1 Quantum Phase Estimation

We know that the quantum phase estimation algorithm is a quantum algorithm to estimate the phase corresponding to an eigenvalue of a given unitary operator. Since the eigenvalues of a unitary operator have unit modulus, they are characterized by their phase, meaning we can say the algorithm retrieves either the phase or the eigenvalue itself.

Let U be a unitary operator acting on an m-qubit register. Thus if $|\psi\rangle$ is an eigenvector of U, then $U|\psi\rangle = e^{2\pi i\theta}|\psi\rangle$ for some $\theta \in \mathbb{R}$. Due to the periodicity of the complex exponential, we can always assume $0 \leq \theta < 1$. However in the given homework the eigenvalue equation is $U|\psi\rangle = e^{i\theta}|\psi\rangle$ and $0 \leq \theta < 2\pi$. So to keep consistency I will use $U|\psi\rangle = e^{2\pi i\frac{\theta}{2\pi}}|\psi\rangle$, where $0 \leq \theta < 2\pi$ and $0 \leq \frac{\theta}{2\pi} < 1$. The algorithm returns an approximation for θ, with high probability.

2 Mathematical Development

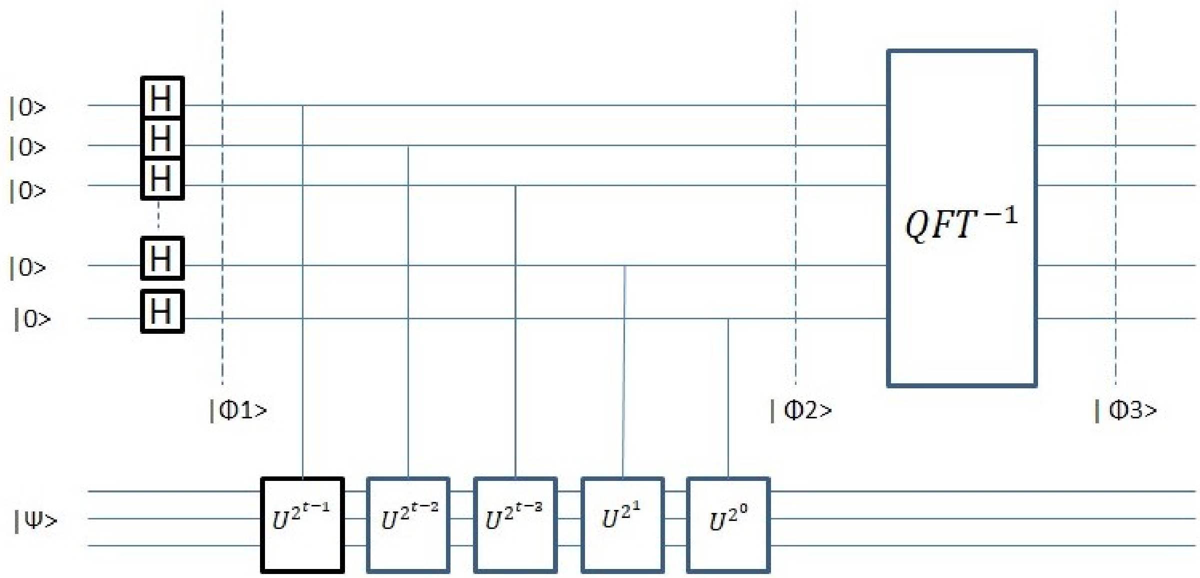

Figure 1: Quantum Phase Estimation Circuit

The input consists of two registers : the upper t qubits comprise the first register, and the lower m qubits are the second register.

The initial state of the system is: $|0\rangle^{\otimes t}|\psi\rangle$
After applying t-bit Hadamard gate operation $H^{\otimes t}$ on the first register, the state becomes:

$$|\phi_1\rangle = \frac{1}{2^{\frac{t}{2}}}(|0\rangle + |1\rangle)^{\otimes t}|\psi\rangle = \frac{1}{2^{t/2}}\sum_{j=0}^{2^t-1}|j\rangle|\psi\rangle. \tag{1}$$

