Quantum Computing with superconducting qubits: Applications in Chemistry and Physics

Ivano Tavernelli

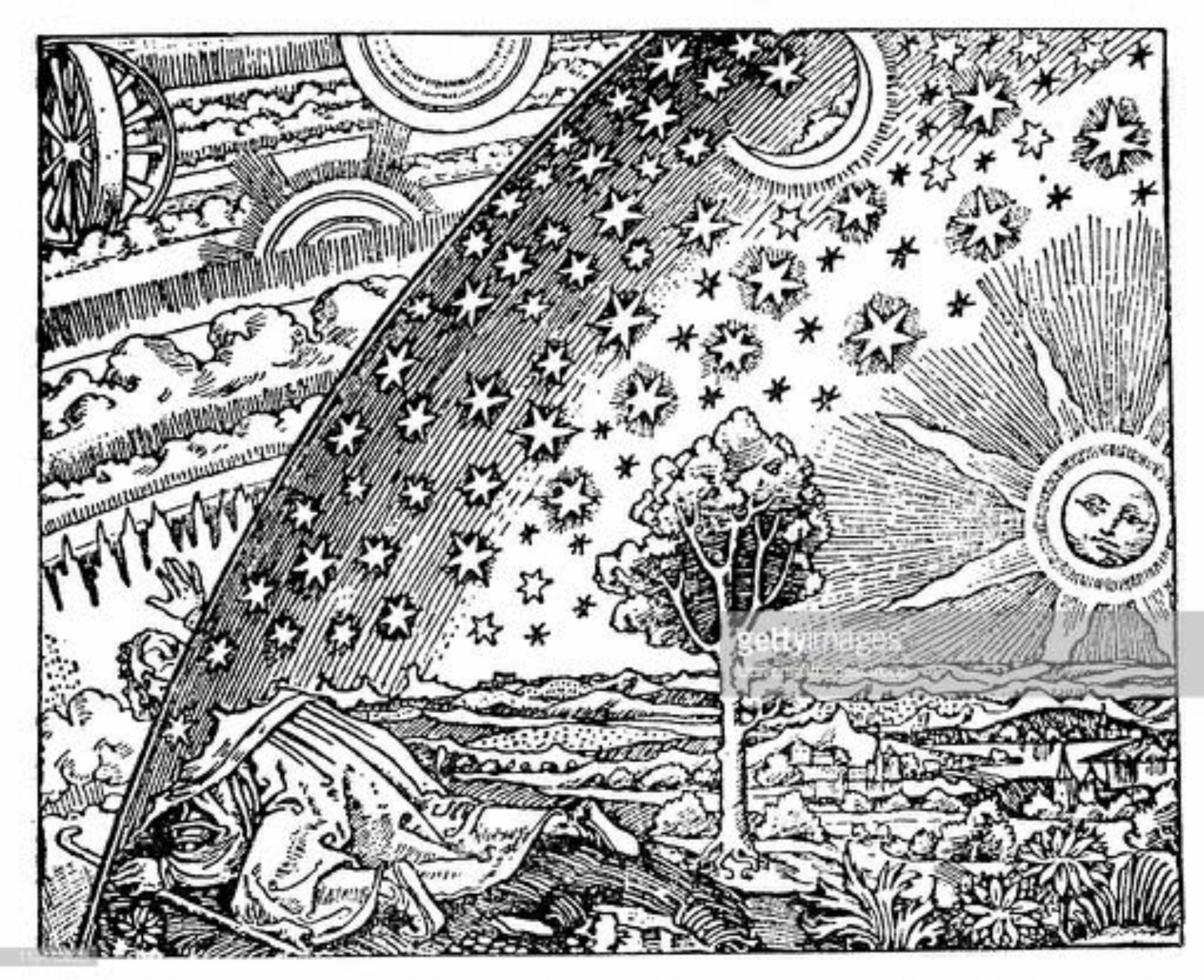
IBM Research - Zurich

PhD colloquium, University of Pavia, Italy

February 14, 2019

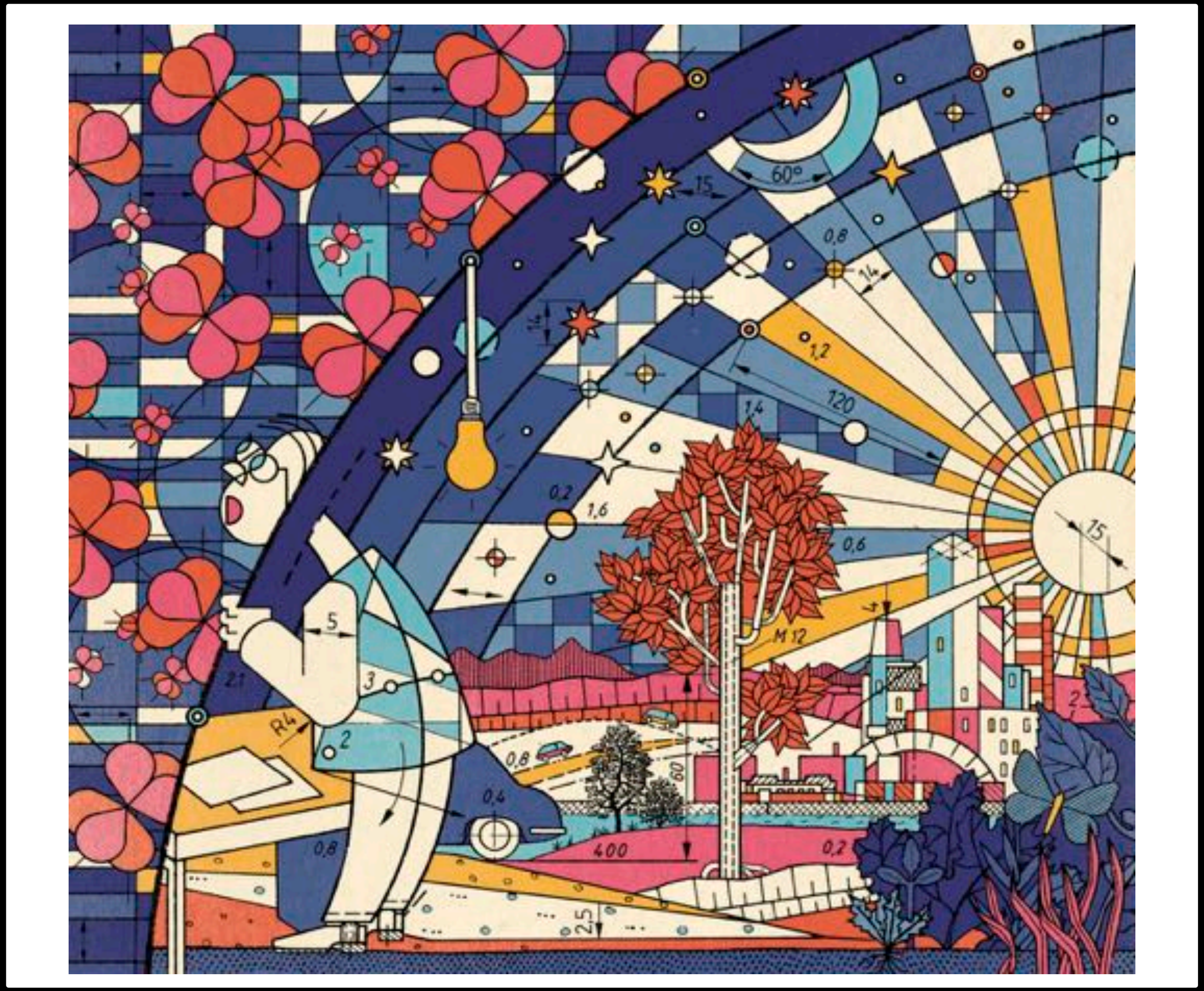
New opportunities

A look into the new cosmology



Medieval conception of the universe (Woodcut)

A look into (quantum) technology



By Christian Gralingen

Outline

Why quantum computing?

Quantum Logic

The IBM Q Hardware & Software

Applications

- Quantum chemistry
- Many-body physics
- Optimization

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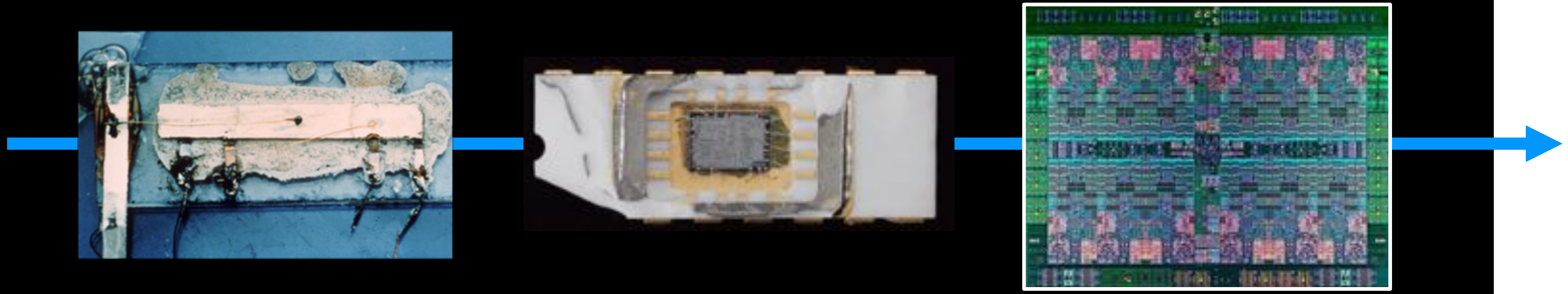
Future of computing



1958

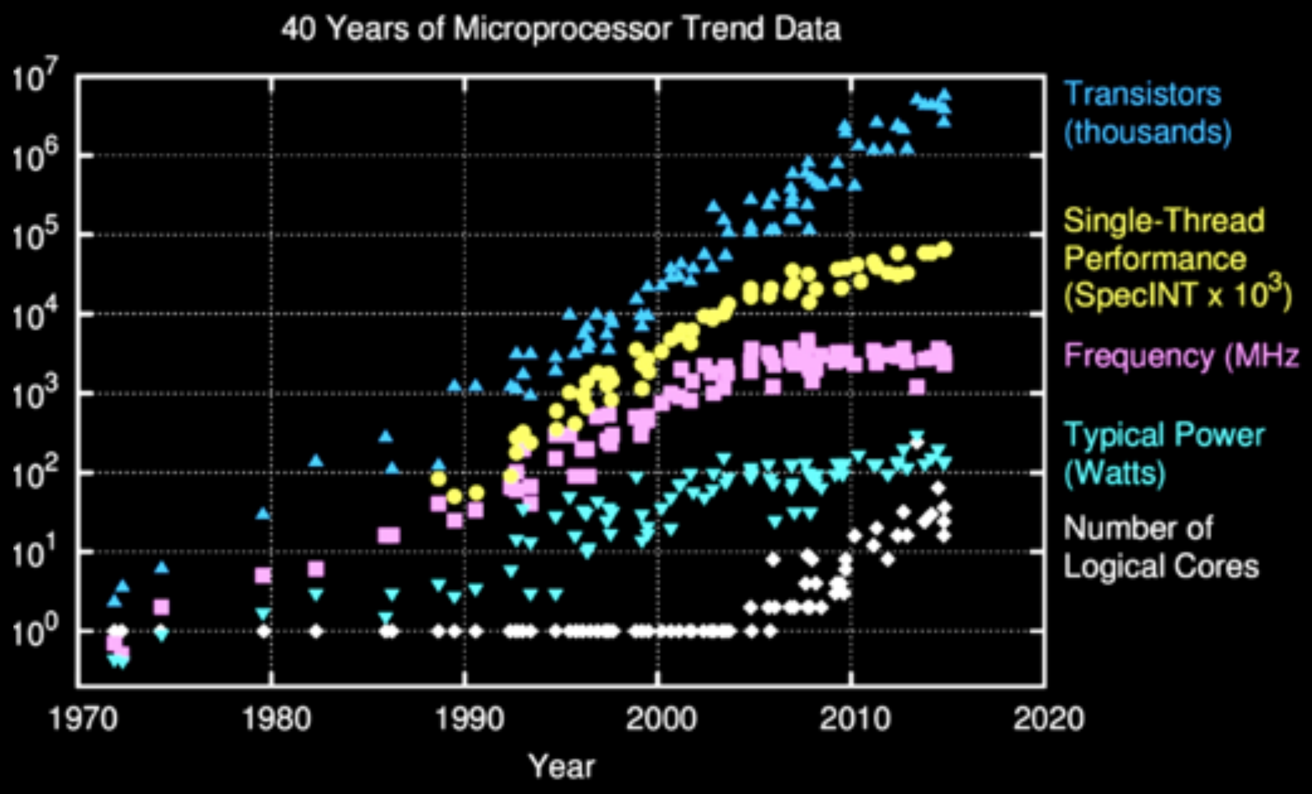
First integrated circuit
Size ~$1cm^2$
2 Transistors

1971

Moore's Law is Born
Intel 4004
2,300 transistors

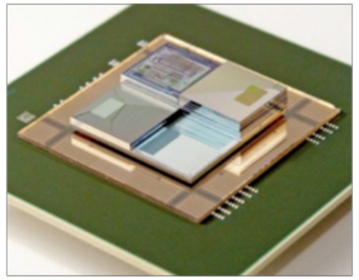
2014

IBM P8 Processor ~ 650 mm^2
22 nm feature size, 16 cores
> 4.2 Billion Transistors



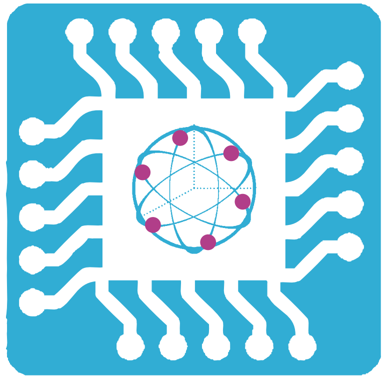
Alternative (co-existing) architectures:

next generation systems (3D/hybrid)



neuromorphic (cognitive)

quantum computing



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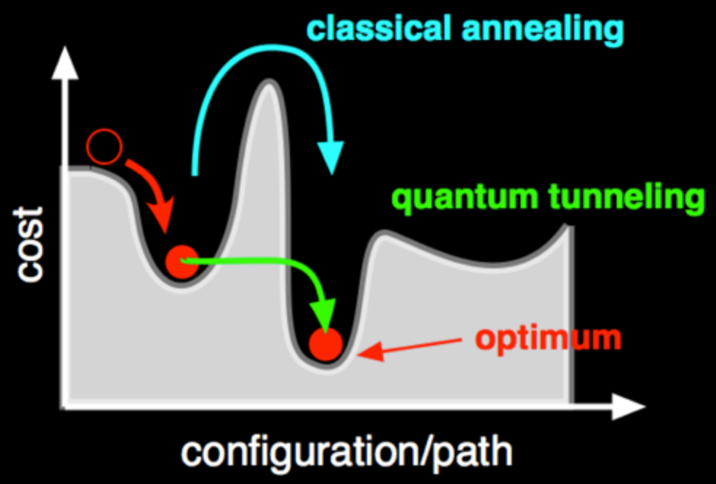
Types of Quantum Computing

Quantum Annealing

Optimization Problems

- Machine learning
- Fault analysis
- Resource optimization
- etc…

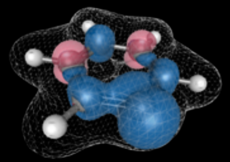


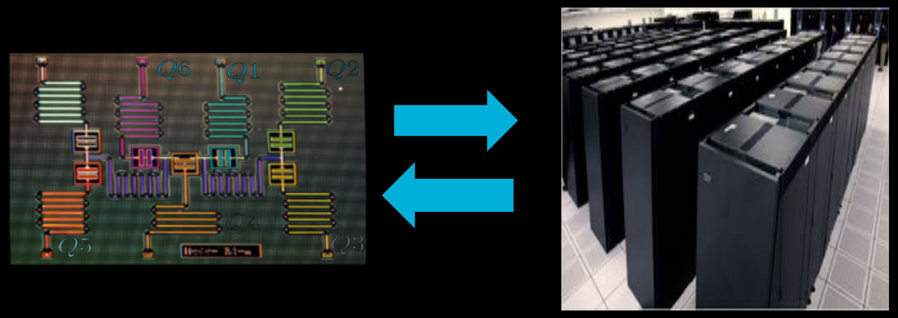
Many 'noisy' qubits can be built; large problem class in optimization; amount of quantum speedup unclear

Approximate NISQ-Comp.

Simulation of Quantum Systems, Optimization

- Material discovery
- Quantum chemistry
- Optimization (logistics, time scheduling,…)
- Machine Learning



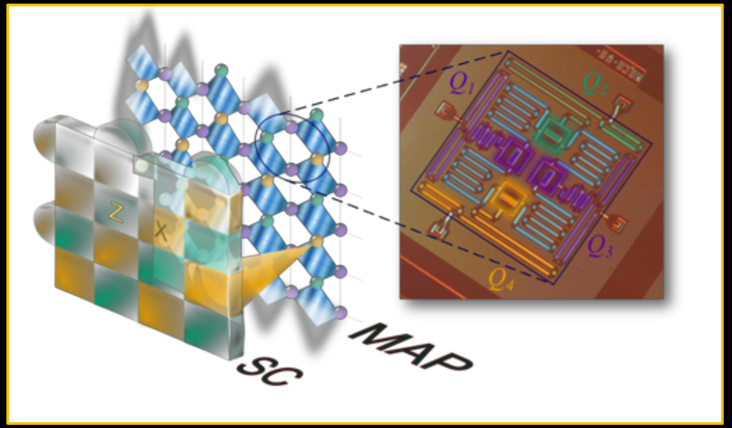


Hybrid quantum-classical approach; already 50-100 "good" physical qubits could provide quantum speedup.

Fault-tolerant Universal Q-Comp.

Execution of Arbitrary Quantum Algorithms

- Algebraic algorithms (machine learning, cryptography,…)
- Combinatorial optimization
- Digital simulation of quantum systems



Surface Code: Error correction in a Quantum Computer

Proven quantum speedup; error correction requires significant qubit overhead.

Types of Quantum Computing

Quantum Annealing

Optimization Problems

- Machine learning
- Fault analysis
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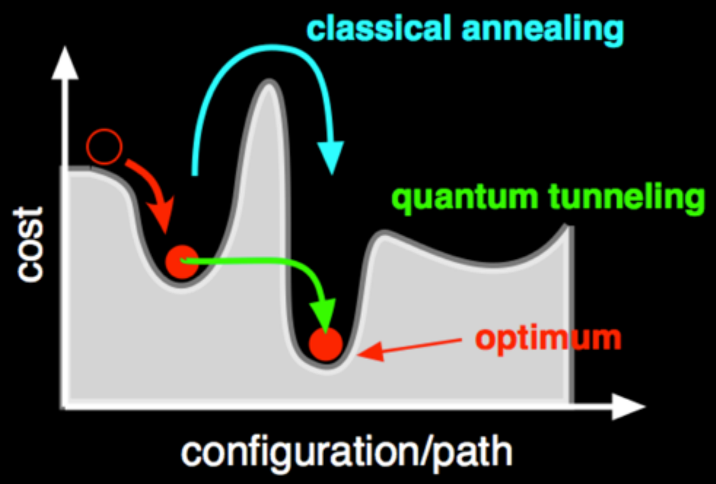
- etc…



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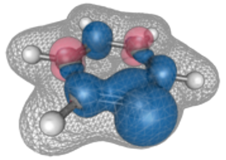

- Material discovery
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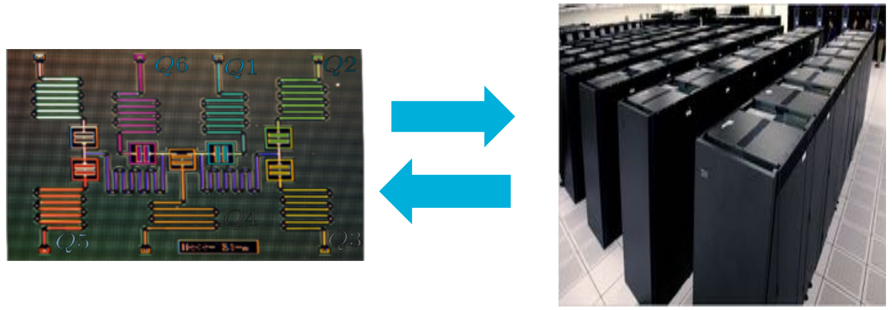
- Optimization
  (logistics, time scheduling,…)
- Machine Learning



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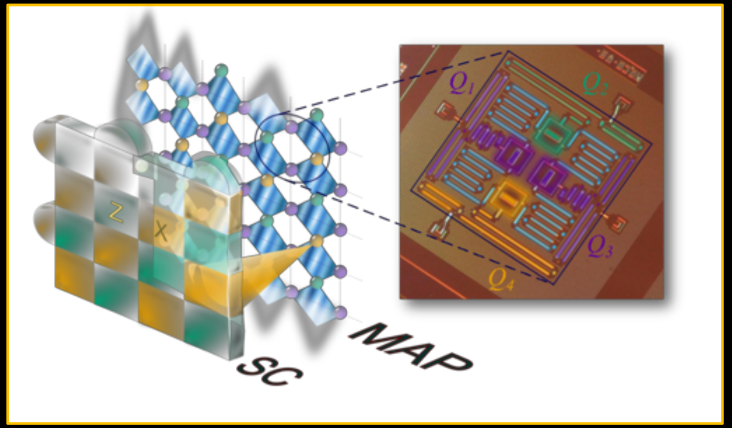

