Experiment 1: Quantum Measurement
Group 3

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Contents

1 Introduction

Quantum computers can outperform classical ones in specific tasks where their nature can be properly utilized for speeding up the computations. In particular, quantum computers are well suited for simulating the behavior of different quantum systems. In this experiment we are going to simulate hyperfine splitting in the hydrogen atom - separation of the ground state of the electron into four different substates caused by the interaction between spins of the electron and the proton. [1] We would construct a set of quantum circuits modeling the system, run the model on the AER simulator to get the expected values of energy for each state, then run the model on several IBM quantum computer backends and compare energies we obtained to the expected values. We would then run a set of calibration circuits on all the used backends to get the information on measurement errors, and use that information to perform error compensation on the results obtained by the model.

2 Experiment setup

2.1 Measuring the state of the qubit

To experimentally get the expectation value of $\hat{Z}$ it's enough to measure the qubit in computational basis, but for $\hat{X}$ and $\hat{Z}$ we need to measure the qubit in X and Y bases respectively. To achieve that, we need to rotate the qubit's state vector in the right way, effectively mapping states of the chosen basis basis into $|0\rangle$ and $|1\rangle$. For X basis we can achieve such rotation by applying the Hadamard gate: $H\left|+\right\rangle = |0\rangle\,, H\left|-\right\rangle = |1\rangle$. For Y basis we apply $S^\dagger$ gate before the Hadamard gate: $HS^\dagger\left|R\right\rangle = |0\rangle\,, HS^\dagger\left|L\right\rangle = |1\rangle$. [3] Therefore

$$\langle\hat{Z}\rangle = \langle\psi|\hat{Z}|\psi\rangle = \langle\psi|0\rangle\,\langle 0|\psi\rangle - \langle\psi|1\rangle\,\langle 1|\psi\rangle = |\,\langle 0|\psi\rangle\,|^2 - |\,\langle 1|\psi\rangle\,|^2$$

$$\langle\hat{X}\rangle = \langle\psi|\hat{X}|\psi\rangle = \langle\psi|\hat{H}\hat{Z}\hat{H}|\psi\rangle = \langle\psi|\hat{H}|0\rangle\,\langle 0|\hat{H}|\psi\rangle - \langle\psi|\hat{H}|1\rangle\,\langle 1|\hat{H}|\psi\rangle = |\,\langle 0|\hat{H}|\psi\rangle\,|^2 - |\,\langle 1|\hat{H}|\psi\rangle\,|^2$$

$$\langle\hat{Y}\rangle = \langle\psi|\hat{X}|\psi\rangle = \langle\psi|\hat{S}\hat{H}\hat{Z}\hat{H}\hat{S}^\dagger|\psi\rangle = \langle\psi|\hat{S}\hat{H}|0\rangle\,\langle 0|\hat{H}\hat{S}^\dagger|\psi\rangle - \langle\psi|\hat{S}\hat{H}|1\rangle\,\langle 1|\hat{H}\hat{S}^\dagger|\psi\rangle = |\,\langle 0|\hat{H}\hat{S}^\dagger|\psi\rangle\,|^2 - |\,\langle 1|\hat{H}\hat{S}^\dagger|\psi\rangle\,|^2$$

We defined the functions x_measurement and y_measurement to measure a qubit in X and Y basis, and then tested them on AER simulator by first choosing a random pure state for a qubit (using random_comp_coeff() function), then measuring this state several times in X, Y and Z bases and reconstructing the state based on this measurement.

2.2 Measuring the energy

We can calculate the energy of the state $|\psi\rangle$ as the expectation value of the Hamiltonian:

$\hat{\mathcal{H}} = A\{\hat{X}_e \otimes \hat{X}_p + \hat{Y}_e \otimes \hat{Y}_p + \hat{Z}_e \otimes \hat{Z}_p\}$, where $A = 1.47e^{-6}eV$ [4] $E = \langle\hat{\mathcal{H}}\rangle = A\{\langle\hat{X}_e \otimes \hat{X}_p\rangle + \langle\hat{Y}_e \otimes \hat{Y}_p\rangle + \langle\hat{Z}_e \otimes \hat{Z}_p\rangle\}$.
We can calculate the expectation value of the tensor products of Pauli operators as:

$\langle\hat{Z}_e \otimes \hat{Z}_p\rangle = \langle\psi|\hat{Z}_e \otimes \hat{Z}_p|\psi\rangle = \langle\psi|\,(|0\rangle\langle 0|-|1\rangle\langle 1|)\otimes(|0\rangle\langle 0|-|1\rangle\langle 1|)\,|\psi\rangle = \langle\psi|\,(|0\rangle\langle 0|\otimes|0\rangle\langle 0| - |0\rangle\langle 0|\otimes|1\rangle\langle 1| - |1\rangle\langle 1|\otimes|0\rangle\langle 0| + |1\rangle\langle 1|\otimes|1\rangle\langle 1|)\,|\psi\rangle = |\,\langle 00|\psi\rangle\,|^2 - |\,\langle 01|\psi\rangle\,|^2 - |\,\langle 10|\psi\rangle\,|^2 + |\,\langle 11|\psi\rangle\,|^2$

