

INTRODUCTION TO GATE-BASED QUANTUM COMPUTING

JUNIQ Summer School on Quantum Information Processing 2023

28 AUGUST 2023 I DR. DENNIS WILLSCH









Lecture Notes: Programming Quantum Computers

https://arxiv.org/pdf/2201.02051.pdf





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1. Quantum Bits and Quantum Gates

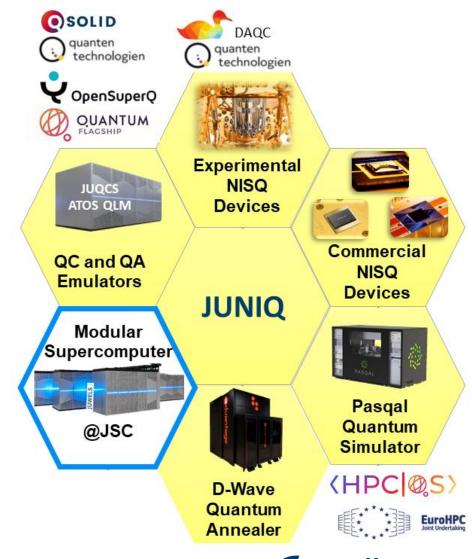




Lecture Notes: Programming Quantum Computers

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- 1. Quantum Bits and Quantum Gates
- 2. Programming and Simulating Quantum Circuits

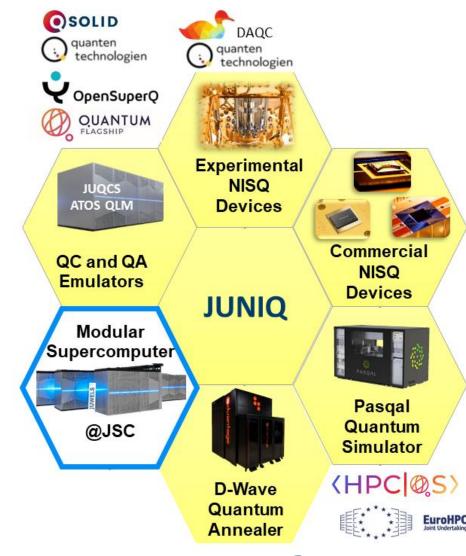




Lecture Notes: Programming Quantum Computers

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- 1. Quantum Bits and Quantum Gates
- 2. Programming and Simulating Quantum Circuits
- 3. Applications:
 - 1. Quantum Fourier Transform
 - 2. Quantum Adder
 - 3. Quantum Approximate Optimization Algorithm





A single qubit



A single qubit

> Definition of a single qubit

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



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Computational basis states:

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

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Digital computer: Bit



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Digital computer: Bit



Quantum computer: Quantum Bit = Qubit

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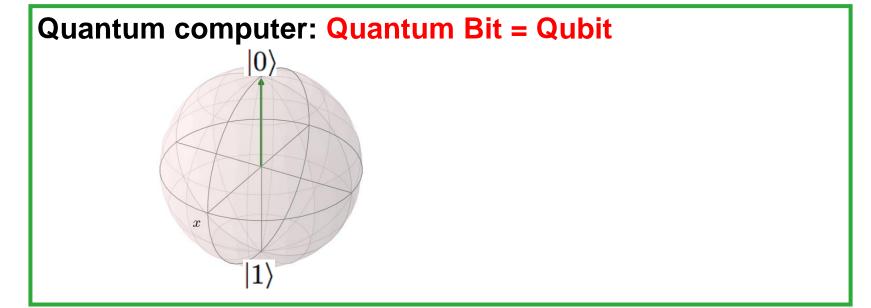
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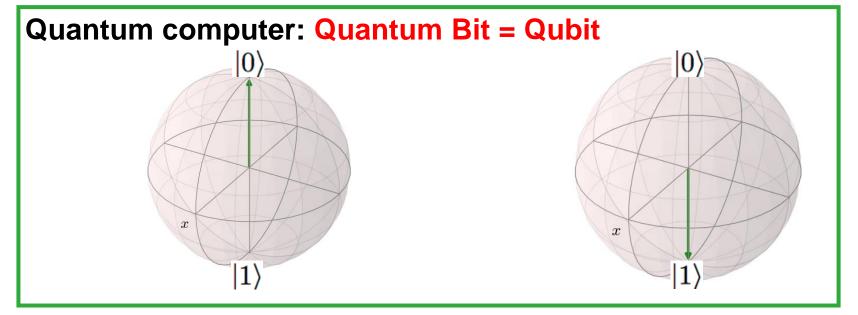
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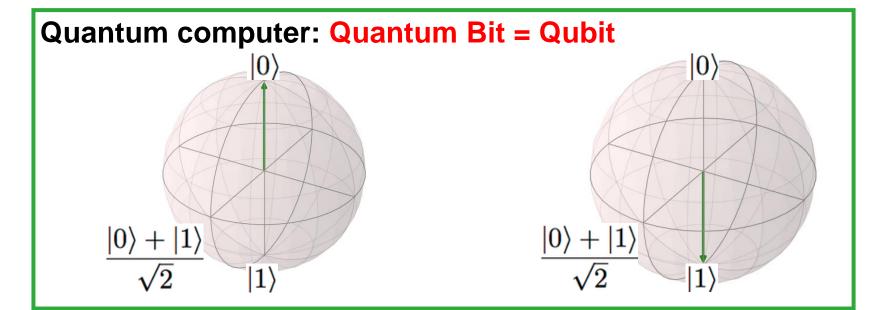
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$$\langle \psi | = (\psi_0^*, \ \psi_1^*)$$



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

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> Representation on the Bloch sphere

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

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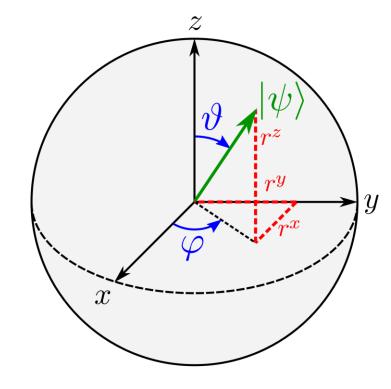
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> Evaluation of the Cartesian coordinates

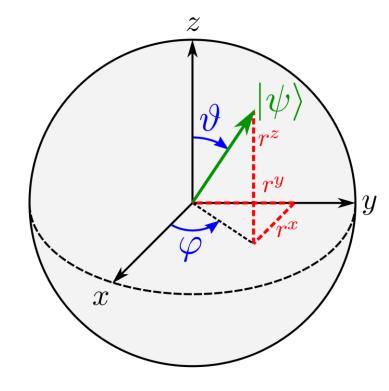
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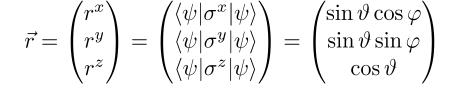
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 $\vec{r} = \begin{pmatrix} r^x \\ r^y \\ r^z \end{pmatrix} = \begin{pmatrix} \langle \psi | \sigma^x | \psi \rangle \\ \langle \psi | \sigma^y | \psi \rangle \\ \langle \psi | \sigma^z |_{y/\lambda} \end{pmatrix} = \begin{pmatrix} \sin \vartheta \cos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

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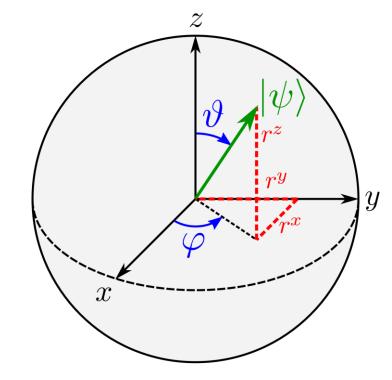
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$$|\psi\rangle \equiv e^{i\Phi}|\psi\rangle$$



