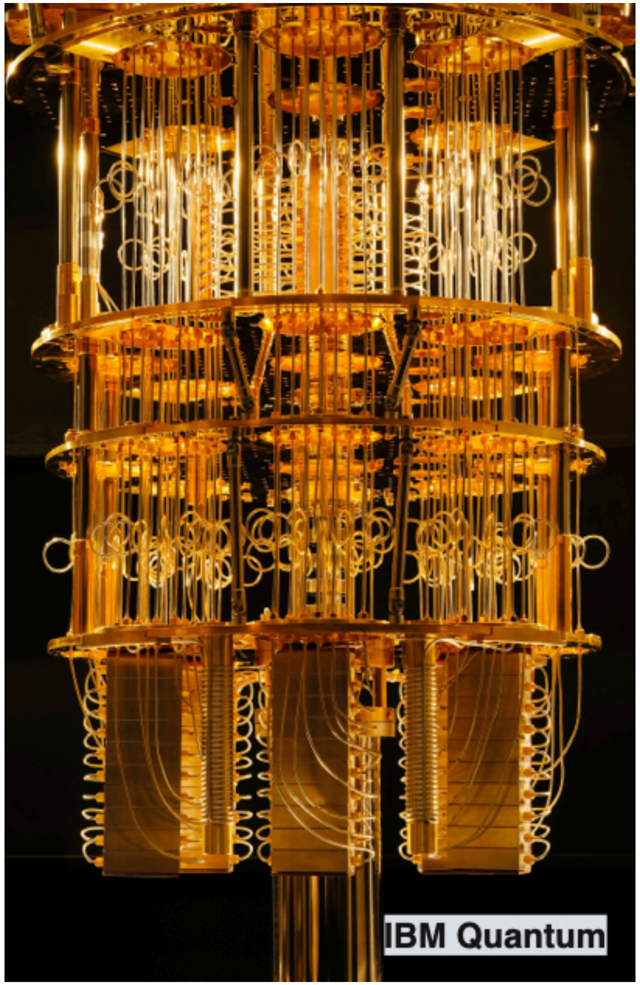
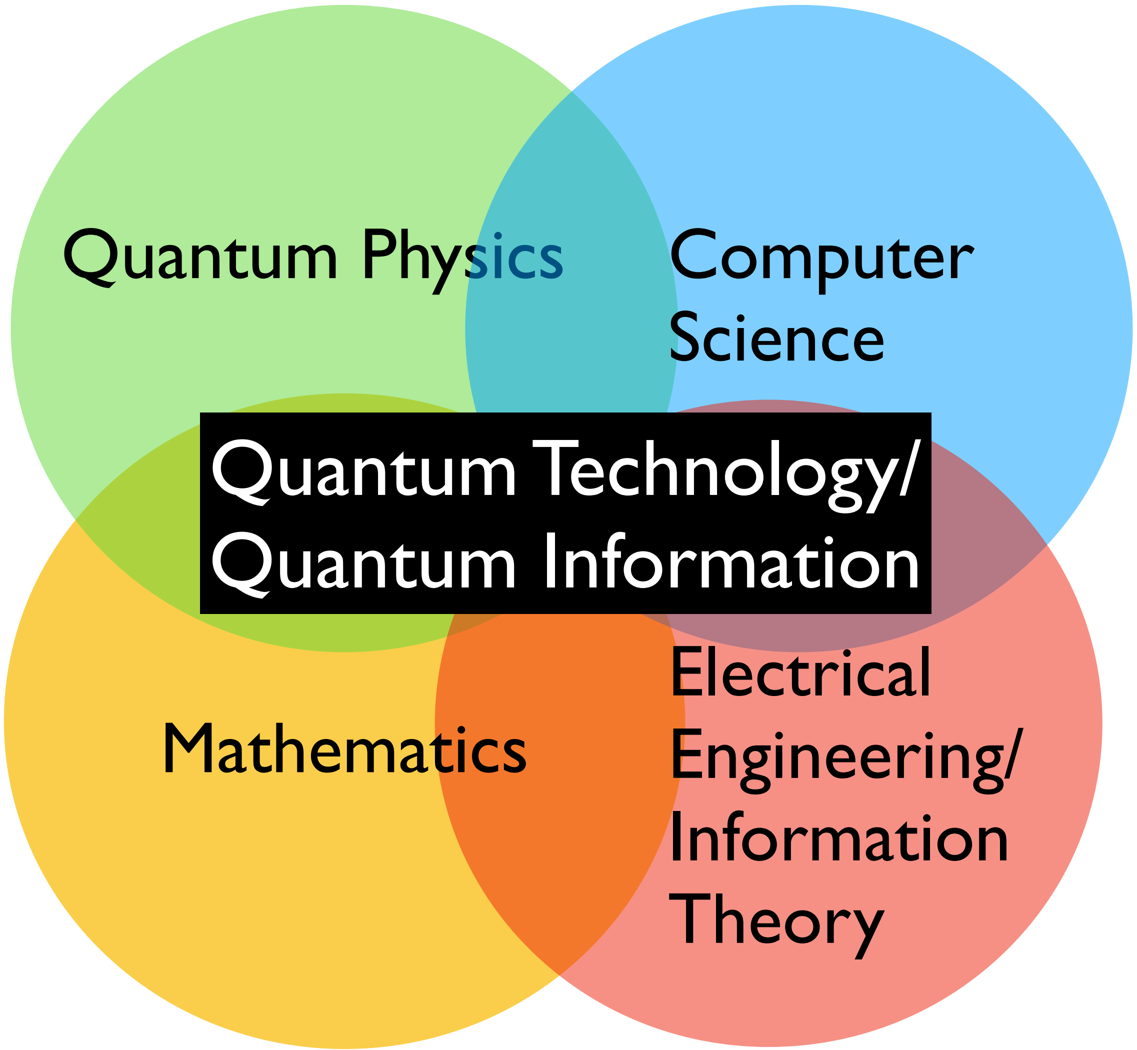
Applications of Quantum Computing: From Material Simulation to Quantum Optimization and „Quantum Machine Learning“



Sabine Tornow, MUAS

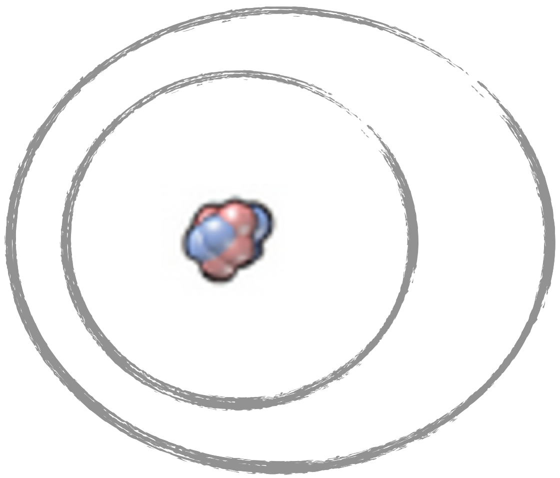
Thanks to: CODE FI, Universität der Bundeswehr München

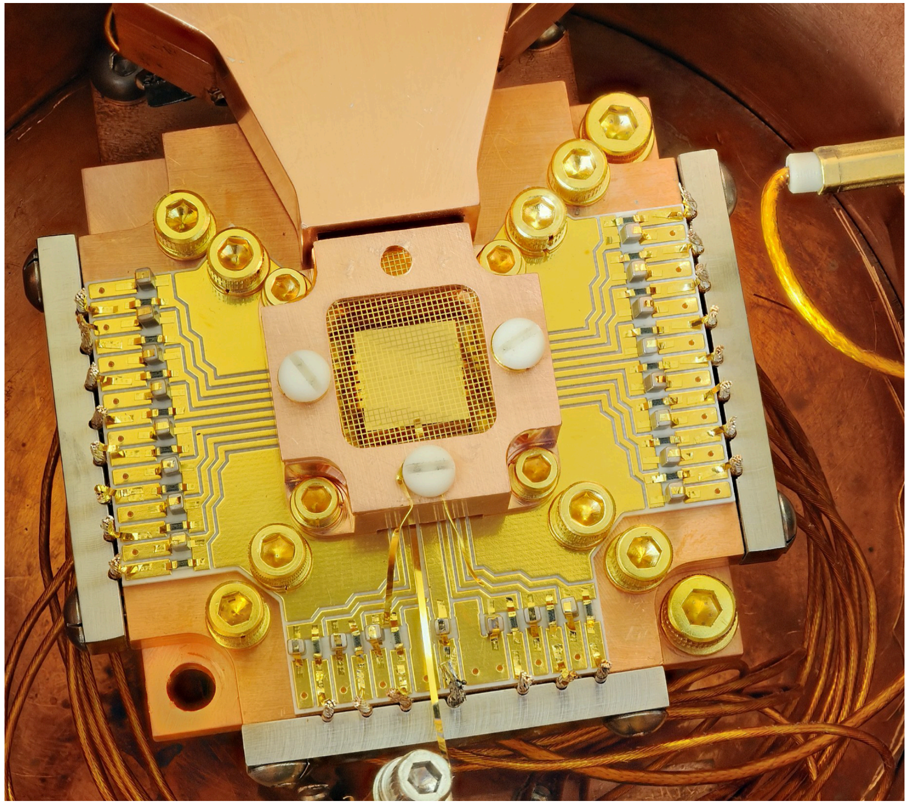
QUANTUM INFORMATION



If information is represented by a quantum system then it is by definition quantum information

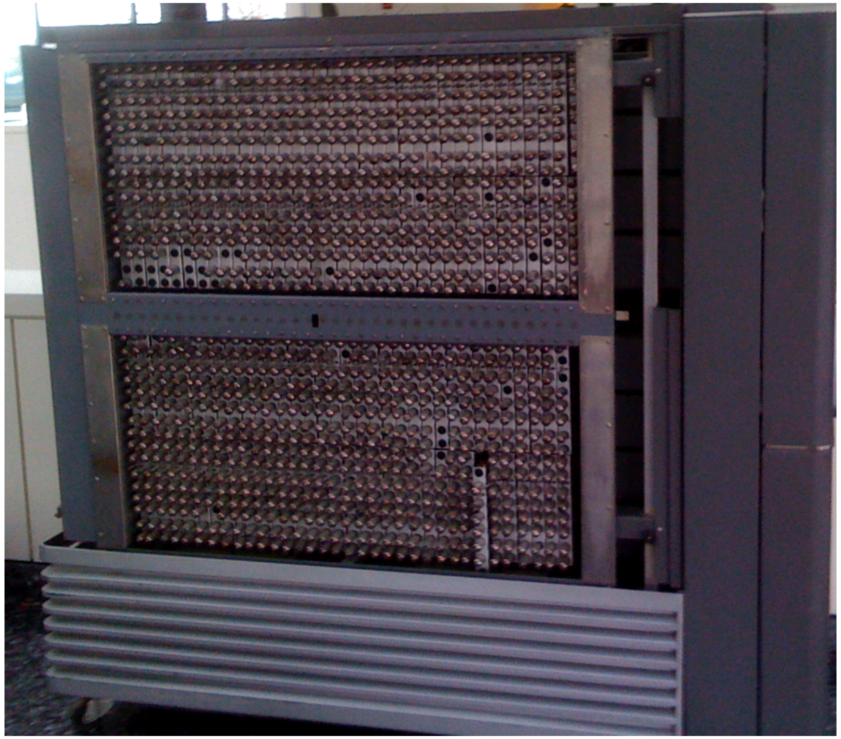
FIRST AND SECOND QUANTUM REVOLUTION



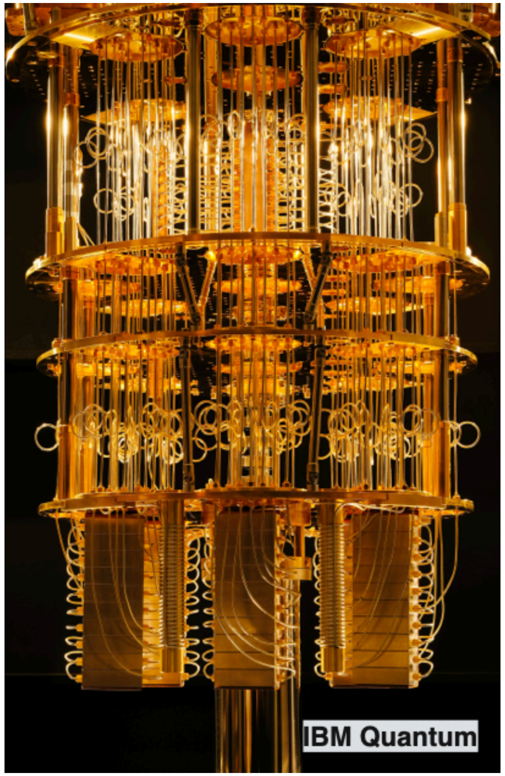


Wikipedia: Chip ion trap for quantum computing from 2011 at NIST.

WHERE DO WE STAND?



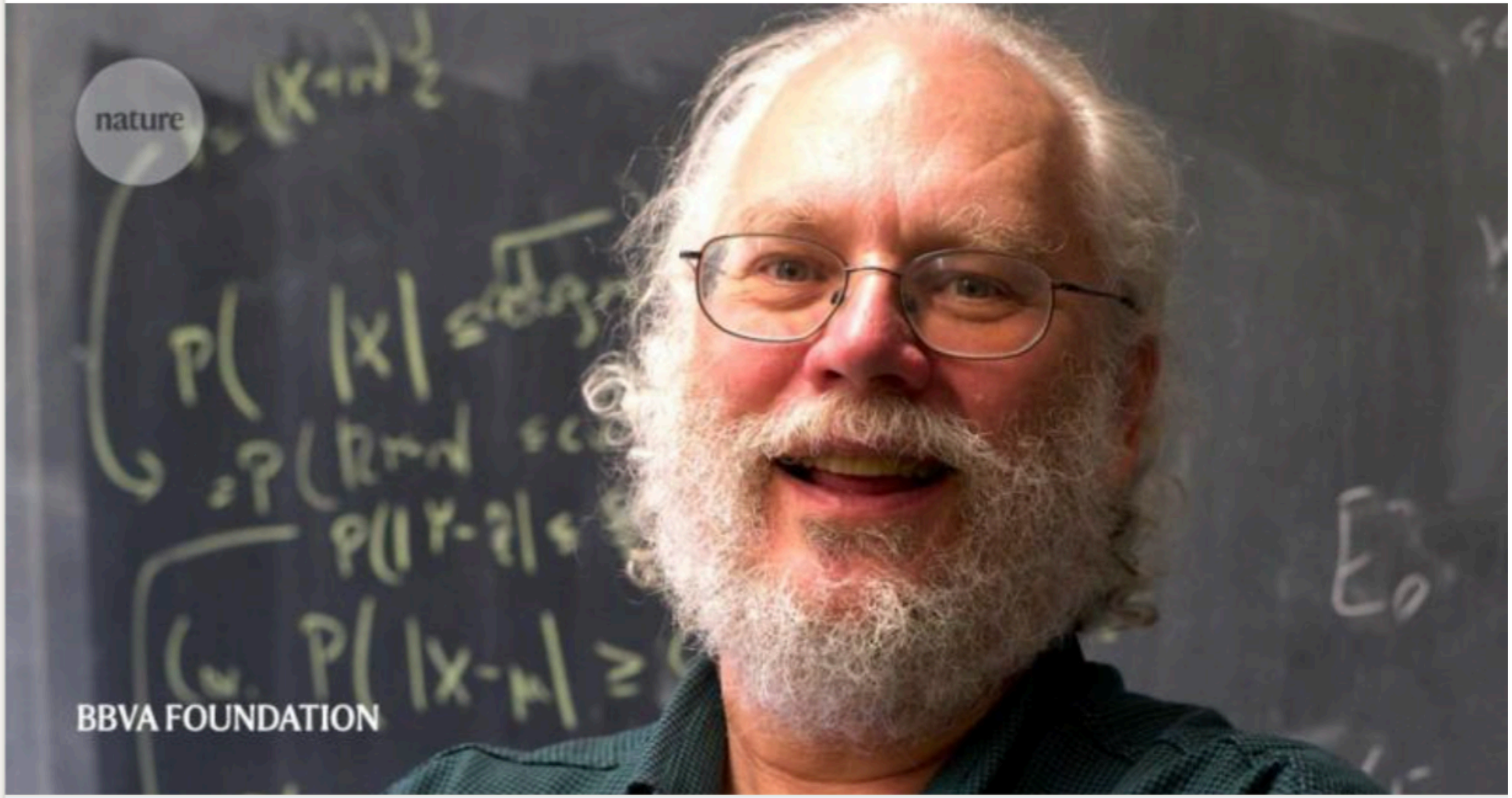
IBM 701



QUANTUM COMPUTERS ARE GOOD AT

- Quantum Physics/Quantum Chemistry
- Factoring
- Linear Algebra
- Searching
- Optimization
- Sampling
- Accelerating machine learning

Quantum computing is at the same time an enabler for incredible opportunities as well as one of the most unexpected threats to cybersecurity.



