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A Quantum-Walk-Unitary HHL Matrix Equation Solver and Its Challenges in the NISQ Era

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Outline

I. Motivation
II. The HHL algorithm
III. The QWU-HHL algorithm
IV. The challenge in the NISQ era

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I. Motivation

- Why do we want to leverage the power of quantum computers?
  - Computational electromagnetic answer the quest of electromagnetic simulation for complex geometries
  - A main contributor to the simulation time: Solving large matrix equations with N unknowns
  - Differential-equation-based methods: Sparse matrix equations

    Conjugate Gradient Method: $O(N)$
  - Moment Method: Dense matrix equations

    Fast Algorithms: $O(N\log N)$
- The HHL quantum matrix equation solver: $O(\log N)$

Outline

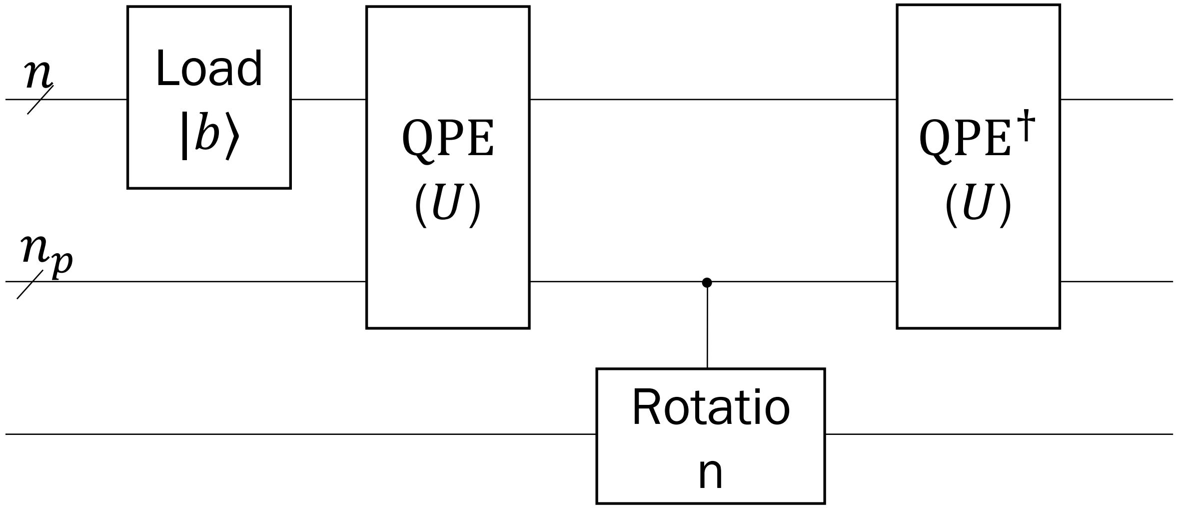
II. The HHL Algorithm

- Name comes from the acronym of its authors: [Harrow, Hassidim, Llyod, 2009, https://arxiv.org/abs/0811.3171]
- Problem Statement: Given a Hermitian matrix A and a normalized right-hand-side vector $|b\rangle$, *prepare* a quantum state $|x\rangle$ (up to a normalization factor) such that $A|x\rangle = |b\rangle$

- Complexity: $O(\log(N)\, s^2\kappa^2/\epsilon)$
  - N: matrix dimension
  - s: the number of nonzero elements per row/column
  - ϵ: desired accuracy