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The qubit

Bloch Sphere representation

one bit	one qubit
0 , 1	$\|0\rangle$, $\|1\rangle$

Qubit: linear superposition

$$|\psi\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|1\rangle$$

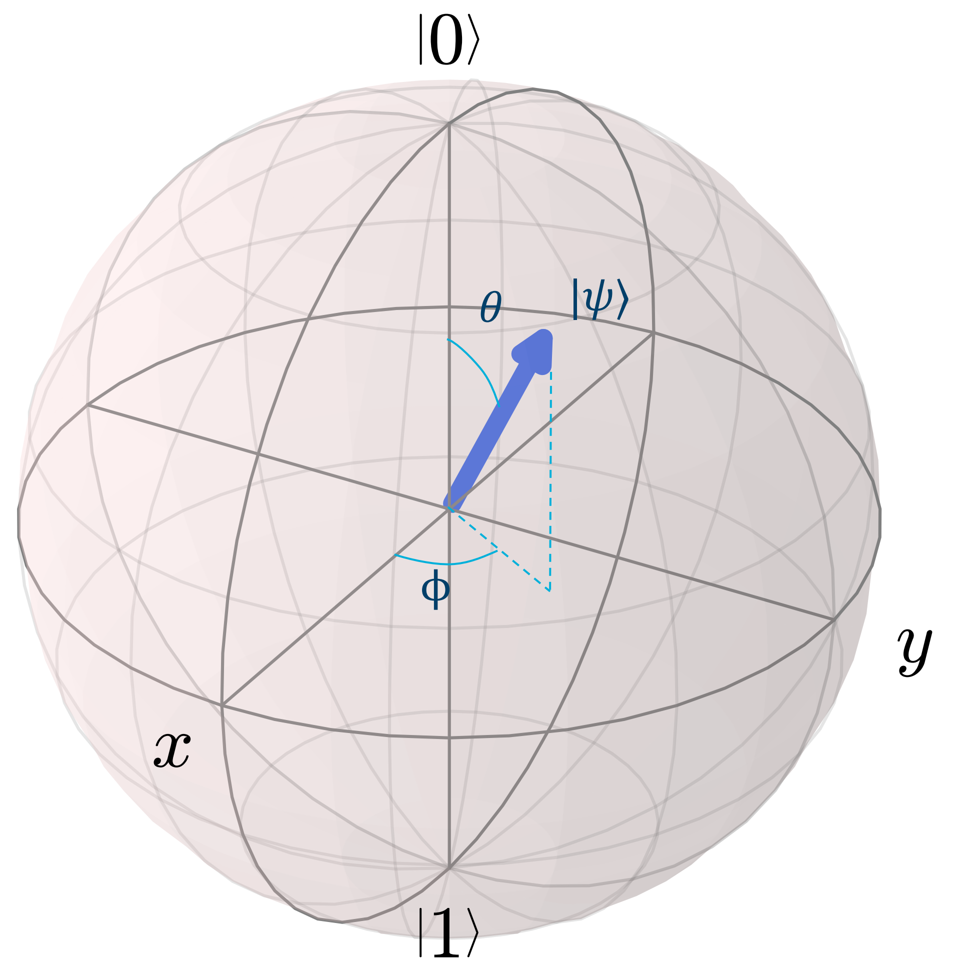
with

$$|\alpha_0|^2 + |\alpha_1|^2 = 1$$

Shown here is the state

$$|\psi\rangle = 0.95|0\rangle + (0.18 + 0.25i)|1\rangle$$

90.25 % of the measurements give $|0\rangle$ and 9.75 % give $|1\rangle$



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Single-qubit gates

$|0\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$|1\rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

X

X gate (σ_x matrix)

$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $\quad |0\rangle \rightarrow |1\rangle$, $\; |1\rangle \rightarrow |0\rangle$

Z

Z gate (σ_z matrix)

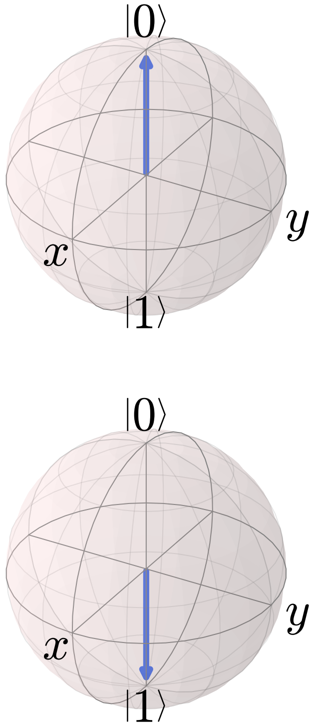
$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ $\quad |0\rangle \rightarrow |0\rangle$, $\; |1\rangle \rightarrow -|1\rangle$

H

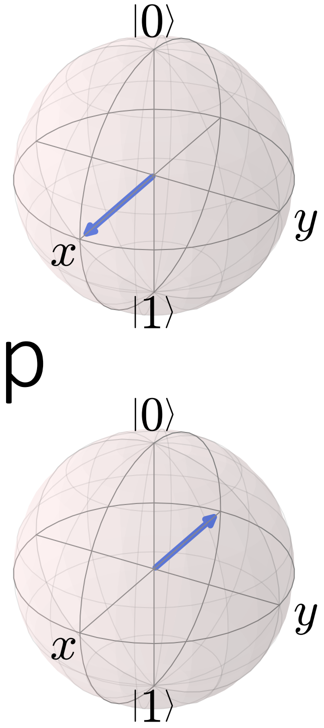
Hadamard gate

$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$ $\quad |0\rangle \rightarrow \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$, $\; |1\rangle \rightarrow \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$

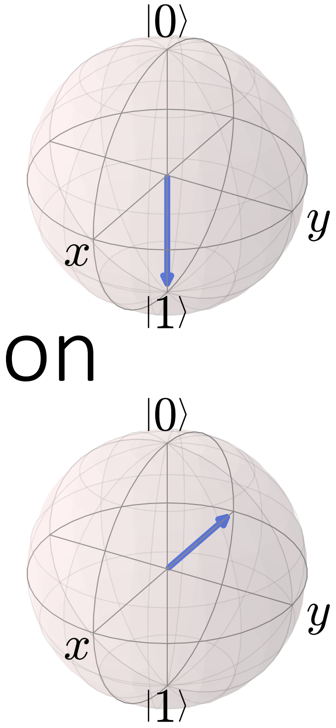
Bit-flip



Phase-flip



Superposition



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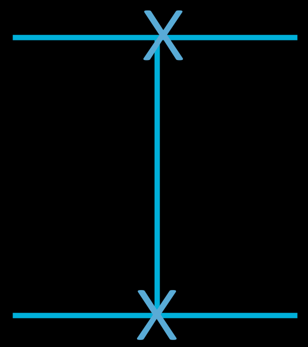
Two-qubit gates - entanglement

SWAP gate

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

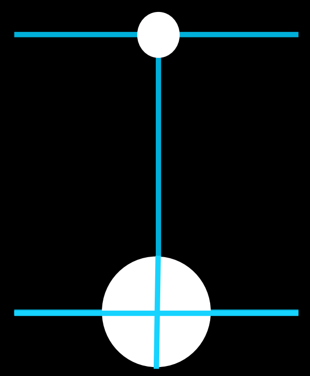
$$\begin{aligned} |00\rangle &\rightarrow |00\rangle \\ |01\rangle &\rightarrow |10\rangle \\ |10\rangle &\rightarrow |01\rangle \\ |11\rangle &\rightarrow |11\rangle \end{aligned}$$



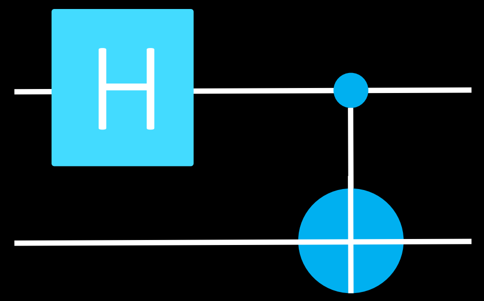
Controlled NOT gate (CNOT)

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

$$\begin{aligned} |00\rangle &\rightarrow |00\rangle \\ |01\rangle &\rightarrow |01\rangle \\ |10\rangle &\rightarrow |11\rangle \\ |11\rangle &\rightarrow |10\rangle \end{aligned}$$



Preparation of a Bell's state



The simplest entangled state

$$|00\rangle \rightarrow \frac{1}{\sqrt{2}}(|00\rangle + |10\rangle) \rightarrow \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) = |\psi_{\mathrm{Bell}}\rangle$$

Hadamard **CNOT**

Given two qubits $|\psi_1\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle$ and $|\psi_2\rangle = \beta_0|0\rangle + \beta_1|1\rangle$ a Bell state cannot be represented as product state $|\psi_1\rangle \cdot |\psi_2\rangle = \alpha_0\beta_0|00\rangle + \alpha_0\beta_1|01\rangle + \alpha_1\beta_0|10\rangle + \alpha_1\beta_1|11\rangle \neq |\psi_{\mathrm{Bell}}\rangle$

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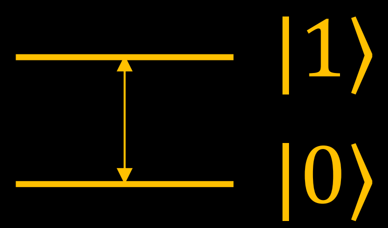
Physical qubit realizations

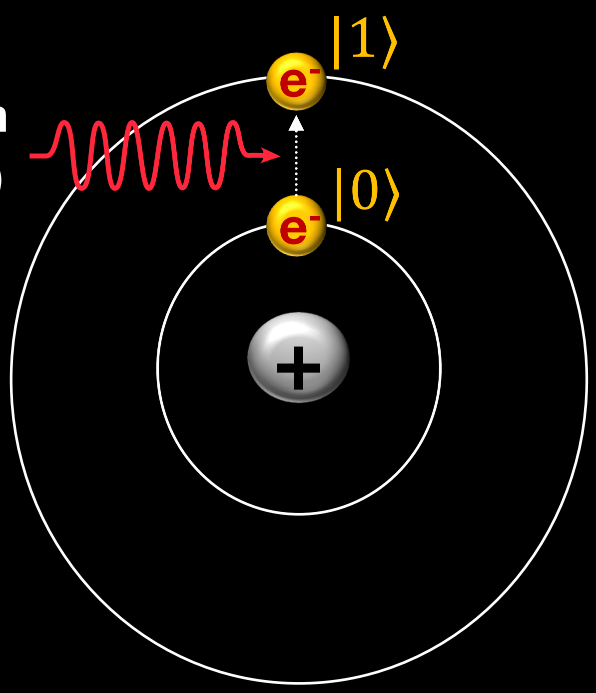
Quantum Bits:

Two-Level Systems

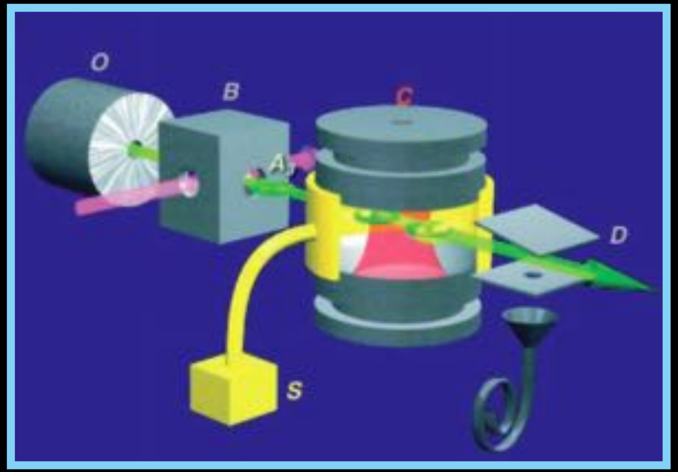


Example:
Atom orbitals with different energetic levels

Photon (Laser)



Neutral Atoms



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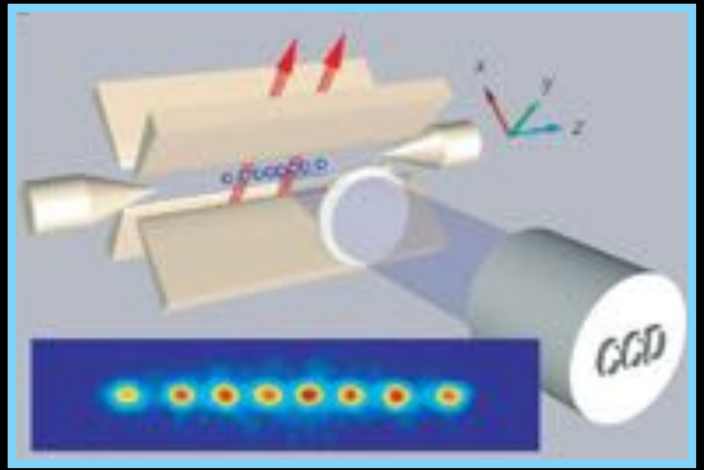
Ion Traps



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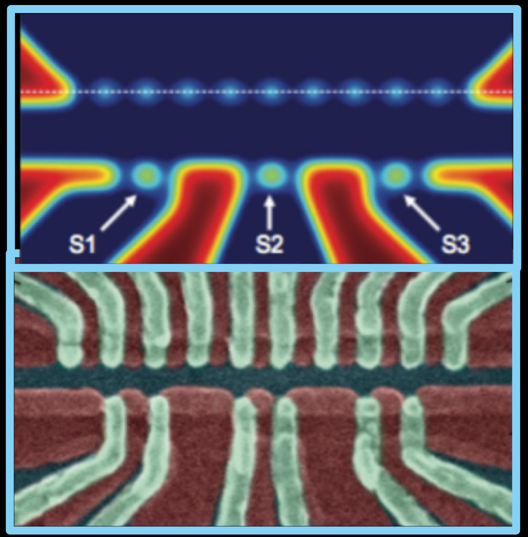
Quantum Dots



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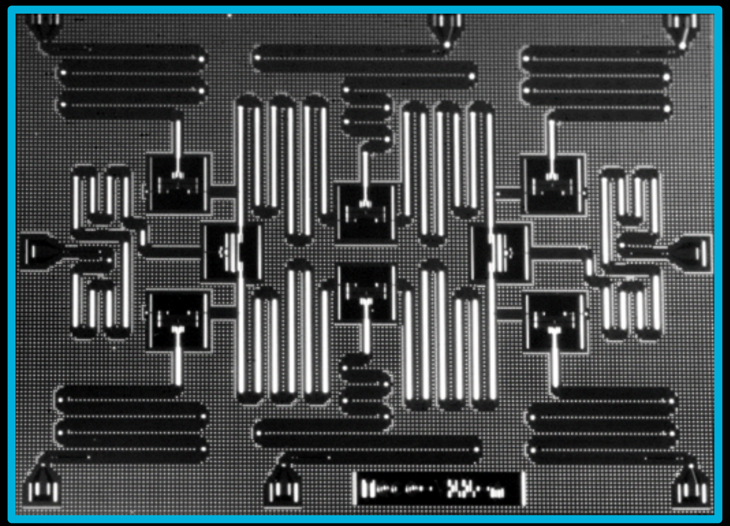
Superconducting Circuits



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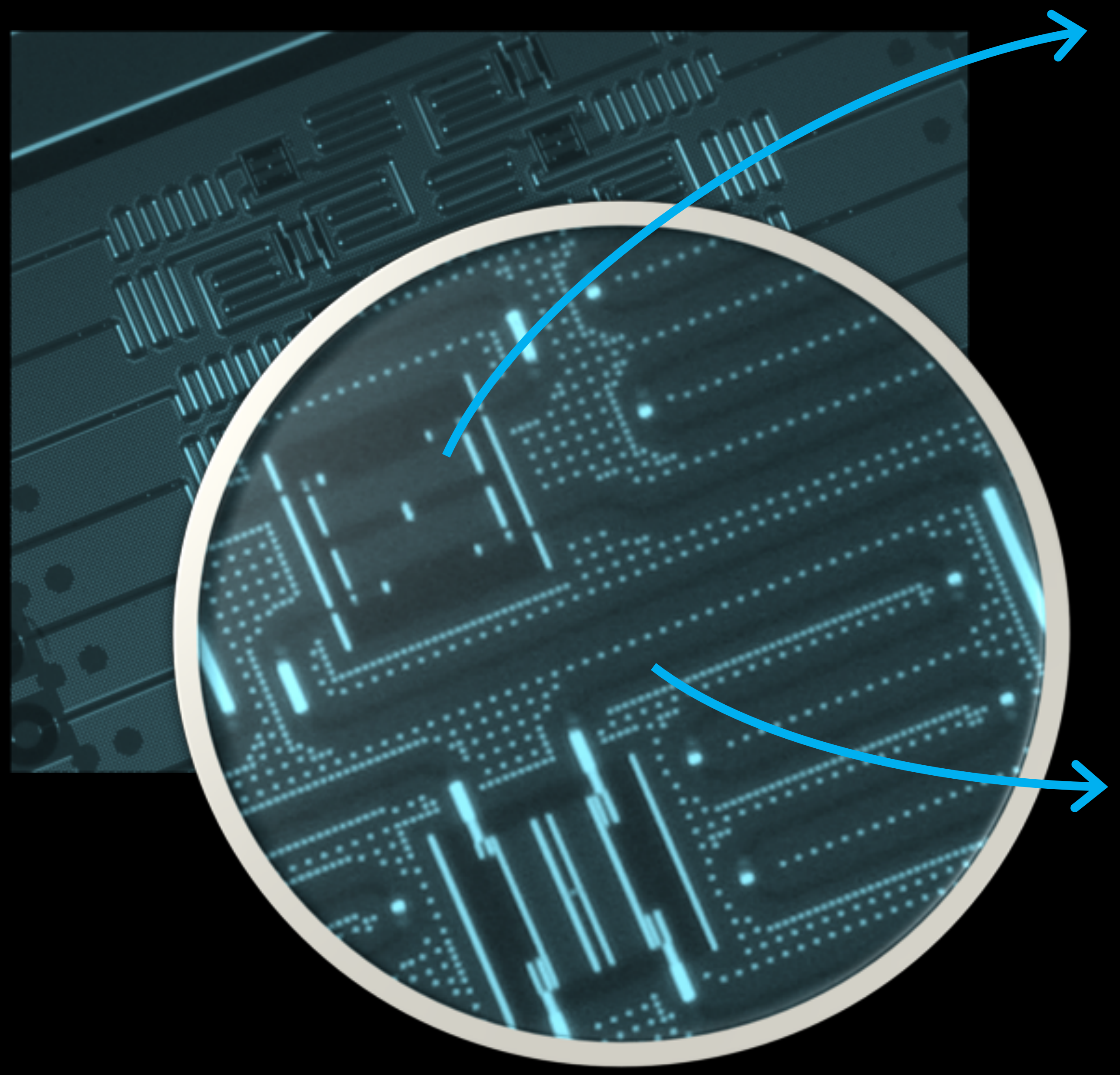
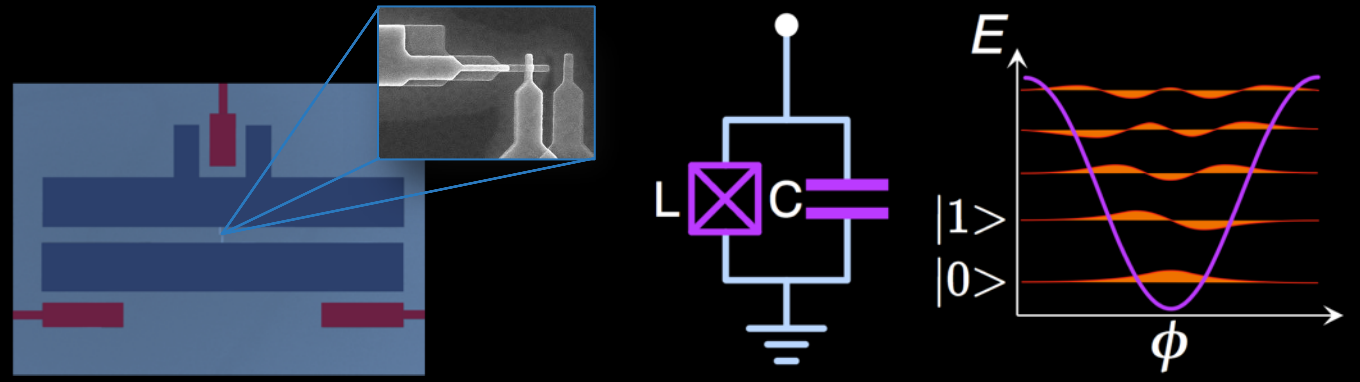
IBM: Superconducting Qubit Processor



Superconducting qubit (transmon):

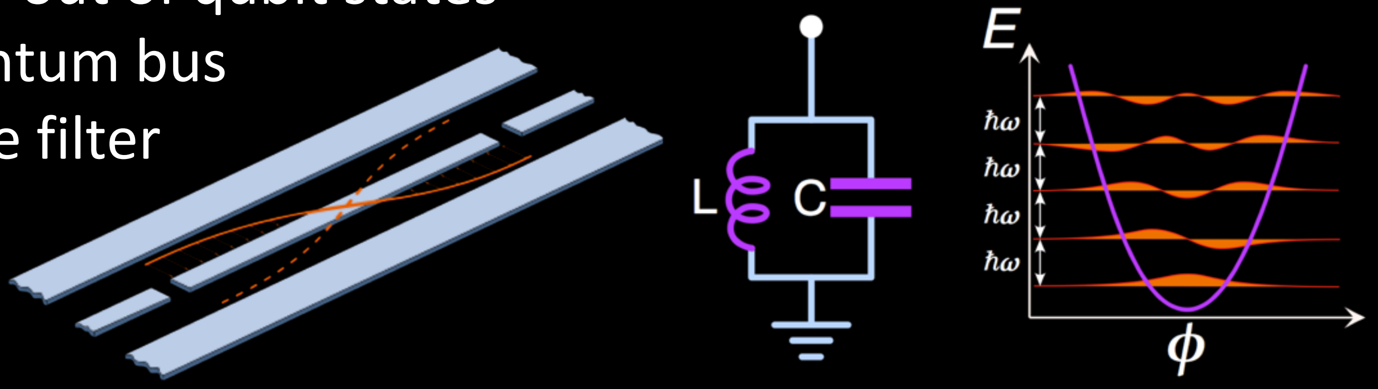
- quantum information carrier
- nearly dissipationless →
  T_1, T_2 ~ 70 µs lifetime, 50MHz clock speed



$E_{01} \approx 5\ \text{GHz} \approx\ 240\ \text{mK}$

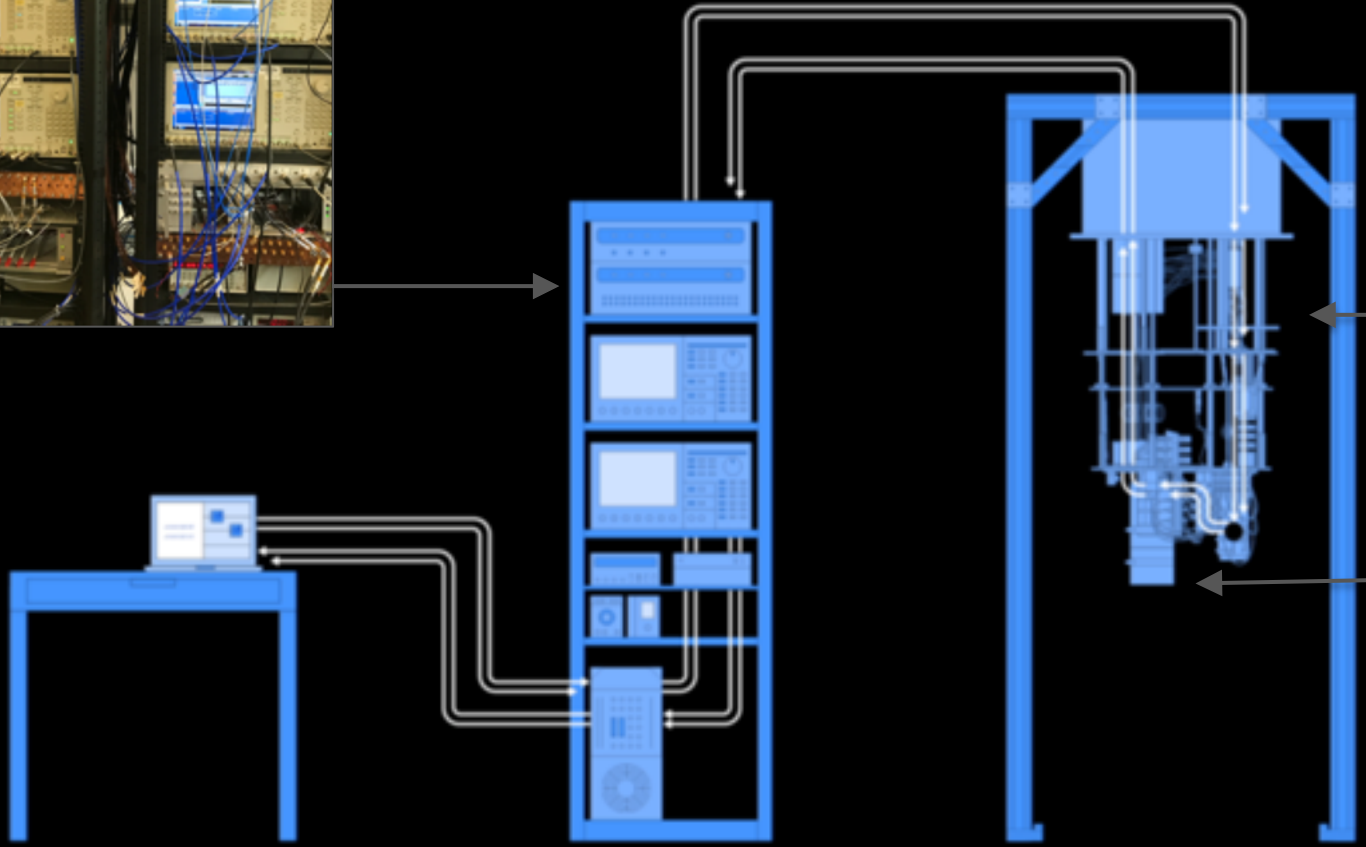
Microwave resonator as:

