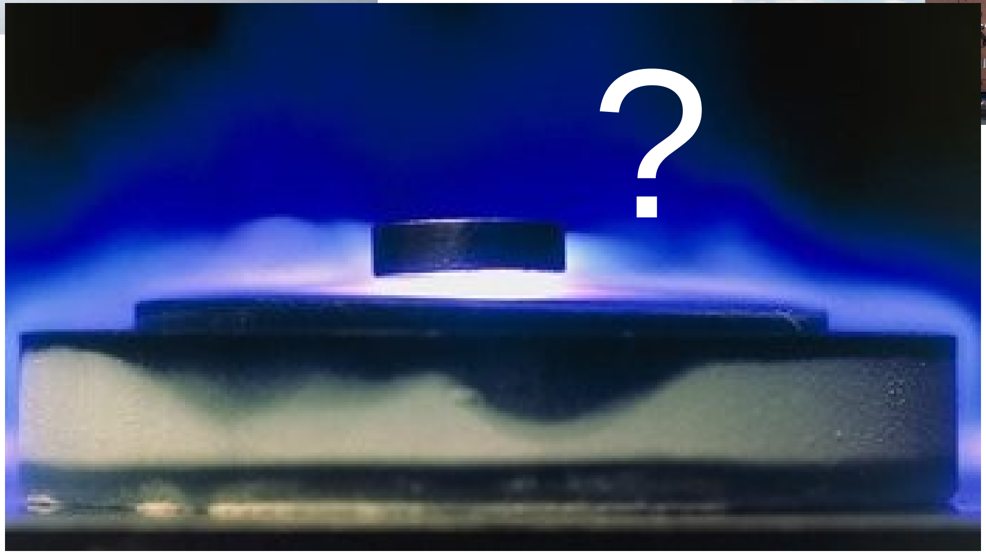
INTRODUCTION TO QUANTUM COMPUTING

FROM THE PERSPECTIVE OF A SOLID STATE PHYSICIST

- **Motivation**
- **Why are some problems so difficult to solve ?**
- **How can we use quantum objects to do computations**

Fabian Eickhoff, SC-HPC, 06.09.2023

MOTIVATION



- We can simulate the behavior of complex macroscopic objects
- We do not understand some properties of small materials

- Why is it so more difficult ?
- How difficult to simulate it ?

MOTIVATION

Spoiler:

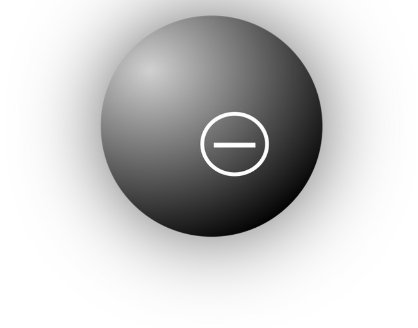
the reason why these problems are so difficult
is the same that makes quantum computers superior to classical ones

- We can simulate the behavior of complex macroscopic objects
- We do not understand some properties of small materials

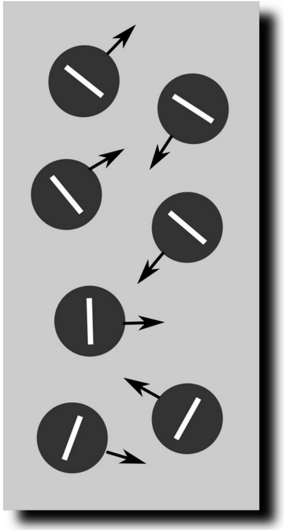
- Why is it so more difficult ?
- How difficult to simulate it ?

THE FUNDAMENTAL PROPERTIES OF ELECTRONS

Elektron

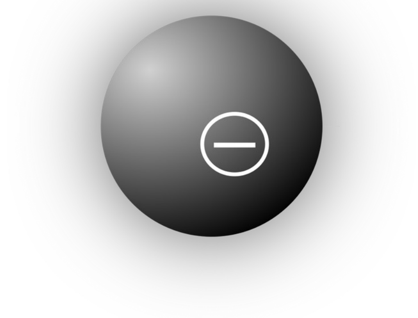


metal - free charge carriers

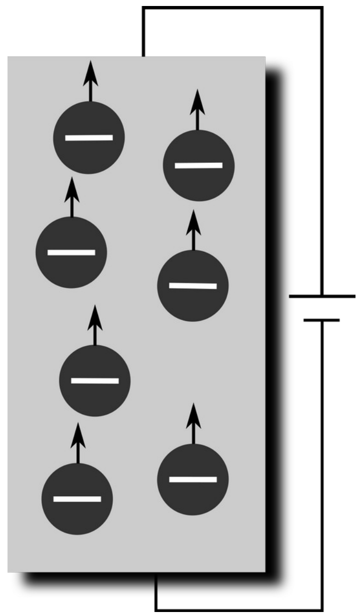


THE FUNDAMENTAL PROPERTIES OF ELECTRONS

Elektron



metal - free charge carriers



THE FUNDAMENTAL PROPERTIES OF ELECTRONS

Electric charge

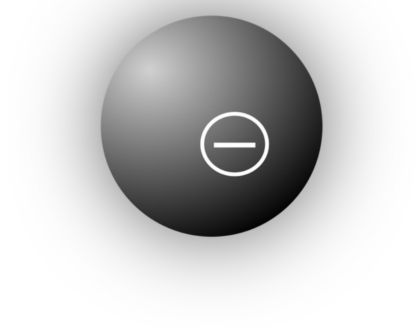
Control of the charge degree of freedom

Electronics

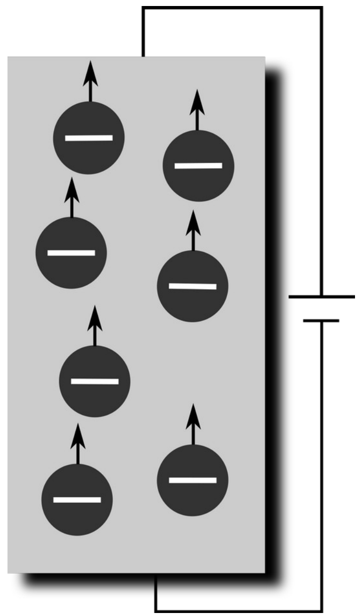
Electrical Components

Digital World

Elektron



metal - free charge carriers



THE FUNDAMENTAL PROPERTIES OF ELECTRONS

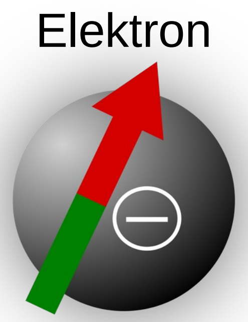
Electric charge

Control of the charge
degree of freedom

Electronics

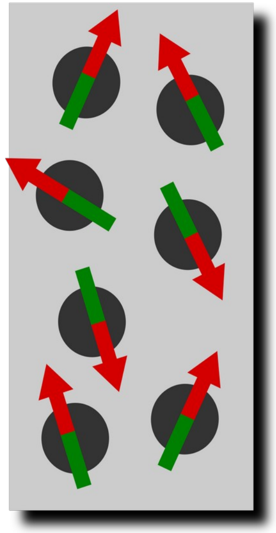
Electrical Components

Digital World



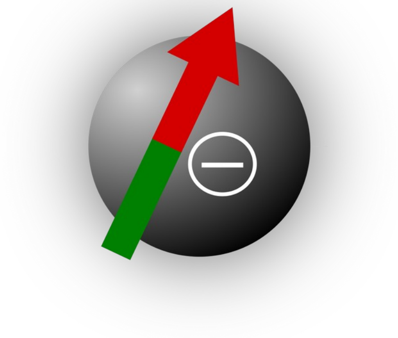
Intrinsic angular momentum - Spin
(one possibility to realize a qubit)

Paramagnetic metal - free charge carriers



THE FUNDAMENTAL PROPERTIES OF ELECTRONS

Elektron



Electric charge

Control of the charge degree of freedom

Electronics

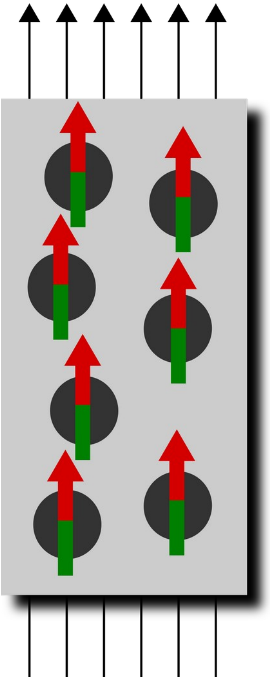
Electrical Components

Digital World

Intrinsic angular momentum - Spin

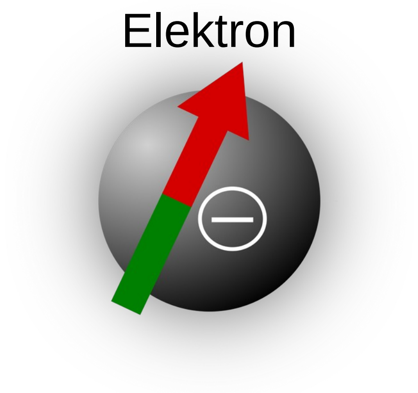
(one possibility to realize a qubit)

