MULT90063: Assignment 1

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Problem 1a: Bloch sphere form. Consider the following single qubit state $|\psi\rangle = a_0 |0\rangle + a_1 |1\rangle$ where the amplitudes are given in polar form as: $(|a_0| = 0.383, \theta_0 = \pi)$ and $(|a_1| = 0.924, \theta_0 = -\pi/2)$ As per the definition given in the lectures, convert to Bloch sphere form specifying the Bloch angles θ_B and ϕ_B. Plot on the Bloch sphere.

Answer. The Bloch sphere form of a quantum state $|\psi\rangle$ is parameterised by the angles θ_B and ϕ_B, which respectively represent the colatitude with respect to the z-axis, and the longitude with respect to the x-axis.

$$\begin{aligned}
|\psi\rangle &= 0.383 \cdot e^{i\pi} |0\rangle + 0.924 \cdot e^{-i\frac{\pi}{2}} |1\rangle \\
&= e^{i\pi}(0.383 |0\rangle + 0.924 \cdot e^{-i\frac{3\pi}{2}} |1\rangle) \\
&= \cos\left(\frac{0.7498\pi}{2}\right) |0\rangle + \sin\left(\frac{0.7498\pi}{2}\right) e^{-i\frac{3\pi}{2}} |1\rangle
\end{aligned}$$

Thus, $\theta_B = 0.7498\pi$ and $\phi_B = -\frac{3\pi}{2}$. $|\psi\rangle$ is visualised on the Bloch sphere below

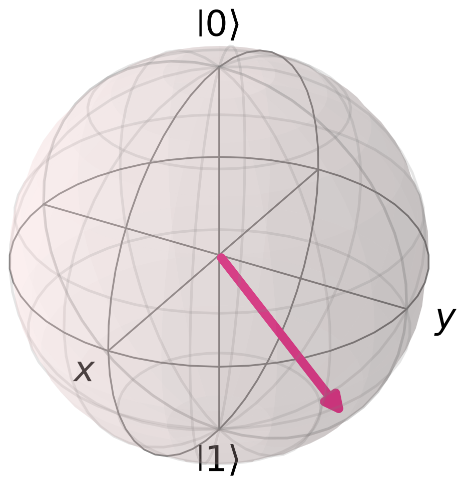


Figure 1: Bloch Sphere representation of $|\psi\rangle = \cos\left(\frac{0.7498\pi}{2}\right) |0\rangle + \sin\left(\frac{0.7498\pi}{2}\right) e^{-i\frac{3\pi}{2}} |1\rangle$

Problem 1b: General rotation. Consider single-qubit operations in matrix form, corresponding to rotations by angle θ_R about X, Y or Z axes. Explain how these operators are related to the familiar Pauli matrices, X, Y and Z given in lectures.

Answer. The relation between the provided general rotation operators and Pauli matrices is demonstrated by the following expression, achieved through exponentiation of the Pauli vector:

$$e^{i\theta(\hat{n}\cdot\sigma)} = I\cos(\theta) + i(\hat{n}\cdot\sigma)\sin(\theta), \tag{1}$$

where $(\sigma = \sigma_x \hat{x} + \sigma_y \hat{y} + \sigma_z \hat{z})$ is the Pauli vector, and $\hat{n} = n_x \hat{x} + n_y \hat{y} + n_z \hat{z}$ is a unit vector.

The above equation (1) can be derived using taylor series expansion of $e^{i\theta(\hat{n}\cdot\sigma)}$.

$$\begin{aligned}
e^{i\theta(\hat{n}\cdot\sigma)} &= I + i\theta\hat{n}\cdot\sigma - \frac{\theta^2}{2!}(\hat{n}\cdot\sigma)^2 - i\frac{\theta^3}{3!}(\hat{n}\cdot\sigma)^3 + \cdots + i^n\frac{\theta^n}{n!}(\hat{n}\cdot\sigma)^n \\
&= \sum_{n=0}^{\infty}\frac{(-1)^n(\theta\hat{n}\cdot\sigma)^{2n}}{(2n)!} + i\sum_{n=0}^{\infty}\frac{(-1)^n(\theta\hat{n}\cdot\sigma)^{2n+1}}{(2n+1)!}
\end{aligned}$$

Note that all even powers of the inner product of $\hat{n}$ and σ are equal to the identity matrix, such that $(\hat{n}\cdot\sigma)^{2n} = I$, for all $n \in \mathbb{Z}_0^+$, and all odd powers give $(\hat{n}\cdot\sigma)^{2n+1} = \hat{n}\cdot\sigma$, for all $n \in \mathbb{Z}_0^+$. Thus, we have

$$\begin{aligned}
e^{i\theta(\hat{n}\cdot\sigma)} &= I\sum_{n=0}^{\infty}\frac{(-1)^n\theta^{2n}}{(2n)!} + i(\hat{n}\cdot\sigma)\sum_{n=0}^{\infty}\frac{(-1)^n\theta^{2n+1}}{(2n+1)!} \\
&= I\cos(\theta) + i(\hat{n}\cdot\sigma)\sin(\theta)
\end{aligned}$$

