INTRODUCTION TO GATE-BASED QUANTUM COMPUTING

JUNIQ Spring School on Quantum Computing 2025

31 MARCH 2025 I DR. DENNIS WILLSCH

Lecture Notes:
Programming Quantum Computers
https://arxiv.org/pdf/2201.02051.pdf

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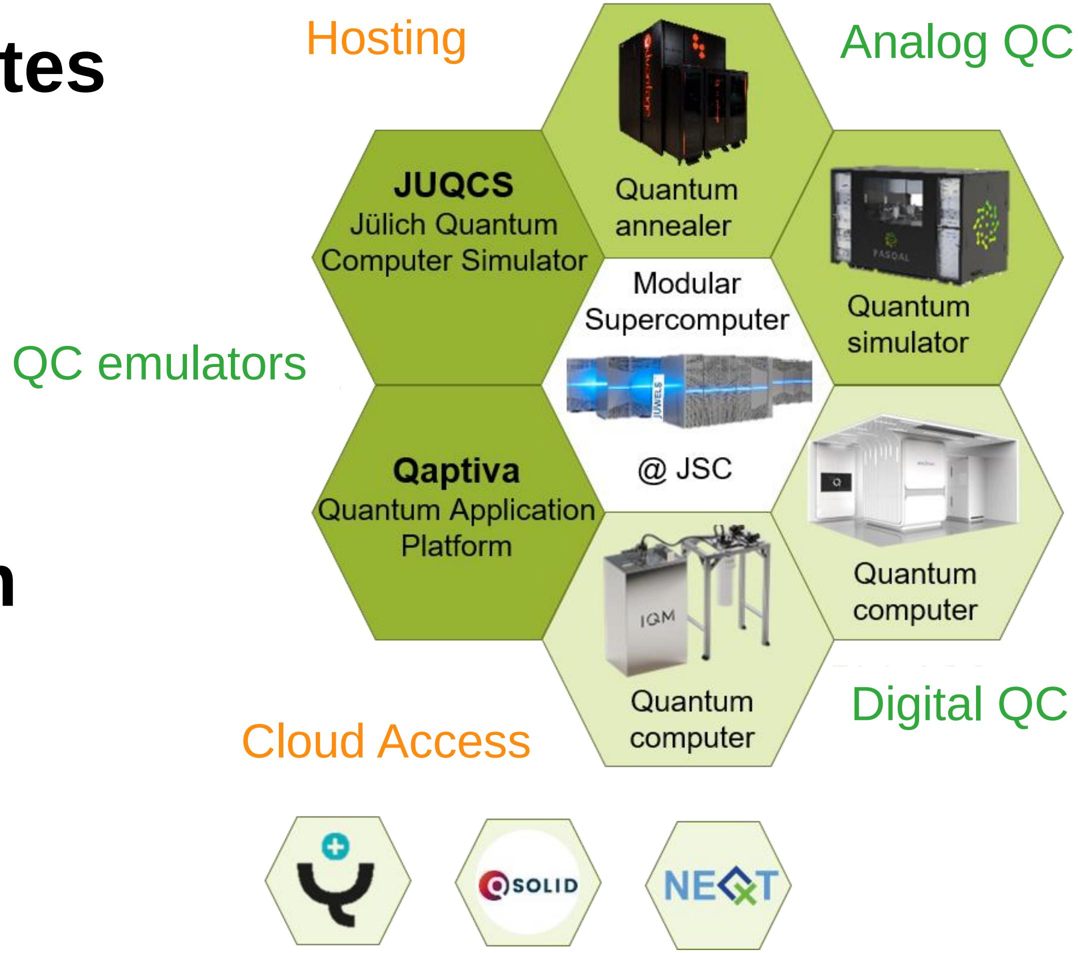


QUANTUM BITS AND QUANTUM GATES

A single qubit

- Definition of a single qubit

$$|\psi\rangle = \psi_0 \, |0\rangle + \psi_1 \, |1\rangle = \begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix}$$

Computational basis states:

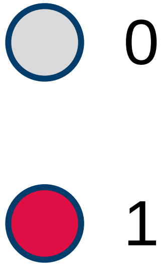
$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Important qubits:

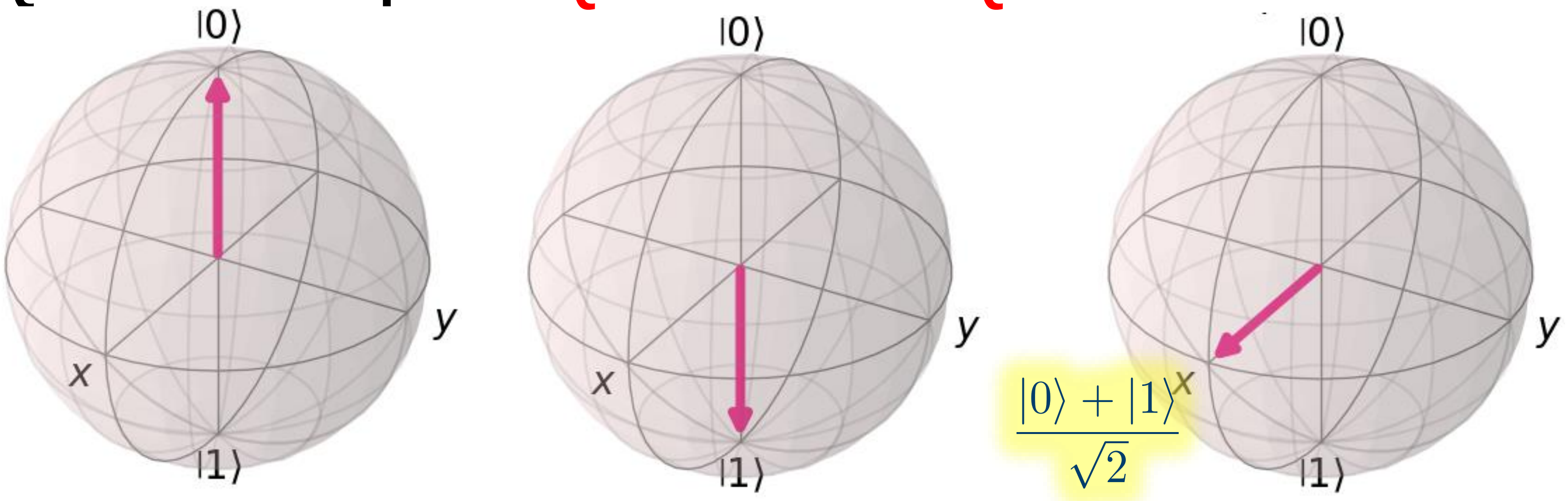
$$|+\rangle = \frac{1}{\sqrt{2}} |0\rangle + \frac{1}{\sqrt{2}} |1\rangle$$

