① Quantum Fourier Transform

(a) Recap: discrete Fourier transform (DFT).

- Used in a lot of places!
  - Signal processing — identifying frequency components of a signal. (audio and video processing)
  - Machine learning — feature extraction
  - Scientific Computing — Solving differential equations numerically.
- **Definition**: for a signal $\{x_k\}_{k=0}^{N-1}$, its DFT is

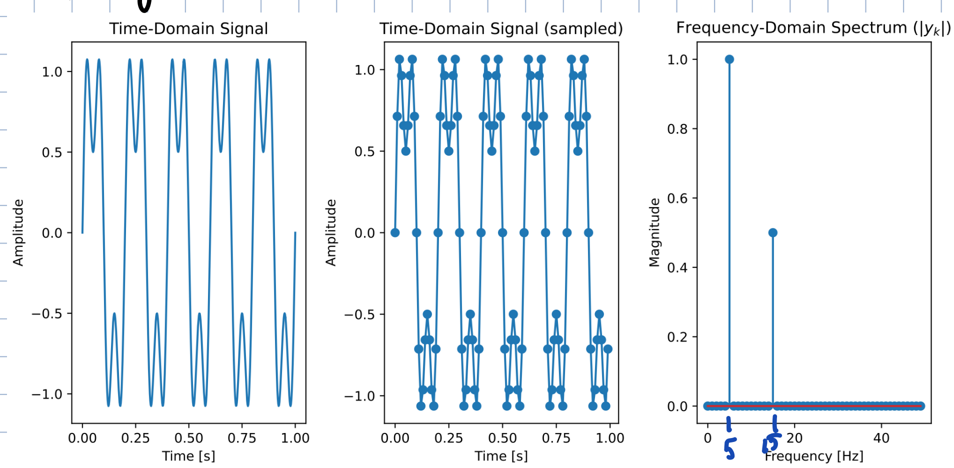
$$y_k = \frac{1}{\sqrt{N}} \sum_{k'=0}^{N-1} x_{k'} \, e^{\frac{2\pi i k' k}{N}} \qquad e^{2\pi i x} = \cos(2\pi x) + i\sin(2\pi x)$$

- **Example**: consider a signal of two sine waves put together:

$$x(t) = \sin(2\pi f_1 t) + \frac{1}{2}\sin(2\pi f_2 t)$$

frequencies

  - $f_1 = 5$ Hz
  - $f_2 = 15$ Hz
  - Sampling rate: $f_s = 100$ Hz $\Rightarrow$ 100 samples total (in 1 sec.)



(b) The Quantum Version! (Quantum Fourier Transform $\equiv$ QFT).

- $y_k = \frac{1}{\sqrt{N}} \sum_{k'=0}^{N-1} x_{k'} e^{\frac{2\pi i k' k}{N}} \longrightarrow \underbrace{Q}_{\text{QFT matrix}} |k\rangle = \frac{1}{\sqrt{d}} \sum_{k'=0}^{d-1} e^{\frac{2\pi i k k'}{d}} |k'\rangle$ (action on basis vectors).

$$|\psi\rangle = \sum_{k=0}^{d-1} x_k |k\rangle \Rightarrow Q|\psi\rangle = \sum_{k=0}^{d-1} x_k Q|k\rangle = \sum_{k=0}^{d-1} x_k \frac{1}{\sqrt{d}} \sum_{k'=0}^{d-1} e^{\frac{2\pi i k k'}{d}} |k'\rangle$$

$$= \sum_{k'=0}^{d-1} \Big(\underbrace{\frac{1}{\sqrt{d}} \sum_{k=0}^{d-1} x_k e^{\frac{2\pi i k k'}{d}}}_{\equiv y_{k'}} \Big) |k'\rangle$$

$$|\psi\rangle = \frac{1}{\sqrt{N}} \sum_{k=0}^{d-1} x_k |k\rangle$$
$$N = \sum_{k=0}^{d-1} |x_k|^2$$