Pauli matrices:

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



Gates as rotations on the Bloch sphere



Gates as rotations on the Bloch sphere

> Rotations around the axes of the Bloch sphere

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

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

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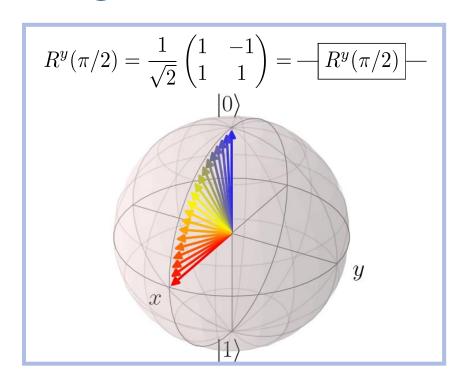
Gates as rotations on the Bloch sphere

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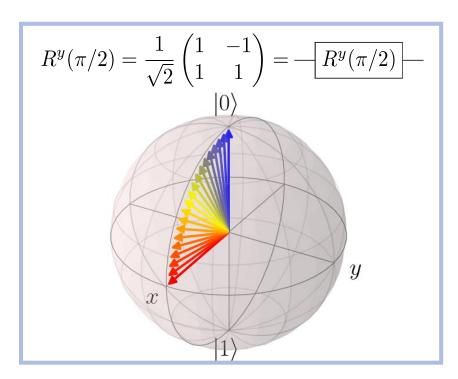
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General rotation gate

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





Gates as rotations on the Bloch sphere

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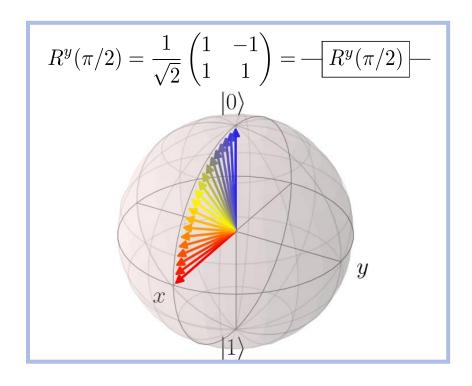
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Standard gate set:

$$X = \sigma^x$$

$$Y = \sigma^y$$

$$Z = \sigma^z$$

$$H = rac{1}{\sqrt{2}} egin{pmatrix} 1 & 1 \ 1 & -1 \end{pmatrix}$$

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

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



Multiple qubits



Multiple qubits

➤ Multi-qubit state

$$|\psi\rangle = \sum_{j=0}^{2^{n}-1} \psi_{j} |j\rangle = \psi_{0} |0\cdots00\rangle + \psi_{1} |0\cdots01\rangle + \cdots + \psi_{2^{n}-1} |1\cdots11\rangle = \begin{pmatrix} \psi_{0} \\ \psi_{1} \\ \vdots \\ \psi_{2^{n}-1} \end{pmatrix}$$



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$$|q_0q_1\rangle = |q_0\rangle \otimes |q_1\rangle \quad A \otimes B = \begin{pmatrix} a_{00}B & a_{01}B & \cdots \\ a_{10}B & a_{11}B & \cdots \\ \vdots & \ddots & \ddots \end{pmatrix}$$

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$$|\phi\rangle = |\phi\rangle \otimes |\phi$$

➤ Important two-qubit gates

$$egin{pmatrix} |00
angle & |01
angle & |10
angle & |11
angle \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

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$$CNOT = CX = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} = \begin{bmatrix} 100 & |010| & |110| & |110| \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} = \begin{bmatrix} 100 & |010| & |110| & |110| \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} = \begin{bmatrix} 100 & |010| & |110| & |110| \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$

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Tensor product
$$|q_0q_1\rangle=|q_0\rangle\otimes|q_1
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$$Z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} =$$

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Page 6

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$$CU = \begin{pmatrix} I & 0 \\ 0 & U \end{pmatrix} = \boxed{\begin{matrix} & & \\ & & U \end{matrix}}$$

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$$|mportant two-qubit gates$$

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Important two-qubit gates

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$$CZ = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} = \begin{array}{c} & \\ & \\ \end{array}$$

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

$$CU = \begin{pmatrix} I & 0 \\ 0 & U \end{pmatrix} = \boxed{\begin{matrix} I \\ U \end{matrix}}$$

General controlled gates

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

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General controlled gates

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

Computational basis states:

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

$$|q_0q_1\rangle = |q_0\rangle \otimes |q_1\rangle$$
 $A \otimes B = \begin{pmatrix} a_{00}B & a_{01}B & \cdots \\ a_{10}B & a_{11}B & \\ \vdots & & \ddots \end{pmatrix}$

$$CU = \begin{pmatrix} I & 0 \\ 0 & U \end{pmatrix} = \boxed{\begin{array}{c} \\ U \\ \end{array}}$$

