EEEN40690 Quantum Computing

Midterm Project
Variational Quantum Eigensolver and the Hydrogen Molecule

Instructions

- This is the midterm project. This accounts for 30% of the marks for this module.
- In your report, please provide answers to the questions. Explain clearly how the answers are obtained and what are their meaning or interpretation. Include relevant intermediate steps of the solution and explain your approach.
- Make sure that the report is readable, and the graphs (if any) are presented according to scientific/engineering standards.
- Some of the questions are open-ended and include a research component. Please formulate clearly your hypothesis and explain what will prove (or disprove) your hypothesis. Make sure that you provide sufficient evidence (analytical results, numerical results, modelling and simulations, evidence from the literature) to support your answer to open-ended or research problems.
- The report must be submitted online through UCD Brightspace:

  My Brightspace → EEEN40690 → Assessment → Assignments → Midterm
- Late submissions will be accepted but a penalty will apply. In the case of late submissions, this module applies the standard UCD policy.
- Plagiarism and copying are offences under the terms of the Student Code, and you should be aware of the possible consequences.

Aim

The midterm project provides exposure to one of the most useful problems in quantum computing, the estimation of the hamiltonian groundstate energy. To complete this mideterm you should be familiar with the following topics:

- Quantum circuit representation of unitary operations
- Basis transformations between the bases noted on the Bloch sphere
- How to describe the state of a multi-qubit system when we only perform measurement on one qubit
- How to recognise some common error channels in their quantum gate representation
- The diagonalisation of a hamiltonian to find its eigenvalues and eigenvectors
- Computation of the expectation value from only measurement outputs in the computational basis of $|0\rangle$ and $|1\rangle$.

Notes

- We label the qubits in our circuit from top to bottom, starting at 0. They are arranged left to right in tensor products.

- We use the concept of Pauli-strings extensively in this project. A Pauli string is a tensor product of Pauli gates or operators. For example;

$$Z_0 \otimes Z_1$$

is a valid Pauli string, applying the Pauli-Z gate to qubits 0 and 1. This is typically shortened with the following notation, dropping the tensor product;

$$Z_0 Z_1$$

Finally, in the case of the identity matrix, it is typically omitted from the Pauli string. For example, $Z_0 \otimes \mathbb{I}_1 \otimes Z_2$ can be written as $Z_0 Z_2$ for a 3 qubit system, with the identity implied.

- We build up understanding of how to measure the expectation of an arbitrary Pauli-string before then measuring the expectation of the hydrogen molecule hamiltonian.
- **When asked for the expectation value we are concerned with measurement outcomes, and not building an evolution operator out of the Hamiltonian. Keep this in mind throughout the project.**

Problems

We are going to build a quantum circuit to estimate the ground state energy of the hydrogen molecule, H_2, hamiltonian. This hamiltonian is obtained from a quantum chemistry method known as the Hartree-Fock approximation. We provide you with this hamiltonian written in the basis of Pauli strings. We start by building simple 2 qubit circuits and finish with the hydrogen molecule. Elements of this project are inspired by the results presented in reference [1].

1. Consider the following two qubit hamiltonian $\hat{H}_a$:

$$\hat{H}_a = Z_0 \otimes Z_1$$

where Z_0, Z_1 represent the Pauli-Z operator applied to qubits 0 and 1 respectively. Given an arbitrary two qubit state vector $|\psi\rangle$, we can compute the expectation value of the hamiltonian as follows:

$$\langle\psi| \hat{H}_a |\psi\rangle$$

If we can only perform measurements on the qubits in the Z-basis, $\{|0\rangle, |1\rangle\}$, how can we use the measurement outcomes on the two qubits to calculate the expectation value of $\hat{H}_a$?

2. How can we now calculate the expecation for a hamiltonian with Pauli matrices other than Z? For example, consider the following 3 qubit hamiltonian:

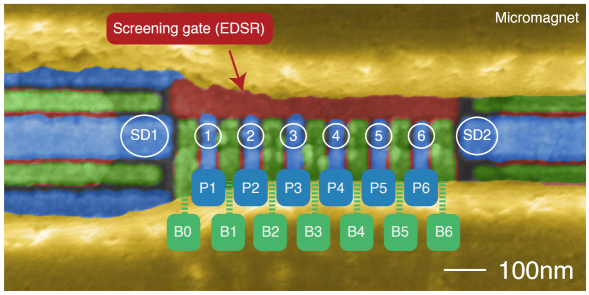
$$\hat{H}_c = X_0 \otimes Y_1 \otimes Z_2$$

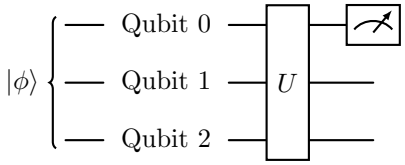
Given that we can only perform measurments in the Z-basis, you will need to perform basis transformations on some of the qubits prior to measurment. Recall the following relations, where H is the hadamard gate, X, Y, Z are the Pauli matrices, and $S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$ is the phase gate:

$$HZH = X, \; SHZHS^\dagger = Y$$

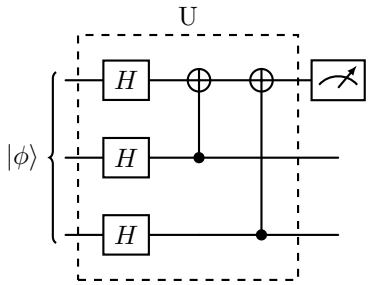
You should show and explain your approach and include any appropriate gate diagrams, mathematics, and scripts.