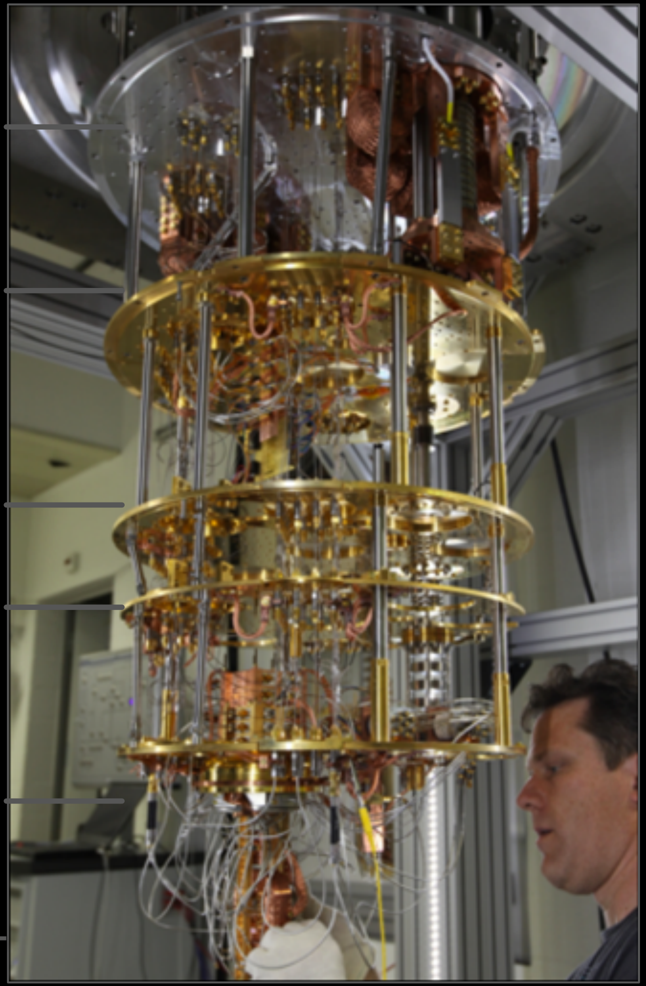
- read-out of qubit states
- quantum bus
- noise filter



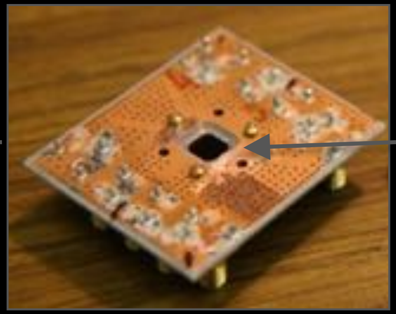
Inside an IBM Q quantum computing system

Microwave electronics

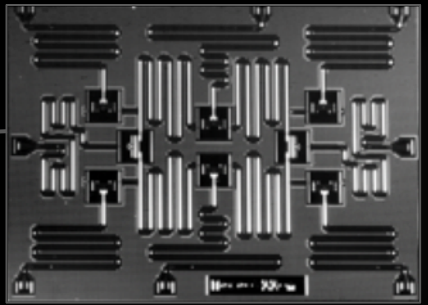




Refrigerator to cool qubits to 10 - 15 mK with a mixture of ^3He and ^4He



PCB with the qubit chip at 15 mK protected from the environment by multiple shields

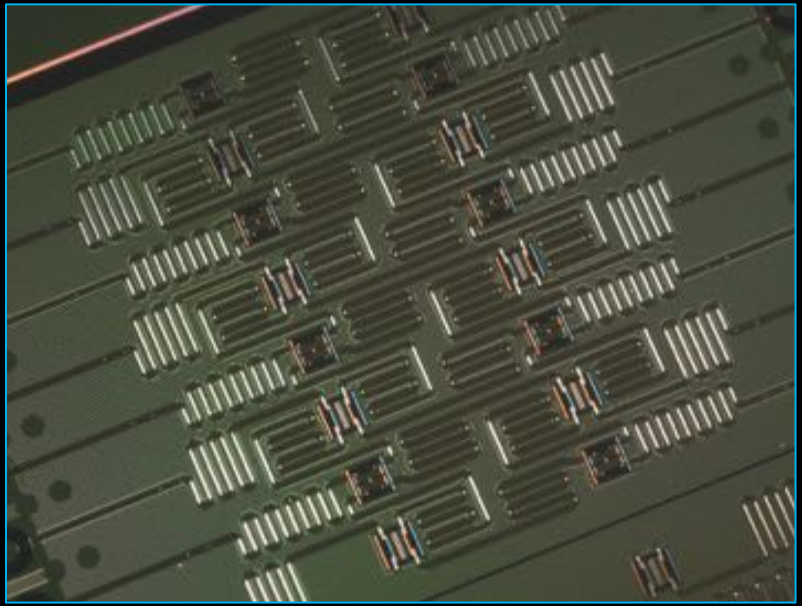


Chip with superconducting qubits and resonators

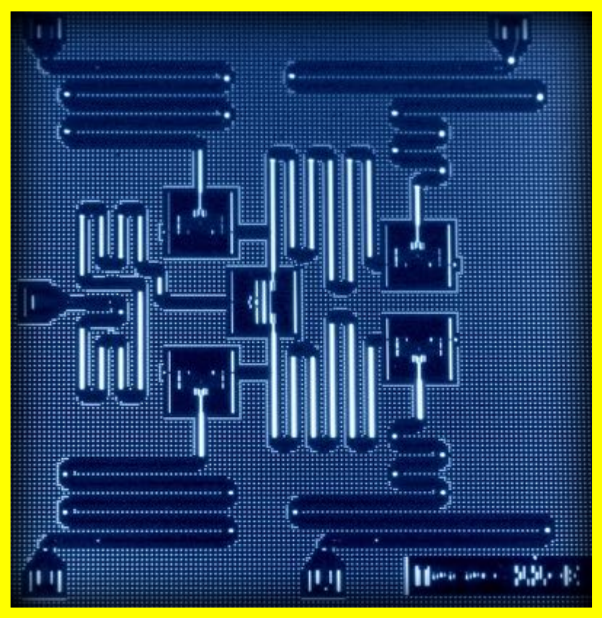
IBM qubit processor architectures

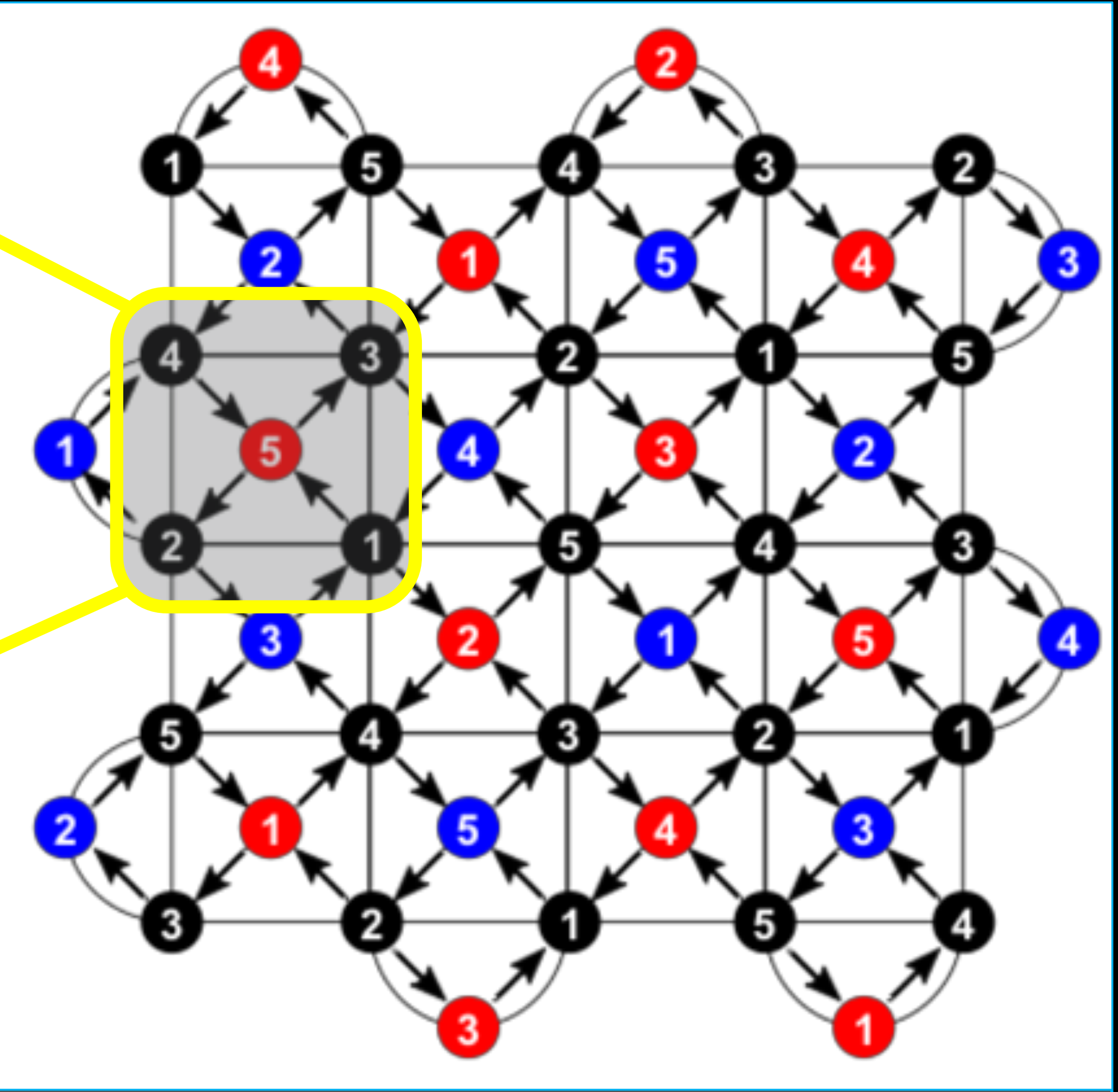
IBM Q experience (publicly accessible)

16 Qubits (2017)



5 Qubits (2016)

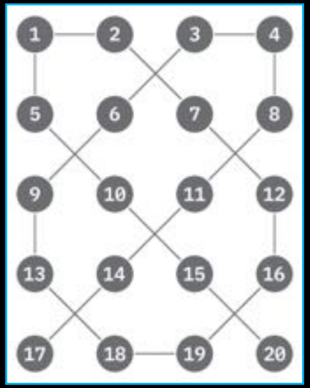




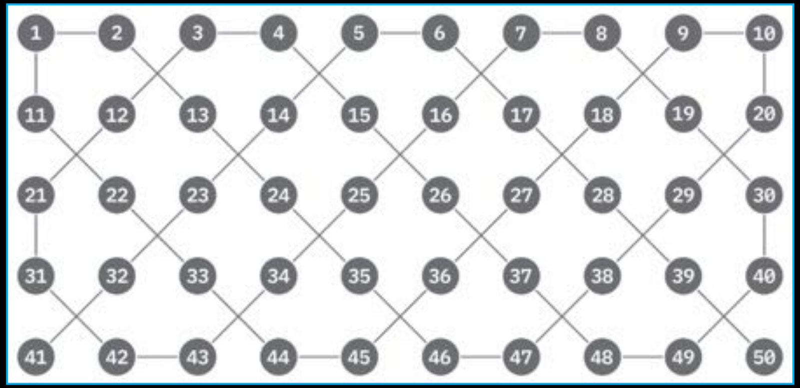
Latticed arrangement for scaling

IBM Q commercial

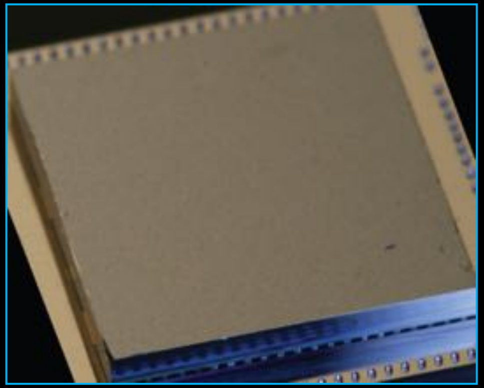
20 Qubits



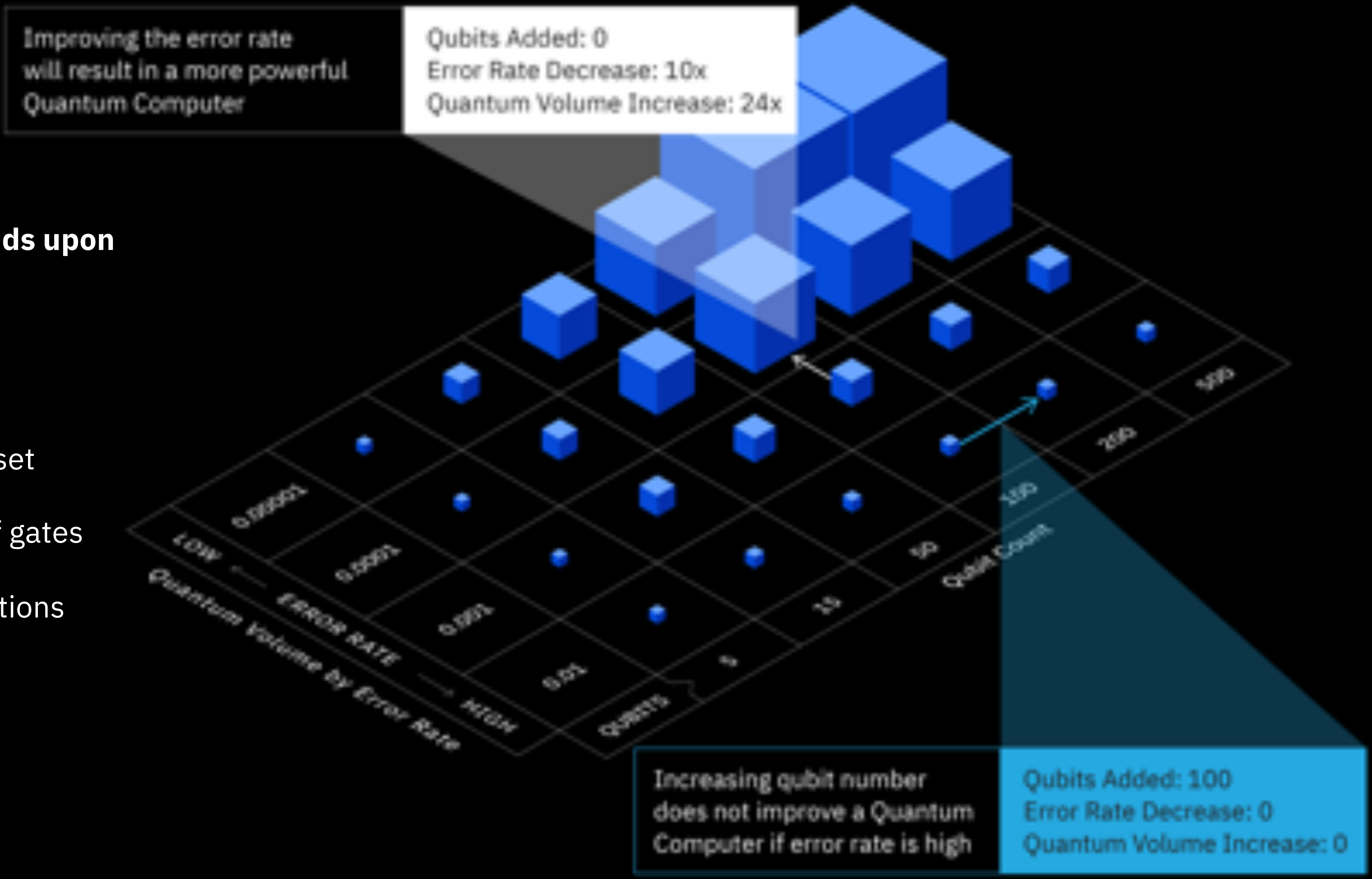
50 Qubit architecture



Package



The power of quantum computing is more than the number of qubits



Quantum Volume depends upon

Number of physical QBs

Connectivity among QBs

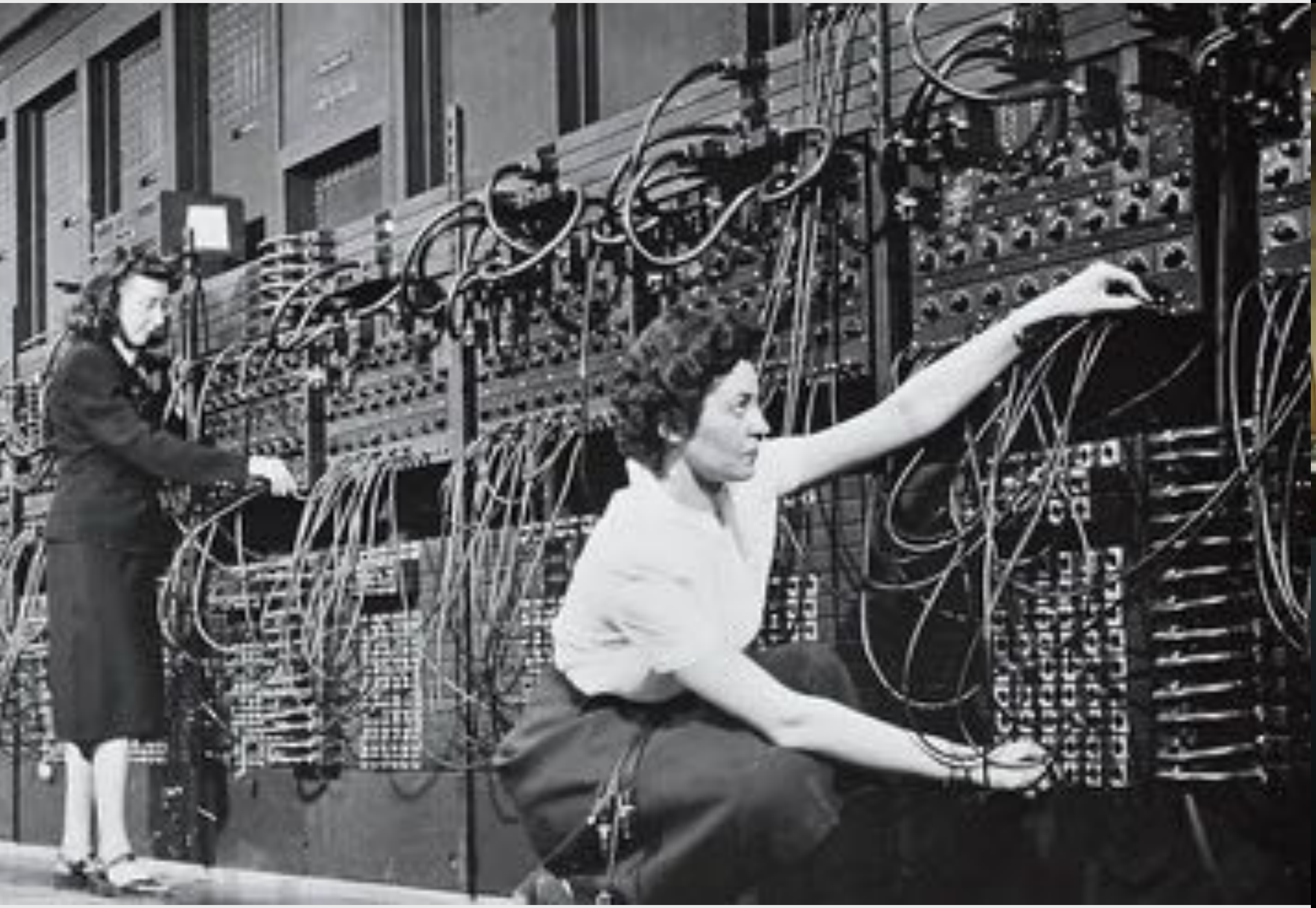
Available hardware gate set

Error and decoherence of gates

Number of parallel operations

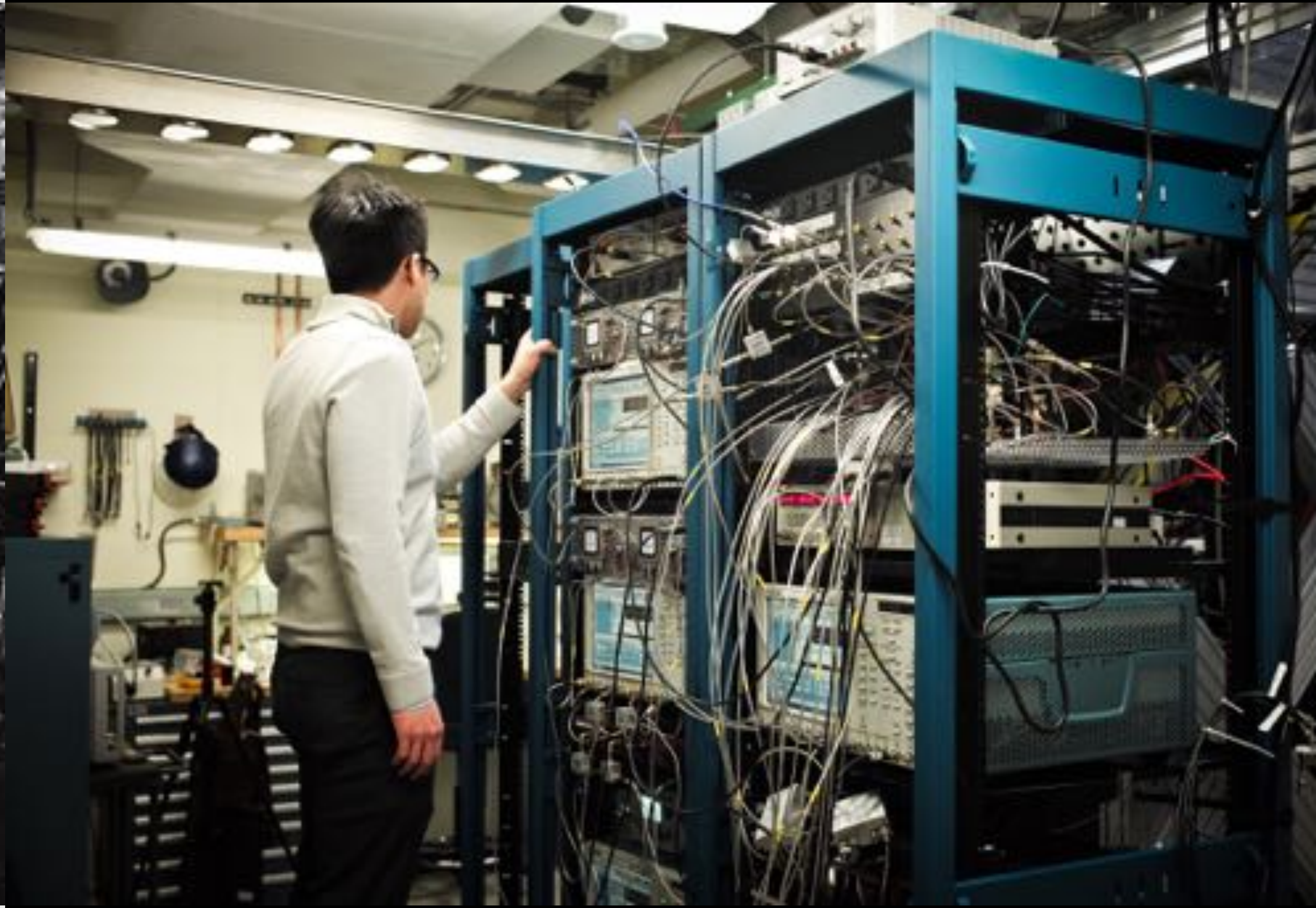
ENIAC

One of the earliest electronic general-purpose computers in 1946



IBM Q Experience in 2016

First cloud quantum computing device



"We've come a long way from then, providing the most advanced and most used quantum computers on the cloud" (2018)