Here j is decimal equivalent of t-bit binary number for example $|2\rangle = |00...010\rangle$. Let U be a unitary operator with eigenvector $|\psi\rangle$ such that $U|\psi\rangle = e^{2\pi i\frac{\theta}{2\pi}}|\psi\rangle$. Thus,

$$U^{2^j}|\psi\rangle = e^{2\pi i\frac{2^j\theta}{2\pi}}|\psi\rangle$$

The transformation implemented on the two registers by the controlled gates applying $U, U^2, U^{2^2}, \dots, U^{2^{t-1}}$ is

$$|k\rangle|\psi\rangle \mapsto |k\rangle U^k|\psi\rangle$$

Let us see what happens to the first register when we apply controlled U operation on each qubit.

$$U^{2^j}H|0\rangle|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle U^{2^j}|\psi\rangle + |1\rangle U^{2^j}|\psi\rangle) = \frac{1}{\sqrt{2}}(|0\rangle|\psi\rangle + e^{2\pi i\frac{2^j\theta}{2\pi}}|1\rangle|\psi\rangle) = \frac{1}{\sqrt{2}}(|0\rangle + e^{2\pi i\frac{2^j\theta}{2\pi}}|1\rangle) \otimes |\psi\rangle$$

So if we take the whole register the output after controlled-U operations will be the following :

$$|\phi_2\rangle = \frac{1}{\sqrt{2}}(|0\rangle + e^{2\pi i\frac{2^{t-1}\theta}{2\pi}}|1\rangle) \otimes \frac{1}{\sqrt{2}}(|0\rangle + e^{2\pi i\frac{2^{t-2}\theta}{2\pi}}|1\rangle) \otimes ... \otimes \frac{1}{\sqrt{2}}(|0\rangle + e^{2\pi i\frac{2^{1}\theta}{2\pi}}|1\rangle) \otimes \frac{1}{\sqrt{2}}(|0\rangle + e^{2\pi i\frac{2^{0}\theta}{2\pi}}|1\rangle) \otimes |\psi\rangle \tag{2}$$

This expression of $|\phi_2\rangle$ is equivalent to $\frac{1}{\sqrt{2^t}}\sum_{j=0}^{2^t-1} e^{2\pi ij\frac{\theta}{2\pi}}|j\rangle|\psi\rangle$ where j is decimal equivalent of binary bitstring.

3 Quantum Fourier Transform

First let us understand what quantum fourier transform does to a quantum circuit.

$$QFT|x\rangle = \frac{1}{2^{\frac{t}{2}}}\sum_{y=0}^{2^t-1} e^{2\pi i\frac{xy}{2^t}}|y\rangle \tag{3}$$

This y is also decimal equivalent of binary number and t is umber of qubits. It is easy to get that $QFT|0\rangle = |+\rangle$ and $QFT|1\rangle = |-\rangle$ which means basically operating on a single qubit state it acts like an hadamard operation or you could say transform computational basis to fourier basis. Now we will see if instead of 1-qubit $|0\rangle$ state, we have a t-qubit state how QFT transforms the circuit. We can convert decimal y into binary y i.e $|y\rangle = |y_1y_2y_3...y_t\rangle$ using $y = 2^{t-1}y_1 + 2^{t-2}y_2 + ... + 2^0y_t = \sum_{k=1}^{t} y_k2^{t-k}$. Now

$$\begin{aligned}
QFT|x\rangle &= \frac{1}{2^{\frac{t}{2}}}\sum_{y=0}^{2^t-1} e^{2\pi ix(\sum_{k=1}^{t} y_k2^{t-k})\frac{1}{2^t}}|y_1y_2y_3...y_t\rangle \\
&= \frac{1}{2^{\frac{t}{2}}}\sum_{y_1=0}^{1}\sum_{y_2=0}^{1}...\sum_{y_t=0}^{1}\prod_{k=1}^{t} e^{2\pi ixy_k2^{t-k}\frac{1}{2^t}}|y_1y_2y_3...y_t\rangle \\
&= \frac{1}{2^{\frac{t}{2}}}\prod_{k=1}^{t}\sum_{y_1=0}^{1}\sum_{y_2=0}^{1}...\sum_{y_t=0}^{1} e^{2\pi i\frac{xy_k}{2^k}}|y_1y_2y_3...y_t\rangle \\
&= \frac{1}{2^{\frac{t}{2}}}\prod_{k=1}^{t}\left[\sum_{y_1=0}^{1}\sum_{y_2=0}^{1}...\sum_{y_t=0}^{1}|y_1\rangle|y_2\rangle|y_3\rangle...|y_t\rangle e^{2\pi i\frac{xy_k}{2^k}}\right] \\
&= \frac{1}{2^{\frac{t}{2}}}\left(\sum_{y_1=0}^{1} e^{2\pi i\frac{xy_1}{2^1}}|y_1\rangle\right)\left(\sum_{y_2=0}^{1} e^{2\pi i\frac{xy_2}{2^2}}|y_2\rangle\right)...\left(\sum_{y_t=0}^{1} e^{2\pi i\frac{xy_t}{2^t}}|y_t\rangle\right) \\
&= \frac{1}{2^{\frac{t}{2}}}\left(|0\rangle + e^{2\pi i\frac{x}{2^1}}|1\rangle\right)\left(|0\rangle + e^{2\pi i\frac{x}{2^2}}|1\rangle\right)...\left(|0\rangle + e^{2\pi i\frac{x}{2^t}}|1\rangle\right)
\end{aligned} \tag{4}$$