Quantum-computing pioneer warns of complacency over Internet security

nature.com • Lesedauer: 5 Min.

"I think the only obstruction to replacing RSA with a secure post-quantum cryptosystem will be will-power and programming time. I think it's something we know how to do; it's just not clear that we'll do it in time."

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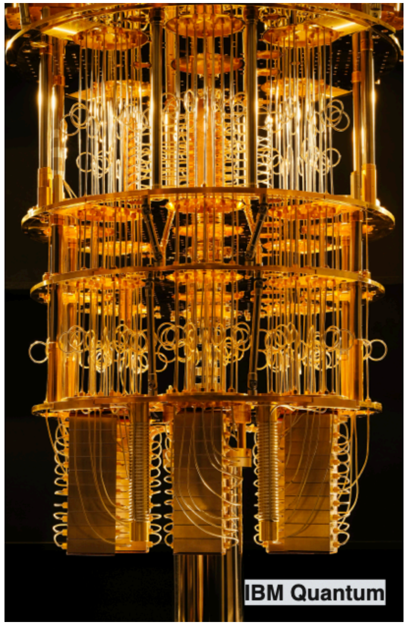
Present quantum hardware enables development of quantum heuristics

https://quantumalgorithmzoo.org

QUANTUM COMPUTING



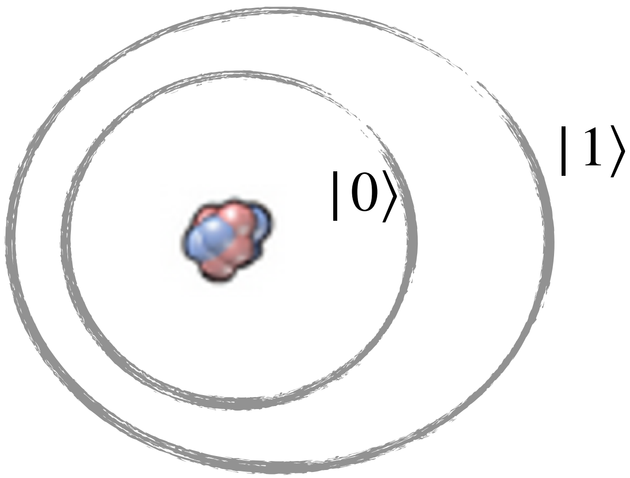
1. Quantum Computing

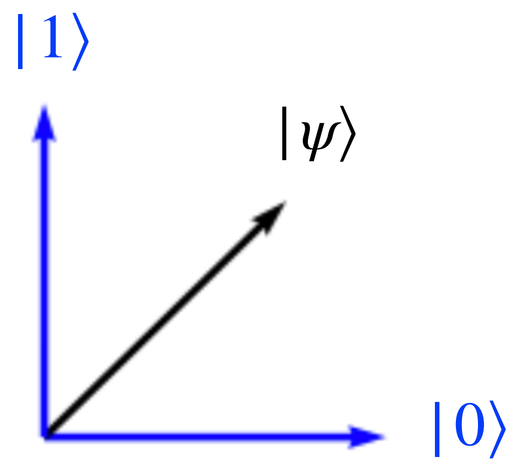
2. Applications:

   - Material Simulation/Open Quantum Systems
   - Optimisation
   - Machine Learning

3. Error mitigation

QUBIT





SUPERPOSITION

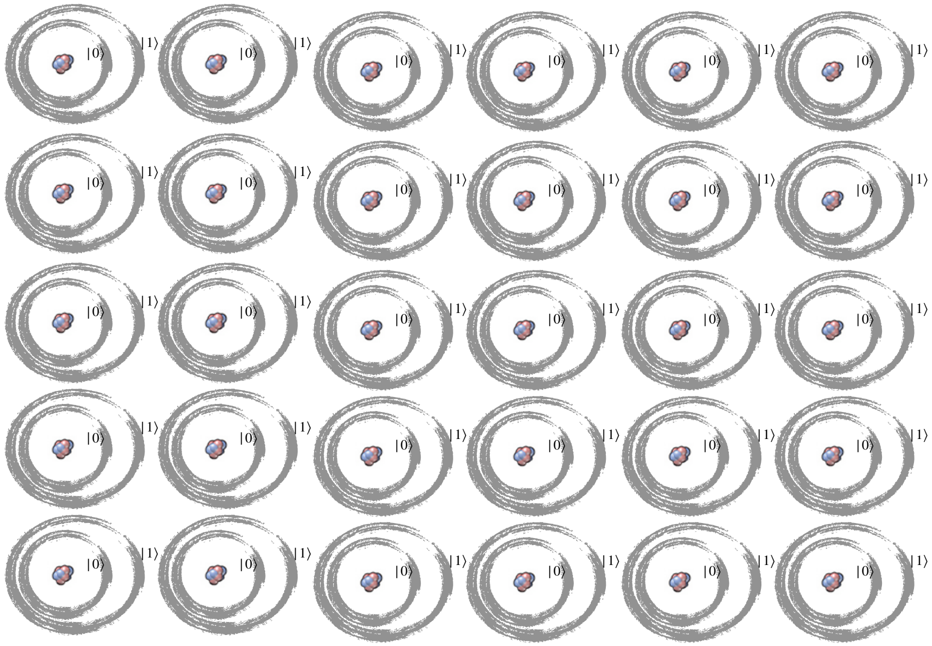
$$|\psi\rangle = a_0|0\rangle + a_1|1\rangle,$$

$$a_0, a_1 \in \mathbb{C},$$

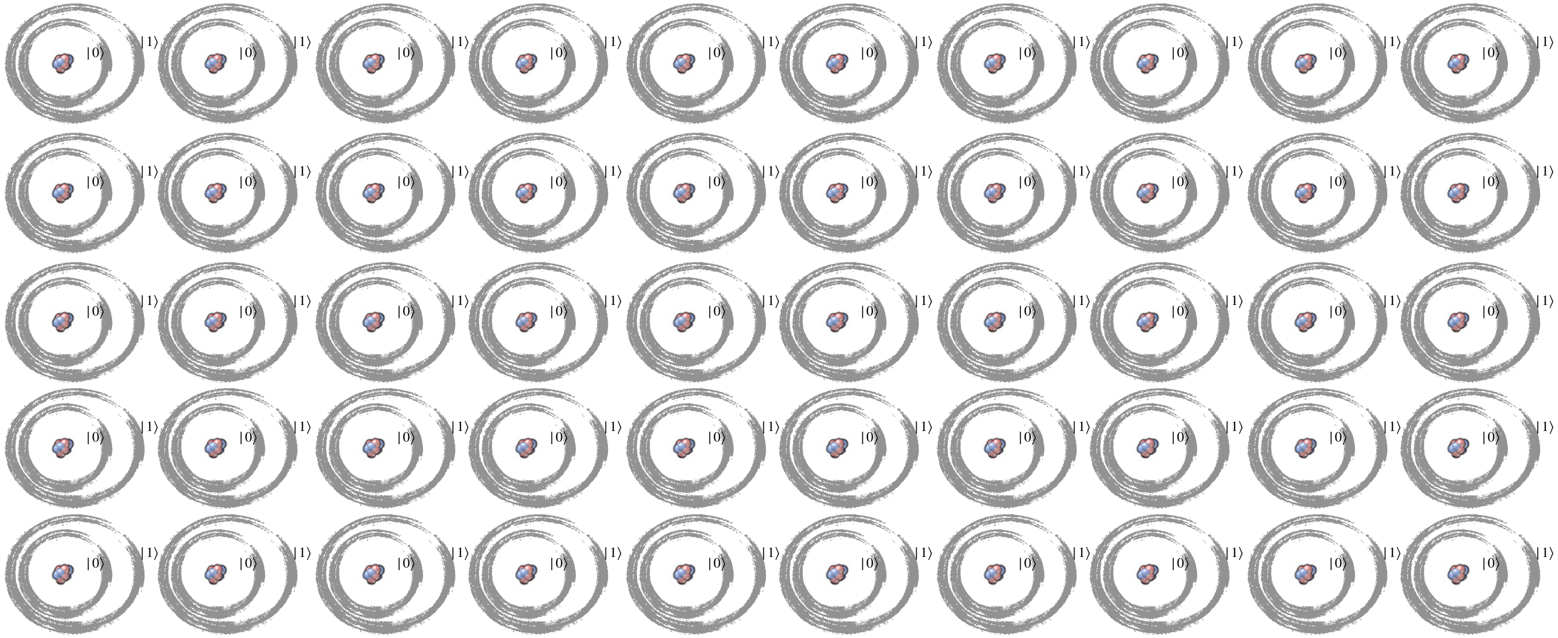
$$|\psi\rangle = \begin{pmatrix} a_0 \\ a_1 \end{pmatrix}$$

$$\sum_{k=0}^{n-1} |a_k|^2 = 1$$

SIMULATING A QUANTUM SYSTEM ON CLASSICAL COMPUTERS



SIMULATING A QUANTUM SYSTEM ON CLASSICAL COMPUTERS



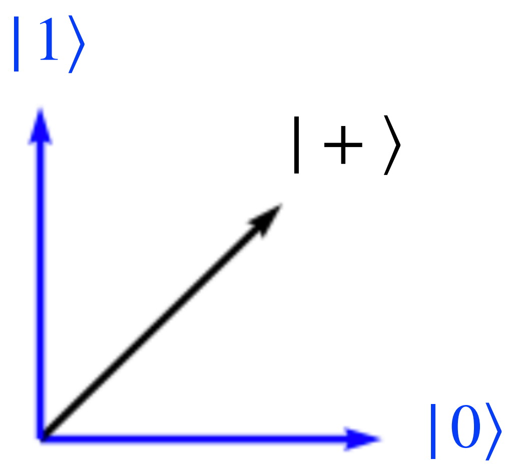
Sabine Tornow

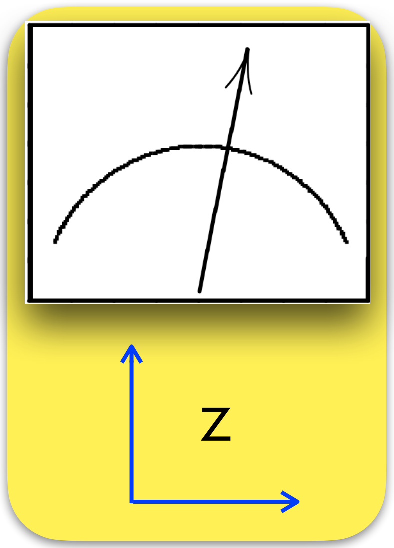
Z-MEASUREMENT

State prepared in:

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

Superposition





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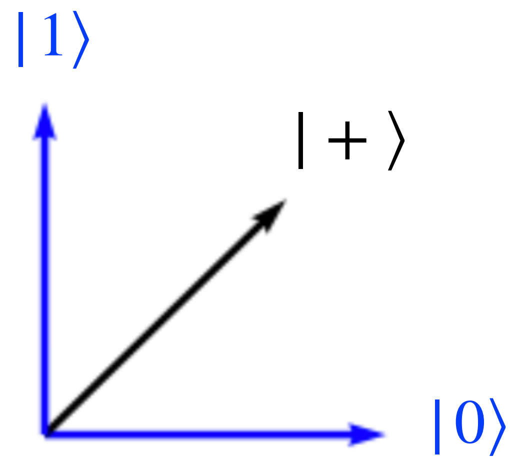

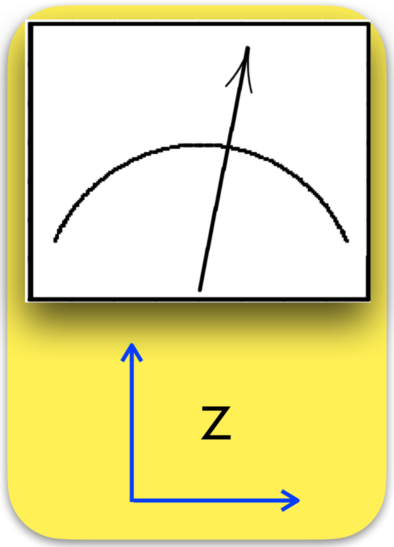

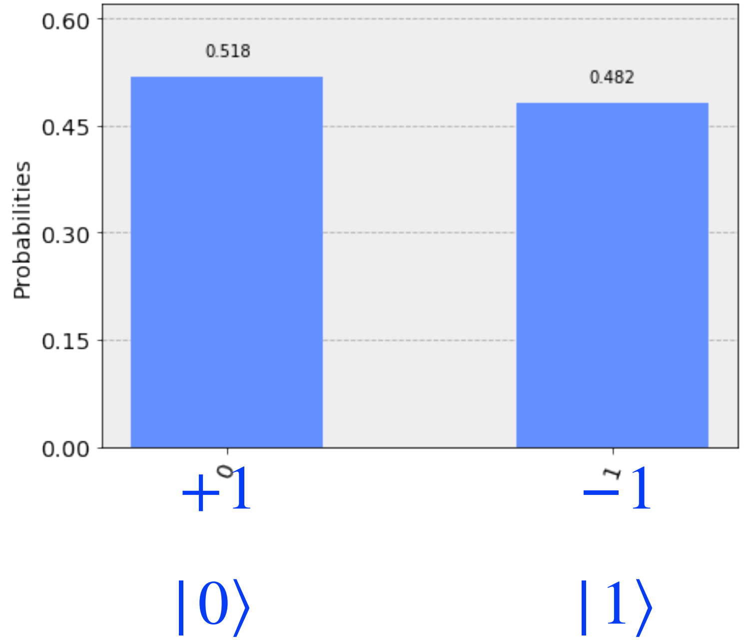

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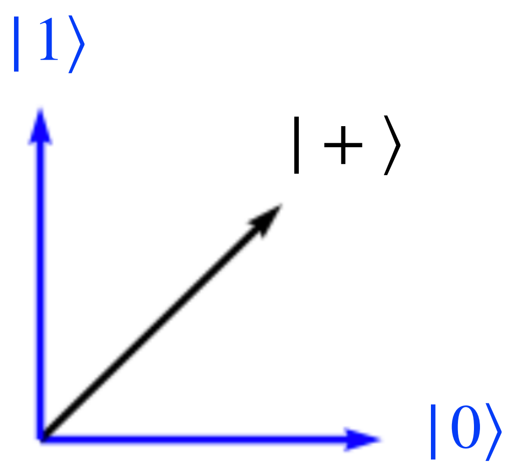
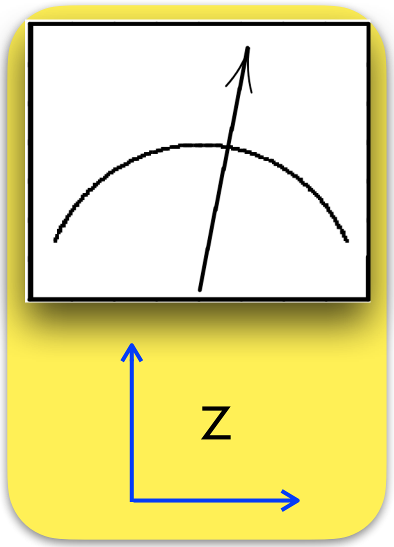
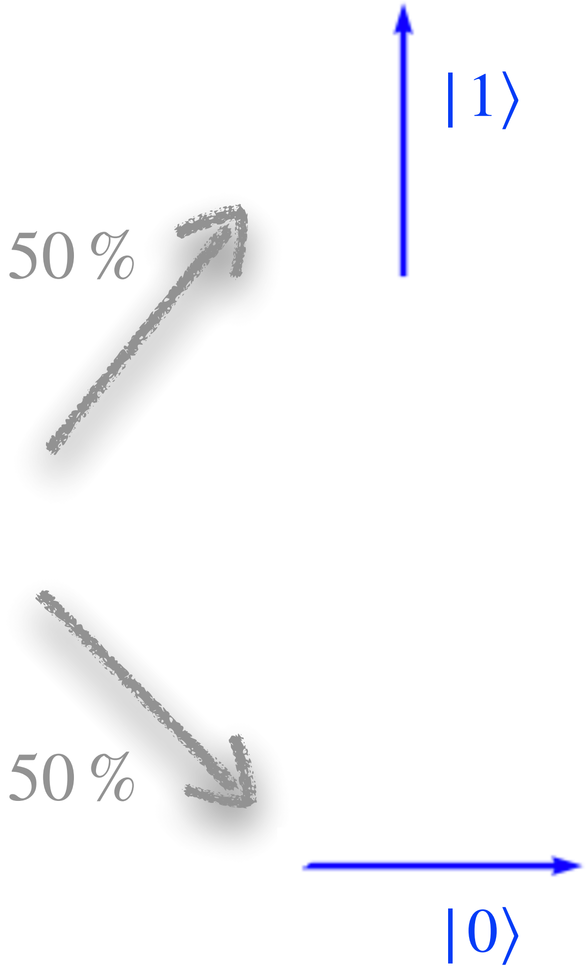