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

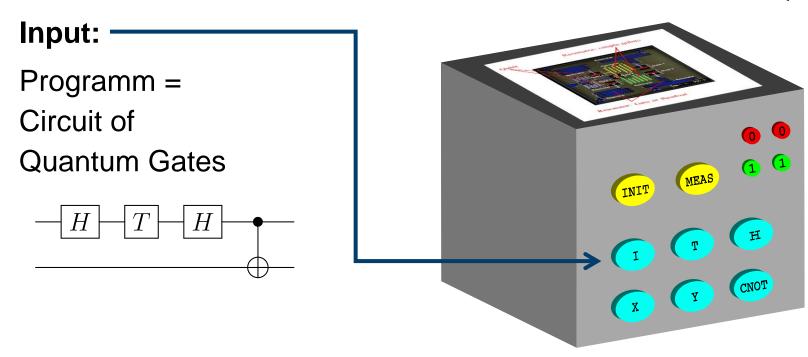


PROGRAMMING AND SIMULATING QUANTUM CIRCUITS





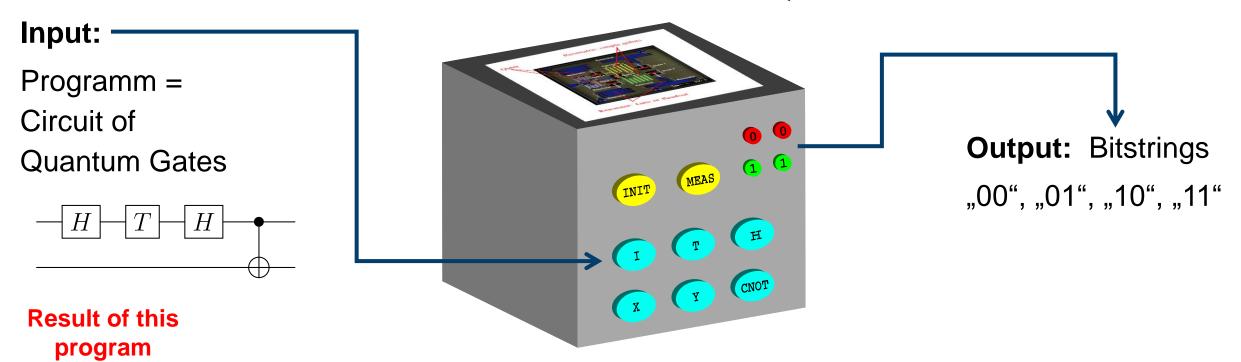
PROGRAMMING AND SIMULATING QUANTUM CIRCUITS







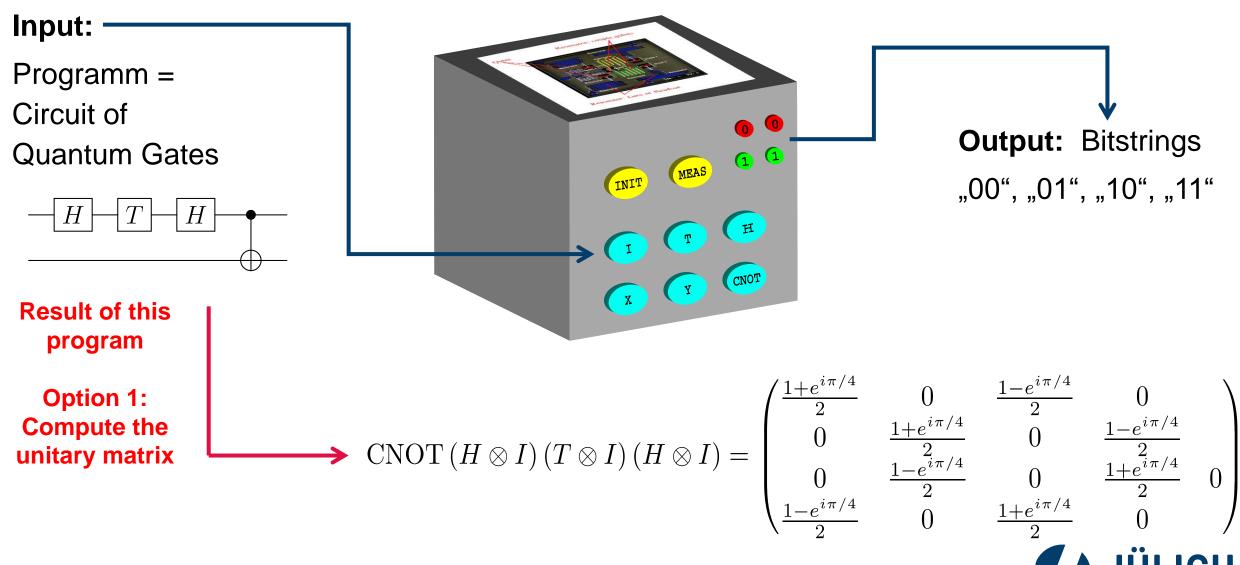




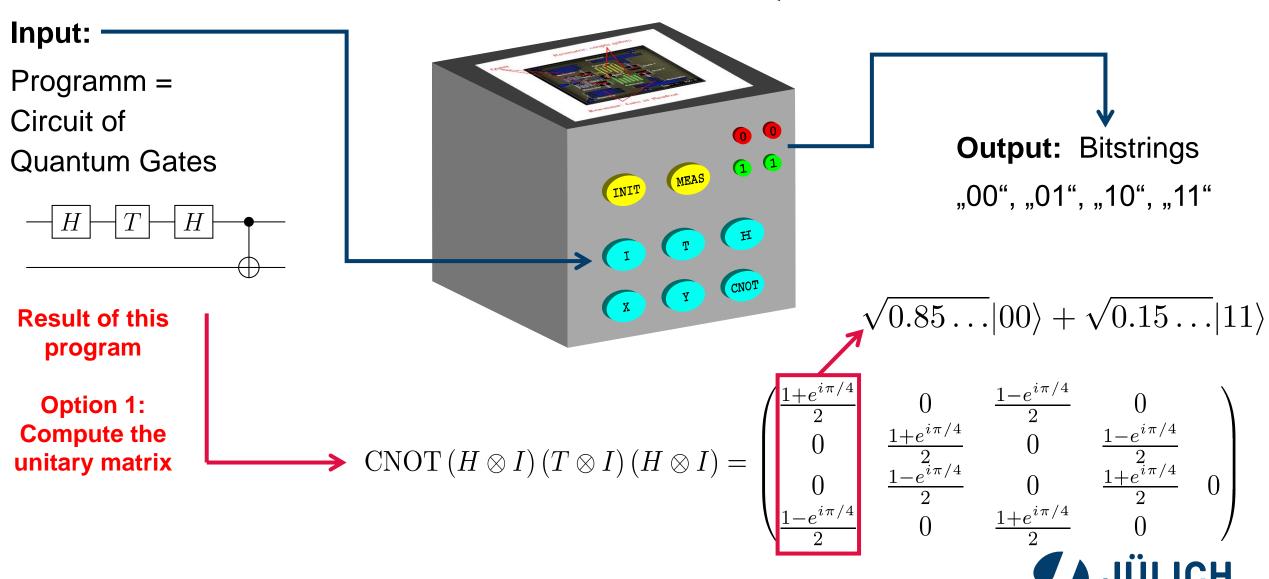
Page 7

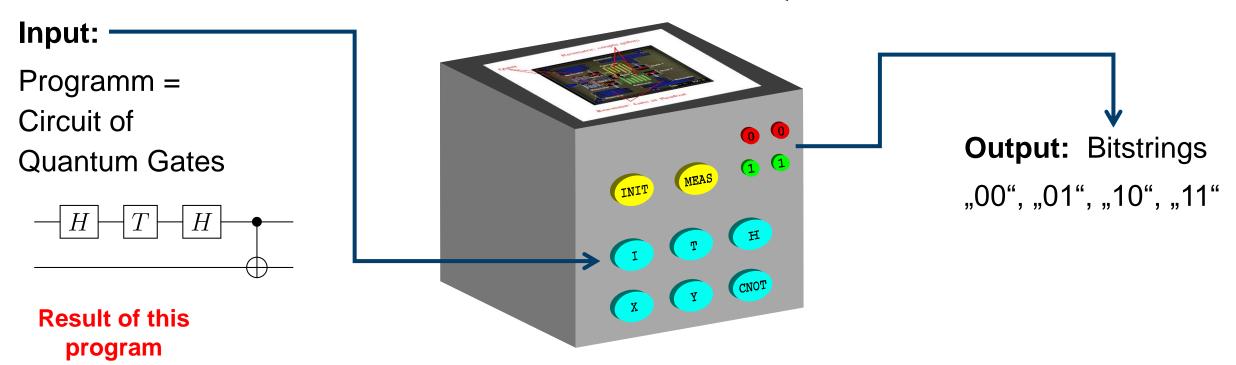
Option 1: Compute the unitary matrix







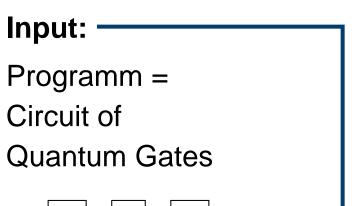




Page 8

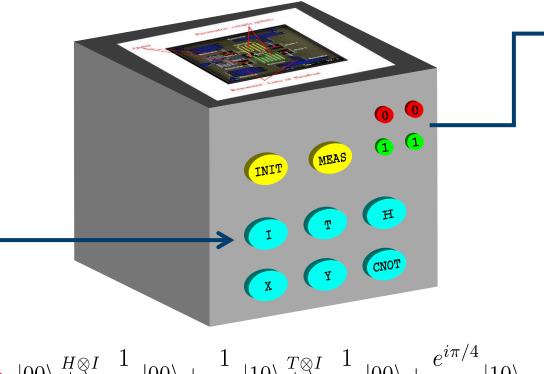
Option 2: Track the unitary transformations