Now we know that QFT is an unitary operation, meaning by pushing in the output of QFT operation as the input of QFT^{-1}, we can get our input state of the QFT. Before I go into inverse quantum Fourier transform, I want to show similarity between Eqn(2) and Eqn(4) if we express the phase in binary format. For Eqn(4) lets express x in binary $x = x_1x_2x_3...x_t$. We calculate

$$\frac{x}{2^t} = \frac{1}{2^t}\left(x_1 2^{t-1} + x_2 2^{t-2} + ... + x_t 2^0\right) = \frac{x_1}{2^1} + \frac{x_2}{2^2} + ... + \frac{x_t}{2^t}$$

$$= 0.x_1 + 0.0x_2 + 0.00x_3 + ... + 0.00..0x_t = 0.x_1x_2x_3...x_t$$

Now we apply this on complex exponential and see what happens :

$$e^{2\pi i \frac{x}{2^1}} = e^{2\pi i(x_1x_2x_3...x_{t-1}.x_t)} = e^{2\pi i(x_1x_2x_3...x_{t-1})}e^{2\pi i(0.x_t)} = e^{2\pi i(0.x_t)}$$

This happen because $x_1x_2x_3...x_{t-1}$ in decimal is an integer and $e^{2\pi n i} = 1$ if n is integer. Similarly we have

$$e^{2\pi i \frac{x}{2^2}} = e^{2\pi i(0.x_{t-2}x_t)} \qquad ; \qquad e^{2\pi i \frac{x}{2^{t-1}}} = e^{2\pi i(0.x_2x_3...x_t)}$$

So we can rewrite Eqn(4) by using the above expressions :

$$= \frac{1}{2^{\frac{t}{2}}}\left(|0\rangle + e^{2\pi i(0.x_t)}|1\rangle\right)\left(|0\rangle + e^{2\pi i(0.x_{t-1}x_t)}|1\rangle\right)...\left(|0\rangle + e^{2\pi i(0.x_1x_2x_3...x_t)}|1\rangle\right) \tag{5}$$

Now if we look at Eqn(2) $\frac{\theta}{2\pi}$ is in binary $0.\theta_1\theta_2...\theta_t$ meaning $2^{t-1} \times 0.\theta_1\theta_2...\theta_t = \theta_1\theta_2...\theta_{t-1}.\theta_t$. So we can rewrite the equation as

$$|\phi_2\rangle = \frac{1}{\sqrt{2}}(|0\rangle + e^{2\pi i(\theta_1\theta_2...\theta_{t-1}.\theta_t)}|1\rangle)\otimes\frac{1}{\sqrt{2}}(|0\rangle + e^{2\pi i(\theta_1\theta_2...\theta_{t-2}.\theta_{t-1}\theta_t)}|1\rangle)\otimes...\otimes\frac{1}{\sqrt{2}}(|0\rangle + e^{2\pi i(0.\theta_1\theta_2...\theta_t)}|1\rangle)\otimes|\psi\rangle$$

$$|\phi_2\rangle = \frac{1}{2^{\frac{t}{2}}}\left(|0\rangle + e^{2\pi i(0.\theta_t)}|1\rangle\right)\otimes\left(|0\rangle + e^{2\pi i(0.\theta_{t-1}\theta_t)}|1\rangle\right)\otimes...\otimes\left(|0\rangle + e^{2\pi i(0.\theta_1\theta_2...\theta_t)}|1\rangle\right)\otimes|\psi\rangle \tag{6}$$