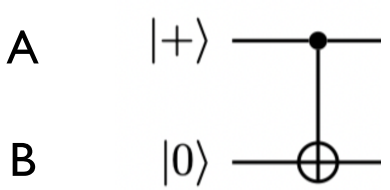


ENTANGLEMENT

Most remarkable manifestation of quantum information is

Entanglement (Verschränkung)

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

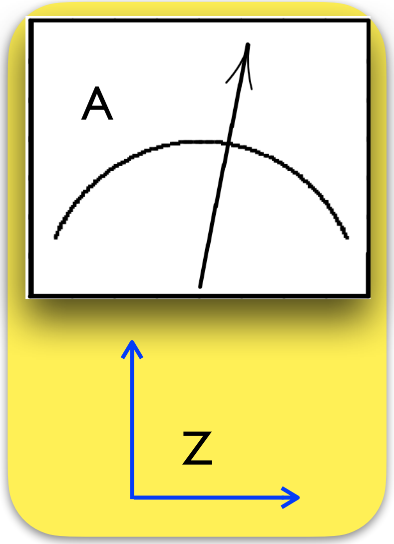


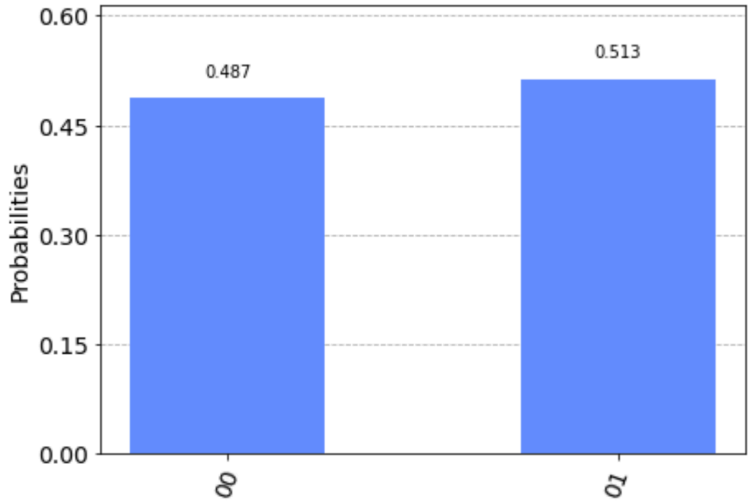
$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle_A \otimes |0\rangle_B + |1\rangle_A \otimes |1\rangle_B\right)$$

This state of two qubits behaves in ways that cannot be explained by supposing that each qubit has a state of its own.

ENTANGLEMENT

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle_A \otimes |0\rangle_B + |1\rangle_A \otimes |1\rangle_B\right)$$





ENTANGLEMENT

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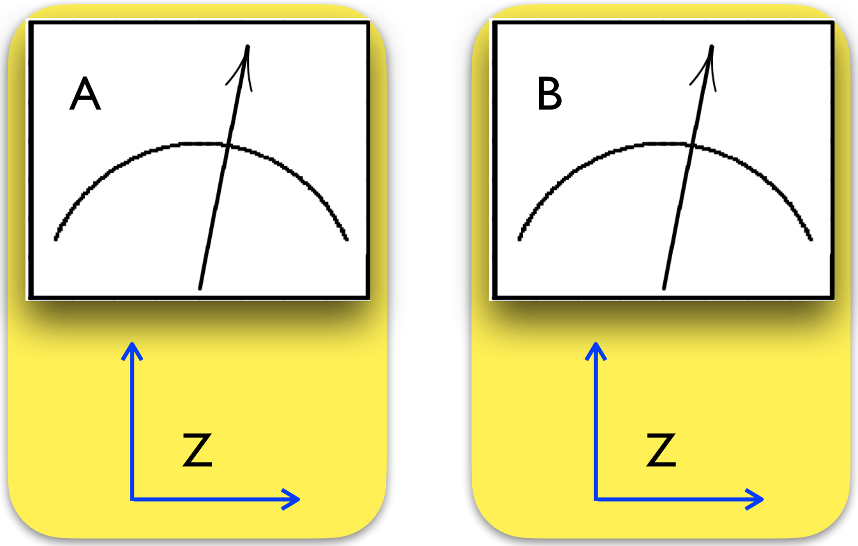
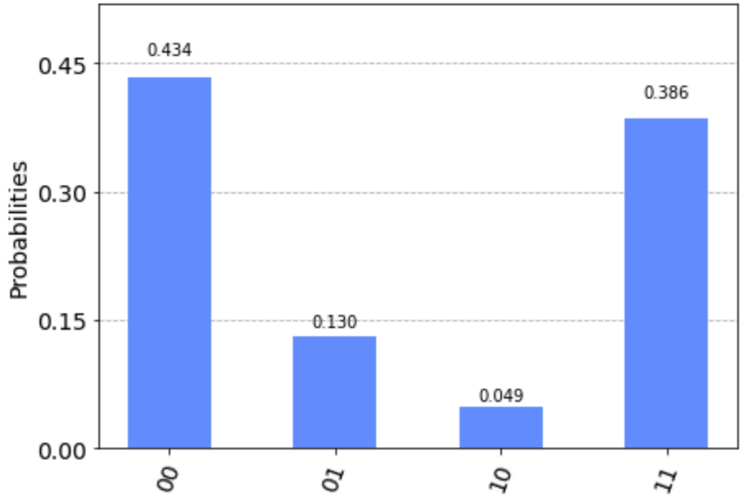
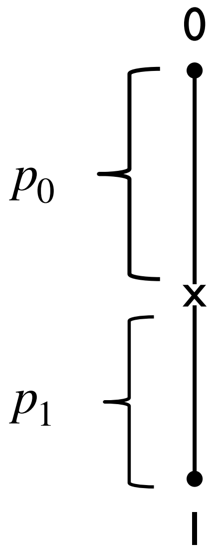
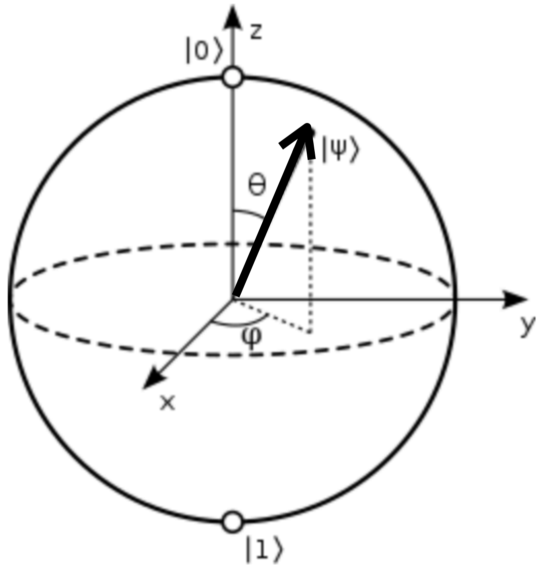




COMPARISON BETWEEN QUANTUM INFORMATION AND DISCRETE CLASSICAL PROBABILITY





Qubit: $|\psi\rangle = a|0\rangle + b|1\rangle$

Probability p_0 (p_1) that bit is 0 (1)

Probability $|a|^2$ that state is in $|0\rangle$
$|b|^2$ that state is in $|1\rangle$

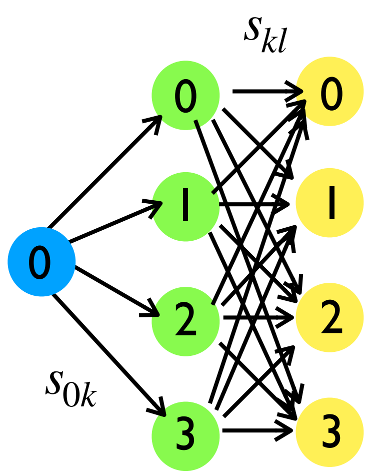
CLASSICAL PROBABILITY THEORY

State: probability vector $\begin{pmatrix} p_0 \\ p_1 \\ p_2 \\ p_3 \end{pmatrix}$ $\qquad \sum p_n = 1, \;\; 0 \leq p_n \leq 1, \;\; p_n \in \mathbb{R}$

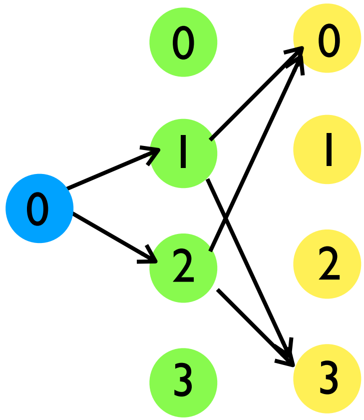
Time evolution:

$$\begin{pmatrix} s_{00} & s_{01} & s_{02} & s_{03} \\ s_{10} & s_{11} & s_{12} & s_{13} \\ s_{20} & s_{21} & s_{22} & s_{23} \\ s_{30} & s_{31} & s_{32} & s_{33} \end{pmatrix} \begin{pmatrix} p_0 \\ p_1 \\ p_2 \\ p_3 \end{pmatrix}$$

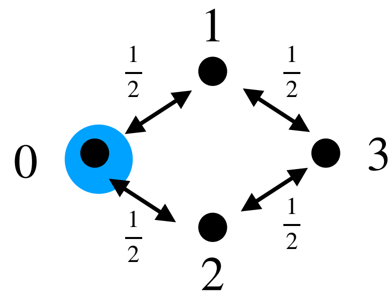
Stochastic matrix



CLASSICAL PROBABILITY THEORY (EXAMPLE)

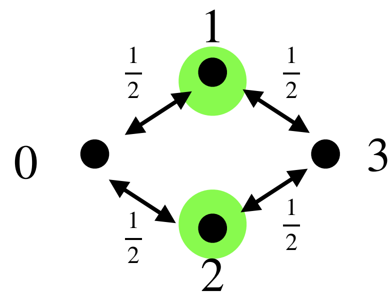


$$\begin{pmatrix} 0 & 1/2 & 1/2 & 0 \\ 1/2 & 0 & 0 & 1/2 \\ 1/2 & 0 & 0 & 1/2 \\ 0 & 1/2 & 1/2 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$



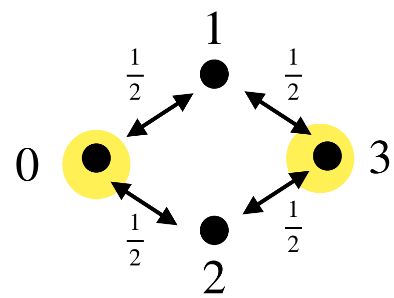
After the first time step

$$\begin{pmatrix} 0 & 1/2 & 1/2 & 0 \\ 1/2 & 0 & 0 & 1/2 \\ 1/2 & 0 & 0 & 1/2 \\ 0 & 1/2 & 1/2 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}$$

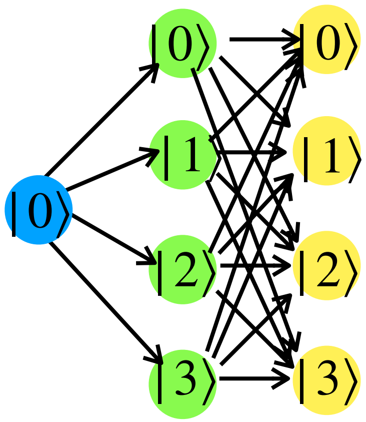


After the second time step

$$\begin{pmatrix} 0 & 1/2 & 1/2 & 0 \\ 1/2 & 0 & 0 & 1/2 \\ 1/2 & 0 & 0 & 1/2 \\ 0 & 1/2 & 1/2 & 0 \end{pmatrix} \frac{1}{2} \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$



QUANTUM INFORMATION



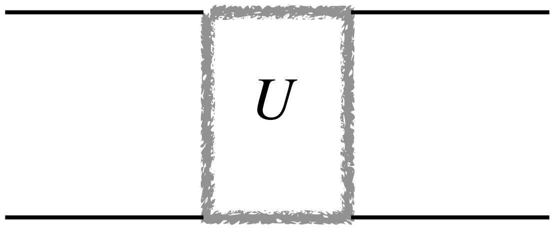
State: vector of probability amplitudes $\begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix}$

$a_n \in \mathbb{C}$

$0 \leq |a_n|^2 \leq 1$

$$\begin{pmatrix} u_{00} & u_{01} & u_{02} & u_{03} \\ u_{10} & u_{11} & u_{12} & u_{13} \\ u_{20} & u_{21} & u_{22} & u_{23} \\ u_{30} & u_{31} & u_{32} & u_{33} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix}$$

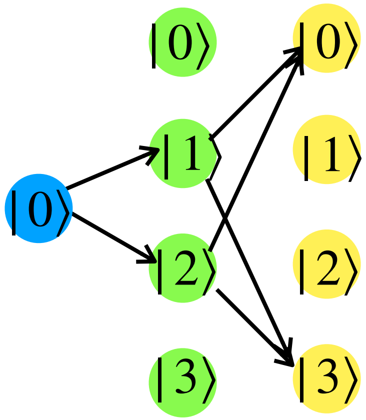
$|\psi\rangle$



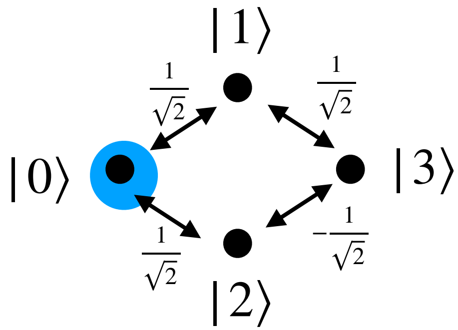
$|\psi'\rangle$

$$|\psi'\rangle = U|\psi\rangle$$

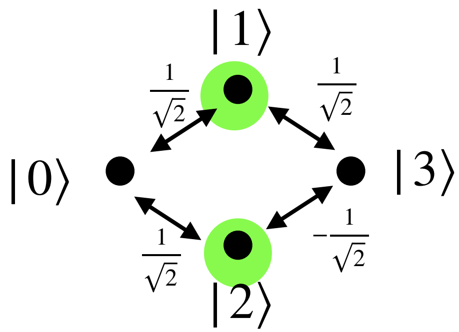
QUANTUM INFORMATION (EXAMPLE)