Paramagnetic metal - free charge carriers



THE FUNDAMENTAL PROPERTIES OF ELECTRONS

Electric charge

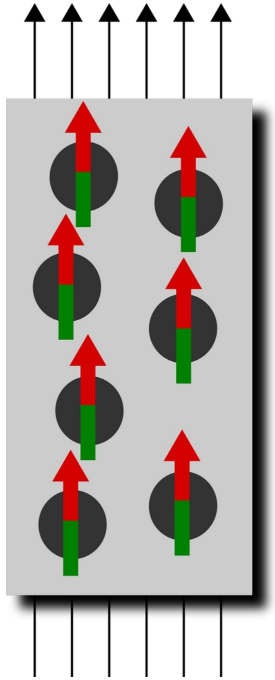


Intrinsic angular momentum - Spin
(one possibility to realize a qubit)

Control of the charge degree of freedom

Control of the spin degree of freedom

Paramagnetic metal - free charge carriers



Electronics

Spintronics

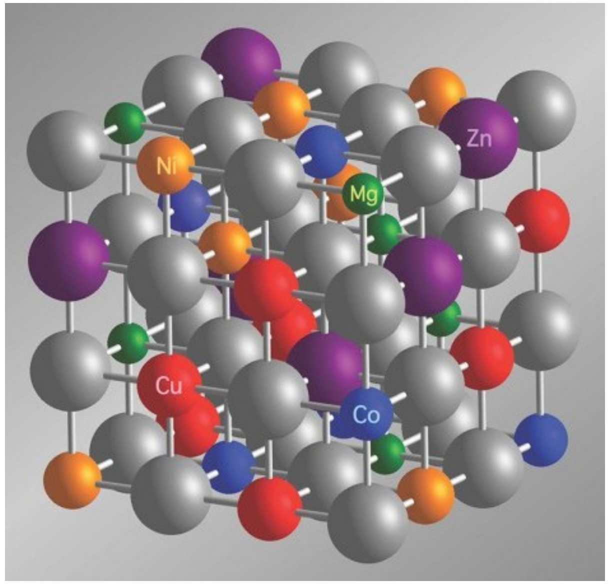
Electrical Components

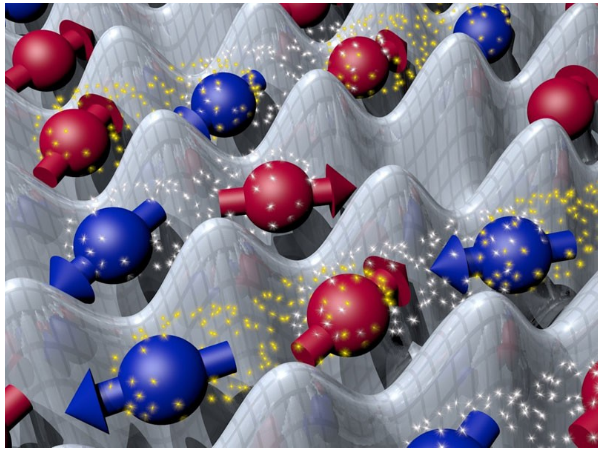
Electrical Components
+
Spin based Components

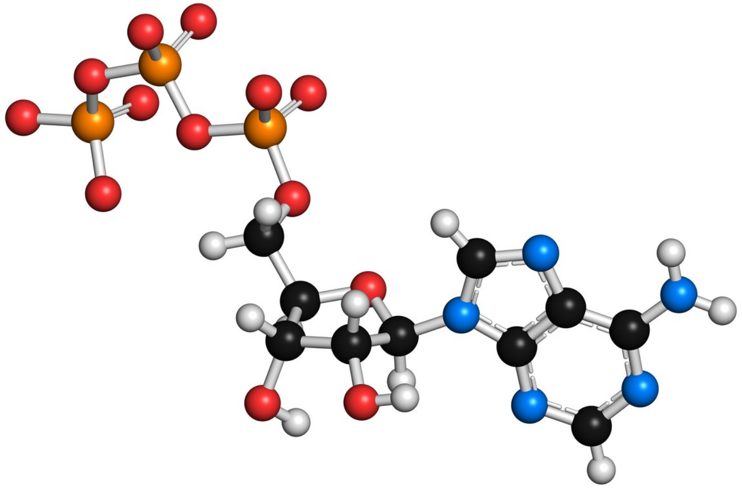
Digital World

New age of Technology

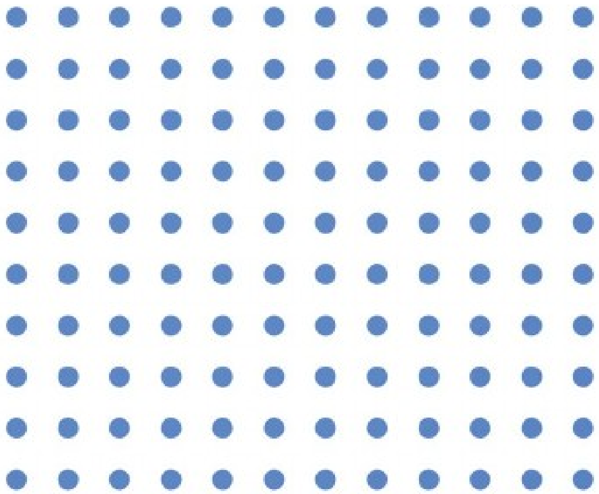
MODELS – Physical Systems







Lattice Models



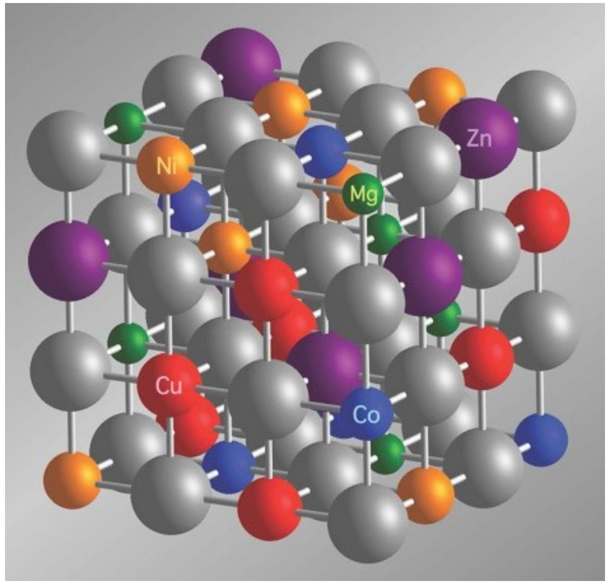
- Discretization of space
- Interactions among constituents

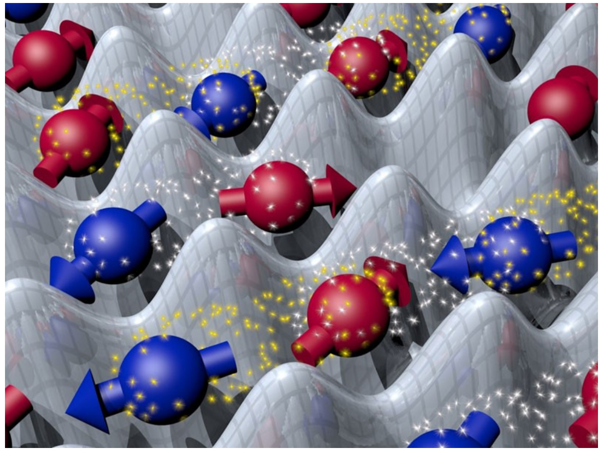
Energy of different configurations

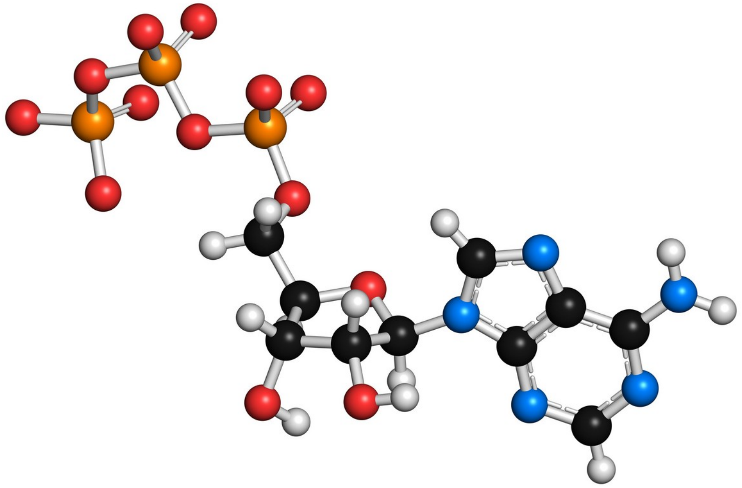
Hamiltonian: $H = \dots$

(cost function)