$$|-\rangle = \frac{1}{\sqrt{2}} |0\rangle - \frac{1}{\sqrt{2}} |1\rangle$$

Digital computer: Bit



Quantum computer: Quantum Bit = Qubit



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QUANTUM BITS AND QUANTUM GATES

A single qubit

➢ Definition of a single qubit

$$|\psi\rangle = \psi_0\,|0\rangle + \psi_1\,|1\rangle = \begin{pmatrix}\psi_0\\ \psi_1\end{pmatrix}$$

Normalization:

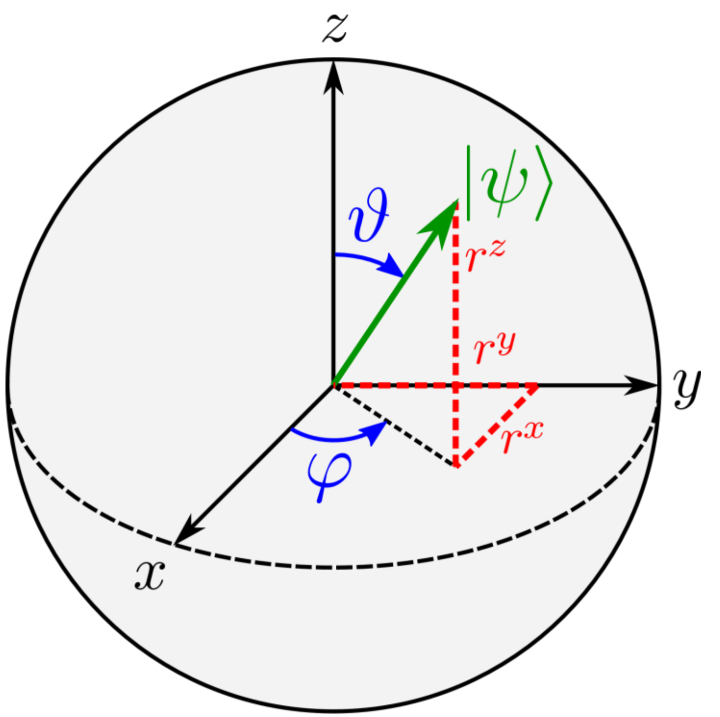
$$\langle\psi|\psi\rangle = |\psi_0|^2 + |\psi_1|^2 = 1$$
$$\langle\psi| = (\psi_0^*,\ \psi_1^*)$$

➢ Representation on the Bloch sphere

$$|\psi\rangle = \cos\frac{\vartheta}{2}\,|0\rangle + e^{i\varphi}\sin\frac{\vartheta}{2}\,|1\rangle = \begin{pmatrix}\cos\frac{\vartheta}{2}\\ e^{i\varphi}\sin\frac{\vartheta}{2}\end{pmatrix}$$

Global phase:

$$|\psi\rangle \equiv e^{i\Phi}|\psi\rangle$$



➢ Evaluation of the Cartesian coordinates

$$\vec{r} = \begin{pmatrix}r^x\\ r^y\\ r^z\end{pmatrix} = \begin{pmatrix}\langle\psi|\sigma^x|\psi\rangle\\ \langle\psi|\sigma^y|\psi\rangle\\ \langle\psi|\sigma^z|\psi\rangle\end{pmatrix} = \begin{pmatrix}\sin\vartheta\cos\varphi\\ \sin\vartheta\sin\varphi\\ \cos\vartheta\end{pmatrix}$$

Pauli matrices:

$$\sigma^x = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} \quad \sigma^y = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} \quad \sigma^z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

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QUANTUM BITS AND QUANTUM GATES

Gates as rotations on the Bloch sphere

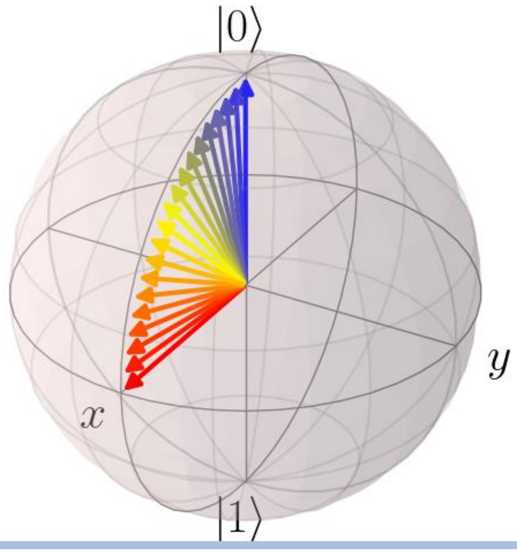
- Rotations around the axes of the Bloch sphere

$$R^x(\theta) = e^{-i\theta\sigma^x/2} = \begin{pmatrix} \cos(\theta/2) & -i\sin(\theta/2) \\ -i\sin(\theta/2) & \cos(\theta/2) \end{pmatrix}$$

$$R^y(\theta) = e^{-i\theta\sigma^y/2} = \begin{pmatrix} \cos(\theta/2) & -\sin(\theta/2) \\ \sin(\theta/2) & \cos(\theta/2) \end{pmatrix}$$

$$R^z(\theta) = e^{-i\theta\sigma^z/2} = \begin{pmatrix} \exp(-i\theta/2) & 0 \\ 0 & \exp(i\theta/2) \end{pmatrix}$$

$$R^y(\pi/2) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} = -\boxed{R^y(\pi/2)}-$$