Result of this program

Option 2: Track the unitary transformations



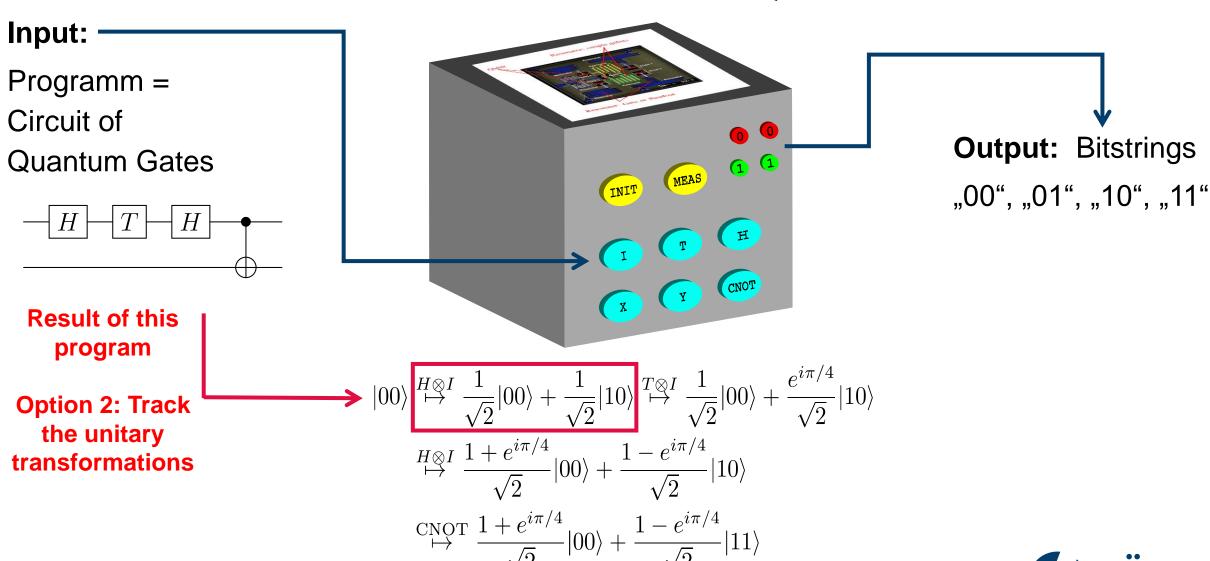
$$\stackrel{H\otimes I}{\longrightarrow} \frac{1 + e^{i\pi/4}}{\sqrt{2}} |00\rangle + \frac{1 - e^{i\pi/4}}{\sqrt{2}} |10\rangle$$

$$\stackrel{\text{CNOT}}{\longrightarrow} \frac{1 + e^{i\pi/4}}{\sqrt{2}} |00\rangle + \frac{1 - e^{i\pi/4}}{\sqrt{2}} |11\rangle$$

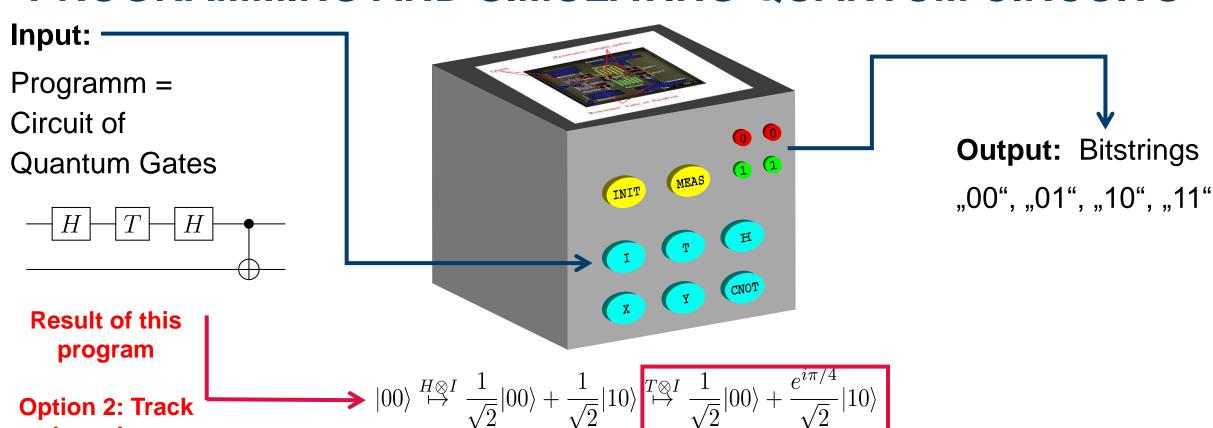
JÜLICH Forschungszentrum

Output: Bitstrings

"00", "01", "10", "11"





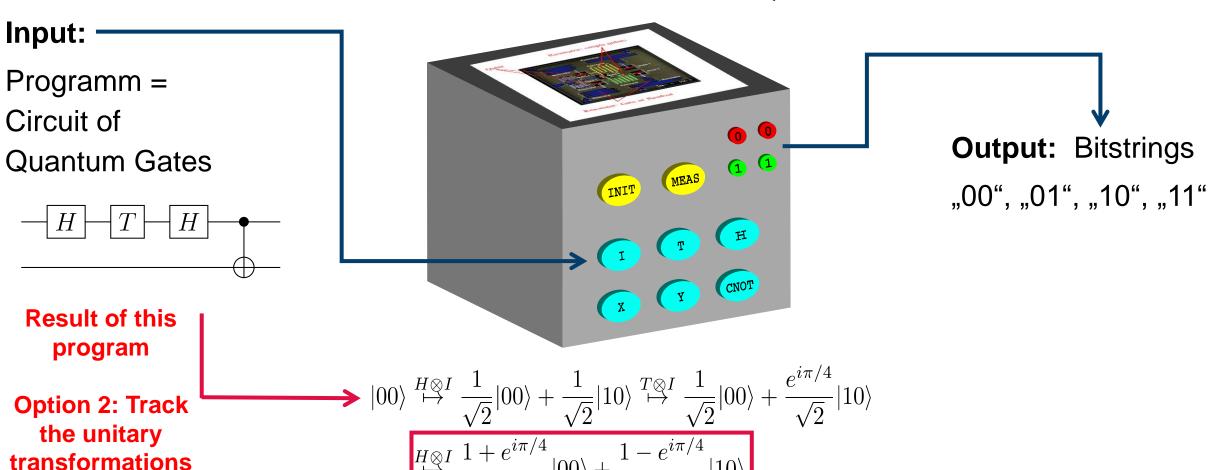


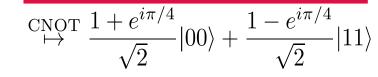
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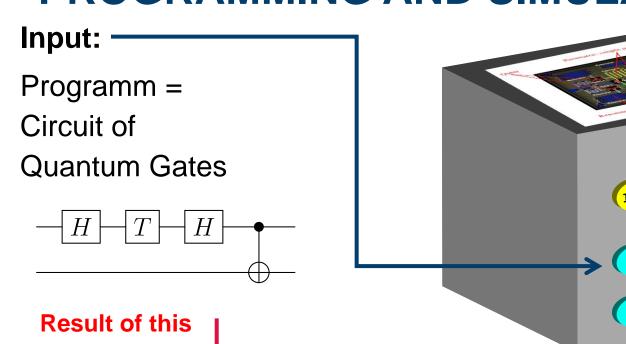
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program

Option 2: Track the unitary transformations

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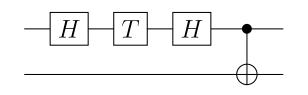
Dr. Dennis Willsch