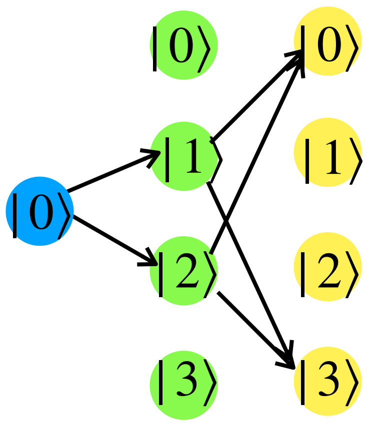
$$\begin{pmatrix} 0 & 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & 0 & 0 & 1/\sqrt{2} \\ 1/\sqrt{2} & 0 & 0 & -1/\sqrt{2} \\ 0 & 1/\sqrt{2} & -1/\sqrt{2} & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$



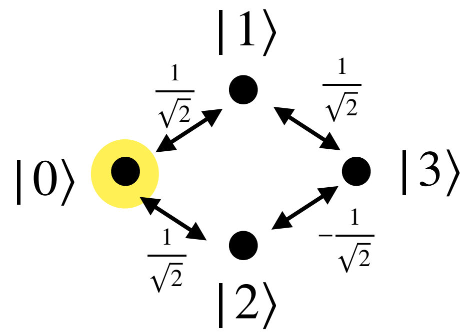
$$\begin{pmatrix} 0 & 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & 0 & 0 & 1/\sqrt{2} \\ 1/\sqrt{2} & 0 & 0 & -1/\sqrt{2} \\ 0 & 1/\sqrt{2} & -1/\sqrt{2} & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}$$



QUANTUM INFORMATION (EXAMPLE)



$$\begin{pmatrix} 0 & 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & 0 & 0 & 1/\sqrt{2} \\ 1/\sqrt{2} & 0 & 0 & -1/\sqrt{2} \\ 0 & 1/\sqrt{2} & -1/\sqrt{2} & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

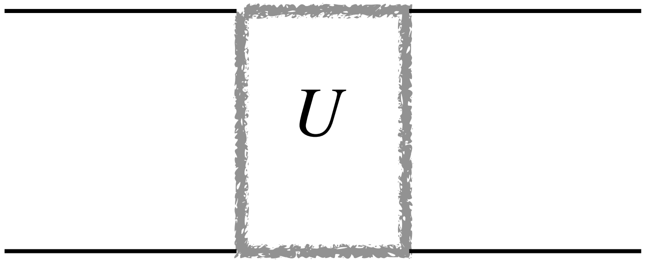


The system is again in state $|0\rangle$.

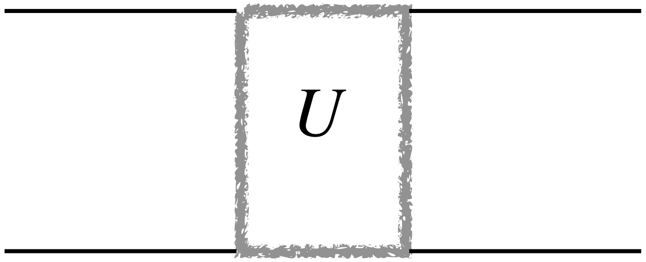
The system is never in state $|3\rangle$ (interference).

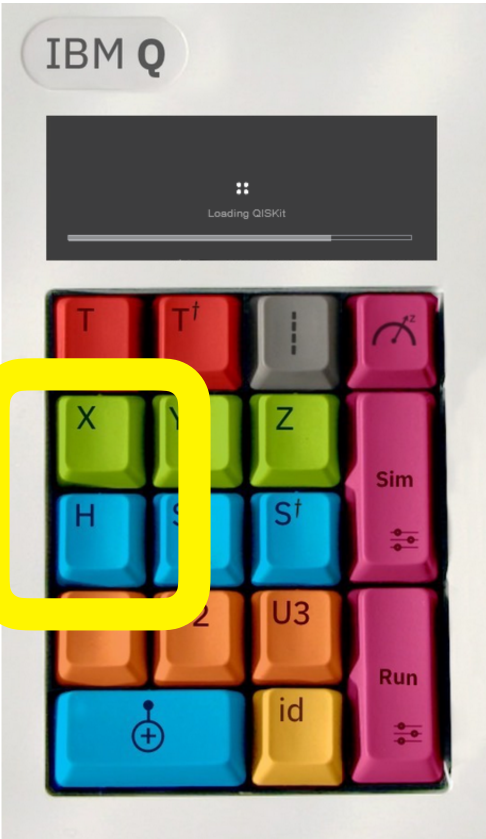
Quantum computing is reversible.

QUANTUM COMPUTING / QUANTUM GATES



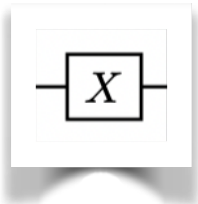
QUANTUM COMPUTING / QUANTUM GATES

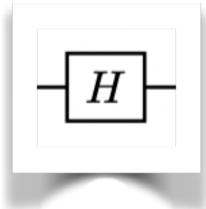




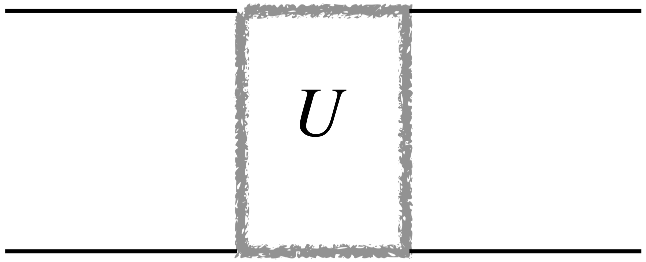
$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

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

$|0\rangle$  $|1\rangle$

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

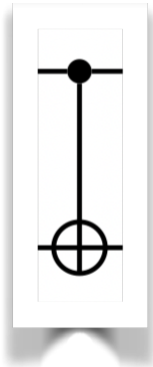
QUANTUM COMPUTING / QUANTUM GATES



$$CNOT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

Control $|+\rangle$

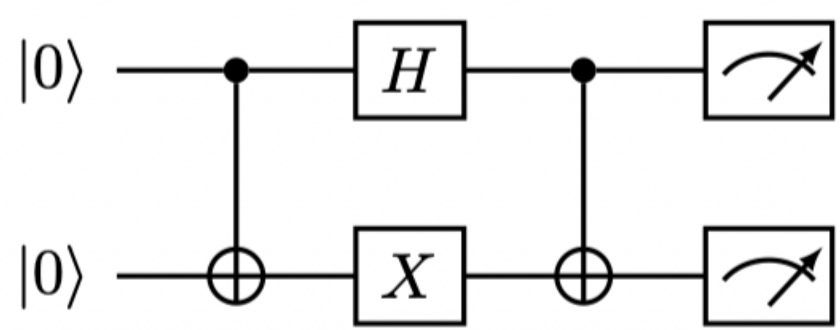
Target $|0\rangle$



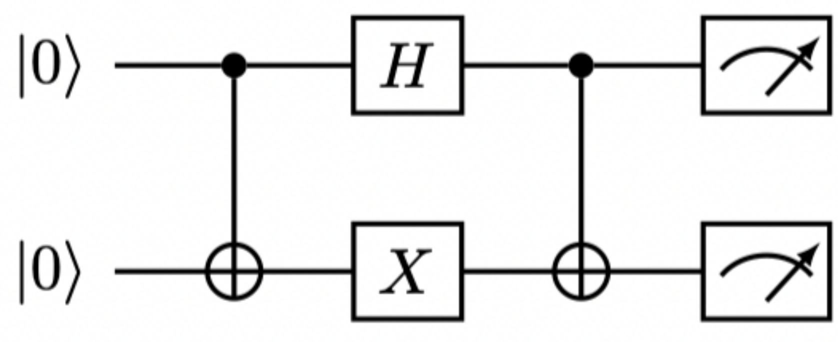
$$\frac{1}{\sqrt{2}}\left(|00\rangle + |11\rangle\right)$$

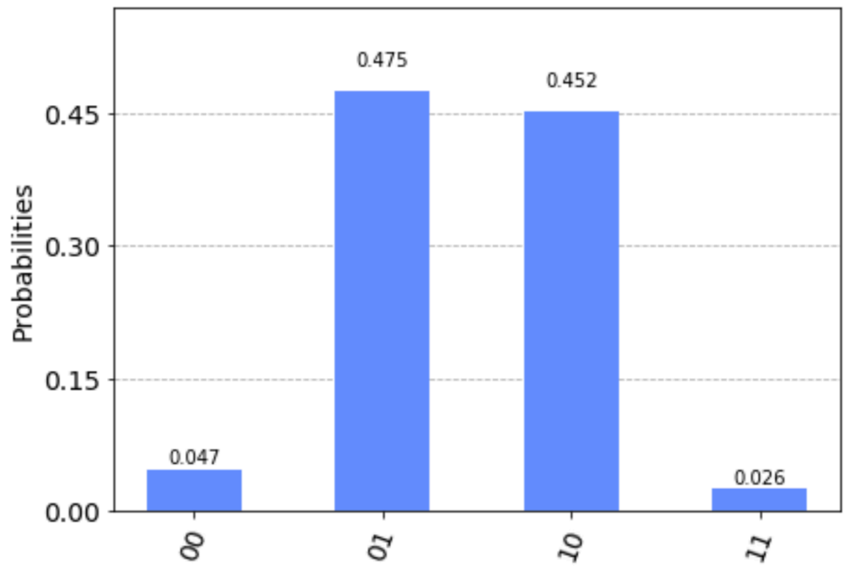
QUANTUM COMPUTING PRINCIPLE

1. Prepare the quantum computer in an initial state: $|\psi\rangle = |00...0\rangle = |0\rangle \otimes |0\rangle \ldots \otimes |0\rangle$
2. Apply gates (multiplication with a unitary matrix)
3. Perform a measurement



$$\begin{pmatrix} 0 & 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & 0 & 0 & 1/\sqrt{2} \\ 1/\sqrt{2} & 0 & 0 & -1/\sqrt{2} \\ 0 & 1/\sqrt{2} & -1/\sqrt{2} & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}$$





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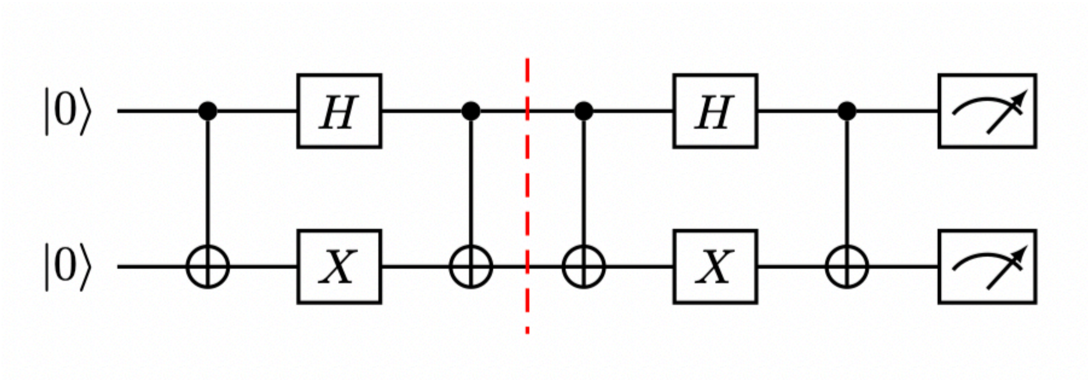
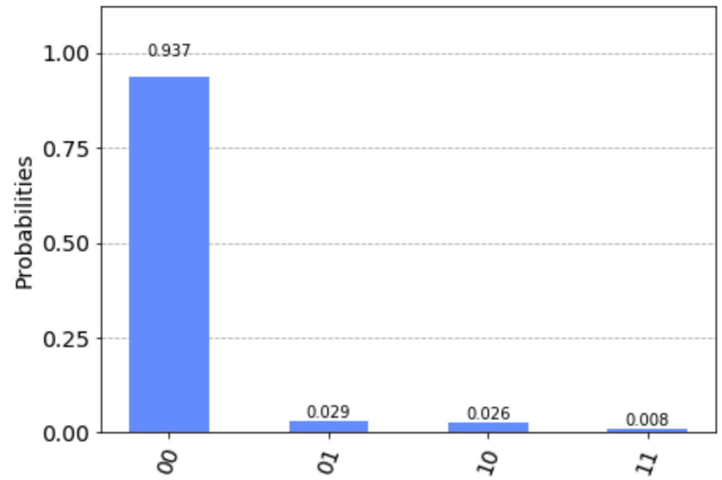
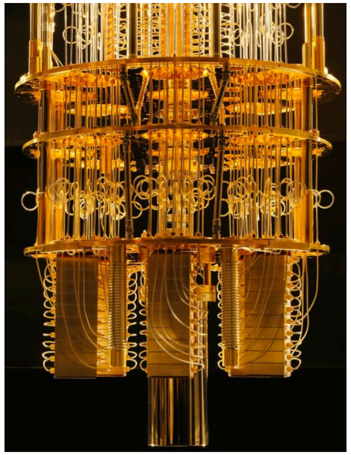




QUANTUM COMPUTER/ CLASSICAL COMPUTER

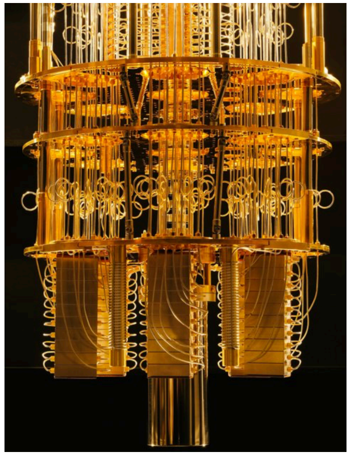


N qubits with 2^N states at the same time

$$|\psi\rangle = a_0|0\rangle + a_1|1\rangle + a_2|2\rangle + a_3|3\rangle + a_4|4\rangle + a_5|5\rangle + a_6|6\rangle + a_7|7\rangle$$

N bits with 2^N states, one at a time

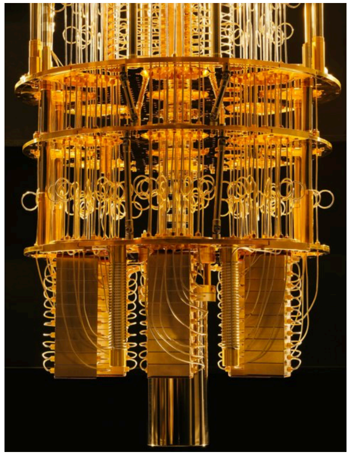
QUANTUM COMPUTER/ CLASSICAL COMPUTER



A qubit does not need to have a definite value until it is measured

A bit always has a definite value

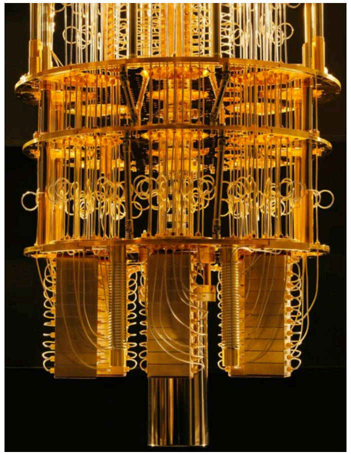
QUANTUM COMPUTER/ CLASSICAL COMPUTER



A qubit in an unknown state cannot be copied

A bit can be copied

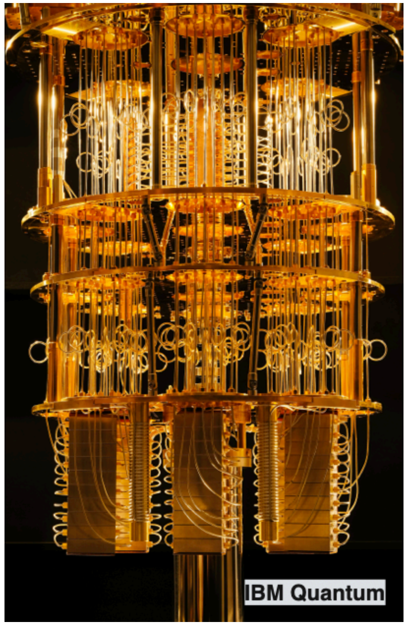
QUANTUM COMPUTER/ CLASSICAL COMPUTER



Reading a qubit may change its state (if the qubit being read is entangled with another qubit, reading one of the qubits will affect the other)