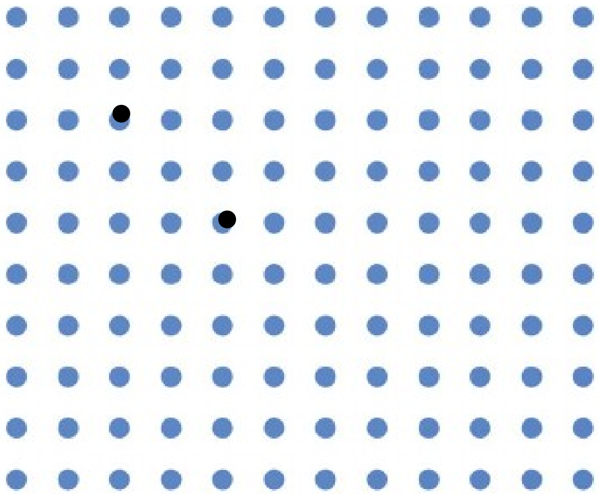
MODELS – Physical Systems







Lattice Models



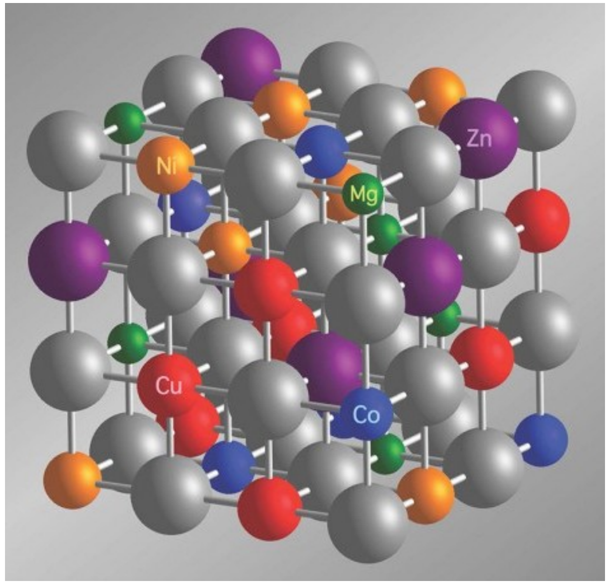
- Discretization of space
- Interactions among constituents

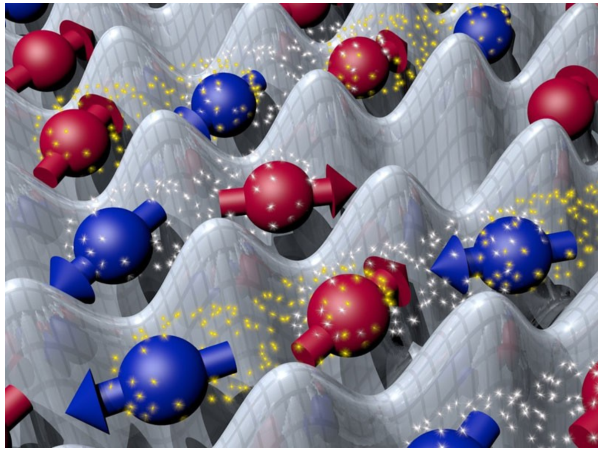
Energy of different configurations

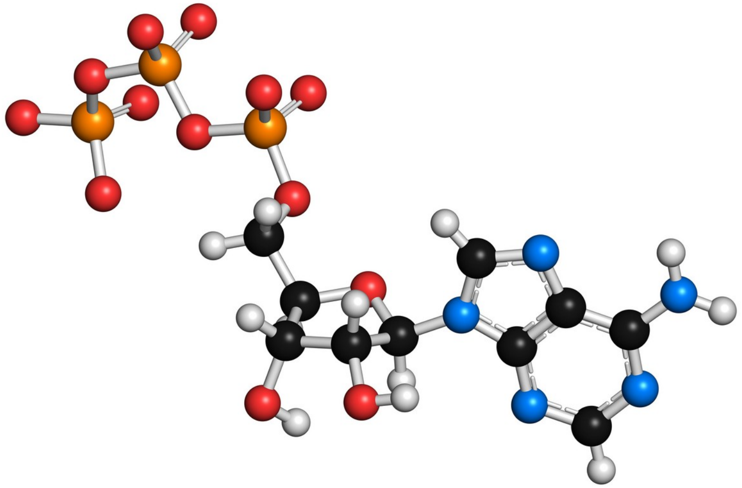
Hamiltonian: $H = \ldots$

(cost function)

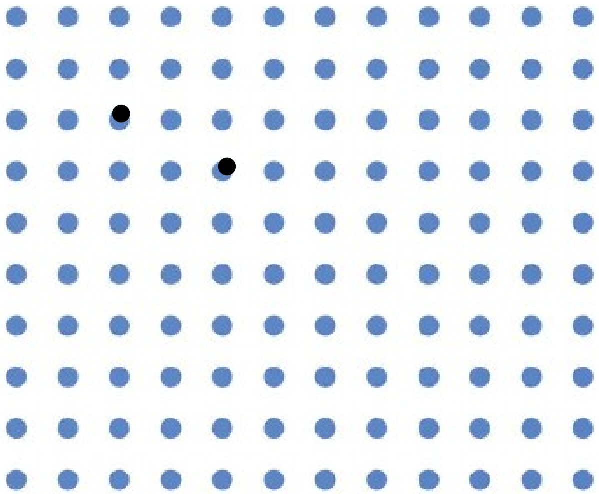
MODELS – Physical Systems







Lattice Models



- Discretization of space
- Interactions among constituents

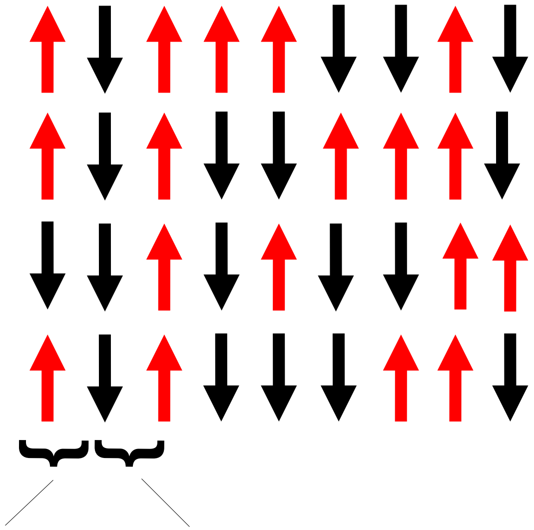
Energy of different configurations

Hamiltonian: $H = \ldots$

(cost function)

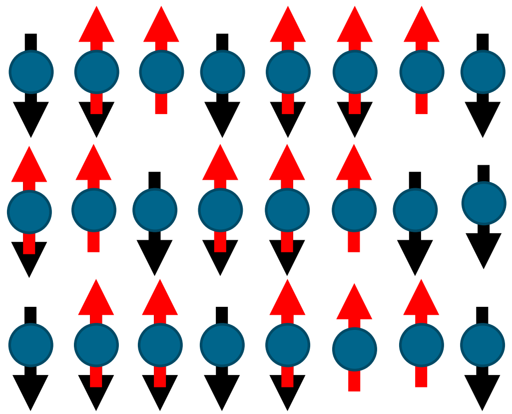
SPIN SYSTEMS – zero temperature

Classical



$$E = E(1,2) + E(2,3) + ... = H(\mathrm{conf})$$

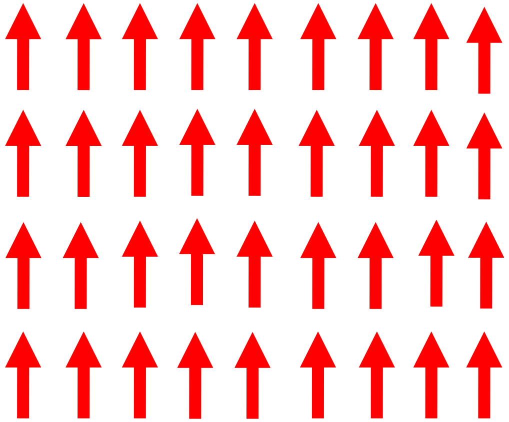
Quantum



$$E = H(\mathrm{conf})$$

- Local interactions
- Zero temperature
  - ➢ solution of the problem = find configuration that minimizes energy

CLASSICAL SYSTEMS – Example

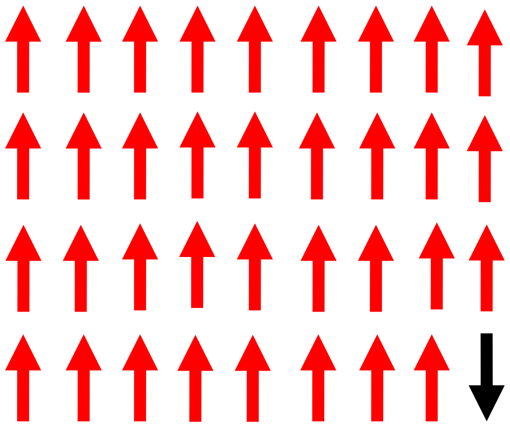


$$E = E(1,2) + E(2,3) + \ldots$$

Configuration	Energy
000…000	0.351
000…001	0.296
000…010	-0.256
000…011	-0.555
…	…
111…111	0.654

