Implementing quantum state tomography in IBM-Q using expectation values

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Abstract

We discuss a method of performing quantum state tomography by finding out expectation values of the Pauli operators and using the data to construct the approximate density matrix of the state initially provided, either pure or mixed. The method is first constructed for any abstract qubits and then experimentally implemented on the IBM-Q Experence. We also discuss about a method to construct some given density matrices on the IBM quantum computer, which although incomplete, might be helpful for developing such techniques in future.

1 Introduction

Quantum State tomography is the process of reconstructing the density matrix representing the unknown state given to the user. Given an unknown pure or mixed state, there are certain methods that one could use to get back the density matrix of the state. Here, we discuss about an algorithm which involves calculating expectation values of Pauli operators to determine the density matrix of the unknown state. All of our discussion here is limited to the case of a single qubit but it can definitely be generalized for arbitrary n-qubits.

The density matrix approach is completely equivalent to the state vector approach since both give the same results, but the density matrix approach is often preferred when dealing with both pure and mixed states. The density matrix for a system can be described as

$$\rho = \sum_i p_i \left|\psi_i\right\rangle \left\langle\psi_i\right|$$

where $|\psi_i\rangle$ are the pure states combining to form the mixed state and p_i is the fraction of that pure state in the system. For a density matrix, the condition $\mathrm{tr}(\rho)=1$ is always satisfied. For pure states, $\mathrm{tr}(\rho^2)=1$ while for mixed states, $\mathrm{tr}(\rho^2)<1$.

2 Expectation Values

The expectation value of an operator $\hat{O}$ for some state $|\psi\rangle$ is defined as

$$\langle\hat{O}\rangle = \langle\psi|\hat{O}|\psi\rangle$$

The expectation value is the probabilistic expected value of the measurements of an experiment. It can be thought of as an average of all the possible outcomes of a measurement as weighted by their likelihood. So, for example, if in an experiment, we measure the state of the qubit, we will either get $|0\rangle$ or $|1\rangle$ which are the eigenbasis of the system in which we am measuring. Now if the state of the qubit is described as

$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle$$

then the probability of getting the result of getting $|0\rangle$ is $|\alpha|^2$ and the probability of getting the result $|1\rangle$ is $|\beta|^2$. If measuring state $|0\rangle$ corresponds to an eigenvalue c_0 and measuring $|1\rangle$ corresponds to an eigenvalue c_1 i.e.

$$\hat{M}\,|0\rangle = c_0\,|0\rangle \qquad \hat{M}\,|1\rangle = c_1\,|1\rangle$$

where $\hat{M}$ is the measurement operator. Since the expectation value is the weighted sum of all the measurements, we can say that the expectation value for this measurement operator is

$$\langle\hat{M}\rangle = |\alpha|^2 c_0 + |\beta|^2 c_1$$

2.1 Calculating expectation values using a single measurement device

Usually while calculating the expectation value of an operator, we need a device which could make measurements in the basis of the eigenvalues of the operator. For example, if we have a state $|\psi\rangle = \alpha\,|0_z\rangle + \beta\,|1_z\rangle = \alpha\,|0\rangle + \beta\,|1\rangle$ (for simplicity, we write $|0_z\rangle$=$|0\rangle$ and $|1_z\rangle$=$|1\rangle$) written in $|0\rangle$ and $|1\rangle$ basis which are eigen values of the σ_z Pauli operator, then we can straightaway determine the expectation value since the measurement is either going to give the result +1 (eigenvalue of $|0\rangle$) or -1 (eigenvalue of $|1\rangle$) because the measurement device itself is only capable of measuring in only these two states.

