Experiment 1: Quantum Measurement
PHYS-C0258: Quantum Labs

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Objectives: Measure the state of the qubit in X- and Y-bases, in addition to standard computational basis (Z-basis). Use this scheme of measurement in different bases to measure the expectation value of the Pauli operators. By utilizing the techniques developed, estimate the energy levels of the hydrogen ground state (hyperfine splitting) using IBMQ simulator and by running the circuit on an IBM quantum computer. Finally, perform simple error mitigation methods to improve the results obtained from the quantum computer.

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1 Introduction

Quantum computers can potentially outperform classical computers in certain computational tasks by leveraging quantum mechanical phenomena like superposition and entanglement. In particular, they are a natural choice for simulating many-body quantum dynamics that otherwise would be intractable for any classical computers.

In this experiment, we simulate the energy levels of a bipartite system using an operational superconducting-circuit based quantum computer from IBM [2], [3]. We estimate the energy levels of the hydrogen ground state using IBMQ simulator and by running the circuit on a physical hardware. Expectantly, we observe the hyperfine splitting of the energy levels of the hydrogen ground state.

To achieve this, we begin by mapping the Hamiltonian describing the electron-proton interaction in the Hydrogen atom to two-qubits quantum circuit. We estimate the energy levels by measuring the expectation value of the Hamiltonian, which requires us to evaluate the expectation value of the Pauli operators. Additionally, we need to create user-defined functions to facilitate measurement in X- and Y-bases in order to evaluate all the Pauli operators. Due to Heisenberg uncertainty of non-commuting observables, we would need to evaluate the same circuit multiple times to obtain the expectation value of all the Pauli operators. Furthermore, we perform standard noise mitigation techniques to improve the measured energies.

2 Hyperfine Splitting in Hydrogen

One of the interesting applications of quantum mechanics is the description of hyperfine splitting observed in Hydrogen ground state [1]. The ground state of the Hydrogen atom does not correspond to a single well-defined energy state due to the spins of the electron and the proton. Instead, there are four distinct states resulting from different spin combinations of the electron and the proton. Three of these states, called *triplet* state, have the same energy and one of the states, called *singlet* state, has three times lower energy than the triplet state.
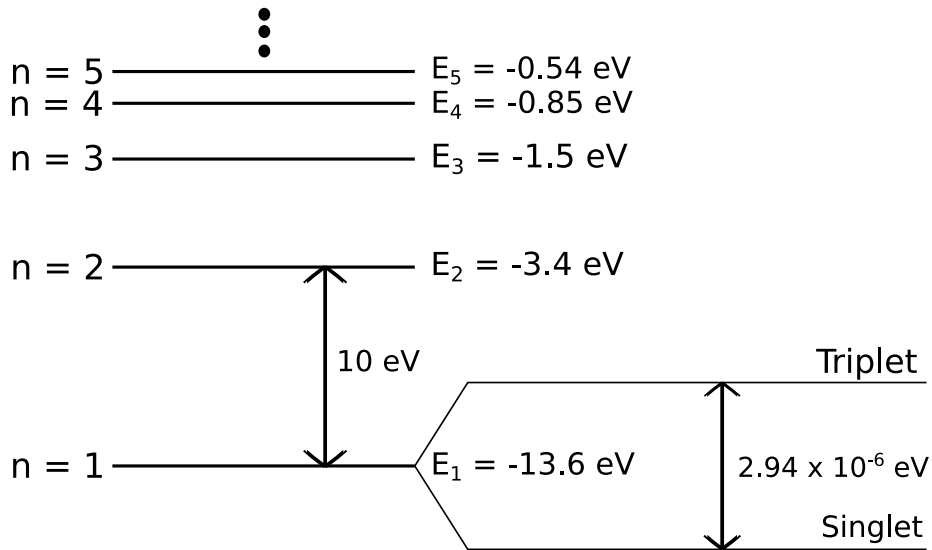

Figure 1: Energy spectrum of the Hydrogen atom. The energy difference of hyperfine splitting of the ground state is much smaller than the transition between the ground and the first excited state (Figure not to scale).