3. Now consider the situation where we have only have a single measurement device, and again, it can only measure in the Z-basis. A physical motivation for this situation is found in many quantum hardware implementations. One example we consider is the 6 qubit processor presented in [2]. A scanning electron microscope image of the Si/SiGe heterostructure is shown below on the left. Both SD1 and SD2 represent measurement devices that can sense the state of the spin in the spin qubits numbered 1-6. Consider after manufacturing that SD2 is not functioning and so we can only perform measurement with SD1. We also limit ourselves to just qubits 1-3. Therefore, we draw our equivalent circuit on the right, relabelling the qubits starting from 0:





We have some initial 3 qubit state $|\phi\rangle$, which could be entangled. U is a unitary transformation prior to measurement on only qubit 0. U is chosen to implement any desired Pauli string measurement, from which we can construct expectations. For example, if we would like to measure the expectation of $X_0 \otimes X_1 \otimes X_2$, we will need to transform this to $Z_0 \otimes \mathbb{I}_1 \otimes \mathbb{I}_2$ to reflect the fact we can only perform Z-basis measurements on qubit 0. In this case U is implemented as follows:



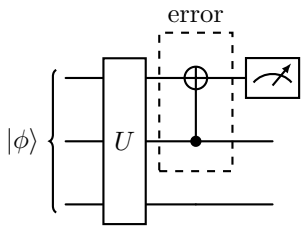
(a) You should first confirm that the transform above allows us to measure the expectation of $X_0 \otimes X_1 \otimes X_2$ by measuring qubit 0 only. You can do this mathematically or through a script, whichever you prefer.

(b) Suggest transformations for the following Pauli strings and compute their expectation:

$$X_0 \otimes Y_1 \otimes Z_2,\ Y_0 \otimes Y_1 \otimes Y_2,\ Z_0 \otimes Z_1 \otimes X_2$$

(c) What is the output density matrix given we are only able to perform a measurement on qubit 0 for the three unitary transformations you suggested?

(d) Consider now that qubit 1 inadvertently interacts with qubit 0 after the unitary basis transform. This causes an error in the state of qubit 0. We model the interaction like so:



What kind of error is this? How does this error affect the expectation value of the three Pauli strings in part (b)?

4. The hamiltonian for the hydrogen molecule in the Pauli basis can be written as follows, where the identity $\mathbb{I}$ applies to all 4 qubits.:

$$\begin{aligned}\hat{H}^a_{\text{hyd}} = c_1\mathbb{I} + c_2Z_2 + c_2Z_3 + c_3Z_0 + c_3Z_1 \\ + c_4Z_2Z_3 + c_5Z_1Z_3 + c_5Z_0Z_2 + c_6Z_1Z_2 + c_6Z_0Z_3 + c_7Z_0Z_1 \\ + c_8X_0X_1Y_2Y_3 + c_8Y_0Y_1X_2X_3 + c_9X_0Y_1Y_2X_3 + c_9Y_0X_1X_2Y_3\end{aligned}$$

The values of $c_1, c_2, \cdots, c_9$ can be obtained from a Hartree Fock simulation of the hydrogen molecule. They are found as follows:

$$\begin{array}{lll} c_1 = -0.138754 & c_2 = -0.152989 & c_3 = +0.164190 \\ c_4 = +0.144579 & c_5 = +0.111373 & c_6 = +0.146726 \\ c_7 = +0.169348 & c_8 = -0.035353 & c_9 = +0.035353 \end{array}$$

All of the above values are given as multiples of $E_h = 27.211eV$, the Hartree energy. These coefficients are a function of the bond length between the two hydrogren atoms in the molecule. These are the values for bond length $R = 1.40a_0$, where $a_0 = 5.2918 \times 10^{-11}m$ is the atomic unit of length.

(a) You should first diagonalise H^a_{hyd} and identify its ground state energy and eigenvector. Given the matrix is not too large this should be easily done on a classical computer. We will use the answer here to compare to that computed by the quantum circuit we construct.

(b) Construct the set of unitary transformations you would need to calculate the expectation of each Pauli string in $\hat{H}^a_{\text{hyd}}$ given that you can perform a measurement on all 4 qubits in the Z-basis. You should display these in quantum gate notation. Explain your methodology for how you would then compute the expectation of $\hat{H}^a_{\text{hyd}}$ given some statevector $|\psi\rangle$.

(c) You are given the following trial wavefunction:

$$|\psi(\theta)\rangle = \cos(\theta)\,|0011\rangle - \sin(\theta)\,|1100\rangle$$

Find the value of θ for which the expectation value of $\hat{H}^a_{\text{hyd}}$ is a minimum. This is your ground state energy, what is the associated ground state statevector? Does this match what you found in part (a)?

Hint: One possible solution is to sweep θ from 0 to 2π and find the minimum value of the expectation. A more sophisticated algorithm would use closed loop feedback using classical optimisation on the value θ. You are welcome to use any method.

References

[1] P. J. J. O'Malley et al., "Scalable Quantum Simulation of Molecular Energies," Phys. Rev. X, vol. 6, no. 3, p. 031007, Jul. 2016, doi: 10.1103/PhysRevX.6.031007.

[2] S. G. J. Philips et al., "Universal control of a six-qubit quantum processor in silicon," arXiv:2202.09252 [cond-mat, physics:quant-ph], Feb. 2022, Accessed: Feb. 21, 2022. [Online]. Available: http://arxiv.org/abs/2202.09252