Now suppose you want to measure the expectation value of the same state for the operator σ_x which has the eigenvectors $|0_x\rangle$ and $|1_x\rangle$, then we know that we can rewrite the state $|\psi\rangle$ in the form of $|0_x\rangle$ and $|1_x\rangle$ such that

$$|\psi\rangle = \gamma\,|0_x\rangle + \delta\,|1_x\rangle$$

but if our measuring device has a limited capability of taking measurements only in the σ_z basis, then we would somehow need to convert our state vector such that

it has the same coefficients γ and δ but with the eigenvectors $|0\rangle$ and $|1\rangle$

$$|\psi'\rangle = \gamma\,|0\rangle + \delta\,|1\rangle$$

by applying some unitary operation $\hat{U}$ such that it could be implemented as some unitary time evolution quantum gate.

$$\hat{U}\,|\psi\rangle = \hat{U}(\alpha\,|0\rangle + \beta\,|1\rangle) = |\psi'\rangle = \gamma\,|0\rangle + \delta\,|1\rangle$$

So, our requirement is to find such a general unitary operation $\hat{U}$ which could calculate expectation value of any given Hermitian operator.

Using our previous example as a base, we see that to convert a vector from σ_z basis to σ_x basis, we need a basis transformation from σ_x basis to σ_z basis.

2.2 Finding the change of basis matrix

Since understanding this part is easier using an example, we continue with the above example. Expressing the Pauli matrices in the $|0\rangle$,$|1\rangle$ basis

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \;\; \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \;\; \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \;\; \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

f The eigenvectors of the σ_z are

$$|v_0; +1\rangle = |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |v_1; -1\rangle = |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

and the eigenvectors of σ_x are

$$|w_0; +1\rangle = |0_x\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad |w_1; -1\rangle = |1_x\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

So, we know how the eigenvectors of σ_x are expressed in terms of eigenvectors of σ_z. So we have a change of basis matrix C to convert a vector from σ_x basis to σ_z basis i.e. to convert a vector from $|0_x\rangle$,$|1_x\rangle$ basis to $|0\rangle$,$|1\rangle$ basis.

$$C = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

But, we actualy need a matrix to convert a vector from σ_z basis to σ_x basis i.e. to convert a vector from $|0\rangle$,$|1\rangle$ basis to $|0_x\rangle$,$|1_x\rangle$ basis, which would be the inverse of the change of basis matrix

$$C^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

which co-incidentally comes out to be the same as C in this case. Thus, we have come up with a way to convert a state in $|0\rangle$,$|1\rangle$ basis such that its coefficients come out to be the same as in the case when the state is written in $|0_x\rangle$,$|1_x\rangle$ basis.

Therefore, in general, if we have a Hermitian operator $\hat{O}$ whose expectation value we want to find, we first find out the eigenvectors $|v_i\rangle$'s of the operator and write a change of basis matrix C whose columns represent the eigenvectors $|v_i\rangle$ and then find the inverse change of basis matrix C^{-1}. Multiplying the given state $|\psi\rangle$ with this inverse change of basis matrix C^{-1} would yield the required state which then can be measured in $|0\rangle$ and $|1\rangle$ basis.

$$\hat{C}\,|\psi\rangle = \hat{C}(\alpha\,|0\rangle + \beta\,|1\rangle) = |\psi'\rangle = \gamma\,|0\rangle + \delta\,|1\rangle$$

$$\langle\hat{O}\rangle = |\gamma|^2 v_0 + |\delta|^2 v_1$$

where v_0 and v_1 are the eigenvalues of their respective eigenvectors $|v_0\rangle$ and $|v_1\rangle$.

Also, we claim that this C^{-1} matrix is a unitary matrix, so it can be implemented as a quantum logic gate.

Proof:

Let C be the change of basis matrix whose columns represent eigenvectors of the operator $\hat{O}$.

$$C = \begin{pmatrix} |v_0\rangle & |v_1\rangle & |v_2\rangle & \dots \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix} \; C^\dagger = \begin{pmatrix} \langle v_0| & \dots \\ \langle v_1| & \dots \\ \langle v_2| & \dots \\ \vdots & \dots \end{pmatrix}$$

$$C^\dagger C = \begin{pmatrix} \langle v_0| & \dots \\ \langle v_1| & \dots \\ \langle v_2| & \dots \\ \vdots & \dots \end{pmatrix} \begin{pmatrix} |v_0\rangle & |v_1\rangle & |v_2\rangle & \dots \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & \dots \\ 0 & 1 & 0 & \dots \\ 0 & 0 & 1 & \dots \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix} = I$$

since $\sum_i \sum_j \langle v_i|v_j\rangle = \delta_{ij}$ (from the result that columns of the change of basis matrix are orthonormal eigenvectors) where δ_{ij} is the Kronecker delta function.