As this Eqn(6) is similar to Eqn(5), this is the reason that after using $|\phi_2\rangle$ as input of QFT^{-1} we will get output $0.\theta_1\theta_2...\theta_t$, thus our phase will be determined.
Now we can use inverse QFT on $|\phi_2\rangle = \frac{1}{\sqrt{2^t}}\sum_{j=0}^{2^t-1} e^{2\pi i j\frac{\theta}{2\pi}}|j\rangle|\psi\rangle$

$$QFT^{-1}|j\rangle = \frac{1}{2^{\frac{t}{2}}}\sum_{y=0}^{2^t-1} e^{-2\pi i\frac{jy}{2^t}}|y\rangle \tag{7}$$

$$\therefore QFT^{-1}|\phi_2\rangle = \frac{1}{\sqrt{2^t}}\sum_{j=0}^{2^t-1} e^{2\pi i j\frac{\theta}{2\pi}}\left(\frac{1}{2^{\frac{t}{2}}}\sum_{y=0}^{2^t-1} e^{-2\pi i\frac{jy}{2^t}}|y\rangle\right)$$

$$|\phi_3\rangle = \frac{1}{2^t}\sum_{y=0}^{2^t-1}\sum_{j=0}^{2^t-1} e^{-2\pi i j\left(\frac{y}{2^t}-\frac{\theta}{2\pi}\right)}|y\rangle|\psi\rangle \tag{8}$$

This $|\phi_3\rangle$ is the final state of the system. It can be seen that this state from the output of the first register is nothing but $\sum_{y=0}^{2^{t-1}} c_y|y\rangle$ where, $c_y = \frac{1}{2^t}\sum_{j=0}^{2^t-1} e^{-2\pi i j\left(\frac{y}{2^t}-\frac{\theta}{2\pi}\right)}$. So probability of getting a certain $|y\rangle$ is given by

$$\Pr(y) = |c_y|^2 = \left|\frac{1}{2^t}\sum_{j=0}^{2^t-1} e^{-2\pi i j\left(\frac{y}{2^t}-\frac{\theta}{2\pi}\right)}\right|^2.$$

$$= \left| \frac{1}{2^t} \left(\frac{e^{-2\pi i (\frac{y}{2^t} - \frac{\theta}{2\pi}) 2^t} - 1}{e^{-2\pi i (\frac{y}{2^t} - \frac{\theta}{2\pi})} - 1} \right) \right|^2$$

$$= \frac{1}{(2^t)^2} \left| \frac{e^{\frac{-2\pi i}{2} (\frac{y}{2^t} - \frac{\theta}{2\pi}) 2^t}}{e^{\frac{-2\pi i}{2} (\frac{y}{2^t} - \frac{\theta}{2\pi})}} \right|^2 \left| \left(\frac{e^{\frac{-2\pi i}{2} (\frac{y}{2^t} - \frac{\theta}{2\pi}) 2^t} - e^{\frac{2\pi i}{2} (\frac{y}{2^t} - \frac{\theta}{2\pi}) 2^t}}{e^{\frac{-2\pi i}{2} (\frac{y}{2^t} - \frac{\theta}{2\pi})} - e^{\frac{2\pi i}{2} (\frac{y}{2^t} - \frac{\theta}{2\pi})}} \right) \right|^2$$

$$= \frac{1}{(2^t)^2} \frac{\sin^2 \left(\frac{2\pi}{2} \left(\frac{y}{2^t} - \frac{\theta}{2\pi} \right) 2^t \right)}{\sin^2 \left(\frac{2\pi}{2} \left(\frac{y}{2^t} - \frac{\theta}{2\pi} \right) \right)}$$

$$= \frac{1}{(2^t)^2} \frac{1 - \cos \left(2\pi \left(\frac{y}{2^t} - \frac{\theta}{2\pi} \right) 2^t \right)}{1 - \cos \left(2\pi \left(\frac{y}{2^t} - \frac{\theta}{2\pi} \right) \right)}$$

$$= \frac{1}{(2^t)^2} \left(\frac{1 - \cos \left(\frac{2\pi 2^t}{2^t} \left(y - \frac{\theta 2^t}{2\pi} \right) \right)}{1 - \cos \left(\frac{2\pi}{2^t} \left(y - \frac{\theta 2^t}{2\pi} \right) \right)} \right)$$

$$\therefore \Pr(y) = \frac{1}{M^2} \left(\frac{1 - \cos \left(\frac{2\pi M}{M} \left(y - \frac{\theta M}{2\pi} \right) \right)}{1 - \cos \left(\frac{2\pi}{M} \left(y - \frac{\theta M}{2\pi} \right) \right)} \right) \quad where, \;\; M = 2^t \tag{9}$$

