Quantum Algorithms

Phase estimation, Hamiltonian simulation & linear system "solving"

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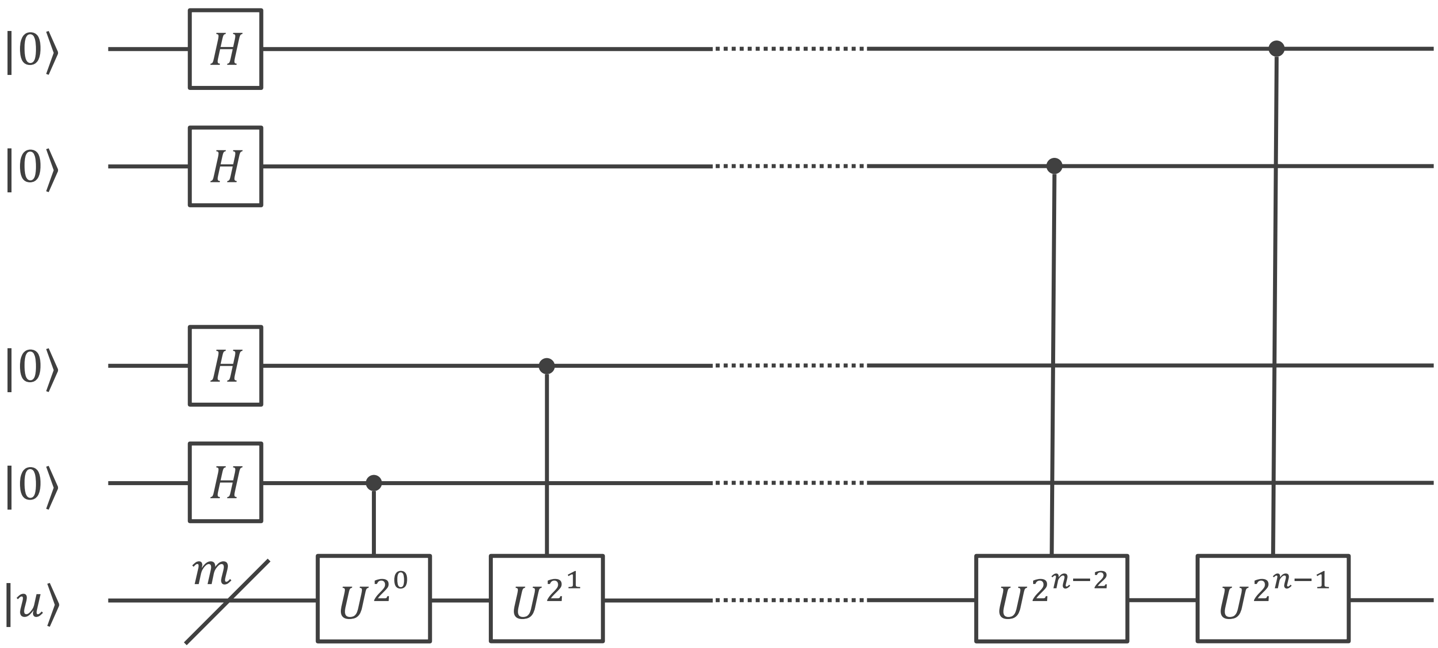
Quantum phase estimation

- Unitary operator U
- Eigenvector $|u\rangle$ with eigenvalue $\mathrm{e}^{\mathrm{i}\phi}$, where $\phi \in [0, 2\pi)$
- Our goal: find $\mathrm{e}^{\mathrm{i}\phi}$, or estimate ϕ (precision to n-qubits)

- Controlled-U^{2^j} gate:

$$CU^{2^j}\left[\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |u\rangle\right] = \frac{1}{\sqrt{2}}\left(|0\rangle + \mathrm{e}^{\mathrm{i}2^j\phi}|1\rangle\right) \otimes |u\rangle$$

