Leibniz Supercomputing Centre
of the Bavarian Academy of Sciences and Humanities

The Quantum Fourier Transform

From Mathematical Formulation to Quantum Circuits

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Introduction

Why the QFT in CUDA-Q?

- **The Quantum Fourier Transform is a core building block in several applications:** Shor's Algorithm, Phase Estimation (QPE), and HHL.

https://quantumalgorithmzoo.org

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- **Bridging Theory and Code:** Moving from the discrete math of state vectors to optimized CUDA-Q kernels.

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- **Performance at Scale:** Why SDK choice matters—leveraging CPU/GPU backends for simulation and execution.

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- **Bridging Theory and Code:** Moving from the discrete math of state vectors to optimized CUDA-Q kernels.
- **Performance at Scale:** Why SDK choice matters—leveraging CPU/GPU backends for simulation and execution.
- **Learning by Doing:** Mastering CUDA-Q Python API through modular circuit design.

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Roadmap of this section

📚 Quantum Circuit, Basis and Binary Number System

Quantum Fourier Transform

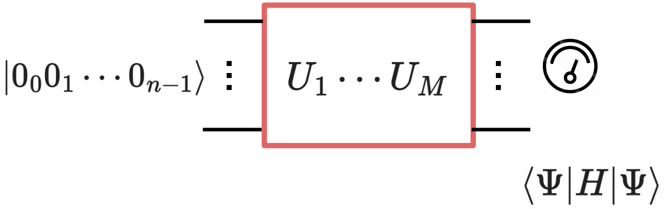
Quantum Phase Estimation

Implementations in CUDA-Q

Quantum Circuit Model

State Preparation and Measurements

Complexity of quantum algorithms



Simulation of circuits is difficult

$$|\Psi\rangle = \sum_{j_0 \cdots j_{n-1}} \underbrace{a_{j_0 \cdots j_{n-1}}}_{2^n} |j_0 j_1 \cdots j_{n-1}\rangle$$

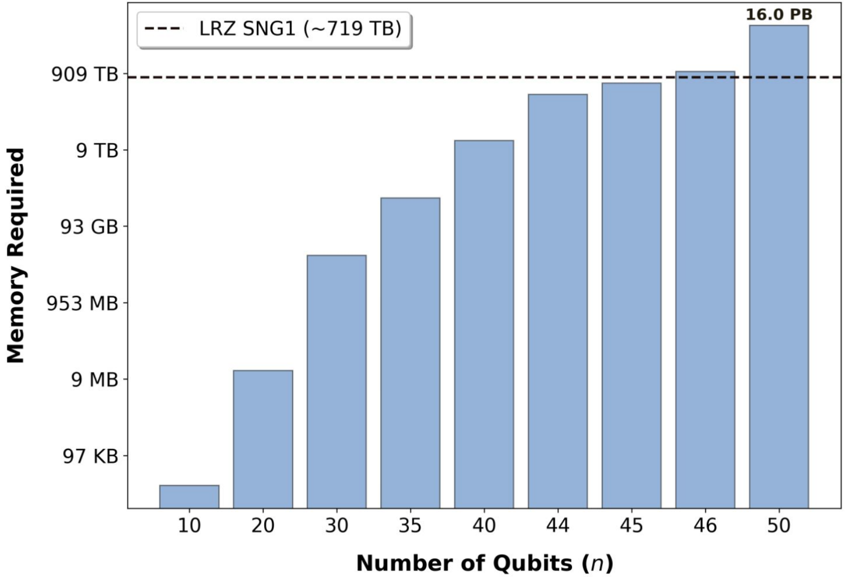


Fig. Memory required for state vector simulations of quantum circuits.