So $C^\dagger C = I$ implies $C^\dagger = C^{-1}$. Now we know from the properties of matrices that $(C^\dagger)^{-1} = (C^{-1})^\dagger$. Also,$C^\dagger = C^{-1}$ since $CC^\dagger = I$.

$$(C^{-1})^\dagger = (C^\dagger)^{-1} = (C^{-1})^{-1}$$

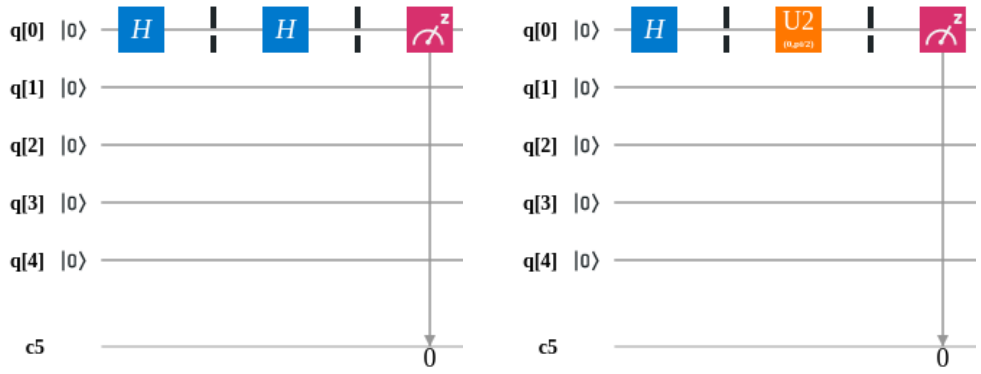
Therefore, we can see that $(C^{-1})^\dagger = (C^{-1})^{-1}$ which means that C^{-1} is a **unitary operation**.

2.3 Calculating expectation values on IBM-Q Experience

Using the above algorithm on the IBM quantum computer, we can experimentally calculate the expectation values of the given Hermitian operators. To test our algorithm we will calculate the expectation values of σ_x and σ_y for the state $|\psi\rangle=\frac{1}{\sqrt{2}}|0\rangle+\frac{1}{\sqrt{2}}|1\rangle$.
Theoretically, using the definition of expectation values as $\langle\hat{O}\rangle=\langle\psi|\hat{O}|\psi\rangle$, we find that

$$\langle\sigma_x\rangle=\langle\psi|\sigma_x|\psi\rangle=1 \qquad \langle\sigma_y\rangle=\langle\psi|\sigma_y|\psi\rangle=0$$

Now using the IBM Quantum Computer, we can verify and compare the results calculated experimentally with the theoretically calculated values. The quantum circuits for these tests are shown in Figure 1 below .



(a) Circuit for calculation of $\langle\sigma_x\rangle$. (b) Circuit for calculation of $\langle\sigma_y\rangle$.

Figure 1: Quantum Circuits setup on IBM-Q Experience.

Here, we are calculating the expectation values $\langle\sigma_x\rangle$ and $\langle\sigma_y\rangle$ for the state $|\psi\rangle=\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle)$ which obtained by applying Hadamard gate (H) on the state $|0\rangle$ of the qubit q1.
For the calculation of expectation value of σ_x, we first need to find the eigenvalues and eigenvectors of σ_x which come out to be

$$|x_0;+1\rangle=|0_x\rangle=\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \qquad |x_1;-1\rangle=|1_x\rangle=\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$$

where +1 and -1 are the eigenvalues of x_0 and x_1. So, our inverse change of basis matrix C^{-1} is

$$C=\frac{1}{\sqrt{2}}\begin{pmatrix}1&1\\1&-1\end{pmatrix} \implies C^{-1}=\frac{1}{\sqrt{2}}\begin{pmatrix}1&1\\1&-1\end{pmatrix}$$

Interestingly, our inverse change of basis matrix here can be directly used since it is nothing but Hadamard gate, which is directly available for use in IBM-Q Experience.