Using this expression, one may recover the general rotation operators by substituting in appropriate values for the unit vector $\hat{n}$, and applying a global phase of $e^{i\frac{\pi}{2}}$ (let $\theta = \frac{\theta_R}{2}$, for consistency of notation).

$$\begin{aligned}
\hat{n} = (1,0,0) \rightarrow e^{i\theta(\hat{n}\cdot\sigma)} &= I\cos(\theta) + iX\sin(\theta) = e^{i\frac{\pi}{2}}\begin{bmatrix}\cos(\theta) & -i\sin(\theta) \\ -i\sin(\theta) & \cos(\theta)\end{bmatrix} \\
\hat{n} = (0,1,0) \rightarrow e^{i\theta(\hat{n}\cdot\sigma)} &= I\cos(\theta) + iY\sin(\theta) = e^{i\frac{\pi}{2}}\begin{bmatrix}\cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta)\end{bmatrix} \\
\hat{n} = (0,0,1) \rightarrow e^{i\theta(\hat{n}\cdot\sigma)} &= I\cos(\theta) + iZ\sin(\theta) = e^{i\frac{\pi}{2}}\begin{bmatrix}\cos(\theta) - i\sin(\theta) & 0 \\ 0 & \cos(\theta) + i\sin(\theta)\end{bmatrix}
\end{aligned}$$

Problem 1c: Rotations on the Quantum User Interface (QUI). In the QUI, consider a rotation around the $(1,1,0)$-axis by $\pi/2$ with global phase set to 0. Use the QUI to perform the rotation to the computational states $|0\rangle$ and $|1\rangle$ individually and hence determine the 2x2 matrix representation for this rotation. Submit appropriate screenshots with your answers. Explain quantitatively (using diagrams) how the operation moves the state on the Bloch Sphere.

Answer. Individually rotating the computational state $|0\rangle$ and $|1\rangle$ by $\frac{\pi}{2}$ around the $(1,1,0)$-axis yields

$$\begin{aligned}
R_{(1,1,0)}\left(\frac{\pi}{2}\right)|0\rangle &= \begin{bmatrix} r_1 & r_2 \\ r_3 & r_4 \end{bmatrix}\begin{bmatrix}1 \\ 0\end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ \frac{1}{\sqrt{2}} - \frac{i}{\sqrt{2}} \end{bmatrix} \\
R_{(1,1,0)}\left(\frac{\pi}{2}\right)|1\rangle &= \begin{bmatrix} r_1 & r_2 \\ r_3 & r_4 \end{bmatrix}\begin{bmatrix}0 \\ 1\end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix} -\frac{1}{\sqrt{2}} + \frac{i}{\sqrt{2}} \\ 1 \end{bmatrix}
\end{aligned}$$

Thus, we have

$$r_1 = \frac{1}{\sqrt{2}},\ \ r_2 = \frac{1}{\sqrt{2}}(-\frac{1}{\sqrt{2}} + \frac{i}{\sqrt{2}}),\ \ r_3 = \frac{1}{\sqrt{2}}(\frac{1}{\sqrt{2}} - \frac{i}{\sqrt{2}}),\ \ r_4 = \frac{1}{\sqrt{2}}$$

and the rotation operator $R_{(1,1,0)}\left(\frac{\pi}{2}\right)$ is given by

$$R_{(1,1,0)}\left(\frac{\pi}{2}\right) = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & -\frac{1}{\sqrt{2}} + \frac{i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} - \frac{i}{\sqrt{2}} & 1 \end{bmatrix}$$

The action of $R_{(1,1,0)}\left(\frac{\pi}{2}\right)$ on a state results in a $\frac{\pi}{2}$ rotation around the axis $(-\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}, 0)$. Figure 3 provides a visual representation of this rotation on the Bloch sphere.

