

# Efficient Classical Simulation of the Quantum Fourier Transform

	Asmus Tørsleff	asmt@itu.dk (asmus.torsleff@gmail.com)
Supervisor	Michael Kastoryano	micka@itu.dk
Co-Supervisor	Nutan Limaye	nuli@itu.dk

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# 1 Motivation

The Fourier transform is one of the most widely applicable procedures, used in anything from signal processing and AI to seismology. Therefore, it is of interest to explore different ways of computing it.

A variant of it; the discrete Fourier transform takes several equally spaced points on a function and transforms them into shifts and frequencies for a linear combination of phase shifted sinus functions of different frequencies. We can also do the opposite.

We can use this e.g., to remove an annoying high pitch noise in a recording: We sample the sound wave, do the Fourier transformation to get the frequencies involved, take out the higher pitched ones and do the inverse Fourier transform to recover the sound wave, now without the high-pitched noise.

There are many ways of computing this discrete Fourier transform, one of the more well-known approaches is the fast Fourier transform (FFT), which has been our most efficient way of computing it for a while. There is an analogous algorithm designed for quantum computers namely the quantum Fourier transform (QFT).

In addition to its standalone value, it is also widely used as a component of other quantum algorithms such as Shor's algorithm, and is therefore an interesting subject of improvement. The QFT has a significantly better time complexity, but only when run on a quantum computer. The QFT takes  $O(n^2)$  quantum gates and FFT takes  $O(\log_2(2^n)2^n) = O(n2^n)$  [3] classical logic gates to compute for  $2^n$  amplitudes or data points. For the QFT  $n$  corresponds to the required number of qubits.

Recently there has been advancements in simulating the QFT approximately on classical computers, while retaining some of this speedup, which is what this project focuses on. This has been shown in the paper[2] which will be referred to as 'the paper' in this paper. We will go through the math needed to implement two different simulations of the QFT, one exact and one approximate but vastly faster and more memory efficient. The first only uses basic matrix math, the second requires a basic understanding of tensor networks which we will try to provide. This project also includes code implementing all the math touched upon by this paper and is intended as a learning resource, this means that the formulas shown will often not be the pretty derivations seen elsewhere but will seek to represent the individual bits that went into constructing them.

In the section 2 we will show how to use matrix math to simulate the QFT, and in section 3 we will show how to compute an exponentially close approximation using tensors. We will then compare the time taken, the memory used and the approximation error between the approaches in section 4. In the appendix there will be example calculations for many of the equations shown later in this paper.

## 2 Dense Simulation

We want to simulate applying the QFT to some state, for this we need a way to represent the QFT and the state. In this section we will work towards representing the QFT circuit as a matrix and the state as a vector.

### 2.1 Representing a one qubit state

In classical computation a bit can either be 1 or 0, in quantum systems however a qubit has a certain probability of collapsing to either one or zero at a given time. To simulate this, we use a vector to represent a qubit or a system of qubits, we denote this using Dirac notation. In Dirac notation we have a bra  $\langle|$  and a ket  $| \rangle$ , generally a bra denotes a row vector and a ket denotes a column vector. To extract the probabilities of a qubit or system of qubits collapsing to one state or the other we take the norm squared of the entries in the vector, the sum of these must be 1 to be a valid state.

$$|1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Figure 1: A qubit with a probability of 1 of collapsing to one

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

Figure 2: A qubit with a probability of 1 of collapsing to zero

$$\begin{aligned} |+\rangle &= \sqrt{0.5}(|0\rangle + |1\rangle) = \begin{bmatrix} \sqrt{0.5} \\ \sqrt{0.5} \end{bmatrix} \\ |-\rangle &= \sqrt{0.5}(|0\rangle - |1\rangle) = \begin{bmatrix} \sqrt{0.5} \\ -\sqrt{0.5} \end{bmatrix} \end{aligned}$$

Figure 3: Qubits with a probability of 0.5 of collapsing to zero and one

In general, a qubit  $\begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \alpha |0\rangle + \beta |1\rangle$  has a probability of  $|\alpha|^2$  of collapsing to zero and  $|\beta|^2$  of collapsing to one. Since we use a vector of complex numbers  $|x|^2 = xx^*$  denotes the norm squared, where if  $x = a + bi$  then  $x^*$  is the complex

conjugate of  $x$ ,  $x^* = a - bi$ . For readability's sake we will not write  $+bi$  after a number if  $b = 0$ , you can assume all numbers in vectors and matrices are complex.

If we look at these vectors in a coordinate system, where the  $z$  axis is the imaginary axis, they all lie on a unit circle.

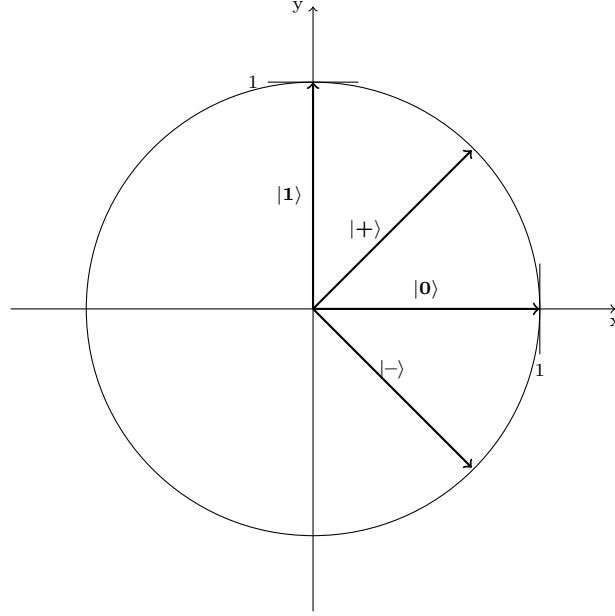


Figure 4: 'Bloch circle' with vectors  $|1\rangle$ ,  $|+\rangle$ ,  $|0\rangle$  and  $|-\rangle$  plotted

In reality we often use complex numbers with a non-zero imaginary part in the vectors, which results in the qubit states instead lying on the unit sphere, this is known as the Bloch sphere. The  $z$  axis is called the phase and generally has no impact on the probabilities of collapsing to a certain state, however it can be used to hold extra information before the qubit is collapsed, this can be useful in computations.

## 2.2 Multiple qubit states

$|1+-\rangle$  denotes a system collapsing to either  $|100\rangle$ ,  $|101\rangle$ ,  $|110\rangle$  or  $|111\rangle$  with probability 0.25. If we want to compute the state vector for the whole system, we take the Kronecker product[5], sometimes called the tensor product, of the vectors representing the individual qubits in the system. The Kronecker product of two matrix like objects consists of duplicating the second object for every entry in the first object and then scaling every value in the duplicate by the entry in the first object.

$$\begin{aligned}
& \begin{bmatrix} a_{00} & a_{01} & a_{02} \\ a_{10} & a_{11} & a_{12} \end{bmatrix} \otimes \begin{bmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \\ b_{20} & b_{21} \end{bmatrix} = \\
& \begin{bmatrix} a_{00} \begin{bmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \\ b_{20} & b_{21} \end{bmatrix} & a_{01} \begin{bmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \\ b_{20} & b_{21} \end{bmatrix} & a_{02} \begin{bmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \\ b_{20} & b_{21} \end{bmatrix} \\ a_{10} \begin{bmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \\ b_{20} & b_{21} \end{bmatrix} & a_{11} \begin{bmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \\ b_{20} & b_{21} \end{bmatrix} & a_{12} \begin{bmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \\ b_{20} & b_{21} \end{bmatrix} \end{bmatrix} = \\
& \begin{bmatrix} a_{00}b_{00} & a_{00}b_{01} & a_{01}b_{00} & a_{01}b_{01} & a_{02}b_{00} & a_{02}b_{01} \\ a_{00}b_{10} & a_{00}b_{11} & a_{01}b_{10} & a_{01}b_{11} & a_{02}b_{10} & a_{02}b_{11} \\ a_{00}b_{20} & a_{00}b_{21} & a_{01}b_{20} & a_{01}b_{21} & a_{02}b_{20} & a_{02}b_{21} \\ a_{10}b_{00} & a_{10}b_{01} & a_{11}b_{00} & a_{11}b_{01} & a_{12}b_{00} & a_{12}b_{01} \\ a_{10}b_{10} & a_{10}b_{11} & a_{11}b_{10} & a_{11}b_{11} & a_{12}b_{10} & a_{12}b_{11} \\ a_{10}b_{20} & a_{10}b_{21} & a_{11}b_{20} & a_{11}b_{21} & a_{12}b_{20} & a_{12}b_{21} \end{bmatrix}
\end{aligned}$$