Computational Basis Representation

Basis and Binary Numbers

$$|\Psi\rangle = \sum_{j_0\cdots j_{n-1}} a_{j_0\cdots j_{n-1}} |j_0 j_1 \cdots j_{n-1}\rangle$$

Binary to decimal conversion:

$$j = j_0 2^{n-1} + j_1 2^{n-2} + \cdots j_{n-1} 2^0$$

$$|\Psi\rangle = \sum_{j=0}^{N-1} a_j |j\rangle$$

Example

Bell State

order-2 tensor

$$|\Psi\rangle = a_{00}|00\rangle + a_{11}|11\rangle$$

vector representation

$$|\Psi\rangle = a_0|0\rangle + a_3|3\rangle$$

Binary to decimal conversion:

$$1 \cdot 2^1 + 1 \cdot 2^0 = 3$$

$$0 \cdot 2^1 + 0 \cdot 2^0 = 0$$

Computational Basis Representation

Basis and Binary Numbers

$$|\Psi\rangle = \sum_{j_0 \cdots j_{n-1}} a_{j_0 \cdots j_{n-1}} |j_0 j_1 \cdots j_{n-1}\rangle$$

Elements of the computational basis can also represent *fractional values*

$$0.j_0 j_1 \cdots j_{n-1} = \frac{j_0}{2} + \frac{j_1}{4} + \cdots \frac{j_{n-1}}{2^n}$$

simplified notation of a fraction

Example

Transform the bits of a computational basis formed by 3 qubits to a fraction:

$$|010\rangle \longrightarrow 0.010 \equiv \frac{0}{2} + \frac{1}{4} + \frac{0}{8} = 0.25$$

😇 don't panic now if you see this

$$\exp(2\pi\, 0.j_0\, j_1\, j_2) \equiv \exp(2\pi\, \theta)$$

Mathematical Definition of the QFT

Action of QFT on Basis States

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

💡 Because the QFT is linear, knowing how the basis transforms tells us how any general function transforms.

Mathematical Definition of the QFT

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Transformation of the expansion coefficients

$$\begin{cases} [0, \cdots, 1, \cdots, 0] \rightarrow [y_0, y_1, \cdots, y_{N-1}] \\ y_k = \frac{1}{\sqrt{N}} e^{2\pi ijk/N} \end{cases}$$

💡 Coefficients transform similarly to the classical Discrete Fourier Transform

Mathematical Definition of the QFT

Action of QFT on Basis States

QFT on a basis results in tensor product of qubit states. Here binary fractions are formed from the bits associated to the transformed computational basis | j ⟩.

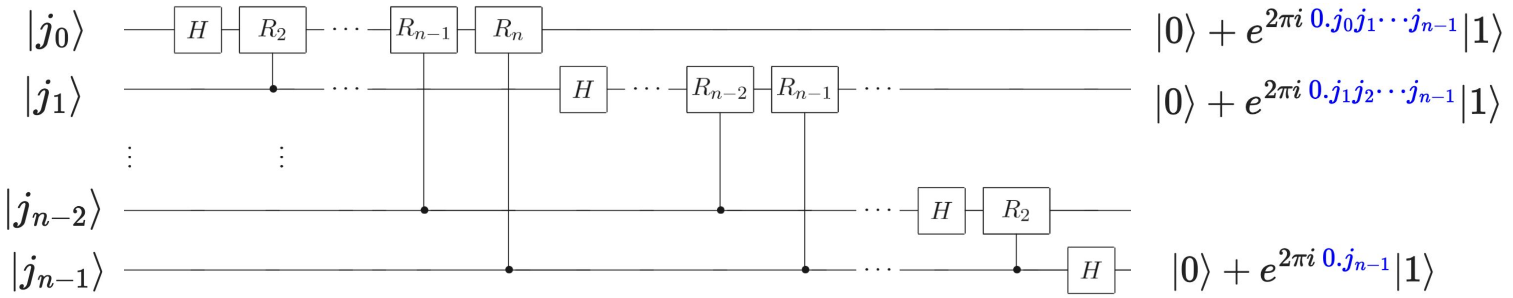
$$|j\rangle \longrightarrow \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{2\pi i jk/N} |k\rangle$$

$$\longrightarrow 1/\sqrt{N}\ \underbrace{\left(|0\rangle + e^{2\pi i\, 0.j_0 j_1 \cdots j_{n-1}}|1\rangle\right)}_{\text{qubit 0}} \underbrace{\left(|0\rangle + e^{2\pi i\, 0.j_1 j_2 \cdots j_{n-1}}|1\rangle\right)}_{\text{qubit 1}} \cdots \underbrace{\left(|0\rangle + e^{2\pi i\, 0.j_{n-1}}|1\rangle\right)}_{\text{qubit (n-1)}}$$