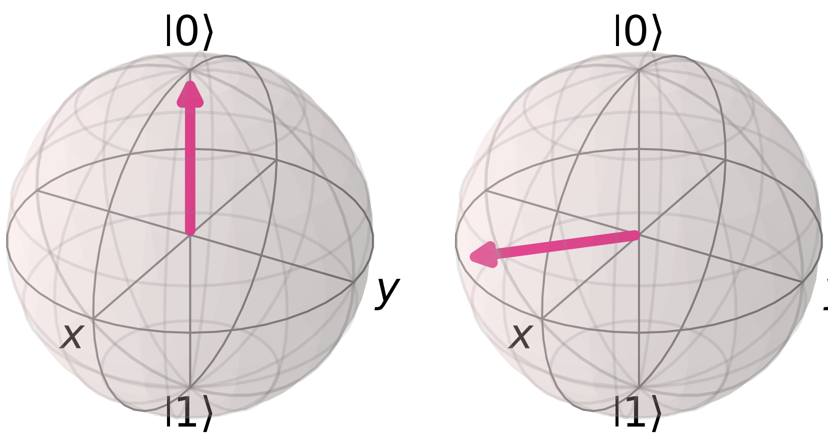


Figure 2: Visual representation of applying $R_{(1,1,0)}\left(\frac{\pi}{2}\right)$ to computational state $|0\rangle$ on the Bloch sphere. Left: original state $|0\rangle$. Right: resulting state after rotation $R_{(1,1,0)}\left(\frac{\pi}{2}\right)|0\rangle$.

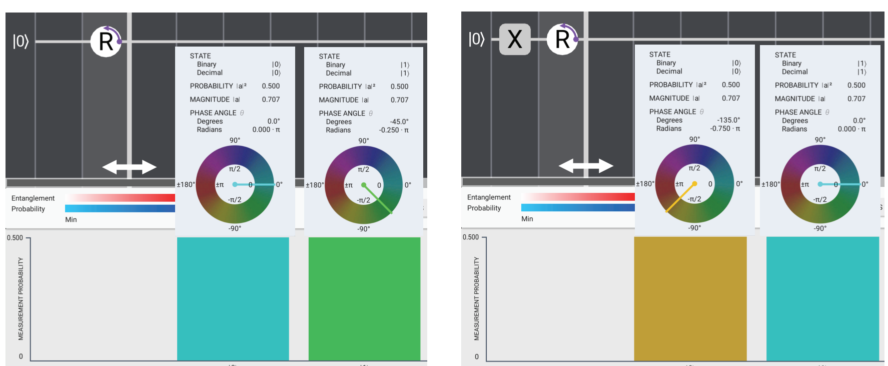


Figure 3: Screenshots from Quantum User Interface (QUI), applying $R_{(1,1,0)}\left(\frac{\pi}{2}\right)$ to computational states $|0\rangle$ (left) and $|1\rangle$ (right).

Problem 2a: Actions on single qubit. Write down the action of H, T and $T^\dagger$ on an arbitrary single qubit state in ket notation.

Answer. Let $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ represent an arbitrary single qubit, where $|\alpha|^2 + |\beta|^2 = 1$.

The action of a Hadamard gate on an arbitrary qubit $|\psi\rangle$ is given by

$$\begin{aligned} H|\psi\rangle &= \frac{1}{\sqrt{2}}(\alpha|0\rangle + \beta|0\rangle + \alpha|1\rangle - \beta ket1) \\ &= \frac{1}{\sqrt{2}}\Big(\alpha(|0\rangle + |1\rangle) + \beta(|0\rangle - |1\rangle)\Big) \\ &= \alpha|+\rangle + \beta|-\rangle \end{aligned}$$

The action of a T gate on an arbitrary qubit $|\psi\rangle$ is given by

$$\begin{aligned} T|\psi\rangle &= \alpha|0\rangle + \beta e^{i\frac{\pi}{4}}|1\rangle \\ &= \alpha|0\rangle + \frac{\beta}{\sqrt{2}}(1+i)|1\rangle \end{aligned}$$

The action of a $T^\dagger$ gate on an arbitrary qubit $|\psi\rangle$ is given by

$$\begin{aligned} T^\dagger|\psi\rangle &= \alpha|0\rangle + \beta e^{-i\frac{\pi}{4}}|1\rangle \\ &= \alpha|0\rangle + \frac{\beta}{\sqrt{2}}(1-i)|1\rangle \end{aligned}$$

Problem 2b: Toffoli gate decomposition. Starting from the initial 3-qubit state $|111\rangle$ (ordering: top-middle-lower), and staying in ket notation, trace through each step of the circuit to verify the output produced.

Answer. The circuit commences with quantum state $|\psi\rangle_0 = |1\rangle \otimes |1\rangle \otimes |1\rangle$. Step 1: apply a Hadamard gate to the third qubit

$$\begin{aligned} |\psi_1\rangle &= H_3|\psi_0\rangle \\ &= |1\rangle \otimes |1\rangle \otimes |-\rangle \end{aligned}$$

Step 2: apply a CNOT gate with the second qubit as the control, and the third qubit as the target

$$\begin{aligned} |\psi_2\rangle &= CNOT_{2,3}|\psi_1\rangle \\ &= |1\rangle \otimes |1\rangle \otimes -|-\rangle \end{aligned}$$

Step 3: apply a $T^\dagger$ gate to qubit 3

$$\begin{aligned} |\psi_3\rangle &= T_3^\dagger|\psi_2\rangle \\ &= |1\rangle \otimes |1\rangle \otimes -\frac{1}{\sqrt{2}}(|0\rangle - e^{-i\pi/4}|1\rangle) \end{aligned}$$