System 1 – IBM January 2019

IBM Q

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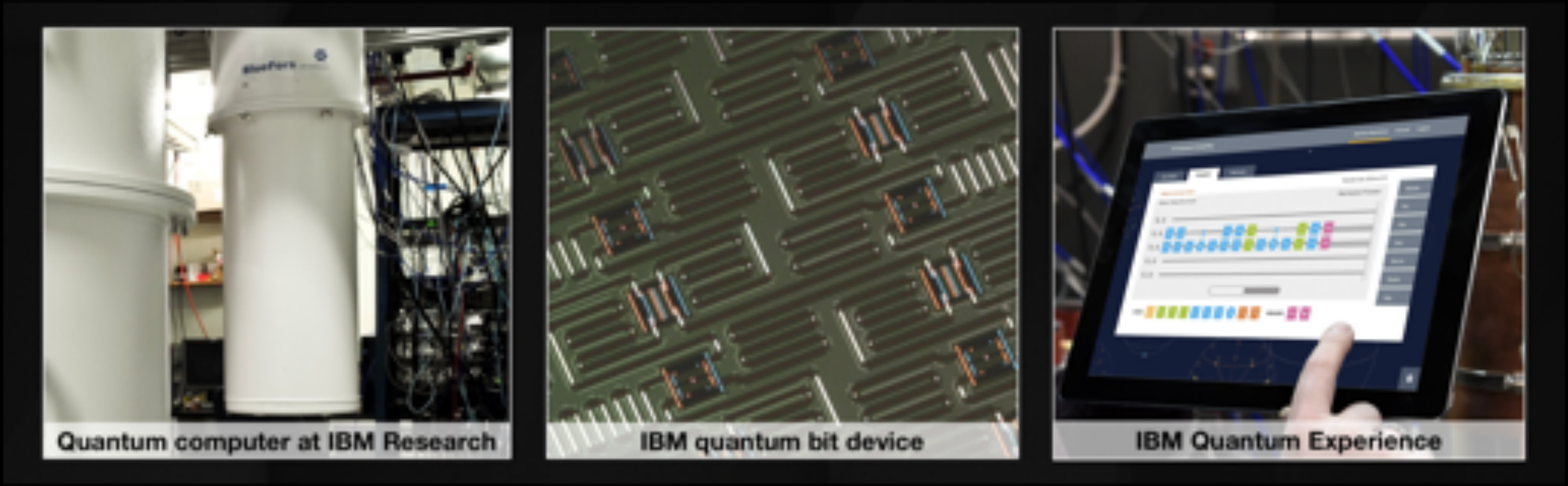
IBM released the IBM **Q** Experience in 2016



In May 2016, IBM made a quantum computing platform available via the IBM Cloud, giving students, scientists and enthusiasts hands-on access to run algorithms and experiments

IBM released the IBM **Q** Experience in 2016

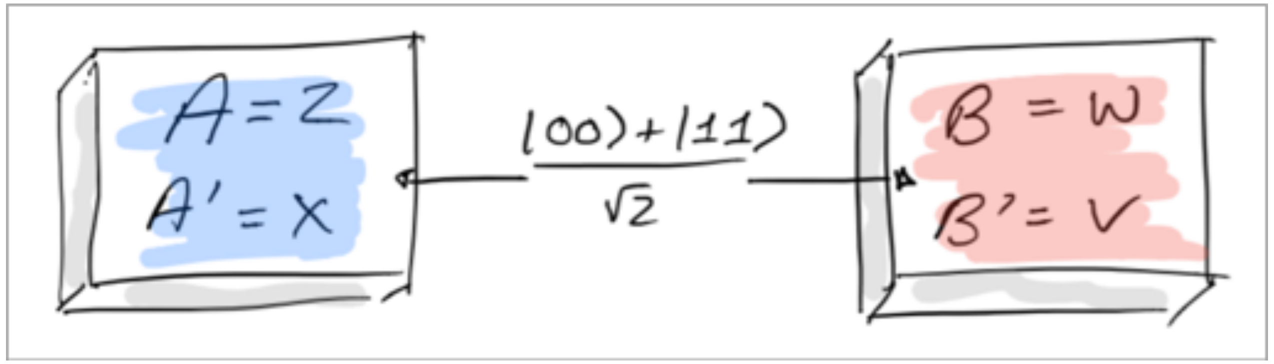
QX is a fantastic tool for teaching.

Proving Bell's inequality using IBM QX is a few minutes task.

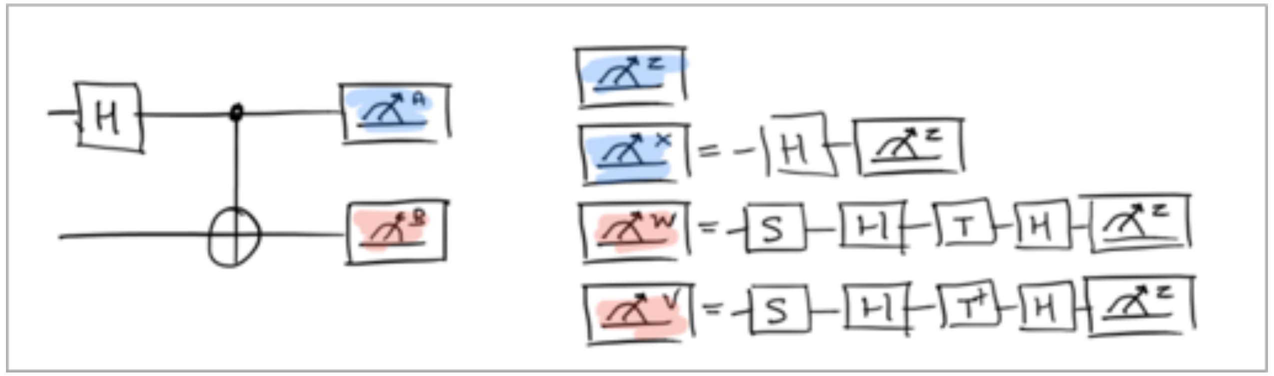
With QX you have access to a 'quantum laboratory' from home.

Test simple quantum algorithms without the need to learn any programming language.

... but you may need more ....



$$C = \langle AB \rangle - \langle AB' \rangle + \langle A'B \rangle + \langle A'B' \rangle$$



Belltest: 8192 shots May 2nd 11:44pm

	P(00)	P(11)	P(01)	P(10)	⟨AB⟩
ZW	0.434	0.380	0.070	0.116	0.629
ZV	0.409	0.415	0.100	0.076	0.648
XW	0.452	0.375	0.090	0.083	0.654
XV	0.110	0.077	0.451	0.36	-0.626

$|C| = 2.56 \pm 0.03$

Qiskit Community

A place for Qiskitters

Qiskit community

Qiskit is driven by our avid community of Qiskitters! We are committed to our goal of bringing quantum computing to people of all backgrounds, and are always excited to hear your feedback directly from you. There are many ways to stay informed, contribute to, and collaborate on Qiskit.

- Slack
- GitHub
- Stack Exchange
- Twitter
- Medium
- YouTube
- Facebook

Qiskit building the software for tomorrow's computers.

IBM Q

The IBM Q Experience has seen extraordinary adoption

First quantum computer on the cloud

> 100,000 users

All 7 continents

> 5.2 Million experiments run

> 120 papers

> 1500 colleges and universities, 300 high schools, 300 private institutions

IBM Q Experience executions on real quantum computers (not simulations)

May 11, 2018

IBM Q16

IBM Q5

Qiskit

high level quantum applications:
chemistry, optimization, AI, finance

state characterization,
error mitigation,
optimal control

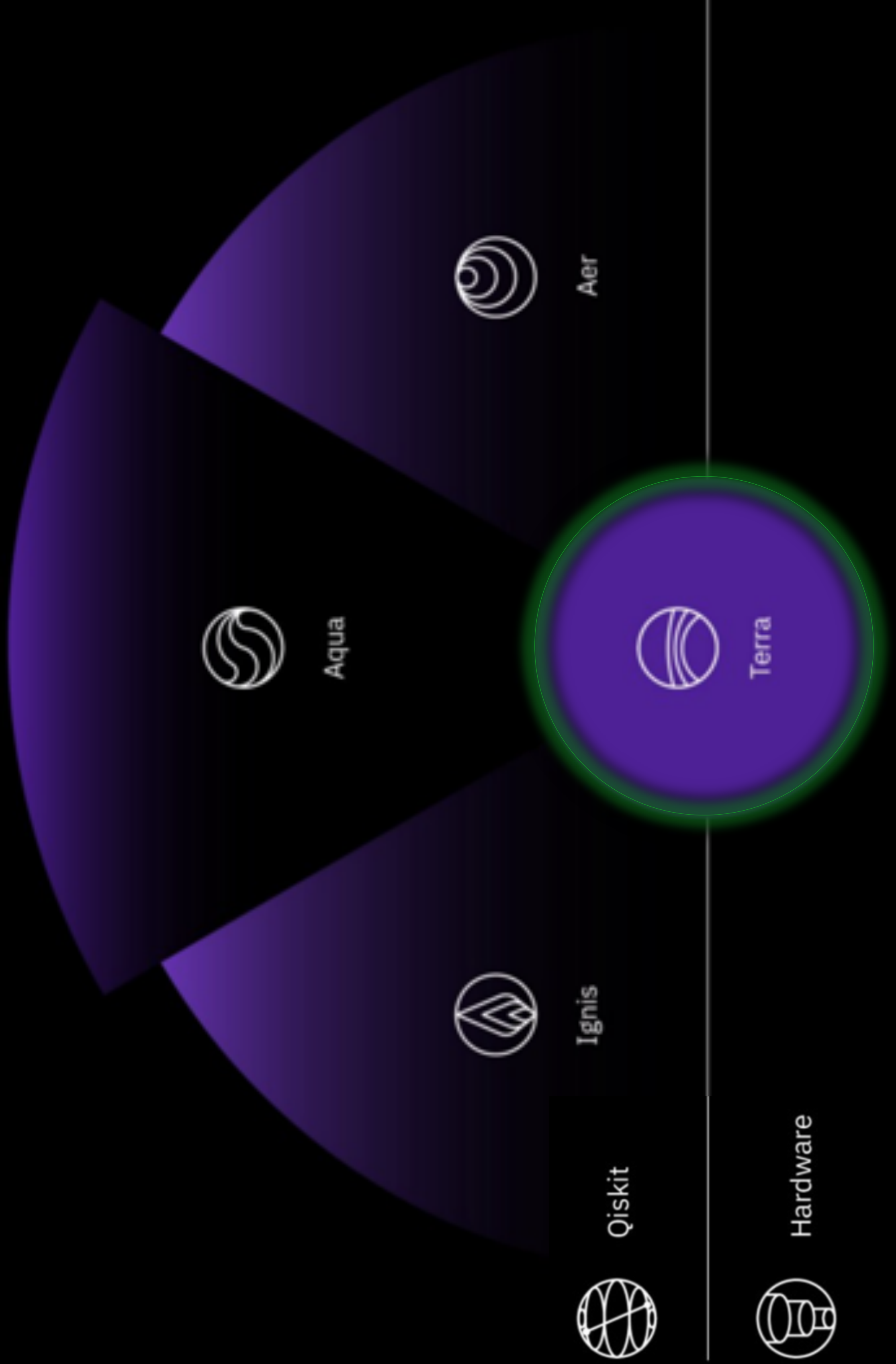
classical simulation of
quantum circuits

core programming tools and API to hardware

QISKit: Terra

Stack

- **Terra inputs**
  Quantum circuit, pulse scheduler
- **Transpiler**
  Optimization passes, pass manager
- **QObj**
  OpenQASM, OpenPulse
- **Backend**
  Device, simulator
  Provider
  Local, IBM Q, third party
- **Job**
- **Result**
  Counts, Statevector, Unitary



Panagiotis Barkoutsos - bpa@zurich.ibm.com

QISKit: Aqua

Stack

Aqua applications domains
Chemistry, AI, Optimization, Finance

Translators

Quantum algorithms

Adaptive
VQE, QAOA.Variational, QSVM.Variational, VQE2QPE

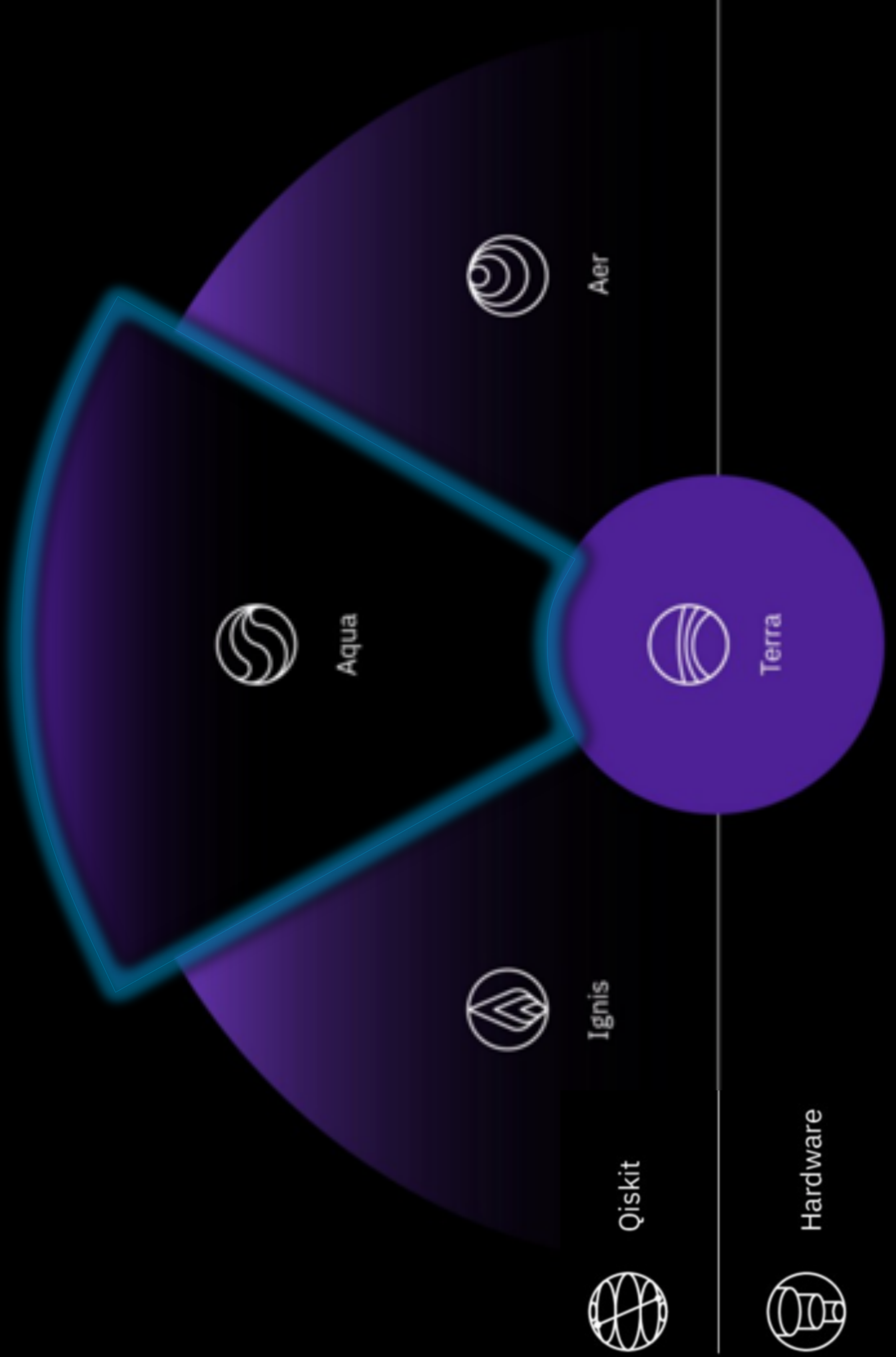
Many-sample
EOH, QSVM.Kernel

Single-sample
QPE, IQPE, Grover

Qiskit Terra

Backend
Device, simulator

Provider
Local, IBM Q, third party



Available for free:
https://quantumexperience.ng.bluemix.net/qx/editor

IBM QX Devices

Outline

Why quantum computing?

Quantum Logic

The IBM Q Hardware & Software

Applications

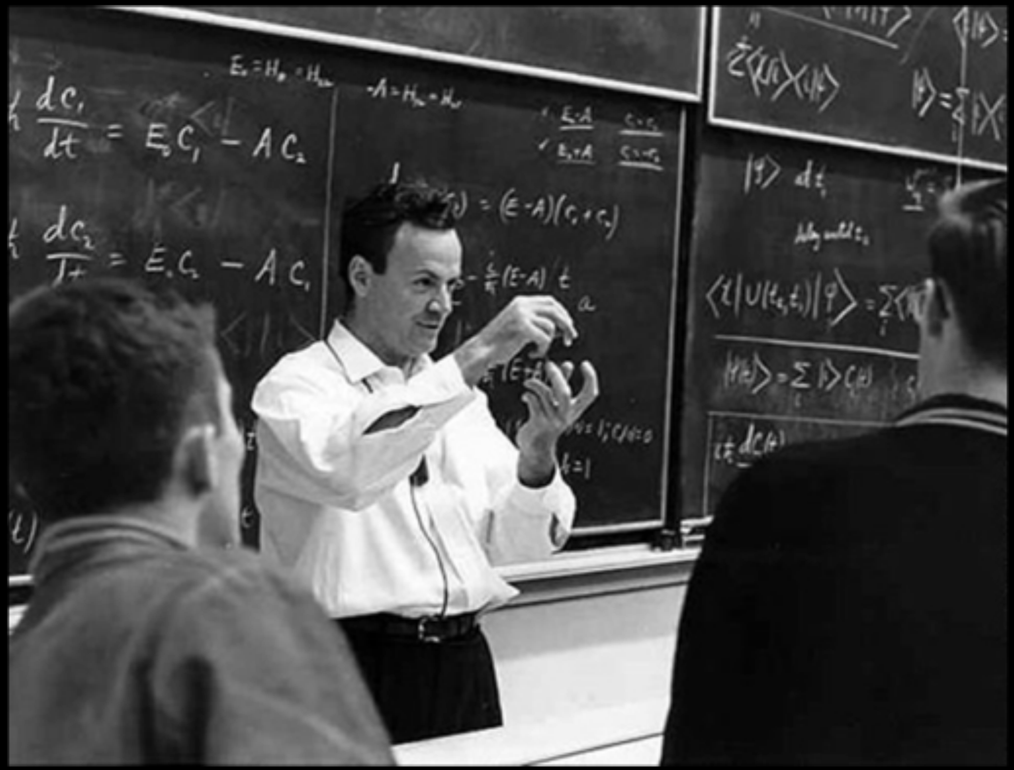
- Quantum chemistry
- Many-body physics
- Classical optimization

Quantum Chemistry & Physics

“I'm not happy with all the analyses that go with just the classical theory, *because nature isn't classical*, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical ...”

International Journal of Theoretical Physics, VoL 21, Nos. 6/7, 1982

Simulating Physics with Computers
Richard P. Feynman



Possible application areas for quantum computing

We believe the following areas might be useful to explore for the early applications of quantum computing:

Chemistry

Material design, oil and gas, drug discovery

Artificial Intelligence

Classification, machine learning, linear algebra

Financial Services

Asset pricing, risk analysis, rare event simulation

Quantum chemistry: Where is it a challenge?