Algorithm (I)



$$\Rightarrow \frac{1}{\sqrt{2^n}}\left(|0\rangle + \mathrm{e}^{\mathrm{i}2^{n-1}\phi}|1\rangle\right) \otimes \cdots \otimes \left(|0\rangle + \mathrm{e}^{\mathrm{i}\phi}|1\rangle\right) \otimes |u\rangle = \frac{1}{\sqrt{2^n}}\sum_{k=0}^{2^n-1} \mathrm{e}^{\mathrm{i}k\phi}|k\rangle \otimes |u\rangle$$

Algorithm (II)

- Write ϕ as

$$\phi = 2\pi\left(\frac{a}{2^n} + \delta\right)$$

- First register:

$$\frac{1}{\sqrt{2^n}}\sum_k \mathrm{e}^{\mathrm{i}k\phi}|k\rangle = \frac{1}{\sqrt{2^n}}\sum_k \mathrm{e}^{\frac{2\pi \mathrm{i}ka}{2^n}}\mathrm{e}^{2\pi \mathrm{i}k\delta}|k\rangle$$

- Apply inverse Quantum Fourier transform:

$$\frac{1}{2^n}\sum_x\left(\sum_k \mathrm{e}^{\frac{2\pi \mathrm{i}ka}{2^n}}\mathrm{e}^{2\pi \mathrm{i}k\delta}\right)\mathrm{e}^{\frac{-2\pi \mathrm{i}kx}{2^n}}|x\rangle = \frac{1}{2^n}\sum_x\sum_k \mathrm{e}^{\frac{-2\pi \mathrm{i}k}{2^n}(x-a)}\mathrm{e}^{2\pi \mathrm{i}k\delta}|x\rangle$$

Algorithm (III)

- Perform a *measurement* on the first register:

$$P(a) = \left|\left\langle a\left|\frac{1}{2^n}\sum_x\sum_k \mathrm{e}^{\frac{-2\pi\mathrm{i}k}{2^n}(x-a)}\mathrm{e}^{2\pi\mathrm{i}k\delta}\right|x\right\rangle\right|^2 = \frac{1}{2^{2n}}\left|\sum_k \mathrm{e}^{2\pi\mathrm{i}k\delta}\right|^2$$

$$= \begin{cases} 1, & \delta = 0 \\ \dfrac{1}{2^{2n}}\left|\dfrac{1-\alpha^{2n}}{1-\alpha}\right|^2, & \delta \neq 0 \end{cases}$$

where $\alpha = \mathrm{e}^{2\pi\mathrm{i}\delta}$.

- Note that

$$P(a|\delta \neq 0) = \frac{1}{2^{2n}}\left|\frac{1-\alpha^{2n}}{1-\alpha}\right|^2 \geqslant \frac{4}{\pi^2} \approx 0.4053$$

Eigensystem solving

- $|\psi\rangle$ instead of eigenvector $|u\rangle$:

$$|\psi\rangle \to |\Psi\rangle = \frac{1}{\sqrt{2^n}} \sum_{k=0}^{2^n-1} |k\rangle \otimes U^k|\psi\rangle, \qquad U = \mathrm{e}^{-\frac{\mathrm{i}H\Delta t}{\hbar}}$$

- Expand with eigenvector $|\phi_\alpha\rangle$:

$$|\psi\rangle = \sum_\alpha \lambda_\alpha |\phi_\alpha\rangle, \qquad U\,|\phi_\alpha\rangle = \mathrm{e}^{-\frac{\mathrm{i}\omega_\alpha \Delta t}{\hbar}}\,|\phi_\alpha\rangle$$

- Then

$$|\Psi\rangle = \frac{1}{\sqrt{2^n}} \sum_k |k\rangle \sum_\alpha \lambda_\alpha \mathrm{e}^{-\frac{\mathrm{i}\omega_\alpha k\Delta t}{\hbar}} |\phi_\alpha\rangle$$

- After Fourier transformation: peaks at ω_α

Hamiltonian simulation

- Schrödinger's equation:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\psi(x,t)\rangle = H|\psi(x,t)\rangle$$

with Hamiltonian

$$H = H_0 + V(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial t^2} + V(x)$$

- "Solve" it:

$$|\psi(x,t)\rangle = \mathrm{e}^{-\frac{\mathrm{i}Ht}{\hbar}}|\psi(x,t)\rangle$$

