle$. By optimizing the parameters accordingly, we can search (approximately) the whole orthogonal complement of $|000\rangle$ to find the second lowest eigenvalue and the corresponding eigenvector.

If the eigenvector of the ground state is not $|000\rangle$, one has to perform a basis transformation. If the ground state has been computed beforehand with the VQE with the ansatz V, the state $V(\theta_*) = |\psi_0\rangle$ approximates the eigenvector of the ground state (with θ_* being the optimized parameter). We can map the state $|\psi_0\rangle$ to the state $|000\rangle$ by applying the inverse of $V(\theta_*)$ (that is $V^\dagger(\theta_*)$) to $|\psi\rangle$. After that, we apply our previously explained ansatz to $|000\rangle$ which results in a state that is in the orthogonal complement of $|000\rangle$. Since unitary matrices (such as $V(\theta_*)$) map orthonormal bases to orthonormal bases, applying $V(\theta_*)$ maps the orthogonal complement of $|000\rangle$ to the orthogonal complement of $|\psi_0\rangle$.

To summarize, the following steps have to be performed to compute the spectral gap of a given Hamiltonian:

- Compute the ground state with the VQE with the ansatz V and store the optimized parameter θ_*
- Compute the excited state with the VQE with the ansatz described below:
  - The initial state is $|0...0\rangle$
  - Apply $V^\dagger(\theta_*)$
  - Apply the controlled ansatz U twice, with multicontrolled X gates in-between (as described above)
  - Apply $V(\theta_*)$
- Compute the difference of the ground state and excited state

Note that the ansatz V and U do not have to have the same circuit architecture.

2.2 Generalization and optimization of the circuit

Let $n+1$ be the number of qubits in a circuit. We denote a computational basis state with $|q_n \dots q_1\rangle|q_0\rangle$, where $q_0, \dots, q_n \in \{0, 1\}$. The idea behind using the multi-controlled X gates between the controlled ansätze is to leave the state $|0 \dots 0\rangle|1\rangle$ untouched and to swap the state of the qubit q_0 if at least one $q_i = 1$ for $i = 1, \dots, n$. More precisely, after applying the first controlled ansatz we have the state $(U|0 \dots 0\rangle)|1\rangle$. Depending on the parameters of U this state can be in a superposition of $|0 \dots 0\rangle|1\rangle, \dots, |1 \dots 1\rangle|1\rangle$, but the amplitudes of the computational basis states with $q_0 = 0$ are zero. After applying the multi-controlled X gates we have a superposition of the states $|0 \dots 0\rangle|1\rangle, |0 \dots 0\rangle|0\rangle, \dots, |1 \dots 1\rangle|0\rangle$. The state $|0 \dots 0\rangle|1\rangle$ is the only state with $q_0 = 1$ and applying the controlled ansatz again gives us a superposition of all computational basis states except $|0 \dots 0\rangle$.

What the operation of the multicontrolled X gates does is basically an OR operation on the qubits $q_1, ..., q_n$, i.e.

$$\text{sequence of multicontrolled-X } |q_n \dots q_1\rangle|0\rangle = |q_n \dots q_1\rangle|q_n \text{ OR } \dots \text{ OR } q_1\rangle.$$

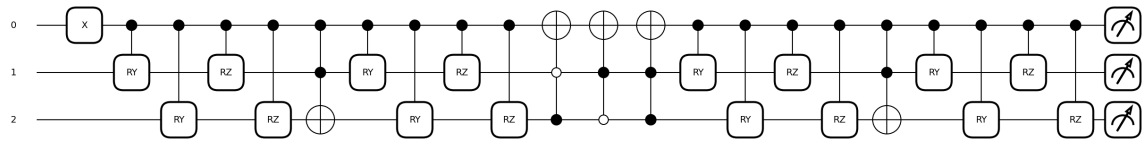

Figure 2: The ansatz of the experiment with $|000\rangle$ as eigenvector of the ground state.