Solving interacting fermionic problems is at the core of most challenges in computational physics and high-performance computing:

$$H_{\mathrm{el}} = -\frac{1}{2}\sum_{i=1}^{N}\nabla_i^2 - \sum_{i=1}^{N_{\mathrm{el}}}\sum_{A=1}^{N_{\mathrm{nu}}}\frac{Z_A}{r_{iA}} + \sum_{i=1,j>i}^{N_{\mathrm{el}},N_{\mathrm{el}}}\frac{1}{r_{ij}}$$

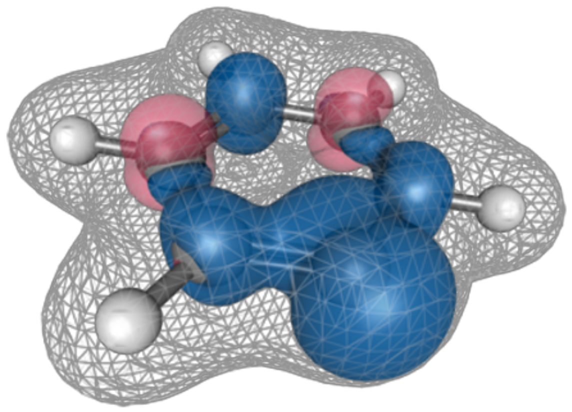
Full CI (exact):

Classical $\mathcal{O}(\exp(N))$

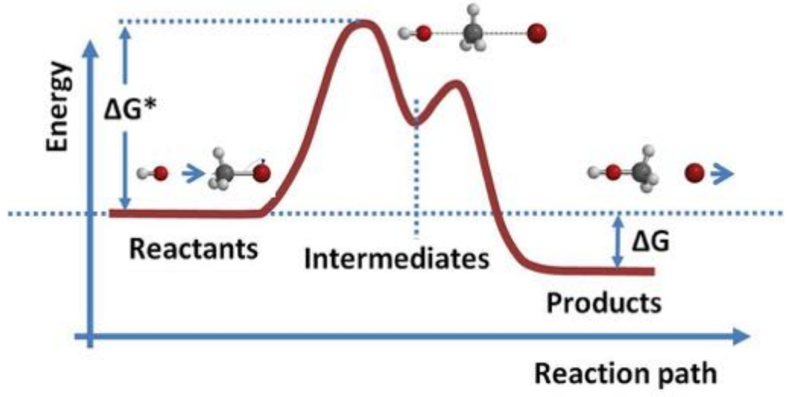
Quantum $\mathcal{O}(N^4)$

Sign problem: Monte-Carlo simulations of fermions are NP-hard [Troyer &Wiese, PRL 170201 (2015)]

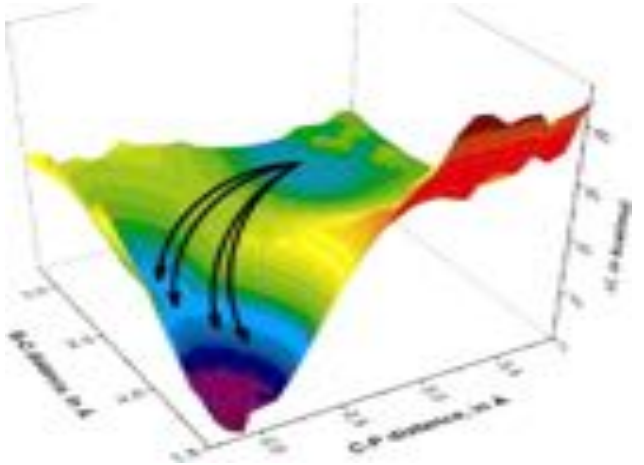
molecular structure



reaction rates



reaction pathways



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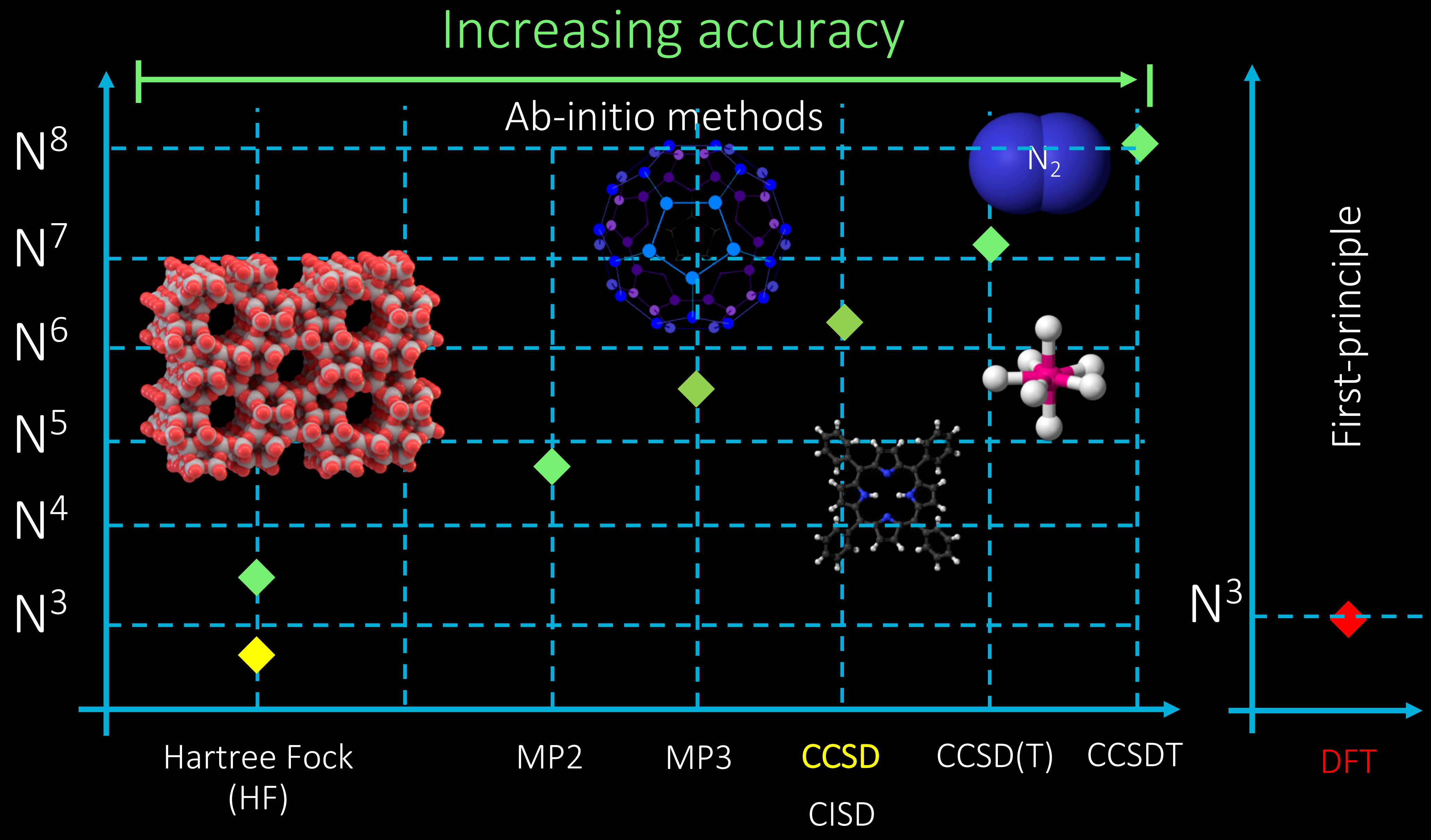
Quantum chemistry – Why a challenge?

Classically, several approximations have been derived to break the exponential scaling



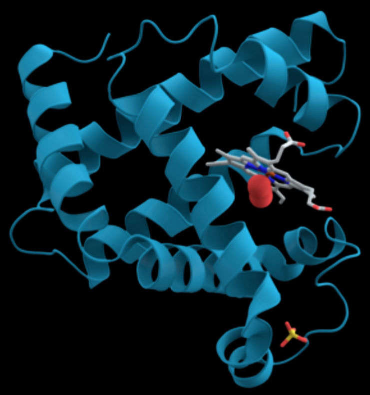
MP: Moller-Plesset

CC: Coupled Cluster

CC: Coupled Cluster

DFT: Density Functional Theory

N: Number of electrons (basis functions)



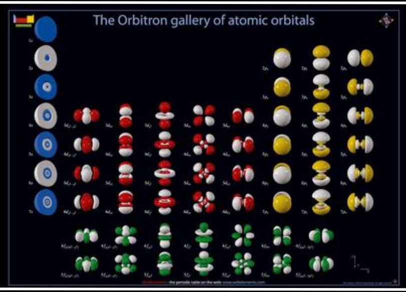
◆ Formal scaling ◆ Practical (implementation)

Quantum chemistry – the VQE approach

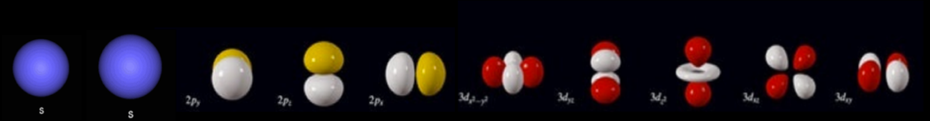
Generate the orbitals
(classical algorithms)
Compute the system Hamiltonian

Hartree Fock equation

$$F(\{\phi_i(r)\})\phi_i(r) = \epsilon_i\phi_i(r)$$

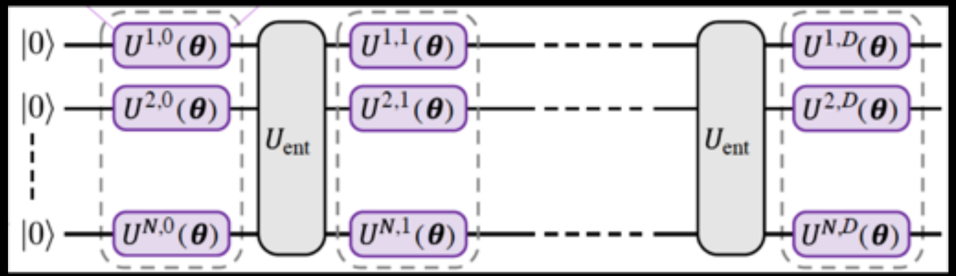


Encode the wavefunction in the qubit space.
(Parametrized by the qubit angles, $\boldsymbol{\theta}_i$)



$$\begin{aligned}|\psi(\theta)\rangle = \theta_1|1 \; 1 \; 1 \; 1 \; 0 \; 0 \; 0 \; 0 \; 0 \; 0\rangle &+ \\ \theta_2|1 \; 1 \; 1 \; 0 \; 1 \; 0 \; 0 \; 0 \; 0 \; 0\rangle &+ \\ \cdots & \\ \theta_{10}|1 \; 1 \; 0 \; 1 \; 0 \; 0 \; 0 \; 0 \; 1 \; 0\rangle &+ \\ \cdots & \\ \theta_{N_c}|0 \; 0 \; 0 \; 0 \; 0 \; 0 \; 1 \; 1 \; 1 \; 1\rangle & \end{aligned}$$

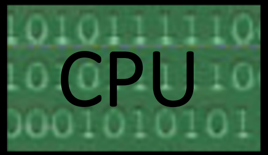
Evaluate the energy on a quantum circuit



$\longrightarrow |\psi(\theta)\rangle \quad E(\theta)$

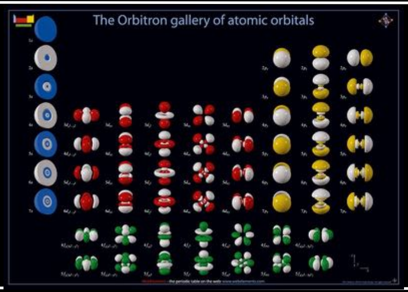
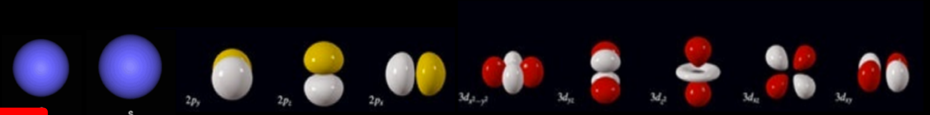
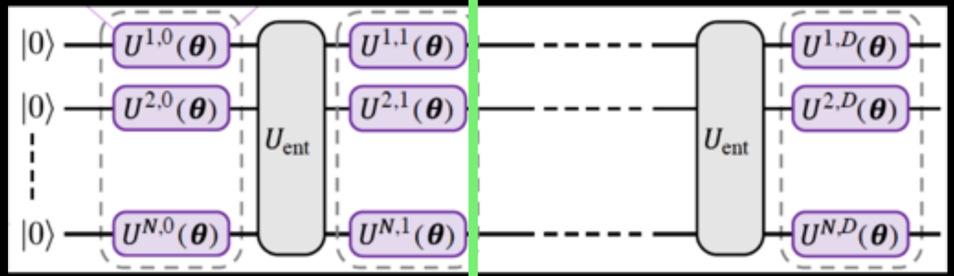
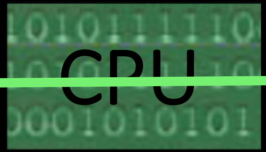
Minimize the energy in a classical device

$E(\theta)$
$\{\theta_1, \theta_2, \ldots, \theta_{N_c}\} \longrightarrow$



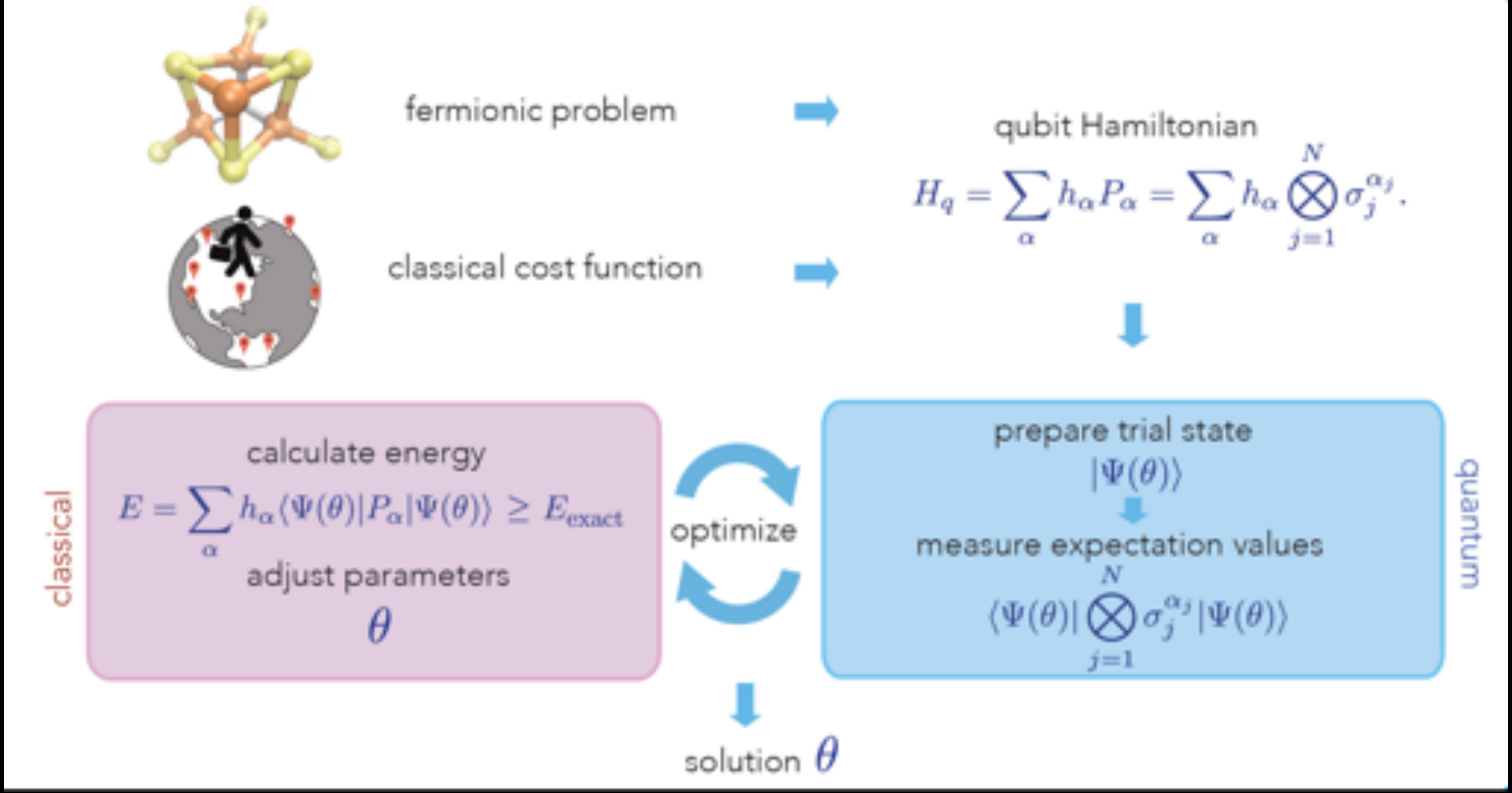
$\longrightarrow \{\theta'_1, \theta'_2, \ldots, \theta'_{N_c}\}$

Quantum chemistry – the VQE approach

Generate the orbitals (classical algorithms) Compute the system Hamiltonian	Hartree Fock equation $F(\{\phi_i(r)\})\phi_i(r) = \epsilon_i \phi_i(r)$ 
Encode the wavefunction in the qubit space. (Parametrized by the qubit angles, $\boldsymbol{\theta}_i$)	 $\|\psi(\theta)\rangle = \theta_1\|1\ 1\ 1\ 1\ 0\ 0\ 0\ 0\ 0\ 0\rangle + \theta_2\|1\ 1\ 1\ 0\ 1\ 0\ 0\ 0\ 0\ 0\rangle + \cdots + \theta_{10}\|1\ 1\ 0\ 1\ 0\ 0\ 0\ 0\ 1\ 0\rangle + \cdots + \theta_{N_c}\|0\ 0\ 0\ 0\ 0\ 0\ 1\ 1\ 1\ 1\rangle$
Evaluate the energy on a quantum circuit	 $\longrightarrow \|\psi(\theta)\rangle \quad E(\theta)$
Minimize the energy in a classical device	$E(\theta)$ $\{\theta_1, \theta_2, \ldots, \theta_{N_c}\}$ →  → $\{\theta'_1, \theta'_2, \ldots, \theta'_{N_c}\}$

Quantum chemistry – The quantum algorithm

The quantum-classical approach: Variational Quantum Eigensolver

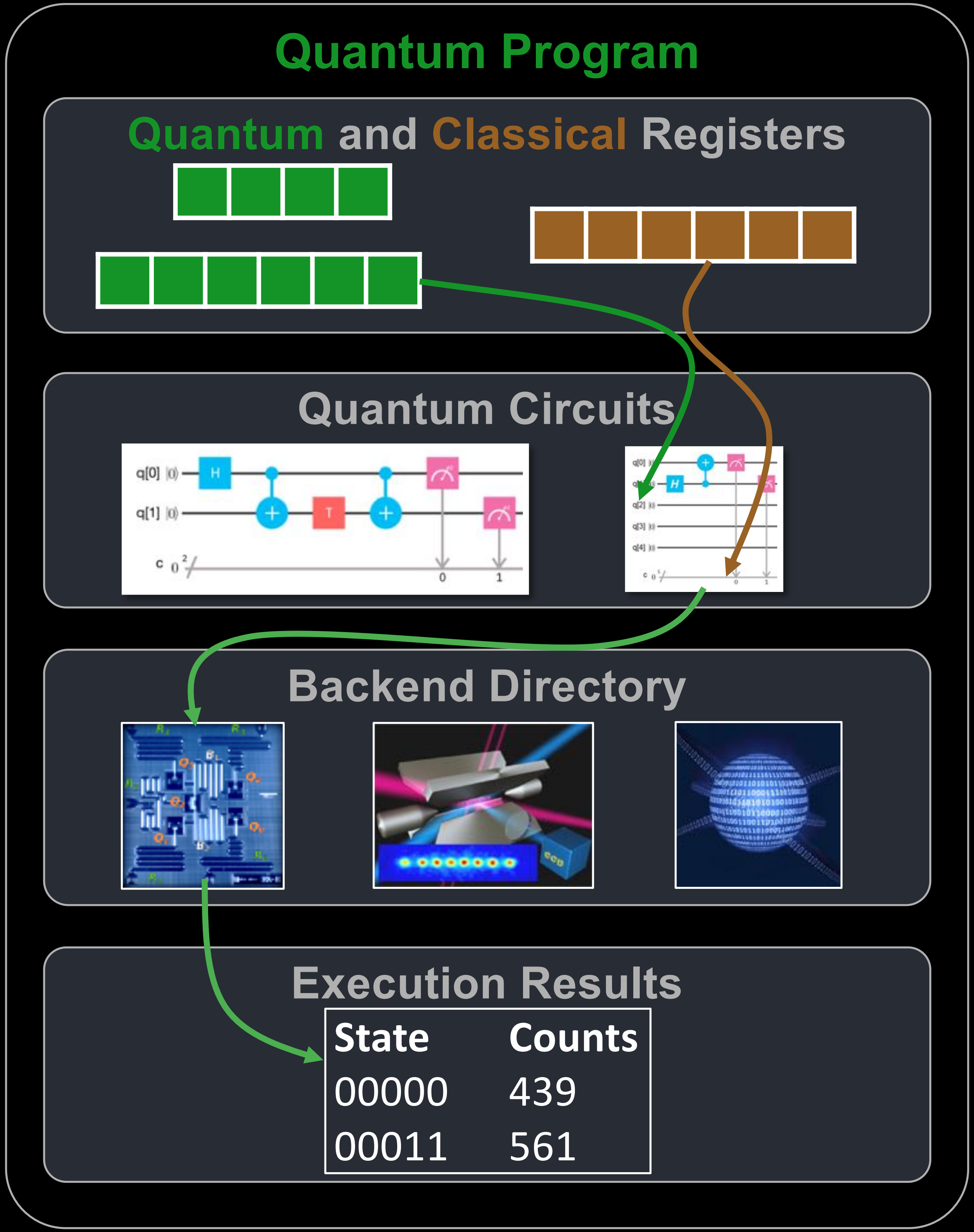


QISKit: Basic workflow

At the highest level, quantum programming in QISKit is broken up into three parts:

1. **Building** quantum circuits
2. **Compiling** quantum circuits to run on a specific backend
3. **Executing** quantum circuits on a backend and analyzing results

Important: Step 2 (compiling) can be done automatically so that a basic user only needs to deal with steps 1 and 3.