- General rotation gate

$$R^{\vec{n}}(\theta) = e^{-i\theta\vec{n}\cdot\vec{\sigma}/2} = \cos\frac{\theta}{2}\, I - i\sin\frac{\theta}{2}\, \vec{n}\cdot\vec{\sigma}$$

Standard gate set:

$$X = \sigma^x \qquad Y = \sigma^y \qquad Z = \sigma^z$$

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \qquad S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \qquad T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix}$$

QUANTUM BITS AND QUANTUM GATES

Multiple qubits

- Multi-qubit state

$$|\psi\rangle = \sum_{j=0}^{2^n-1} \psi_j |j\rangle = \psi_0 |0\cdots 00\rangle + \psi_1 |0\cdots 01\rangle + \cdots + \psi_{2^n-1} |1\cdots 11\rangle = \begin{pmatrix} \psi_0 \\ \psi_1 \\ \vdots \\ \psi_{2^n-1} \end{pmatrix}$$

Computational basis states:

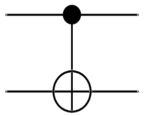
$$|00\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad |01\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad |10\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \quad |11\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

Tensor product

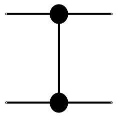
$$|q_0 q_1\rangle = |q_0\rangle \otimes |q_1\rangle \qquad A \otimes B = \begin{pmatrix} a_{00}B & a_{01}B & \cdots \\ a_{10}B & a_{11}B & \\ \vdots & & \ddots \end{pmatrix}$$

- Important two-qubit gates

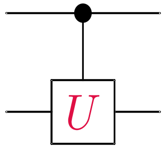
$$\mathrm{CNOT} = \mathrm{CX} = \begin{array}{c} \begin{matrix} |00\rangle & |01\rangle & |10\rangle & |11\rangle \end{matrix} \\ \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \end{array} =$$



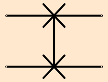
$$\mathrm{CZ} = \begin{array}{c} \begin{matrix} |00\rangle & |01\rangle & |10\rangle & |11\rangle \end{matrix} \\ \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \end{array} =$$



$$\mathrm{C}U = \begin{pmatrix} I & 0 \\ 0 & U \end{pmatrix} =$$



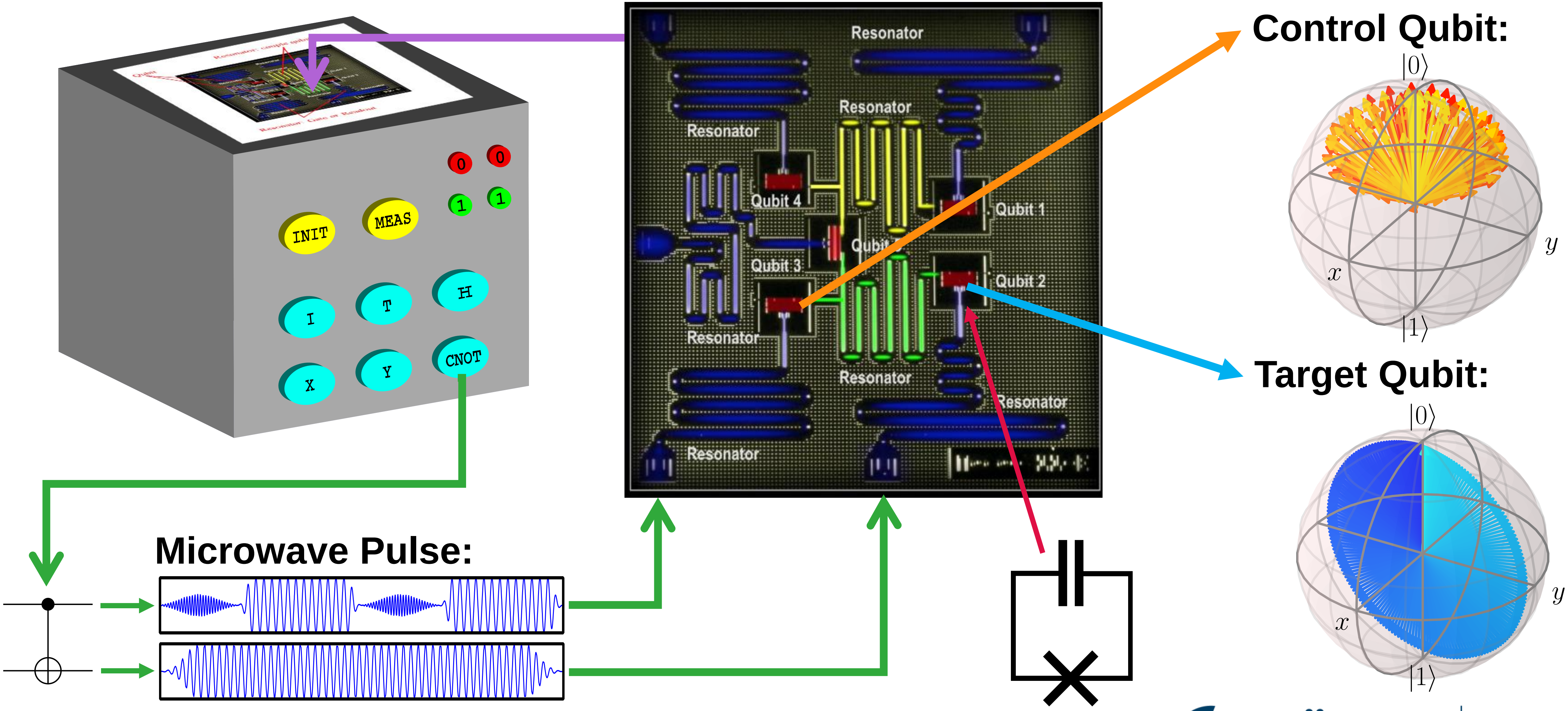
$$\mathrm{SWAP} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} =$$