This is the probability of measuring a certain $|y\rangle$.

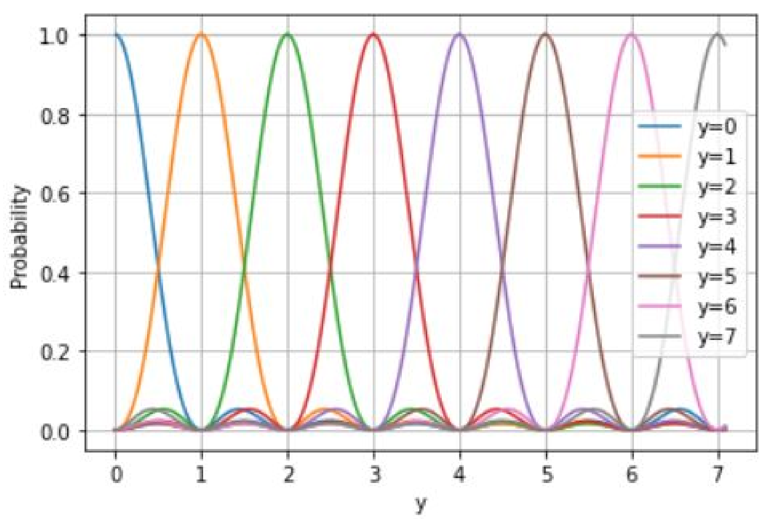

Figure 2: Plot of Probability function P(y) for one eigenstate $|y\rangle$. Plots are reaching peaks when $y = \frac{\theta M}{2\pi}$

4 General Case

Now for general case where $|\psi_k\rangle = \sum_k a_k|\psi_k\rangle$ is a superposition of a number of states we will derive the expressions as before. Here

$$|\phi_1\rangle = \frac{1}{2^{\frac{t}{2}}}(|0\rangle + |1\rangle)^{\otimes t} \sum_k a_k|\psi_k\rangle = \frac{1}{2^{t/2}} \sum_{j=0}^{2^t-1} |j\rangle \sum_k a_k|\psi_k\rangle. \tag{10}$$

We know $U^j \sum_k a_k|\psi_k\rangle = \sum_k a_k e^{2\pi ij\frac{\theta_k}{2\pi}}|\psi_k\rangle$ and after applying the unitary operations we get $|\phi_2\rangle$ -

$$|\phi_2\rangle = \frac{1}{2^{t/2}} \sum_{j=0}^{2^t-1} |j\rangle \otimes U^j \sum_k a_k|\psi_k\rangle$$

$$|\phi_2\rangle = \frac{1}{2^{t/2}} \sum_{j=0}^{2^t-1} |j\rangle \otimes \sum_k a_k e^{2\pi ij\frac{\theta_k}{2\pi}}|\psi_k\rangle$$

Now applying IQFT as before we get :

$$QFT^{-1}|\phi_2\rangle = |\phi_3\rangle = \frac{1}{2^{t/2}} \sum_{j=0}^{2^t-1} \left(\frac{1}{2^{\frac{t}{2}}} \sum_{y=0}^{2^t-1} e^{-2\pi i\frac{jy}{2^t}}|y\rangle \right) \otimes \sum_k a_k e^{2\pi ij\frac{\theta_k}{2\pi}}|\psi_k\rangle$$

$$\therefore |\phi_3\rangle = \frac{1}{2^t} \sum_{j=0}^{2^t-1} \left(\sum_{y=0}^{2^t-1} e^{-2\pi i\frac{jy}{2^t}}|y\rangle \right) \otimes \sum_k a_k e^{2\pi ij\frac{\theta_k}{2\pi}}|\psi_k\rangle \tag{11}$$