Similiarly, we need the eigenvectors and eigenvalues of σ_y operator which come out to be

$$|y_0; +1\rangle = |0_y\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ i\end{pmatrix} \qquad |y_1; -1\rangle = |1_y\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -1\end{pmatrix}$$

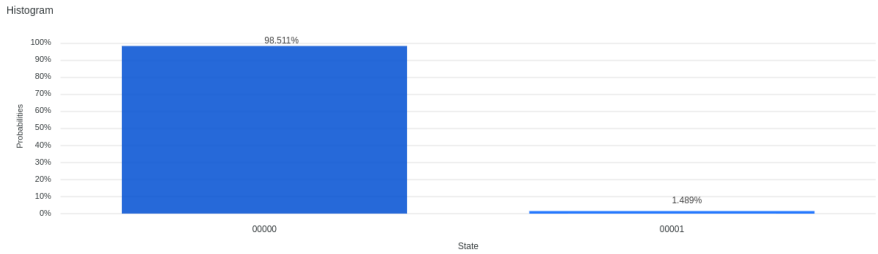
So the inverse change of basis matrix would be

$$C = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ i & -i\end{pmatrix} \implies C^{-1} = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & -i\\ 1 & i\end{pmatrix}$$

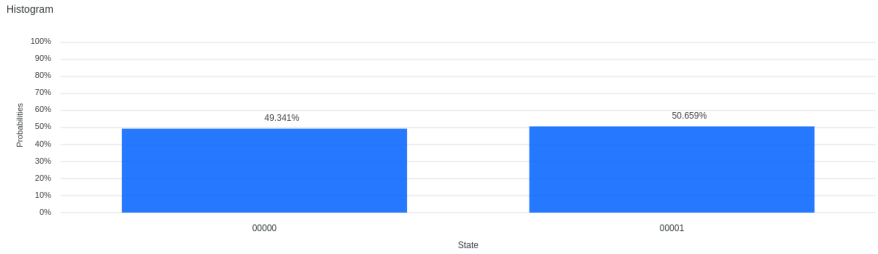
This unitary operation can be implemented using the $U_2(\phi, \lambda)$ gate where we can substitute $\phi = 0$ and $\lambda = \pi/2$. The U_2 gate is defined as

$$U_2(\phi, \lambda) = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & -e^{i\lambda}\\ e^{i\phi} & e^{i(\lambda+\phi)}\end{pmatrix}$$

So putting $\phi = 0$ and $\lambda = \pi/2$ gives the same matrix as C^{-1}. The results obtained are shown in Figure 2 below-



(a) Probabilities for eigenvalues of σ_x.



(b) Probabilities for eigen values of σ_y.

Figure 2: Probabilities for Quantum Circuits given in Fig. 1.

Now from the probabilities obtained from the measurements, we can calculate the expectation values as follows-

$$\langle \hat{O} \rangle = |\alpha|^2 v_0 + |\beta|^2 v_1$$

where $|\alpha|^2$ and $|\beta|^2$ are probabilities of eigenvalues v_0 and v_1 respectively.

So from the data, the experimentally calculated expectation values are-

$$\langle \sigma_x \rangle_{experimental} = (0.98511)(+1) + (0.01489)(-1) = \textbf{0.97033}$$

$$\langle \sigma_y \rangle_{experimental} = (0.49341)(+1) + (0.50659)(-1) = \textbf{-0.01318}$$

which are very close to their theoretically calculated values-

$$\langle \sigma_x \rangle_{theoretical} = \langle \psi | \sigma_x | \psi \rangle = \mathbf{1} \qquad \langle \sigma_y \rangle_{theoretical} = \langle \psi | \sigma_y | \psi \rangle = \mathbf{0}$$

3 Quantum State Tomography

Quantum State Tomography is the process of reconstructing a density matrix after applying some operations on the given unknown source state. The state to be determined can be either mixed or pure state. **Pure states** are systems consisting of only a single type of quantum states whereas **mixed states** are systems consisting of mixtures of quantum states.