Figure 5: Example of taking the Kronecker product of two matrices

$$\begin{aligned}
& |1+-\rangle = |1\rangle \otimes |+\rangle \otimes |-\rangle = \\
& \begin{bmatrix} 0 \\ 1 \end{bmatrix} \otimes \begin{bmatrix} \sqrt{0.5} \\ \sqrt{0.5} \end{bmatrix} \otimes \begin{bmatrix} \sqrt{0.5} \\ -\sqrt{0.5} \end{bmatrix} = \\
& \begin{bmatrix} 0 \begin{bmatrix} \sqrt{0.5} \begin{bmatrix} \sqrt{0.5} \\ -\sqrt{0.5} \end{bmatrix} \\ \sqrt{0.5} \begin{bmatrix} \sqrt{0.5} \\ -\sqrt{0.5} \end{bmatrix} \end{bmatrix} \\ 1 \begin{bmatrix} \sqrt{0.5} \begin{bmatrix} \sqrt{0.5} \\ -\sqrt{0.5} \end{bmatrix} \\ \sqrt{0.5} \begin{bmatrix} \sqrt{0.5} \\ -\sqrt{0.5} \end{bmatrix} \end{bmatrix} \end{bmatrix} = \begin{bmatrix} 0 \begin{bmatrix} 0.5 \\ -0.5 \\ 0.5 \\ -0.5 \end{bmatrix} \\ 1 \begin{bmatrix} 0.5 \\ -0.5 \\ 0.5 \\ -0.5 \end{bmatrix} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0.5 \\ -0.5 \\ 0.5 \\ -0.5 \end{bmatrix} = \\
& 0 \cdot |000\rangle + 0 \cdot |001\rangle + 0 \cdot |010\rangle + 0 \cdot |011\rangle + \\
& 0.5 \cdot |100\rangle - 0.5 \cdot |101\rangle + 0.5 \cdot |110\rangle - 0.5 \cdot |111\rangle
\end{aligned}$$

Figure 6: Using the Kronecker product to compute the state vector for the system in state  $|1+-\rangle$

If we square this vector, equivalent to taking the norm squared when the imaginary parts are zero, we get the probability corresponding to each state.

$$| |1+-\rangle |^2 = \begin{bmatrix} 0^2 \\ 0^2 \\ 0^2 \\ 0^2 \\ 0.5^2 \\ -0.5^2 \\ 0.5^2 \\ -0.5^2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0.25 \\ 0.25 \\ 0.25 \\ 0.25 \end{bmatrix}$$

Figure 7: Squaring entries in the state vector to obtain probabilities of the system being in each state, the  $i$ 'th entry in the vector is the probability of the system being in state  $|i\rangle$  if you write  $i$  in binary using 3 digits.

### 2.3 Manipulating qubits

In traditional electrical circuits we use logic gates such as NOT, AND, OR, NAND, etc. to manipulate bits. In quantum circuits some common gates are Pauli-X (X, bit flip or NOT), I (identity), H (Hadamard), CNOT (CX or controlled not), etc. In the same way we represent the state of a quantum system as a vector, we can represent a gate that operates on a state as a matrix.

$$\mathbf{I} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \mathbf{X} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \mathbf{H} = \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} \\ \sqrt{0.5} & -\sqrt{0.5} \end{bmatrix} \quad \mathbf{R}_n = \begin{bmatrix} 1 & 0 \\ 0 & e^{\frac{2\pi i}{2^n}} \end{bmatrix}$$

Figure 8: Matrixes corresponding to  $\mathbf{I}$ ,  $\mathbf{X}$ ,  $\mathbf{H}$  and  $\mathbf{R}_n$  gates, which act on a single cubit.

If we wish to apply a gate to a qubit in a system, we do so by doing matrix multiplication between the state and the gate.

$$\mathbf{I} |0\rangle = |0\rangle \quad \mathbf{I} |1\rangle = |1\rangle$$

Figure 9: Applying  $\mathbf{I}$  gate to the states  $|0\rangle$  and  $|1\rangle$ .

$$\mathbf{X} |0\rangle = |1\rangle \quad \mathbf{X} |1\rangle = |0\rangle$$

Figure 10: Applying  $\mathbf{X}$  gate to the states  $|0\rangle$  and  $|1\rangle$ .

$$\mathbf{H}|0\rangle = |+\rangle \quad \mathbf{H}|1\rangle = |-\rangle$$

Figure 11: Applying  $\mathbf{H}$  gate to the states  $|0\rangle$  and  $|1\rangle$ .

$$\mathbf{R}_2|0\rangle = |0\rangle \quad \mathbf{R}_2|1\rangle = \begin{bmatrix} 0 \\ i \end{bmatrix}$$

Figure 12: Applying  $\mathbf{R}_2$  gate to the states  $|0\rangle$  and  $|1\rangle$ .

$$\mathbf{CX}|00\rangle = |00\rangle \quad \mathbf{CX}|01\rangle = |01\rangle \quad \mathbf{CX}|10\rangle = |11\rangle \quad \mathbf{CX}|11\rangle = |10\rangle$$

Figure 13: Applying  $\mathbf{CX}$  gate to the states  $|00\rangle$ ,  $|01\rangle$ ,  $|10\rangle$  and  $|11\rangle$ .

See appendix 6.2 for detailed calculations of these applications.

Here we see that applying  $\mathbf{I}$  does not change the state. Applying  $\mathbf{X}$  takes the state to the same state but reversed. Applying  $\mathbf{H}$  takes the state into a super position of  $|1\rangle$  and  $|0\rangle$ . Applying  $\mathbf{R}_n$  changes the phase of the cubit but not the chance of it collapsing to something. A key property of quantum gates is that they are reversible, and in fact their own inverses.

$$\mathbf{I}(\mathbf{I}|0\rangle) = |0\rangle \quad \mathbf{I}(\mathbf{I}|1\rangle) = |1\rangle$$

Figure 14: Applying  $\mathbf{I}$  gate to the states  $|0\rangle$  and  $|1\rangle$  twice.

$$\mathbf{X}(\mathbf{X}|0\rangle) = |0\rangle \quad \mathbf{X}(\mathbf{X}|1\rangle) = |1\rangle$$

Figure 15: Applying  $\mathbf{X}$  gate to the states  $|0\rangle$  and  $|1\rangle$  twice.

$$\mathbf{H}(\mathbf{H}|0\rangle) = |0\rangle \quad \mathbf{H}(\mathbf{H}|1\rangle) = |1\rangle$$

Figure 16: Applying  $\mathbf{H}$  gate to the states  $|0\rangle$  and  $|1\rangle$  twice.



$$\mathbf{R}_2(\mathbf{R}_2|0\rangle) = |0\rangle \quad \mathbf{R}_2(\mathbf{R}_2|1\rangle) = |1\rangle$$

Figure 17: Applying  $\mathbf{R}_2$  gate to the states  $|0\rangle$  and  $|1\rangle$  twice.

$$\mathbf{CX}(\mathbf{CX}|00\rangle) = |00\rangle \quad \mathbf{CX}(\mathbf{CX}|01\rangle) = |01\rangle \quad \mathbf{CX}(\mathbf{CX}|10\rangle) = |10\rangle \quad \mathbf{CX}(\mathbf{CX}|11\rangle) = |11\rangle$$

Figure 18: Applying  $\mathbf{CX}$  gate to the states  $|00\rangle$ ,  $|01\rangle$ ,  $|10\rangle$  and  $|11\rangle$  twice.

This makes any quantum circuit constructed using these gates reversible.