And, similarly:

$\langle\hat{X}_e \otimes \hat{X}_p\rangle = \langle\psi|\hat{X}_e \otimes \hat{X}_p|\psi\rangle = \langle\psi|(\hat{H}_e \otimes \hat{H}_p)(\hat{Z}_e \otimes \hat{Z}_p)(\hat{H}_e \otimes \hat{H}_p)|\psi\rangle = |\,\langle 00|(\hat{H}_e \otimes \hat{H}_p)|\psi\rangle\,|^2 - |\,\langle 01|(\hat{H}_e \otimes \hat{H}_p)|\psi\rangle\,|^2 - |\,\langle 10|(\hat{H}_e \otimes \hat{H}_p)|\psi\rangle\,|^2 + |\,\langle 11|(\hat{H}_e \otimes \hat{H}_p)|\psi\rangle\,|^2 = |\,\langle 00|\phi\rangle\,|^2 - |\,\langle 01|\phi\rangle\,|^2 - |\,\langle 10|\phi\rangle\,|^2 + |\,\langle 11|\phi\rangle\,|^2$, where $|\phi\rangle = (\hat{H}_e \otimes \hat{H}_p)\,|\psi\rangle$

$\langle\hat{Y}_e \otimes \hat{Y}_p\rangle = \langle\psi|\hat{Y}_e \otimes \hat{Y}_p|\psi\rangle = \langle\psi|(\hat{S}_e \otimes \hat{S}_p)(\hat{H}_e \otimes \hat{H}_p)(\hat{Z}_e \otimes \hat{Z}_p)(\hat{H}_e \otimes \hat{H}_p)(\hat{S}_e^\dagger \otimes \hat{S}_p^\dagger)|\psi\rangle = |\,\langle 00|(\hat{H}_e \otimes \hat{H}_p)(\hat{S}_e^\dagger \otimes \hat{S}_p^\dagger)|\psi\rangle\,|^2 - |\,\langle 01|(\hat{H}_e \otimes \hat{H}_p)(\hat{S}_e^\dagger \otimes \hat{S}_p^\dagger)|\psi\rangle\,|^2 - |\,\langle 10|(\hat{H}_e \otimes \hat{H}_p)(\hat{S}_e^\dagger \otimes \hat{S}_p^\dagger)|\psi\rangle\,|^2 + |\,\langle 11|(\hat{H}_e \otimes \hat{H}_p)(\hat{S}_e^\dagger \otimes \hat{S}_p^\dagger)|\psi\rangle\,|^2 = |\,\langle 00|\theta\rangle\,|^2 - |\,\langle 01|\theta\rangle\,|^2 - |\,\langle 10|\theta\rangle\,|^2 + |\,\langle 11|\theta\rangle\,|^2$, where $|\theta\rangle = (\hat{S}_e^\dagger \otimes \hat{S}_p^\dagger)(\hat{H}_e \otimes \hat{H}_p)\,|\psi\rangle$

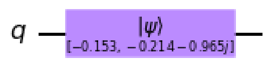
Therefore, to compute the energy value for every state $|\psi\rangle \in \{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$ we need to prepare several quantum circuits, each measuring one state in one of the bases, and then run them several times to compute the expectation values and then the final values of energy. As there are 4 possible states and 3 bases, we have to run 12 circuits in total. We first run those circuits on the AER simulator, so we can get the expected value of energy for every state. We would also use those values to calculate the wavelength of the light emitted when transitioning from one of the triplet states to singlet, expecting to arrive at 21.1 cm hydrogen line wavelength.

2.3 Executing the circuits on Quantum Computer

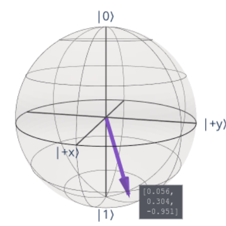
Now we will run the same circuits on the real quantum computers [2] and see, how well the energy value computed while running the model on the real quantum hardware matches the prediction. We would run the model on several IBM quantum backends, picking the qubits with the best CNOT error for each, and compare the results. We would calculate errors for energy of each state, as well as error for the emitted wavelength.
We would also try to apply a quantum error mitigation technique: run a set of calibration circuits on every backend and use the results to create a matrix characterizing the readout error, then use the inverse of this matrix to remove the error from the measured results. Note that this error mitigation technique only allows to combat readout errors, but can do nothing against other types of errors.