Step 4: apply a CNOT gate with the first qubit as the control, and the third qubit as the target

$$\begin{aligned} |\psi_4\rangle &= CNOT_{1,3}|\psi_3\rangle \\ &= |1\rangle \otimes |1\rangle \otimes \frac{1}{\sqrt{2}}(e^{-i\pi/4}|0\rangle - |1\rangle) \end{aligned}$$

Step 5: apply a T gate to qubit 3

$$\begin{aligned}
|\psi_5\rangle &= T_3 |\psi_4\rangle \\
&= |1\rangle \otimes |1\rangle \otimes \frac{1}{\sqrt{2}}(e^{-i\pi/4} |0\rangle - e^{i\pi/4} |1\rangle)
\end{aligned}$$

Step 6: apply a CNOT gate with the second qubit as the control, and the third qubit as the target

$$\begin{aligned}
|\psi_6\rangle &= CNOT_{2,3} |\psi_5\rangle \\
&= |1\rangle \otimes |1\rangle \otimes -\frac{1}{\sqrt{2}}(e^{i\pi/4} |0\rangle - e^{-i\pi/4} |1\rangle)
\end{aligned}$$

Step 7: apply a $T^\dagger$ gate to qubit 3

$$\begin{aligned}
|\psi_7\rangle &= T_3^\dagger |\psi_6\rangle \\
&= |1\rangle \otimes |1\rangle \otimes -\frac{1}{\sqrt{2}}(e^{i\pi/4} |0\rangle - e^{-i\pi/2} |1\rangle)
\end{aligned}$$

Step 8: apply a CNOT gate with the first qubit as the control, and the third qubit as the target

$$\begin{aligned}
|\psi_8\rangle &= CNOT_{1,3} |\psi_7\rangle \\
&= |1\rangle \otimes |1\rangle \otimes \frac{1}{\sqrt{2}}(e^{-i\pi/2} |0\rangle - e^{i\pi/4} |1\rangle)
\end{aligned}$$

Step 9: apply T gates to qubits 2 and 3

$$\begin{aligned}
|\psi_9\rangle &= T_2 T_3 |\psi_8\rangle \\
&= |1\rangle \otimes e^{i\pi/4} |1\rangle \otimes \frac{1}{\sqrt{2}}(e^{-i\pi/2} |0\rangle - e^{i\pi/2} |1\rangle) \\
&= |1\rangle \otimes e^{i\pi/4} |1\rangle \otimes \frac{e^{-i\pi/2}}{\sqrt{2}}(|0\rangle - e^{i\pi} |1\rangle) \\
&= |1\rangle \otimes e^{i\pi/4} |1\rangle \otimes e^{-i\pi/2} |+\rangle
\end{aligned}$$

Step 10: apply a CNOT gate with the first qubit as the control, and the second qubit as the target, and apply a Hadamard gate to qubit 3

$$\begin{aligned}
|\psi_{10}\rangle &= CNOT_{1,2} H_3 |\psi_9\rangle \\
&= |1\rangle \otimes e^{i\pi/4} |0\rangle \otimes e^{-i\pi/2} |0\rangle
\end{aligned}$$

Step 11: apply a T gate to qubit 1, and a $T^\dagger$ gate to qubit 2

$$\begin{aligned}
|\psi_{11}\rangle &= T_1 T_2^\dagger |\psi_{10}\rangle \\
&= e^{i\pi/4} |1\rangle \otimes e^{i\pi/4} |0\rangle \otimes e^{-i\pi/2} |0\rangle
\end{aligned}$$

Step 12: apply a CNOT gate with the first qubit as the control, and the second qubit as the target

$$\begin{aligned}
|\psi_{12}\rangle &= CNOT_{1,2}\,|\psi_{11}\rangle \\
&= e^{i\pi/4}\,|1\rangle \otimes e^{i\pi/4}\,|1\rangle \otimes e^{-i\pi/2}\,|0\rangle \\
&= e^{i\pi/4}e^{i\pi/4}e^{-i\pi/2}\,|110\rangle \\
&= |110\rangle
\end{aligned}$$

Problem 3a: Oracle construction. Construct an oracle with five qubits, which identifies (i.e. applies a phase to) numbers in the set $(1, 3, 7, 22, 25)$. You may use multiply controlled operations. Optimise your circuit to use as few operations as possible. Briefly describe your implementation of this circuit including any optimisations which you have made.