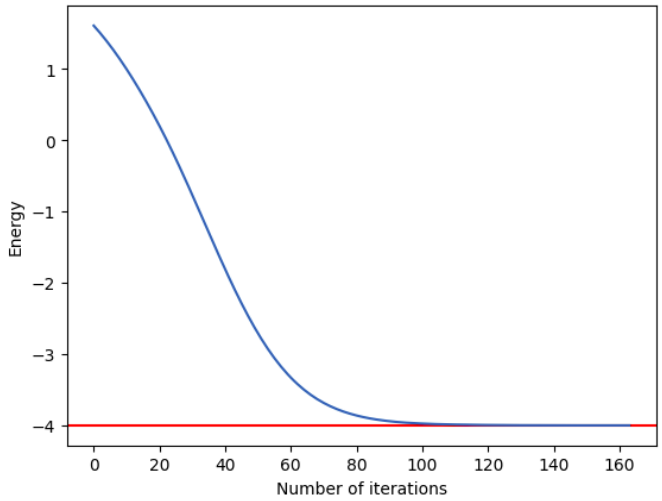

Figure 3: The convergence plot of the experiment with $|000\rangle$ as eigenvector of the ground state. The red line indicates the correct eigenvalue -4.

Implementing this directly in a quantum circuit is very inefficient since the number of controlled X gates increases exponentially with the number of qubits (for $n+1$ qubits we need $2^n - 1$ multicontrolled X gates!). However, by applying De Morgan's laws we see that

$$q_n \text{ OR } \ldots \text{ OR } q_1 = \neg(\neg q_n \text{ AND } \ldots \text{ AND } \neg q_1).$$

Implementing the second term requires only one multicontrolled-X gate and $2n$+1 X gates.

Another aspect for potential optimization is the possibility of the usage of different ansätze when computing the ground state and excited state. For example one could use a chemistry-inspired ansatz to compute the ground state and to perform the basis transformation in the circuit for the excited state, while using a hardware-efficient ansatz for computing the excited state.

3 Experiments

In all our experiments we use a statevector simulator. The small experiments have been performed on the local harddrive, while the more compute intensive experiments have been performed within an Amazon Braket notebook instance. The code and results of the experiments are in the provided jupyter notebooks.

To test our ideas we perform experiments with 3 qubits with a custom defined Hamiltonian. We use a diagonal matrix as our Hamiltonian with the lowest eigenvalue in the first row and column. That means, the eigenvector for the ground state is $|000\rangle$. We construct the orthogonal ansatz as described above and compute the excited state (i.e. the second lowest eigenvalue) with the VQE. We use the AdamOptimizer with a step size of 0.01 and a convergence tolerance of 10^{-6}. Fig. 2 shows the ansatz used, and Fig. 3 shows the convergence plot. We can clearly see that the VQE converges to the correct solution.

To test our ansatz with the basis transformation, in our next experiment we define a diagonal matrix as our Hamiltonian with the lowest value **not** being in the first row and column, i.e. the eigenvector is not $|000\rangle$. We first compute the ground state and then the excited state. We use the AdamOptimizer with a step size of 0.01 and a convergence tolerance of 10^{-6} as well. Fig. 4 shows the ansatz used, and Fig.

6 and 5 shows the convergence plots. We can see that the VQE converges very slowly for the excited state, which might be due to the increased complexity of the cost function.

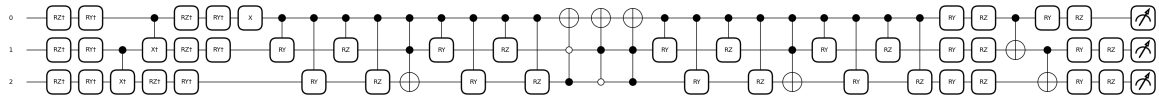

Figure 4: The ansatz of the the VQE to compute the excited state.