This $|\phi_3\rangle$ is the final state of the system. Now probability of getting a certain state $|y_0\rangle$ is

$$Pr(y_0) = |\langle y_0|\phi_2\rangle|^2 = \langle \phi_2|y_0\rangle\langle y_0|\phi_2\rangle$$

$$Pr(y_0) = (\frac{1}{2^t})^2 \sum_{j'=0}^{2^t-1} \left(\sum_{y=0}^{2^t-1} e^{2\pi i\frac{j'y}{2^t}} \langle y|y_0\rangle \right) \sum_{k'} a_{k'} e^{-2\pi ij'\frac{\theta'_k}{2\pi}} \langle \psi_{k'}| \sum_{j=0}^{2^t-1} \left(\sum_{y=0}^{2^t-1} e^{-2\pi i\frac{jy}{2^t}} \langle y|y_0\rangle \right) \sum_k a_k e^{2\pi ij\frac{\theta_k}{2\pi}}|\psi_k\rangle$$

$$Pr(y_0) = \frac{1}{(2^t)^2} \sum_{j'=0}^{2^t-1} e^{2\pi i\frac{j'y_0}{2^t}} \sum_{j=0}^{2^t-1} e^{-2\pi i\frac{jy_0}{2^t}} \sum_{k'} a_{k'} e^{-2\pi ij'\frac{\theta'_k}{2\pi}} \langle \psi_{k'}| \sum_k a_k e^{2\pi ij\frac{\theta_k}{2\pi}}|\psi_k\rangle$$

$$Pr(y_0) = \frac{1}{(2^t)^2} \sum_{j'=0}^{2^t-1} e^{2\pi i\frac{j'y_0}{2^t}} \sum_{j=0}^{2^t-1} e^{-2\pi i\frac{jy_0}{2^t}} \sum_{k'} \sum_k a_k a_{k'} e^{-2\pi ij'\frac{\theta_{k'}}{2\pi}} e^{2\pi ij\frac{\theta_k}{2\pi}} \langle \psi_{k'}|\psi_k\rangle$$

Considering orthogonality of ψ_k i.e. $\langle \psi_{k'}|\psi_k\rangle = \delta_{kk'}$ we get

$$Pr(y_0) = \frac{1}{(2^t)^2} \sum_{j'=0}^{2^t-1} e^{2\pi i\frac{j'y_0}{2^t}} \sum_{j=0}^{2^t-1} e^{-2\pi i\frac{jy_0}{2^t}} \sum_k a_k^2 e^{-2\pi ij'\frac{\theta_k}{2\pi}} e^{2\pi ij\frac{\theta_k}{2\pi}}$$

$$Pr(y_0) = \frac{1}{(2^t)^2}\sum_k a_k^2 \left(\sum_{j'=0}^{2^t-1} e^{2\pi i j'\left(\frac{y_0}{2^t}-\frac{\theta_k}{2\pi}\right)} \sum_{j=0}^{2^t-1} e^{-2\pi i j\left(\frac{y_0}{2^t}-\frac{\theta_k}{2\pi}\right)}\right)$$

$$Pr(y_0) = \frac{1}{(2^t)^2}\sum_k a_k^2 \left(\frac{e^{-2\pi i(\frac{y}{2^t}-\frac{\theta}{2\pi})2^t}-1}{e^{-2\pi i(\frac{y}{2^t}-\frac{\theta}{2\pi})}-1}\right)^2$$

$$Pr(y_0) = \frac{1}{(2^t)^2}\sum_k a_k^2 \left(\frac{1-\cos\left(\frac{2\pi 2^t}{2^t}\left(y_0-\frac{\theta_k 2^t}{2\pi}\right)\right)}{1-\cos\left(\frac{2\pi}{2^t}\left(y_0-\frac{\theta_k 2^t}{2\pi}\right)\right)}\right)$$

$$Pr(y_0) = \frac{1}{M^2}\sum_k a_k^2 \left(\frac{1-\cos\left(\frac{2\pi M}{M}\left(y_0-\frac{\theta_k M}{2\pi}\right)\right)}{1-\cos\left(\frac{2\pi}{M}\left(y_0-\frac{\theta_k M}{2\pi}\right)\right)}\right) \qquad where, \quad M = 2^t \tag{12}$$

This is the probability of measuring a certain $|y_0\rangle$.

