## Quantum computing and quantum machine learning: <br> Introduction

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| Airbus Quantum Computing Challenge <br> Bringing flight physics into the Quantum Era |  |  |  |  |  |  |  |  |  |  |
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| ZEITT <br> olitik Gesellschaft Wirtschaft Kultur • Wissen Gesundheit • Digital Campus • Arbeit Sport ZEITmagazin • mehr • |  |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |  |
| Technologie <br> Bund investiert zwei Milliarden Euro für Quantencomputer <br> Innerhalb von fünf Jahren soll in Deutschland ein Quantencomputer entstehen. Mithilfe von Qubits erzielt die Technologie weit höhere Leistungen als herkömmliche Rechner. <br> 11. Mai 2021, 11:29 Uhr / Quelle: ZEIT ONLINE, dpa, kzi / $\square$ |  |  |  |  |  |  |  |  |  |  |

## The future is Quantum.




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## Application fields


[https://www.bcg.com/de-
de/publications/2019/quantum-computers create-value-when

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## Emerging technology:

## Quantum computing

Quantum computing (QC) has the potential to lead to disruptive changes in many industrial areas:

- Simulation of quantum mechanical systems
- (Development of new drugs, chemical sector with battery development, ...)
- Optimization problems (Logistics, production, pharma,...)
- Quantum machine learning (Computer vision, mobility,...)


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## Applications in particle physics

a
Odd lattice sites
$\stackrel{\bullet}{n} \cong \stackrel{\uparrow}{n} \cong \operatorname{vac} L_{n}=L_{n-1}$
$\mathrm{O}_{n} \cong \underset{n}{\Omega} \cong e^{-} \quad L_{n}=L_{n-1}-1$
Even lattice sites
$\stackrel{\hat{n}}{n} \cong e^{+} \quad L_{n}=L_{n-1}+1$
$\mathrm{O}_{n} \cong \underset{n}{n} \cong$ vac $L_{n}=L_{n-1}$
d


## Lattice QCD

- fundamental interactions in discretized space


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## Is it all just a hype?

„We help companies make better decisions in less time with quantum-hybrid computing"
"Quantum computing has the potential to drive the major breakthroughs needed to help solve the climate crisis."
"Much like artificial intelligence in its early days, the reputation of quantum computing has been tarnished by grand promises and few concrete results. Talk of quantum computers is often closely flanked by promises of polynomialtime solutions to NP-Hard problems and other such implausible appeals to blind optimism.."

## What quantum computing might be able to do and what not:

## QC will not replace classical computers.

- QC are expected to lead to exponential or polynominal speed-up for certain calculations (or more precisely subroutines).
Academic quantum advantage has been claimed.
A practical quantum advantage has not been shown yet.
- A claim on quantum utility has been made recently.


## Plan for the lectures

1. Intro to quantum computing (Jeanette)
2. Fault-tolerant quantum computing (Federico)
3. Introduction to NISQ quantum computing (Jeanette)
4. Quantum computing for optimization problems (Federico)
5. Quantum machine learning (Jeanette)

Lectures interleaved with tutorials (typically first lecture, then tutorial)


## Jeanette

## Searches for SUSY + DM, additional Higgs bosons @ ATLAS -> Quantum computing @ Fraunhofer/LMU



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## Introduction to quantum computing

1. What is quantum computing?
2. Basics:
a) History
b) Current research questions in quantum computing
c) Definitions
d) What is a qubit?
3. One and multi-qubit gates, simple algorithms

because nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy.

Richard Feynman, Simulating Physics with Computers, International Journal of Theoretical Physics 21, 467 (1982)

## History of QC



Fig. 3.3 Timeline of quantum computing and quantum machine learning
[M. Schuld \& F. Petruccione, Machine Learning with Quantum Computers, Springer 2021]

## Research questions

- What is quantum information?
- Can we build a computer based on quantum systems?
- How can we then formulate algorithms on such systems?
- What does quantum theory mean for the limits of what is computable?
- What distinguishes quantum computers from classical ones?
- With first small and noisy quantum computers starting to be available: for what can we use them? (Now and in perspective)
- How can we control their imperfection?

Research topics of Jeanette's department

- How to organise the interplay between classical and quantum computers?