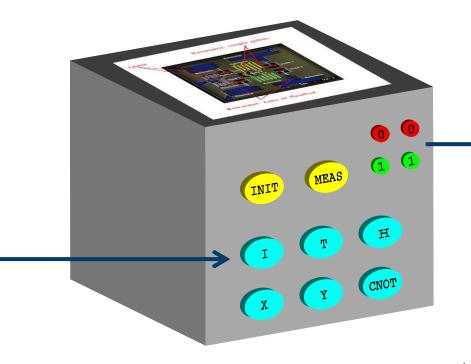
Programm = Circuit of

Quantum Gates



Result of this program

Option 2: Track the unitary transformations

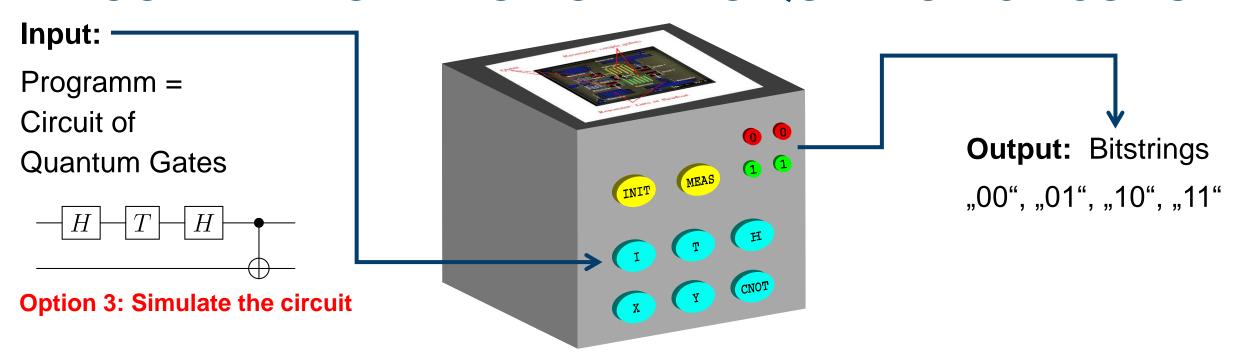


Output: Bitstrings

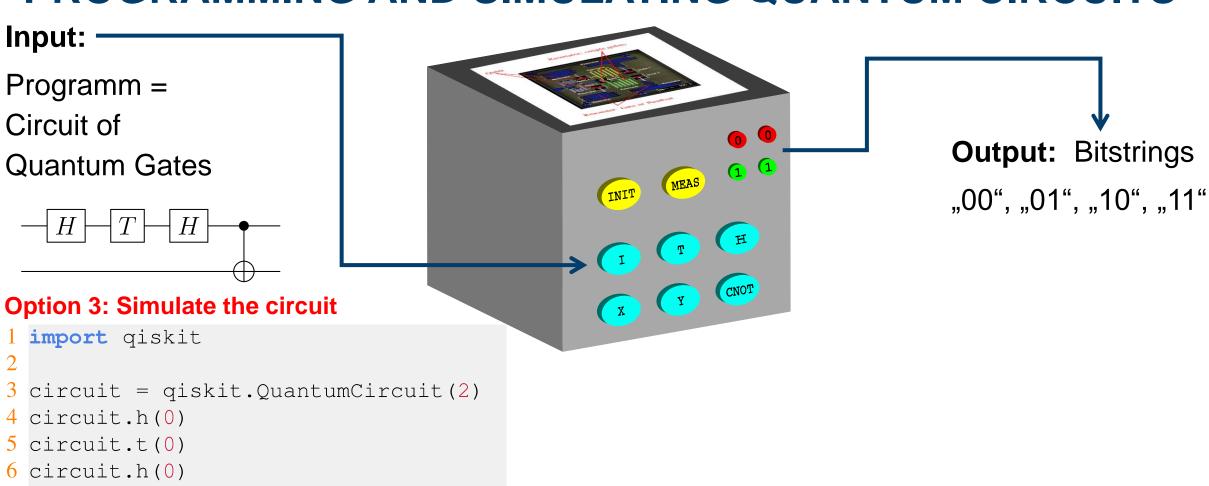
$$\sqrt{0.85\dots}|00\rangle + \sqrt{0.15\dots}|11\rangle$$

$$\stackrel{H\otimes I}{\mapsto} \frac{1+e^{i\pi/4}}{\sqrt{2}}|00\rangle + \frac{1-e^{i\pi/4}}{\sqrt{2}}|10\rangle$$

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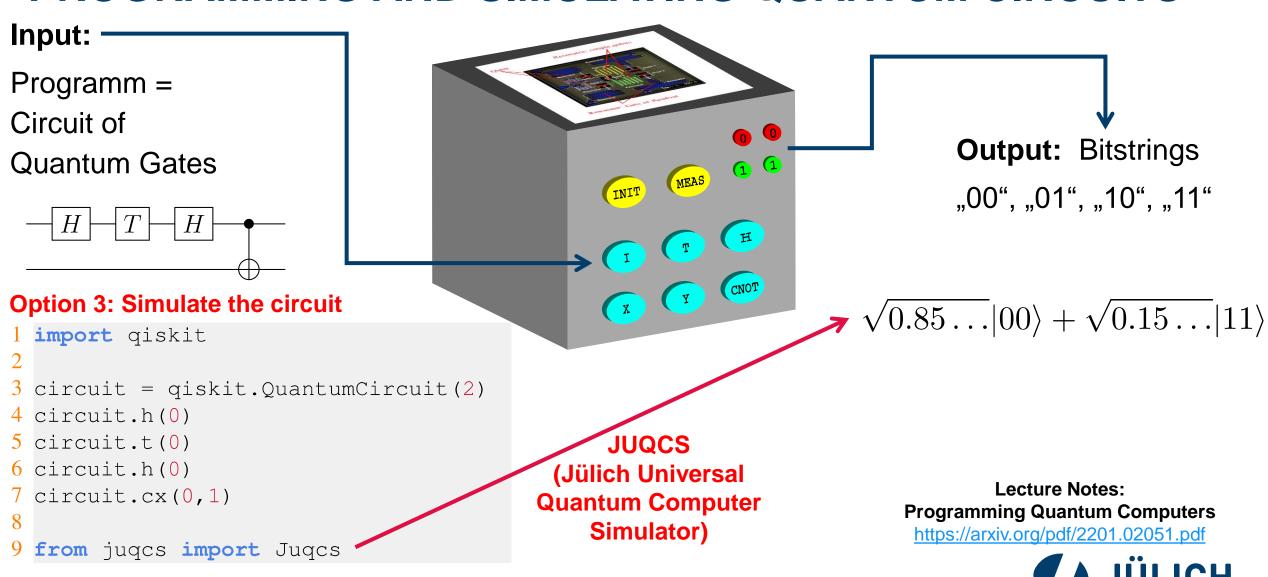


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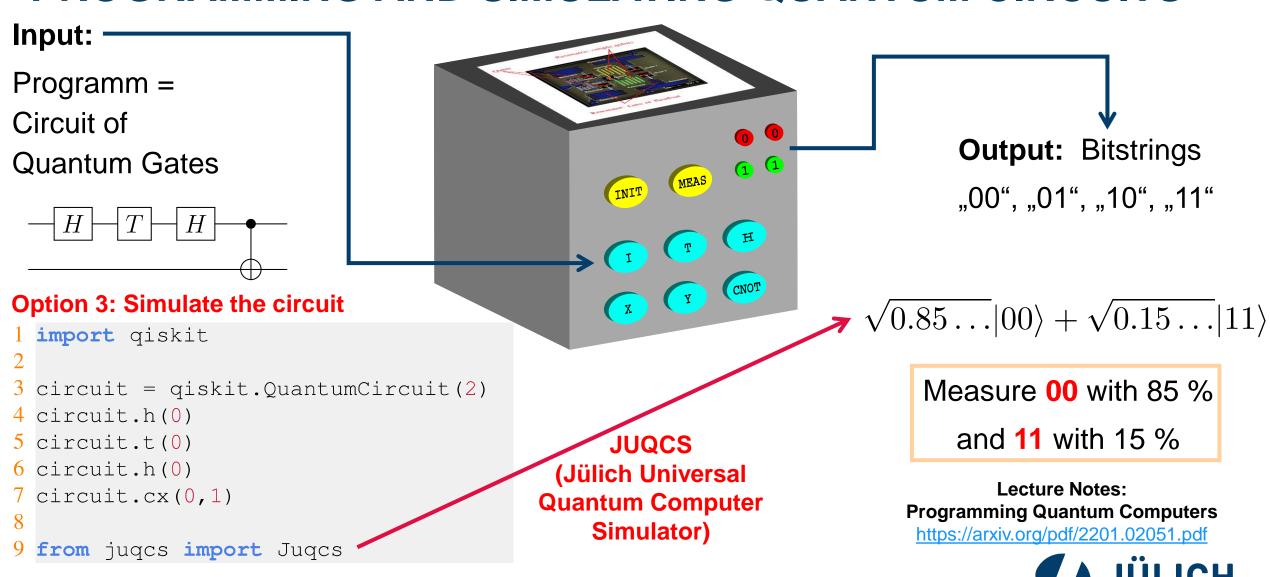