## 2.4 Manipulating qubits individually

We have seen how we apply a gate to a system of qubits the same size as the gate. If we want to apply a gate to the  $i$ 'th qubit we construct a gate the same size as the system which acts with identity on every other qubit. We again use the Kronecker product for this.

$$(\mathbf{I} \otimes \mathbf{I} \otimes \mathbf{X})|000\rangle = |001\rangle$$

Figure 19: Applying  $\mathbf{X}$  to the first qubit in a 3-qubit system.

$$(\mathbf{I} \otimes \mathbf{X} \otimes \mathbf{I})|000\rangle = |010\rangle$$

Figure 20: Applying  $\mathbf{X}$  to the second qubit in a 3-qubit system.

$$(\mathbf{X} \otimes \mathbf{I} \otimes \mathbf{I})|000\rangle = |100\rangle$$

Figure 21: Applying  $\mathbf{X}$  to the third qubit in a 3-qubit system.

If we want to apply multiple gates at a time, we just replace the corresponding  $\mathbf{I}$  gates.

$$(\mathbf{X} \otimes \mathbf{I} \otimes \mathbf{H})|000\rangle = |10+\rangle$$

Figure 22: Applying  $\mathbf{X}$  to the thrid qubit and  $\mathbf{H}$  to the first qubit in a 3-qubit system.

See calculations in appendix 6.3.

In general, we can construct and apply any number of gates,  $U_0, U_1, \dots, U_n$ , to a state  $|\Psi\rangle$  in sequence, this is in essence our quantum circuit. And because of the associative nature of matrix multiplication, we can combine the entire circuit before applying it to different states! This saves tremendous amounts of resources when doing repetitive computations.

$$U_0 U_1 \dots U_n |\Psi\rangle = \left( \prod_{i=0}^n U_i \right) |\Psi\rangle$$

Figure 23: Associative nature of matrix multiplication.

$$\mathbf{U} = \mathbf{CX}(\mathbf{I} \otimes \mathbf{H})(\mathbf{I} \otimes \mathbf{X}) = \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} & 0 & 0 \\ -\sqrt{0.5} & \sqrt{0.5} & 0 & 0 \\ 0 & 0 & -\sqrt{0.5} & \sqrt{0.5} \\ 0 & 0 & \sqrt{0.5} & \sqrt{0.5} \end{bmatrix}$$

Figure 24: Computing a matrix representation of a circuit,  $\mathbf{U}$ , that first applies  $\mathbf{X}$  then  $\mathbf{H}$  to the first qubit then  $\mathbf{CX}$  to the first and second qubit.

$$\begin{aligned} \mathbf{U}|00\rangle &= |0-\rangle \\ \mathbf{U}|01\rangle &= |0+\rangle \\ \mathbf{U}|10\rangle &= -|1-\rangle \\ \mathbf{U}|11\rangle &= |1+\rangle \end{aligned}$$

Figure 25: Applying the circuit represented by the matrix  $\mathbf{U}$  from figure 24 to different states.

## 2.5 Controlled gates

We have described the  $\mathbf{R}_n$  gate but for the *QFT* circuit we need it controlled by another qubit. We can construct a controlled gate out of any other gate, we simply take the gate that should happen if the control qubit is  $|0\rangle$  and place it in the top left quadrant of a matrix, then place what should happen if it is  $|1\rangle$  in the bottom right quadrant. This can be expressed like so:

$$\begin{aligned} \mathbf{CU}_{1,2} &= |0\rangle\langle 0| \otimes \mathbf{I} + |1\rangle\langle 1| \otimes \mathbf{U} = \\ &\begin{bmatrix} 1 & \\ 0 & \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & \end{bmatrix} \otimes \mathbf{I} + \begin{bmatrix} 0 & \\ 1 & \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 0 & \end{bmatrix} \otimes \mathbf{U} = \\ &\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \otimes \mathbf{I} + \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \otimes \mathbf{U} \end{aligned}$$

Figure 26: Constructing a controlled gate  $\mathbf{CU}_{1,2}$  from a gate  $\mathbf{U}$  where the first qubit controls the second.

$$\begin{aligned} \mathbf{CU}_{2,1} &= \mathbf{I} \otimes |0\rangle\langle 0| + \mathbf{U} \otimes |1\rangle\langle 1| = \\ &\mathbf{I} \otimes \begin{bmatrix} 1 & \\ 0 & \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & \end{bmatrix} + \mathbf{U} \otimes \begin{bmatrix} 0 & \\ 1 & \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 0 & \end{bmatrix} = \\ &\mathbf{I} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + \mathbf{U} \otimes \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \end{aligned}$$

Figure 27: Constructing a controlled gate  $\mathbf{CU}_{2,1}$  from a gate  $\mathbf{U}$  where the second qubit controls the first.

In our case the controlling qubit is always after the  $\mathbf{R}_n$  gate so we only need the second formula. It is important to note that the controlled gate,  $\mathbf{U}$  in the examples, can be of any size, therefore it is not an issue that some of the controlled gates have 'empty' wires between them for example here is the result for a  $\mathbf{CR}_{3,1}$  gate.

$$\begin{aligned}
\mathbf{C}\mathbf{R}_{3,1} &= \mathbf{I} \otimes \mathbf{I} \otimes |0\rangle\langle 0| + \mathbf{R}_3 \otimes \mathbf{I} \otimes |1\rangle\langle 1| = \\
&\mathbf{I} \otimes \mathbf{I} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + \mathbf{R}_3 \otimes \mathbf{I} \otimes \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} = \\
&\mathbf{I} \otimes \mathbf{I} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + \mathbf{R}_3 \otimes \mathbf{I} \otimes \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}
\end{aligned}$$

Figure 28: Constructing a controlled gate  $\mathbf{C}\mathbf{R}_{3,1}$  from a gate  $\mathbf{R}_3$  where the second qubit controls the first.

$|\Psi\rangle\langle\Psi|$  is often called a projection on  $\Psi$ .

## 2.6 The Quantum Fourier Transform

Now we can represent a state as a vector and we have the building blocks for representing the QFT as a matrix. The  $QFT_n$  circuit applies the QFT to a  $n$ -qubit state and looks like this:

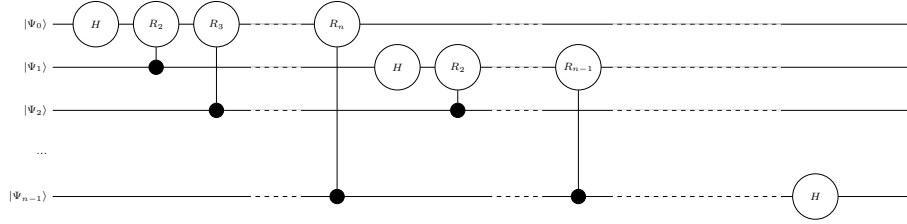


Figure 29: Circuit diagram of  $QFT_n$ .

In essence this circuit diagram can be read:

1. apply the  $\mathbf{H}$  gate to the first qubit.
2. apply the  $\mathbf{R}_2$  gate to the first qubit controlled by the second qubit.
3. apply the  $\mathbf{R}_3$  gate to the first qubit controlled by the third qubit.
4. ...
5. apply the  $\mathbf{R}_n$  gate to the first qubit controlled by the last qubit.
6. apply the  $\mathbf{H}$  gate to the second qubit.
7. apply the  $\mathbf{R}_2$  gate to the second qubit controlled by the third qubit.
8. ...
9. apply the  $\mathbf{R}_{n-1}$  gate to the second qubit controlled by the last qubit.

10. ...

11. apply the **H** gate to the last qubit.