- The QFT matrix is unitary! Let $\omega = e^{\frac{2\pi i}{d}}$, $\bar{\omega} = e^{\frac{-2\pi i}{d}} = \omega^{-1}$

$$\cos\left(\frac{2\pi}{d}\right) + i \sin\left(\frac{2\pi}{d}\right)$$

$$Q = \frac{1}{\sqrt{d}} \sum_{k,k'=0}^{d-1} \omega^{kk'} |k\rangle\langle k'|$$

$$QQ^\dagger = \left(\frac{1}{\sqrt{d}} \sum_{k,k'=0}^{d-1} \omega^{kk'} |k\rangle\langle k'| \right) \left(\frac{1}{\sqrt{d}} \sum_{j,j'=0}^{d-1} \omega^{-jj'} |j'\rangle\langle j| \right)$$

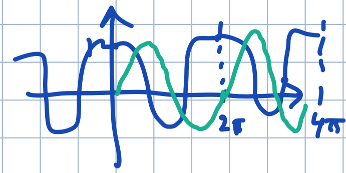
$$= \frac{1}{d} \sum_{k,k'=0}^{d-1} \sum_{j,j'=0}^{d-1} \omega^{kk'} \omega^{-jj'} |k\rangle \underbrace{\langle k'|j'\rangle}_{=\delta_{j',k'}} \langle j|$$

$$= \frac{1}{d} \sum_{k,k'=0}^{d-1} \sum_{j=0}^{d-1} \omega^{kk'} \omega^{-jk'} |k\rangle\langle j|$$

$$= \sum_{k,j=0}^{d-1} \Big(\underbrace{\frac{1}{d} \sum_{k'=0}^{d-1} \omega^{k'(k-j)}}_{} \Big) |k\rangle\langle j|$$

$\to \delta_{j,k}$

$$= \frac{1}{d}\sum_{k'=0}^{d-1} e^{\frac{2\pi i}{d} k' \underbrace{(k-j)}_{\equiv x}}$$



$\circledast$ If $x=0 \to \frac{1}{d}\sum_{k'=0}^{d-1}(1) = 1$

$\circledast$ If $x\neq 0 \to \frac{1}{d}\sum_{k'=0}^{d-1} \omega^{k'x} \to (\omega^x)^{k'}$

$$(\omega^x)^d = e^{\frac{2\pi i x}{d}\cdot d} = e^{2\pi i x} = \underbrace{\cos(2\pi x)}_{=1\ \forall x} + i\underbrace{\sin(2\pi x)}_{=0\ \forall x}$$

$\downarrow$

$=1$

$$= \frac{1}{d}\underbrace{\sum_{k'=0}^{d-1}(\omega^x)^{k'}} = \frac{1-(\omega^x)^d}{1-\omega} = 0.$$

Finite geometric series! $\sum_{k'=0}^{d-1} r^{k'} = \frac{1-r^d}{1-r}$

$\circledast$ So $\frac{1}{d}\sum_{k'=0}^{d-1}\omega^{k'(k-j)} = \delta_{j-k,0} = \delta_{j,k}$

$$\Rightarrow QQ^\dagger = \sum_{k,j=0}^{d-1}\underbrace{\left(\frac{1}{d}\sum_{k'=0}^{d-1}\omega^{k'(k-j)}\right)}_{\delta_{k,j}} |k\rangle\langle j| = \mathbb{1} \checkmark$$

Similarly, $Q^\dagger Q = \mathbb{1}$.

$$Q = \frac{1}{\sqrt{d}}\begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & \omega & \omega^2 & \cdots & \omega^{d-1} \\ 1 & \omega^2 & \omega^4 & \cdots & \omega^{2(d-1)} \\ \vdots & \vdots & & & \\ 1 & \omega^{d-1} & \omega^{2(d-1)} & \cdots & \omega^{(d-1)^2} \end{pmatrix}$$

Note: for $d=2$, $\omega = e^{\frac{2\pi i}{2}} = e^{\pi i} = -1 \Rightarrow Q = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & \omega \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \rightarrow$ Hadamard!