Any general quantum system can be described using a density matrix which in its most general form for a single qubit can be written as

$$\rho = \frac{I + a\sigma_x + b\sigma_y + c\sigma_z}{2}$$

where $a = \langle \sigma_x \rangle$, $b = \langle \sigma_y \rangle$, $c = \langle \sigma_z \rangle$ and I is the identity matrix.

Using the method discussed in the previous section, we can calculate the expection values $\langle \sigma_x \rangle$, $\langle \sigma_y \rangle$ and $\langle \sigma_z \rangle$ and hence, determine the density matrix of the unknown quantum state (mixed or pure).

3.1 Performing quantum state tomography of a Bell state subsystem

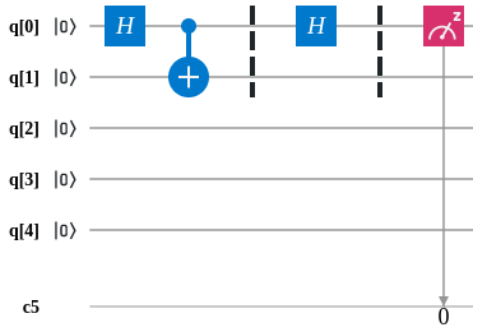
To check our hypothesis, we will try to determine the density matrix for the subsystem (first qubit) of the prepared Bell state. The Bell state we prepare is the β_{00} state

$$\beta_{00} = \frac{|0_A 0_B\rangle + |1_A 1_B\rangle}{\sqrt{2}}$$

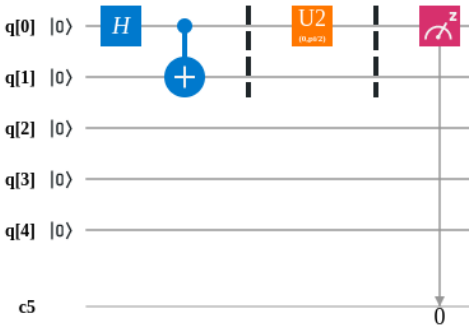
where A represents the first qubit and B represents the second qubit.

To prepare the Bell state β_{00}, we first apply Hadamard(H) gate on the first qubit and then apply CNOT gate to it with the first qubit as the control qubit.

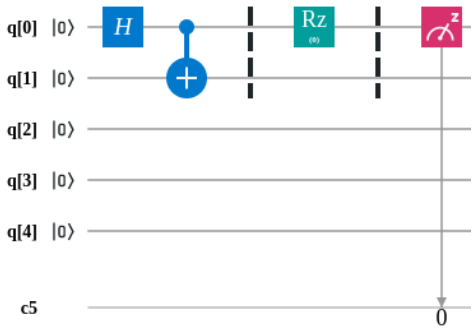
The circuits for measuring the expectation values on β_{00} are shown below in Figure 3.



(a) Circuit for calculation of $\langle\sigma_x\rangle$.



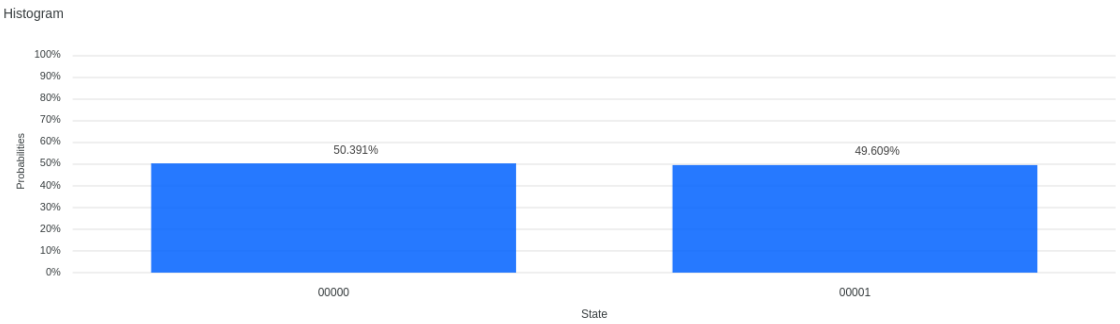
(b) Circuit for calculation of $\langle\sigma_y\rangle$.