3 Results

3.1 Measuring the state of the qubit



(a) Initial state



(b) Reconstructed state

$\phi = atan2(y, x) \approx 5.034$, $\theta = atan2(y, z) \approx 4.904$
$a = \cos\frac{\theta}{2} \approx -0.811, b = e^(i\phi) * \sin\frac{\theta}{2} \approx 0.112 - 0.574$, which is approximately equal to the initial state.

3.2 Measuring the energy

After running the circuits on the AER simulator, we get the expectation value for the energy of the triplet states as $1.470 * 10^{-6}eV$, and for singlet state as $-4.410 * 10^{-6}eV$ and 21.1 cm for the emission wavelength

3.3 Executing the circuits on Quantum Computer

We executed the circuits on several quantum backends, and got the following energy values:

Table 1: Estimated values for energies from different backends

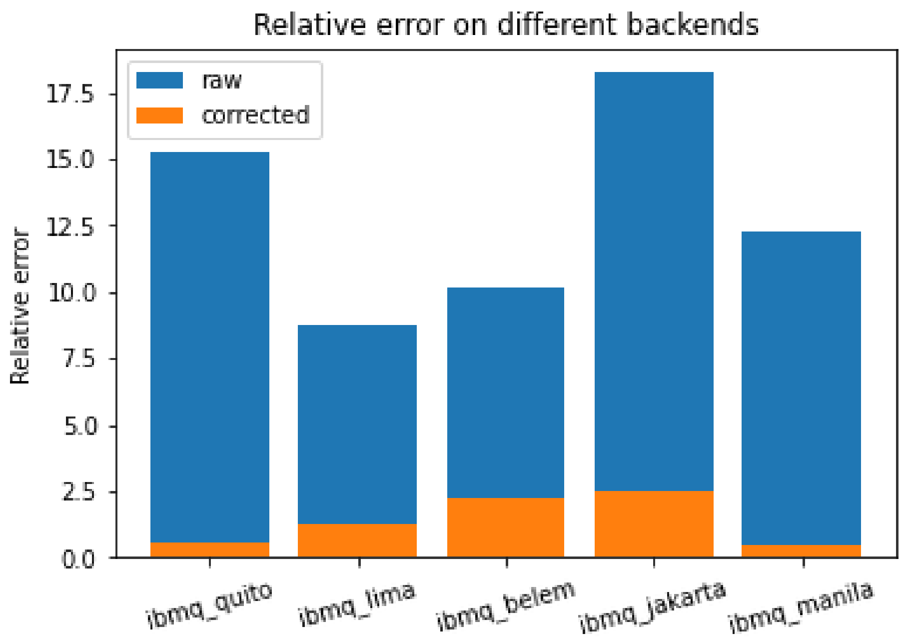
	$\|00\rangle$	$\|01\rangle$	$\|10\rangle$	$\|11\rangle$
ibmq_quito	1.27E-06 eV	1.23E-06 eV	1.24E-06 eV	-3.72E-06 eV
ibmq_lima	1.35E-06 eV	1.37E-06 eV	1.30E-06 eV	-4.04E-06 eV
ibmq_belem	1.35E-06 eV	1.30E-06 eV	1.32E-06 eV	-3.93E-06 eV
ibmq_jakarta	1.20E-06 eV	1.26E-06 eV	1.15E-06 eV	-3.62E-06 eV
ibmq_manila	1.31E-06 eV	1.28E-06 eV	1.25E-06 eV	-3.95E-06 eV

After executing the calibration circuits and applying the filters, we got the following results:

Table 2: Estimated values for energies from different backends, corrected

	$\|00\rangle$	$\|01\rangle$	$\|10\rangle$	$\|11\rangle$
ibmq_quito	1.47E-06 eV	1.45E-06 eV	1.47E-06 eV	-4.37E-06 eV
ibmq_lima	1.48E-06 eV	1.48E-06 eV	1.42E-06 eV	-4.37E-06 eV
ibmq_belem	1.47E-06 eV	1.42E-06 eV	1.43E-06 eV	-4.28E-06 eV
ibmq_jakarta	1.45E-06 eV	1.48E-06 eV	1.38E-06 eV	-4.35E-06 eV
ibmq_manila	1.48E-06 eV	1.47E-06 eV	1.48E-06 eV	-4.38E-06 eV

We also computed mean errors before and after the error mitigation:



4 Conclusion

As we can see, even modern days, noisy intermediate-scale quantum computers can be helpful in modelling tasks. Thanks to error mitigation techniques, errors of those simulations are quite small, which enables the use of their results in many spheres.

5 References

List of references

[1] Laure Mercier Aashish Sah. "Experiment 1: Quantum Measurement". In: *PHYS-C0258: Quantum Labs* ().

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

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

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

6 Appendix A: IBM Quantum Lab notebook

The appendix is included as a separate file