This is all well and good, but how does this circuit end up performing a discrete Fourier transform? The definition of the DFT is given by this formula:

$$X_k = \sum_{n=0}^{N-1} x_n \cdot e^{-\frac{i2\pi}{N}kn}$$

where  $x$  is the input vector and  $X$  is the output vector, the subscripts are used for indexing in the vectors.

$$x_n = \frac{1}{N} \sum_{k=0}^{N-1} X_k \cdot e^{\frac{i2\pi}{N}kn}$$

This is the inverse DFT. The QFT acts on a state  $|x\rangle = |x_0, x_1, \dots, x_{N-1}\rangle$  and transforms it into the state  $|y\rangle = |y_0, y_1, \dots, y_{N-1}\rangle$ , the transformation is exactly:

$$y_k = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} x_n e^{\frac{i2\pi}{N}kn}$$

We see that it is equivalent to the inverse DFT. The QFT applied to a state is also sometimes written as

$$\text{QFT} |x_1 x_2 \dots x_n\rangle = \frac{1}{\sqrt{N}} (|0\rangle + e^{2\pi i [0.x_n]} |1\rangle) \otimes (|0\rangle + e^{2\pi i [0.x_{n-1}x_n]} |1\rangle) \otimes \dots \otimes (|0\rangle + e^{2\pi i [0.x_1 x_2 \dots x_n]} |1\rangle)$$

where  $[b_0.b_1b_2b_3\dots b_n] = \sum_{i=0}^n \frac{b_i}{2^i}$ , so a binary number[7]. If we don't apply the swaps in the end of the QFT we get

$$\text{QFT} |x_1 x_2 \dots x_n\rangle = \frac{1}{\sqrt{N}} (|0\rangle + e^{2\pi i [0.x_1 x_2 \dots x_n]} |1\rangle) \otimes \dots \otimes (|0\rangle + e^{2\pi i [0.x_{n-1}x_n]} |1\rangle) \otimes (|0\rangle + e^{2\pi i [0.x_n]} |1\rangle)$$

But how does the circuit laid out above result in this formula? Let us first look at  $QFT_1 |x_1\rangle$ , which is just **H**  $|x_1\rangle$  this can be written as  $\frac{1}{\sqrt{2}}(|0\rangle + e^{\frac{2\pi i}{2^1}x_1} |1\rangle)$ . We see here that if  $x_1$  is 1 we have  $\frac{1}{\sqrt{2}}(|0\rangle + e^{\pi i} |1\rangle)$  and if it is 0 we have  $\frac{1}{\sqrt{2}}(|0\rangle + e^0 |1\rangle)$  which is equivalent to  $\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) = H |1\rangle$  and  $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = H |0\rangle$ . To make the equation match the one from the definition we can say  $\frac{1}{\sqrt{2}}(|0\rangle + e^{\frac{2\pi i}{2^1}x_1} |1\rangle) = \frac{1}{\sqrt{2}}(|0\rangle + e^{2\pi i \frac{x_1}{2^1}} |1\rangle) = \frac{1}{\sqrt{2}}(|0\rangle + e^{2\pi i [0.x_1]} |1\rangle)$ .

For the case of  $QFT_2 |x_1, x_2\rangle$  we have that  $x_2$  is transformed in the same way as  $x_1$  in  $QFT_1$  and  $x_1$  is now transformed like so **H**  $|x_1\rangle$  if  $x_2 = 0$  and **HR**  $|x_1\rangle$  if  $x_2 = 1$ . This can be expressed like so  $\frac{1}{\sqrt{2}}(|0\rangle + e^{\frac{2\pi i}{2^1}x_1} e^{\frac{2\pi i}{2^2}x_2} |1\rangle) = \frac{1}{\sqrt{2}}(|0\rangle + e^{\frac{2\pi i}{2^1}x_1 + \frac{2\pi i}{2^2}x_2} |1\rangle) = \frac{1}{\sqrt{2}}(|0\rangle + e^{2\pi i [0.x_1 x_2]} |1\rangle)$ . If we put this together we get  $\frac{1}{\sqrt{2}}(|0\rangle + e^{2\pi i [0.x_1 x_2]} |1\rangle) \otimes \frac{1}{\sqrt{2}}(|0\rangle + e^{2\pi i [0.x_2]} |1\rangle) = \frac{1}{\sqrt{2^2}}(|0\rangle + e^{2\pi i [0.x_1 x_2]} |1\rangle) \otimes (|0\rangle + e^{2\pi i [0.x_2]} |1\rangle)$ .

For the case of  $QFT_3 |x_1, x_2, x_3\rangle$  we have that  $x_2$  and  $x_3$  is transformed in the same way as  $x_1$  and  $x_2$  in  $QFT_2$  and  $x_1$  is now transformed like so  $\mathbf{H} |x_1\rangle$  if  $x_2 = x_3 = 0$ ,  $\mathbf{HR}_2 |x_1\rangle$  if  $x_2 = 1, x_3 = 0$ ,  $\mathbf{HR}_3 |x_1\rangle$  if  $x_2 = 0, x_3 = 1$  and  $\mathbf{HR}_2\mathbf{R}_3 |x_1\rangle$  if  $x_2 = x_3 = 1$ . This can be expressed with  $\frac{1}{\sqrt{2^1}}(|\mathbf{0}\rangle + e^{\frac{2\pi i}{2^1}x_1} e^{\frac{2\pi i}{2^2}x_2} e^{\frac{2\pi i}{2^3}x_3} |\mathbf{1}\rangle) = \frac{1}{\sqrt{2^1}}(|\mathbf{0}\rangle + e^{\frac{2\pi i}{2^1}x_1 + \frac{2\pi i}{2^2}x_2 + \frac{2\pi i}{2^3}x_3} |\mathbf{1}\rangle) = \frac{1}{\sqrt{2^1}}(|\mathbf{0}\rangle + e^{2\pi i[0.x_1x_2x_3]} |\mathbf{1}\rangle)$ .

This pattern continues in a sort of recursive definition of  $QFT_n$  in terms of  $QFT_{n-1}$  and one 'step' affecting the first qubit.

## 2.7 Putting it all together

With these tools we can now create a formula for constructing a n-qubit state and a n-qubit QFT circuit.

$$|\Psi\rangle = |\Psi_1\Psi_2..\Psi_n\rangle = \bigotimes_{i=1}^n |\Psi_i\rangle$$

Figure 30: Constructing the state vector for the n-qubit state  $|\Psi\rangle$ .

$$I(k) = \begin{cases} \bigotimes_{i=k}^1 \mathbf{I} & \text{if } k \geq 1 \\ [1] & \text{otherwise} \end{cases}$$

$$STEP(i, n) = \begin{cases} \prod_{j=i}^2 (I(i) \otimes (\mathbf{I} \otimes I(j-2) \otimes |\mathbf{0}\rangle \langle \mathbf{0}| + \mathbf{R}_j \otimes I(j-2) \otimes |\mathbf{1}\rangle \langle \mathbf{1}|) \otimes I(n-i-j)) & \text{if } i \geq 2 \\ [1] & \text{otherwise} \end{cases}$$

$$QFT(n) = \prod_{i=n-1}^0 (STEP(n-i, n) (I(i) \otimes \mathbf{H} \otimes I(n-i-1)))$$

Figure 31: Constructing the matrix for the n-qubit QFT.

This can be turned into pseudo-code:

---

```

STATE(psi)
1  r = [1]
2  for each digit d in psi do:
3      if d = 1
4          r = r ⊗  $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$ 
5      else if d = 0
6          r = r ⊗  $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ 
7  return r

```

---



---

```

I(k)
1  r = [1]
2  id =  $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ 
3  while k ≥ 1 do:
4      r = r ⊗ id
5      k = k - 1
6  return r

STEP(i, n)
1  j = i
2  r = [1]
3  id =  $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ 
4  p0 =  $\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$ 
5  p1 =  $\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$ 
6  while j ≥ 2 do:
7      rj =  $\begin{bmatrix} 1 & 0 \\ 0 & e^{\frac{2\pi i}{2^j}} \end{bmatrix}$ 
8      r = r · (I(i) ⊗ (id ⊗ I(j - 2) ⊗ p0 + rj ⊗ I(j - 2) ⊗ p0) ⊗ I(n - i - j))
9      j = j - 1
10 return r

QTF(n)
1  r = I(n)
2  had =  $\begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} \\ \sqrt{0.5} & -\sqrt{0.5} \end{bmatrix}$ 
3  i = n - 1
4  while i ≥ 0 do:
5      r = r · STEP(n - i, n) · (I(i) ⊗ had ⊗ I(n - i - 1))
6      i = i - 1
7  return r

```

---

An example application could be  $QFT(4) \cdot STATE(0010)$ . Now we move on to show how we construct and apply the circuit using tensor networks.