from jugcs import Jugcs

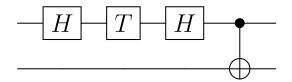
circuit.cx(0,1)



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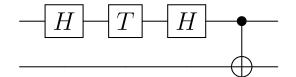
Simulation with Qiskit Aer





Simulation with Qiskit Aer

qasm_simulator

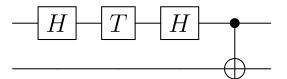


```
{'00': 856, '11': 144}
```



Simulation with Qiskit Aer

qasm_simulator

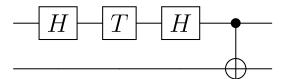


```
import qiskit
circuit = qiskit.QuantumCircuit(2)
circuit.h(0)
circuit.t(0)
circuit.h(0)
circuit.cx(0,1)
circuit.measure all()
backend = qiskit.Aer.get backend('qasm simulator')
result = qiskit.execute(circuit.reverse bits(),__
                       backend=backend,
                       shots=1000).result()
result.get counts()
{'00': 856, '11': 144}
                 Measure 00 with 85 %
                    and 11 with 15 %
```



Simulation with Qiskit Aer

qasm_simulator



statevector_simulator

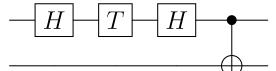
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result = giskit.execute(circuit.reverse bits(),
                       backend=backend,
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result.get counts()
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                    and 11 with 15 %
```

```
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 = qiskit.execute(circuit.reverse bits(),
                       backend=backend).result()
result.get statevector()
array([0.85355339+0.35355339j, 0.
                                       +0.j
                +0.j , 0.14644661-0.35355339j])
      0.
```



Simulation with Qiskit Aer

qasm_simulator _____



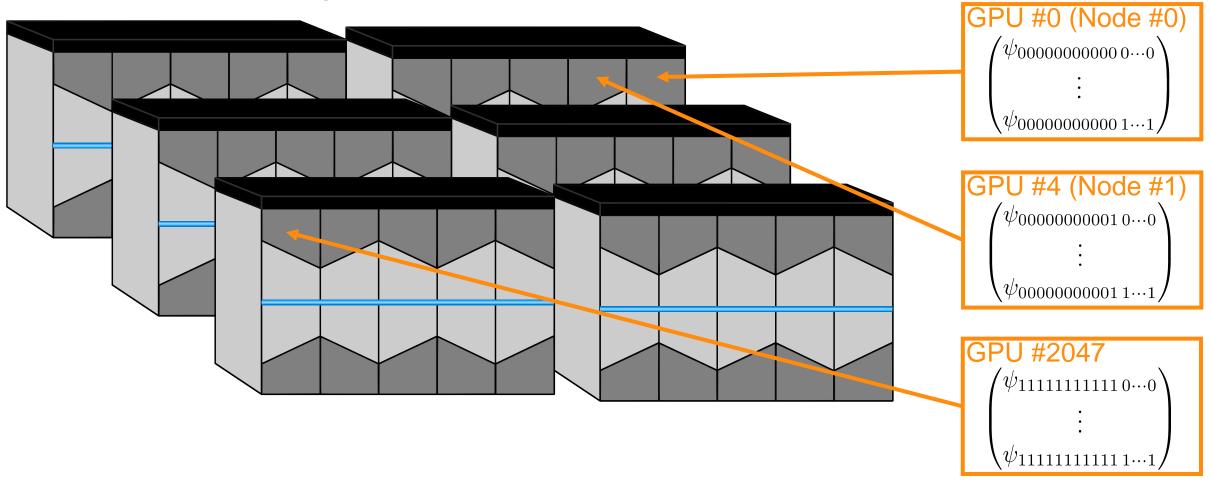
statevector_simulator

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                                         +0.j
                             , 0.14644661-0.35355339j])
      0.
                +0.j
       \sqrt{0.85...|00} + \sqrt{0.15...|11}
```