- There are 2^N different configurations
- Impossible to solve if $N = \mathcal{O}(100)$

CLASSICAL SYSTEMS – Example

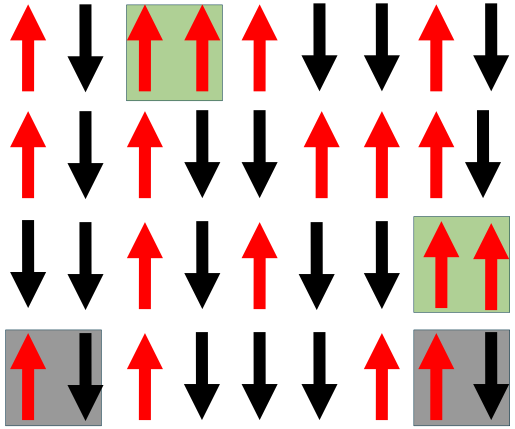


$$E = E(1,2) + E(2,3) + \dots$$

Configuration	Energy
000…000	0.351
000…001	0.296
000…010	-0.256
000…011	-0.555
…	…
111…111	0.654

- There are 2^N different configurations
- Impossible to solve if $N = \mathcal{O}(100)$

CLASSICAL SYSTEMS – Example

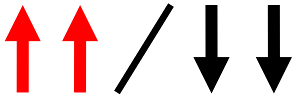


$$E = E(1,2) + E(2,3) + \ldots$$

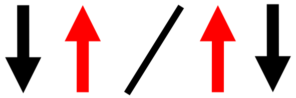
Configuration	Energy
000…000	-1000 ←
000…001	-998
000…010	-997
010…101	+1000
…	…
111…111	-1000 ←

Ferromagnetic groundstate

Symmetries: Translation invariance, Rotation invariance,…

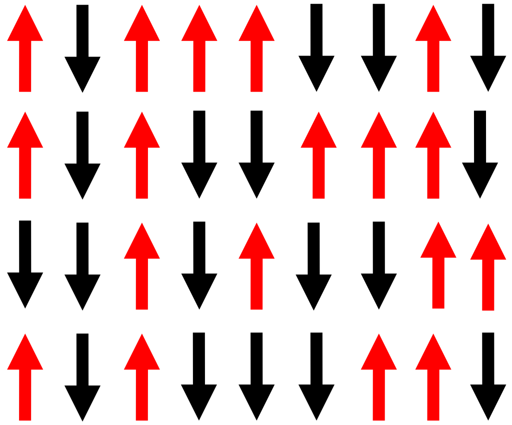


$$E = -1$$



$$E = +1$$

CLASSICAL SYSTEMS – Example

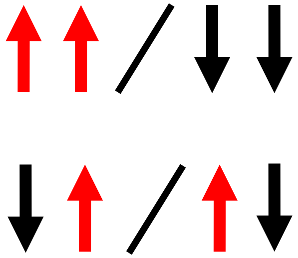


$$E = E(1,2) + E(2,3) + \dots$$

Configuration	Energy
000…000	+1000
000…001	+998
000…010	+997
010…101	-1000 ←
…	…
111…111	+1000

Antiferromagnetic groundstate

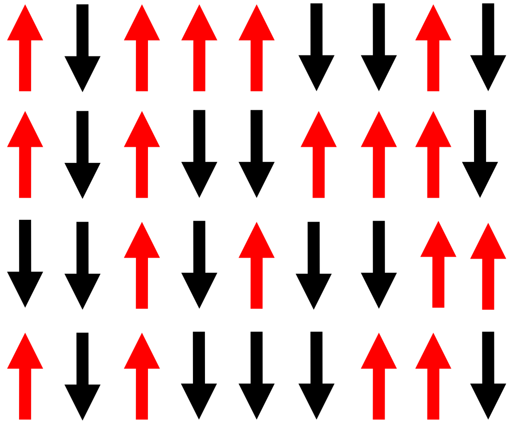
Symmetries: Translation invariance, Rotation invariance,…



$$E = +1$$

$$E = -1$$

CLASSICAL SYSTEMS – Example

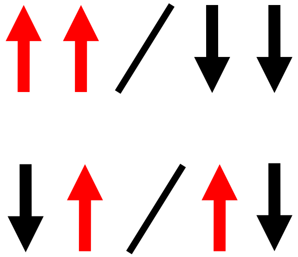


$$E = E(1,2) + E(2,3) + \ldots$$

Configuration	Energy
000…000	+1000
000…001	+998
000…010	+997
010…101	-1000
…	…
111…111	+1000

Antiferromagnetic groundstate

Symmetries: Translation invariance, Rotation invariance,…



$$E = +1$$

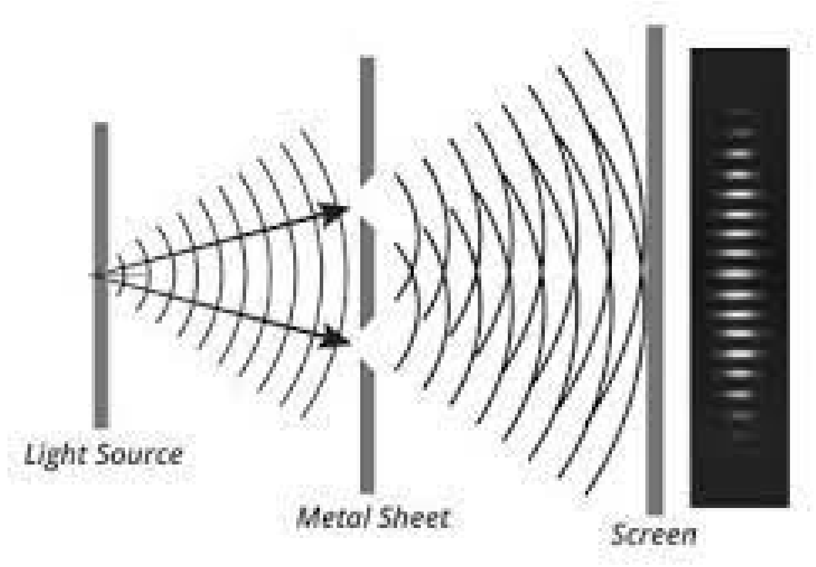
$$E = -1$$

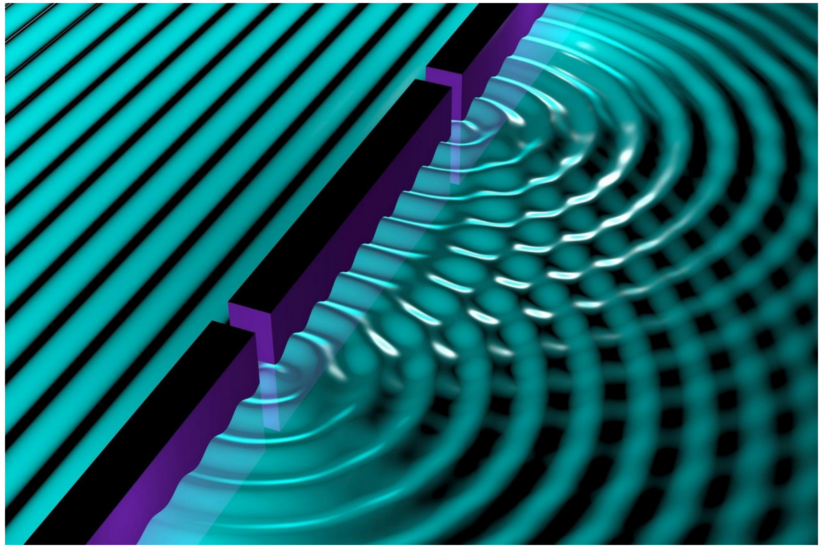
Conclusion:

- Classical systems are difficult to simulate
- Practical problems – it is relatively simple to find the solution
- There exist numerical methods for finite temperature