- General controlled gates

$$\mathrm{C}U_{i_1 i_2} |q_0 \cdots q_{n-1}\rangle = \begin{cases} |q_0 \cdots q_{n-1}\rangle & (\text{if } q_{i_1} = 0) \\ |q_0 \cdots q_{i_2-1}\rangle \left(U |q_{i_2}\rangle\right) |q_{i_2+1} \cdots q_{n-1}\rangle & (\text{if } q_{i_1} = 1) \end{cases}$$

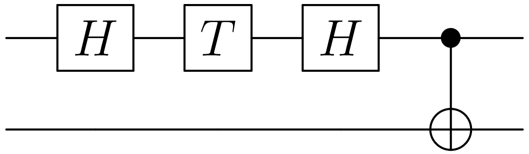
INTERLUDE: SUPERCONDUCTING QUANTUM COMPUTERS

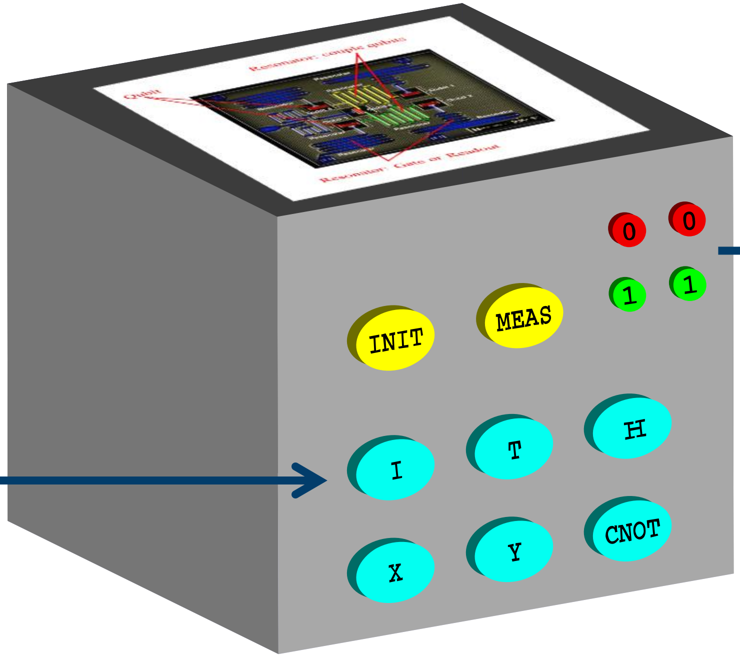


PROGRAMMING AND SIMULATING QUANTUM CIRCUITS

Input:

Program = Circuit of Quantum Gates





Output: Bitstrings

„00“, „01“, „10“, „11“

$$\sqrt{0.85\ldots}|00\rangle + \sqrt{0.15\ldots}|11\rangle$$

Result of this program

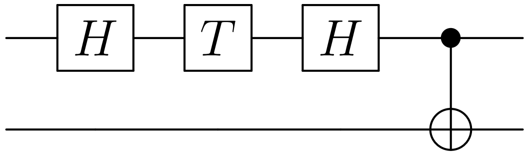
Option 1: Compute the unitary matrix

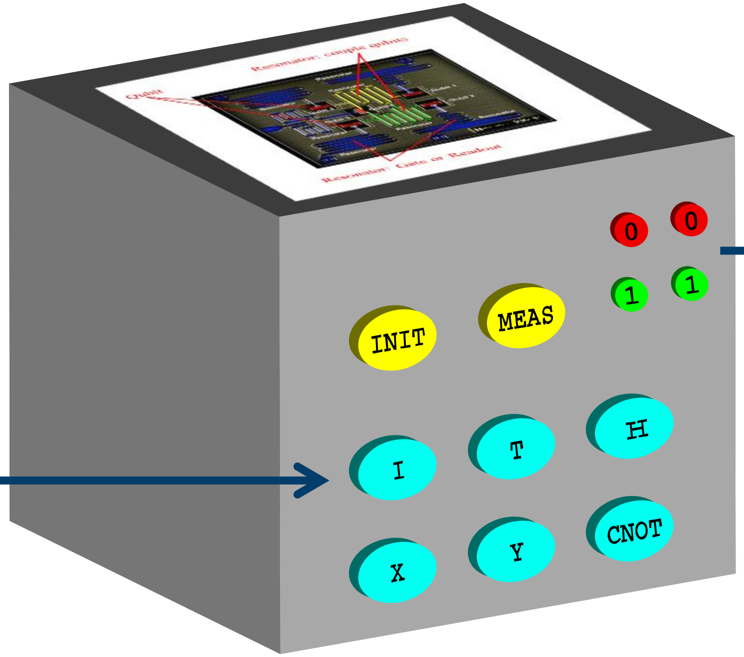
$$\mathrm{CNOT}\,(H \otimes I)\,(T \otimes I)\,(H \otimes I) = \begin{pmatrix} \frac{1+e^{i\pi/4}}{2} & 0 & \frac{1-e^{i\pi/4}}{2} & 0 \\ 0 & \frac{1+e^{i\pi/4}}{2} & 0 & \frac{1-e^{i\pi/4}}{2} \\ 0 & \frac{1-e^{i\pi/4}}{2} & 0 & \frac{1+e^{i\pi/4}}{2} \\ \frac{1-e^{i\pi/4}}{2} & 0 & \frac{1+e^{i\pi/4}}{2} & 0 \end{pmatrix}$$