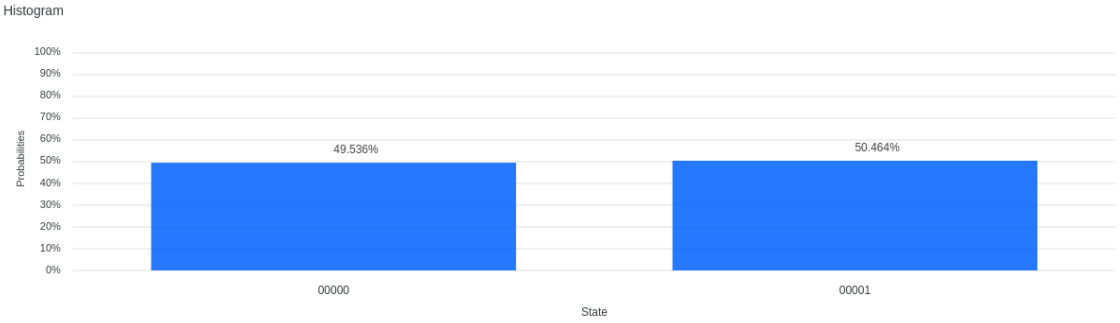
(c) Circuit for calculation of $\langle\sigma_z\rangle$.

Figure 3: Quantum Circuits for QST of subsystem A of β_{00} on IBM-Q Experience.

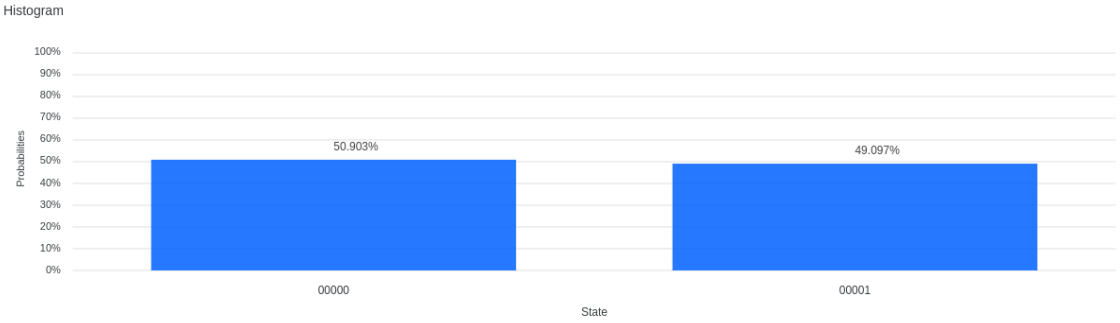
The measurement operation along z is applied only on the first qubit since we are only determining the density matrix of the first qubit's subsystem A. Now calculating the expectation values $\langle\sigma_x\rangle$, $\langle\sigma_y\rangle$ and $\langle\sigma_z\rangle$ for the subsystem A using the previously developed algorithm, we get the results of probabilities as shown in Figure 4 on the next page.



(a) Probabilities for eigenvalues of σ_x.



(b) Probabilities for eigen values of σ_y.



(c) Probabilities for eigen values of σ_z.

Figure 4: Probabilities for Quantum Circuits given in Fig. 3.

From the experimental data, we calculate the expectation values of σ_x, σ_y and σ_z by again using the formula discussed in Section 2.3

$$\langle\sigma_x\rangle_{experimental} = (0.50391)(+1) + (0.49606)(-1) = \mathbf{0.00785}$$
$$\langle\sigma_y\rangle_{experimental} = (0.49536)(+1) + (0.50464)(-1) = \mathbf{-0.00928}$$
$$\langle\sigma_z\rangle_{experimental} = (0.50903)(+1) + (0.49097)(-1) = \mathbf{0.01806}$$

So, determining the density matrix using the description given in the introduction of this section-

$$\rho = \frac{I + a\sigma_x + b\sigma_y + c\sigma_z}{2}$$

Here, a = 0.00785, b = -0.00928 and c=0.01806. Therefore-

$$\rho = \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} + \frac{0.00785}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} + \frac{-0.00928}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} + \frac{0.01806}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

$$\rho = \frac{1}{2}\begin{pmatrix}1.01086 & 0.00785 + 0.0928i\\ 0.00785 - 0.0928i & 0.98194\end{pmatrix} = \begin{pmatrix}0.50903 & 0.003925 + 0.0464i\\ 0.003925 - 0.0464i & 0.49097\end{pmatrix}$$