Registers

IO/Input register	I
Clock/Phase register	C
Ancilla	A

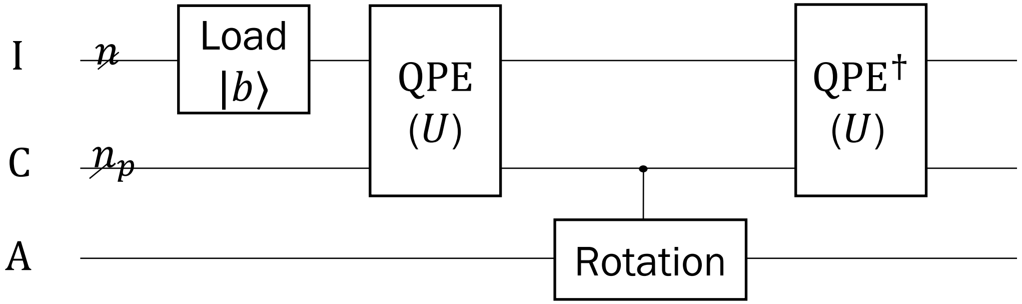


II. The HHL Algorithm: Insights

- Quantum supremacy

Quantum superposition allows n qubits to represent 2^n numbers, which needs 2^n classical bits to represent

- The idea of HHL

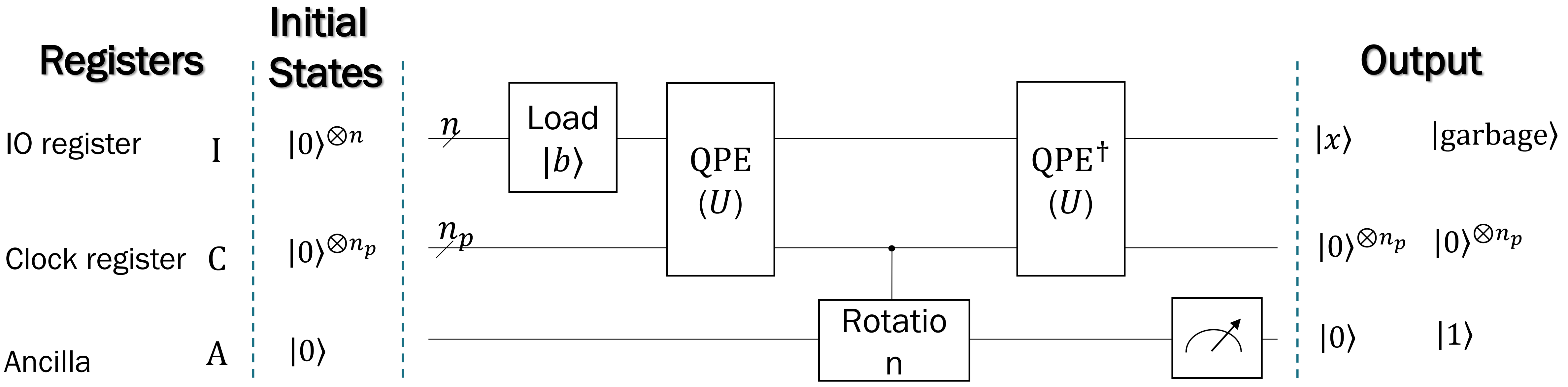


Solve the matrix equation via eigendecomposition:

There are methods to find (QPE) and invert (controlled rotation) the eigenvalues quantum mechanically

- The Quantum Phase Estimation (QPE) is the core of the HHL algorithm, and is the erroneous step in the HHL algorithm
  - The unitary U is implemented as $U = e^{iAt}$ via Hamiltonian simulation in classical HHL
  - The number of qubits n_p is chosen according to the required accuracy $\epsilon_{QPE} = 2^{-m}$ and success probability p: $n_p = m + \lceil \log(2 + 1/2p) \rceil$ [Nielsen, Chuang, 2010]
- The controlled rotation is a simplified block of "do something to the eigenvalue", i.e., $f(\lambda)$ can be implemented for other algorithm and HHL chooses $f(\lambda) = 1/\lambda$ [Harrow, Hassidim, Llyod, 2009]

II. The HHL Algorithm



- The desired output $|x\rangle$ is distinguished from the $|\text{garbage}\rangle$ via the state of the ancilla.
- The output is stored as a quantum state. If one needs classical information for post-processing, one can only retrieve that as the expectation of a measurement operator $\langle x|M|x\rangle$, where M is the measurement operator.
- The unitary U is a choice up to the user. The eigenvalues and eigenvectors of U and the Hermitian matrix A need to be closely related so that the eigendecomposition can be achieved quantum mechanically.