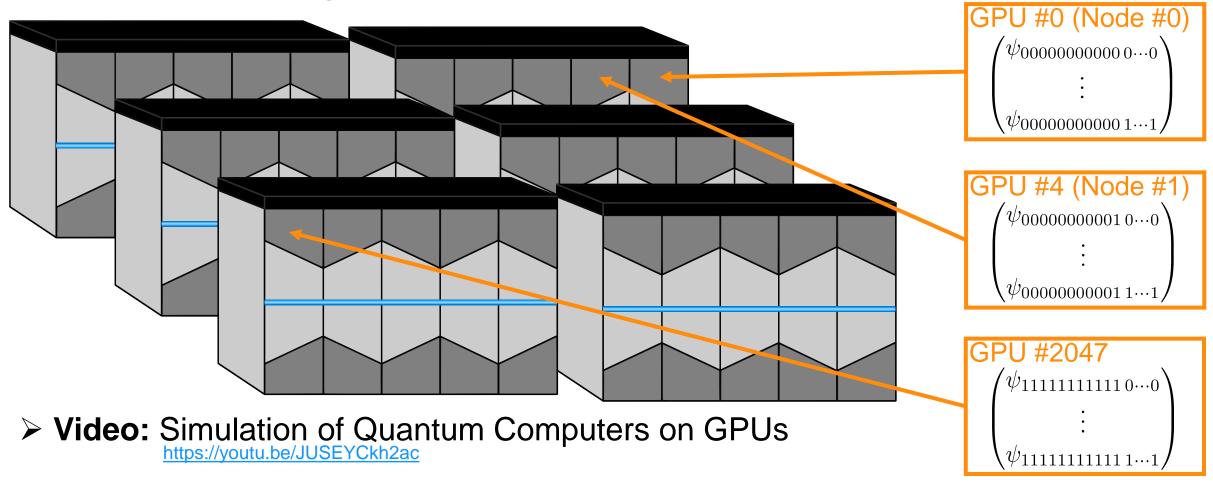
SIMULATING QUANTUM CIRCUITS

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



SIMULATING QUANTUM CIRCUITS

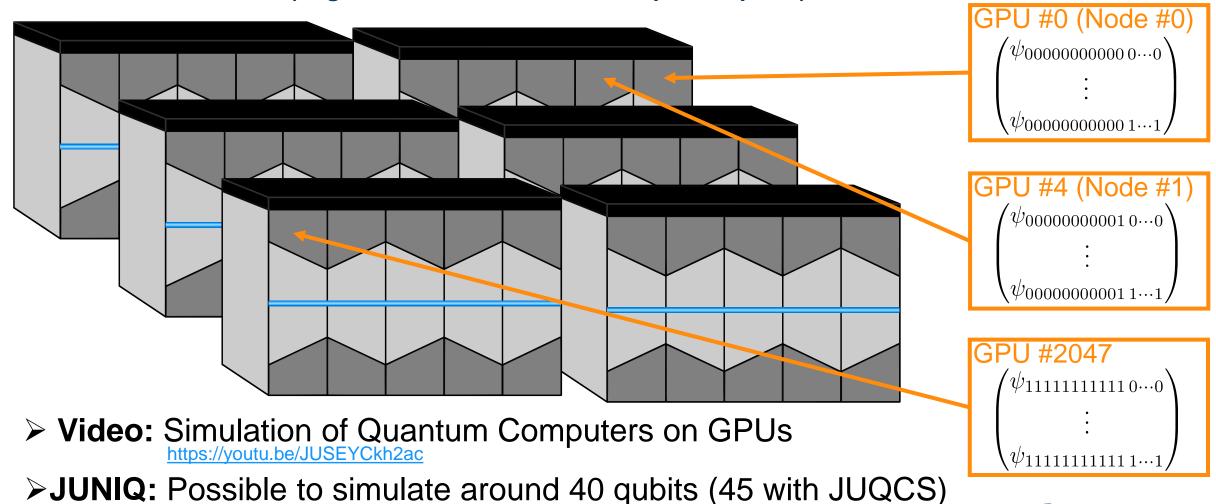
Simulation with JUQCS (large-scale simulations on a supercomputer)





SIMULATING QUANTUM CIRCUITS

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



Page 11

https://juniq.fz-juelich.de

An operation to move registers into phases and back



An operation to move registers into phases and back

> The formal definition of the QFT is:

$$|q_0q_1q_2\cdots\rangle \stackrel{\text{QFT}}{\mapsto} \sum_{q_0'q_1'q_2'\cdots} e^{2\pi i (q_0q_1q_2\cdots) (q_0'q_1'q_2'\cdots)/2^N} |q_0'q_1'q_2'\cdots\rangle$$



An operation to move registers into phases and back

> The formal definition of the QFT is:

> Intuition:

$$|j\rangle \leftrightarrow \sum_{j'} e^{2\pi i j j'/2^n} |j'\rangle$$

$$|q_0q_1q_2\cdots\rangle \stackrel{\text{QFT}}{\mapsto} \sum_{q_0'q_1'q_2'\cdots} e^{2\pi i (q_0q_1q_2\cdots)(q_0'q_1'q_2'\cdots)/2^N} |q_0'q_1'q_2'\cdots\rangle$$

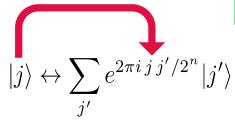
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> Implementation for two qubits:

$$|q_2\rangle$$
 H S H H



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 H S H H

Verification:

SWAP
$$(I \otimes H)$$
 CS $(H \otimes I) |q_2q_3\rangle \propto$

$$|00\rangle$$
 $|01\rangle$ $|10\rangle$ $|11\rangle$

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

rification:
$$SWAP (I \otimes H) CS (H \otimes I) |q_2q_3\rangle \propto \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & i & -1 & -i \\ 1 & -1 & 1 & -1 \\ 1 & -i & -1 & i \end{pmatrix} |q_2q_3\rangle = \sum_{q_2'q_3'} e^{2\pi i \, (q_2q_3) \, (q_2'q_3')/4} |q_2'q_3'\rangle$$

An operation to move registers into phases and back

The formal definition of the QFT is:

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$$e^{2\pi i (q_2 q_3) 0/4} |0\rangle$$

$$+ e^{2\pi i (q_2 q_3) 1/4} |1\rangle$$

$$+ e^{2\pi i (q_2 q_3) 2/4} |2\rangle$$

$$+ e^{2\pi i (q_2 q_3) 3/4} |3\rangle$$

A nice application of the QFT



A nice application of the QFT

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

$$|q_0q_1\rangle|q_2q_3\rangle$$

$$\mapsto$$

$$|q_0q_1\rangle|q_0q_1+q_2q_3\rangle$$



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Page 13

> Such a modulo-4 adder would also work on superpositions



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



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$$\mapsto$$

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

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

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

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

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



A nice application of the QFT



A nice application of the QFT

➤ Idea: → The QFT converts between registers and phases



A nice application of the QFT

- ➤ Idea: → The QFT converts between registers and phases
 - → By using bitwise phase shifts, we can implement the addition in the exponent



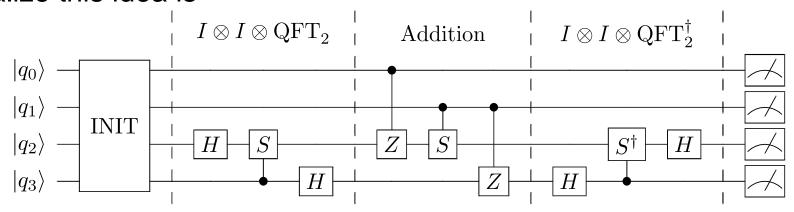
A nice application of the QFT

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 - → This is automatically modulo 4



A nice application of the QFT

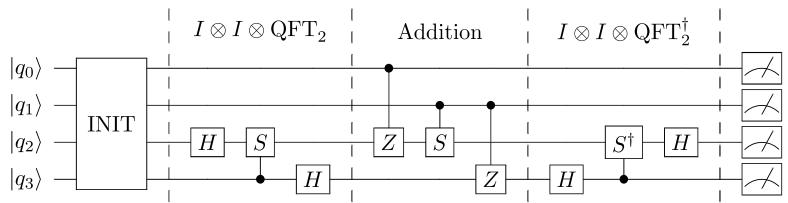
- ➤ Idea: → The QFT converts between registers and phases
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A nice application of the QFT

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Page 14

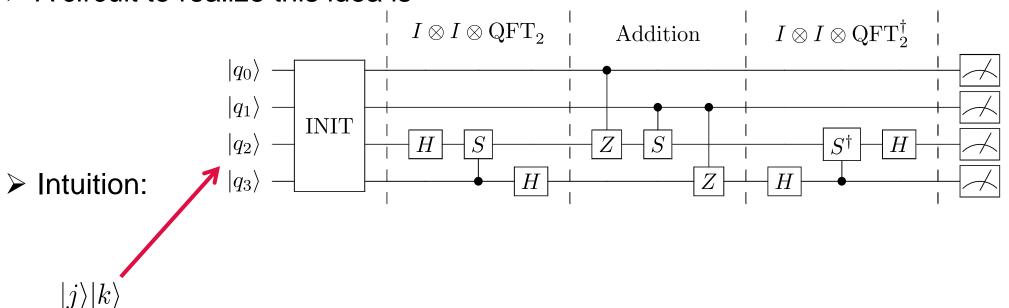


A nice application of the QFT

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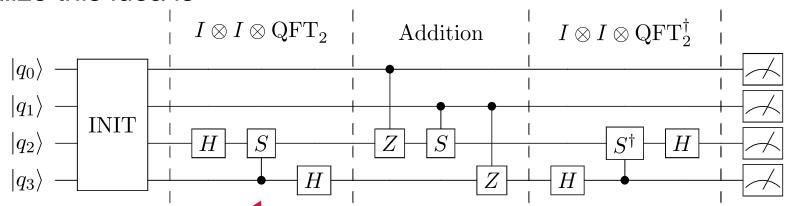
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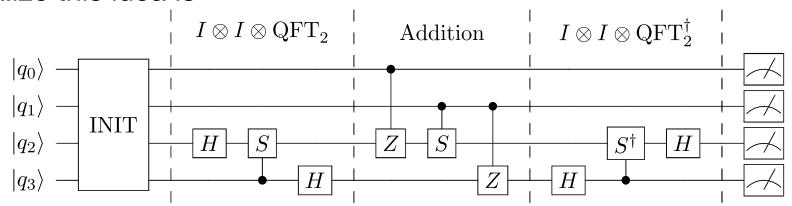