Answer. Let $S = \{1, 3, 7, 22, 25\}$ denote the set of solutions. Let $M = |S|$ denote the cardinality of S. We can construct an oracle to apply a phase to the computational states $|i\rangle\, \forall i \in S$ using a series of X gates and controlled-Z gates. The general intution of an example (non-optimised) circuit is as follows:

Given a target $S' \in S$, we first apply X gates to flip all qubits corresponding to 0-valued bits in the binary representation of S'. Then, we apply a controlled-Z gate (controlled on $|1\rangle$ state) with any given qubit as a target, and all remaining qubits as controls. This controlled-Z gate flips the phase of the target qubit if the input state ψ_0 matches the binary representation of S'. We then revert each qubit back to it's initial computational state using X gates. In this way, we construct a complete circuit by chaining M components, where the action of each component is such that it applies a phase to a unique computational state $S' \in S$.

One can optimise this circuit to use only controlled-Z gates, by methodically setting the control computational states to match the binary representations of solutions in S. For example, one could detect an input string 00001 ($S' = 1$) using a CNOT gate that is controlled by the $|0\rangle$ state in the first four qubits, and the $|1\rangle$ state in the final qubit. This optimised circuit[1] achieves the target function of the Oracle in five operations.

Problem 3b: Grover's algorithm (single iteration). Use the oracle which you constructed in part (a) to implement a single iteration of Grover's algorithm, starting from an equal superposition, and calculate the probability of measuring a number which is in the given set of numbers at the output. Show your working.

Answer. Continue with the same notation as part (a), with $S = \{1, 3, 7, 22, 25\}$ denoting the set of solutions and $M = |S|$ denoting the cardinality of S. We begin with an initial state in equal superposition

$$|\phi\rangle = \frac{1}{\sqrt{N}} \sum_{i=0}^{N-1} |i\rangle$$

[1] Access this circuit at `https://qui.science.unimelb.edu.au/circuits/642e4c77d5f0500054592227`

We can rewrite this state using a convenient two-dimensional basis of solutions, $|a\rangle$, and non-solutions, $|b\rangle$

$$
\begin{aligned}
|a\rangle &= \frac{1}{\sqrt{M}} \sum_{i \in S} |i\rangle\,, \quad |b\rangle = \frac{1}{\sqrt{N-M}} \sum_{i \notin S} |i\rangle \\
|\Phi_0\rangle &= \alpha\,|a\rangle + \beta\,|b\rangle\,, \quad \text{where} \\
\alpha &= \frac{\sqrt{M}}{\sqrt{N}}, \quad \beta = \frac{\sqrt{N-M}}{\sqrt{N}}
\end{aligned}
$$

In this basis, the initial state $|\Phi_0\rangle$ forms an angle $\theta = \arcsin\left(\frac{\sqrt{M}}{\sqrt{N}}\right)$ with the horizontal axis, and each iteration of Grover's algorithm increases this angle by exactly 2θ. After one iteration of Grover's algorithm, the initial state $|\Phi_0\rangle = (1, \theta)$ in polar form is modified to $|\Phi_1\rangle = (1, 3\theta)$.

One can calculate the probability of measuring a solution $S' \in S$ by projecting $|\Phi_1\rangle$ on to the vertical axis

$$
\begin{aligned}
Pr(S') &= \arcsin(3\theta) \\
&= \arcsin\left(\frac{3\sqrt{5}}{\sqrt{32}}\right) \\
&\approx 0.9388
\end{aligned}
$$

Problem 3c: Grover's algorithm (optimal iterations). How many iterations of Grover's algorithm are required to give the highest probability of success using your oracle? Use the geometric picture and show your working.

Answer. Continung with the two-dimensional geometric representation $|\Phi_0\rangle = \alpha\,|a\rangle + \beta\,|b\rangle$, the probability of measuring a solution $S' \in S$ is maximised when $\alpha = 1$, which occurs when the angle between the $|\Phi\rangle$ and the horizontal-axis is $\frac{\pi}{2}$.

Moreover, we know that each iteration of Grover's algorithm increases the angle between the $|\Phi\rangle$ and the horizontal-axis by $\frac{\theta}{2}$. Thus, we can calcuate the number of steps, n, that maximises the probability of measuring a solution $S' \in S$ by solving

$$
\begin{aligned}
(2n+1)\theta &= \frac{\pi}{2} \\
2n+1 &\approx 3.8654 \\
n &\approx 1.4327
\end{aligned}
$$

Thus, the probability of measuring a solution in S is maximised at a quantity between one and two iterations. Given that iterations can only be performed in whole numbers, one can determine the optimal number of iterations by comparing α after one and two iterations.