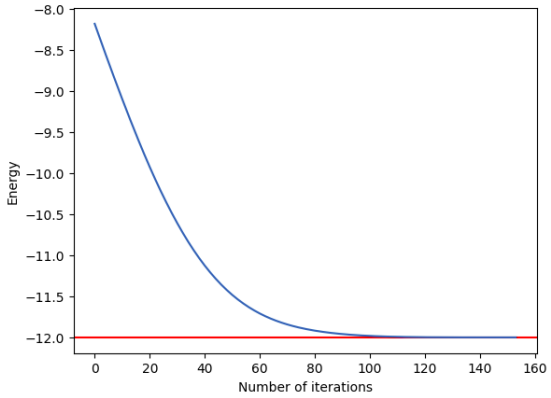

Figure 5: The convergence plot of the computation of the ground state. The red line indicates the correct eigenvalue.

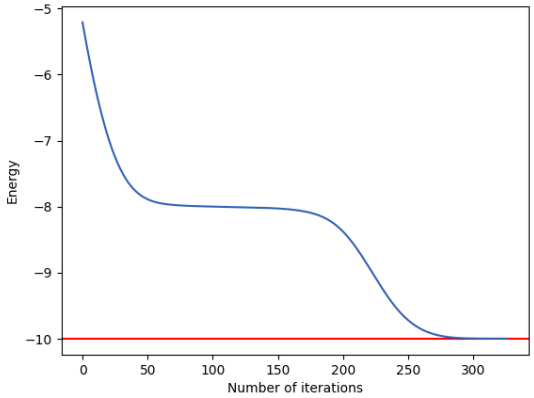

Figure 6: The convergence plot of the computation of the excited state with basis transformation. The red line indicates the correct eigenvalue -10.

3.1 Hydrogen

We compute the ground state and first excited state of the hydrogen molecule H_2 with a bond length of 0.742. We use the basis STO-3G and optimize the VQE with the QNG optimizer. In Fig. 7 - 9 we can see that the VQE converges to the correct eigenvalues.

3.2 Helium

For the helium molecule we do not compute the ground state but use the result of the VQE which is provided in the Pennylane dataset. We approximate the first excited state of the helium molecule with a bond length of 5.2. We use the basis 6-31G and optimize the VQE with the QNG optimizer. In Fig. 10 we can see that the VQE converges to the correct value with a total error of -0.055.

4 Conclusion

In this project we proposed a novel ansatz that is able to compute the first excited state of a Hamiltonian. To see how the results scale with an increased number of qubits, further experiments have to be performed.

References

[SN22] Kyle Sherbert and Marco Buongiorno Nardelli. Orthogonal-ansatz vqe: Locating excited states without modifying a cost-function. *arXiv preprint arXiv:2204.04361*, 2022.

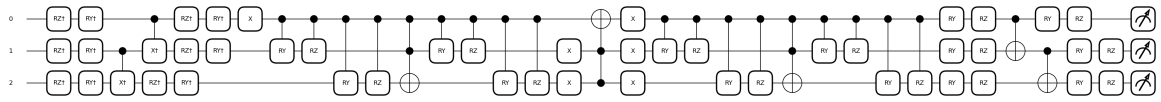

Figure 7: The ansatz of the VQE to compute the first excited state of the hydrogen molecule.

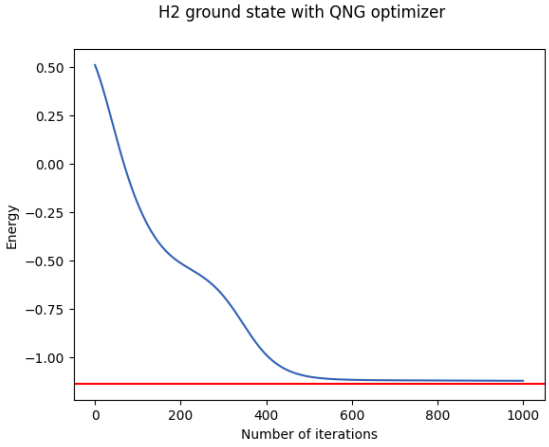

Figure 8: The convergence plot of the computation of the ground state. The red line indicates the correct value.