Nielsen & Chuang, *Quantum Comp. & Quantum Info.* (2010)

Mathematical Definition of the QFT

Circuit for the Quantum Fourier Transform



$$H = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

Hadamard gate
(denoted h in CUDA-Q)

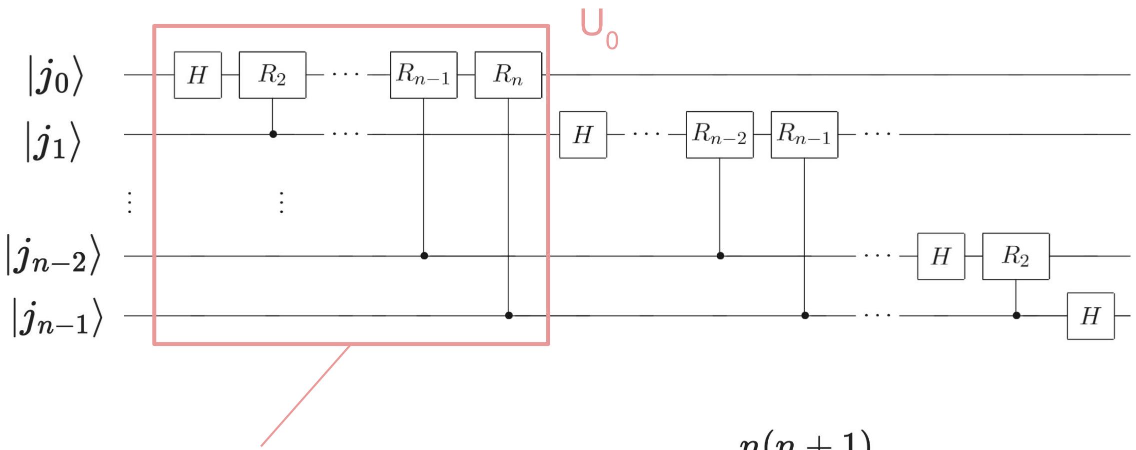
$$R_k \equiv \begin{bmatrix} 1 & 0 \\ 0 & e^{2\pi i/2^k} \end{bmatrix}$$

Single qubit phase shift
(denoted r1 in CUDA-Q)