- Let $d = 2^n$, $\omega = e^{\frac{2\pi i}{2^n}} \longrightarrow$ What is a circuit representation of QFT?

Use the binary representation of $0, 1, 2, \ldots, 2^n - 1$

e.g., $n = 3$:

0	$\rightarrow$	000
1	$\rightarrow$	001
2	$\rightarrow$	010
3	$\rightarrow$	011
4	$\rightarrow$	100
5	$\rightarrow$	101
6	$\rightarrow$	110
7	$\rightarrow$	111

$\in \{0, 1, 2, \ldots, 7\}$

$k \rightarrow (k_1, k_2, k_3)$

$k = k_1 \cdot 4 + k_2 \cdot 2 + k_3 \cdot 1$

⊛ In general: $k = \sum_{l=1}^{n} 2^{n-l} k_l$

$$Q|j\rangle = \frac{1}{\sqrt{2^n}} \sum_{k=0}^{2^n - 1} e^{\frac{2\pi i jk}{2^n}} |k\rangle$$

$$\Rightarrow Q|j_1, j_2, \ldots, j_n\rangle = \frac{1}{\sqrt{2^n}} \sum_{k_1, k_2, \ldots, k_n \in \{0,1\}} e^{\frac{2\pi i}{2^n} j (k_1 2^{n-1} + k_2 2^{n-2} + \cdots + k_n)} |k_1, k_2, \ldots, k_n\rangle$$

$$= \frac{1}{\sqrt{2^n}} \sum_{k_1 \in \{0,1\}} \sum_{k_2 \in \{0,1\}} \cdots \sum_{k_n \in \{0,1\}} e^{\frac{2\pi i}{2^n} j k_1 2^{n-1}} e^{\frac{2\pi i}{2^n} j k_2 2^{n-2}} \cdots e^{\frac{2\pi i}{2^n} j k_n} |k_1, k_2, \ldots, k_n\rangle$$

$$= \left(\frac{1}{\sqrt{2}} \sum_{k_1 \in \{0,1\}} e^{\frac{2\pi i}{2^n} j k_1 2^{n-1}} |k_1\rangle \right) \left(\frac{1}{\sqrt{2}} \sum_{k_2 \in \{0,1\}} e^{\frac{2\pi i}{2^n} j k_2 2^{n-2}} |k_2\rangle \right) \cdots \left(\frac{1}{\sqrt{2}} \sum_{k_n \in \{0,1\}} e^{\frac{2\pi i}{2^n} j k_n} |k_n\rangle \right)$$

$$= \left(\frac{1}{\sqrt{2}} \sum_{k_1 \in \{0,1\}} e^{2\pi i k_1 \frac{j}{2}} |k_1\rangle \right) \left(\frac{1}{\sqrt{2}} \sum_{k_2 \in \{0,1\}} e^{2\pi i k_2 \frac{j}{2^2}} |k_2\rangle \right) \cdots \left(\frac{1}{\sqrt{2}} \sum_{k_n \in \{0,1\}} e^{2\pi i k_n \frac{j}{2^n}} |k_n\rangle \right)$$