II. The HHL Algorithm-Improvements

- Most HHL improvements the result (achieving better complexity) or removes the requirements [Dervovic et al, 2018, https://arxiv.org/abs/1802.08227]
  - Reduce the complexity dependence on the condition number from κ^2 to $\kappa \log^3 \kappa$ [Ambainis, https://arxiv.org/abs/1010.4458]
  - Reduce the complexity dependence on the precision from $\mathrm{ploy}(1/\epsilon)$ to $\mathrm{ploy}\log(1/\epsilon)$ [Childs et al, 2017, https://doi.org/10.1137/16M1087072]
  - Removes the requirement on the sparsity of the Hamiltonian matrix A [Wossnig et al, 2018, https://doi.org/10.1103/PhysRevLett.120.050502]
- Most improvements leaves the unitary U in the QPE untouched, with the necessity of Hamiltonian simulation
- Hamiltonian simulations are not trivial, and if we do not need it explicitly, can we remove it in the HHL process?

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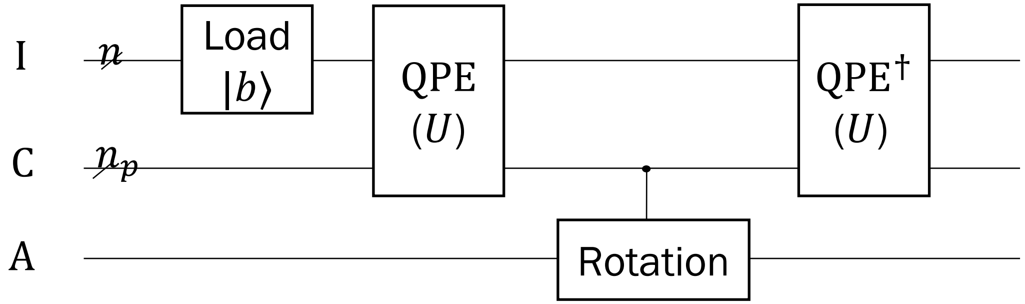
III. The QWU-HHL Algorithm

- The Hamiltonian simulation is not a necessary explicit step
  - The whole QPE block is for the purpose of estimating the eigenvalues of A
  - The Hamiltonian simulation (implementation of $U = e^{iAt}$) is needed because the eigenvalue and eigenvector relationship between e^{iAt} and A is straightforward

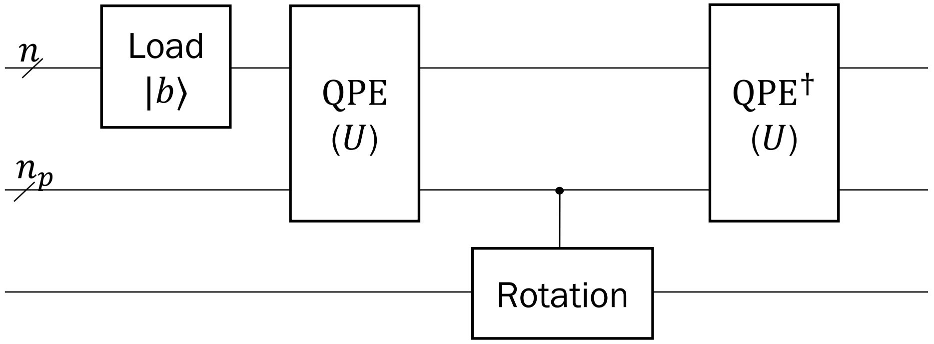


Operator	Eigenvector	Eigenvalue
A	$\|u\rangle$	λ
$U = e^{iAt}$	$\|u\rangle$	$e^{i2\pi\tilde{\theta}} = e^{i\lambda t}$

- Popular Hamiltonian simulation methods include
  - Decomposition of the Hamiltonian [Low et al, 2023, https://arxiv.org/abs/2211.09133v2]: difficult to apply to a general Hamiltonian
  - Quantum-walk-based methods [Berry, Childs 2012, https://arxiv.org/abs/0910.4157v4]