This experimentally determined matrix is very close to the actual value of the theoretically determined density matrix. So theoretically, the density matrix for the subsystem A's qubit is-

$$\rho_{AB} = \begin{pmatrix}1 & 0 & 0 & 1\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 1 & 0 & 0 & 1\end{pmatrix} \implies \rho_A = tr_B(\rho_{AB}) = \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = \begin{pmatrix}0.5 & 0\\ 0 & 0.5\end{pmatrix}$$

which is very nearly the same as the experimental density matrix.

$$\rho^2 = \begin{pmatrix}0.26129 & 0.00392 + 0.0464i\\ 0.00392 - 0.0464i & 0.24322\end{pmatrix} \qquad tr(\rho^2) = 0.50451 < 1$$

So, the subsystem A is a mixed state which is expected since the two qubits are entangled with each other in β_{00} state. Hence, we have determined a method to do quantum state tomography of some unknown quantum state and determine its density matrix by calculating the expectation values for σ_x, σ_y and σ_z.

4 Proposing a method to prepare density matrices on a quantum computer

Suppose we have to construct some given density matrix for some subsystem of an entangled quantum system. Let the state of that entangled system be represented as-

$$|\xi\rangle = \alpha\,|00\rangle + \beta\,|01\rangle + \gamma\,|10\rangle + \delta\,|11\rangle$$

So, the density matrix of the whole system can be written as -

$$\rho = |\xi\rangle\langle\xi| = \begin{pmatrix} |\alpha|^2 & \alpha\beta^* & \alpha\gamma^* & \alpha\delta^* \\ \beta\alpha^* & |\beta|^2 & \beta\gamma^* & \beta\delta^* \\ \gamma\alpha^* & \gamma\beta^* & |\gamma|^2 & \gamma\delta^* \\ \delta\alpha^* & \delta\beta^* & \delta\gamma^* & |\delta|^2 \end{pmatrix}$$

Taking the partial trace to get the density matrix of subsystem 1-

$$\rho_1 = \begin{pmatrix} |\alpha|^2 + |\beta|^2 & \alpha\gamma^* + \beta\delta^* \\ \gamma\alpha^* + \delta\beta^* & |\gamma|^2 + |\delta|^2 \end{pmatrix}$$

Since $\alpha, \beta, \gamma, \delta$ are complex numbers, we can write them as

$$\alpha = a + ib \qquad \alpha = c + id \qquad \alpha = e + if \qquad \delta = g + ih$$

Putting the values of the above complex numbers into the density matrix ρ_1, we get

$$\rho_1 = \begin{pmatrix} a^2 + b^2 + c^2 + d^2 & (ae + bf + cg + dh) + i(be + dg - af - ch) \\ (ae + bf + cg + dh) - i(be + dg - af - ch) & e^2 + f^2 + g^2 + h^2 \end{pmatrix}$$

Now, if I have to prepare some general density matrix of the form

$$\rho_1 = \begin{pmatrix} A & B + iC \\ B - iC & 1 - A \end{pmatrix}$$

I will get four equations with 8 unknowns-

$$a^2 + b^2 + c^2 + d^2 = A$$
$$ae + bf + cg + dh = B$$
$$be + dg - af - ch = C$$
$$e^2 + f^2 + g^2 + h^2 = 1 - A$$

Since many different states can form the same density matrices, this result is correct since we can have infinite number of solutions for α, β, γ and δ. Of the many α, β, γ and δ, we only need one of the solutions to construct the required density matrix. Preparing the required generic or seperable state to create that density matrix for the system is another task to be handled. But, the most important task is to somehow find any one solution to these equations which is yet to be completed.

5 References

[1] Nielsen, Michael A.; Chuang, Isaac L. (2010). Quantum Computation and Quantum Information (2nd ed.). Cambridge: Cambridge University Press.

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