QUANTUM SYSTEMS

Double slit experiment – particle wave duality

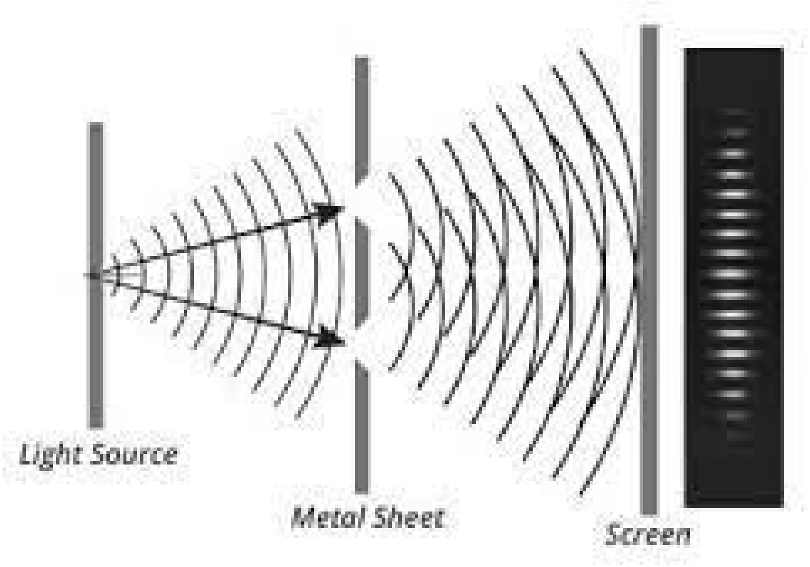


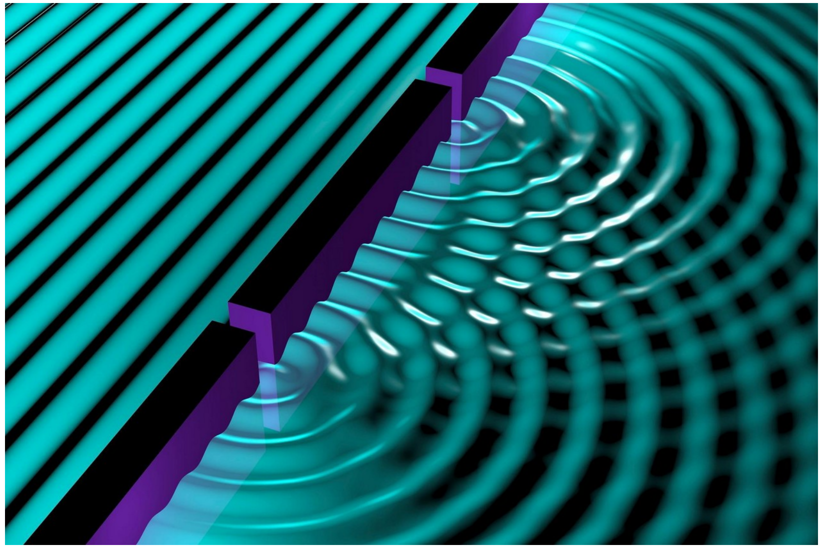


- Waves passing a double slit show a typical interference pattern
- However, the same pattern is observed if single electrons are used (or even atoms and molecules)

QUANTUM SYSTEMS

Double slit experiment – particle wave duality





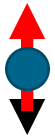
- Waves passing a double slit show a typical interference pattern
- However, the same pattern is observed if single electrons are used (or even atoms and molecules)

If we throw a classical stone: $\vec{x} = f_{\mathrm{Newton}}(t)$ - The stone is at ***a specific position*** at each point in time

If we throw a QM stone: $\mathrm{prob}[\vec{x}] = |\Psi_{\mathrm{SGL}}(\vec{x}, t)|^2$ - The stone is at ***multiple positions*** at each point in time

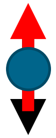
QUANTUM SYSTEMS

Superposition of states:

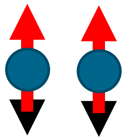
		Classical (Bits)	Quantum mechanical (Qubits)
System:		$\|0\rangle,\ \|1\rangle$	$c_0\|0\rangle + c_1\|1\rangle$

QUANTUM SYSTEMS

Superposition of states:

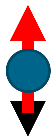
	Classical (Bits)	Quantum mechanical (Qubits)
System: 	$\vert 0\rangle,\ \vert 1\rangle$	$c_0\vert 0\rangle + c_1\vert 1\rangle$

Entaglement of spins:

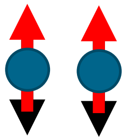
System: 	$\vert 0,0\rangle,\ \vert 0,1\rangle$ $\vert 1,0\rangle,\ \vert 1,1\rangle$	$c_0\vert 0,0\rangle + c_1\vert 0,1\rangle + c_2\vert 1,0\rangle + c_3\vert 1,1\rangle$

QUANTUM SYSTEMS

Superposition of states:

		Classical (Bits)	Quantum mechanical (Qubits)
System:		$\|0\rangle,\ \|1\rangle$	$c_0\|0\rangle + c_1\|1\rangle$

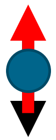
Entaglement of spins:

System:		$\|0,0\rangle,\ \|0,1\rangle$ $\|1,0\rangle,\ \|1,1\rangle$	$c_0\|0,0\rangle + c_1\|0,1\rangle + c_2\|1,0\rangle + c_3\|1,1\rangle$

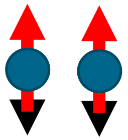
Question:
How many bits do we need to write down a general classical / QM state composed of N spins ?

QUANTUM SYSTEMS

Superposition of states:

		Classical (Bits)	Quantum mechanical (Qubits)
System:		$\|0\rangle, \|1\rangle$	$c_0\|0\rangle + c_1\|1\rangle$

Entaglement of spins:

		Classical	Quantum mechanical
System:		$\|0,0\rangle, \|0,1\rangle$ $\|1,0\rangle, \|1,1\rangle$	$c_0\|0,0\rangle + c_1\|0,1\rangle + c_2\|1,0\rangle + c_3\|1,1\rangle$

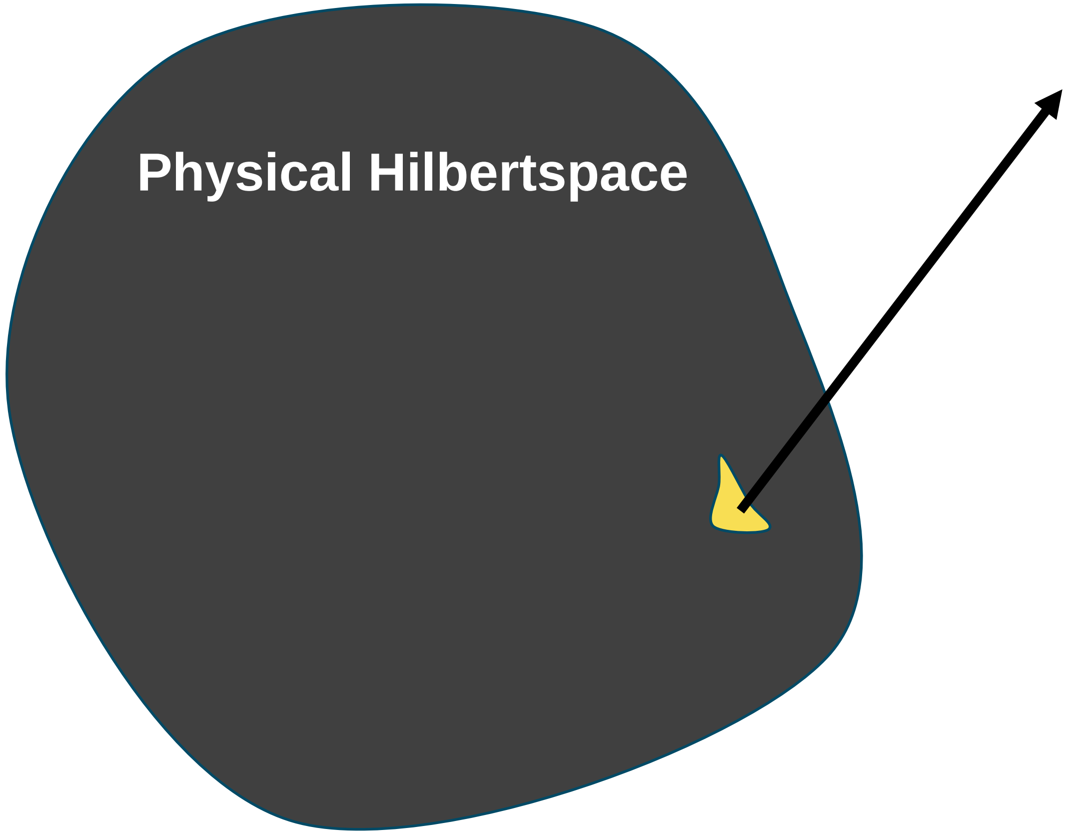
Question:
How many bits do we need to write down a general classical / QM state composed of N spins ?

Classical: N

Quantum mechanical: $\mathcal{O}(2^N)$ → 70 spins need $2^{70} \approx 10^{21}$ numbers = 1 zettabyte

→ **Amount of digital data in the world**

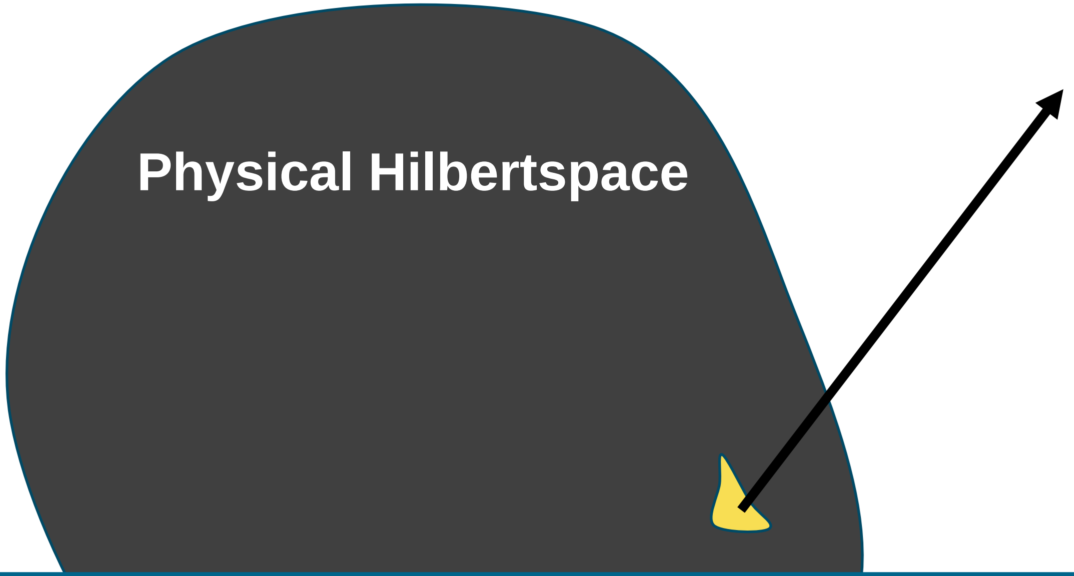
How to solve QM problems ?