Spatial discretization

- Suppose $-d \leqslant x \leqslant d$:

$$|\psi(x,t)\rangle \approx \left|\tilde{\psi}(t)\right\rangle = \frac{1}{\mathcal{N}} \sum_{i=0}^{2^n-1} \psi(x_i,t)\,|i\rangle$$

where

$$x_i = \left(i + \frac{1}{2}\right)\Delta - d, \qquad \Delta = \frac{2d}{2^n}$$

- A good approximation if $\Delta \ll \xi$

Time integration

- Time-evolution of wave function:

$$|\psi(x, t+\epsilon)\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(H_0+V)\epsilon}|\psi(x,t)\rangle$$

- Trotter decomposition:

$$\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(H_0+V)\epsilon} = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H_0\epsilon}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}V\epsilon} + \mathcal{O}(\epsilon^2)$$

- Note that $[H_0, V] \neq 0$
- Fourier transformation (diagonalization):

$$-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x} = \mathcal{F}^{-1}k\mathcal{F} \Longrightarrow \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\widehat{H}_0\epsilon} = \mathcal{F}^{-1}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\frac{\hbar^2k^2}{2m}\epsilon}\mathcal{F}$$

Time integration (continued)

- Apply l times to get $|\psi(x, t = l\epsilon)\rangle$:

$$\mathcal{F}^{-1} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\frac{\hbar^2 k^2}{2m}\epsilon}\,\mathcal{F}\;\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}V\epsilon}$$

- Summarize: simulation = QFT + diagonal operator $\mathrm{e}^{\mathrm{i}cf(x)}$
- Implementation:

$$\begin{matrix} |0\rangle \\ \otimes \\ |x\rangle \end{matrix} \xrightarrow{f} \begin{matrix} |f(x)\rangle \\ \otimes \\ |x\rangle \end{matrix} \longrightarrow \begin{matrix} \mathrm{e}^{\mathrm{i}cf(x)}|f(x)\rangle \\ \otimes \\ |x\rangle \end{matrix} \xrightarrow{f^{-1}} \begin{matrix} \mathrm{e}^{\mathrm{i}cf(x)}|0\rangle \\ \otimes \\ |x\rangle \end{matrix} = \begin{matrix} |0\rangle \\ \otimes \\ \mathrm{e}^{\mathrm{i}cf(x)}|x\rangle \end{matrix}$$

More details

$$
\begin{matrix} |0\rangle \\ \otimes \\ |x\rangle \end{matrix}
\xrightarrow{f}
\begin{matrix} |f(x)\rangle \\ \otimes \\ |x\rangle \end{matrix}
\longrightarrow
\begin{matrix} \mathrm{e}^{\mathrm{i}cf(x)}|f(x)\rangle \\ \otimes \\ |x\rangle \end{matrix}
\xrightarrow{f^{-1}}
\begin{matrix} \mathrm{e}^{\mathrm{i}cf(x)}|0\rangle \\ \otimes \\ |x\rangle \end{matrix}
=
\begin{matrix} |0\rangle \\ \otimes \\ \mathrm{e}^{\mathrm{i}cf(x)}|x\rangle \end{matrix}
$$

1. Function evaluation: $\mathcal{O}(2^n)$ generalized C^n-NOT gates
   - More efficient for specific structures (e.g. potential V in QM)
2. Perform $|y\rangle \to \mathrm{e}^{\mathrm{i}cy}|y\rangle$ with m single-qubit R_z gates:

$$\exp \mathrm{i}cy = \exp \sum_{j=0}^{m-1} \mathrm{i}cy_j 2^j = \prod_{j=0}^{m-1} \exp\left(\mathrm{i}cy_j 2^j\right)$$

with

$$R_z\left(c2^j\right) = \begin{pmatrix} 1 & \\ & \mathrm{e}^{\mathrm{i}c2^j} \end{pmatrix}$$

Linear system "solving"

- Given a matrix $\boldsymbol{A}$ and a vector $\boldsymbol{b}$, find a vector $\boldsymbol{x}$ such that $\boldsymbol{Ax} = \boldsymbol{b}$
- Instead of $\boldsymbol{x}$ itself, we want to know $\boldsymbol{x}^\dagger \boldsymbol{M} \boldsymbol{x}$
- Runtime: $\mathcal{O}(\kappa^2 \log N)$
- Classical: $\mathcal{O}(\kappa N)$ or $\mathcal{O}(\sqrt{\kappa} N)$ if positive semidefinite
  - Exponentially speed-up!

