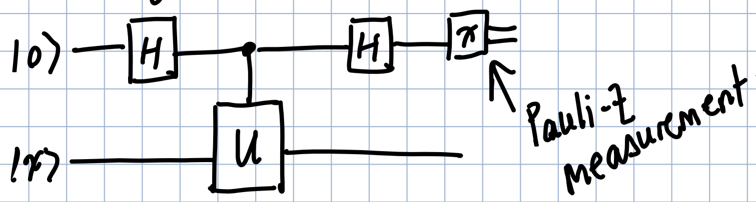
① Recap: Hadamard Test.

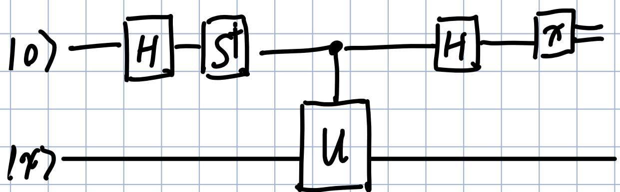
Estimating $\langle\psi|U|\psi\rangle$, where U is a unitary and $|\psi\rangle$ is a state vector.



$$\Pr[0] = \frac{1}{2}\left(1 + \mathrm{Re}(\langle\psi|U|\psi\rangle)\right), \quad \Pr[1] = \frac{1}{2}\left(1 - \mathrm{Re}(\langle\psi|U|\psi\rangle)\right).$$

$$S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \Rightarrow S^\dagger = \begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix}$$

For the imaginary part:



$$\Pr[0] = \frac{1}{2}\left(1 + \mathrm{Im}(\langle\psi|U|\psi\rangle)\right)$$

$$\Pr[1] = \frac{1}{2}\left(1 - \mathrm{Im}(\langle\psi|U|\psi\rangle)\right).$$

⊛ In both cases, we have $\Pr[0] = \frac{1}{2}(1+\alpha)$, $\Pr[1] = \frac{1}{2}(1-\alpha)$, where α is unknown. To estimate α, we do the following procedure:

For $i = 1, 2, \ldots, N$ ($N \equiv$ # of samples / # of times we run the quantum circuit).

- Each time we get outcome "0" → record $x_i = 1$
- Each time we get outcome "1" → record $x_i = -1$
- Do this N times, then take the sample mean/average: $\hat{x}_N = \frac{1}{N}\sum_{i=1}^{N} x_i$ → Sample mean

$\Big\}$ → ⊛ This defines a random variable X:

$$\Pr[X = \pm 1] = \frac{1}{2}(1 \pm \alpha)$$

This defines a random variable $\hat{X}_N = \frac{1}{N}\sum_{i=1}^{N} X_i$. $\hat{X}_N$ is an unbiased estimator of X:

$$\underbrace{\mathbb{E}[\hat{X}_N]}_{\text{True mean}} = \frac{1}{N}\sum_{i=1}^{N} \underbrace{\mathbb{E}[X_i]}_{=\mathbb{E}[X]\ \forall i,\ \text{b/c all samples are independent and identical.}} = \frac{1}{N}\sum_{i=1}^{N} \mathbb{E}[X] = \mathbb{E}[X].$$

$\mathbb{E}[X] = (+1)\cdot \Pr[X=+1] + (-1)\cdot \Pr[X=-1] = \frac{1}{2}(1+\alpha) - \frac{1}{2}(1-\alpha) = \alpha.$

- As $N \to \infty$, $\hat{X}_N \to \mathbb{E}[X] = \alpha$ (law of large numbers).

  ⊛ So the sample average approaches the true (unknown) value of α!

② Motivation: Expectation values

- Why do we care about quantities of the form $\langle \psi | U | \psi \rangle$?

  B/c they can be used to compute expectation values of observables.

- Observable: Any Hermitian operator (recall: M Hermitian $\Leftrightarrow M^\dagger = M$)

  ⊛ Fact from linear algebra: Every Hermitian operator can be diagonalized

  $$M = \sum_{i=1}^{d} \lambda_i |v_i\rangle\langle v_i|,$$ where: λ_i : eigenvalues (real numbers). $|v_i\rangle$: orthonormal eigenvectors.

  $$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = |0\rangle\langle 0| - |1\rangle\langle 1|$$

  $$\boxed{\sum_{i=1}^{d} |v_i\rangle\langle v_i| = \mathbb{1}}$$

  ⊛ Axiom of quantum mechanics: every physical quantity corresponds to a Hermitian operator (e.g., position, momentum, energy...).

  The eigenvalues are the possible values of the quantity

  We get the value of the quantity through measurement.

- For an observable/Hermitian operator M, the corresponding measurement is given by the eigenvectors. ($\{|v_i\rangle\langle v_i|\}$ is the POVM.)

- For a state ρ, the probability that it has value λ_i is

$\Pr[i] = \mathrm{Tr}[|v_i\rangle\langle v_i|\rho]$ (Born rule). $= \langle v_i|\rho|v_i\rangle$

The expected value of the observable is:

$$\langle M\rangle_\rho = \sum_{i=1}^{n} \lambda_i \Pr[i] = \sum_{i=1}^{n} \lambda_i \mathrm{Tr}[|v_i\rangle\langle v_i|\rho] = \mathrm{Tr}\Big[\big(\underbrace{\sum_{i=1}^{n} \lambda_i |v_i\rangle\langle v_i|}_{M}\big)\rho\Big] = \mathrm{Tr}[M\rho].$$

Definition of expectation value!