Operations used in the circuit

Mathematical Definition of the QFT

Complexity Analysis of the Quantum Fourier Transform

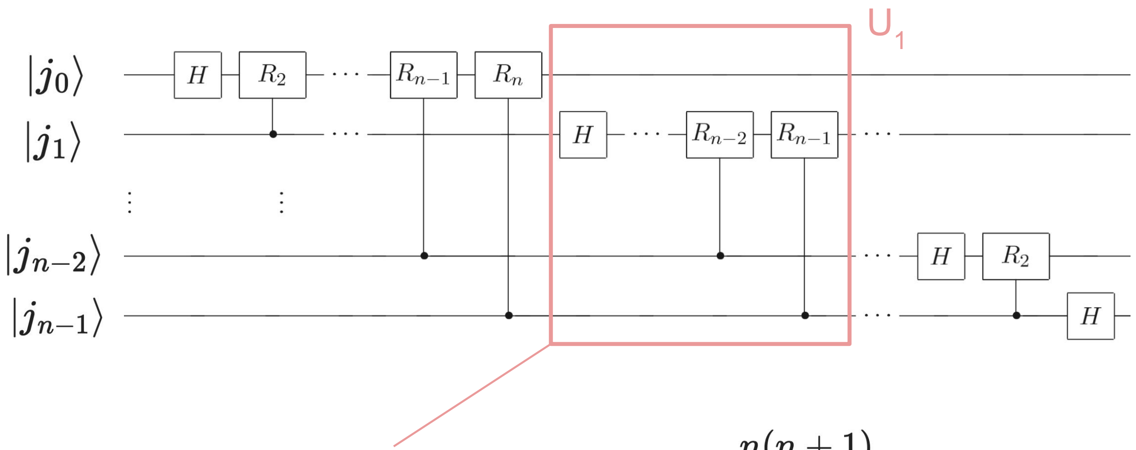


Gate count: $n + (n-1) + (n-2) + \cdots 1 = \dfrac{n(n+1)}{2}$

Complexity: $O(n^2)$

Mathematical Definition of the QFT

Complexity Analysis of the Quantum Fourier Transform



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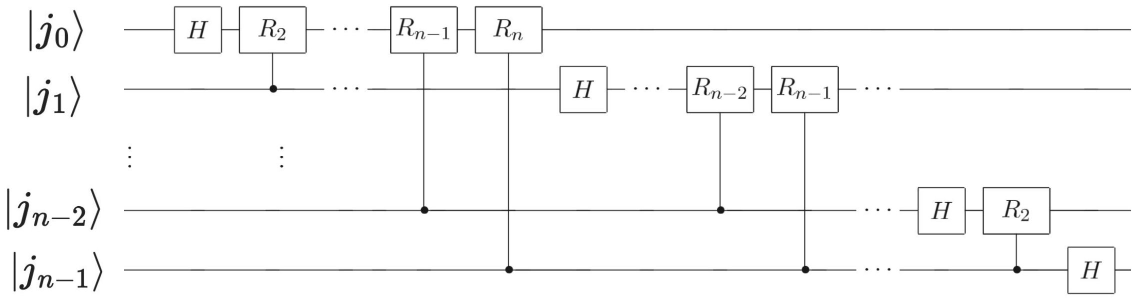

Gate count: $n + (n-1) + (n-2) + \cdots 1 = \frac{n(n+1)}{2}$

$U_{n-1} \cdots U_0$

Complexity: $O(n^2)$

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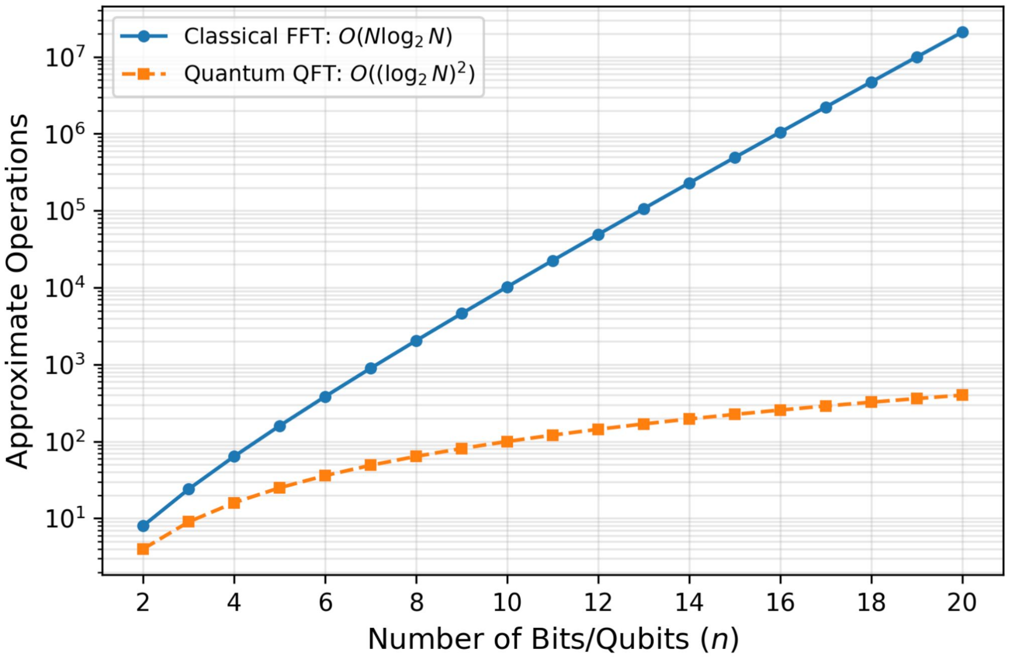
Complexity Analysis of the Quantum Fourier Transform



