

# Homework 7 (part 2)

## CSE 490q

**Due:** Fri, Dec 4th by 11pm PST

In this part of the assignment, you will simulate a piece of the molecule.

## 1 Setup

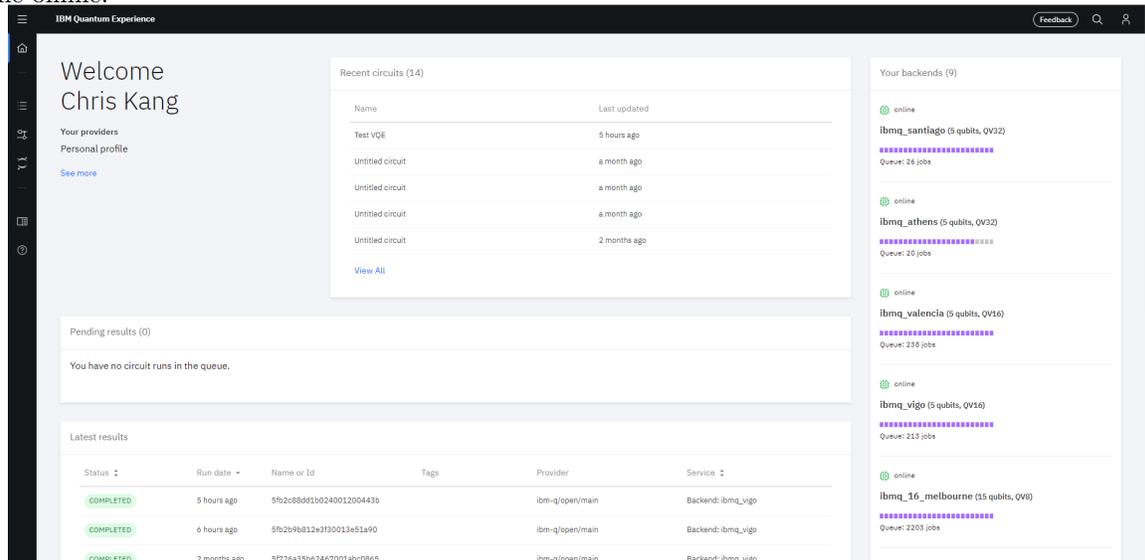
These are the setup steps in order to start running a quantum program!

**Register for an IBM Q account:**

1. Go to <https://quantum-computing.ibm.com/>
2. You can register for an account with your CSE Google account / Github / IBMid (...if you'd like to make one? I guess?)

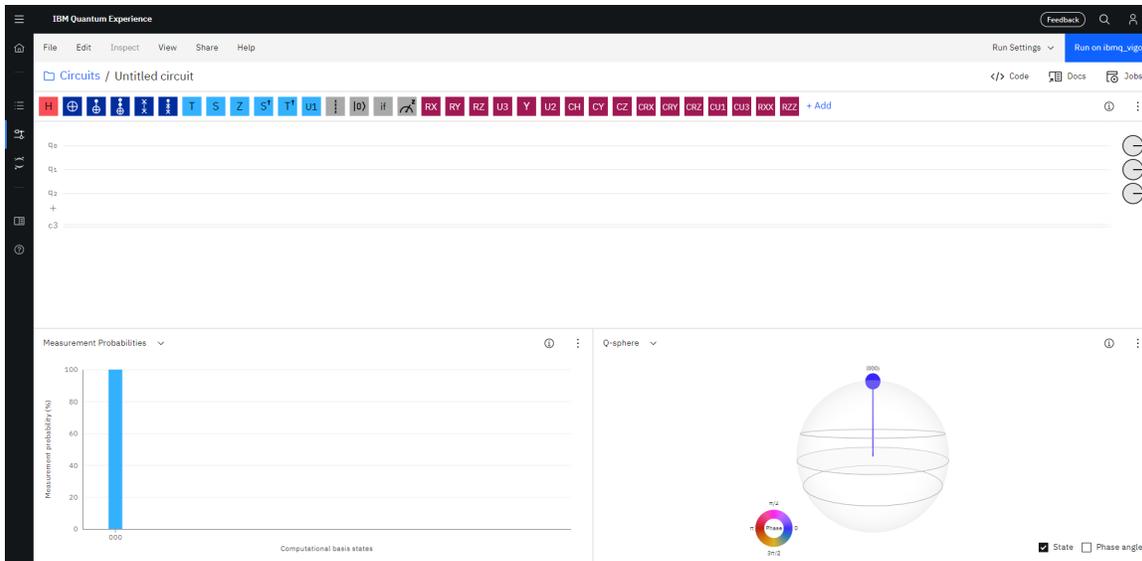
**Become familiar with IBM Q Online**

While the components integrate with QISKit in Python, all of the experiments we'd like to run can be done online.