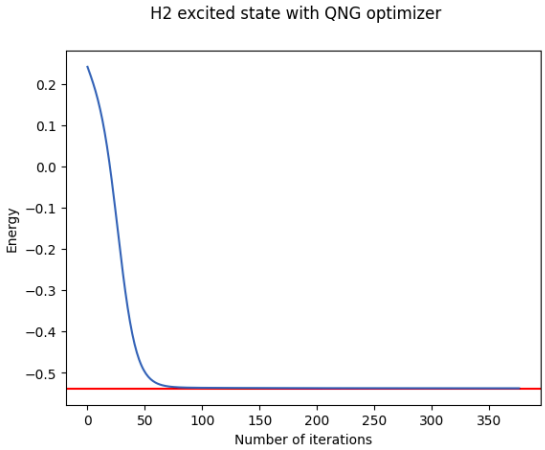

Figure 9: The convergence plot of the computation of the excited state of the hydrogen molecule. The red line indicates the correct value.

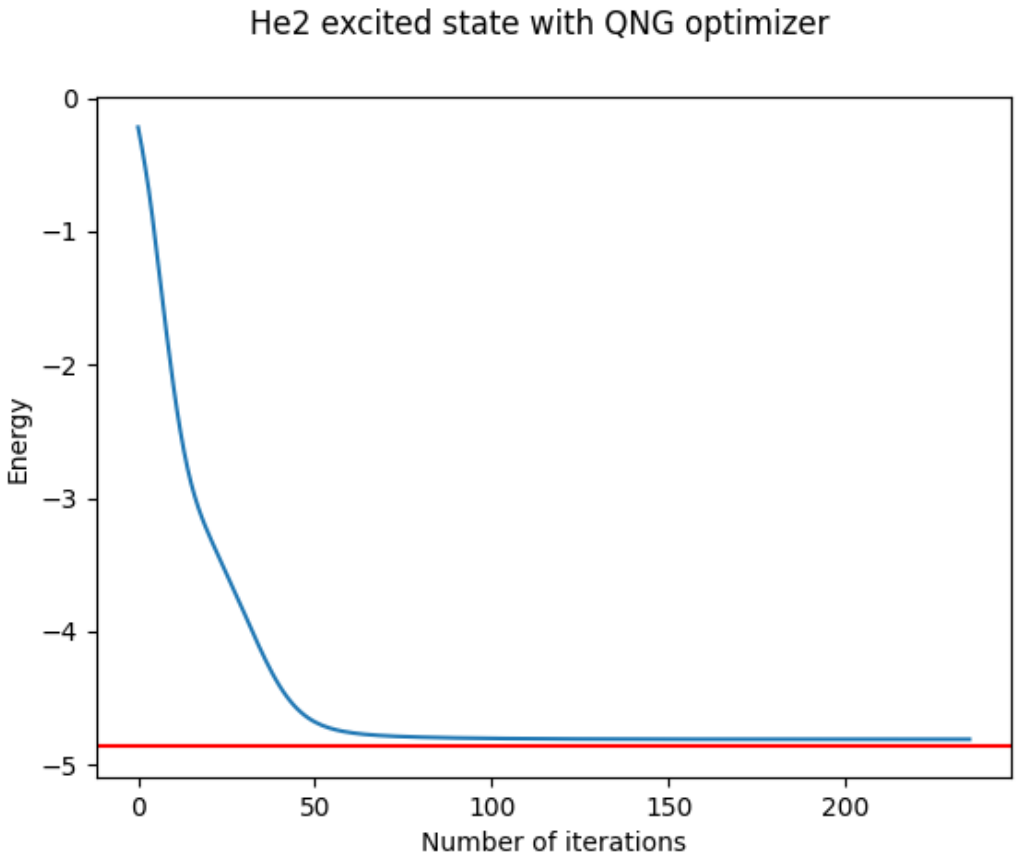

Figure 10: The convergence plot of the computation of the excited state of the helium molecule. The red line indicates the correct value.