Reference: A. W. Harrow et. al., *Quantum Algorithm for Linear Systems of Equations*, Phys. Rev. Lett. 103, 150502 (2009)

Basic idea

- Suppose $\boldsymbol{A}$ is Hermitian
- Represent $\boldsymbol{b}$ as:

$$|b\rangle = \sum_i b_i \, |i\rangle$$

- Hamiltonian simulation:
  - Apply $\mathrm{e}^{\mathrm{i}\boldsymbol{A}t}$ to $|b\rangle$
  - Decompose $|b\rangle$ in the eigen-basis of $\boldsymbol{A}$
  - Via quantum phase estimation
- After decomposition:

$$\approx \sum_j \beta_j |u_j\rangle \otimes |\lambda_j\rangle$$

- Linear map (rotation):

$$|\lambda_j\rangle \rightarrow C\lambda_j^{-1}|\lambda_j\rangle$$

- Uncompute $|\lambda_j\rangle$ register, left with a state proportional to

$$\sum_j \beta_j \lambda_j^{-1} |u_j\rangle = A^{-1}|b\rangle = |x\rangle$$

Algorithm (I) – initialization

- $\boldsymbol{A}$ (Hermitian, with s sparse) → unitary operator $\mathrm{e}^{\mathrm{i}\boldsymbol{A}t}$
- Time complexity: $\tilde{O}(s^2 t \log N)$
- If $\boldsymbol{A}$ is not Hermitian?
  - Define

$$\widetilde{\boldsymbol{A}} = \begin{pmatrix} \mathbf{0} & \boldsymbol{A} \\ \boldsymbol{A}^\dagger & \mathbf{0} \end{pmatrix}$$

  - Solve equation

$$\widetilde{\boldsymbol{A}}\boldsymbol{y} = \begin{pmatrix} \boldsymbol{b} \\ \mathbf{0} \end{pmatrix} \implies \boldsymbol{y} = \begin{pmatrix} \mathbf{0} \\ \boldsymbol{x} \end{pmatrix}$$

- An efficient procedure to prepare $|b\rangle$

Algorithm (II) – phase estimation

- State: ancilla $\otimes$ register $\otimes$ memory
- Initial state: $|0\rangle_{\mathrm{A}} \otimes |0\rangle_{\mathrm{R}} \otimes |b\rangle_{\mathrm{M}}$
- Phase estimation:

$$|b\rangle_{\mathrm{M}} = \sum_j \beta_j |u_j\rangle, \qquad A|u_j\rangle = \lambda_j |u_j\rangle$$

- Let

$$|0\rangle_{\mathrm{R}} \to |\Psi_0\rangle_{\mathrm{R}} := \sqrt{\frac{2}{T}} \sum_{\tau=0}^{T-1} \sin \frac{\pi\left(\tau + \frac{1}{2}\right)}{T} |\tau\rangle$$

Algorithm (III) – Hamiltonian evolution

- Apply on $|\Psi_0\rangle_\mathrm{R} \otimes |b\rangle_\mathrm{M}$:

$$\sum_{\tau=0}^{T-1} |\tau\rangle\langle\tau| \otimes \mathrm{e}^{\frac{\mathrm{i}A\tau t_0}{T}}, \qquad t_0 = \mathcal{O}\left(\frac{\kappa}{\epsilon}\right)$$

We have

$$|\Psi_0\rangle_\mathrm{R} \otimes \mathrm{e}^{\frac{\mathrm{i}A\tau t_0}{T}} |b\rangle_\mathrm{M} = \sum_j |\Psi_0\rangle_\mathrm{R} \otimes \beta_j \mathrm{e}^{\frac{\mathrm{i}\lambda_j t_0}{T}\tau} |u_j\rangle_\mathrm{M}$$