## A few basic definitions

Qubit: A quantum system associated with two measurable states

Quantum computer (QC): Physical implementation of $n$ qubits with precise control on the evolution of the system

Quantum algorithm (QAlg): Controlled manipulations of a quantum system with subsequent measurement to retrieve information from the system

Quantum gates: Manipulation that act on one or two, ... qubits

A quantum algorithm can be formulated as quantum circuits of elementary gates

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## In a nutshell: What is quantum computing?

A classical bit can be either 0 or 1 .
A Quantum Bit ( $\wedge=$ Qubit) is the superposition of two states |0> und |1> at the same time:

$$
\begin{gathered}
a|0>+b| 1> \\
\text { with }|a|^{2}+|b|^{2}=1
\end{gathered}
$$

But: When measuring the qubit, only the classical states 0 and 1 can be measured, i.e. 0 is measured with a probability of $|a|^{2}$ and 1 with a probability of $|b|^{2}$
A quantum computer returns probabilistic results.


Qubit: Bloch sphere $=$

## The formal mathematical definition

A qubit is the fundamental unit of quantum information.
At any given time, it is in a superposition state represented by a linear combination of Dirac vectors $\mid 0>$ and $\mid 1>$ in $\mathbb{C}^{2}$ :

$$
|\psi>=a| 0>+b \mid 1>\text { where }|a|^{2}+|b|^{2}=1
$$

## And $a, b \in \mathbb{C}$

The vectors |0> and |1> form an orthonormal basis of a two-dimensional Hilbert space -> Computational basis.
$a$ and $b$ are called probability amplitudes.
$\mid 0>$ and $\mid 1>$ can be represented as the standard basis states of $\mathbb{C}^{2}$ :

$$
\left|0>=\binom{1}{0} \in \mathbb{C}^{2}, \quad\right| 1>=\binom{0}{1} \in \mathbb{C}^{2}
$$

## A qubit in polar form

We can rewrite a qubit in polar form:

$$
|\psi>=a| 0>+b\left|1>=r_{1} e^{\varphi_{1} i}\right| 0>+r_{2} e^{\varphi_{2} i} \mid 1>
$$

Furthermore, we can identify two quantum states if they only differ by a multiple of a complex unit, i.e. by a factor $e^{i \varphi}$ for $0 \leq$ $\varphi<2 \pi$.

That means the above qubit is effectively the same as:

$$
\left|\psi>=r_{1}\right| 0>+r_{2} e^{\left(\varphi_{2}-\varphi_{1}\right) i} \mid 1>
$$

$r_{1}$ and $r_{2}$ are in $\mathbb{R}$ and $r_{1}{ }^{2}+r_{2}{ }^{2}=1$.

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## Mapping to the Bloch sphere

We can find $0 \leq \theta \leq \pi$ so that

$$
r_{1}=\cos \frac{\theta}{2} \text { and } r_{2}=\sin \frac{\theta}{2}
$$

With this:

$$
\left.\left|\psi>=\cos \left(\frac{\theta}{2}\right)\right| 0>+\sin \left(\frac{\theta}{2}\right) e^{\varphi i} \right\rvert\, 1>
$$

Using this, we can use a non-linear projection to get from the threedimensional surface of the hypershere in $\mathbb{C}^{2}$ (that one can think of as $\mathbb{R}^{4}$ ) to a two-dimensional surface of a Bloch sphere in $\mathbb{R}^{2}$. The main point why this does work is because we can ignore global phases.


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## Basic operations acting on one qubit