To describe this bipartite system, we need to choose a suitable basis states. As we know from linear algebra that there is no unique basis states for describing any system. Thus, we pick a basis that utilizes the spin states of both the electron and the proton. That is, both being spin one-half particles, we can define 4-dimensional Hilbert space $\mathcal{H} = \mathcal{H}_e \otimes \mathcal{H}_p$, which is formed from the tensor product of two-dimensional Hilbert spaces describing both the electron and the proton.

$$
\begin{aligned}
&State\ 1: |++\rangle\,;\text{electron } up,\ \text{proton } up\\
&State\ 2: |+-\rangle\,;\text{electron } up,\ \text{proton } down\\
&State\ 3: |-+\rangle\,;\text{electron } down,\ \text{proton } up\\
&State\ 4: |--\rangle\,;\text{electron } down,\ \text{proton } down,
\end{aligned}
\tag{1}
$$

where we have used a shorthand notation $|++\rangle = |+\rangle \otimes |+\rangle$. That is, the first +/- symbol refers to the electron spin states and the second symbol refers to the proton spin states.

We can write down an arbitrary two-qubit state as a linear combination of

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these basis states:

$$|\psi\rangle = |++\rangle \langle + + |\psi\rangle + |+-\rangle \langle + - |\psi\rangle$$
$$+ |+-\rangle \langle + - |\psi\rangle + |--\rangle \langle - - |\psi\rangle. \qquad (2)$$

From introductory quantum mechanics course, we found out that the Hamiltonian of a single, spin one-half particle can be expressed in terms of Pauli/sigma operators/matrices. Similarly, we can also write down the Hamiltonian of a bipartite system as a sum of tensor product of Pauli operators defined on Hilbert spaces of the electron and the proton:

$$\hat{H} = A\{\hat{X}_e \otimes \hat{X}_p + \hat{Y}_e \otimes \hat{Y}_p + \hat{Z}_e \otimes \hat{Z}_p\}, \qquad (3)$$

where $\{\hat{X}_e, \hat{Y}_e, \hat{Z}_e\} \in \hat{\mathcal{H}}_e$, $\{\hat{X}_p, \hat{Y}_p, \hat{Z}_p\} \in \hat{\mathcal{H}}_p$, and $\{\hat{X}_e \otimes \hat{X}_p, \hat{Y}_e \otimes \hat{Y}_p, \hat{Z}_e \otimes \hat{Z}_p\} \in \hat{\mathcal{H}}$. The constant A is given by the product of the magnetic moments of the electron and the proton over the distance between them in the Hydrogen atom.

Having the basis states and the Hamiltonian ready, we can solve the Schrödinger equation and obtain the energy levels of the Hydrogen ground state, analytically. This is not something we will do in the lab assignment, even though solving this analytically is a fun exercise. Instead, we will now use this mathematical description to simulate the energy levels of the Hydrogen ground state using IBMQ.

One final note, in order to obtain the energies, you must evaluate the expectation value of the Hamiltonian, which yields,

$$E = \langle\hat{H}\rangle = A\{\langle\hat{X}_e \otimes \hat{X}_p\rangle + \langle\hat{Y}_e \otimes \hat{Y}_p\rangle + \langle\hat{Z}_e \otimes \hat{Z}_p\rangle\}. \qquad (4)$$

For a detailed analytical solution, see here

3 Simulating with IBMQ

We realize that both the electron and the proton are spin one-half particles, similar to a superconducting qubit. Thus, we require a minimum of two-qubit quantum processor, with one qubit acting as an electron and the other as a proton, to simulate the energy levels of the Hydrogen ground state. Luckily, all of the quantum processors offered by IBMQ contains 5 qubits or more.

The experiment is divided into three distinct tasks. Below, you can find a summary of the lab assignment. A detailed instructions is provided in the jupyter notebook **Exp1_QuantumMeasurement.ipynb**. All the tasks that you need to carry out is included in the notebook.