Reading one bit does not change its value and has no effect on any other

QUANTUM COMPUTING



1. Quantum Computing

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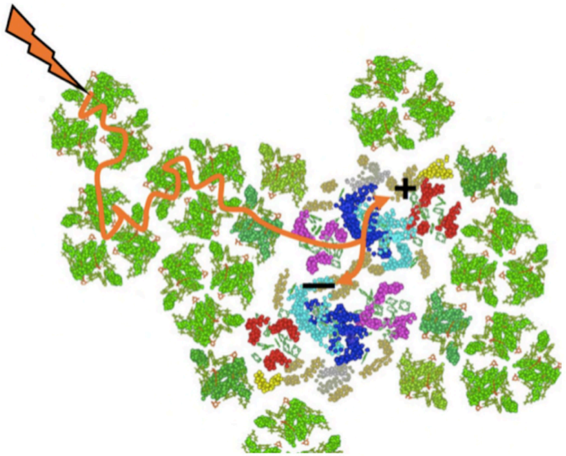
OPEN QUANTUM SYSTEMS ON THE QUANTUM COMPUTER

Physical System

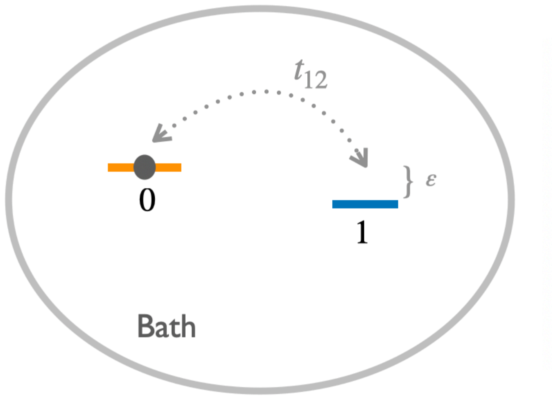


http://pubs.rsc.org | doi:10.1039/C1FD00078K

understanding would have many relevant applications, e.g., energy storage

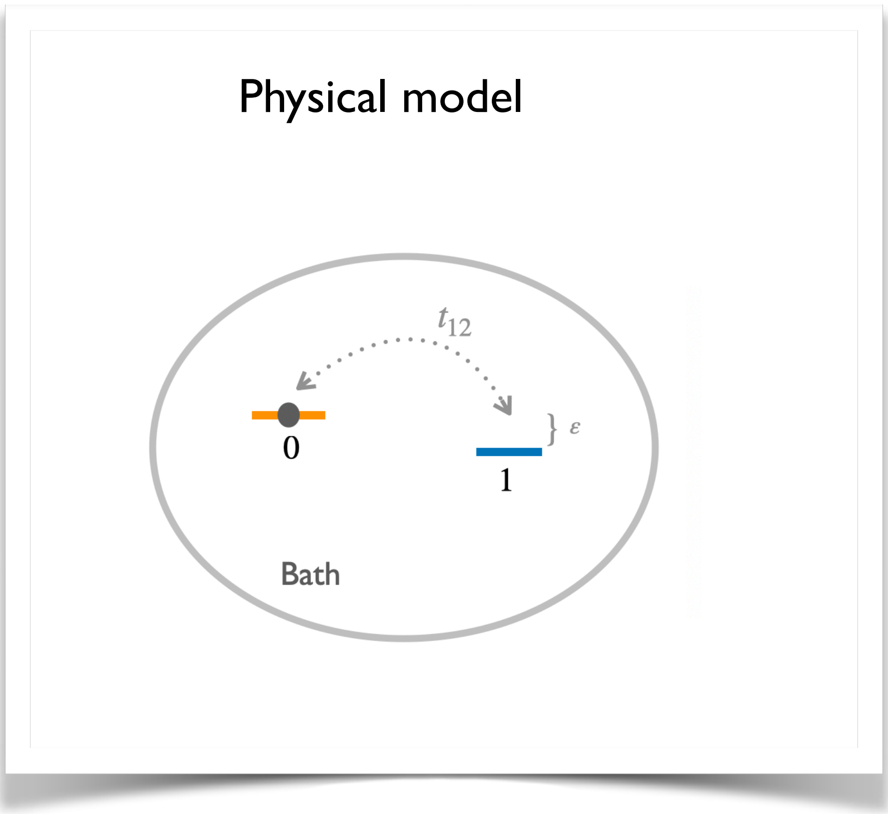
exponential growth of variables, efficiently simulating quantum many-body systems is hard on a classical computer

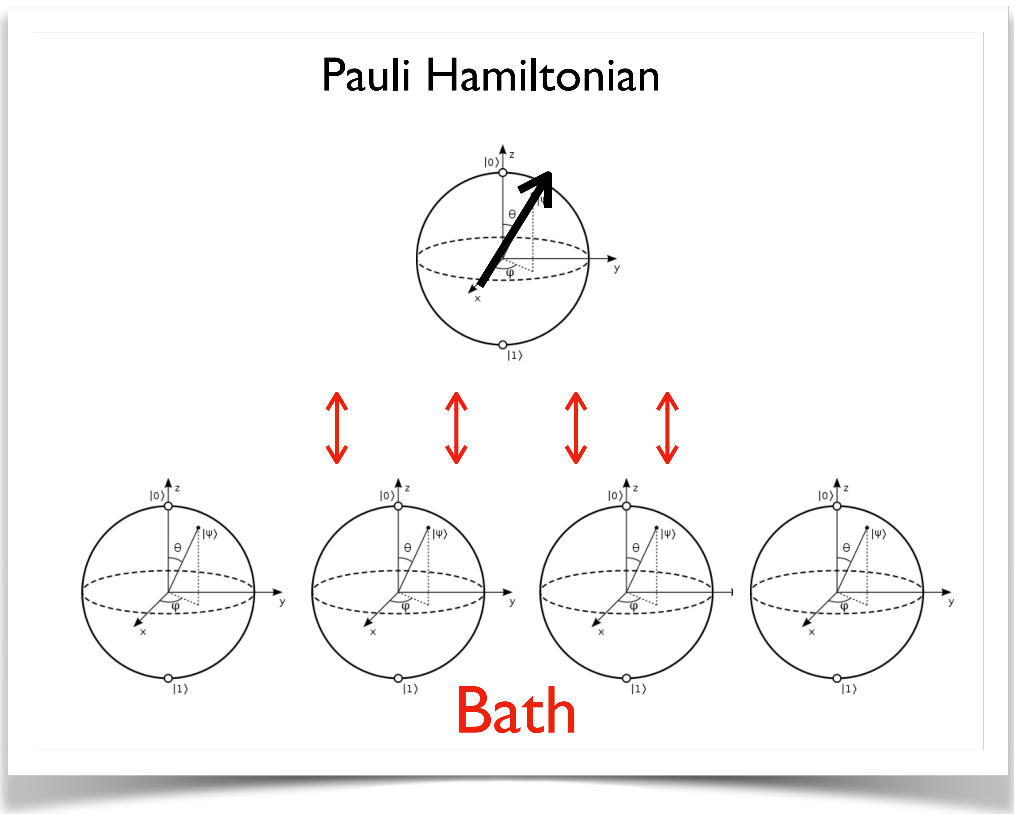
Physical model



Dissipative two-electron transfer: A numerical renormalization group study, Sabine Tornow, Ralf Bulla, Frithjof B. Anders, and Abraham Nitzan Phys. Rev. B **78**, 035434

OPEN QUANTUM SYSTEMS ON THE QUANTUM COMPUTER



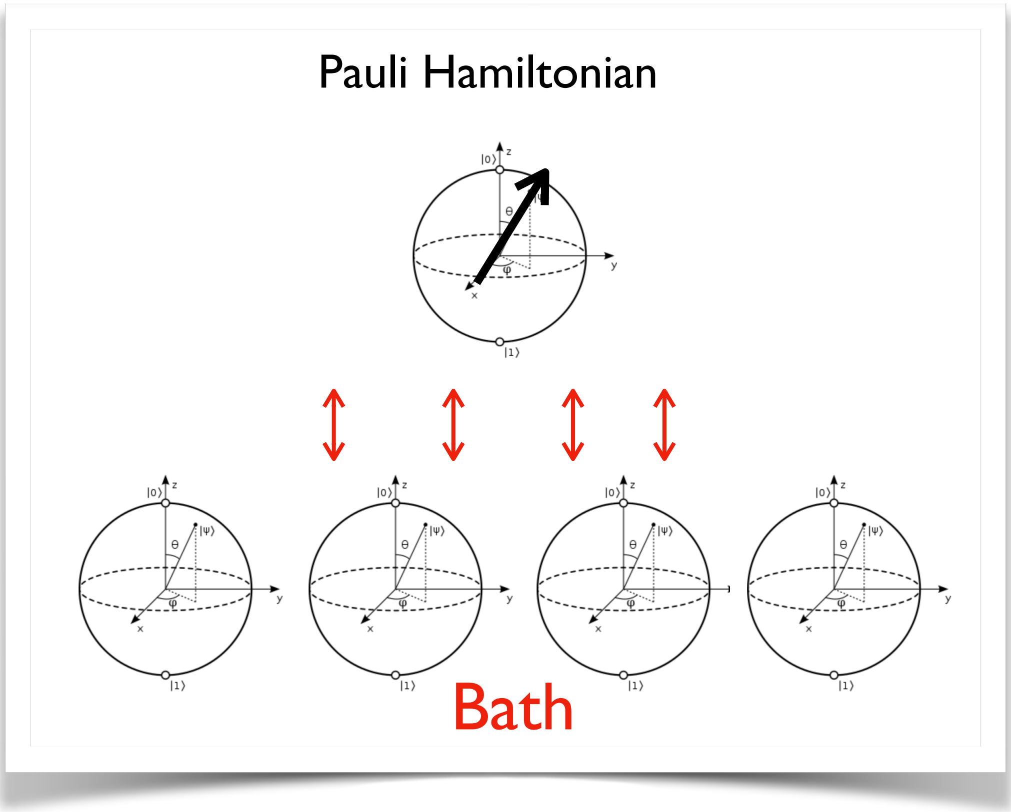


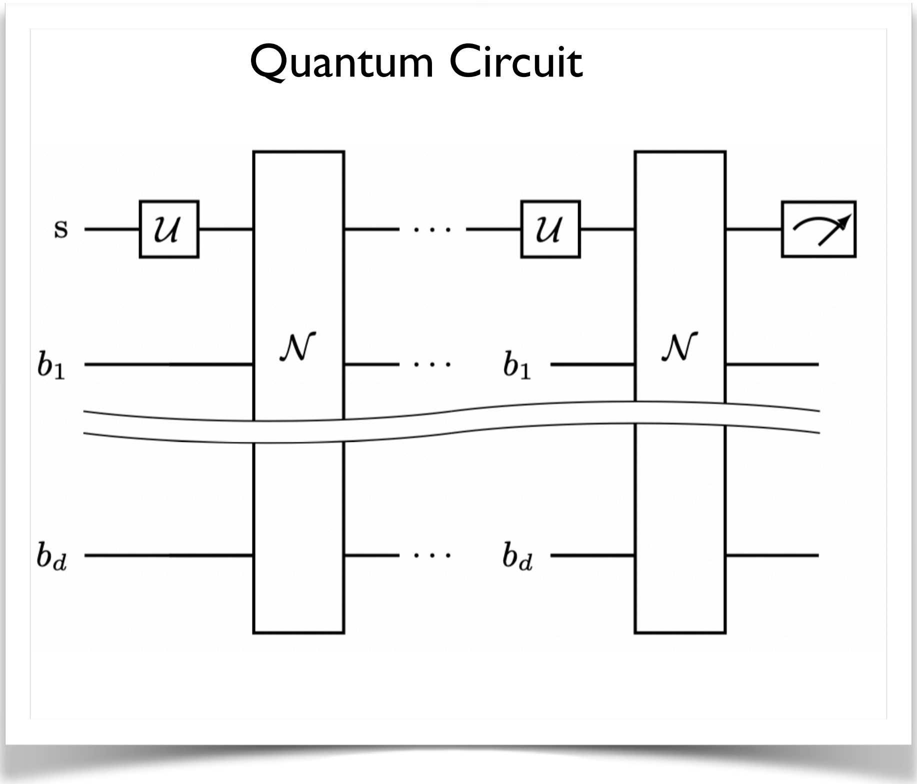
$$H_{sys} = -\,t_{12}\ \sigma_x + \epsilon\ \sigma_z$$

$$H_{\text{sys-bath}} = \sum_{k=1}^{n} g\ (\sigma_x \otimes \sigma_{x,k} + \sigma_y \otimes \sigma_{y,k})$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$
$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$
$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