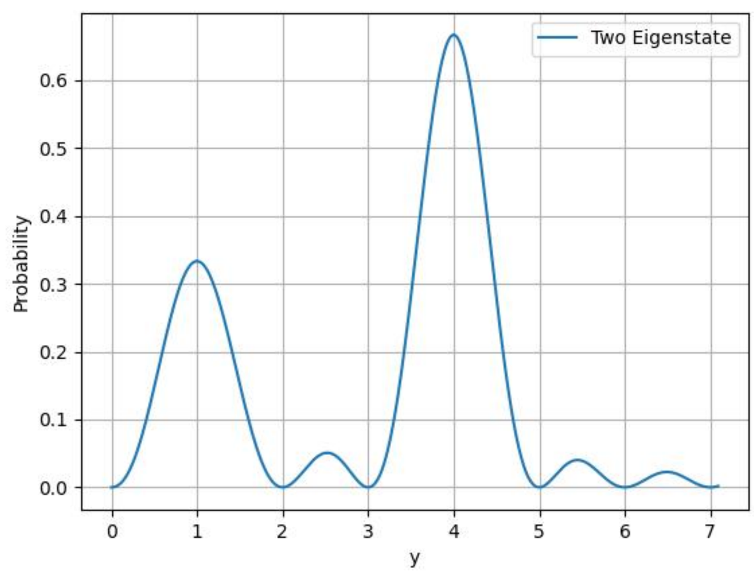

Figure 3: Plot of probability distribution function $P(y,\theta)$ for two eigenstates with phases $(\pi/4, \pi)$ and $a_k = \left(\frac{1}{\sqrt{3}}, \sqrt{\frac{2}{3}}\right)$. Plots are reaching peaks with an amplitude a_k^2 if $y_0 = \frac{\theta_k M}{2\pi}$.

4.1 Density Matrix :

The density matrix is defined as $\rho = \sum_i p_i|\psi_i\rangle\langle\psi_i|$ where ψ_i's are the quantum states with different probability amplitude p_i. However in our case there is only one state $|\phi_3\rangle$, so the density matrix is given by $\rho = |\phi_3\rangle\langle\phi_3|$.

$$\therefore \rho = |\phi_3\rangle\langle\phi_3|$$

$$= \left(\frac{1}{M} \sum_{j=0}^{M-1} \left(\sum_{x=0}^{M-1} e^{-2\pi i \frac{jx}{M}} |x\rangle \right) \otimes \sum_k a_k e^{2\pi i j \frac{\theta_k}{2\pi}} |\psi_k\rangle \right) \left(\frac{1}{M} \sum_{j'=0}^{M-1} \left(\sum_{y=0}^{M-1} e^{2\pi i \frac{j' y}{M}} \langle y| \right) \otimes \sum_{k'} a_{k'} e^{-2\pi i j' \frac{\theta_{k'}}{2\pi}} \langle \psi_{k'}| \right)$$

$$= \frac{1}{M^2} \sum_k \sum_{k'} a_k a_{k'} \sum_{x=0}^{M-1} \sum_{j=0}^{M-1} e^{-2\pi i j \left(\frac{x}{M} - \frac{\theta_k}{2\pi} \right)} \sum_{y=0}^{M-1} \sum_{j'=0}^{M-1} e^{2\pi i j' \left(\frac{y}{M} - \frac{\theta_{k'}}{2\pi} \right)} |x\rangle\langle y| \otimes |\psi_k\rangle\langle\psi_{k'}|$$

$$= \frac{1}{M^2} \sum_k \sum_{k'} a_k a_{k'} \left[\sum_{x=0}^{M-1} \frac{e^{-2\pi i \left(\frac{x}{M} - \frac{\theta_k}{2\pi} \right) M} - 1}{e^{-2\pi i \left(\frac{x}{M} - \frac{\theta_k}{2\pi} \right)} - 1} \right] \left[\sum_{y=0}^{M-1} \frac{e^{2\pi i \left(\frac{y}{M} - \frac{\theta_{k'}}{2\pi} \right) M} - 1}{e^{2\pi i \left(\frac{y}{M} - \frac{\theta_{k'}}{2\pi} \right)} - 1} \right] |x\rangle\langle y| \otimes |\psi_k\rangle\langle\psi_{k'}|$$