3.1 Measuring the state of a qubit

Fundamental to the operation of a quantum computer is the ability to compute the Bloch components of a qubit or qubits. These components correspond to the expectation values of the Pauli operators **X**,**Y**,**Z**, and are important quantities for applications such as quantum chemistry and optimization. Unfortunately, it is impossible to simultaneously compute these values (Heisenberg uncertainty relationship of non-commuting operators/observables), thus requiring many executions of the same circuit. In addition, measurements are restricted to the

computational basis (Z-basis) so that each Pauli needs to be rotated to the standard basis to access the x and y components. In this task, you will implement the following:

- Derive the expression for expectation values of Pauli operators for a single-qubit case. We will use this idea in deriving the expectation values of Pauli operators for two-qubit case.

- Create the X-measurement function, *x_measurement(qc, qbit, cbit)*, to measure the expectation value of Pauli X operator.

- Create the Y-measurement function, *y_measurement(qc, qbit, cbit)*, to measure the expectation value of Pauli Y operator.

- Verify your implementation by comparing the results with the help of analytical tools.

3.2 Measuring energy levels of the hydrogen ground state

The energy of a quantum system can be estimated by measuring the expectation value of its Hamiltonian (4), which is a Hermitian operator, through the procedure we outlined in subsection 3.1.

In this part, we evaluate the energy difference among these four states, which is from the *hyperfine splitting*, by computing the energy expectation value for the system of two spins with the Hamiltonian expressed in Pauli operators (3). In this task, you will:

- Derive the expression for expectation values of Pauli operators for a two-qubit state. As we saw in the theory section, evaluating the energies essentially means measuring the expectation value of Pauli operators. *Hint: Use the distributive property when evaluating the tensor product of outer products, express the outer product in matrix form, and calculate the tensor product using matrix method, for ex:* $\begin{bmatrix} a & b \\ c & d \end{bmatrix} \otimes \begin{bmatrix} x & y \\ z & w \end{bmatrix} =$
$\begin{bmatrix} a \cdot \begin{bmatrix} x & y \\ z & w \end{bmatrix} & b \cdot \begin{bmatrix} x & y \\ z & w \end{bmatrix} \\ c \cdot \begin{bmatrix} x & y \\ z & w \end{bmatrix} & d \cdot \begin{bmatrix} x & y \\ z & w \end{bmatrix} \end{bmatrix}$. *Also, remember* $|+-\rangle = |+\rangle \otimes |-\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes$
$\begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \cdot \begin{bmatrix} 0 \\ 1 \end{bmatrix} \\ 0 \cdot \begin{bmatrix} 0 \\ 1 \end{bmatrix} \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$.

- Construct the circuits to prepare four different bell (entangled) states.

- Use the X- and Y- measurement functions from subsection 3.1 to measure the expectation values of Pauli X and Y for both qubits.

- Verify you obtain the correct wavelength of the emission from the transition between the triplet states and singlet state.

3.3 Executing the circuits on a IBM quantum computer

In this part, we execute the same circuit created in subsection 3.2 on a physical hardware. You will conduct following steps in this task:

- Load your IBMQ account, choose a proper backend such that the readout error and CNOT error for a given quantum processor is minimum.

- Run the circuits on different available backends and record the results. Perform some statistical analysis on the data and state your observations in the report.

- Carry out error mitigation techniques to improve the measured energies for the singlet and triplet states. Note that, we will only improve errors resulting from spontaneous decay (finite T1 time).

- Calculate the relative errors of the energies with and without the implementation of error mitigation techniques.

Side note

Suggestion: Instead of tackling the whole assignment at once, follow the notebook code blocks and write unit tests or run your functions on a separate notebook to make sure your codes are doing exactly what it is supposed to. In case of doubt, always ask for help from your group members or the TA. You can also find relevant information from qiskit webpage [3].

You will give a presentation and write a report for this lab assignment. Use the templates provided to you for both preparing the presentation and writing the report. You will deliver jupyter notebook ***Exp1_QuantumMeasurement.ipynb*** and the report by the deadline (one week from starting the experiment). Make sure to reserve the time by email for the presentation.

References

[1] Richard Feynman, Robert Leighton, and Sands Matthew. *The Feynman lectures on physics.* Addison-Wesley Pub. Co., 1963.

[2] IBM. *IBM Quantum Computing.* https://quantum-computing.ibm.com/, 2021.

[3] Qiskit. *Qiskit.* https://qiskit.org/, 2021.