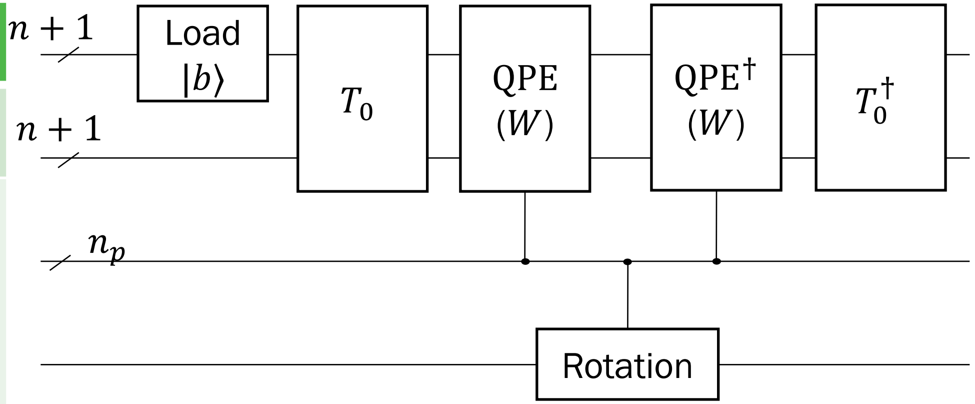
III. The QWU-HHL Algorithm

- Inspired by the quantum-walk-based Hamiltonian simulation, we use the quantum walk operator W as the unitary
  - $W \triangleq iS(2TT^\dagger - I)$
  - $T \triangleq \sum_{j=1}^{N} |j\rangle|\phi_j\rangle\langle j|$
  - $S \triangleq \sum_{j=1}^{N} \sum_{k=0}^{N-1} |k\rangle|j\rangle\langle j|\langle k|$



Classical HHL

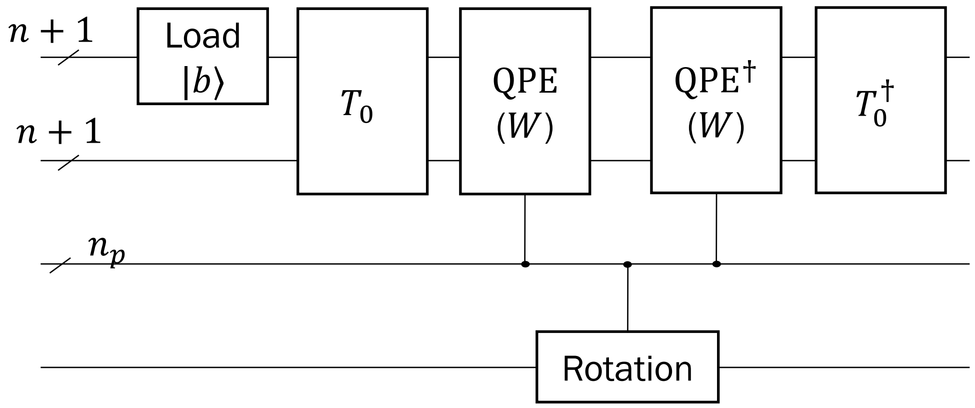
Operator	Eigenvector	Eigenvalue
A	$\|u_j\rangle$	λ_j
W	$\|v_j^{\pm}\rangle = \frac{1 + i\mu_j^{\pm} S}{\sqrt{2(1-\hat{\lambda}_j^2)}} T\|u_j\rangle$	$\mu_j^{\pm} = i\hat{\lambda}_j \pm \sqrt{1-\hat{\lambda}_j^2}$ where $\hat{\lambda}_j = \frac{\lambda_j}{X}$, $X \triangleq \max_{j,k}\|H_{jk}\|$



QWU-HHL

III. The QWU-HHL Algorithm

- In the definition,
  - $W \triangleq iS\left(2TT^{\dagger} - I\right)$
  - $T \triangleq \sum_{j=1}^{N} |j\rangle|\phi_j\rangle\langle j|$
  - $S \triangleq \sum_{j=1}^{N} \sum_{k=0}^{N-1} |k\rangle|j\rangle\langle j|\langle k|$
- T is the mapping from $\mathbb{C}^N$ to $\mathbb{C}^N \otimes \mathbb{C}^N$ as the eigenvector of W lives in the latter
- S is the swapping operator