PROGRAMMING AND SIMULATING QUANTUM CIRCUITS

Input:

Programm =
Circuit of
Quantum Gates





Output: Bitstrings

„00“, „01“, „10“, „11“

$$\sqrt{0.85\ldots}|00\rangle + \sqrt{0.15\ldots}|11\rangle$$

Result of this program

Option 2: Track the unitary transformations

$$|00\rangle \overset{H\otimes I}{\longmapsto} \frac{1}{\sqrt{2}}|00\rangle + \frac{1}{\sqrt{2}}|10\rangle$$

$$\overset{T\otimes I}{\longmapsto} \frac{1}{\sqrt{2}}|00\rangle + \frac{e^{i\pi/4}}{\sqrt{2}}|10\rangle$$

$$\overset{H\otimes I}{\longmapsto} \frac{1+e^{i\pi/4}}{2}|00\rangle + \frac{1-e^{i\pi/4}}{2}|10\rangle \overset{\mathrm{CNOT}}{\longmapsto} \frac{1+e^{i\pi/4}}{2}|00\rangle + \frac{1-e^{i\pi/4}}{2}|11\rangle$$

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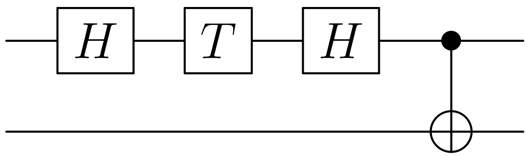
PROGRAMMING AND SIMULATING QUANTUM CIRCUITS

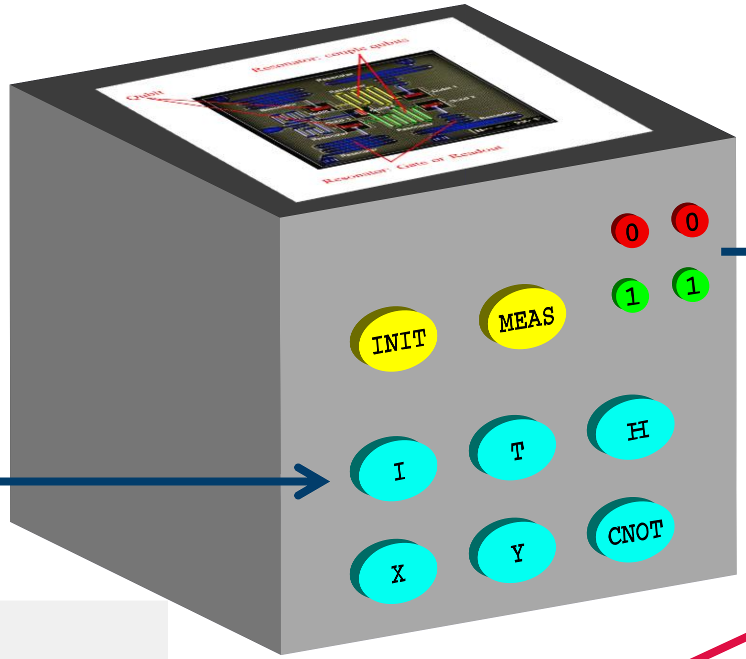
Input:

Programm =

Circuit of

Quantum Gates





Output: Bitstrings

„00“, „01“, „10“, „11“

$$\sqrt{0.85\ldots}|00\rangle + \sqrt{0.15\ldots}|11\rangle$$

Measure **00** with 85 %

and **11** with 15 %

Option 3: Simulate the circuit

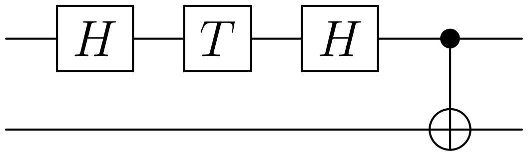
```python
import qiskit

circuit = qiskit.QuantumCircuit(2)
circuit.h(0)
circuit.t(0)
circuit.h(0)
circuit.cx(0,1)

from juqcs import Juqcs
```

JUQCS (Jülich Universal Quantum Computer Simulator)

Python Package qiskit-juqcs: https://pypi.org/project/qiskit-juqcs/

PROGRAMMING AND SIMULATING QUANTUM CIRCUITS

Simulation with Qiskit Aer



qasm_simulator

```python
import qiskit
circuit = qiskit.QuantumCircuit(2)
circuit.h(0)
circuit.t(0)
circuit.h(0)
circuit.cx(0,1)
circuit.measure_all()

backend = qiskit.Aer.get_backend('qasm_simulator')
result = backend.run(circuit,
                     shots=1000).result()
result.get_counts()
```

```
{'00': 846, '11': 154}
```

Measure **00** with 85 %

and **11** with 15 %

statevector_simulator

```python
import qiskit
circuit = qiskit.QuantumCircuit(2)
circuit.h(0)
circuit.t(0)
circuit.h(0)
circuit.cx(0,1)


backend = qiskit.Aer.get_backend('statevector_simulator')
result = backend.run(circuit.reverse_bits()).result()

result.get_statevector()
```

```
Statevector([0.85355339+0.35355339j, 0.        +0.j        ,
             0.        +0.j        , 0.14644661-0.35355339j],
```