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$$|j\rangle|k\rangle \mapsto |j\rangle \left(\sum_{k'} e^{2\pi i \, k \, k'/2^n} |k'\rangle\right)$$

A nice application of the QFT

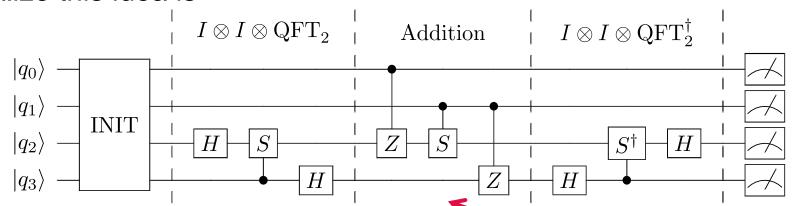
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$$|j\rangle|k\rangle \mapsto |j\rangle \left(\sum_{k'} e^{2\pi i \, k \, k'/2^n} |k'\rangle\right) = \sum_{k'} e^{2\pi i \, k \, k'/2^n} |j\rangle|k'\rangle$$

A nice application of the QFT

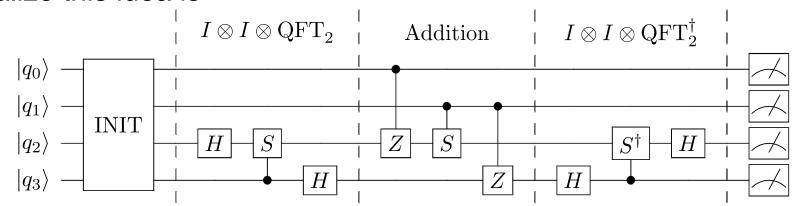
- ➤ Idea: → The QFT converts between registers and phases
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$$|j\rangle|k\rangle\mapsto|j\rangle\left(\sum_{k'}e^{2\pi i\,k\,k'/2^n}|k'\rangle\right)=\sum_{k'}e^{2\pi i\,k\,k'/2^n}|j\rangle|k'\rangle\mapsto\sum_{k'}e^{2\pi i\,(j+k)\,k'/2^n}|j\rangle|k'\rangle$$

A nice application of the QFT

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

A very brief overview of the QAOA

> Say we want to find the minimum of the function

$$E(q_0, \dots, q_{n-1}) = \sum_{i,j} q_i Q_{ij} q_j$$



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A very brief overview of the QAOA

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> Say we want to find the minimum of the function

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

"QUBO" (q = 0,1)



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Combinatorial optimization problem

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 \Leftrightarrow "QUBO" (q = 0,1)

- $E(s_0, \dots, s_{n-1}) = \sum_{i < j} h_i s_i + \sum_{i < j} J_{ij} s_i s_j$
 - "Ising" (s = +1,-1)

- Combinatorial optimization problem
 - → discrete optimization is hard!



A very brief overview of the QAOA

> Say we want to find the minimum of the function

$$E(q_0,\ldots,q_{n-1}) = \sum_{i,j} q_i Q_{ij} q_j \qquad \Leftrightarrow \qquad E(s_0,\ldots,s_{n-1}) = \sum_i h_i s_i + \sum_{i < j} J_{ij} s_i s_j$$
 "QUBO" (q = 0,1)

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

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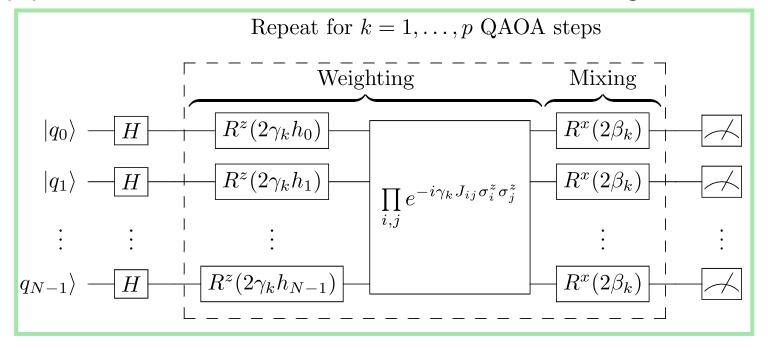


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➤ Look at p=1 QAOA step

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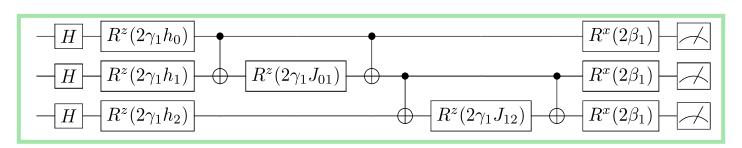
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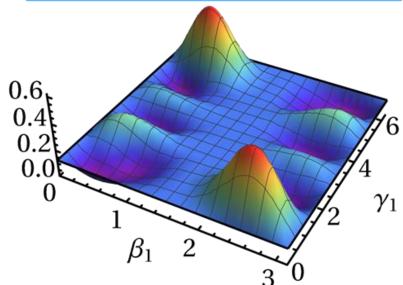
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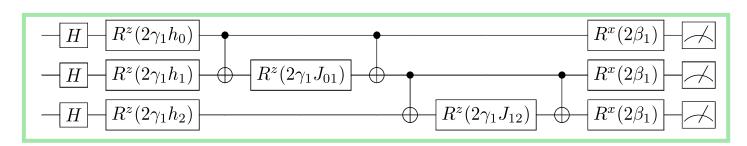
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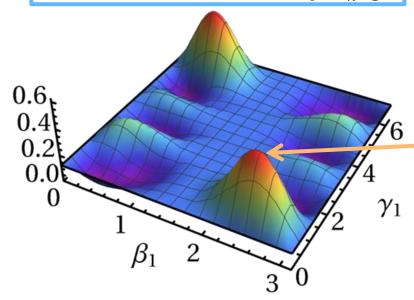
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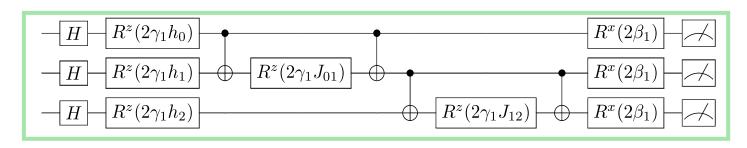
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Success probability $|\psi_{q_0^*\cdots q_{n-1}^*}|^2$





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



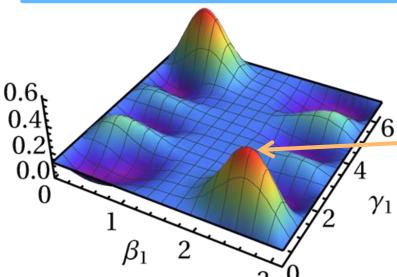
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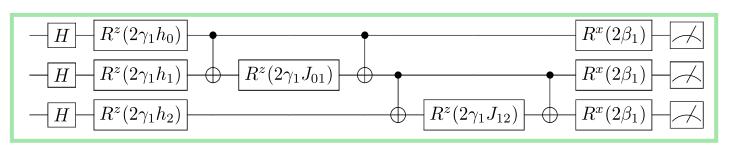
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➤ Look at p=1 QAOA step

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



➤ Will be a central topic of this School ©



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THANK YOU FOR YOUR ATTENTION

> Further information:

Programming Quantum Computers:

> JUQCS: Video

> JUQCS: Paper

https://arxiv.org/pdf/2201.02051.pdf

https://youtu.be/JUSEYCkh2ac

https://doi.org/10.1016/j.cpc.2022.108411