### 3 Tensor Network Simulation

Tensors[1] are mathematical objects with a lot in common with  $n$ -dimensional arrays. Some examples of tensors you are probably familiar with, a rank 0 tensor is just a scalar, a rank 1 tensor is a vector, a rank 2 tensor is a matrix, and so on. The rank of the tensor tells you how many indices you need to describe a single element in the tensor e.g., you need 1 index to tell which element in a vector you are talking about, and you need 2, namely a column and row index to uniquely specify an element in a matrix. Each index has a dimension, for example a rank 2 tensor that is  $m$  by  $n$  would have one index  $i$  with dimension  $n$  and another index  $j$  with dimension  $m$ , we can then label an element in the tensor  $a_{ij}$  where  $i \in \{0, 1, \dots, n-1\}, j \in \{0, 1, \dots, m-1\}$ . If we have more indices, they are sometimes written as  $a_{ij}^{kl}$ . We can use diagrams to draw these tensors, the tensors are represented by red squares and the indices are represented by lines attaching to the square. The shape and colour of the tensors and the position of the lines typically do not matter, what is important is which of them are connected by shared indices.

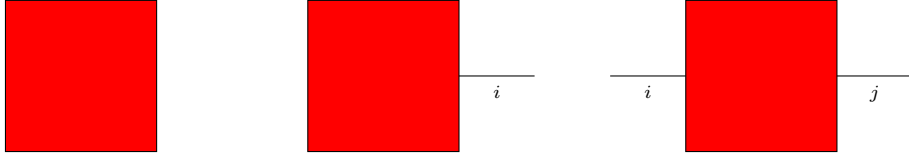


Figure 32: Rank 0, 1 and 2 tensors. Each index is represented by a line.

Often the indices are not labelled on these drawings. If we have two tensors, we can make them share an index if they each have an index with the same dimension. So, if we have two rank 3 tensors, one where the dimensions of the indexes are 2, 3, 5 and another where the dimensions are 1, 4, 3, we can see that they both have an index of dimension 3 so if we wish we can make them share label for this index. Thus, they could have the indices  $i, j, k$  and  $l, m, j$ , notice the reuse of  $j$ .

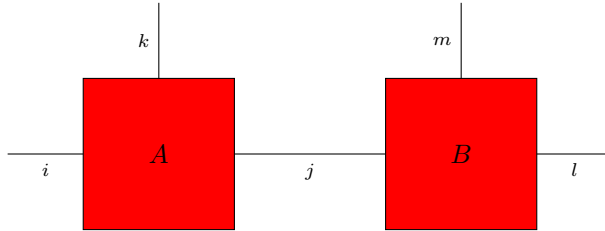


Figure 33: Rank 3 tensors sharing index  $j$ .



### 3.1 Contracting tensors

But what is this good for? In essence, when we make tensors share indices it is a way to symbolise that we are *contracting* them. The actual computation of the contraction can be done at a later point we are just marking our intention. This is important as we might want to build an entire network of tensors and then be strategic about which shared indices we choose to contract. Contracting a shared index is synonymous with computing the product of the two tensors.

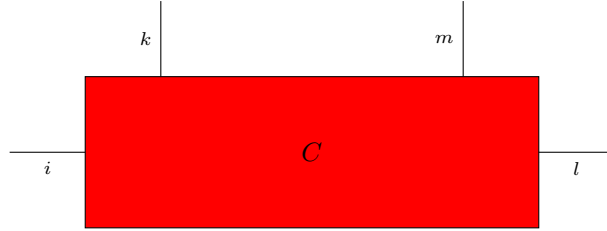


Figure 34: Rank 4 tensor after contracting shared index  $j$  from Figure 33.

In this example we have two tensors A and B where each have elements of the form  $a_{ijk}, b_{lmj}$  resulting in a single tensor C with the elements

$$c_{iklm} = \sum_{x=0}^{dim(j)-1} a_{ikx} b_{lmx}$$

Here  $dim(j) = 3$  and we subtract 1 since the elements are 0 indexed. In *tensor notation* the summation is implicit if there is a shared index in such an equation so we would just write  $c_{iklm} = a_{ijk} b_{lmj}$

### 3.2 Reshaping tensors

$|\Psi\rangle$  is a vector, in other words a rank 1 tensor, but later we are using them as rank 2 and 3 tensors, how can we do so? We can simply add some ranks like so,  $|\Psi\rangle \rightarrow [|\Psi\rangle] \rightarrow [[|\Psi\rangle]]$ , this can be done for the gates as well; we just add indices with dimension 1. The more general rule goes that you can change the rank of the tensor as much as you want as long as the product of the dimensions is the same. By this logic we can always add indices with dimension 1, but we can also split indices in two as long as the product of the dimensions of the new indices equals the old index's dimensions. We can also combine indices. This operation is often called reshaping.

### 3.3 Splitting two qubit gates into two tensors with a shared index

The SVD[6] is a mathematical operation that disassembles a matrix A into a matrix U, a vector of singular values  $\lambda$  and a matrix V, which upholds the

property  $A = U\Lambda Vh$  where  $\Lambda$  is a matrix where the diagonal corresponds to the values of  $\lambda$  and all the other elements are 0, and  $Vh$  is the conjugate transpose of  $V$ .

To take advantage of this we have our 4x4 gates, they have two indices that each have a dimension 4 but we reshape to 4 indices with dimensions 2 - an input for each qubit and an output for each. So if we describe our matrix elements with regards to these indices we can say an element  $a_{i_1 i_2 o_1 o_2}$  is in either the top half or the bottom half depending on  $i_1$ , and in the left half or right half depending on  $o_1$  this gives us a sub matrix that is 2x2, which we divide the same way using  $i_2$  and  $o_2$ . So, our matrix elements are divided like this:

$$\begin{bmatrix} a_{0000} & a_{0001} & a_{0010} & a_{0011} \\ a_{0100} & a_{0101} & a_{0110} & a_{0111} \\ a_{1000} & a_{1001} & a_{1010} & a_{1011} \\ a_{1100} & a_{1101} & a_{1110} & a_{1111} \end{bmatrix}$$

Figure 35: Matrix element indices.

Unfortunately, the SVD splits vertically i.e., in this case we would be splitting the gate between the inputs and outputs, but we are interested in splitting between the two qubits, so  $i_1$  and  $o_1$  are separate from  $i_2$  and  $o_2$ . Luckily, we can just swap around the indices and thus elements beforehand, we just have to remember to swap them back when all is set and done.

$$\begin{bmatrix} a_{0000} & a_{0001} & a_{0100} & a_{0101} \\ a_{0010} & a_{0011} & a_{0110} & a_{0111} \\ a_{1000} & a_{1001} & a_{1100} & a_{1101} \\ a_{1010} & a_{1011} & a_{1110} & a_{1111} \end{bmatrix}$$

Figure 36: Indices swapped.

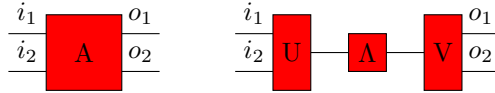


Figure 37: SVD without swapping.

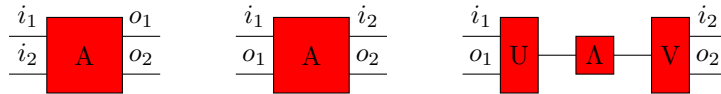


Figure 38: SVD with swapping.

We do though want to express this using two tensors only, but this is fortunately easy as we can just split  $\Lambda$  by squaring every value in it. Now we can contract two indices and get the result we want.

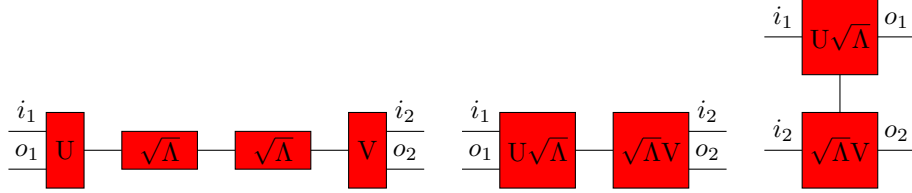


Figure 39: Combine the network from figure 38 into two tensors.