- Perform Fourier transformation:

$$\sum_j \sum_k \alpha_{k|j}\beta_j |k\rangle_\mathrm{R} \otimes |u_j\rangle_\mathrm{M} \sim \sum_j \sum_k \alpha_{k|j}\beta_j |\tilde{\lambda}_k\rangle_\mathrm{R} \otimes |u_j\rangle_\mathrm{M}$$

Algorithm (IV) – controlled rotation

- Apply controlled-$R(\lambda^{-1})$ on

$$\sum_j \sum_k |0\rangle_{\mathrm{A}} \otimes \alpha_{k|j}\beta_j \left|\tilde{\lambda}_k\right\rangle_{\mathrm{R}} \otimes \left|u_j\right\rangle_{\mathrm{M}}$$

We have

$$\sum_j \sum_k \alpha_{k|j}\beta_j \left(\sqrt{1 - \frac{C^2}{\tilde{\lambda}_k^2}} |0\rangle_{\mathrm{A}} + \frac{C}{\tilde{\lambda}_k} |1\rangle_{\mathrm{A}} \right) \otimes \left|\tilde{\lambda}_k\right\rangle_{\mathrm{R}} \otimes \left|u_j\right\rangle_{\mathrm{M}}$$

- Reverse/undo step (II), (III):

$$\left|\tilde{\lambda}_k\right\rangle_{\mathrm{R}} \rightarrow |0\rangle_{\mathrm{R}}$$

Algorithm (V) – measurement

- Assume perfect phase estimation

$$\alpha_{k|j} = \begin{cases} 1, & \tilde{\lambda}_k = \lambda_j; \\ 0, & \text{otherwise.} \end{cases}$$

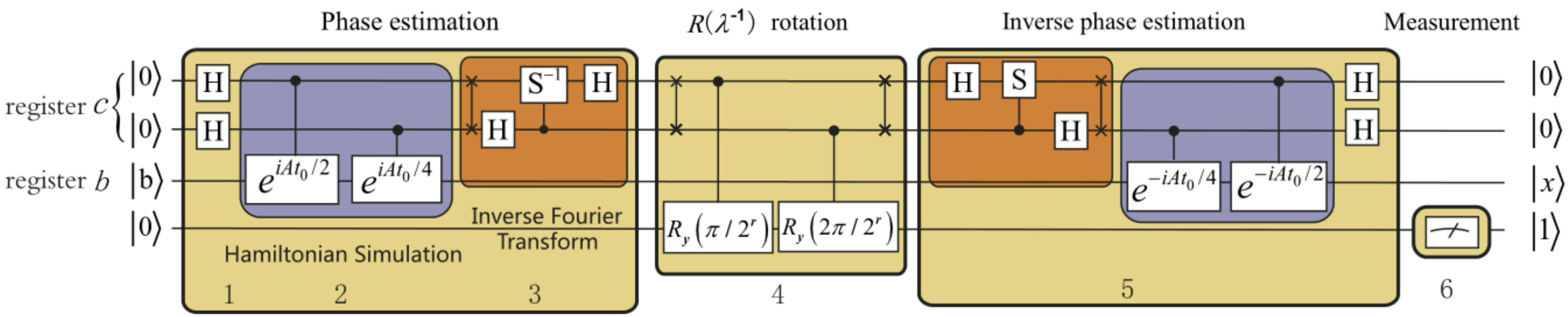
Then

$$\sum_j \beta_j \left(\sqrt{1 - \frac{C^2}{\lambda_k^2}} |0\rangle_{\mathrm{A}} + \frac{C}{\lambda_j} |1\rangle_{\mathrm{A}} \right) \otimes |0\rangle_{\mathrm{R}} \otimes |u_j\rangle_{\mathrm{M}}$$