Consider $n=3$: $\mathcal{Q}|j_1, j_2, j_3\rangle = \left(\frac{1}{\sqrt{2}}\sum_{k_1\in\{0,1\}} e^{2\pi i k_1 \frac{j}{2}}|k_1\rangle\right)\left(\frac{1}{\sqrt{2}}\sum_{k_2\in\{0,1\}} e^{2\pi i k_2 \frac{j}{2^2}}|k_2\rangle\right)\left(\frac{1}{\sqrt{2}}\sum_{k_3\in\{0,1\}} e^{2\pi i k_3 \frac{j}{2^3}}|k_3\rangle\right)$

$$j = 4j_1 + 2j_2 + j_3 \Rightarrow \frac{j}{2} = 2j_1 + j_2 + \frac{j_3}{2}$$

$$\frac{j}{2^2} = \frac{j}{4} = j_1 + \frac{j_2}{2} + \frac{j_3}{4}$$

$$\frac{j}{2^3} = \frac{j}{8} = \frac{j_1}{2} + \frac{j_2}{4} + \frac{j_3}{8}$$

$$\Rightarrow e^{2\pi i k_1 \frac{j}{2}} = \underbrace{e^{2\pi i k_1 (2j_1)}}_{=1}\ \underbrace{e^{2\pi i k_1 j_2}}_{=1}\ e^{2\pi i k_1 \frac{j_3}{2}} = e^{\pi i k_1 j_3} = (-1)^{k_1 j_3}$$

$$e^{2\pi i k_2 \frac{j}{4}} = \underbrace{e^{2\pi i k_2 j_1}}_{=1}\ \underbrace{e^{2\pi i k_2 \left(\frac{j_2}{2}\right)}}_{=(-1)^{k_2 j_2}}\ \underbrace{e^{2\pi i k_2 \left(\frac{j_3}{4}\right)}}_{= e^{\frac{2\pi i}{4} k_2 j_3}}$$

$$e^{2\pi i k_3 \frac{j}{8}} = \underbrace{e^{\frac{2\pi i}{2} k_3 j_1}}_{(-1)^{k_3 j_1}}\ e^{\frac{2\pi i}{4} k_3 j_2}\ e^{\frac{2\pi i}{8} k_3 j_3}$$

Therefore: $\mathcal{Q}|j_1, j_2, j_3\rangle = \left(\frac{1}{\sqrt{2}}\sum_{k_1\in\{0,1\}} (-1)^{k_1 j_3}|k_1\rangle\right)\left(\frac{1}{\sqrt{2}}\sum_{k_2\in\{0,1\}} (-1)^{k_2 j_2} e^{\frac{2\pi i}{4} k_2 j_3}|k_2\rangle\right)$

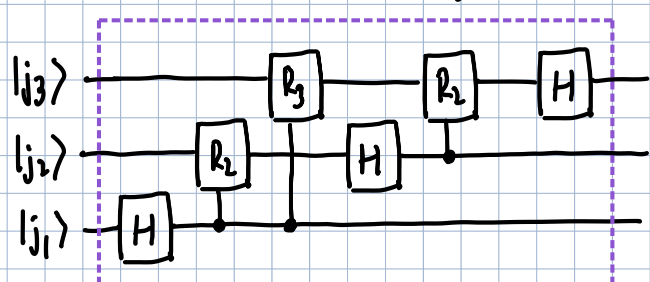
$$\left(\frac{1}{\sqrt{2}}\sum_{k_3\in\{0,1\}} (-1)^{k_3 j_1} e^{\frac{2\pi i}{4} k_3 j_2} e^{\frac{2\pi i}{8} k_3 j_3}|k_3\rangle\right)$$

$$= \frac{1}{\sqrt{2^3}}\sum_{k_1,k_2,k_3\in\{0,1\}} (-1)^{k_1 j_3}(-1)^{k_2 j_2}(-1)^{k_3 j_1} e^{\frac{2\pi i}{4} k_2 j_3} e^{\frac{2\pi i}{4} k_3 j_2} e^{\frac{2\pi i}{8} k_3 j_3}|k_1, k_2, k_3\rangle$$

$$= \tilde{\mathcal{Q}}|j_3, j_2, j_1\rangle$$

$$R_z(\theta) = e^{i\frac{\theta}{2}Z} = \begin{pmatrix}1 & 0\\ 0 & e^{i\frac{\theta}{2}}\end{pmatrix}$$