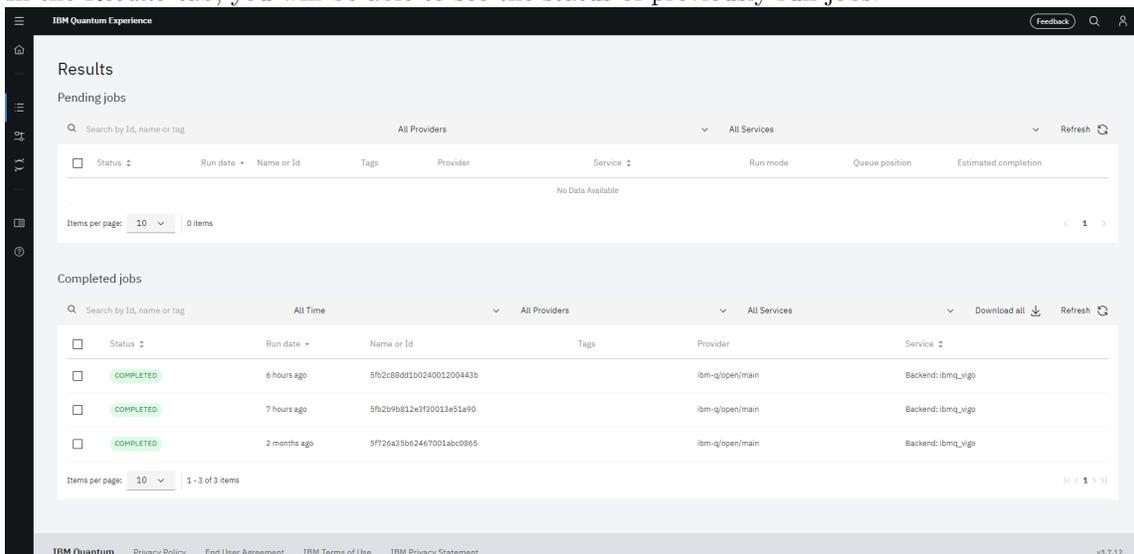
On the left hand bar, there are three segments: Results, Circuit Composer, and Quantum Lab (you can show these titles by clicking the hamburger in the top left). We will be focusing on *Results* and *Circuit Composer*.

In the *Circuit Composer* tab, you can directly create quantum circuits (with the horizontal scores we've used).



1. You can rename the drawing by clicking where it says “Untitled Circuit.”
2. The circuit composer has a variety of gates available; more information is available here: <https://quantum-computing.ibm.com/docs/idx/operations-glossary>.
3. In the bottom left, the measurement probabilities are displayed. These are theoretical and do not account for noise. Similarly, the right side provides a graphical representation of the output states (and does not account for noise).
4. When you are ready, click “Run Settings” and set the number of shots to the maximum of 8192. You should select the device based on which has the fewest number of jobs on the homepage.

Chris is happy to help troubleshoot in office hours and IBM’s help menu is thorough. In the *Results* tab, you will be able to see the status of previously run jobs.



By clicking on the run, you can see the output distribution and further information on the implemented circuit.

**Problem 1 (Setup).** As a simple test, please setup the circuit to construct EPR pair  $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ , run it on either the Santiago / Athens devices, and screenshot both the output and the circuit necessary.

**If you have any questions with this part of the assignment, be sure to ask! If this part is not working correctly, the next parts will not work either.**

Note, when running jobs:

1. DO NOT USE THE STATE VECTOR SIMULATOR, as it is only a simulation
2. If possible, use the Santiago / Athens devices, as they have a higher “Quantum Volume” than other devices (and better overall fidelity). While some of the other devices will work, your results may be less accurate
3. Set the trials to maximum (8192), as it will help us reduce the variance

## 2 Ansatz

In the following section, you will apply the VQE approach upon a simplified, single dimensional ansatz  $|\psi(\theta)\rangle$ . The ansatz will be built using the operations shown in the table below, where the 0th qubit is the first in the ket representation (i.e., a 1 for the 0th qubit would be represented  $|1000\rangle$ ).

| Gate         | Control | Target |
|--------------|---------|--------|
| $Ry(\theta)$ |         | 0      |
| CNOT         | 0       | 1      |
| X            |         | 0      |
| X            |         | 2      |