$$\sqrt{0.85\ldots}|00\rangle + \sqrt{0.15\ldots}|11\rangle$$

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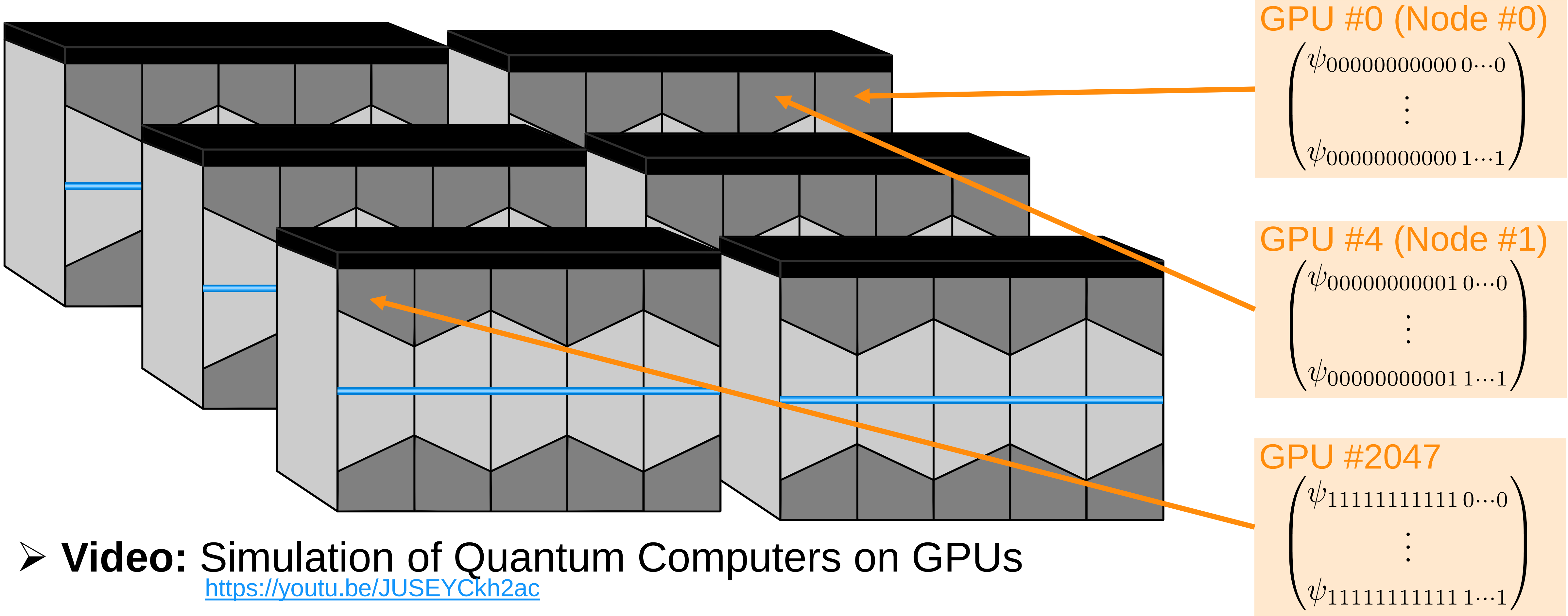
De Raedt et al., CPC **176**, 121 (2007)
De Raedt et al., CPC **237**, 47 (2019)
Willsch et al., CPC **278**, 108411 (2022)

SIMULATING QUANTUM CIRCUITS

Simulation with JUQCS (large-scale simulations on a supercomputer)



- **Video:** Simulation of Quantum Computers on GPUs
  https://youtu.be/JUSEYCkh2ac
- **JUNIQ:** Possible to simulate around 40 qubits (45 with JUQCS-G)
  https://juniq.fz-juelich.de

QUANTUM FOURIER TRANSFORM

An operation to move registers into phases and back

Here happens a multiplication modulo 2^n
→ Can (ab)use QFT for arithmetics!
(addition, multiplication, etc.)

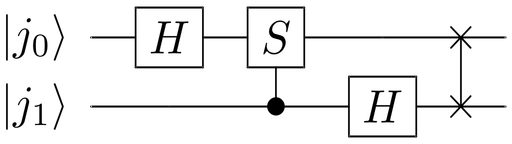
- The formal definition of the QFT is:

$$|j_0 j_1 j_2 \cdots\rangle \overset{\text{QFT}}{\mapsto} \frac{1}{\sqrt{2^n}} \sum_{k_0 k_1 k_2 \cdots} e^{2\pi i\, (j_0 j_1 j_2 \cdots)\cdot(k_0 k_1 k_2 \cdots)/2^n} |k_0 k_1 k_2 \cdots\rangle$$

- Intuition:

$$|j\rangle \leftrightarrow \sum_{k=0}^{2^n-1} e^{2\pi i\, j\, k/2^n} |k\rangle$$

- Implementation for two qubits:



- Verification:

$$\text{SWAP}\,(I \otimes H)\,CS\,(H \otimes I)\,|j_0 j_1\rangle = \frac{1}{2} \begin{array}{cccc} |00\rangle & |01\rangle & |10\rangle & |11\rangle \end{array} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & i & -1 & -i \\ 1 & -1 & 1 & -1 \\ 1 & -i & -1 & i \end{pmatrix} |j_0 j_1\rangle = \frac{1}{2} \sum_{k_0 k_1} e^{2\pi i\, (j_0 j_1)\cdot(k_0 k_1)/4} |k_0 k_1\rangle$$

$$e^{2\pi i\, (j_0 j_1)\cdot 0/4}|0\rangle + e^{2\pi i\, (j_0 j_1)\cdot 1/4}|1\rangle + e^{2\pi i\, (j_0 j_1)\cdot 2/4}|2\rangle + e^{2\pi i\, (j_0 j_1)\cdot 3/4}|3\rangle$$

Draper, arXiv:quant-ph/0008033 (2000)
https://arxiv.org/pdf/2201.02051.pdf

QUANTUM ADDER

A nice application of the QFT

- We are looking for a quantum circuit to implement the following unitary operation

$$|x_0x_1\rangle|y_0y_1\rangle \overset{\mathrm{ADD}_{2+2}}{\longmapsto} |x_0x_1\rangle|\underbrace{y_0y_1 + x_0x_1}_{\text{Sum } s_0s_1}\rangle$$