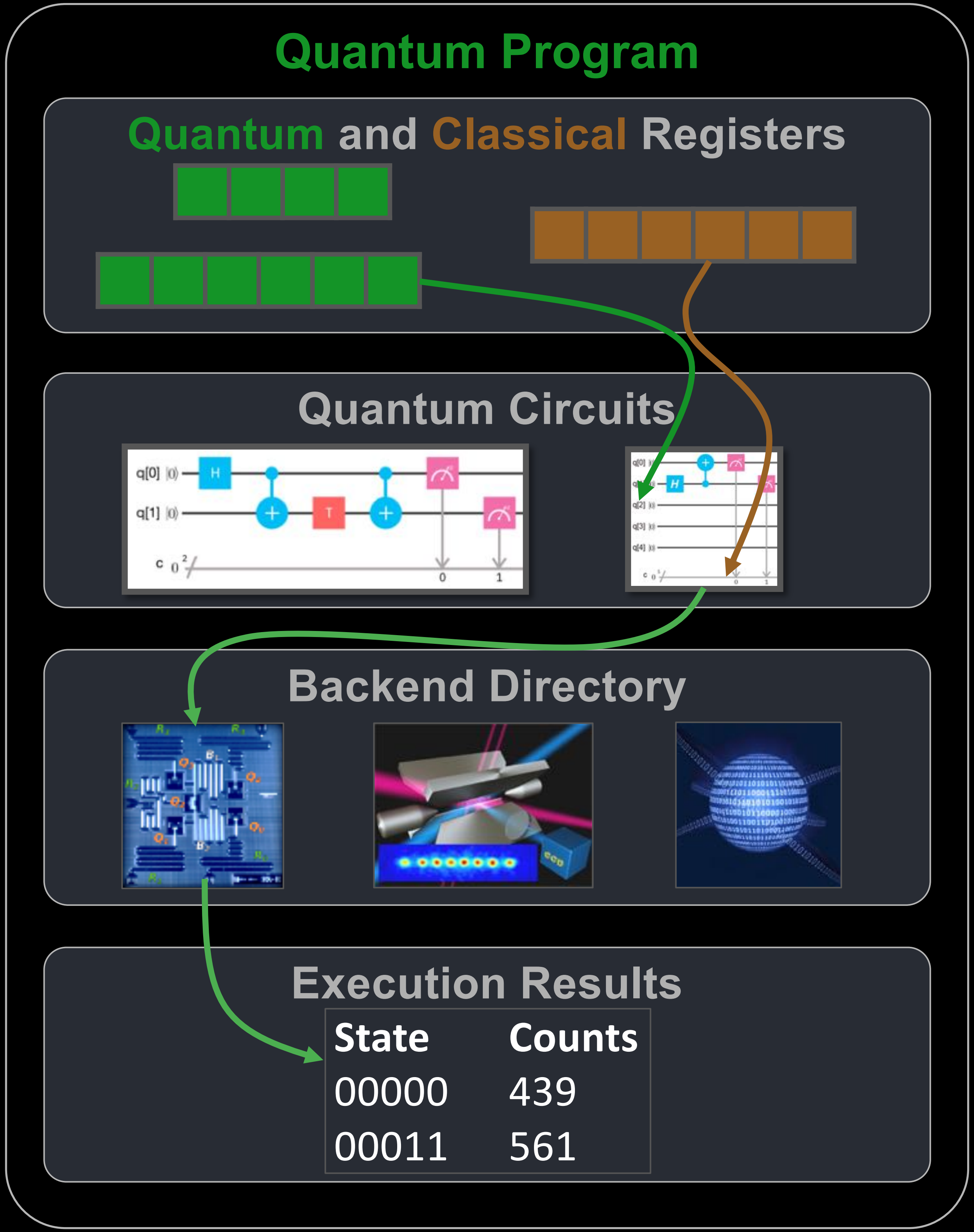


QISKit: Basic workflow

At the highest level, quantum programming in QISKit is broken up into three parts:

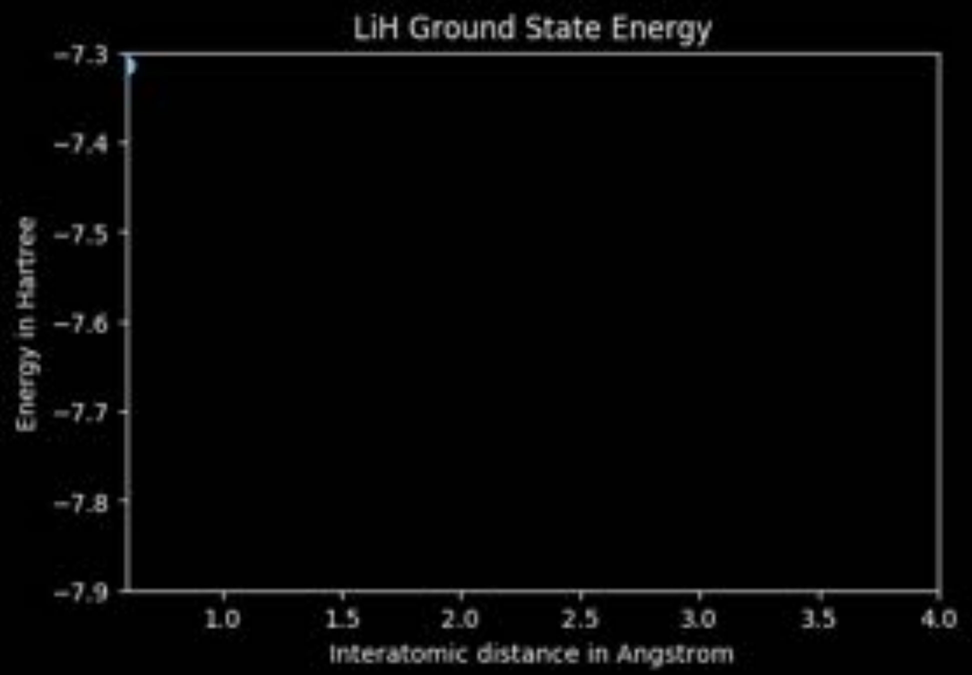
```
[python3] $ pip install qiskit
```

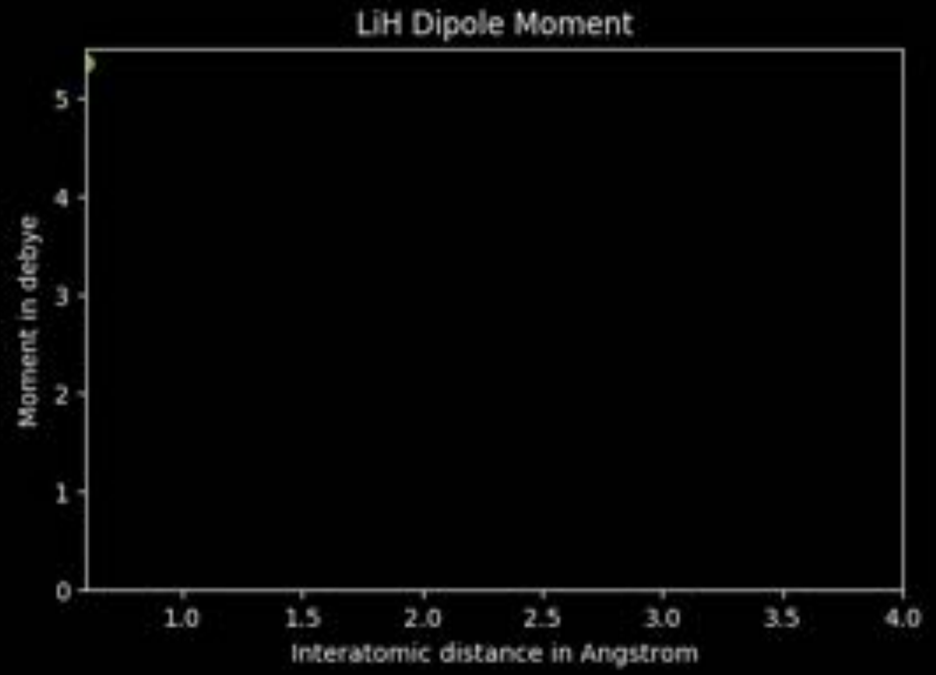
```python
from qiskit import QuantumRegister, ClassicalRegister
from qiskit import QuantumCircuit, Aer, execute

q = QuantumRegister(2)
c = ClassicalRegister(2)
qc = QuantumCircuit(q, c)

qc.h(q[0])
qc.cx(q[0], q[1])
qc.measure(q, c)

backend = Aer.get_backend('qasm_simulator')
job_sim = execute(qc, backend)
sim_result = job_sim.result()

print(sim_result.get_counts(qc))
```



Panagiotis Barkoutsos - bpa@zurich.ibm.com

Qiskit Aqua Chemistry Example






```
import numpy as np
from qiskit_aqua_chemistry import AQUAChemistry

aqua_chemistry_dict = {
  "driver": { "name": "PYSCF" },
  "PYSCF": { "atom": "", "basis": "sto3g" },
  "operator": {
    "name": "hamiltonian",
    "qubit_mapping": "parity",
    "two_qubit_reduction": True,
    "freeze_core": True,
    "orbital_reduction": [-3, -2]
  },
  "algorithm": { "name": "VQE" },
  "optimizer": { "name": "COBYLA", "maxiter": 10000 },
  "variational_form": { "name": "UCCSD" },
  "initial_state": { "name": "HartreeFock" }
}
molecule = "H .0 .0 -{0}; Li .0 .0 {0}"

pts  = [x * 0.1  for x in range(6, 20)]
pts += [x * 0.25 for x in range(8, 16)]
pts += [4.0]
energies = np.empty(len(pts))
distances = np.empty(len(pts))
dipoles = np.empty(len(pts))

for i, d in enumerate(pts):
  aqua_chemistry_dict["PYSCF"]["atom"] = molecule.format(d/2)
  solver = AQUAChemistry()
  result = solver.run(aqua_chemistry_dict)
  energies[i] = result["energy"]
  dipoles[i] = result["total_dipole_moment"] / 0.393430307
  distances[i] = d
```

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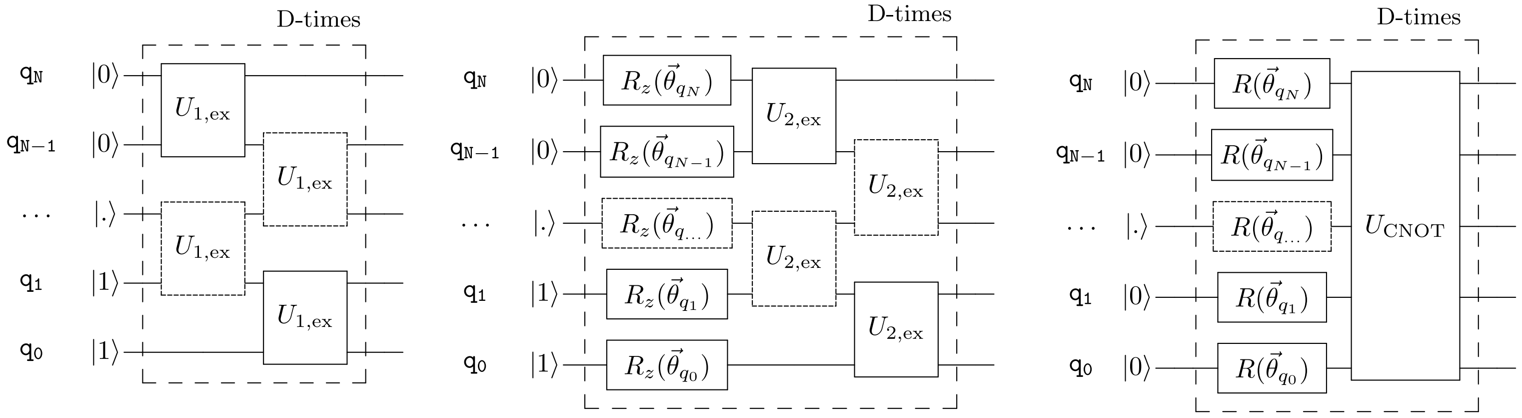
Trial Wavefunctions

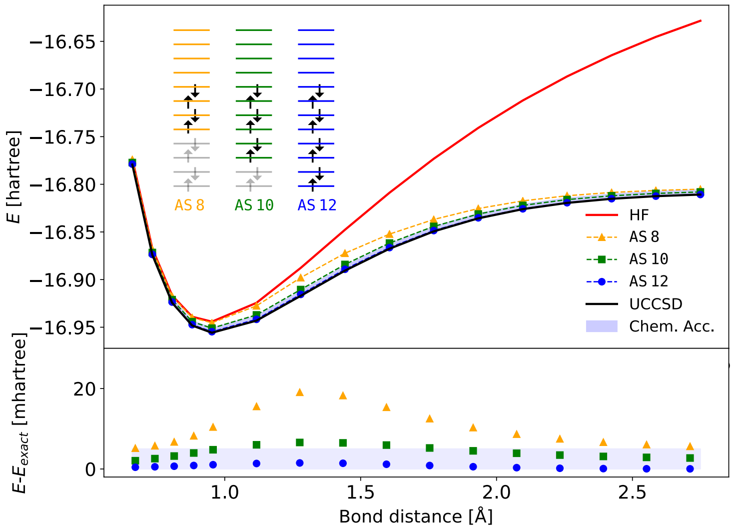
Variational Principle

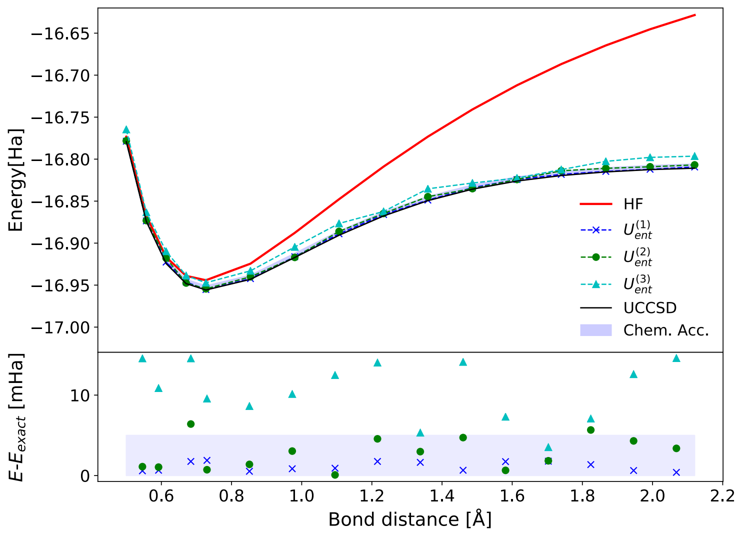
Heuristic Ansatz

$$|\Psi(\vec{\theta})\rangle = \overbrace{\hat{U}^D(\vec{\theta})\hat{U}_{\mathrm{ent}} \dots \hat{U}^1(\vec{\theta})\hat{U}_{\mathrm{ent}}}^{\mathrm{D-times}} \hat{U}^0(\vec{\theta})|\Phi_0\rangle$$

$$U_{1,\mathrm{ex}}(\theta_1,\theta_2) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\theta_1 & e^{i\theta_2}\sin\theta_1 & 0 \\ 0 & e^{-i\theta_2}\sin\theta_1 & -\cos\theta_1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad U_{2,\mathrm{ex}}(\theta) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos 2\theta & -i\sin 2\theta & 0 \\ 0 & -i\sin 2\theta & \cos 2\theta & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$



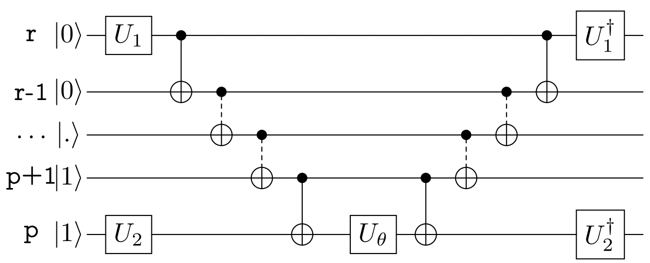




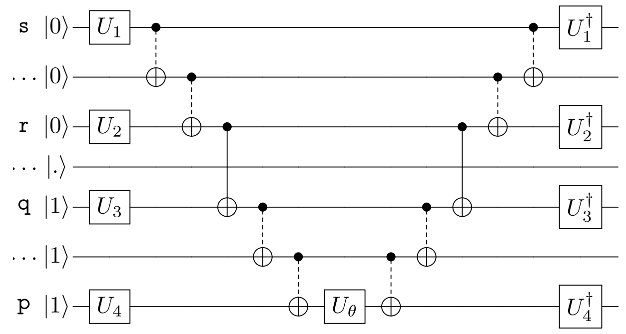
UCCSD Ansatz

$$|\Psi(\vec{\theta})\rangle = e^{\hat{T}(\vec{\theta}) - \hat{T}^\dagger(\vec{\theta})}|\Phi_0\rangle$$

$$\hat{T}_1(\vec{\theta}) = \sum_{i;m} \theta_i^m \, \hat{a}_m^\dagger \hat{a}_i \qquad \hat{T}_2(\vec{\theta}) = \frac{1}{2}\sum_{i,j;m,n} \theta_{i,j}^{m,n} \, \hat{a}_n^\dagger \hat{a}_m^\dagger \hat{a}_j \hat{a}_i$$



$(U_1, U_2) = \{(Y, H), (H, Y)\} \quad \left(\text{where } Y = R_x(-\frac{\pi}{2})\right)$



$(U_1, U_2, U_3, U_4) = \{(H,H,Y,H), (Y,H,Y,Y), (H,Y,Y,Y), (H,H,H,Y), (Y,H,H,H), (H,Y,H,H), (Y,Y,Y,H), (Y,Y,H,Y)\}$

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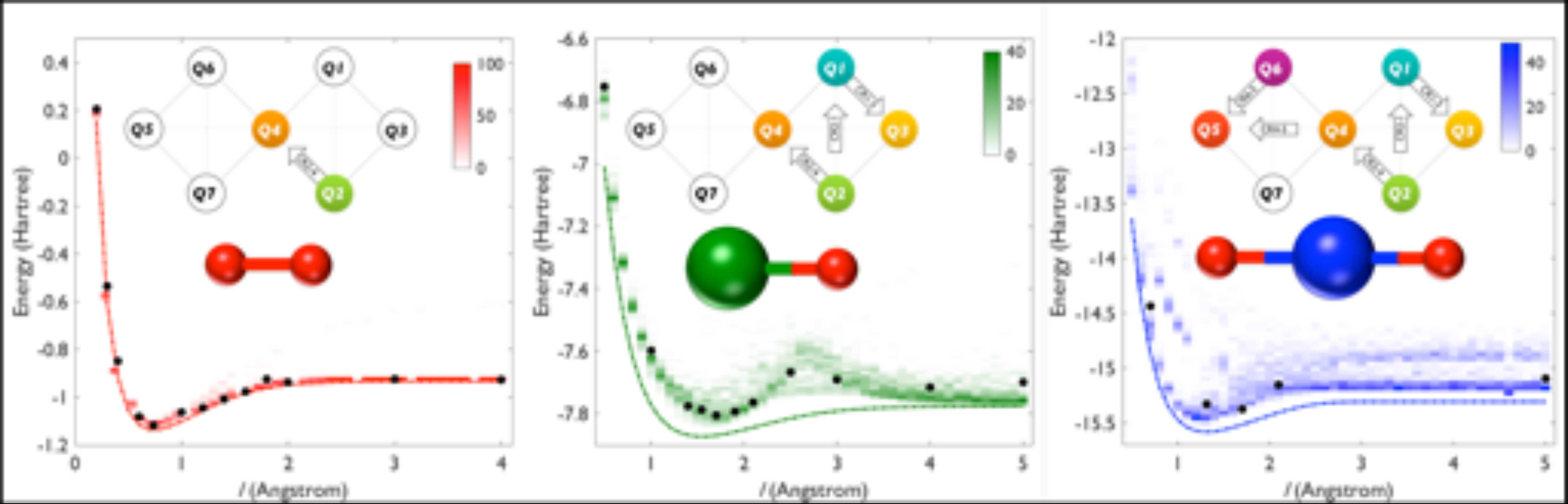
Quantum chemistry – the VQE approach

Ground state-energy of simple molecules



H_2: 2 qubits
5 Pauli terms, 2 sets

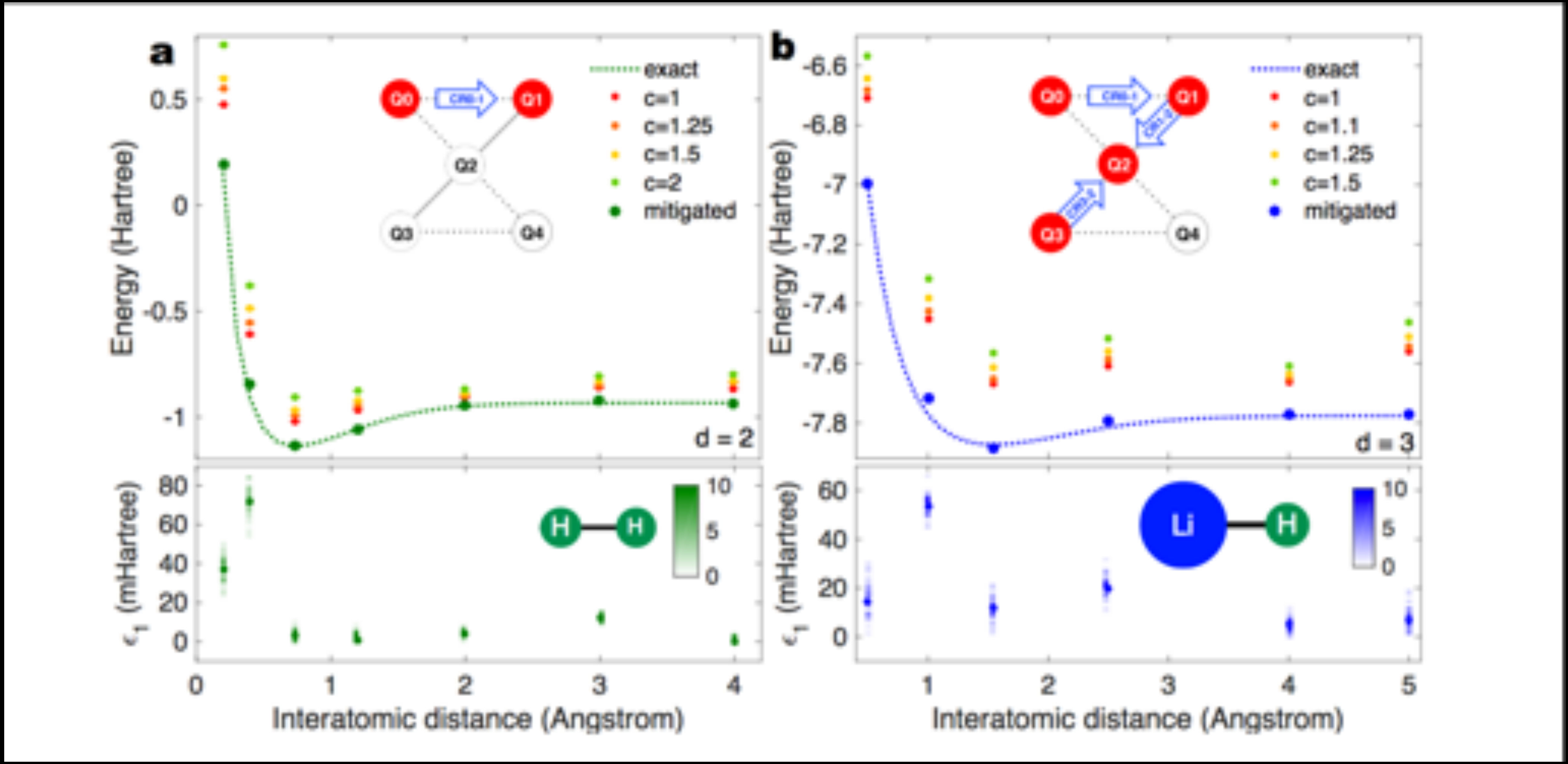
LiH: 4 qubits
100 Pauli terms, 25 sets

BeH_2: 6 qubits
144 Pauli terms, 36 sets

[A. Kandala et al. **Nature 549**, 242-246, 2017]

Quantum chemistry – the VQE approach with error corr.