Table 3.3 Some useful single-qubit logic gates and their representations

| Gate | Circuit representation | Matrix representation | Dirac representation |
| :---: | :---: | :---: | :---: |
| X | - $X$ | $\left(\begin{array}{ll}0 & 1 \\ 1 & 0\end{array}\right)$ | $\|1\rangle\langle 0\|+\|0\rangle\langle 1\|$ |
| Y | $-{ }^{Y}$ | $\left(\begin{array}{cc}0 & -i \\ i & 0\end{array}\right)$ | $i\|1\rangle\langle 0\|-i\|0\rangle\langle 1\|$ |
| Z | $-2-$ | $\left(\begin{array}{cc}1 & 0 \\ 0 & -1\end{array}\right)$ | $\|1\rangle\langle 0\|-\|0\rangle\langle 1\|$ |
| H | - ${ }^{-}$ | $\frac{1}{\sqrt{2}}\left(\begin{array}{cc}1 & 1 \\ 1 & -1\end{array}\right)$ | $\frac{1}{\sqrt{2}}(\|0\rangle+\|1\rangle)\langle 0\|+\frac{1}{\sqrt{2}}(\|0\rangle-\|1\rangle)\langle 1\|$ |
| $S$ | $-5$ | $\frac{1}{\sqrt{2}}\left(\begin{array}{ll}1 & 0 \\ 0 & i\end{array}\right)$ | $\frac{1}{\sqrt{2}}\|0\rangle\langle 0\|+\frac{1}{\sqrt{2}} i\|1\rangle\langle 1\|$ |
| $R$ | $-2$ | $\frac{1}{\sqrt{2}}\left(\begin{array}{lc}1 & 0 \\ 0 & e^{(-i \pi / 4)}\end{array}\right)$ | $\frac{1}{\sqrt{2}}\|0\rangle\langle 0\|+\frac{1}{\sqrt{2}} e^{(-i \pi / 4)}\|1\rangle\langle 1\|$ |

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## Two qubits

Orthonormal basis formed by two qubits:

$$
\begin{aligned}
& \left|\psi>_{1}=a_{1}\right| 0>_{1}+b_{1} \mid 1>_{1}>\text { where }\left|a_{1}\right|^{2}+\left|b_{1}\right|^{2}=1 \\
& \left|\psi>_{2}=a_{2}\right| 0>_{2}+b_{2} \mid 1>_{2}>\text { where }\left|a_{2}\right|^{2}+\left|b_{2}\right|^{2}=1
\end{aligned}
$$

The orthonormal basis is then:

$$
\left|0>_{1} \otimes\right| 0>_{2},\left|0>_{1} \otimes\right| 1>_{2},\left|1>_{1} \otimes\right| 0>_{2},\left|1>_{1} \otimes\right| 1>_{2}
$$

Or in short:

$$
|00>,|01>,|10>,| 11>
$$

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## Example: Representation of numbers

To display numbers from 0 to 15 in bits, we need 4 bits:
0000
0001
0010
0011
0100

1111

Four qubits allow to represent all of these 16 states at the same time:

$$
\begin{aligned}
& |0000>+|0001>+|0010>+| 0011\rangle+| 0100\rangle+|0101\rangle+ \\
& |0110>+|0111>+|1000>+| 1001\rangle+| 1010\rangle+|1011\rangle+ \\
& |1100\rangle+|1101\rangle+|1110\rangle+|1111\rangle
\end{aligned}
$$

$\rightarrow$ Parallelisation of calculations possible.

With n qubits $2^{n}$ states can be represented at the same time.

## Basic operations acting on multiple qubits

| Gate | Circuit representation | Matrix representation |
| :---: | :---: | :---: |
| CNOT |  | $\left(\begin{array}{llll}1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0\end{array}\right)$ |
| SWAP | * | $\left(\begin{array}{llll}1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1\end{array}\right)$ |
| T |  | $\left(\begin{array}{llllllll}1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0\end{array}\right)$ |

Multi-qubit gates are required to entangle qubits (and without entanglement some basic benefit of QC not available).

## Definition:

A 2-qubit state in $\mathbb{C}^{2} \otimes \mathbb{C}^{2}$ is called entangled if and only if it cannot be written as tensor product of two 1 -qubit kets:

$$
\left|\psi_{1}>\otimes\right| \psi_{2}>=\left(a_{1}\left|0>_{1}+b_{1}\right| 1>_{1}\right) \otimes\left(a_{2}\left|0>_{2}+b_{2}\right| 1>_{2}\right)
$$

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## Measurement of a two-qubit system