- Such a modulo-4 adder would also work on superpositions!
- Examples:

$$|2\rangle\,|1\rangle \mapsto |2\rangle\,|3\rangle$$

$$|2\rangle\,\frac{|0\rangle+|1\rangle}{\sqrt{2}} \mapsto |2\rangle\,\frac{|2\rangle+|3\rangle}{\sqrt{2}}$$

$$|2\rangle\,\frac{|0\rangle+|1\rangle+|2\rangle}{\sqrt{3}} \mapsto |2\rangle\,\frac{|2\rangle+|3\rangle+|0\rangle}{\sqrt{3}}$$

$$\frac{|0\rangle+|1\rangle}{\sqrt{2}}\,\frac{|2\rangle+|3\rangle+|0\rangle}{\sqrt{3}} \mapsto \frac{|0\rangle|2\rangle+|0\rangle|3\rangle+|0\rangle|0\rangle+|1\rangle|3\rangle+|1\rangle|0\rangle+|1\rangle|1\rangle}{\sqrt{6}}$$

QUANTUM ADDER

A nice application of the QFT

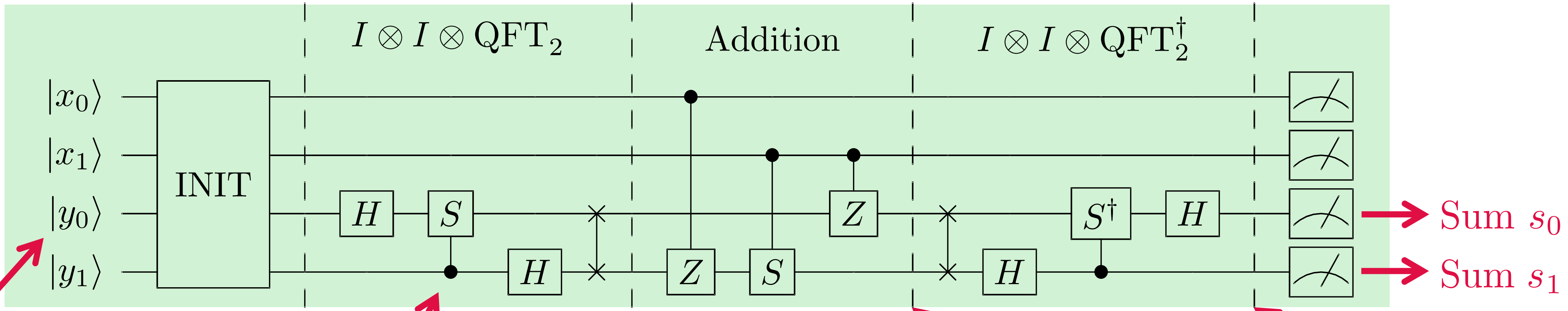
$$|j\rangle \leftrightarrow \sum_{k=0}^{2^n-1} e^{2\pi i\, j\, k/2^n} |k\rangle$$

- Idea: → The QFT converts between registers and phases

  → By using bitwise phase shifts, we can implement the addition in the exponent

  → This is automatically modulo 4 (← periodicity of the complex exponential function)

- A circuit to realize this idea is:



- Intuition:

$$|j\rangle|k\rangle \mapsto |j\rangle\left(\sum_{k'} e^{2\pi i\, k\, k'/2^n}|k'\rangle\right) = \sum_{k'} e^{2\pi i\, k\, k'/2^n}|j\rangle|k'\rangle \mapsto \sum_{k'} e^{2\pi i\,(j+k)\,k'/2^n}|j\rangle|k'\rangle \mapsto |j\rangle|j+k\rangle$$

QUANTUM APPROXIMATE OPTIMIZATION ALGORITHM

A very brief overview of the QAOA

- Say we want to find the minimum of the function

$$E(q_0, \ldots, q_{n-1}) = \sum_{i,j} q_i Q_{ij} q_j \quad \Leftrightarrow \quad E(s_0, \ldots, s_{n-1}) = \sum h_i s_i + \sum_{i<j} J_{ij} s_i s_j$$

"QUBO" (q = 0,1) **"Ising" (s = +1,-1)**

- Combinatorial optimization problem

  → discrete optimization is hard!

- Idea: With a quantum circuit, we can create a superposition

$$|\psi\rangle = \psi_0 |0 \cdots 00\rangle + \cdots + \boxed{\psi_{q_0^* \cdots q_{n-1}^*} |q_0^* \cdots q_{n-1}^*\rangle} + \cdots + \psi_{2^n-1} |1 \cdots 11\rangle$$

Solution to the problem

- Goal: Enhance this term!