Find a good ansatz for the (finite dimensional) Many body wavefunction and opimize it

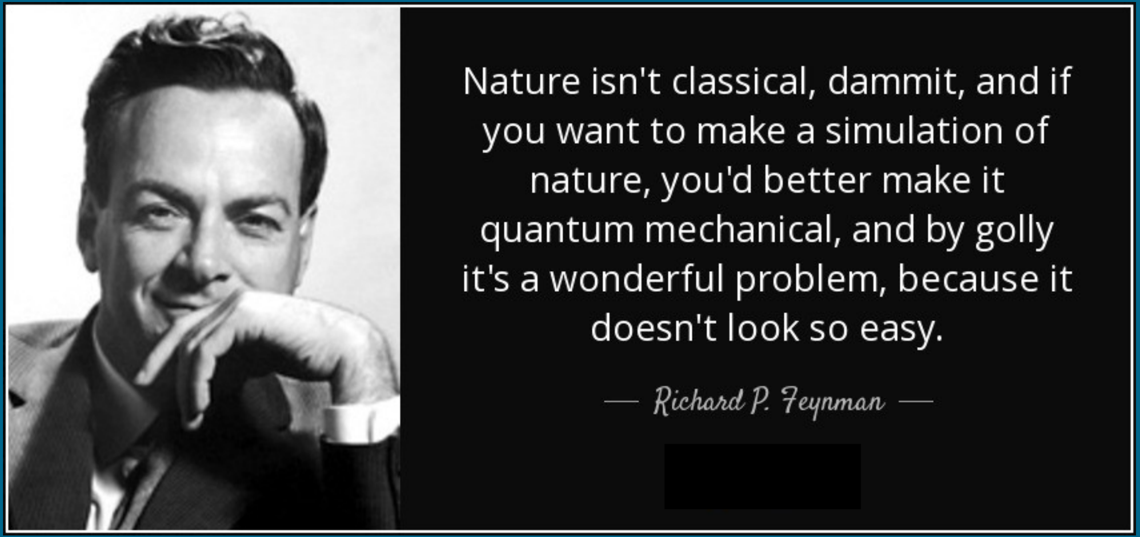
- Density functional theory (*1998 nobel prize in chemestry*)
- Quantum monte carlo
- Density matrix renormalization
- Dynamical mean field theory
- Matrix product states / Tensor networks
- Numerical renormalization group
- …

How to solve QM problems ?



Find a good ansatz for the (finite dimensional) Many body wavefunction and opimize it

- Density functional theory (*1998 nobel prize in chemestry*)
- Variational quantum monte carlo
- Density matrix renormalization
- Dynamical mean field theory
- Matrix product states / Tensor networks
- Numerical renormalization group
- …

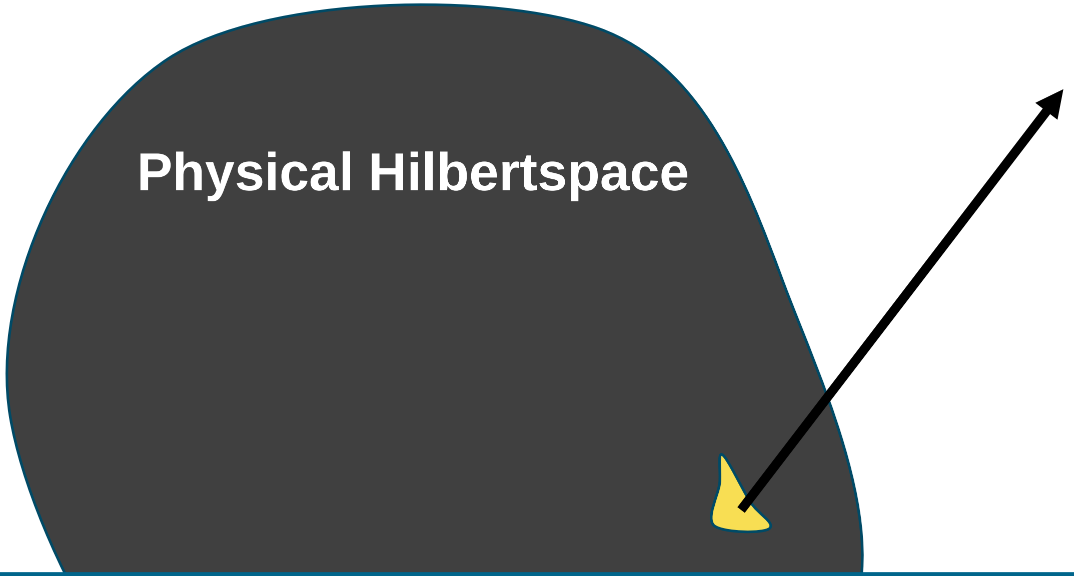


If we want to simulate a system of 300 spins:

Classical computer:
if we would store one bit of information in a single atom the whole (observable) universe wouldn't be enough to represent a single state

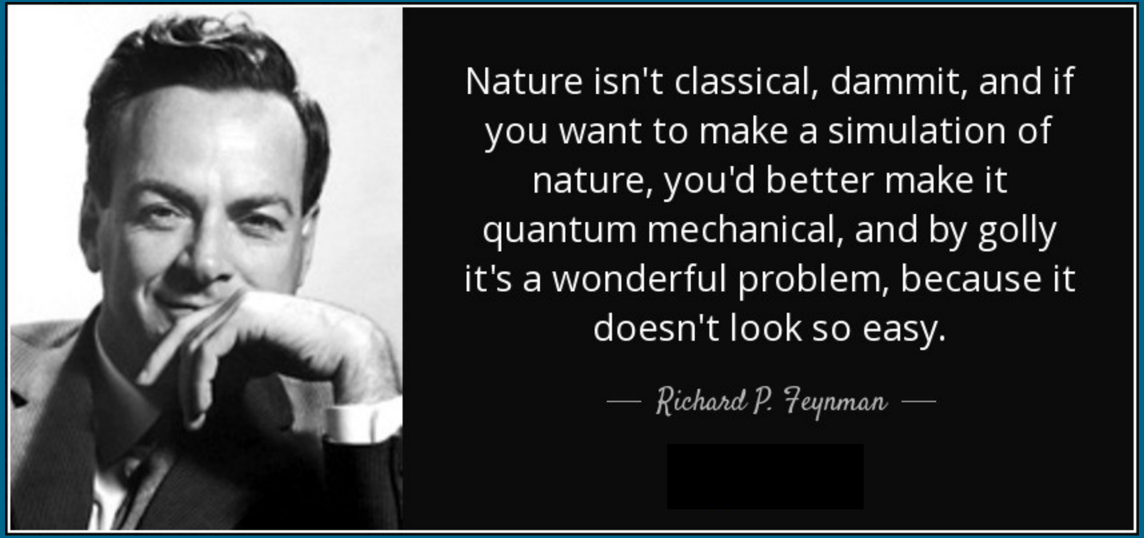
Quantum computer:
how many qubits / atoms do we need?

How to solve QM problems ?