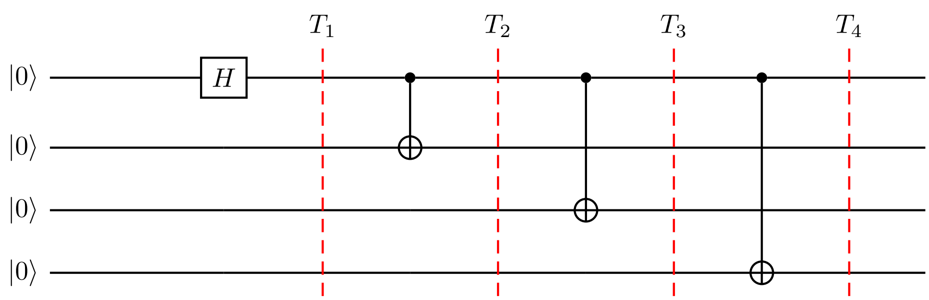
We know from part (b) that $\alpha \approx 0.9388$ after one iteration. After two iterations,

$$\begin{aligned}\alpha &= \arcsin(5\theta) \\ &= \arcsin\left(\frac{5\sqrt{5}}{\sqrt{32}}\right) \\ &\approx 0.8956\end{aligned}$$

Thus, over whole-number iterations, the probability of measuring a solution in S is maximised after one iteration.

Problem 4: Four-qubit GHZ state. Using QUI, create a circuit which constructs the four qubit GHZ state, using only single qubit and two-qubit operations. Optimise the circuit as much as possible. Write down the state at each time-step through the circuit.

Answer. Starting with four qubits initialised in computational state $|0\rangle$, we can construct a four-qubit GHZ state by placing a single qubit in superposition, and then using this superposed qubit as a control for repeated $CNOT$ gates on the remaining three qubits. This results in a maximally entangled state GHZ state, as demonstrated below.



(T_0) We begin with zero-initialised state $|\psi_0\rangle$ comprising four qubits

$$|\psi_0\rangle = |0\rangle \otimes |0\rangle \otimes |0\rangle \otimes |0\rangle$$

(T_1) Apply a Hadamard gate to the first qubit

$$\begin{aligned}|\psi_1\rangle &= H_1 |\psi_0\rangle \\ &= \frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes |0\rangle \otimes |0\rangle \otimes |0\rangle\end{aligned}$$

(T_2) Apply a CNOT gate with the first qubit as the control, and the second qubit as the target

$$\begin{aligned}|\psi_2\rangle &= CNOT_{12} |\psi_1\rangle \\ &= \frac{|00\rangle + |11\rangle}{\sqrt{2}} \otimes |0\rangle \otimes |0\rangle\end{aligned}$$

(T_3) Apply a CNOT gate with the first qubit as the control, and the third qubit as the target

$$\begin{aligned}|\psi_3\rangle &= CNOT_{13}\,|\psi_2\rangle \\ &= \frac{|000\rangle + |111\rangle}{\sqrt{2}} \otimes |0\rangle\end{aligned}$$

(T_4) Apply a CNOT gate with the first qubit as the control, and the fourth qubit as the target, thereby achieving the four-qubit GHZ state

$$\begin{aligned}|\psi_4\rangle &= CNOT_{14}\,|\psi_3\rangle \\ &= \frac{|0000\rangle + |1111\rangle}{\sqrt{2}}\end{aligned}$$

Problem 5a: CHSH inequality (classical states). Suppose that Q, R, S, and T take values $\{\pm 1\}$. Consider the quantity composed of combined operators: $QS + RS + RT - QT$. Note that there is an implied tensor product in these combined operators. In this case, what is the upper bound on the expectation (mean value) of the quantity $QS + RS + RT - QT$? This is called Bell's inequality.

Answer. Since $S, T \in \{-1, 1\}$, we have either $S = T$ or $S = -T$. Now consider the following combination

$$QS + RS + RT - QT = Q(S - T) + R(S + T) \tag{2}$$

In the case $S = T$, $Q(S - T) = 0$, while in the case $S = -T$, $R(S + T) = 0$. In either eventuality, one of the terms on the RHS of equation 2 will become zero, and the remaining term will take the values ± 2. Thus, if the measurement is repeated over n independent trials, the upper bound on the expectation of the measured quantity is given by

$$\langle QS + RS + RT - QT\rangle \leq 2$$

Problem 5b: CHSH inequality (quantum states). Next we consider measuring the expectation value of the quantity $QS + RS + RT - QT$ when Alice and Bob have access to quantum states. What are the eigenvalues for each of Q, R, S, and T? What is the expectation value $\langle QS + RS + RT - QT\rangle$ for the product state $|\psi_{\text{Alice}}\rangle \otimes |\psi_{\text{Bob}}\rangle$? What is the max possible value?

Answer. We can determine the eigenvalues of Alice and Bob's observables (Q, R, S, T) by solving their characteristic equations.