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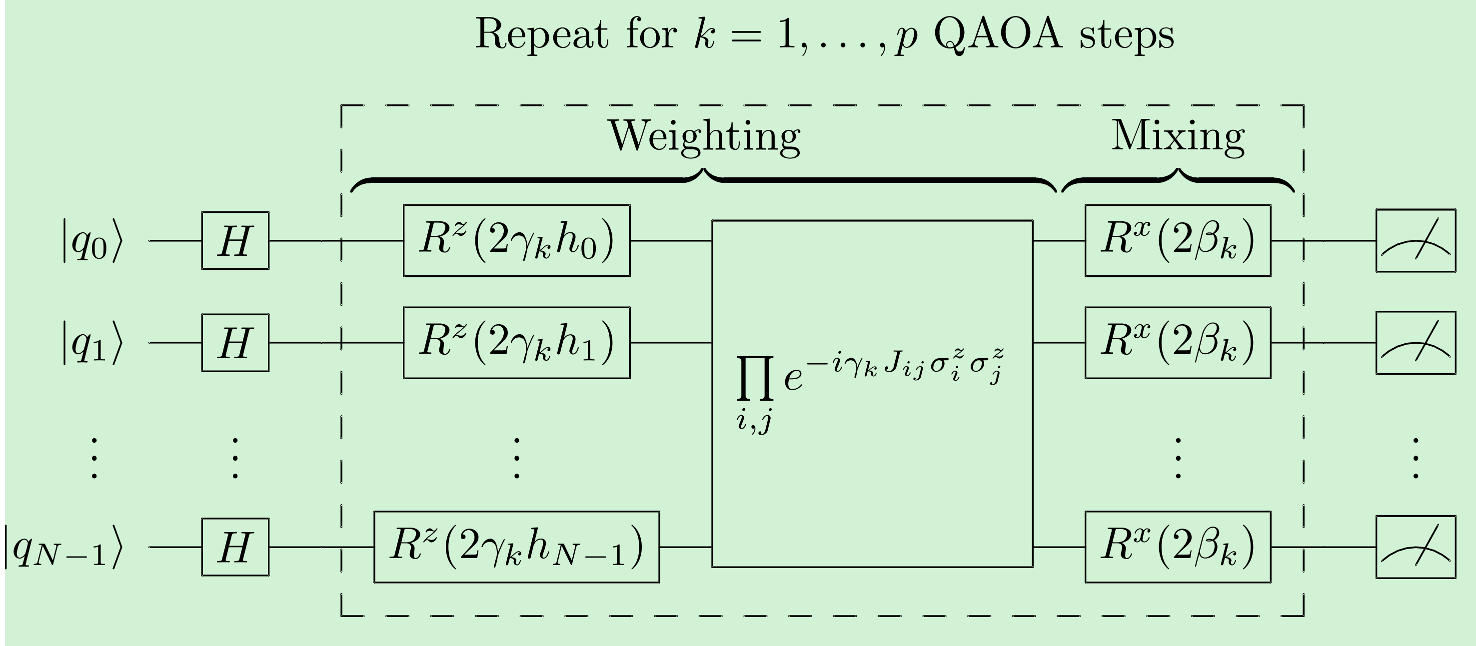
QUANTUM APPROXIMATE OPTIMIZATION ALGORITHM

A very brief overview of the QAOA

- Goal: Enhance this term!

$$|\psi\rangle = \psi_0 |0\cdots 00\rangle + \cdots + \psi_{q_0^*\cdots q_{n-1}^*} |q_0^* \cdots q_{n-1}^*\rangle + \cdots + \psi_{2^n-1} |1\cdots 11\rangle$$

- Make the quantum circuit dependent on real parameters $(\beta_1, \ldots, \beta_p, \gamma_1 \ \ldots, \gamma_p)$
- Hope: these 2p parameters are easier searchable than the original discrete variables



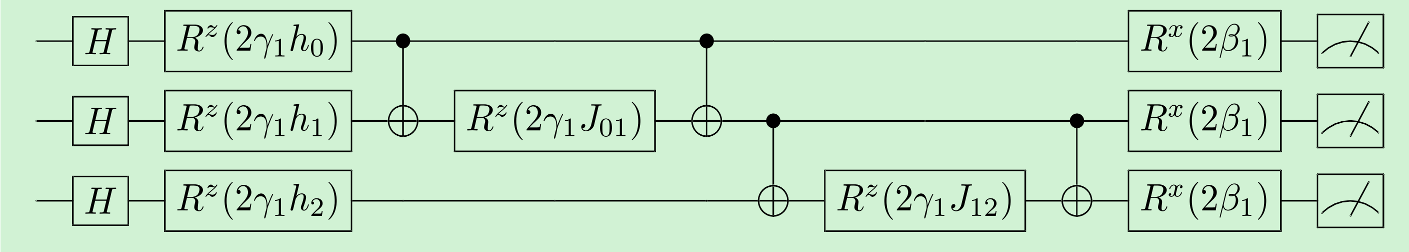
QUANTUM APPROXIMATE OPTIMIZATION ALGORITHM

A very brief overview of the QAOA

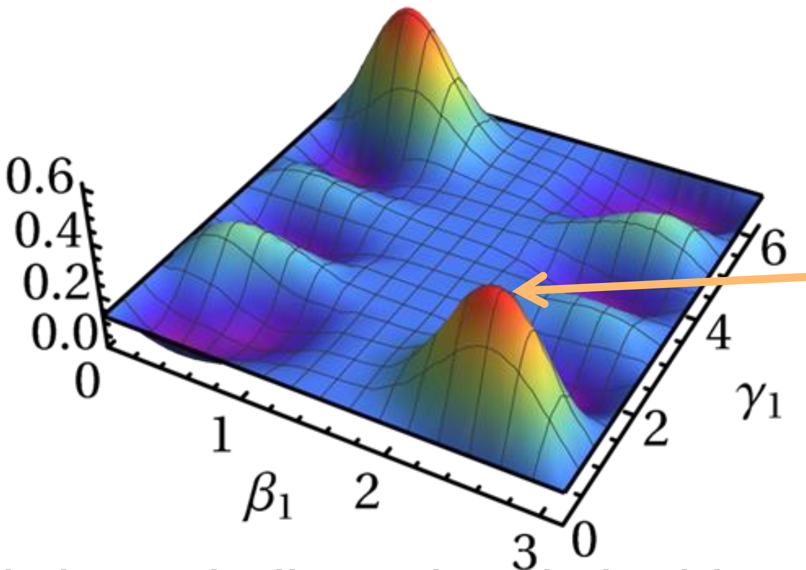
- Goal: Enhance this term!

$$|\psi\rangle = \psi_0 \, |0\cdots 00\rangle + \cdots + \psi_{q_0^*\cdots q_{n-1}^*} \, |q_0^* \cdots q_{n-1}^*\rangle + \cdots + \psi_{2^n-1} \, |1\cdots 11\rangle$$

- Look at p=1 QAOA step



Success probability $|\psi_{q_0^*\cdots q_{n-1}^*}|^2$



There are regions where the success probability is enhanced! How to find them?

- Will be a dedicated topic in this School ☺

THANK YOU FOR YOUR ATTENTION

- Further information:
  - **Programming Quantum Computers:** https://arxiv.org/pdf/2201.02051.pdf
  - **JUQCS:** Video https://youtu.be/JUSEYCkh2ac
  - **JUQCS:** Paper https://doi.org/10.1016/j.cpc.2022.108411