Ground state-energy of simple molecules

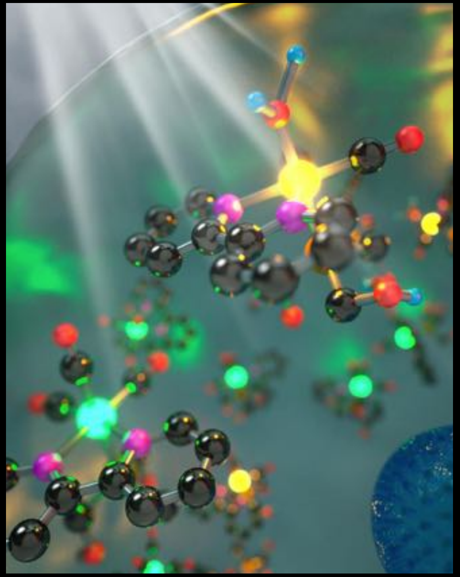


IBM

Quantum chemistry

Excited state energies

Interaction of light with matter:



- Photocatalysis
- Artificial photosynthesis
- Light harvesting

$$H_{el} = -\frac{1}{2}\sum_{i=1}^{N}\nabla_i^2 - \sum_{i=1}^{N_{el}}\sum_{A=1}^{N_{nu}}\frac{Z_A}{r_{iA}} + \sum_{i=1,j>i}^{N_{el},N_{el}}\frac{1}{r_{ij}}$$

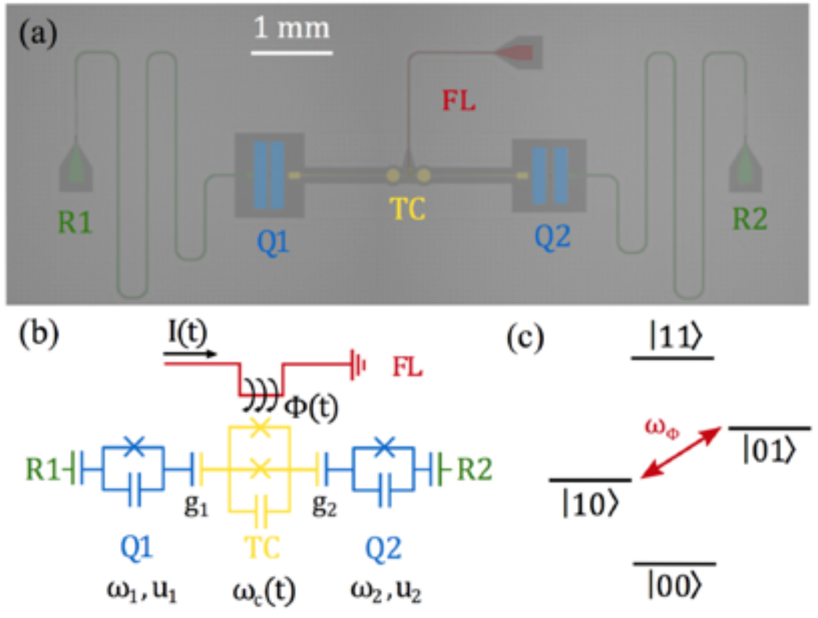
Full CI (exact):
Classical $\mathcal{O}(\exp(N))$
Quantum $\mathcal{O}(N^4)$

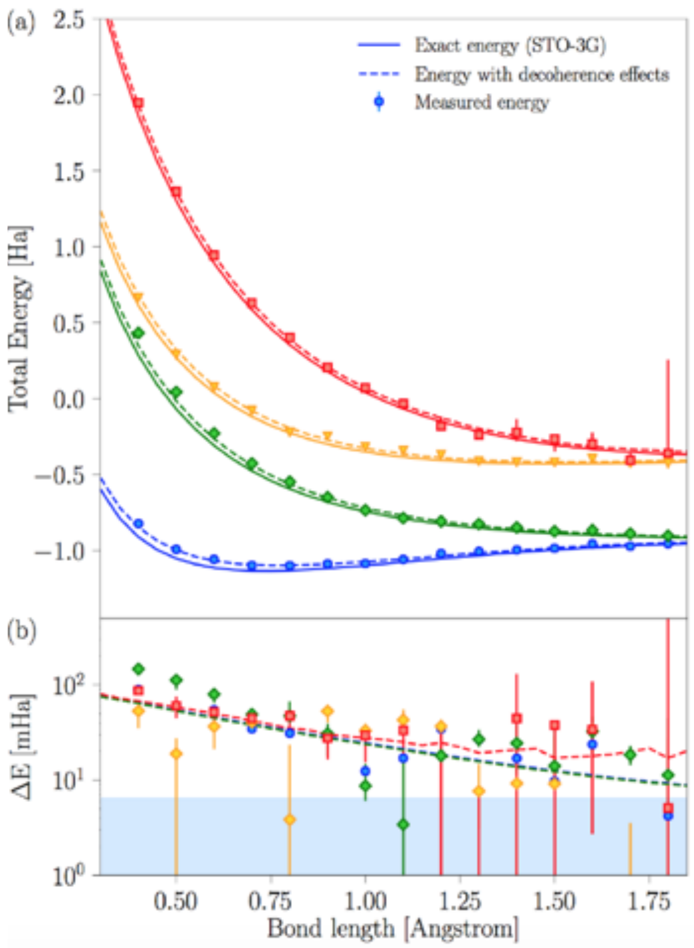
Gate-efficient simulation of molecular eigenstates on a quantum computer

M. Ganzhorn, D.J. Egger, P. Barkoutsos, P. Ollitrault, G. Salis, N. Moll, A. Fuhrer, P. Mueller, S. Woerner, I. Tavernelli and S. Filipp
IBM Research Zurich, Säumerstrasse 4, 8803 Rüschlikon, Switzerland
(Dated: September 14, 2018)

arXiv:1809.05057

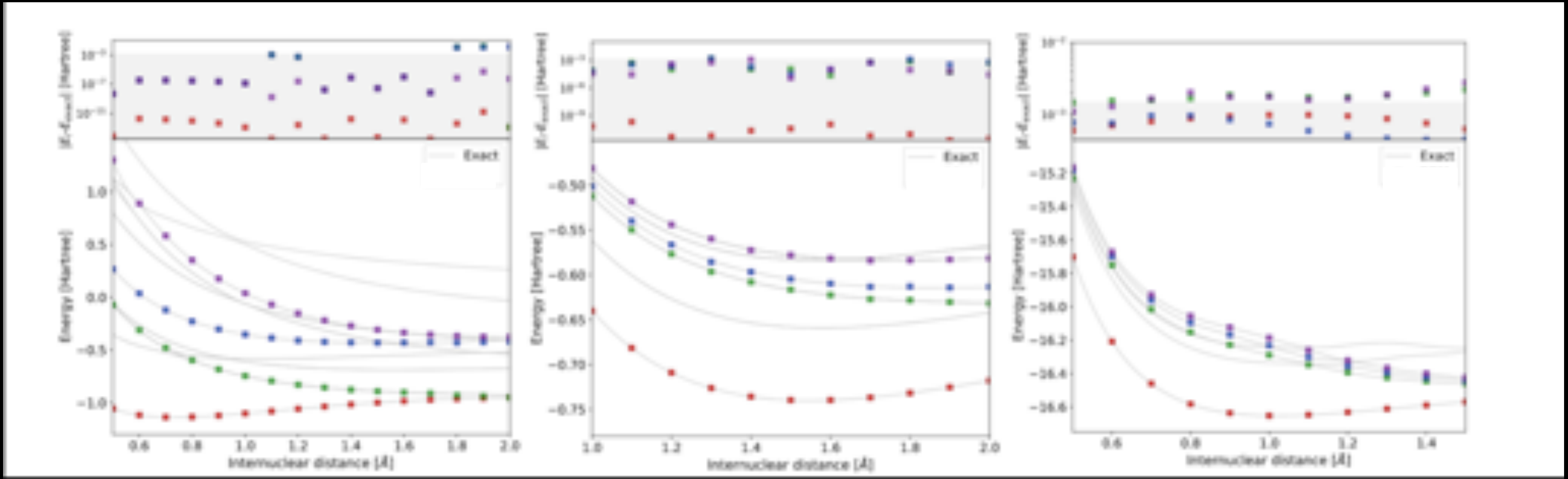
Photochemistry of H_2





Quantum chemistry – Recent and Medium term developments

Example: excited state energies of 2 and 3 atomic systems



(a) H_2 (b) LiH (c) H_2O

Hubbard model

$$H_{\mathrm{Hub}} = -t \sum_{\langle i,j \rangle,\sigma} \left(c^{\dagger}_{j\sigma} c_{i\sigma} + c^{\dagger}_{i\sigma} c_{j\sigma} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

t : hopping term

U : in-site repulsive term

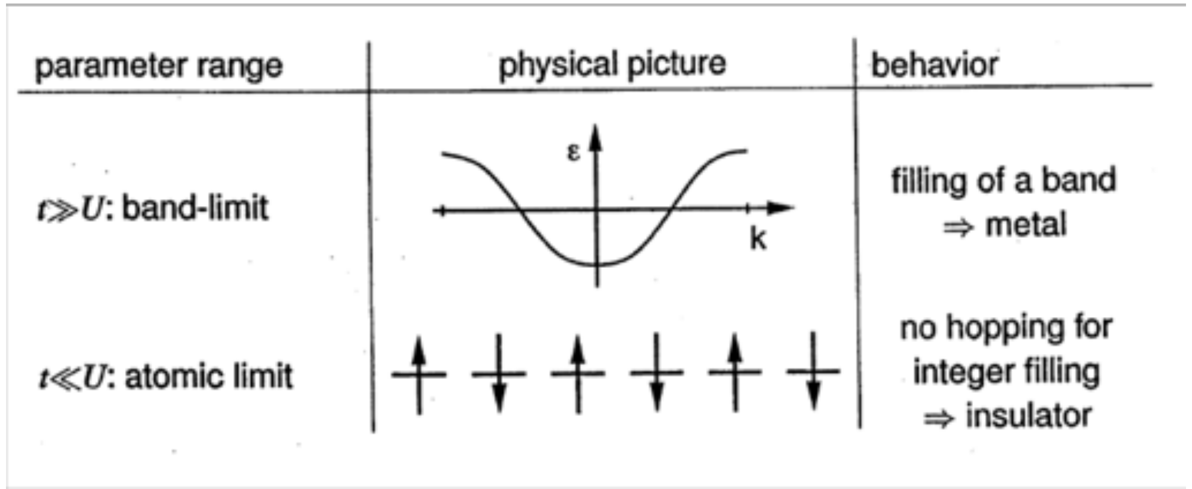
$\langle i,j \rangle$: adjacent sites

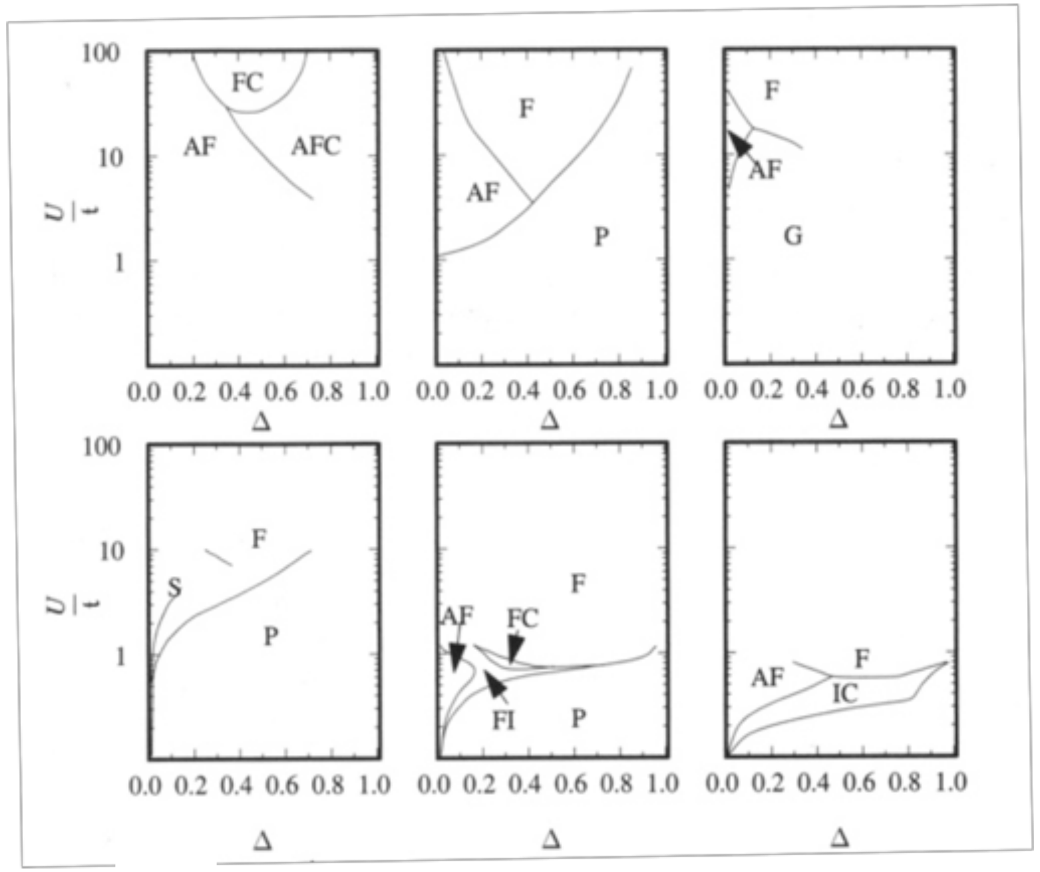
J. Hubbard, Proc. Roy. Soc. London, A266, 238 (1963

Study physical properties with a quantum algorithm:

1. Ground state with VQE
2. Time-dependent properties using time-propagation
3. Excited states and dynamics
4. Phase transitions and statistical physics

At some intermediate value of U/t, there will be a “metal-to-insulator” transition: the „Mott“ transition.





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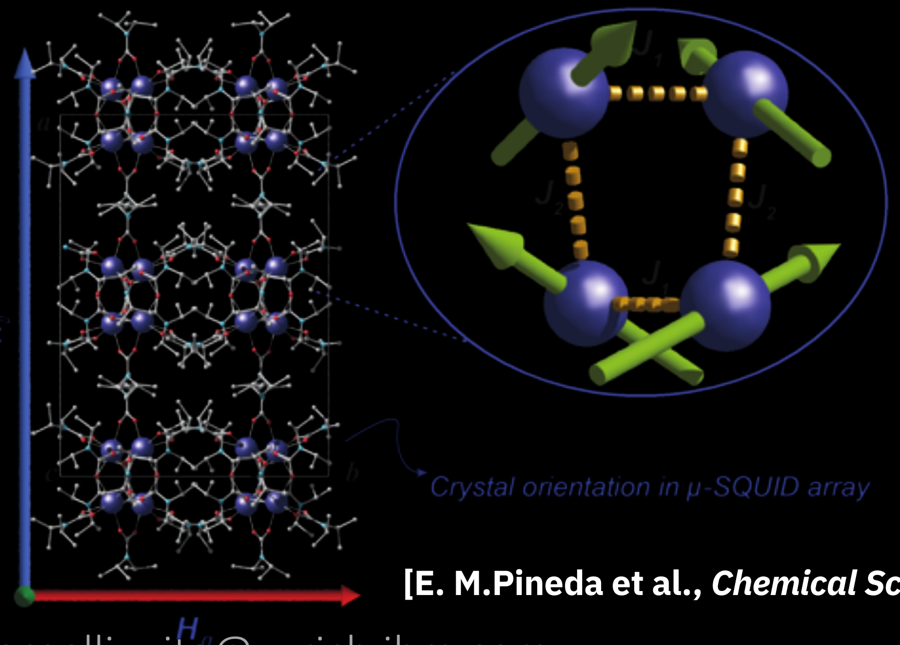
Simulation of molecular magnetic systems

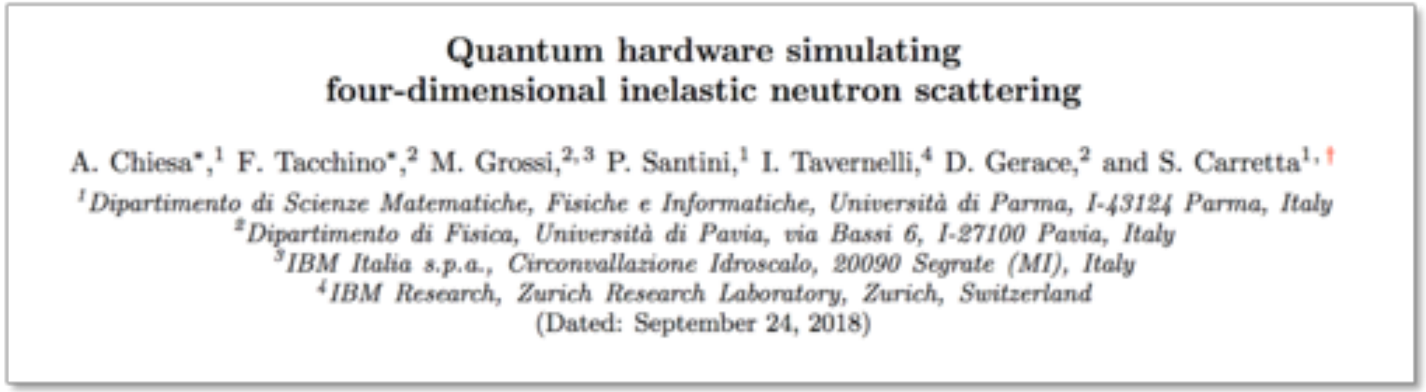
Measuring the spin-spin time-dependent correlation function

$$C_{ij}^{\alpha\beta}(t) = \langle s_i^{\alpha}(t) s_j^{\beta} \rangle$$

scales exponentially with the number of sites.

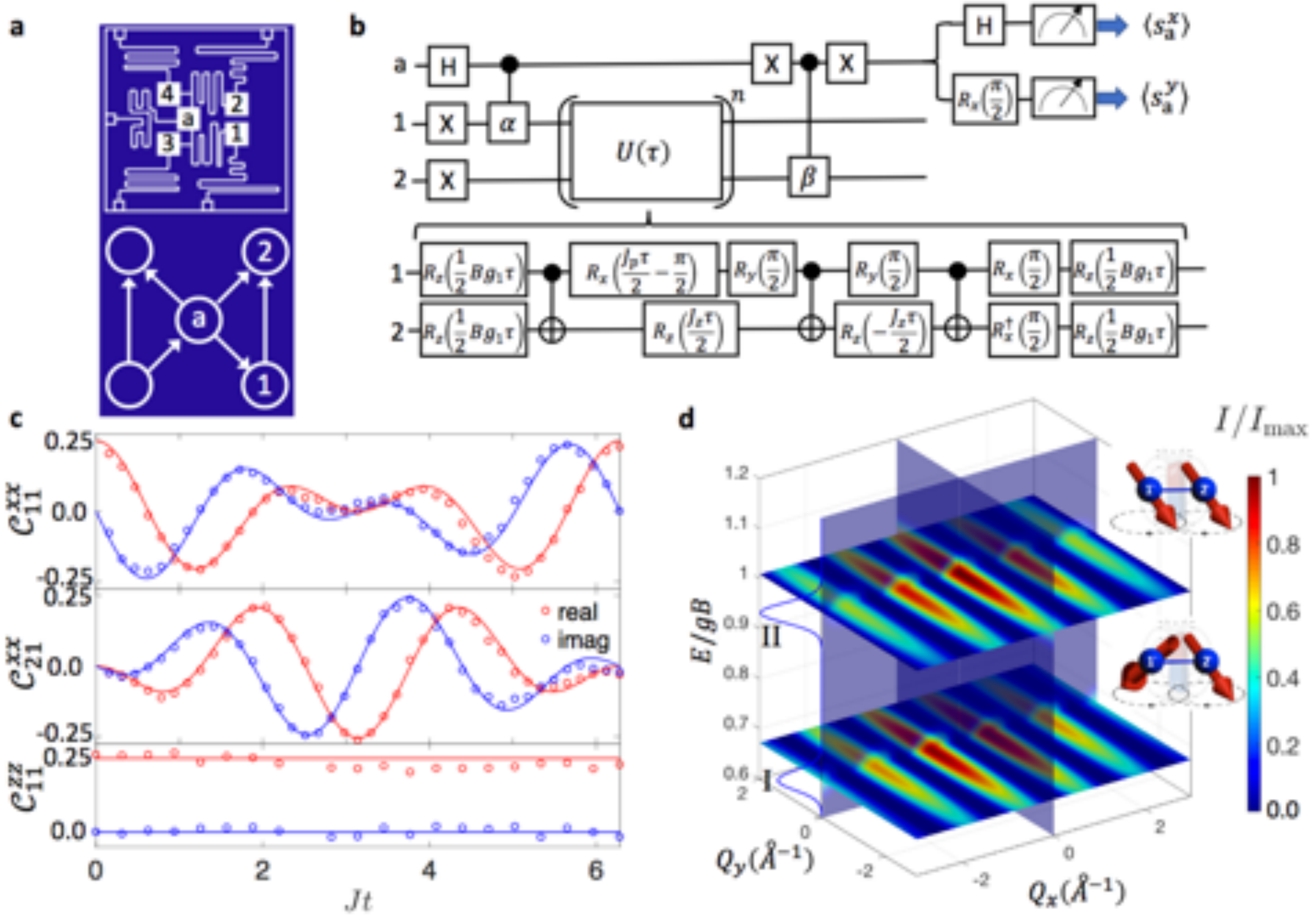


[E. M.Pineda et al., *Chemical Science*, 2017, 8, 1178]


Quantum hardware simulating four-dimensional inelastic neutron scattering

A. Chiesa*,[1] F. Tacchino*,[2] M. Grossi,[2,3] P. Santini,[1] I. Tavernelli,[4] D. Gerace,[2] and S. Carretta[1,†]

[1]Dipartimento di Scienze Matematiche, Fisiche e Informatiche, Università di Parma, I-43124 Parma, Italy
[2]Dipartimento di Fisica, Università di Pavia, via Bassi 6, I-27100 Pavia, Italy
[3]IBM Italia s.p.a., Circonvallazione Idroscalo, 20090 Segrate (MI), Italy
[4]IBM Research, Zurich Research Laboratory, Zurich, Switzerland
(Dated: September 24, 2018)