💡 We have not included sample complexity. What if we use an algorithm that ideally does not requires too many samples?

Fig. Scaling Comparison: Classical FFT vs. Quantum QFT

Applications of QFT

The Quantum Phase Estimation

The Quantum Phase Estimation

Statement of the Problem

Given *U* and one of its eigenstates:

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

goal: compute the phase

$$\phi = 0.j_0\,j_1\ \cdots\ j_{t-1}$$

$$|\phi\rangle \equiv |j\rangle = |j_0 j_i \cdots j_{n-1}\rangle$$

💡 the **basis** that provides the best n-bit approximation of the phase.

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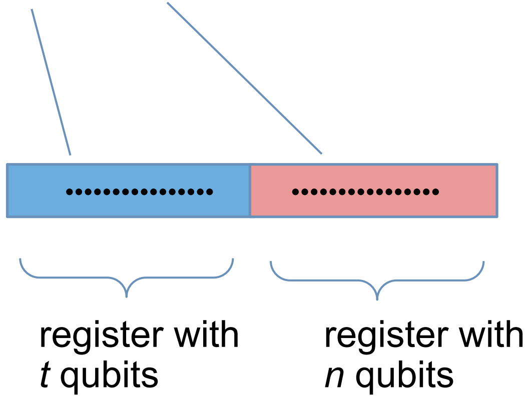
QPE works with 2 registers in the circuit

$$|0\rangle \otimes |u\rangle \longrightarrow |\phi\rangle \otimes |u\rangle$$

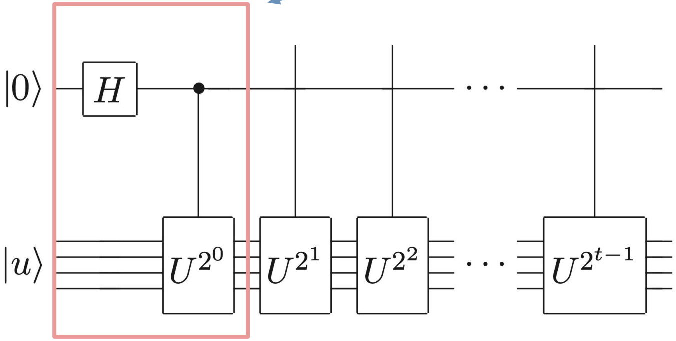


The Quantum Phase Estimation (QPE)

Circuit for the Quantum Phase Estimation

$$CU\left(H|0\rangle \otimes |u\rangle\right) = CU\left[\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |u\rangle\right]$$

$$= \frac{1}{\sqrt{2}}\left(|0\rangle + e^{2\pi i\phi}|1\rangle\right) \otimes |u\rangle$$



💡 this *phase kickback* operation effectively transfers the phase from the second register to the first register.