The eigenvalues of Q are given by

$$\begin{aligned}\det(\lambda I - Z) &= 0 \\ \det\left(\begin{bmatrix}\lambda - 1 & 0 \\ 0 & \lambda + 1\end{bmatrix}\right) &= 0 \\ (\lambda - 1)(\lambda + 1) &= 0 \\ \lambda &= \pm 1\end{aligned}$$

The eigenvalues of R are given by

$$\begin{aligned}
\det(\lambda I - X) &= 0 \\
\det\left(\begin{bmatrix} \lambda & -1 \\ -1 & \lambda \end{bmatrix}\right) &= 0 \\
\lambda^2 - 1 &= 0 \\
\lambda &= \pm 1
\end{aligned}$$

The eigenvalues of S are given by

$$\begin{aligned}
\det\left(\lambda I - \left(-\frac{Z+X}{\sqrt{2}}\right)\right) &= 0 \\
\det\left(\begin{bmatrix} \lambda + \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \lambda - \frac{1}{\sqrt{2}} \end{bmatrix}\right) &= 0 \\
(\lambda + \frac{1}{\sqrt{2}})(\lambda - \frac{1}{\sqrt{2}}) - \frac{1}{2} &= 0 \\
\lambda &= \pm 1
\end{aligned}$$

The eigenvalues of T are given by

$$\begin{aligned}
\det\left(\lambda I - \frac{Z-X}{\sqrt{2}}\right) &= 0 \\
\det\left(\begin{bmatrix} \lambda - \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \lambda + \frac{1}{\sqrt{2}} \end{bmatrix}\right) &= 0 \\
(\lambda - \frac{1}{\sqrt{2}})(\lambda + \frac{1}{\sqrt{2}}) - \frac{1}{2} &= 0 \\
\lambda &= \pm 1
\end{aligned}$$

We calculate the expectation value of $\langle QS + RS + RT - QT \rangle$ with reference to the state $|\psi_{AB}\rangle$ by evaluating the expression

$$\langle QS + RS + RT - QT \rangle = \langle \psi_{AB} | \, QS + RS + RT - QT \, | \psi_{AB} \rangle$$

Let $C = QS + RS + RT - QT$ for brevity of notation. Begin by calculating tensor products

QS, RS, RT and QT

$$QS = Z \otimes -\frac{Z+X}{\sqrt{2}} = -\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & -1 & -1 \\ 0 & 0 & -1 & 1 \end{bmatrix}$$

$$RS = X \otimes -\frac{Z+X}{\sqrt{2}} = -\frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \\ 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \end{bmatrix}$$

$$RT = X \otimes \frac{Z-X}{\sqrt{2}} = -\frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 0 & 1 & -1 \\ 0 & 0 & -1 & -1 \\ 1 & -1 & 0 & 0 \\ -1 & -1 & 0 & 0 \end{bmatrix}$$

$$QT = Z \otimes \frac{Z-X}{\sqrt{2}} = -\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 & 0 & 0 \\ -1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix}$$

Thus, C is given by

$$C = -\sqrt{2} \begin{bmatrix} -1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ -1 & 0 & 0 & -1 \end{bmatrix}$$

Now, we calculate the joint state $|\psi_{AB}\rangle$ as follows

$$\begin{aligned} |\psi_{AB}\rangle &= |\psi_A\rangle \otimes |\psi_B\rangle \\ &= \begin{bmatrix} \cos(\theta_A)\cos(\theta_B) \\ -\cos(\theta_A)\sin(\theta_B) \\ \sin(\theta_A)\cos(\theta_B) \\ -\sin(\theta_A)\sin(\theta_B) \end{bmatrix} \end{aligned}$$

Now, we use the above expressions for C and $|\psi_{AB}\rangle$ to calculate the expectation $\langle C\rangle$

$$\begin{aligned} \langle C\rangle &= \langle\psi_{AB}| \, C \, |\psi_{AB}\rangle \\ &= -\sqrt{2} \begin{bmatrix} \cos(\theta_A)\cos(\theta_B) \\ -\cos(\theta_A)\sin(\theta_B) \\ \sin(\theta_A)\cos(\theta_B) \\ -\sin(\theta_A)\sin(\theta_B) \end{bmatrix}^T \begin{bmatrix} -1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ -1 & 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} \cos(\theta_A)\cos(\theta_B) \\ -\cos(\theta_A)\sin(\theta_B) \\ \sin(\theta_A)\cos(\theta_B) \\ -\sin(\theta_A)\sin(\theta_B) \end{bmatrix} \\ &= \sqrt{2}(-\cos^2(\theta_A)\cos^2(\theta_B) + \cos(\theta_A)\cos(\theta_B)\sin(\theta_A)\sin(\theta_B) \\ &\qquad + \cos^2(\theta_A)\sin^2(\theta_B) + \cos(\theta_A)\sin(\theta_B)\sin(\theta_A)\cos(\theta_B) \\ &\qquad + \sin(\theta_A)\cos(\theta_B)\cos(\theta_A)\sin(\theta_B) + \sin^2(\theta_A)\cos^2(\theta_B) \\ &\qquad + \sin(\theta_A)\sin(\theta_B)\cos(\theta_A)\cos(\theta_B) - \sin^2(\theta_A)\sin^2(\theta_B)) \\ &= -\sqrt{2}\cos(2\theta_A + 2\theta_Y) \end{aligned}$$

Thus, one can see that the maximum possible value for $\langle C \rangle$ is $\sqrt{2}$, which occurs when $(2\theta_A + 2\theta_Y = 1)$.