- Usually measurements in the compuational basis
- Measurements are represented by projections onto the possible eigenspaces:

$$
P_{0}=|0><0| \text { or } P_{1}=|1><1|
$$

- E.g., $p(0)=\operatorname{tr}\left(P_{0}|\psi><\psi|\right)=\langle\psi| P_{0}\left|\psi>=\left|a_{1}\right|^{2}\right.$
- The full oberservable corresponding to the computational basis measurement is the Pauli-z observable:

$$
\sigma_{z}=|0><0|-|1><1|
$$

- With the eigenvalues:

$$
\begin{aligned}
& +1 \text { for |0> } \\
& -1 \text { for |1> }
\end{aligned}
$$

## Measurement in practise

- How to obtain a expectation value? -> Sample. Run a QAlg $s$ times. $s$ is called the number of shots.
- How many shots are required to obtain an estimate $<\sigma_{z}>$ with an error $\varepsilon$ ?
-> Bernoulli experiment
- In case of large $s$ and a probability of $p \approx 0.5$ : Wald interval for $\left\langle\sigma_{z}\right\rangle=0$ :

$$
\varepsilon=z \cdot \sqrt{\frac{\hat{p}(1-\hat{p})}{s}}
$$

With $\hat{p}$ : estimator for the probability
$z$ : confidence level

- $0\left(\varepsilon^{-2}\right)$ samples required for a given $\varepsilon$ and $z$
- Example: $\varepsilon=0.1$ and $z=0.99$ : $s=167$

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## Measurement in practise

- If $\hat{p} \rightarrow 0$ or $\hat{p} \rightarrow 1$ :

The Wald approximation is not valid, instead the Wilson score interval is required:

$$
\varepsilon=\frac{z}{1+\frac{z^{2}}{s}}\left(\frac{\hat{p}(1-\hat{p})}{s}+\frac{z^{2}}{4 s^{2}}\right)^{1 / 2}
$$

=> For $\varepsilon=0.1$ only 27 measurements are required for the same boundaries as before.

[M. Schuld et al, Machine Learning with Quantum Computers, Springer 2021]

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## Why is quantum computing promising?

## Superposition of states

Entanglement of states - i.e. multiple qubits are connected/correlated.

Interference of qubits - i.e. states interfer $\rightarrow$ Enhancement or reduction of states (see Grover!)

Quantum computing could potentially result in an increased computing capacity - thus leads to a more efficient solution of problems.
$\rightarrow$ Simplified processing of complicated datasets, solution of currently unsolvable problems.

However: It is uncertain when the quality of quantum computers will be sufficient to fully profit from these advantages.

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## The flow of a quantum computation

Simplified: Superposition/Entanglement + Interference -> Solution


Superposition of all possibilities

## Quantum circuit

Computation driven interference


Solution
[https://qiskit.org/documentation/qc_intro.html]

## What is a quantum computer?

## Different criteria to assess quality of quantum computer

 + if it is a quantum computer:
## - Universality

- Universal quantum computer? -> Di Vicenzo criteria
- Fidelity (Quality of qubits)
- Scalability (Architecture scalable?)
- Qubits: number, architecture-specific limitations like nearest neighbor connections
- Logical connectivity (two-qubit gates possible for all qubits?)
- Circuit depth (How many operations possible?)


## Di-Vicenzo criteria:

1. Scalable qubit system with distinct qubits?
2. Ability to initialize the state of any qubit to a definite state in the computational basis
3. The qubits must hold their states
4. Ability to apply unitary operators to qubit states and to two qubits at once
5. Ability for ,strong' measurements, i.e. the ability that the measurement measures the state of the qubit for the property being measured

- Cloud access (and availability in general)


## Different QC hardware concept (examples)

## Neutral atoms

- Atom ensemble surrounded by laser system forming an magneto-optical trap, addressable arrays of atoms.
- Requires a specific way of programming (pulser), good connectivity, more native to QUBO formulations?