This whole process is sometimes called the operator Schmidt decomposition[7].

### 3.4 representing a circuit and state using tensors

We can use a tensor network to represent our *QFT* circuit and our state. We will use a matrix product state (MPS) to represent our state, and a matrix product operator (MPO) to represent our circuit, these are just subcategories of tensor networks.

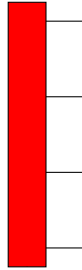


Figure 40: 4-qubit state represented as a tensor (MPS).

Here we have the whole state in one large tensor. This is highly undesirable as this uses a lot of memory, we would rather construct a network of tensors. Let us take the state  $|0010\rangle$  as an example.

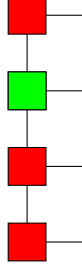


Figure 41: 4-qubit state  $|0010\rangle$  represented as a tensor network (MPS). Red represents  $|0\rangle$  and green  $|1\rangle$ .

Here we reshape the tensors representing each qubit to fit with our network structure. They simply have shared indices of size 1 connecting them. Now let us look at representing the QFT as a MPO:

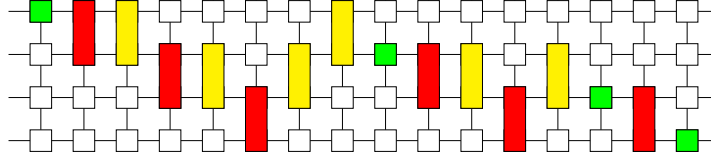


Figure 42:  $QFT_4$  represented as a tensor network (MPO). White represents an identity gate, green a Hadamard gate, red a controlled  $R_x, x \in \{2, 3, 4\}$  gate, and yellow a swap gate.

Now you might ask why we suddenly are using a ton of swap gates, and what are they even. Swap gates simply swap the values of two qubits, so if  $|10\rangle$  goes in  $|01\rangle$  comes out. This is simulated with this matrix, when swapping adjacent qubits as we are.

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Figure 43: SWAP gate matrix.

We do this to avoid having non-local gates in the circuit, such as the controlled  $R_x$  gates we use in the QFT. This was not a concern when doing the dense simulation, but here we have to split everything up into tensors acting on individual qubits and therefore would like smaller gates to start with. The reason we have to split everything up is mostly a limitation of the library[4] we are using for the simulation; it is a perfectly valid tensor network even without splitting every

gate. It does add a cost of slightly less than two swap gates per non-local gate. This low overhead is not something that can be achieved in general, the most general way to make every gate local requires swapping the two qubits with the ones between them until they are adjacent, applying the gate, and then swapping them back to where they came from, this takes swap gates equal to the number of qubits between the two target qubits times two. We are fortunately in a situation where we can do this in a smarter way.

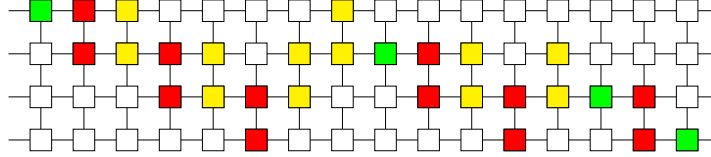


Figure 44:  $QFT_4$  from figure 42 with all two qubit gates split using the operator Schmidt decomposition.

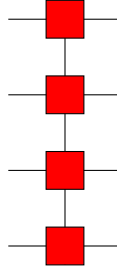


Figure 45:  $QFT_4$  from figure 44 with 'horizontal' shared indices contracted.

We have used the operator Schmidt decomposition to split the two qubit gates such that we can apply them to each of our qubits separately. Now that we have our state MPS and our QFT MPO we can apply the MPO to the MPS by connecting the outputs from the MPS to the inputs of the MPO and contracting those shared indexes. This results in an updated MPS. If we wish to combine two MPOs into one we do the same, just connecting the output of one to the input of another and contracting.

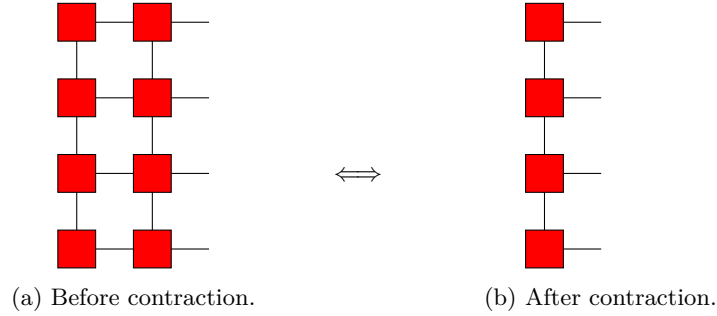


Figure 46: MPO applied to MPS.

After splitting a gate which acts on more than one qubit the index, they share will have a dimension of 1 or larger, and when we contract a MPO like so, we can see that the dimension scales quite quickly, with the layers if we do not do something:

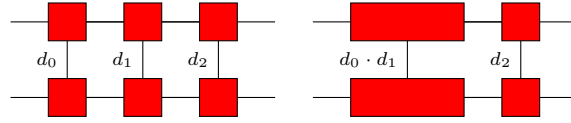


Figure 47: MPO with vertical bond dimensions  $d_i$ .

So, what can we do? We can compress the bonds in our MPO every now and then, to get them back to a manageable size, this is possible since we know our QFT has a fixed max bond dimension. The way we do it is to go through our bonds, e.g. from top to bottom and contract then re-split them using the SVD. This will help, but we can do better if we are willing to pay a little accuracy, we can truncate the singular values to only the ones that contribute the most and cut out those that do not contribute a lot to the result. In the QFT circuit it has been shown that the singular values decrease exponentially so we don't lose much precision.

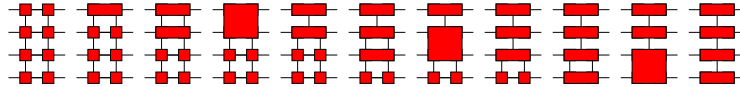


Figure 48: From left to right: Steps in compressing an MPO.

Compressing a MPO takes time, but frees up memory, it is therefore important to weigh these two against each other when implementing such a simulation, as we can get dramatic speedups by sacrificing a little memory, but due to the scaling of the bond dimensions we quickly end up having to compress to not run out of memory.

So far, we have described how to take the vectors and matrix representations of gates and add dimensions to them to make them fit our MPS and MPO representations. We show how to take a matrix for a two-qubit gate and split it into two separate matrices. We show how to contract a tensor network and how to compress an MPO after some number of applications of other MPOs. We use this to represent the QFT as a tensor network using only local gates, using swap gates in the construction.

## 4 Results & Conclusion

During this project I implemented both the dense and tensor network simulations and here are some results, unless otherwise mentioned all tensor network simulations are run with max bond at 32.

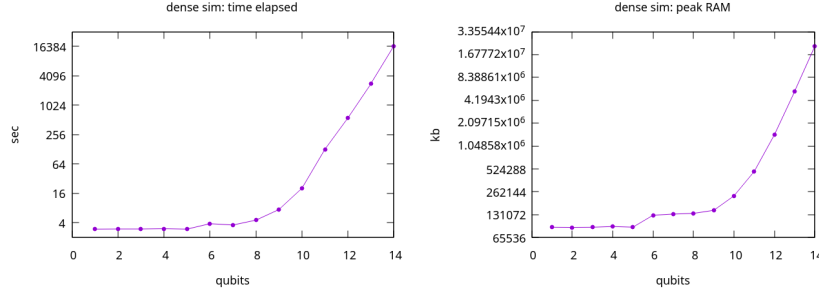


Figure 49: Time and peak RAM usage from constructing the dense matrices, using the approach discussed in section 2.

We see here that both time and memory usage scales faster than quadratic in the number of qubits simulated in the dense simulation. If we look at the tensor network simulation, we see a different picture; time scales quadratically and memory has these spikes but seems to not be affected by the number of qubits after a while. We also notice that before we had to stop at 14 qubits, now we arbitrarily stop at 32 qubits, but if we want, we can run it with 64 qubits in around 30 minutes or larger if we have the time.