⊛ Define the rotation gate $R_k = \begin{pmatrix}1 & 0\\ 0 & e^{\frac{2\pi i}{2^k}}\end{pmatrix}$

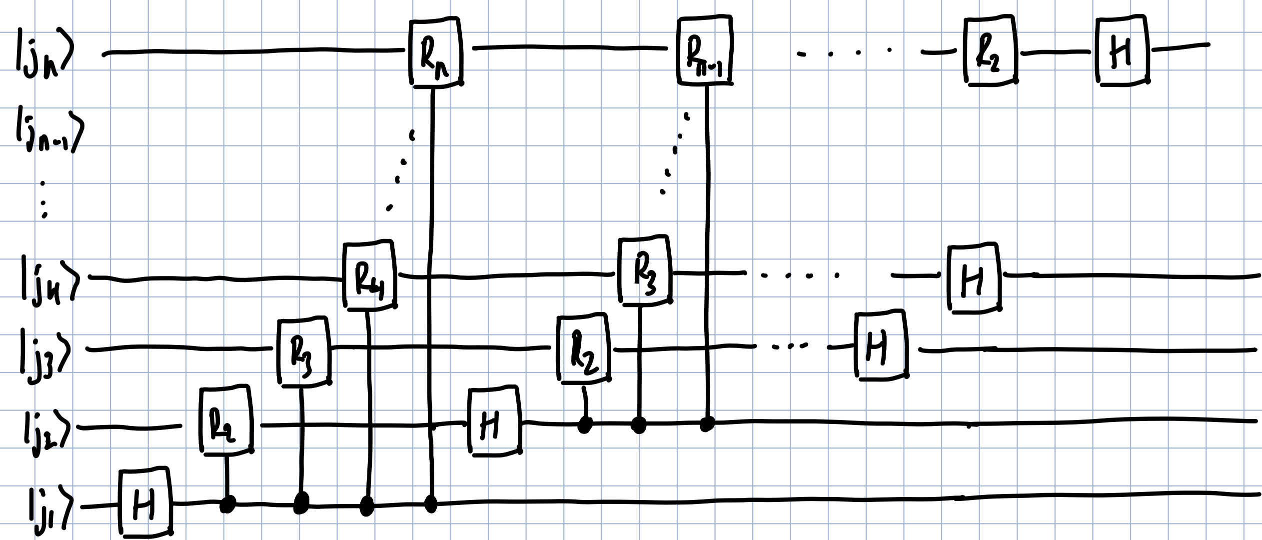


$\tilde{\mathcal{Q}}$

So $Q|j_1,j_2,j_3\rangle = \tilde{Q}|j_3,j_2,j_1\rangle = \tilde{Q}S|j_1,j_2,j_3\rangle$

Permutation of the qubits!

⊛ In general, $\tilde{Q}$ is given by the following circuit.



② The Phase Estimation Algorithm

- An application of the quantum Fourier transform.
- A prominent method in quantum chemistry for finding ground-state energies of molecules.
- Consider a Hamiltonian $H = \sum_{k=1}^{r} \lambda_k |\psi_k\rangle\langle\psi_k|$

Eigenvectors.

Eigenvalues/energies.

A Hermitian operator that describes the energy levels of a many-body quantum system.

The evolution operator is $U = e^{-itH} = \sum_{k=1}^{r} e^{-it\lambda_k} |\psi_k\rangle\langle\psi_k|$