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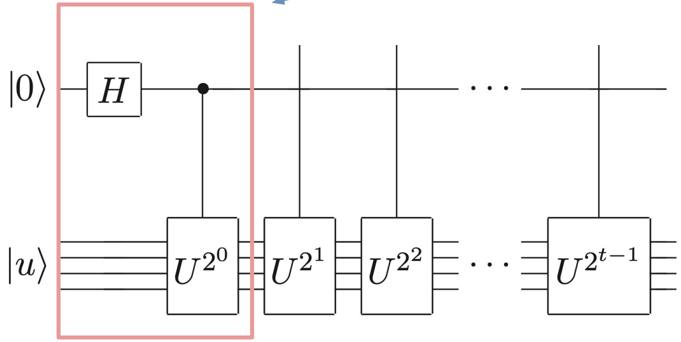

$$|0\rangle + e^{2\pi i\, 0.j_0 j_1 \cdots j_{t-1}}|1\rangle$$

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$$|j\rangle \equiv |\phi\rangle = |j_0\, j_1\, \cdots\, j_{t-1}\rangle$$

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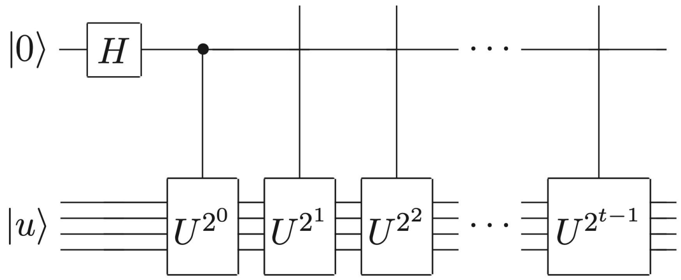

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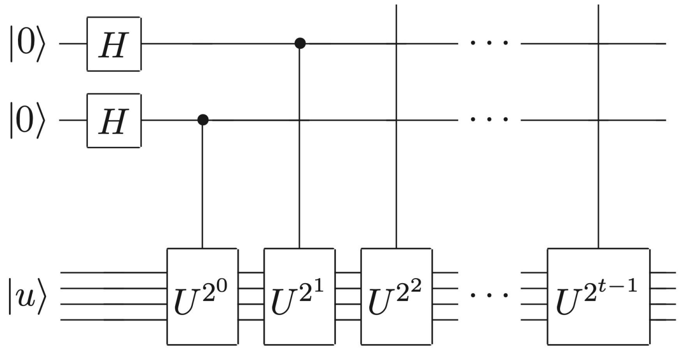

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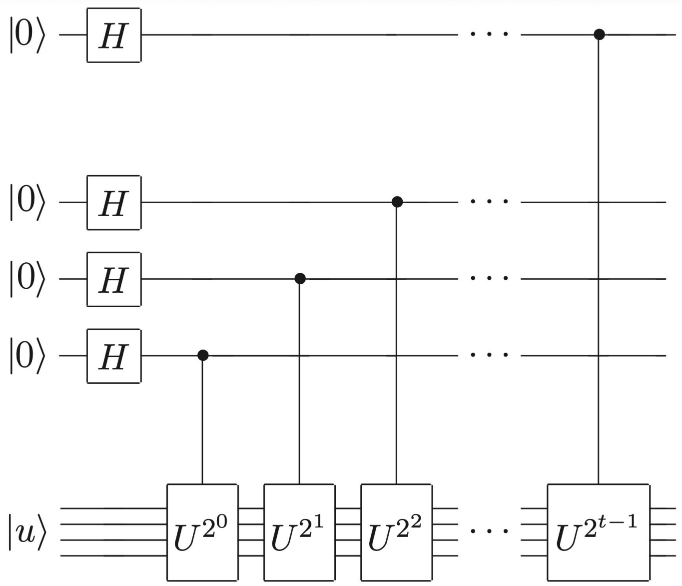

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💡 This is the quantum fourier transform of *j* - the basis that describes the phase.