- Measure on ancilla to get $|1\rangle_{\mathrm{A}}$:

$$\sim \sum_j C \beta_j \lambda_j^{-1} |u_j\rangle \propto |x\rangle$$

Algorithm summary & complexity

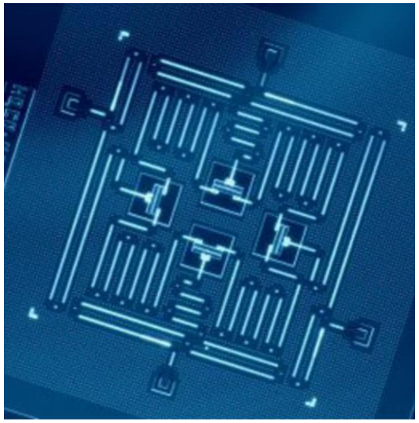


- Phase estimation: $\tilde{\mathcal{O}}(ts^2)$
- Fourier transformation: $\mathcal{O}(\log N)$
- Total: $\tilde{\mathcal{O}}(s^2\kappa^2 \log N/\epsilon)$

Figure from: J. Pan et. al., *Experimental realization of quantum algorithm for solving linear systems of equations*, Phys. Rev. A **89**, 022313 (2014)

Experimental realization*

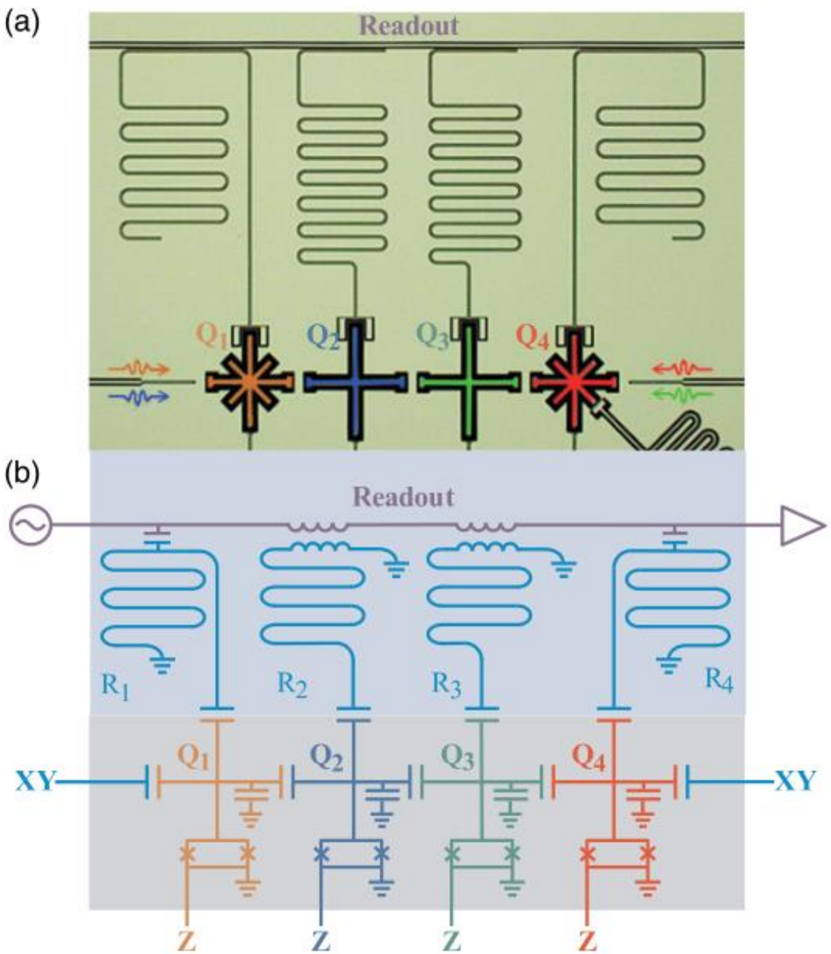
- Superconducting quantum processor
- A quantum linear solver for 2×2 system
- "Four transmon qubits of the Xmon variety"
    - Charge qubit: basis states are charge states
    - Superconducting island + Josephson junction
    - Transmon (2007): "to decrease the sensitivity to charge noise"
    - Xmon (2013): "combines facile fabrication, straightforward connectivity, fast control, and long coherence"