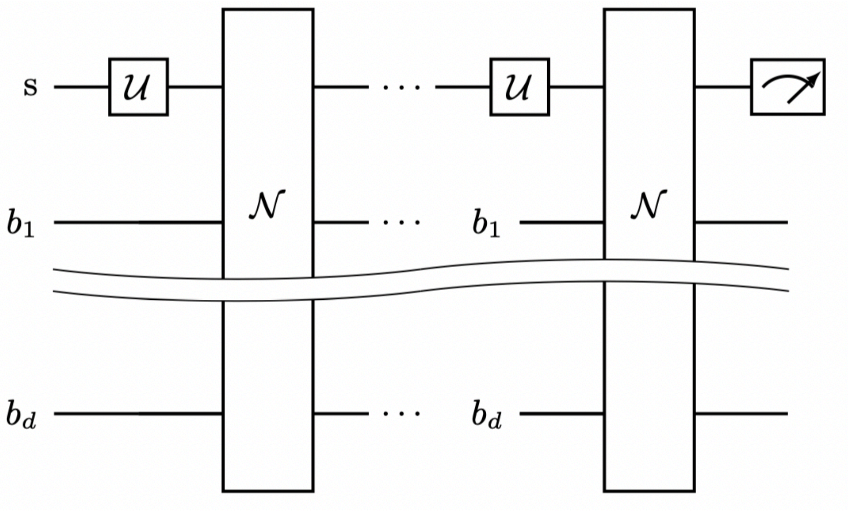
OPEN QUANTUM SYSTEMS ON THE QUANTUM COMPUTER



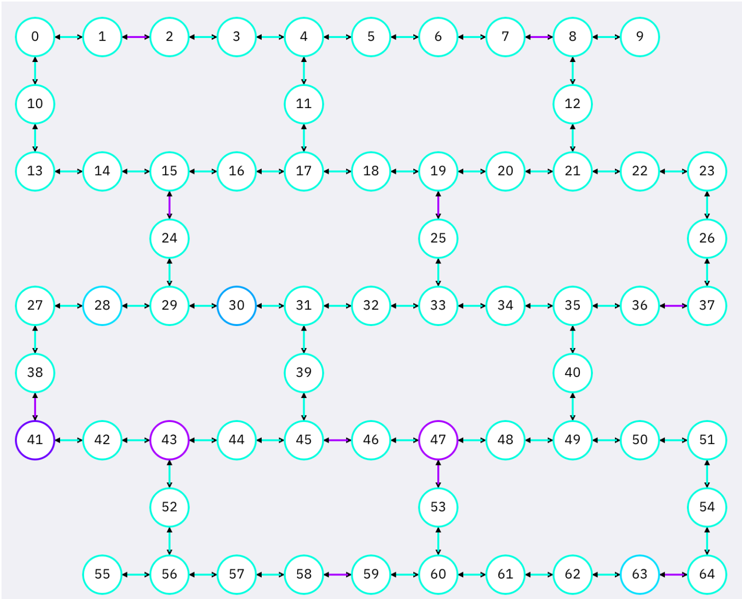


OPEN QUANTUM SYSTEMS ON THE QUANTUM COMPUTER

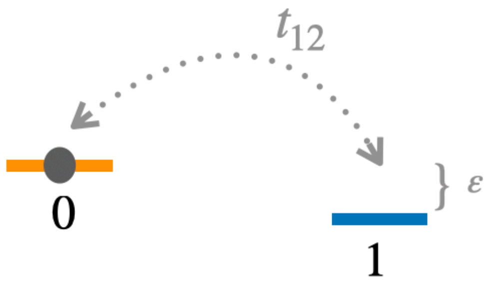
Quantum Circuit

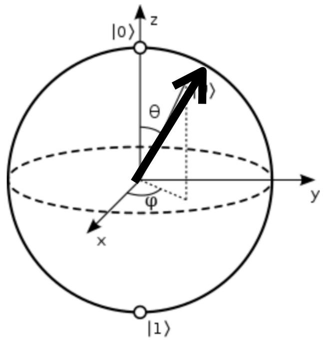


Quantum Chip



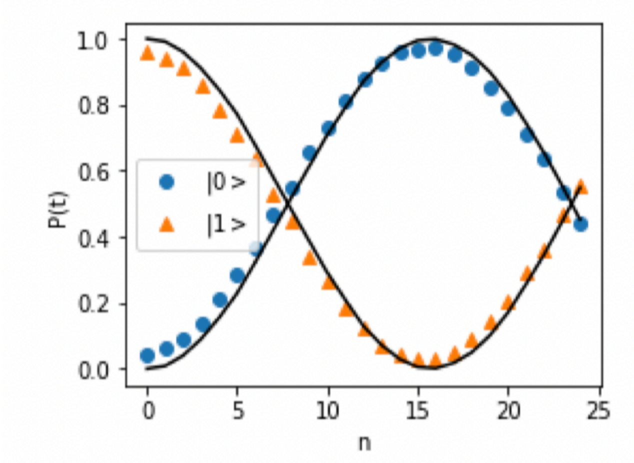
ELECTRON TRANSFER ON THE QUANTUM COMPUTER





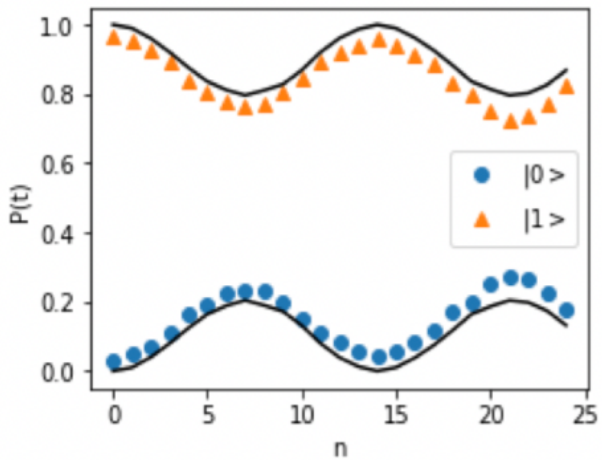
$$\left(-\boxed{R_x(2\ t_{12}\ \Delta t)}-\boxed{R_z(2\ \epsilon\ \Delta t)}- \right)^n$$

Occupation probability $\varepsilon = 0$



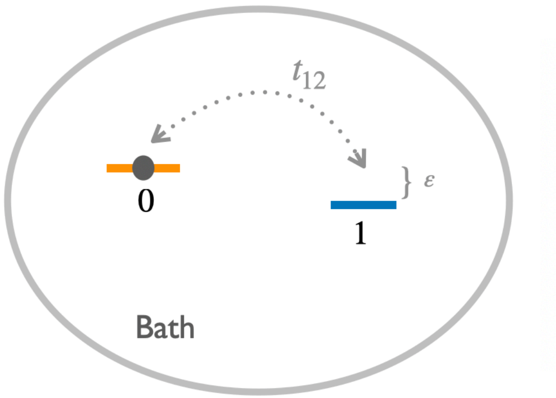
n time steps

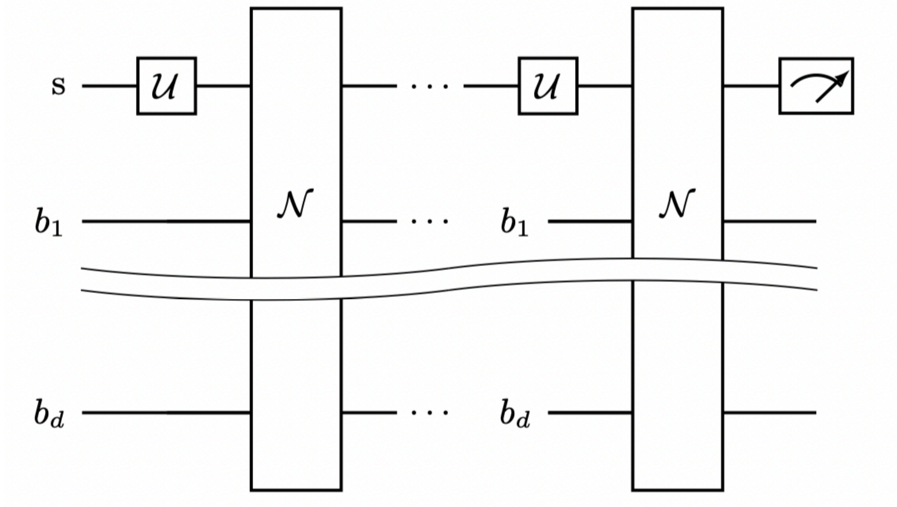
Occupation probability $\varepsilon \neq 0$



n time steps

OPEN QUANTUM SYSTEMS ON THE QUANTUM COMPUTER





Tornow, Gehrke, Helmbrecht, to be published

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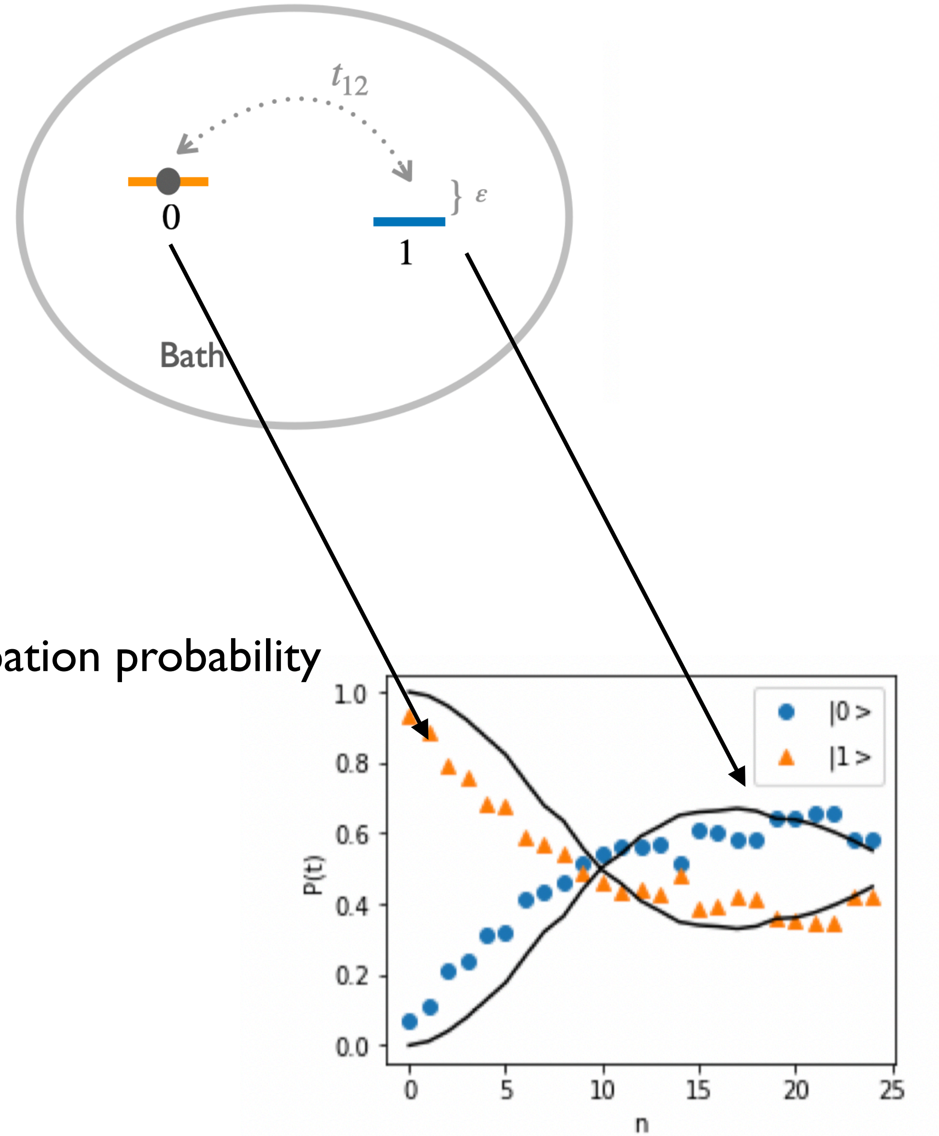
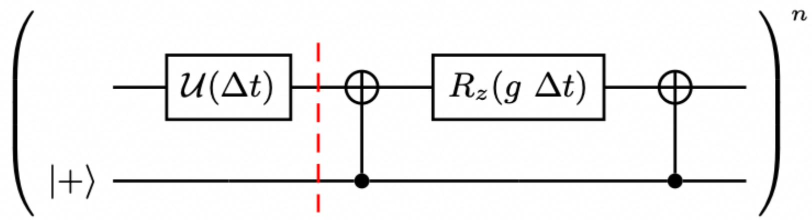


Occupation probability



n time steps

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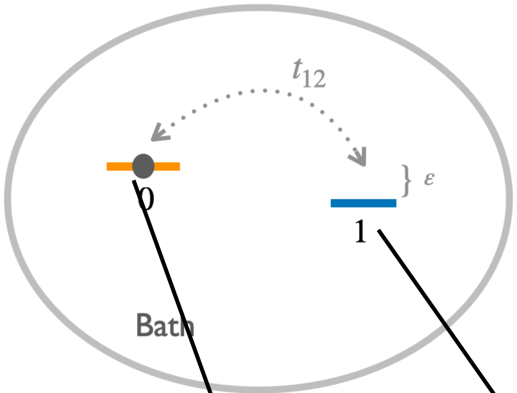
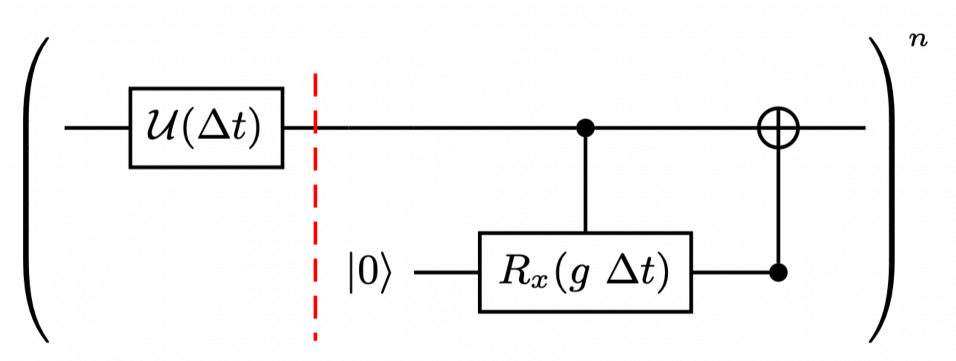
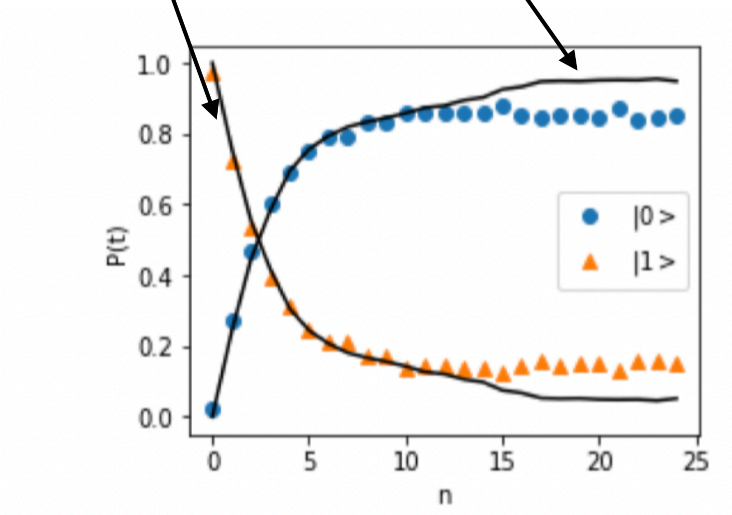




Occupation probability



n time steps

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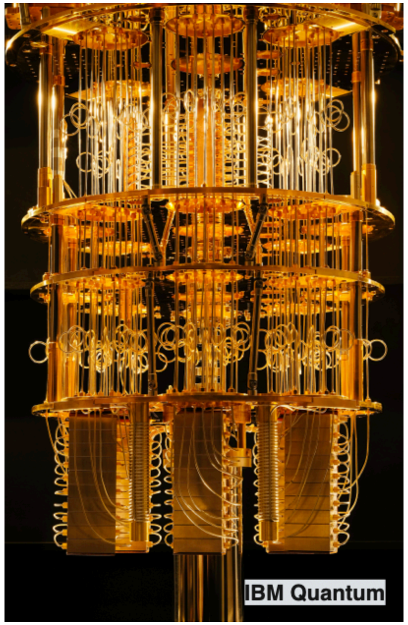
QUANTUM COMPUTING



1. Quantum Computing

2. Applications:

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CLASSICAL DATA ON THE QUANTUM COMPUTER

1. Number encoding: $3 \rightarrow 11 \rightarrow \ |11\rangle$

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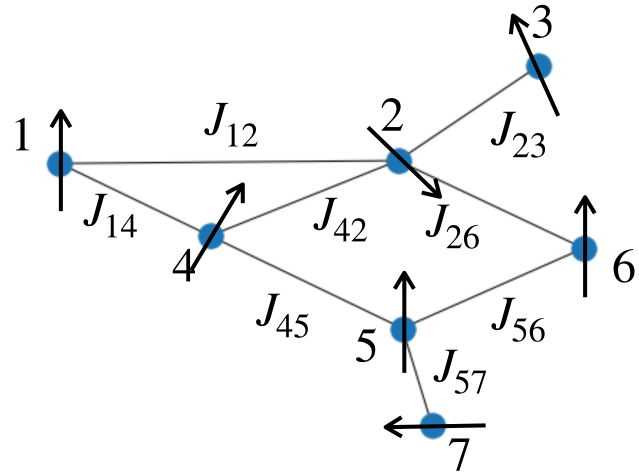
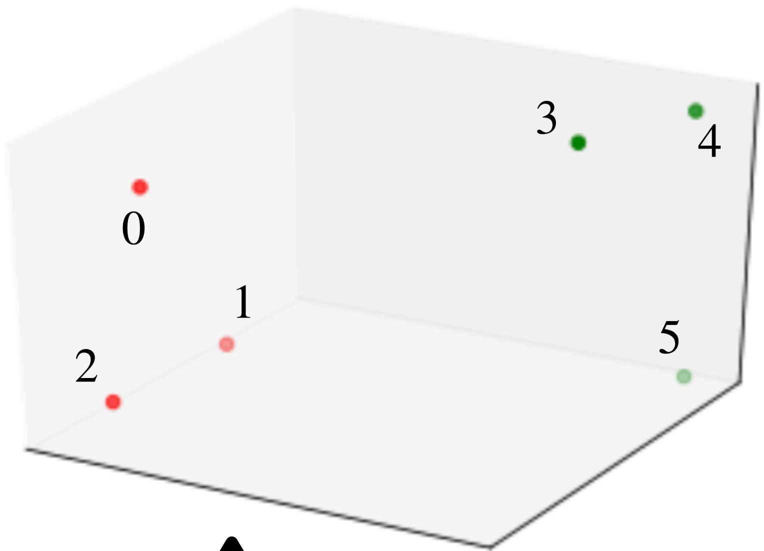
4. Hamiltonian encoding: $H = \sum_k h_k\, \sigma_k - \sum_{<k,l>} J_{kl}\, \sigma_k \otimes \sigma_l$