Problem 5c: CHSH inequality (shared qubits). Now consider the case where Alice and Bob share the state (Alice qubit first, Bob qubit second): $\psi_{AB} = \cos(\phi)\,|01\rangle - \sin(\phi)\,|10\rangle$. For what values of ϕ is the quantity $\langle QS + RS + RT - QT \rangle$ maximum (given the observables in part (b))? What is the significance of such ϕ for the state $|\psi_{AB}\rangle$? How does this value for $\langle QS + RS + RT - QT \rangle$ compare to the value in part (a)? This is the basis of the CHSH inequality.

Answer. Let $C = QS + RS + RT - QT$ for brevity of notation, as above. We begin by calculating the expectation $\langle C \rangle$ as follows

$$\begin{aligned}
\langle C \rangle &= \langle \psi_{AB} | \, C \, | \psi_{AB} \rangle \\
&= -\sqrt{2} \begin{bmatrix} 0 \\ \cos(\phi) \\ -\sin(\phi) \\ 0 \end{bmatrix}^T \begin{bmatrix} -1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ -1 & 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} 0 \\ \cos(\phi) \\ -\sin(\phi) \\ 0 \end{bmatrix} \\
&= \sqrt{2}(\cos(\phi)(cos(\phi) + sin(\phi)) + \sin(\phi)(cos(\phi) + sin(\phi))) \\
&= \sqrt{2}(\cos^2(\phi) + cos(\phi)sin(\phi) + \sin(\phi)cos(\phi) + sin^2(\phi)) \\
&= \sqrt{2}(sin(2\phi) + 1)
\end{aligned}$$

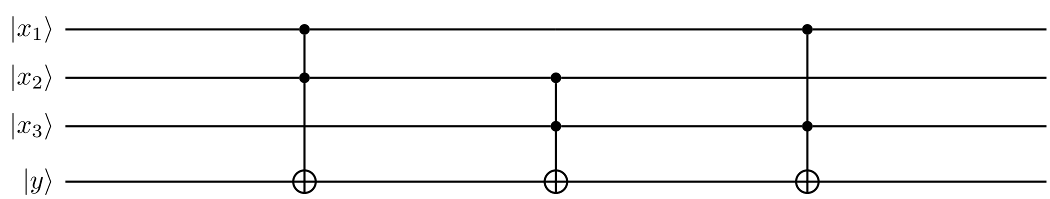
Thus, the quantity $\langle QS + RS + RT - QT \rangle$ is maximised for $\phi = \frac{2n\pi}{4}$, $n \in \mathbb{Z}^+$. As such, the inequality is modified as follows:

$$\langle QS + RS + RT - QT \rangle \leq 2\sqrt{2}$$

This value exceeds the upper bound under classical mechanics, which suggests that observable phenomena are not well-explained by local hidden variables.

Problem 6a: Quantum circuit (3-qubit). Design a quantum circuit that implements $f(x)$ for x represented by $n = 3$ qubits (in ket notation, define the left-most qubit corresponding to the most significant bit). Draw the quantum circuit using one-qubit gates, two-qubit gates and as few Toffoli gates as possible. Explain its working. You may use ancilla qubits.

Answer. Using three input qubits $(|x_1\rangle, |x_2\rangle, |x_3\rangle)$ and one output qubit $|y\rangle$, we can design a simple quantum circuit to implement $f(x)$ using three Toffoli gates.



Each Toffoli gate monitors a unique two-bit pair, and flips the output qubit $|y\rangle$ if both bits in the target pair are set to one. In the event that all three bits are set to one, an odd number of Toffoli gates ensures that the output qubit registers 1.

Note: each Toffoli gate can, in principle, be reproduced using single-qubit gates alone, as in problem (2). As such, this circuit could be reconstructed without explicit use of any Toffoli gates. For brevity of notation, this exercise is avoided.

Problem 6b: Quantum circuit (5-qubit). Work out a 5-bit quantum implementation of $f(x)$ – i.e. if there are more 1's than 0's in the input, your function should return 1, otherwise returns 0. Draw a schematic quantum circuit which demonstrates the working of this function. You do not need to draw the full quantum circuit, a clear strategy that demonstrates the working for 5-qubit inputs is sufficient. You must use only one, two and three-qubit gates. Hint: You may use your 3-bit implementation from part (a) as a black box.

Answer. [Insert Answer]