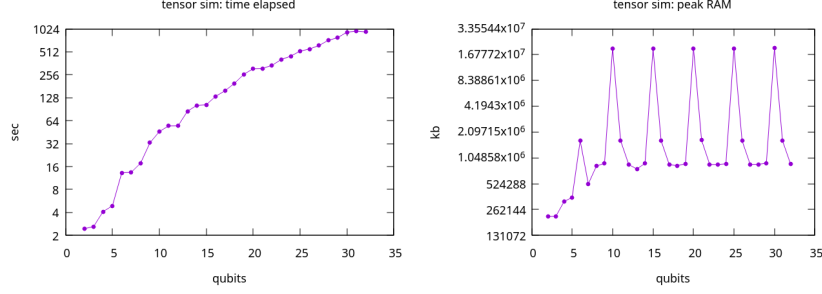


Figure 50: Time and peak RAM usage from constructing the MPOs, using the approach discussed in section 3, compressing after every fifth gate applied.

The spikes stem from only compressing the MPO every five gates, to confirm this we do the same benchmark where we compress every time.

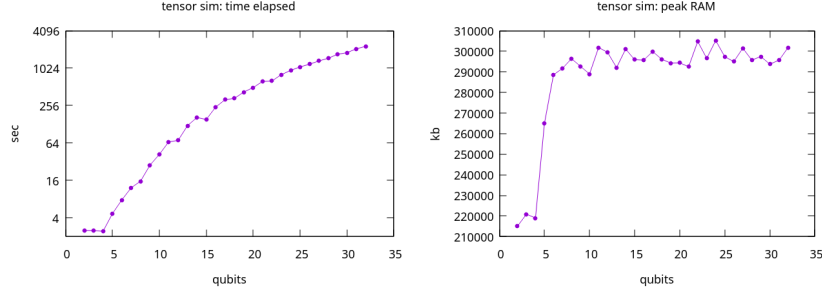


Figure 51: Time and peak RAM usage from constructing the MPOs, using the approach discussed in section 3, compressing after every gate applied.

Here we can see the spikes disappear, but we trade it for more time elapsed about 2.5x for 32 qubits. For 64 qubits with a max bond at 65 the difference is 30 minutes against 1 hour and 40 minutes i.e., a 3.3x speedup gained by skipping some compressions.

Now for the precision, the whole project is built upon the recently proven claim that the singular values are exponentially decreasing in the QFT circuit and therefore we can get most of the precision with a low max bond on the network, here we see a plot of the precision for both the compress every time and every fifth time.



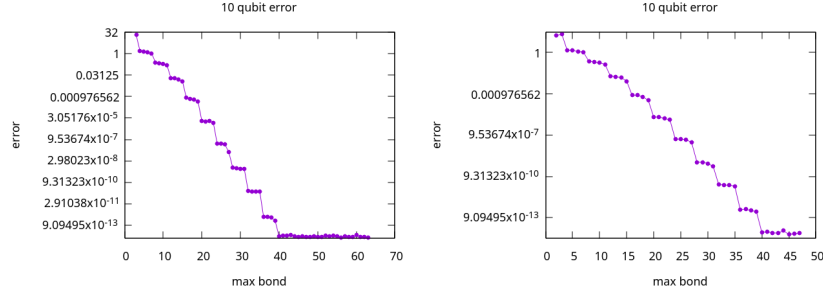


Figure 52: Error obtained by converting the MPO to its dense representation and taking the operator norm of the difference with the exact matrix produced by the dense simulation. Left: compress every time, right: compress every fifth time.

We see here that the error is approximately the same whether we compress every time or every fifth time. We also notice that it decreases less and less and at some point, completely stops improving as we increase the max bond. This is exactly as we expected to see. This is because at some point around a max bond of 40 we keep any relevant data for this circuit even after the compression. If we look at how the memory and time usage is affected by adjusting the max bond, we see that it is a powerful lever for trading precision for performance.

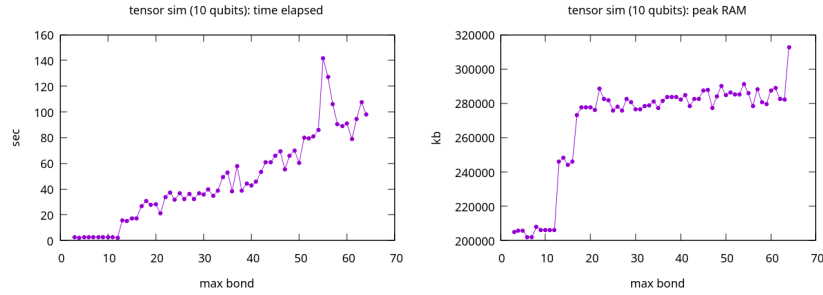


Figure 53: Time and peak RAM usage from constructing the MPOs, using the approach discussed in section 3, compressing after every gate applied.

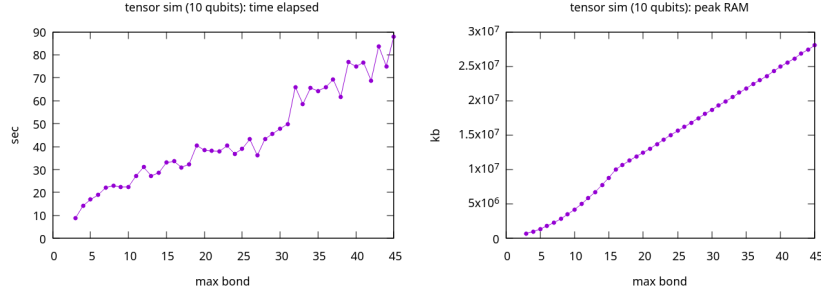


Figure 54: Time and peak RAM usage from constructing the MPOs, using the approach discussed in section 3, compressing after every fifth gate applied.

The reason we do not extend the graph for the benchmark where we compress every fifth time beyond 47 as max bond is because the spikes in memory usage scale with the max bond and the gap between compressions as seen in the peak memory graph in figure 54.

In conclusion I have implemented enough of the ideas from the paper to see the effects play out and it is indeed far more efficient to simulate the QFT using tensor networks, with close to no error.

## 5 Further work & Acknowledgements

I unfortunately did not have time to look into nor implement the zip-up algorithm discussed in the paper which could be something interesting to work on. I would like to acknowledge Michael Kastoryano and Nutan Limaye for their supervision, I would not have been even a third of the way by now without them. I would also like to acknowledge Sebastian Loeschcke for giving a few tips and tricks for working with the python library quimb, which saved me many hours.

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## 6 Appendix

### 6.1 Code

All code used for the project can be found here: <https://github.com/AceMouse/quantum-sim> and in the zip file submitted along with this report.

### 6.2 calculations for section 2.3

$$\begin{aligned}\mathbf{I}|0\rangle &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \cdot 1 + 0 \cdot 0 \\ 0 \cdot 1 + 1 \cdot 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} = |0\rangle \\ \mathbf{I}|1\rangle &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \cdot 0 + 0 \cdot 1 \\ 0 \cdot 0 + 1 \cdot 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} = |1\rangle\end{aligned}$$

Figure 55: Applying  $\mathbf{I}$  gate to the states  $|0\rangle$  and  $|1\rangle$

$$\begin{aligned}\mathbf{X}|0\rangle &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \cdot 1 + 1 \cdot 0 \\ 1 \cdot 1 + 0 \cdot 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} = |1\rangle \\ \mathbf{X}|1\rangle &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \cdot 0 + 1 \cdot 1 \\ 1 \cdot 0 + 0 \cdot 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} = |0\rangle\end{aligned}$$