QWU-HHL

- T translates the initial state of the system (the RHS state) into the eigenbasis of W

$$T|b\rangle = T\sum_{j=1}^{N} \beta_j |u_j\rangle = \sum_{j=1}^{N} \frac{\beta_j}{\sqrt{2\left(1-\hat{\lambda}_j^2\right)}}\left[\left(1+i\hat{\lambda}_j\mu_j^-\right)|v_j^+\rangle + \left(1+i\hat{\lambda}_j\mu_j^+\right)|v_j^-\rangle\right]$$

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IV. The NISQ hardware

- Logical qubits vs physical qubits
  - A logical qubit is a qubit used for programming
    - Typically made out of a collection of physical qubits
    - All qubits referred so far are logical qubits
  - A physical qubit is a quantum realization of a qubit. Physical qubits suffer from decoherence.
- Quantum errors [Devitt et al, https://arxiv.org/abs/0905.2794]
  - Coherent errors: undesired gates applied to the system
  - Environmental decoherence: qubits losing information due to interaction with the environment
  - Measurement, etc.

Proof-of-concept qubits	Potential applications
A few logical qubits	• Quantum Secret Sharing • Quantum Co-processor
~50 logical qubits	• Demonstration of Quantum supremacy
~150 logical qubits	• Quantum Chemistry • Machine Learning
$\sim 10^6$ logical qubits	A full fault-tolerant quantum computer

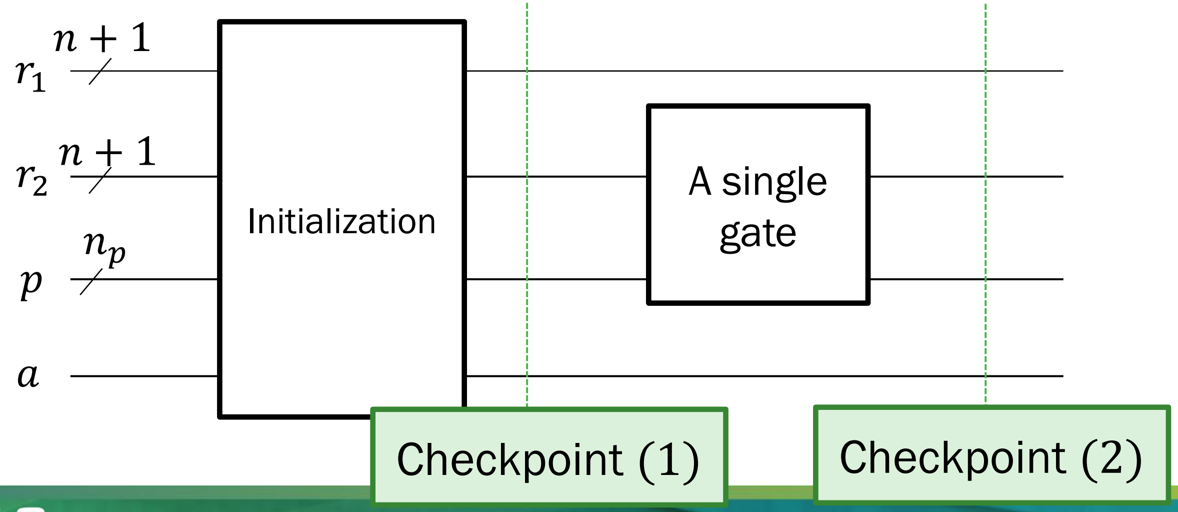
[Fruchtman, Choi, 2016, Technical Roadmap for Fault-Tolerant Quantum Computing]