Find a good ansatz for the (finite dimensional) Many body wavefunction and opimize it

- Density functional theory (*1998 nobel prize in chemestry*)
- Variational quantum monte carlo
- Density matrix renormalization
- Dynamical mean field theory
- Matrix product states / Tensor networks
- Numerical renormalization group
- …



If we want to simulate a system of 300 spins:

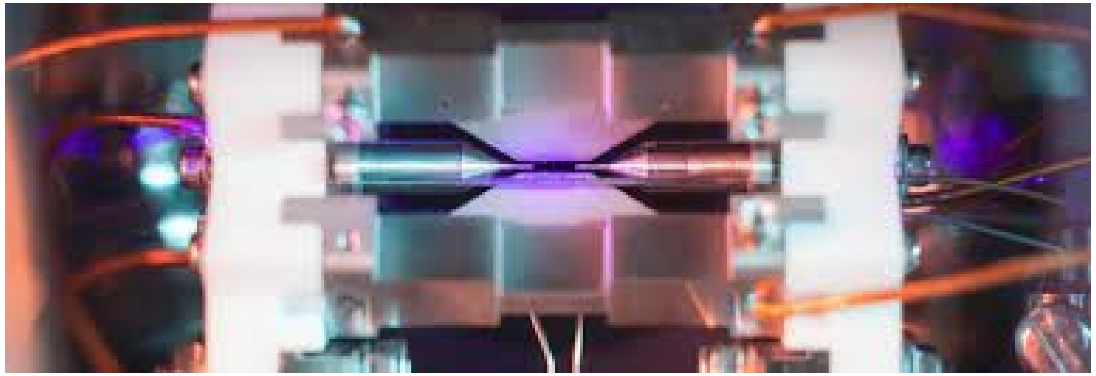
Classical computer:
if we would store one bit of information in a single atom the whole (observable) universe wouldn‘t be enough to represent a single state

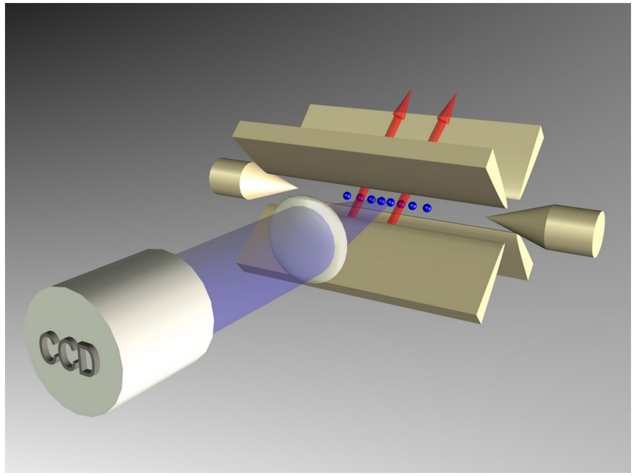
Quantum computer:
how many qubits / atoms do we need? - **300...**

(Digital) QUANTUM COMPUTER – Building blocks

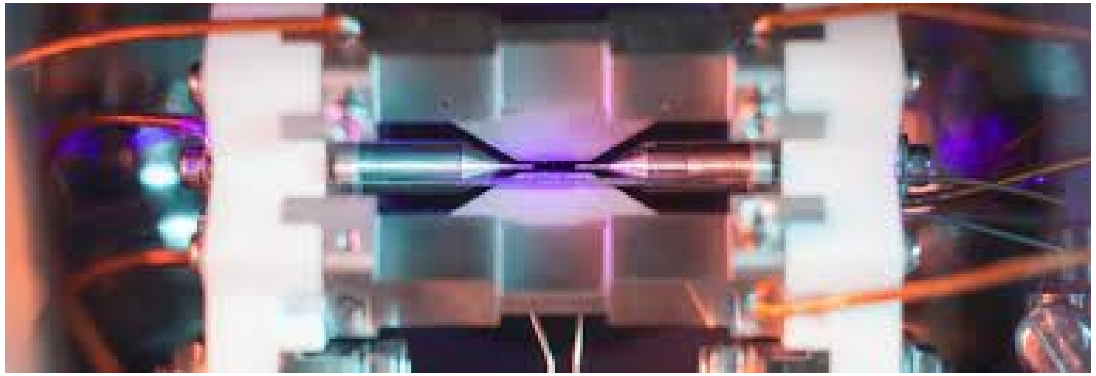
Qubits:

- nitrogen vacancies (spins)
  - Tomorrow: Dr. Gopalakrishnan Balasubramanian (XeedQ)
- superconductors
- trapped ions
- photons
- ...





(Digital) QUANTUM COMPUTER – Building blocks



Qubits:

- nitrogen vacancies (spins)
  - Tomorrow: Dr. Gopalakrishnan Balasubramanian (XeedQ)
- superconductors
- trapped ions
- photons
- ...

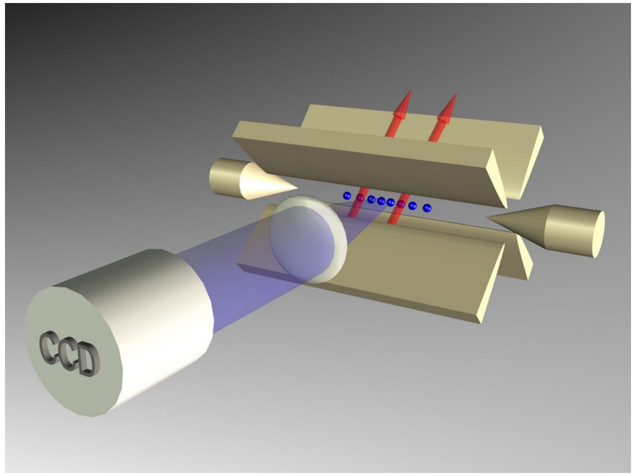
Logic gates – realized for example by laser beams

2^3	2^2	2^1	2^0		
0	1	0	0	=	4

Bit-Flip
(single bit operation)

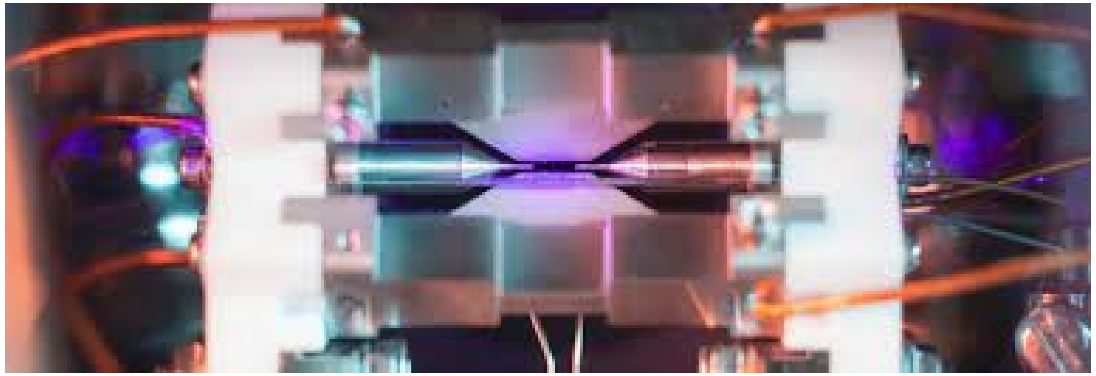
↓

$$0 \quad 1 \quad 1 \quad 0 \quad = \quad 6$$



Operator	Gate(s)		Matrix
Pauli-X (X)	X	⊕	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Y (Y)	Y		$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-Z (Z)	Z		$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard (H)	H		$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Phase (S, P)	S		$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
$\pi/8$ (T)	T		$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$
Controlled Not (CNOT, CX)	● / ⊕		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
Controlled Z (CZ)	● / Z	● / ●	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$

(Digital) QUANTUM COMPUTER – Building blocks



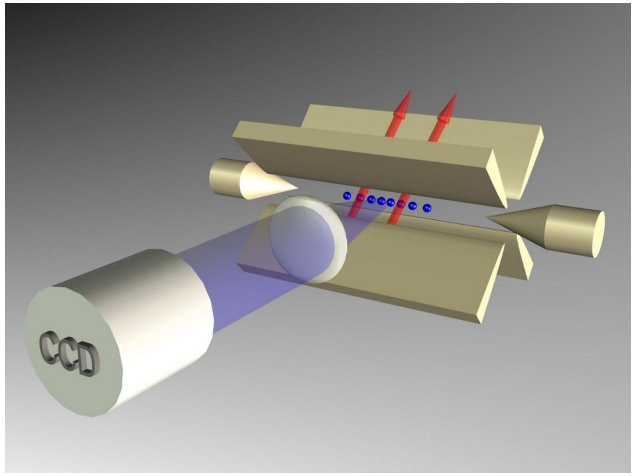
Qubits:

- nitrogen vacancies (spins)
  - ➢ Tomorrow: Dr. Gopalakrishnan Balasubramanian (XeedQ)
- superconductors
- trapped ions
- photons
- ...