L. Henriet et al, Quantum Computing with neutral atoms, arXiv:2006.12326v2


## Superconducting qubits

- Superconducting Josephson junctions at cryogenic temperatures.
" Low connectivity, many SWAP operations needed for highly connected circuits, runtime environments in first attempts available



## Trapped ions

- Ionized atoms trapped in electric potentials to form a line of qubits.
- Can be operated at room temperature, high connectivity, no runtime environment and running jobs relatively manuel



## Source:

 https://www.aqt.eu/ media-press/, Dieter Kühl
## Example for a superconducting chip design




Ibm_cusco

127 qubits
[Visit via the IBM Lab, e.g.
https://quantum-
computing.ibm.com/services/res ources ]


## Classical computers

## Components of a classical computer (simplified):

- Processor (Central Processing Unit - CPU)
- Graphics Processing Unit (GPU) for specialized calculations
- Memory for storing information during the calculation
- Storage for long-term preservation of data


## Difference CPU and GPU:

- CPU good at performing different operations, but then maybe slow
- GPU good for a set of highly optimized operations - for these very fast (matrix multiplication)

Quantum computing to be included in these systems as Quantum Processing Unit


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## Storage of information and operations

A
Microprocessor Chip

## Capacity of storage:

- Measured in terabytes, gigabytes,
- 1 gigabyte $=1000$ megabytes $=\ldots=10^{9}$ bytes
- 1 byte $\wedge=8$ bits

Operations by using transitors

B


3D view of a transistor



The channel is open

## Operations



| INPUT |  | OUTPUT |
| :---: | :---: | :---: |
| A | B |  |
| 0 | 0 | 1 |
| 1 | 0 | 0 |
| 0 | 1 | 0 |
| 1 | 1 | 1 |

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## How to realize an addition

Task:
$0+0=0$
$1+0=1$
$0+1=1$
$1+1=0$ carry 1

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## How to realize an addition

Task:
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$1+0=1$
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Which logical gates are needed?


Almost there!

## How to realize an addition

Task:
$0+0=0$
$1+0=1$
$0+1=1$
$1+1=0$ carry 1

Which logical gates are needed?


Half-Adder

[Source: https://www.101computing.net/binary-additions-using-logic-gates/]

Almost there!

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## The interplay between classical and quantum computers



Classical computer or HPC system

## A word on complexity and what we need to achieve


[R. Sutor, Dancing with Qubits, Packt]

In QC we are interested in achieving at least a polynominal speedup with respect to classical algorithms.

## How to compare algorithms? - The ,Big - O' notation:

Let $f(n)$ and $g(n)$ be functions from positive integers to positive reals. We say $\mathrm{f}=\mathrm{O}(\mathrm{g})$ (which means that " f grows no faster than g ") if there is a constant $\mathrm{c}>0$ such that $f(n) \leq c \cdot g(n)$.

Example: Sorting

Sort $[7,-2,0,3]$ - How do you do it? In general number of swaps $\leq \frac{1}{2} n^{2}$
So $O\left(n^{2}\right)$

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With the advent of near-term quantum devices, this monolithic reliance on complexity theory is slowly changing. Empirical studies and proof-of-principle experiments have to deal with the details of an implementation, and a constant factor in the runtime, for example, if we need $\mathrm{n}=20$ qubits or $\mathrm{cn}=$ $1,000,000 * 20$ qubits (even if the constant $c$ does not grow with the problem size), suddenly becomes crucial. This is an exciting development: classical computer science would be widely decimated (and machine learning hardly existent) if the only algorithms people are interested in were those for which we can prove efficient runtimes on paper.
Maria Schuld et al.

## How to define quantum speedup?

## Terminology developed by T.F. Rnnow et al. to benchmark QCs and quantum algorithms:

## Provable quantum speedup:

- Proof required that there cannot be a classical algorithm that performs as well or better than the considered quantum algorithm
- This is the case for Grover's algorithm -> scales quadratically better than classical, given an oracle to mark the desired state


## Strong quantum speedup:

- Comparison of the quantum algorithm with the best known classical algorithm
- For example Shor's algorithm


## Common quantum speedup:

- Strong quantum speedup relaxed to comparing to best available classical algorithm


## Potential quantum speedup:

- Only comparing two specific algorithms and just referring to this comparison.


## Limited quantum speedup:

- Comparison of two conceptually equivalent algorithms.
- Example: quantum and classical annealing

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## Outlook: A map through fault-tolerant QC



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## Tutorial: the addition on a quantum computer

Tutorials attached to the agenda

## Setup:

- Either linux installation, virtual box with linux installation, or google colab
- Install via pip:
- pip install qiskit
- pip install pennylane
- (and probably a few more things will be requested during the installation process)
- Installation commands in google colab have to be preceeded by a !