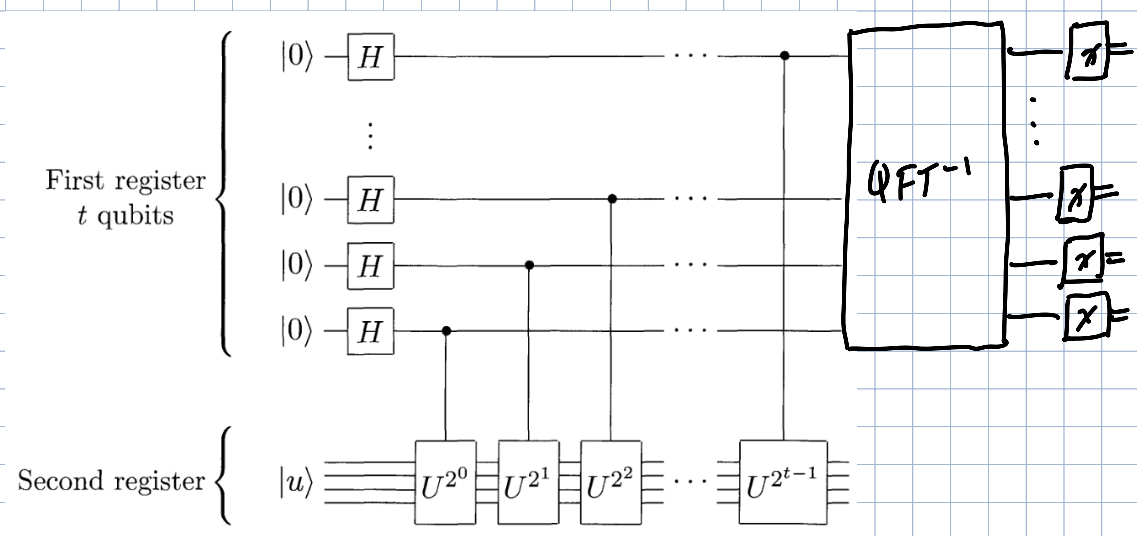
– **Question**: Using these evolutions, can we estimate the λ_k?

(a) Assume we are given $|u\rangle$ s.t. $U|u\rangle = e^{2\pi i\lambda}|u\rangle$, $\underline{\underline{\lambda \in [0,1)}}$

(λ is the unknown "phase", $|u\rangle$ is a given eigenvector.)

Assume also that we can implement the controlled-U^j gate (take this as a black box for now).

(b)



$$|0\rangle^{\otimes t} \otimes |u\rangle \mapsto \frac{1}{\sqrt{2^t}} \sum_{\vec{x}\in\{0,1\}^t} |\vec{x}\rangle \otimes |u\rangle = \frac{1}{\sqrt{2^n}} \sum_{x_1,x_2,\ldots,x_t\in\{0,1\}} |x_1,x_2,\ldots,x_t\rangle \otimes |u\rangle$$

ctrl targ.

$|a\rangle|b\rangle$

$cU(|a\rangle|b\rangle) = |a\rangle U^a|b\rangle$

$$\mapsto \frac{1}{\sqrt{2^t}} \sum_{x_1,x_2,\ldots,x_t\in\{0,1\}} |x_1,x_2,\ldots,x_t\rangle \otimes \underbrace{U^{x_t}|u\rangle}_{\hookrightarrow = e^{2\pi i\lambda x_t}|u\rangle}$$

$U|u\rangle = e^{2\pi i\lambda x_t}|u\rangle$

U^{x_t}

(b/c $|u\rangle$ is an eigenvector!)

$$= \frac{1}{\sqrt{2^t}} \sum_{x_1,x_2,\ldots,x_t\in\{0,1\}} e^{2\pi i\lambda x_t} |x_1,x_2,\ldots,x_t\rangle \otimes |u\rangle$$

$U = \sum_k e^{2\pi i\lambda_k}|\gamma_k\rangle\langle\gamma_k|$

$$\mapsto \frac{1}{\sqrt{2^t}} \sum_{x_1,x_2,\ldots,x_t\in\{0,1\}} e^{2\pi i\lambda x_t} |x_1,x_2,\ldots,x_t\rangle \otimes \underbrace{(U^2)^{x_{t-1}}|u\rangle}_{= e^{2\pi i(2\lambda)x_{t-1}}|u\rangle}$$