**Problem 2 (Ansatz).** Before we do anything, let’s verify the representation of the ansatz. Define the ansatz  $|\psi(\theta)\rangle$  as above, and verify the following expansion of the ansatz:

$$|\psi(\gamma)\rangle = (\cos(\frac{\gamma}{2}) |10\rangle + \sin(\frac{\gamma}{2}) |01\rangle) \otimes |10\rangle \quad (1)$$

Finally, describe the output states of  $|\psi(\alpha)\rangle$ ,  $|\psi(\beta)\rangle$ ,  $|\psi(\omega)\rangle$ , where  $\alpha = 0.4\pi$ ,  $\beta = 0.3\pi$ ,  $\omega = 0$

Recognize that we can interpret this ansatz as denoting an electron as being in a superposition between the 0th and 1st orbital, and a second electron concretely in the 2nd orbital.

### 3 Simulation

**Problem 3** (Simulation!). There are three different properties to simulate: the ansatz, the Hadamard test, and the Paulis.

For the ansatz: given the description of  $|\psi(\theta)\rangle$  above, implement this in the online circuit builder. Make sure to set the correct theta by double clicking on the “Ry” gate when you add it to the circuit. Some things to keep in mind:

1. For the Paulis - make sure you are controlling on the Hadamard test’s ancilla!
2. For the Hadamard test - make sure to measure the ancilla qubit and read it to the classical register. It’s not necessary to measure any of the other output qubits.
3. Begin by simulating this Pauli sequence: **IIII**. (Again, where the qubits are indexed as 0, 1, 2, 3).  
**Hint: this circuit should have a straightforward result**

Repeat the simulation procedure below for EACH of the three values for  $\theta$  ( $\alpha, \beta, \omega$ ).  
Now, simulate ONE of these Pauli sequences. If you were born in the...

| Birth Month            | Simulation Target |
|------------------------|-------------------|
| First quarter (01-03)  | ZIII              |
| Second quarter (04-06) | IZII              |
| Third quarter (07-09)  | IIZI              |
| Fourth quarter (10-12) | IIIZ              |

Now, simulate ONE of these Pauli sequences (**and take a screenshot**). If you were born in the...

| Birth Week          | Simulation Target |
|---------------------|-------------------|
| First week (01-07)  | XXXX              |
| Second week (08-14) | XXYY              |
| Third week (15-21)  | YYXX              |
| Fourth week (22+)   | YYYY              |

Finally, simulate ONE of these Pauli sequences. If you were born on a...

| Birth Week | Simulation Target |
|------------|-------------------|
| Monday     | IIZZ              |
| Tuesday    | IZIZ              |
| Wednesday  | IZZI              |
| Thursday   | ZIIZ              |
| Friday     | ZIZI              |
| Saturday   | ZZII              |
| Sunday     | Any above!        |

You should now have the following results to turn in:

1. **Three screenshots** of the XXXX/XXYY/YYXX/YYYY Pauli circuits and their results
2. **Nine results**, three per each angle

More details will come on the Ed on where to submit your results. Congrats, though - you’ve just used a quantum computer, simulated a portion of a molecule, and understand the theory behind the algorithm!

## 4 Obtaining the Paulis

While we provided the Paulis and the coefficients directly, it's good to also know how they were obtained (via Jordan-Wigner). Notably, this is the full and complete definition of the JW transform (**different from the slides!**):

$$a_p^\dagger = \left( \bigotimes_{l=0}^{p-1} Z_l \right) \otimes \left( \frac{X_p - iY_p}{2} \right) \otimes \left( \bigotimes_{l=p+1}^n I_l \right) \quad (2)$$

$$a_p = \left( \bigotimes_{l=0}^{p-1} Z_l \right) \otimes \left( \frac{X_p + iY_p}{2} \right) \otimes \left( \bigotimes_{l=p+1}^n I_l \right) \quad (3)$$

Essentially, we apply  $Z$  to the first  $p - 1$  qubits, and also apply the Pauli sum to  $p$ , leaving the qubits  $p + 1$  to  $n$  unchanged. This is necessary to correct for a parity factor (aka: the phase of an electron in a higher orbital is dependent upon whether electrons occupy lower orbitals).

There are different term types for a fermionic Hamiltonian, one specifically called the PQQP term:

$$a_p^\dagger a_q^\dagger a_q a_p \quad (4)$$

**Problem 4.** Derive the formulation for the PQQP term in Paulis.