Figure 56: Applying  $\mathbf{X}$  gate to the states  $|0\rangle$  and  $|1\rangle$

$$\begin{aligned}\mathbf{H}|0\rangle &= \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} \\ \sqrt{0.5} & -\sqrt{0.5} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} \sqrt{0.5} \cdot 1 + \sqrt{0.5} \cdot 0 \\ \sqrt{0.5} \cdot 1 - \sqrt{0.5} \cdot 0 \end{bmatrix} = \begin{bmatrix} \sqrt{0.5} \\ \sqrt{0.5} \end{bmatrix} = |+\rangle \\ \mathbf{H}|1\rangle &= \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} \\ \sqrt{0.5} & -\sqrt{0.5} \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} \sqrt{0.5} \cdot 0 + \sqrt{0.5} \cdot 1 \\ \sqrt{0.5} \cdot 0 - \sqrt{0.5} \cdot 1 \end{bmatrix} = \begin{bmatrix} \sqrt{0.5} \\ -\sqrt{0.5} \end{bmatrix} = |-\rangle\end{aligned}$$

Figure 57: Applying  $\mathbf{H}$  gate to the states  $|0\rangle$  and  $|1\rangle$

$$\begin{aligned}\mathbf{R}_2 |0\rangle &= \begin{bmatrix} 1 & 0 \\ 0 & e^{\frac{2\pi i}{2^2}} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \cdot 1 + 0 \cdot 0 \\ 0 \cdot 1 + e^{\frac{2\pi i}{2^2}} \cdot 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} = |0\rangle \\ \mathbf{R}_2 |1\rangle &= \begin{bmatrix} 1 & 0 \\ 0 & e^{\frac{2\pi i}{2^2}} \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \cdot 0 + 0 \cdot 1 \\ 0 \cdot 0 + e^{\frac{2\pi i}{2^2}} \cdot 1 \end{bmatrix} = \begin{bmatrix} 0 \\ e^{\frac{2\pi i}{2^2}} \end{bmatrix} = \begin{bmatrix} 0 \\ i \end{bmatrix}\end{aligned}$$

Figure 58: Applying  $\mathbf{R}_2$  gate to the states  $|0\rangle$  and  $|1\rangle$

$$\begin{aligned}\mathbf{CX} |00\rangle &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} = |00\rangle \\ \mathbf{CX} |01\rangle &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \cdot 0 + 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 0 + 1 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 0 + 0 \cdot 1 + 0 \cdot 0 + 1 \cdot 0 \\ 0 \cdot 0 + 0 \cdot 1 + 1 \cdot 0 + 0 \cdot 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} = |01\rangle \\ \mathbf{CX} |10\rangle &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 1 + 0 \cdot 0 \\ 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 1 + 0 \cdot 0 \\ 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 1 + 1 \cdot 0 \\ 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 1 + 0 \cdot 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} = |11\rangle \\ \mathbf{CX} |11\rangle &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 1 \\ 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 1 \\ 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 1 \\ 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} = |10\rangle\end{aligned}$$

Figure 59: Applying  $\mathbf{CX}$  gate to the states  $|00\rangle$ ,  $|01\rangle$ ,  $|10\rangle$  and  $|11\rangle$

### 6.3 calculations for section 2.4

$$\begin{aligned}
(\mathbf{I} \otimes \mathbf{I} \otimes \mathbf{X})|\mathbf{000}\rangle &= \left( \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \right) \left( \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ 0 \end{bmatrix} \right) = \\
&= \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\ \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\
&= \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \\
&= \begin{bmatrix} 0 \cdot 1 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 1 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = |\mathbf{001}\rangle
\end{aligned}$$

Figure 60: Applying  $\mathbf{X}$  to the first qubit in a 3 qubit system

$$\begin{bmatrix} 0 \cdot 1 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 1 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Figure 61: Applying **X** to the second qubit in a 3 qubit system

$$\begin{bmatrix} 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 \\ 1 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \\ 0 \cdot 1 + 0 \cdot 0 + 0 \cdot 0 + 1 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 + 0 \cdot 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Figure 62: Applying  $\mathbf{X}$  to the thrid qubit in a 3 qubit system



$$(\mathbf{X} \otimes \mathbf{I} \otimes \mathbf{H})|\mathbf{000}\rangle = \left( \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} \\ \sqrt{0.5} & -\sqrt{0.5} \end{bmatrix} \right) \left( \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ 0 \end{bmatrix} \right) =$$

system

$$\begin{aligned}
\mathbf{U} &= \mathbf{CX}(\mathbf{I} \otimes \mathbf{H})(\mathbf{I} \otimes \mathbf{X}) = \\
&\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} \\ \sqrt{0.5} & -\sqrt{0.5} \end{bmatrix} \\ 0 & \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} \\ \sqrt{0.5} & -\sqrt{0.5} \end{bmatrix} \end{bmatrix} \begin{bmatrix} \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} \\ \sqrt{0.5} & -\sqrt{0.5} \end{bmatrix} & 0 \\ 1 & \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} \\ \sqrt{0.5} & -\sqrt{0.5} \end{bmatrix} \end{bmatrix} \begin{bmatrix} 1 & \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\ 0 & \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \end{bmatrix} \begin{bmatrix} 0 & \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\ 1 & \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \end{bmatrix} = \\
&\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} & 0 & 0 \\ \sqrt{0.5} & -\sqrt{0.5} & 0 & 0 \\ 0 & 0 & \sqrt{0.5} & \sqrt{0.5} \\ 0 & 0 & \sqrt{0.5} & -\sqrt{0.5} \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} = \\
&\begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} & 0 & 0 \\ \sqrt{0.5} & -\sqrt{0.5} & 0 & 0 \\ 0 & 0 & \sqrt{0.5} & -\sqrt{0.5} \\ 0 & 0 & \sqrt{0.5} & \sqrt{0.5} \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} = \\
&\begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} & 0 & 0 \\ -\sqrt{0.5} & \sqrt{0.5} & 0 & 0 \\ 0 & 0 & -\sqrt{0.5} & \sqrt{0.5} \\ 0 & 0 & \sqrt{0.5} & \sqrt{0.5} \end{bmatrix}
\end{aligned}$$

Figure 64: Computing a matrix representation of a circuit,  $\mathbf{U}$ , that first applies  $\mathbf{X}$  then  $\mathbf{H}$  to the first qubit then  $\mathbf{CX}$  to the first and second qubit

$$\begin{aligned}
\mathbf{U}|\mathbf{00}\rangle &= \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} & 0 & 0 \\ -\sqrt{0.5} & \sqrt{0.5} & 0 & 0 \\ 0 & 0 & -\sqrt{0.5} & \sqrt{0.5} \\ 0 & 0 & \sqrt{0.5} & \sqrt{0.5} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} \sqrt{0.5} \\ -\sqrt{0.5} \\ 0 \\ 0 \end{bmatrix} = |\mathbf{0-}\rangle \\
\mathbf{U}|\mathbf{01}\rangle &= \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} & 0 & 0 \\ -\sqrt{0.5} & \sqrt{0.5} & 0 & 0 \\ 0 & 0 & -\sqrt{0.5} & \sqrt{0.5} \\ 0 & 0 & \sqrt{0.5} & \sqrt{0.5} \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} \sqrt{0.5} \\ \sqrt{0.5} \\ 0 \\ 0 \end{bmatrix} = |\mathbf{0+}\rangle \\
\mathbf{U}|\mathbf{10}\rangle &= \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} & 0 & 0 \\ -\sqrt{0.5} & \sqrt{0.5} & 0 & 0 \\ 0 & 0 & -\sqrt{0.5} & \sqrt{0.5} \\ 0 & 0 & \sqrt{0.5} & \sqrt{0.5} \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ -\sqrt{0.5} \\ \sqrt{0.5} \end{bmatrix} = -|\mathbf{1-}\rangle \\
\mathbf{U}|\mathbf{11}\rangle &= \begin{bmatrix} \sqrt{0.5} & \sqrt{0.5} & 0 & 0 \\ -\sqrt{0.5} & \sqrt{0.5} & 0 & 0 \\ 0 & 0 & -\sqrt{0.5} & \sqrt{0.5} \\ 0 & 0 & \sqrt{0.5} & \sqrt{0.5} \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \sqrt{0.5} \\ \sqrt{0.5} \end{bmatrix} = |\mathbf{1+}\rangle
\end{aligned}$$

Figure 65: Applying the circuit represented by the matrix  $\mathbf{U}$  from figure 64 to different states