$U^2 = \sum_k e^{2\pi i\lambda_k \cdot 2}|\gamma_k\rangle\langle\gamma_k|$

$\vdots$

$$\mapsto \frac{1}{\sqrt{2^t}} \sum_{x_1,x_2,\dots,x_t\in\{0,1\}} e^{2\pi i(\dots)} \overset{Q^{-1}}{\underbrace{|x_1,x_2,\dots,x_t\rangle}} \otimes |u\rangle$$

$$\sum_{l=1}^{t} 2^{t-l}\lambda x_l \equiv x\lambda \quad \to \quad \lambda\Big(\underbrace{x_1 2^{t-1}+x_2 2^{t-2}+\dots+x_{t-1}\cdot 2+x_t}_{=x}\Big)$$

Now apply the inverse of QFT! Recall that

$$Q|j_1,j_2,\dots,j_t\rangle = \frac{1}{\sqrt{2^t}} \sum_{k_1,k_2,\dots,k_t\in\{0,1\}} e^{\frac{2\pi i}{2^t} j\,(k_1 2^{t-1}+k_2 2^{t-2}+\dots+k_t)} |k_1,k_2,\dots,k_t\rangle$$

$$j=\sum_{l=1}^{t} j_l\, 2^{t-l}$$

Also, Q is unitary, $QQ^\dagger = \mathbb{1} \Rightarrow Q^{-1} = Q^\dagger$

$$Q^{-1}|x_1,x_2,\dots,x_t\rangle = \frac{1}{\sqrt{2^t}} \sum_{k_1,k_2,\dots,k_t\in\{0,1\}} e^{-\frac{2\pi i}{2^t} x\,(k_1 2^{t-1}+k_2 2^{t-2}+\dots+k_t)} |k_1,k_2,\dots,k_t\rangle$$

$$\Rightarrow \frac{1}{\sqrt{2^t}} \sum_{x_1,x_2,\dots,x_t\in\{0,1\}} e^{2\pi i x\lambda}\, Q^{-1}|x_1,x_2,\dots,x_t\rangle \otimes |u\rangle$$

$$= \frac{1}{2^t} \sum_{x_1,\dots,x_t\in\{0,1\}} \sum_{k_1,\dots,k_t\in\{0,1\}} e^{2\pi i x\lambda}\, e^{-\frac{2\pi i}{2^t} x\,(k_1 2^{t-1}+k_2 2^{t-2}+\dots+k_t)} |k_1,k_2,\dots,k_t\rangle \otimes |u\rangle$$

$$\sum_{l=1}^{t} 2^{t-l} k_l = k$$

$$= \sum_{l'=1}^{t-1} 2^{t-l'} x_{l'}$$

$$e^{2\pi i x\lambda}\, e^{-2\pi i x \frac{k}{2^t}} = e^{2\pi i x\left(\lambda - \frac{k}{2^t}\right)}$$

$$= \frac{1}{2^t} \sum_{k=0}^{2^t-1} \left(\sum_{x=0}^{2^t-1} e^{\frac{2\pi i}{2^t} x (2^t \cdot \lambda - k)} \right) |k\rangle \otimes |u\rangle \qquad \left(\sum_{x=0}^{d-1} \omega^{xk} = d \cdot \delta_{k,0} \right)$$

(*) Now, suppose that λ can be represented using t bits exactly:

$$\lambda = \sum_{l=1}^{t} 2^{-l} \lambda_l \Rightarrow 2^t \lambda = \sum_{l=1}^{t} 2^{t-l} \lambda_l$$

Then $\delta_{2^t \lambda, k} \Rightarrow \delta_{\lambda_l, k_l} \quad \forall\, l$

$$= |\lambda\rangle \otimes |u\rangle$$

Binary representation of λ!

Finally, measurement leads to the exact t-bit representation of λ with probability one!