IV. The NISQ hardware

- Today's available quantum hardware is Noisy Intermediate-Scale Quantum (NISQ) hardware [Preskill, 2018, https://arxiv.org/abs/1801.00862]
- The ultimate goal: Fault-tolerant quantum computer
  - low-error logical qubits: Google has demonstrated quantum error correction works in practice: increasing the number of physical qubits in a logical qubit yield a better logical qubit [Google Quantum AI, 2023, https://doi.org/10.1038/s41586-022-05434-1]
  - Many of these qubits: IBM endeavors to make large-scale quantum computers by multi-chip quantum processors with chip-to-chip couplers [IBM development roadmap, IBM Quantum Computing | Roadmap]

IV. QWU-HHL on NISQ Hardware

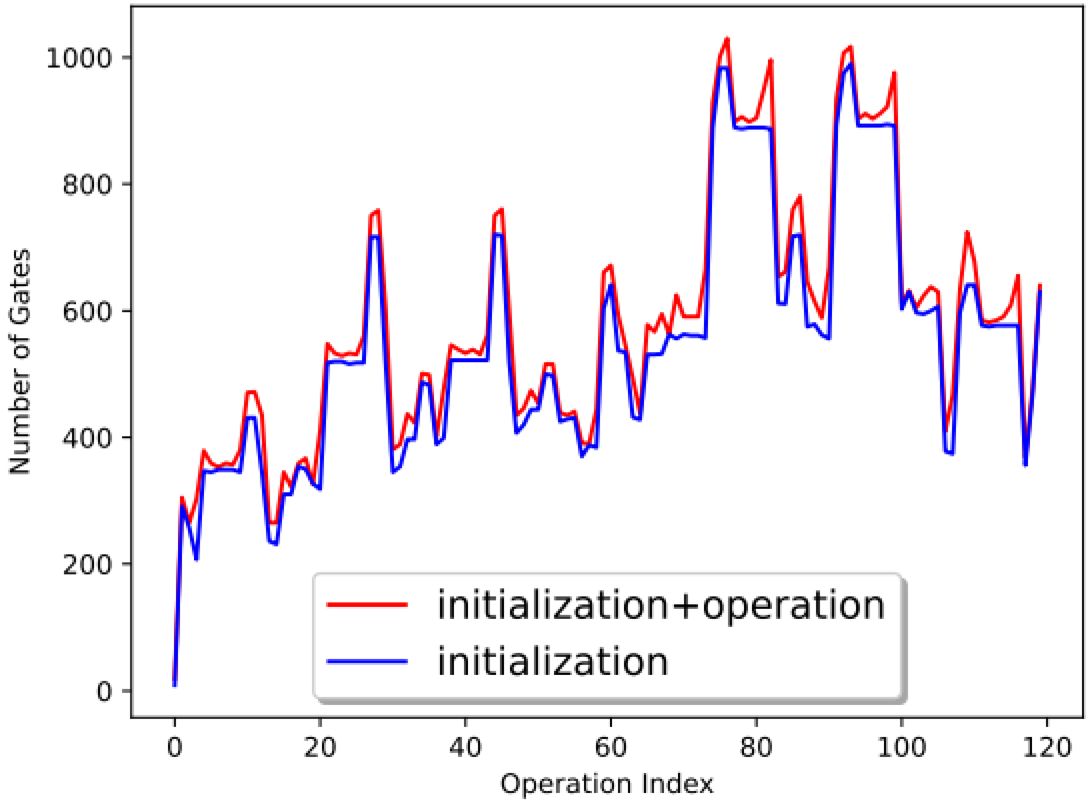
- Unfortunately, Quantum Phase Estimation is not applicable in NISQ hardware
  - IBM Jakarta processor: Median CNOT error = 8.193×10^{-3} (from IBM Lab)
  - 100 CNOT operations in sequence will cause the accuracy to drop below 50%
  - The HHL algorithm requires (tens of) thousands of gates, far beyond the capability of current hardware
- If the whole HHL circuit is too deep, what if we apply only one operation at a time?