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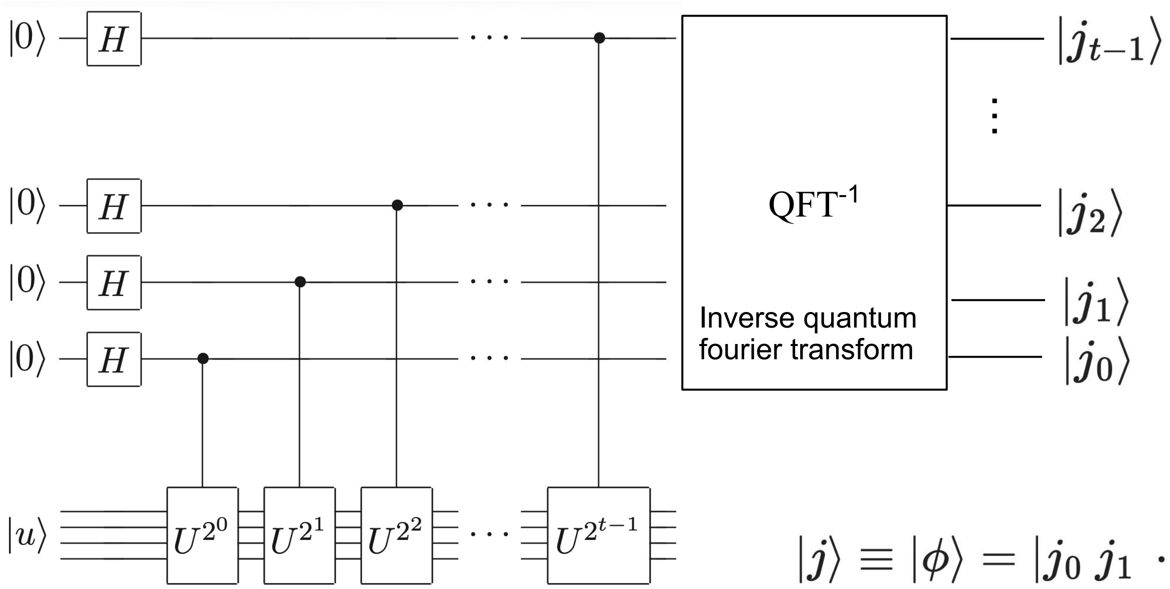
The Quantum Phase Estimation (QPE)

Circuit for the Quantum Phase Estimation



💡 Measurements should indicate the basis *j* as the most probably outcome.

$$|j\rangle \equiv |\phi\rangle = |j_0\, j_1\, \cdots\, j_{t-1}\rangle$$

The Quantum Phase Estimation (QPE)

The QPE in Action: Sampling Eigenvalues

$$e^{-iHt}|\Phi_n\rangle = e^{-i\epsilon_n t}|\Phi_n\rangle = e^{2\pi i\phi_n}|\Phi_n\rangle$$

Imagine that we want the ground state eigenvalue of a Hamiltonian (*H*).

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And that we have a method to construct a “good” Ansatz - overlap with the ground state.

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$$\mathbf{QFE} \cdot |0\rangle \otimes |\tilde{\Psi}\rangle = \sum_m a_m|\phi_m\rangle \otimes |\Phi_m\rangle$$

Imagine that we want the ground state eigenvalue of a Hamiltonian (*H*).

And that we have a method to construct a “good” Ansatz - overlap with the ground state.

💡 QPE will “sample” with some probability the ground states phase associated with the eigenvalue!

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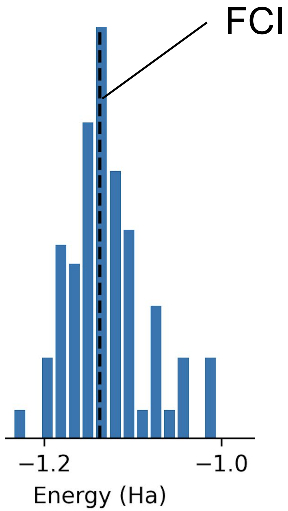

Fig. Sampling the ground state energy of the H2 molecule using STO-3G basis.

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Summary

- **Foundations:** Reviewing quantum circuits, basis states, and binary mapping.
- **The QFT:** Exploring the mechanics of the Quantum Fourier Transform.
- **Applications:** Leveraging the QFT for Quantum Phase Estimation (QPE).

👩🏻‍💻 Now let’s move from theory to implementation with CUDA-Q!