4Q/4B/4R by IBM

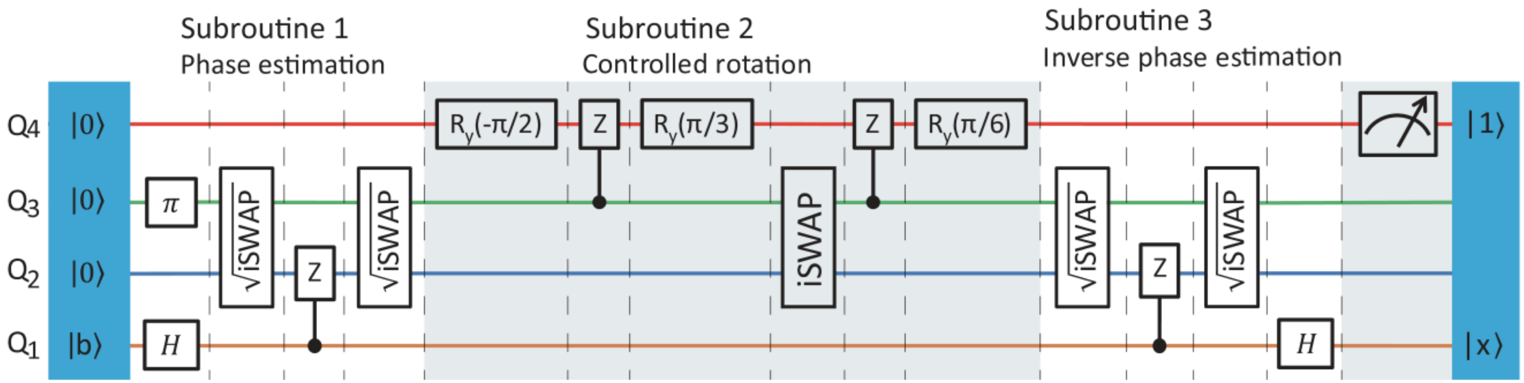
Reference: Y. Zheng et. al., *Solving Systems of Linear Equations with a Superconducting Quantum Processor*, Phys. Rev. Lett. **118**, 210504 (2017)
Figure from: https://www.nature.com/articles/s41534-016-0004-0

Device



- Q_1 to Q_4: four Xmon qubits
- Z: frequency-control line
  - For rotations of the qubit state around the Z axis
- XY: microwave line
  - For single-qubit rotations around X and Y axes
- R_1 to R_4: readout resonators
  - Couple to a common transmission line
  - Enable simultaneous single-shot quantum nondemolition measurement

Circuit



- System matrix $\boldsymbol{A}$:

$$A = \begin{pmatrix} 1.5 & 0.5 \\ 0.5 & 1.5 \end{pmatrix}, \qquad \lambda_1 = 1, \lambda_2 = 2$$

- Can be optimized
- Q_4: ancilla, Q_2Q_3: register, Q_1: memory
- 18 input states in $|b_j\rangle$ on Bloch sphere

Results

- Apply σ_i on $|x\rangle$ (with $|b\rangle = |0\rangle$):

$$\left\{-\frac{3}{8}, 0, \frac{1}{2}\right\}$$

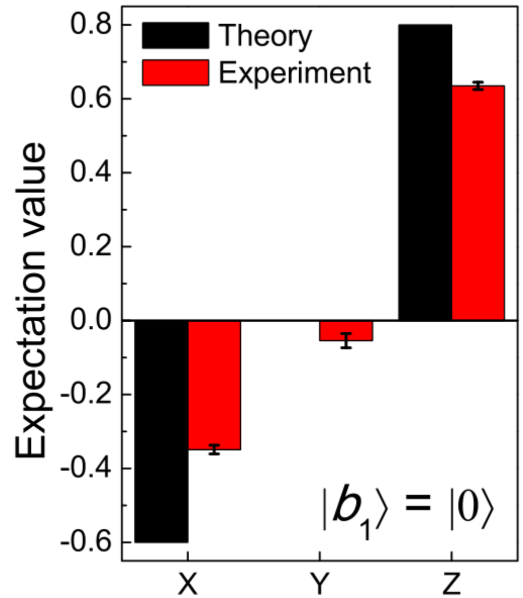
- Output state fidelities:

$$0.840 \pm 0.006 \sim 0.923 \pm 0.008$$

- Quantum process fidelity:

$$0.837 \pm 0.006$$

- Sources of errors:
  - Decoherence
  - Insufficient grounding



Are the expectation values incorrect?

Questions?