My journey through the IBM Quantum Challenge 2021 - Part 2

It took me 2 days to finish the first three questions and now I was up against the final two questions.

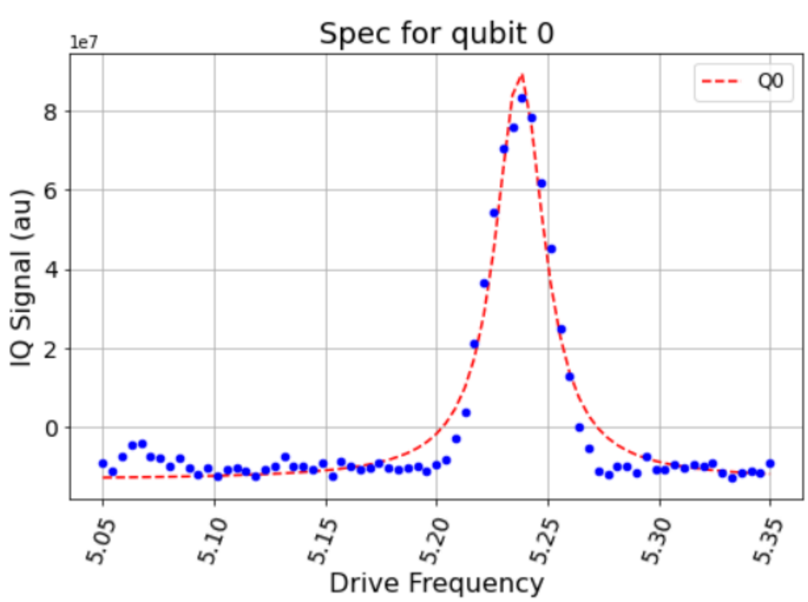
Challenge 4 : Transmon Qubits

My blog post about quantum hardware must have wormed you up to the different types of ways to make physical qubits. Transmon Qubits are currently the most extensively used of all the options available and a lot of corporations have invested heavily in them, including IBM.
The major distinction between classical and quantum physics is that in quantum physics, practically everything is “quantized” (I think that is the reason for the name). To put it another way, properties can only have discrete values. So energy is quantized in levels too, of which the ground state and the first excited state of the Physical Quantum system are used in the creation of qubits.

The 4th challenge was to find the optimum pulse to go from the first excited level to the second excited level. I don't think this is used a lot for real applications but it sure was interesting.

Transition frequency |0> to |1>

The first step is to determine the frequency of transition between the ground and first excited states (|0> to |1>).
This is accomplished by first establishing an array of frequencies between the expected values and then evaluating each choice individually. The data is then used for curve fitting, and the driving frequency is the most optimum frequency for the transition to occur.

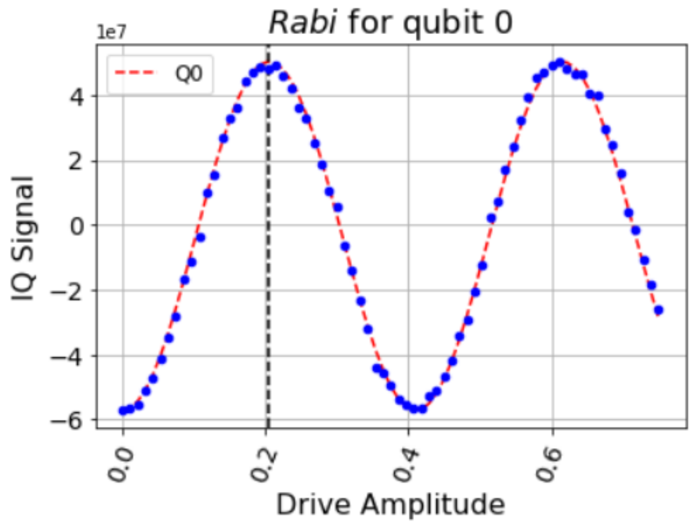


Drive Frequency

For my case the drive frequency came out to be 5.237599 GHz.

Drive Amplitude |0> to |1>

The next step is to determine the pulse's driving amplitude. This needs a technique similar to step one, only this time we incrementally increase the Drive Amplitude until we reach the optimal transition level for evolving |0> to |1>.

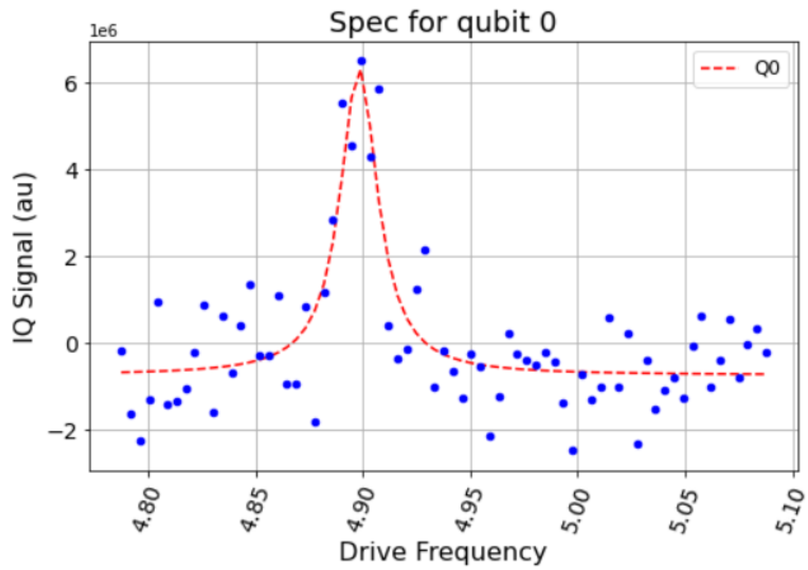


Drive Amplitude

The answer came out to be 0.205 for my case.