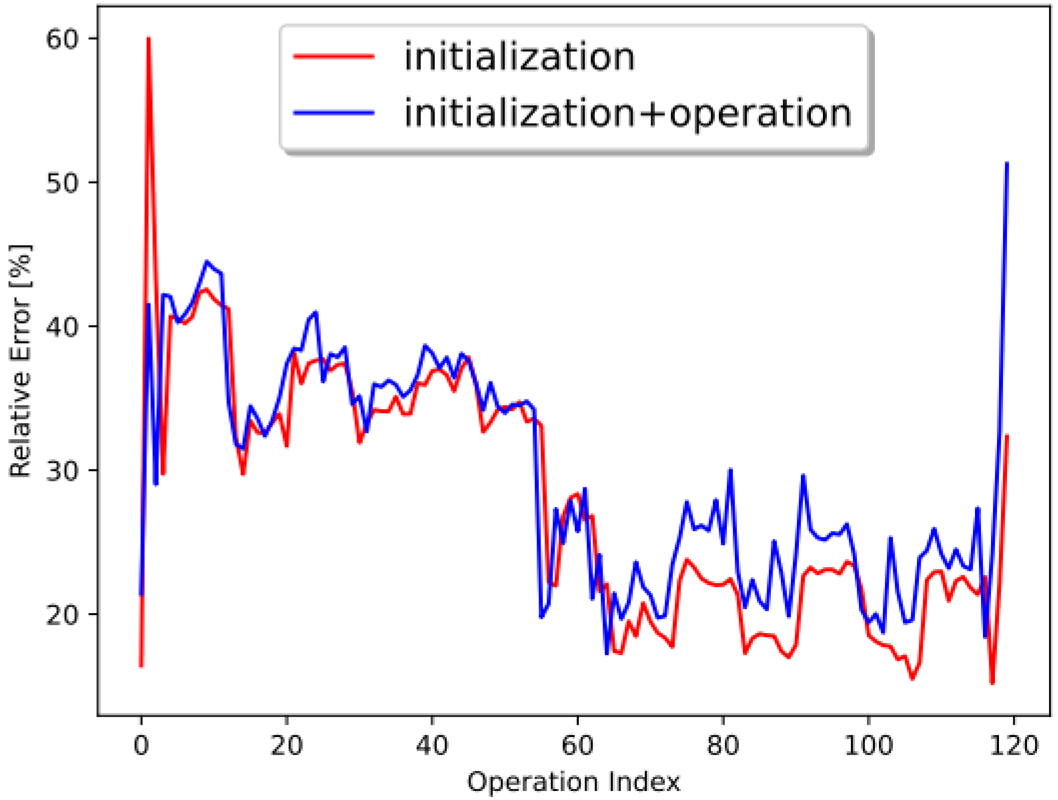


IV. QWU-HHL on NISQ Hardware

- We use an elementary 2×2 matrix equation as an example
  - $A = \begin{bmatrix} -2 & 1 \\ 1 & -2 \end{bmatrix}, |b\rangle = |1\rangle$ as the equal superposition of the eigenvector
  - 7-qubit IBM Jakarta, 1 qubit for all registers except the clock register, which have 2 qubits
  - Eigenphases of W: 0.00, 0.01(repeated twice), 0.10. Exactly representable using 2 qubits
  - 120 fundamental gates in the entire QWU-HHL circuit
- We execute 120 circuits and record the results at the two checkpoints using both an ideal simulator and Jakarta
- On Jakarta, the subcircuit is decomposed into 6 basis gates CX, I, Rz, $\sqrt{X}$, X, and if-else

IV. QWU-HHL on NISQ Hardware





- The final vector is less than 50% accurate
- The initialization is the main error source in the subcircuit
- The re-initialization and division routine is not effective with Qiskit's default initialization functionality

Summary and Future Work

- The QWU-HHL is an improvement to the classical HHL which removes the necessity of Hamiltonian simulation by choosing the quantum walk unitary
- The implementation of HHL is not meaningful in current noisy hardware
- The re-initialization and division routine is not effective with Qiskit's default initialization functionality, more sophisticated initialization schemes need to be investigated
- NISQ-specific HHL [Yalovetzky et al, 2021, https://arxiv.org/abs/2110.15958] is worth studying for deploying HHL to hybrid quantum-classical systems