- If we don't know the eigenvectors (b/c they are hard to get for large matrices!), but we know that M can be written as

$$M = \sum_{j=1}^{k} c_j U_j, \quad \text{then} \quad \langle M\rangle_\gamma = \mathrm{Tr}[M|\gamma\rangle\langle\gamma|]$$

unitaries

$$= \sum_{j=1}^{k} c_j \mathrm{Tr}[U_j |\gamma\rangle\langle\gamma|]$$

$$= \sum_{j=1}^{k} c_j \langle\gamma|U_j|\gamma\rangle$$

Estimate using Hadamard test!

So we estimate each term individually using the Hadamard test and then add to get an overall estimate of the expectation value.

③ Quantum Fourier Transform

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

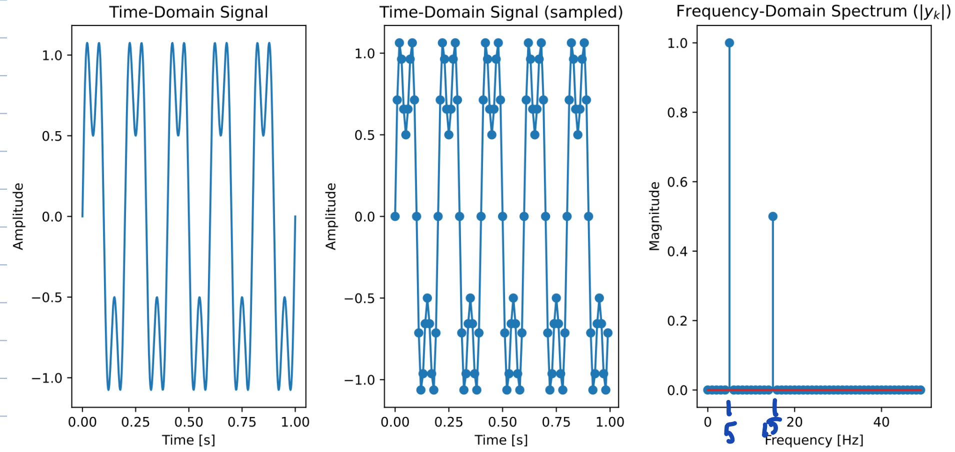
- Used in a lot of places!
  - Signal processing — identifying frequency components of a signal. (audio and video processing)
  - Machine learning — feature extraction
  - Scientific Computing — Solving differential equations numerically.
- Definition: for a signal $\{x_k\}_{k=0}^{N-1}$, its DFT is

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

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

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

  - $f_1 = 5$ 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).

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

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

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

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

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

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

$$\overline{\omega} = \cos\left(\frac{2\pi}{d}\right) - i\sin\left(\frac{2\pi}{d}\right)$$

$$= e^{-\frac{2\pi i}{d}}.$$

$$= \omega^{-1}$$

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

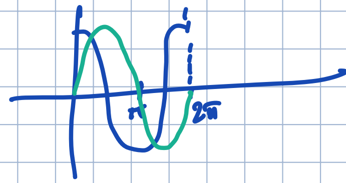
$$= \frac{1}{d} \sum_{k,k'=0}^{d-1} \sum_{j,j'=0}^{d-1} \omega^{kk'} \omega^{-jj'} |k\rangle \underbrace{\langle k'|j'\rangle}_{=\delta_{j',k'}} \langle j|$$

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

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

$\rightarrow \delta_{j,k}$

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



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

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

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

$\downarrow$ $=1$

$\omega = e^{\frac{2\pi i}{d}}$

$\omega^x = e^{\frac{2\pi i x}{d}}$

$\omega^{xd} = e^{2\pi i x}$

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

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

⊛ 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

$\Rightarrow \underbrace{k}_{\in\{0,1,2,\ldots,7\}} \rightarrow (k_1, k_2, k_3)$

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

In general: $k = \sum_{\ell=1}^{n} 2^{n-\ell} k_\ell$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

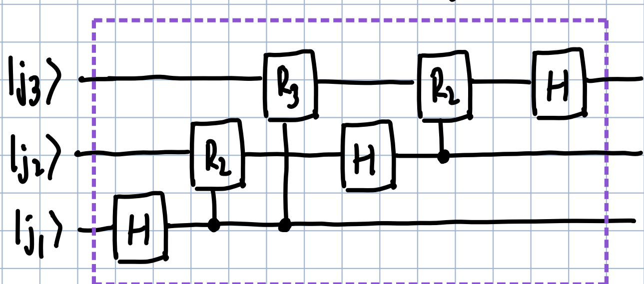
$$= \tilde{\mathcal{Q}}|j_3,j_2,j_1\rangle$$

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

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

$$R_2 = \begin{pmatrix}1 & 0\\ 0 & \underbrace{e^{\frac{2\pi i}{4}}}_{e^{\frac{\pi i}{2}} = i}\end{pmatrix}$$

$$\begin{pmatrix}1 & 0\\ 0 & i\end{pmatrix}$$



$\tilde{\mathcal{Q}}$

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.