Transition Frequency |1> to |2>

Finally lets find the transition frequency for |1> to |2>, this is what we are here for. The same procedure is followed but this is only executed once we have gotten to |1> level.(this is why I went through the trouble above).
Same procedure will be repeated just between 4.8 to 5.1 as the end points this time.



Final solution

The final solution that we get is 4.898233 GHz. This challenge was unscored and honestly this was the one that I enjoyed the most.

Challenge 5: Variational Quantum EigenSolver

VQE is the algorithm which finally made Feynman's dream come true, simulating quantum mechanical systems using Quantum Machines. The algorithm is able to use noisy quantum computers to find the ground state of the molecules. The results hence obtained are similar to experimental results proving the effectiveness of the algorithm.
The success of VQE comes from the fact that it uses the best parts of both Quantum as well as Traditional Computers to solve the problem at hand.The Quantum Processor stores and manipulates the system's wave function, while the Classical Computer optimises the Quantum circuit and analyses the data received to determine the ground state energy.

Let’s take a deeper look into the Variational Quantum Eigensolver.

Some cool Math

The molecular Hamiltonian is given below

$$H = -\sum_{A=1}^{M} \frac{\nabla_A^2}{2M_A} - \sum_{i=1}^{N} \frac{\nabla_i^2}{2} - \sum_{i=1}^{N}\sum_{A=1}^{M} \frac{Z_A}{r_{iA}} + \sum_{B>A} \frac{Z_A Z_B}{R_{AB}} + \sum_{j>i} \frac{1}{r_{ij}}$$

If you look closely each term refers to kinetic or potential energy of the electrons or the nucleus. The wave function is the eigenequation of the Hamiltonian and the different eigenvalues correspond to different energy levels of the system.

$$H|\psi >= E|\psi >$$

So what we want is the minimum possible eigenvalue aka the ground state energy level for this hamiltonian. This is done by representing the wave function (psi) using a quantum circuit which we call the *ansatz.* This circuit is a variational circuit in other words the circuit is formed of rotation gates and CNOTs, the angle of rotation can be varied in order to get the lowest possible value of the eigenvalue.

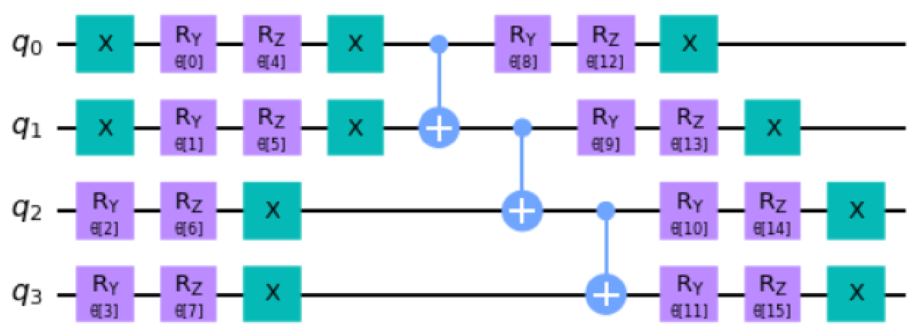
$$H|\psi(\theta) >= E(\theta)|\psi(\theta) >$$

$$E(\theta) =< \psi(\theta)|H|\psi(\theta) >$$

The challenge was to obtain the ground state energy for LiH with a minimum number of CNOT gates. This was the only challenge which actually affected our rank on the leaderboard. And ofcourse your boy was at the top with a score of 3.

Solution

We start by mapping the Molecular Hamiltonian to qubits using one of the mappers provided, I choose the Parity Mapper. Then the next step was to decide on the Ansatz. Initially I started with the UCCSD but the cost was above 200, so after some experimenting and a bit of discussion on the slack channel with other participants. I decided to go with TwoLocal because that uses the minimum number of CNOTs. The main idea is to have a lesser number of CNOTs and more single qubit gates, this will actually make the task of optimizers a bit hard but the noise will decrease. The final ansatz circuit is given below.



Finally after choosing the optimizer as COBYLA (this I choose on the basis of a little experimentation), I got the score 3. Yayy !!!

The challenge was surely hard and time consuming but the amount of knowledge that I gained over those few days was tremendous. And the best part of the challenge was the happiness that you get after you have worked hard. Hopefully this got you familiarized with questions of IQC 2021 and I will meet you all there next year.

Resources

1. https://medium.com/qiskit/ibm-quantum-challenge-2021-heres-what-to-expect-65a303753ffb
2.