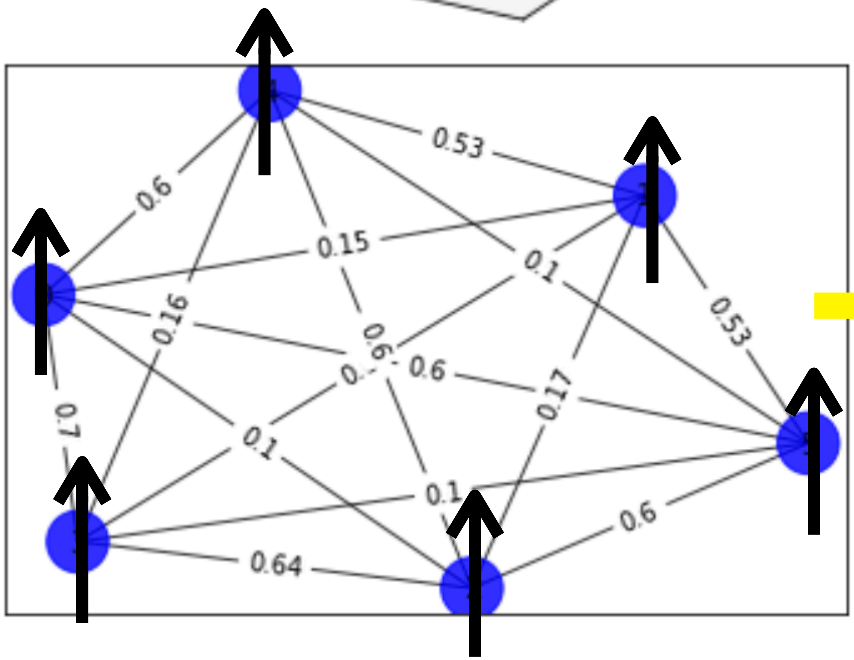


CLUSTERING/OPTIMIZATION



$$J_{kl} =$$

```
[[0.   0.15 0.1  0.7  0.6  0.6 ]
 [0.15 0.   0.17 0.6  0.53 0.53]
 [0.1  0.17 0.   0.64 0.6  0.6 ]
 [0.7  0.6  0.64 0.   0.16 0.1 ]
 [0.6  0.53 0.6  0.16 0.   0.1 ]
 [0.6  0.53 0.6  0.1  0.1  0.  ]]
```



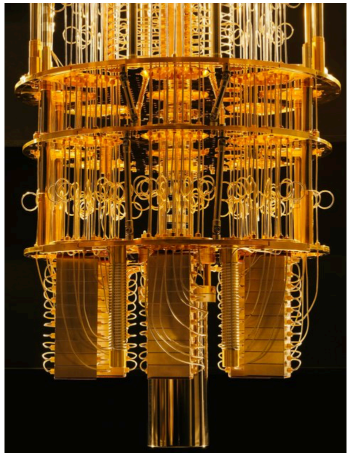
$$H = \sum_{k} h_k \, \sigma_k^x - \sum_{<k,l>} J_{kl} \, \sigma_k^z \otimes \sigma_l^z$$

Tornow, S. & Mewes, H.W. Functional modules by relating protein interaction networks and gene expression. Nucleic Acids Res. 31, 6283-6289

Sabine Tornow

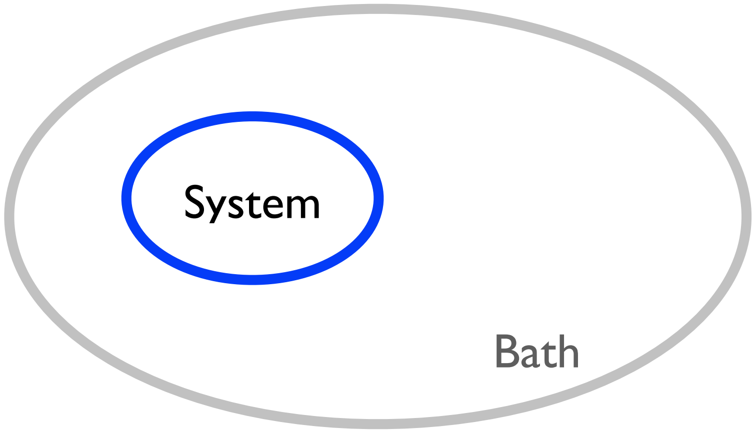
OPTIMIZATION ON A QUANTUM/CLASSICAL COMPUTER

The QC is an open quantum system itself

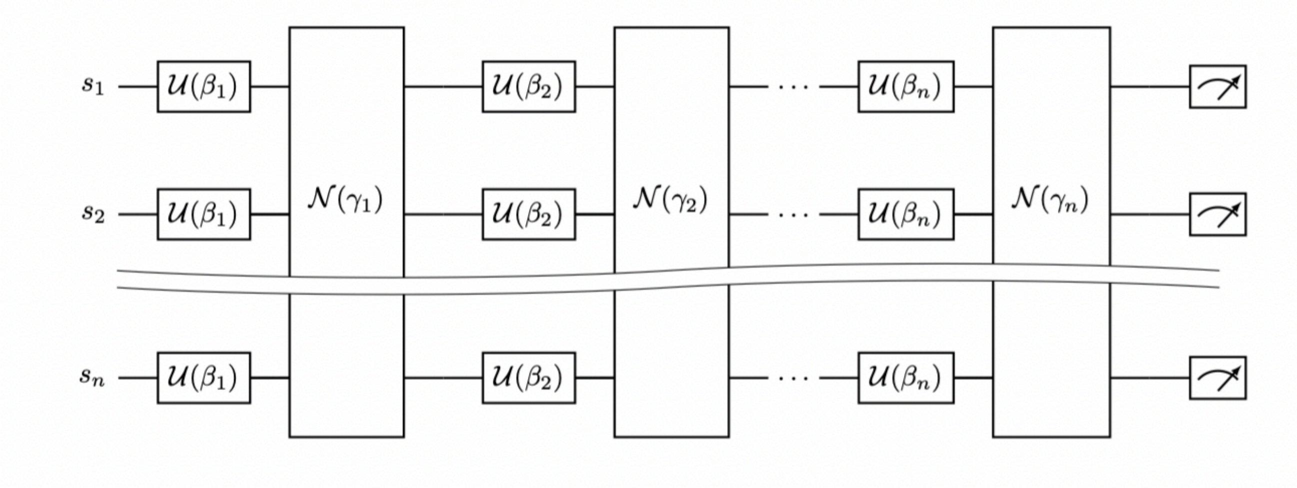


QPU

CPU



QUANTUM APPROXIMATE OPTIMIZATION ALGORITHM

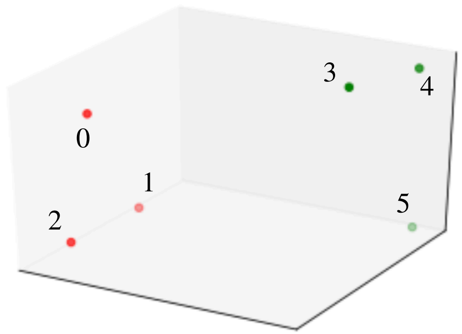


$\langle H \rangle$

Minimize $\langle H \rangle$ by optimising $\vec{\beta}$, $\vec{\gamma}$

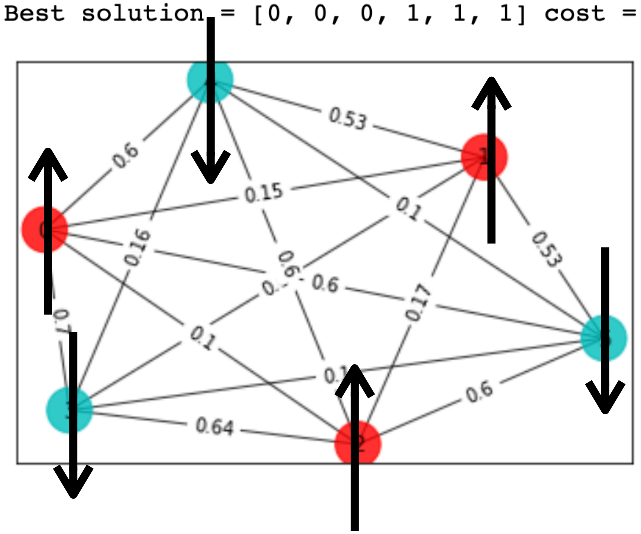
$$\mathcal{U}(\beta) = e^{-iH_0 \cdot \beta} \qquad \mathcal{N}(\gamma) = e^{-iH_1 \cdot \gamma}$$

For the optimal choice of β and γ,
$|\psi\rangle$ corresponds to the lowest energy of H.

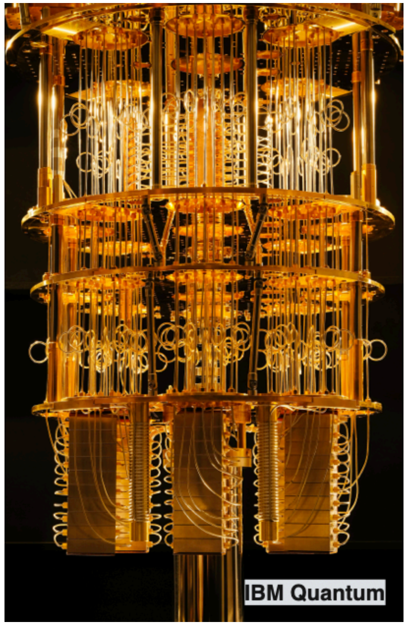


Example: Clustering

```
Best solution = [0, 0, 0, 1, 1, 1] cost = 5.4
```



QUANTUM COMPUTING



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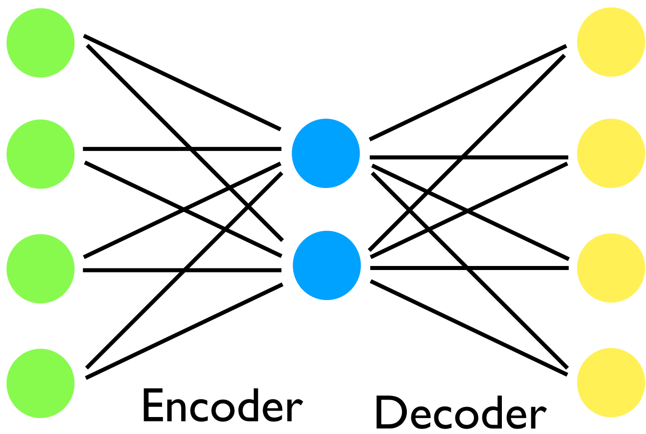
MACHINE LEARNING ON THE QUANTUM COMPUTER



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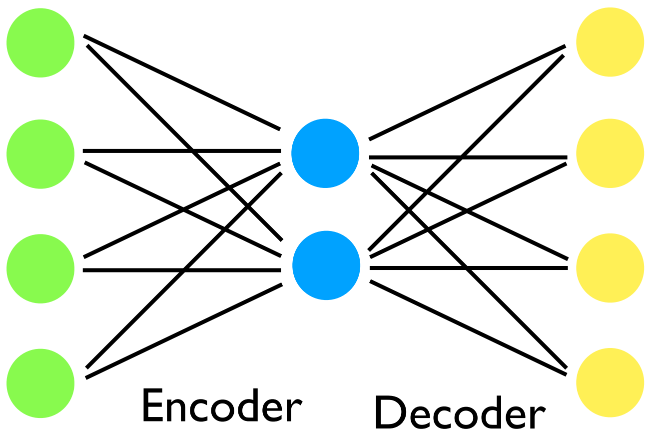
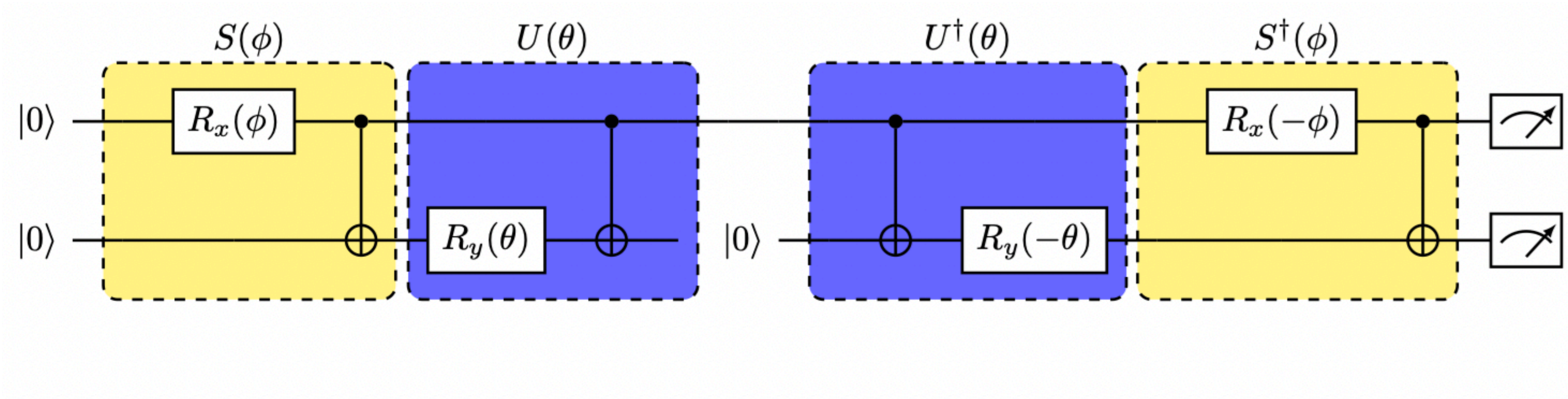
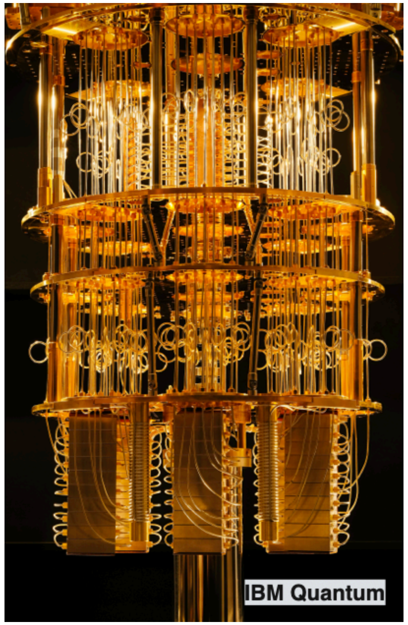