Logic gates – realized for example by laser beams

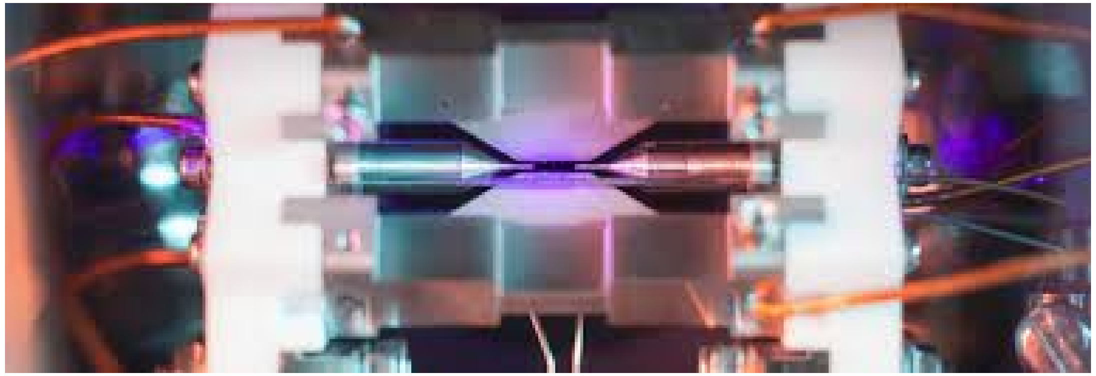
$$\begin{array}{cccccccc} & 2^3 & 2^2 & 2^1 & 2^0 & & \\ \hline & 0 & 1 & 0 & 0 & = & 4 \\ + & 0 & 1 & 1 & 0 & = & 6 \\ \hline & 1 & 0 & 1 & 0 & = & 10 \end{array}$$

Compare two bits
(two bit operations)



Operator	Gate(s)	Matrix
Pauli-X (X)	X, ⊕	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Y (Y)	Y	$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-Z (Z)	Z	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard (H)	H	$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Phase (S, P)	S	$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
$\pi/8$ (T)	T	$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$
Controlled Not (CNOT, CX)	● – ⊕	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
Controlled Z (CZ)	● – Z, ● – ●	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$

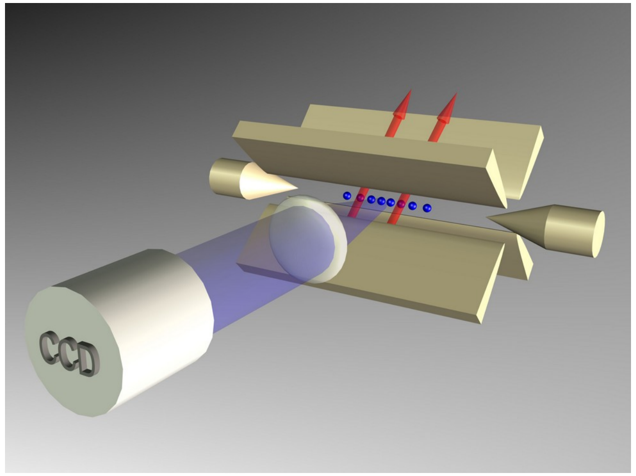
(Digital) QUANTUM COMPUTER – Building blocks



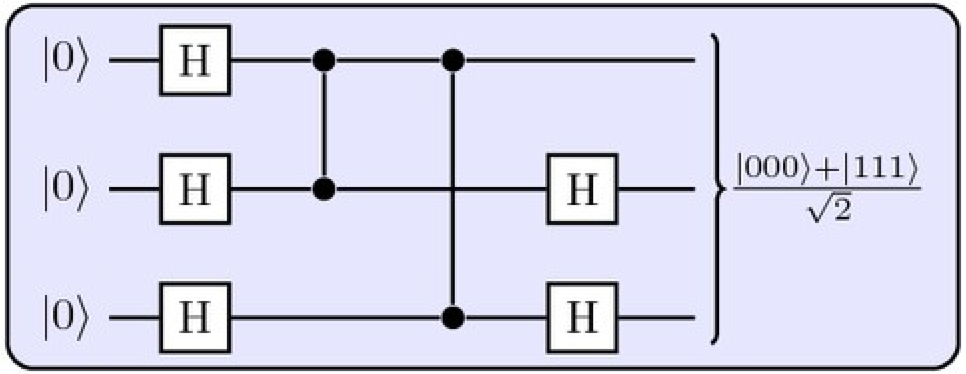
Qubits:

- nitrogen vacancies (spins)
  - ➢ Tomorrow: Dr. Gopalakrishnan Balasubramanian (XeedQ)
- superconductors
- trapped ions
- photons
- ...

Logic gates – realized for example by laser beams



Quantum circuit



Operator	Gate(s)		Matrix
Pauli-X (X)	X	⊕	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Y (Y)	Y		$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-Z (Z)	Z		$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard (H)	H		$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Phase (S, P)	S		$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
$\pi/8$ (T)	T		$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$
Controlled Not (CNOT, CX)	●–⊕		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
Controlled Z (CZ)	●–Z	●–●	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$

QUANTUM COMPUTER – conclusion

Using N (perfect) Qubits and a universal set of quantum logical gates:

- We can prepare a quantum state that represents 2^N N-Bit states *at the same time*

  $|\Psi\rangle = c_0|00...0\rangle + ... + c_{2^N}|11...1\rangle$

- We can perform operations on 2^N N-Bit states *at the same time* (quantum parallelism)

  $\hat{O}|\Psi\rangle = c_0\hat{O}|00...0\rangle + ... + c_{2^N}\hat{O}|11...1\rangle$

↓

Exponential speedup for a ***specific*** set of problems:

- Simulation of quantum mechanical materials
- Prime factorization – Shor‘s algorithm
- …

QUANTUM COMPUTER – conclusion

DLR

Using N (perfect) Qubits and a universal set of quantum logical gates:

- We can prepare a quantum state that represents 2^N N-Bit states *at the same time*
  $|\Psi\rangle = c_0|00...0\rangle + ... + c_{2^N}|11...1\rangle$

- We can perform operations on 2^N N-Bit states *at the same time* (quantum parallelism)
  $\hat{O}|\Psi\rangle = c_0\hat{O}|00...0\rangle + ... + c_{2^N}\hat{O}|11...1\rangle$

Exponential speedup for a ***specific*** set of problems:

- Simulation of quantum mechanical materials
- Prime factorization – Shor‘s algorithm
- …

Difficulties / Drawbacks:

- Mapping between QM and classical world
  - ➢ we need to prepare the quantum state
  - ➢ we can only extract N-bits of information from N-qubits
- Loss of coherence (quantumness) with time
  - ➢ Circuits need to be very short
- Reduced connectivity between qubits
- Number of controlled (logical) qubits is small ~ 50-100

QUANTUM COMPUTER – conclusion

Using N (perfect) Qubits and a universal set of quantum logical gates:

- We can prepare a quantum state that represents 2^N N-Bit states *at the same time*

$$|\Psi\rangle = c_0|00...0\rangle + ... + c_{2^N}|11...1\rangle$$

- We can perform operations on 2^N N-Bit states *at the same time* (quantum parallelism)

$$\hat{O}|\Psi\rangle = c_0\hat{O}|00...0\rangle + ... + c_{2^N}\hat{O}|11...1\rangle$$

Exponential speedup for a ***specific*** set of problems:

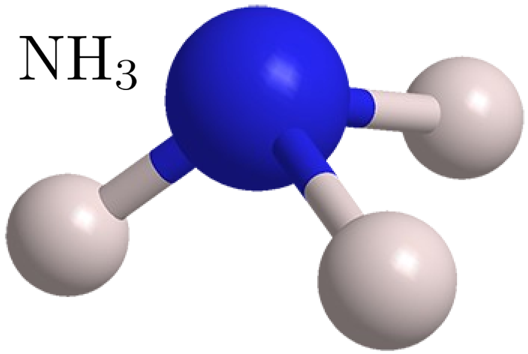
- Simulation of quantum mechanical materials
- Prime factorization – Shor‘s algorithm
- …

Difficulties / Drawbacks:

- Mapping between QM and classical world
  - ➢ we need to prepare the quantum state
  - ➢ we can only extract N-bits of information from N-qubits
- Loss of coherence (quantumness) with time
  - ➢ Circuits need to be very short
- Reduced connectivity between qubits
- Number of controlled (logical) qubits is small ~ 50-100

NITROGEN FIXATION

Ammonia / Ammoniak



- Very common fertilizer
- We woudn‘t have 8 billion people on earth without ammonia
- Its production consums ~2% of world‘s energy (high temperature / high pressure)

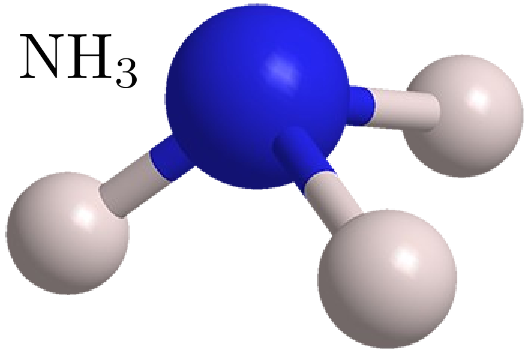
Very inefficient way!

Ammonia plant in india

NITROGEN FIXATION

Ammonia / Ammoniak

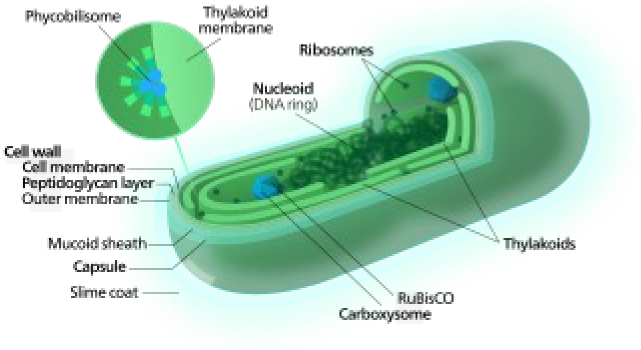
NH_3



- Very common fertilizer
- We woudn‘t have 8 billion people on earth without ammonia
- Its production consums ~2% of world‘s energy (high temperature / high pressure)

Very inefficient way!

Ammonia plant in india



Cyanobacteria spontaneously produce ammonia at room temperature…

… But we still don‘t know how it works since it is a quantum process