QUANTUM COMPUTING



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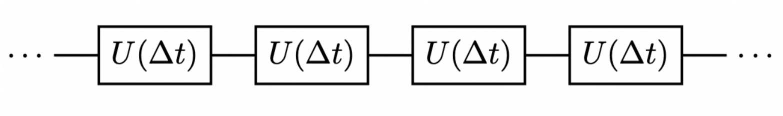
ERROR CORRECTION AND ERROR MITIGATION

- Zero noise extrapolation



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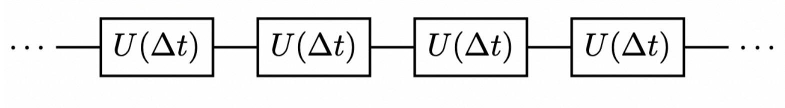

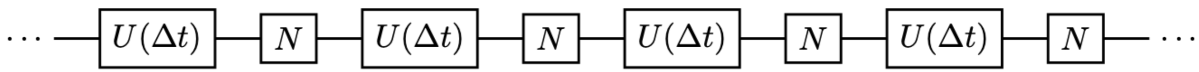

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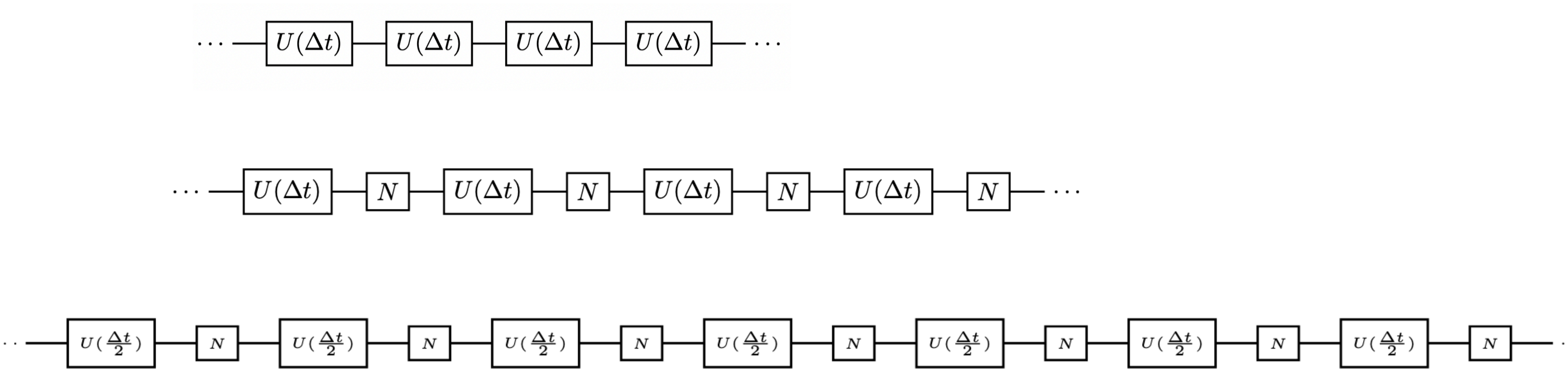
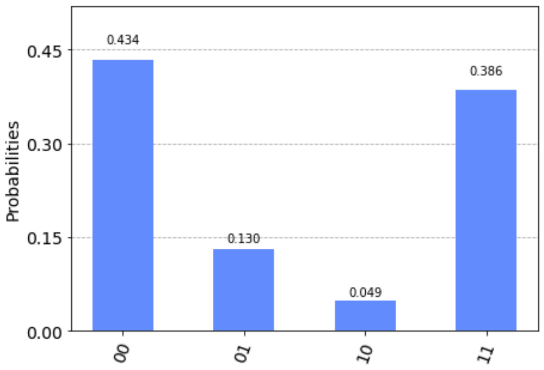


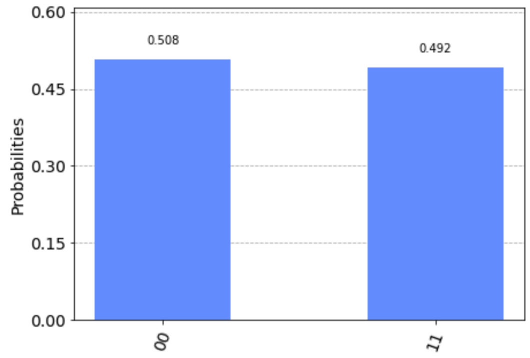
$$N \to 0$$

ERROR CORRECTION AND ERROR MITIGATION

- Machine learning for error mitigation



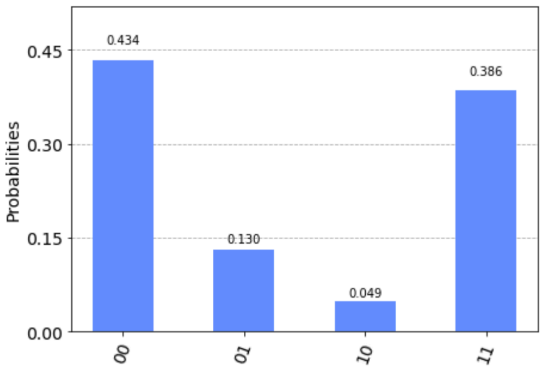
X_{noisy}



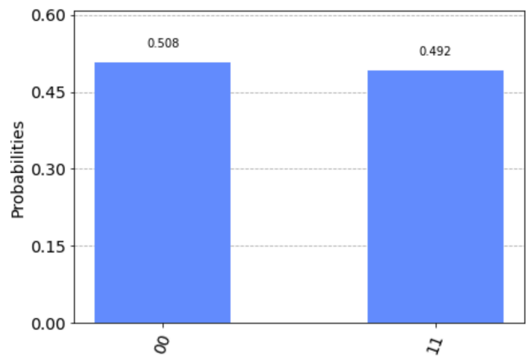
X_{exact}

ERROR CORRECTION AND ERROR MITIGATION

- Machine learning for error mitigation



X_{noisy}



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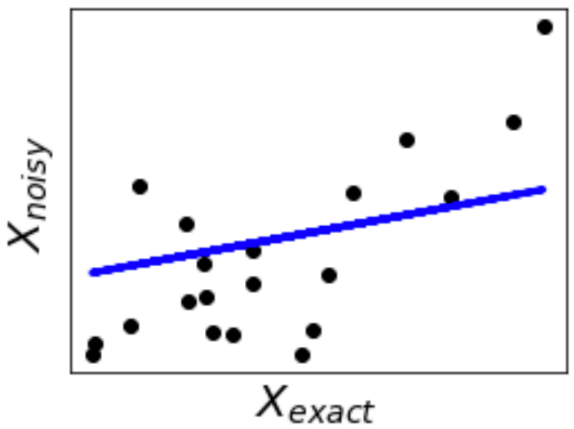
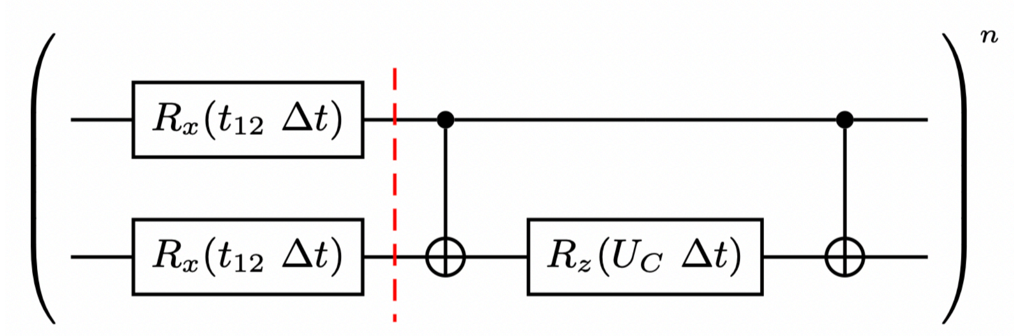
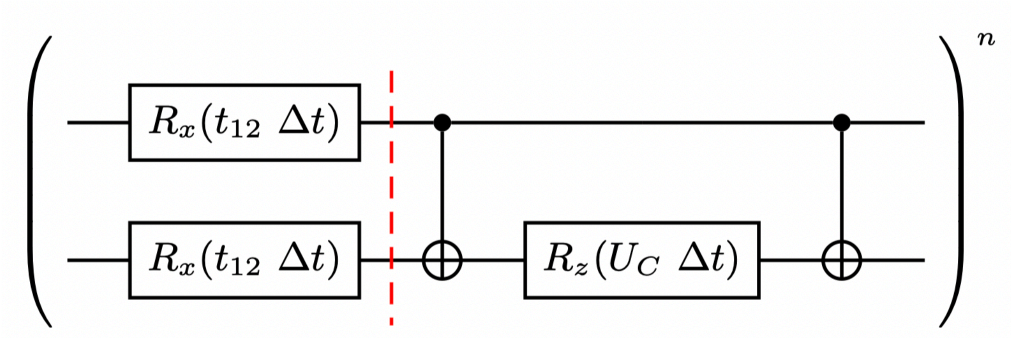




Predict

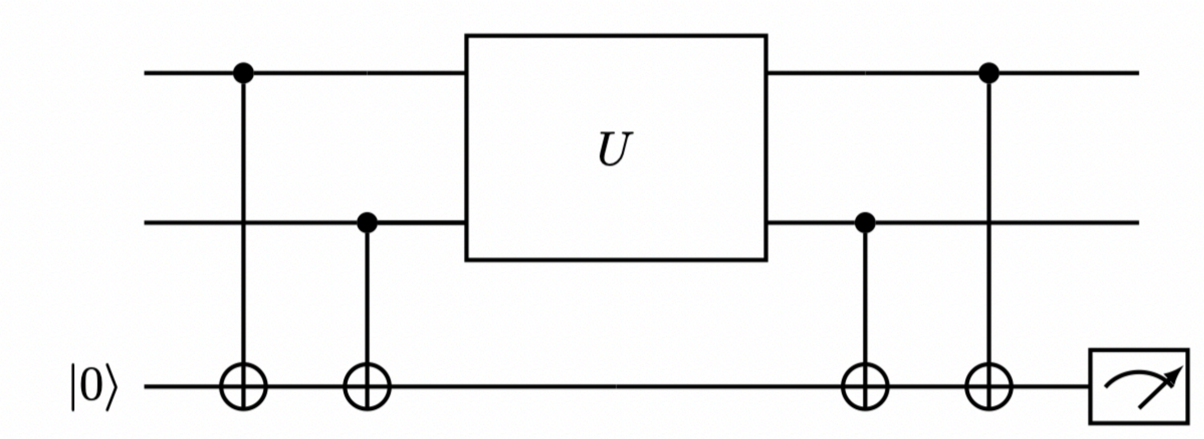
ERROR CORRECTION AND ERROR MITIGATION

- Test symmetry



ERROR CORRECTION AND ERROR MITIGATION

- Quantum error detection

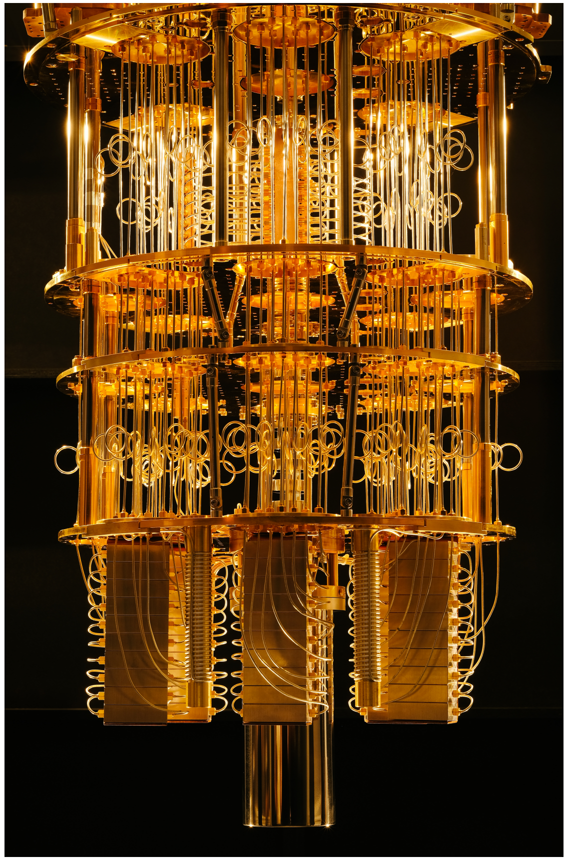


ERROR CORRECTION AND ERROR MITIGATION

- Quantum error correction

QUANTUM COMPUTING

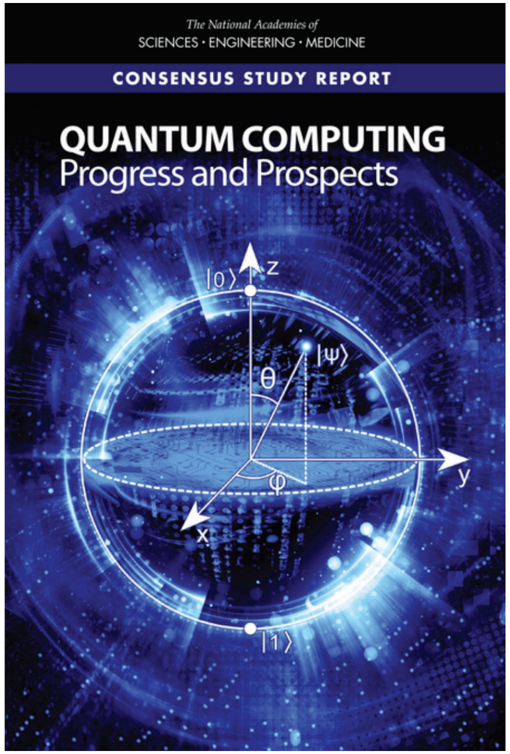
- Emerging quantum hardware enables evaluation of (heuristic) quantum algorithms
- Quantum advantage for near-term devices (NISQ) will only be achieved by error mitigation

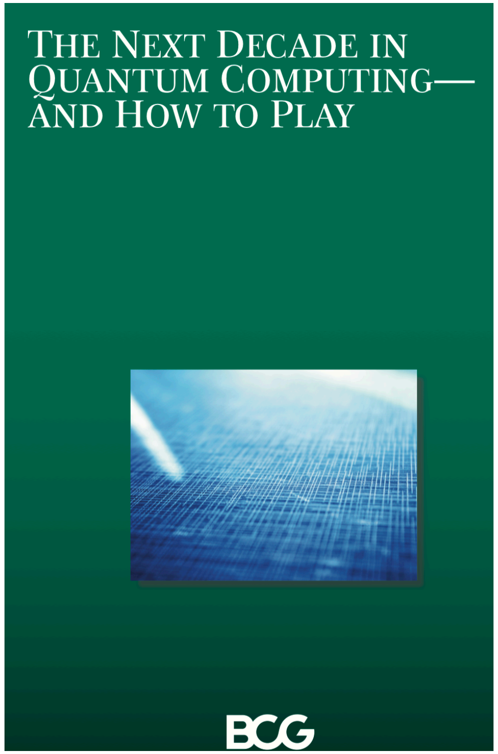


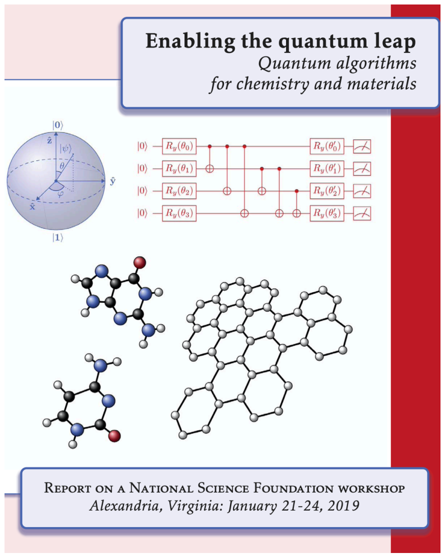
Sabine Tornow, MUAS

Thanks to: CODE FI, Universität der Bundeswehr München

LITERATURE







Qiskit

THE FUTURE IS QUANTUM