Simulation of molecular magnetic systems

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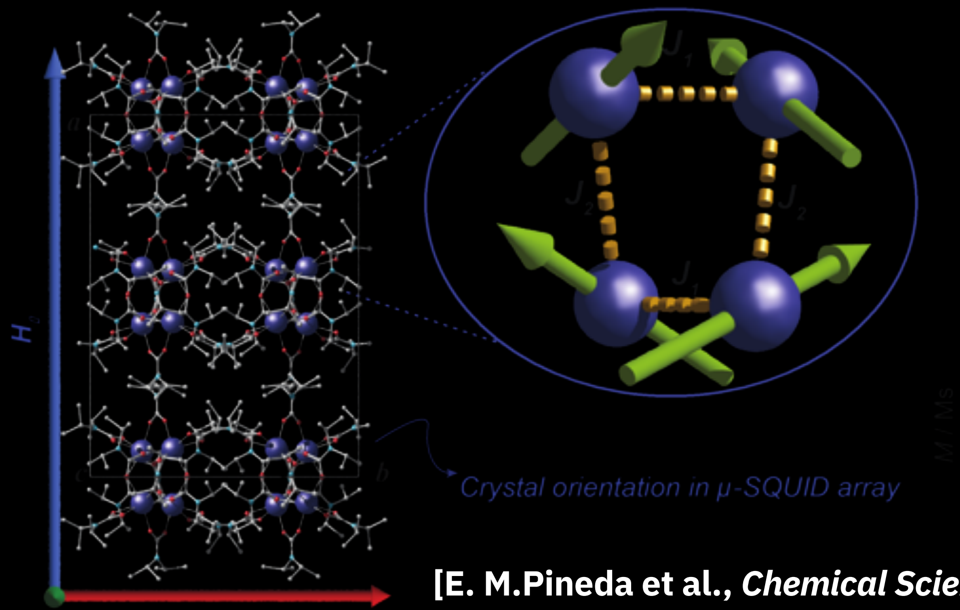
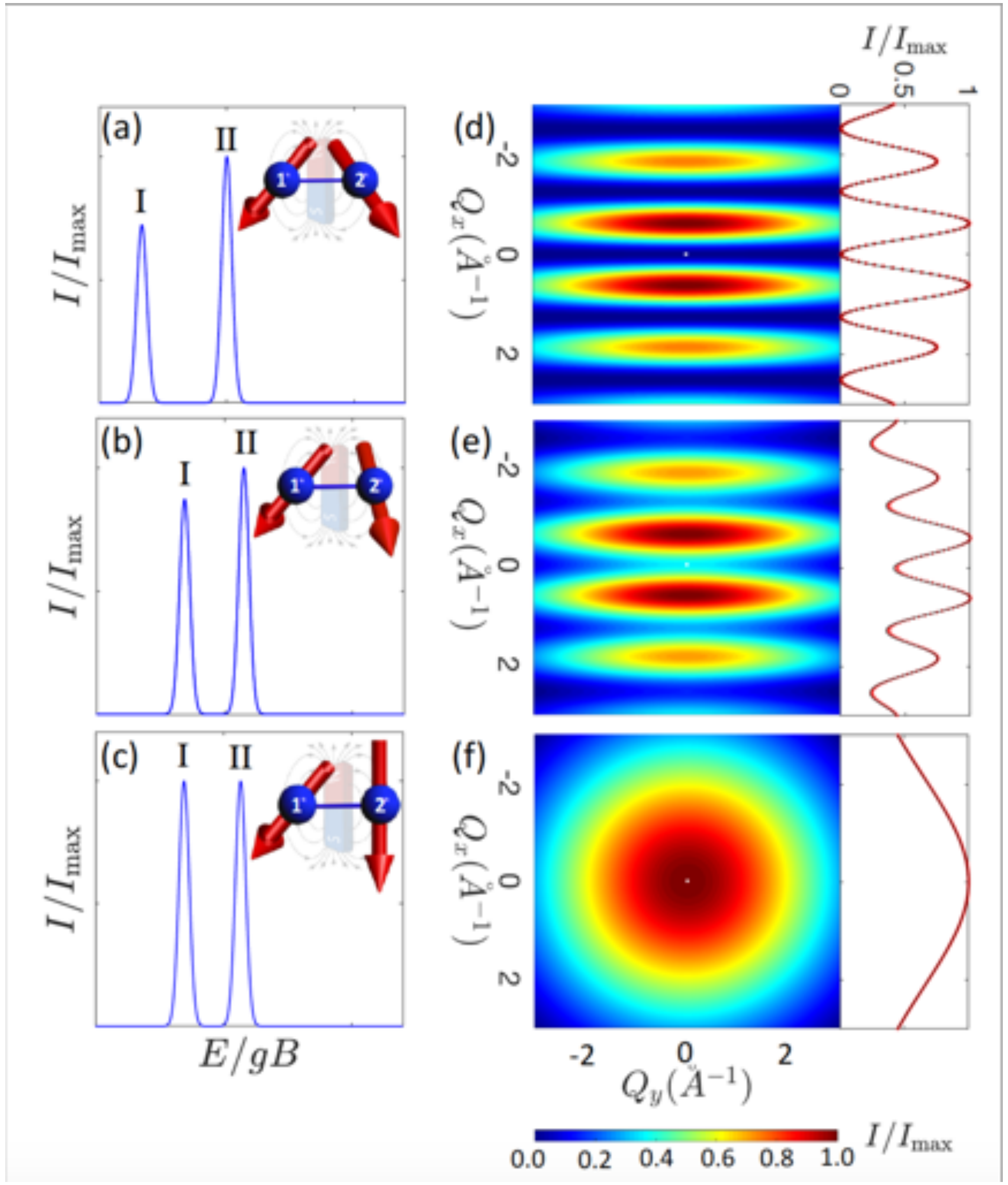


[E. M.Pineda et al., *Chemical Science*, 2017, 8, 1178]



Quantifying entanglement. **(a-c)** Inelastic neutron scattering spectra as a function of the normalized transferred for three different 2 spin system with decreasing entanglement. **(d-f)** Corresponding inelastic neutron scattering signals integrated over Q_z.

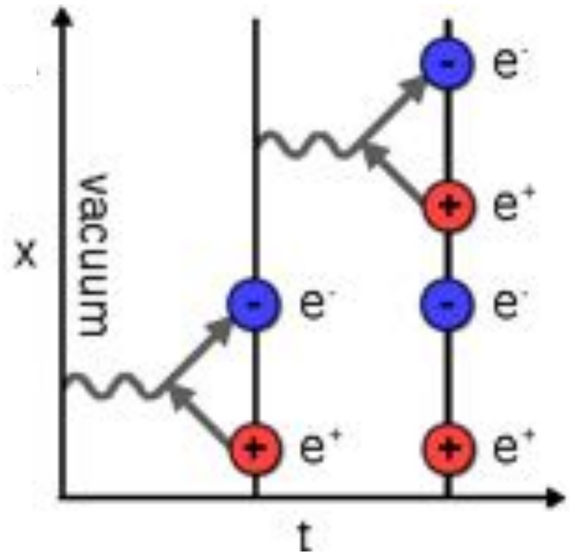
Lattice field theory in HEP

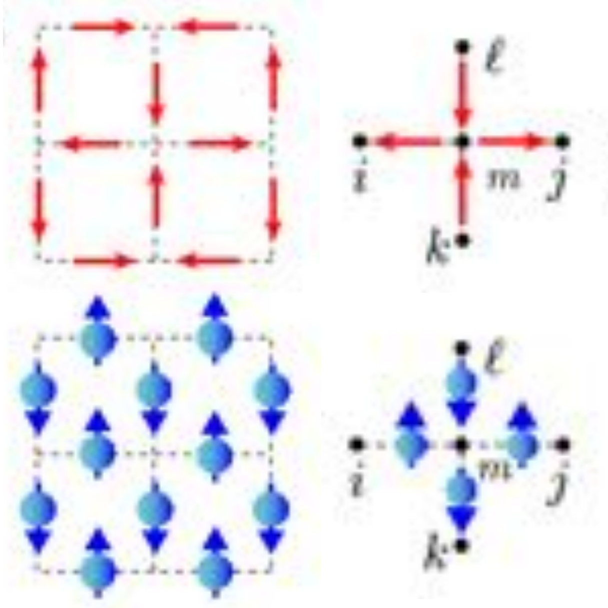
Problem
Real-time propagation of gauge theories is notoriously challenging for classical computers. Digital quantum computers can offer a valid interesting alternative.

Solution strategy (using IBM Q 20-50 qubit devices)

1. Implement fermions and gauge boson in a qubit register (e.g. 1+1 Schwinger model).
2. Static properties: optimization using VQE.
3. Time evolution using the Trotter decomposition of the unitary evolution operator.

(1+1) Schwinger model





E.A. Martinez et al., Nature, 534, 516 (2016)

Outline

Why quantum computing?

Quantum Logic

The IBM Q Hardware & Software

Applications

- Quantum chemistry
- Many-body physics
- Optimization

Polymer folding

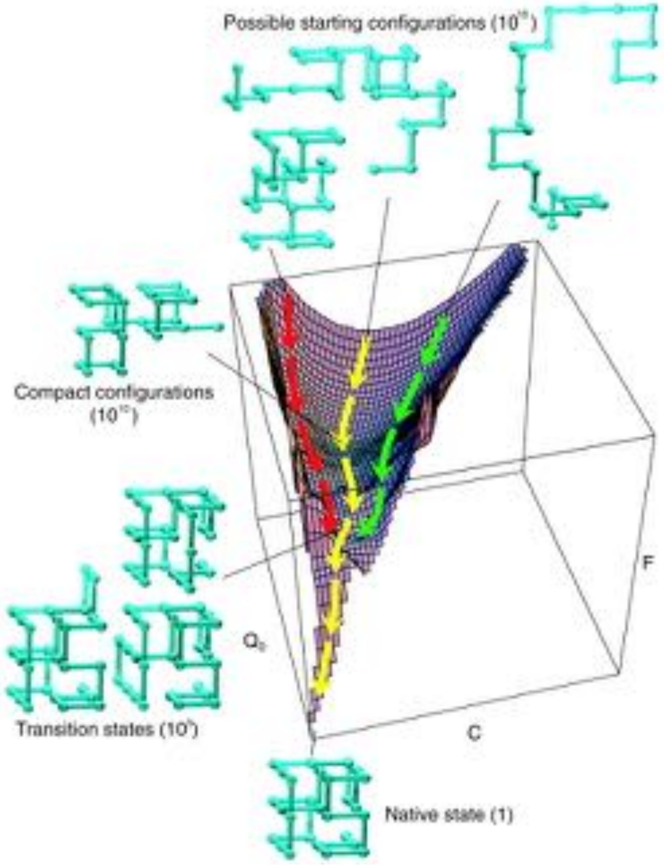
Problem

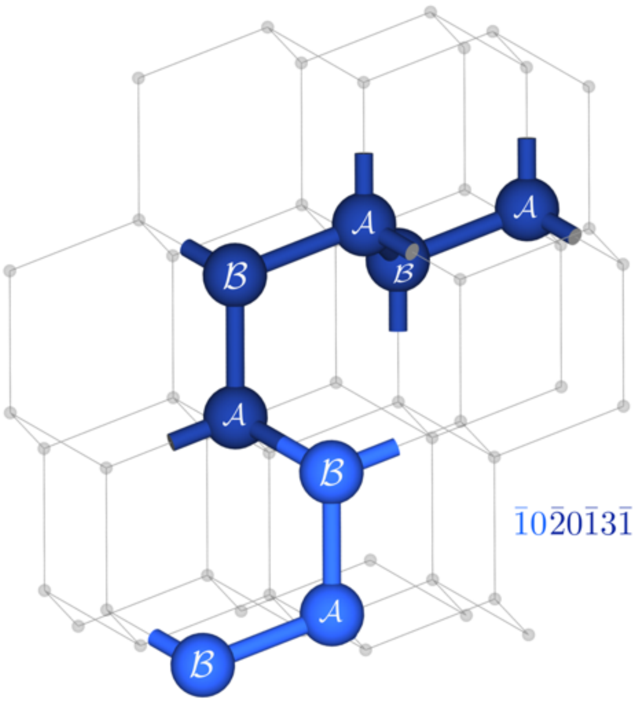
find the folded structure of a linear chain of beads (amino acids, AA) in a regular lattice. This is a simplified model of the more complex protein folding problem.

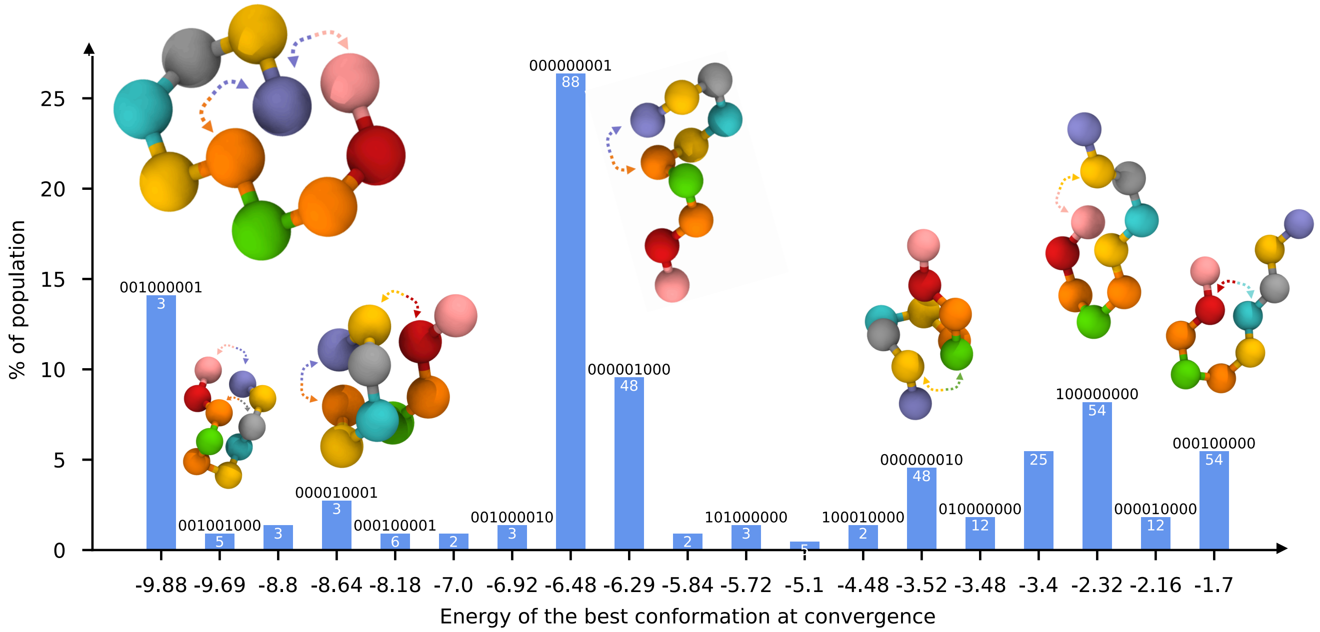
The size of the configuration space scales exponentially with the number of polymer beads (AA).

Solution strategy

assign binary variables to the different beads orientations in the sequence and minimize the string of binaries using the QAOA quantum algorithm and/over Grover’s search. The quantum variables are lattice directions of the bonds.







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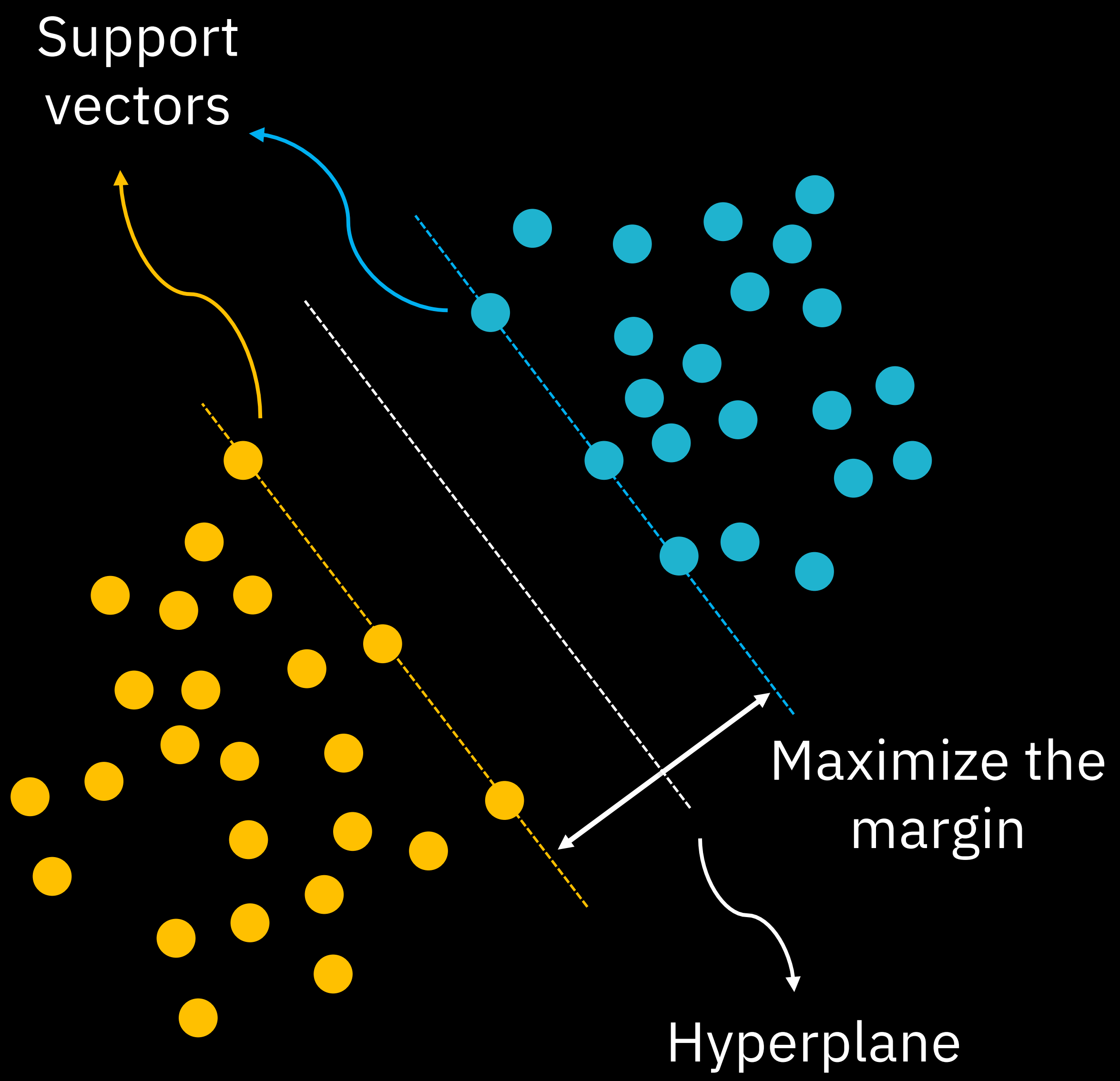
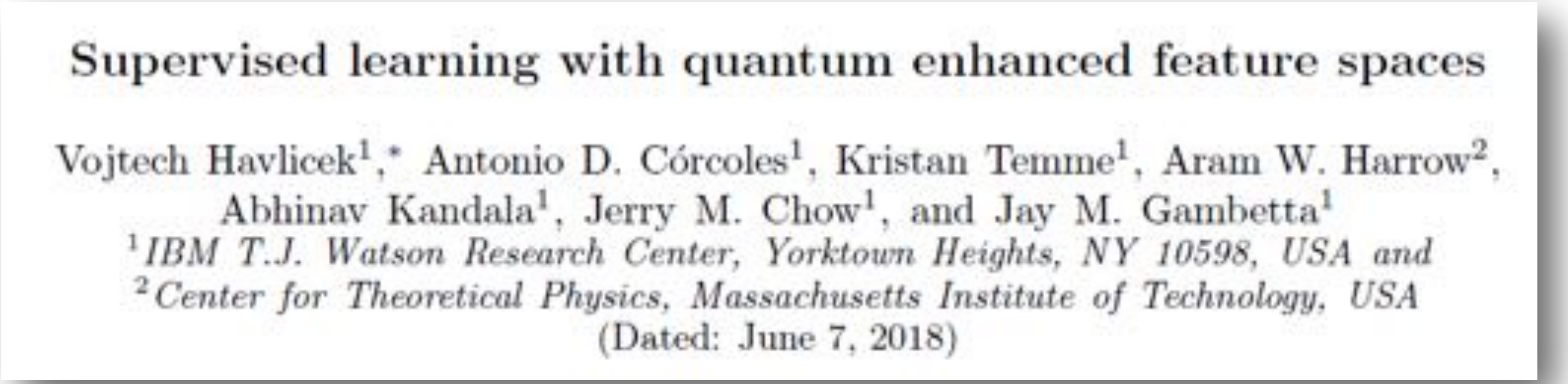
Recent Results by **IBM Research**




Supervised learning with quantum enhanced feature spaces

Vojtech Havlicek[1,*] Antonio D. Córcoles[1], Kristan Temme[1], Aram W. Harrow[2], Abhinav Kandala[1], Jerry M. Chow[1], and Jay M. Gambetta[1]
[1]*IBM T.J. Watson Research Center, Yorktown Heights, NY 10598, USA and*
[2]*Center for Theoretical Physics, Massachusetts Institute of Technology, USA*
(Dated: June 7, 2018)

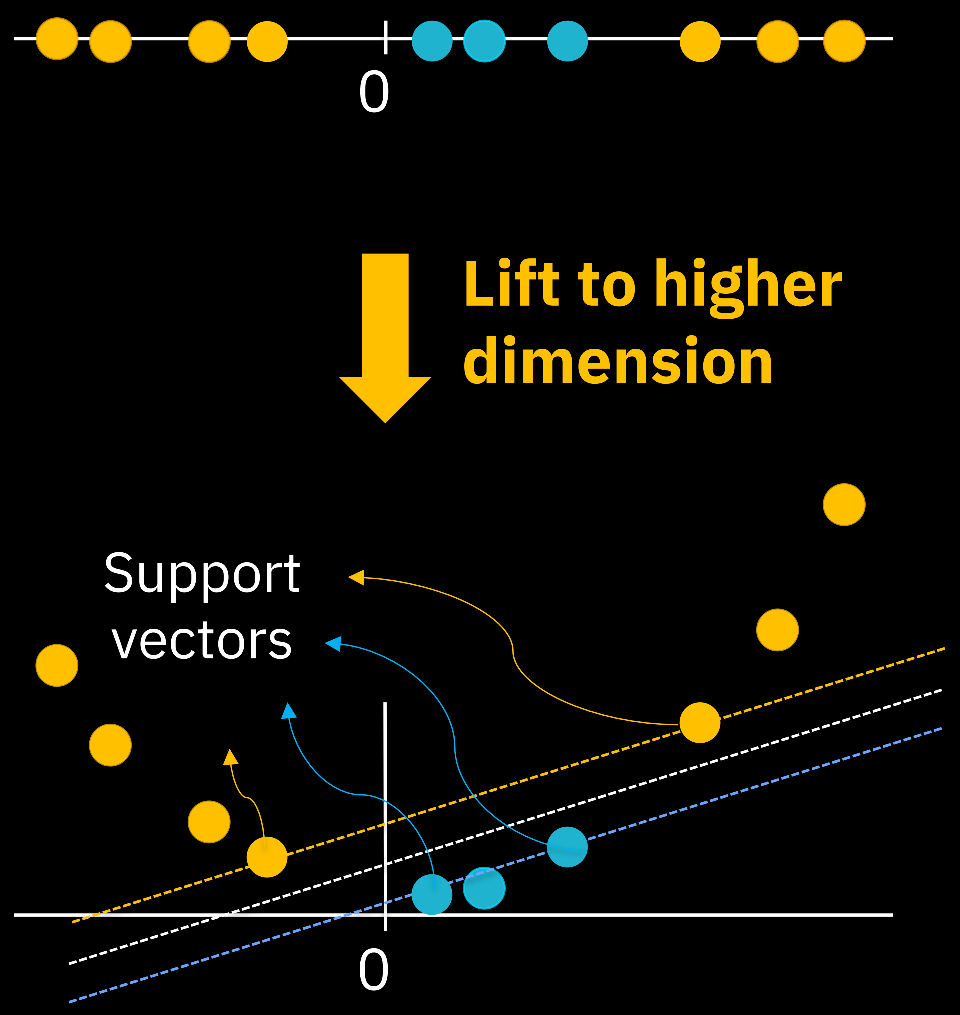
arXiv:1804.11326

Possible applications:

- Customer segmentation
- Image classification
- Fraud detection

Recent Results by **IBM Research**

The data may not be linearly separable



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Possible applications:
- Customer segmentation
- Image classification
- Fraud detection

Quantum Support Vector Machines (SVM) may offer **performance advantages** to classical SVMs by using kernels that cannot be computed efficiently classically

Demonstrated on **real quantum device**

Recent Results by IBM Research

Supervised learning with quantum enhanced feature spaces

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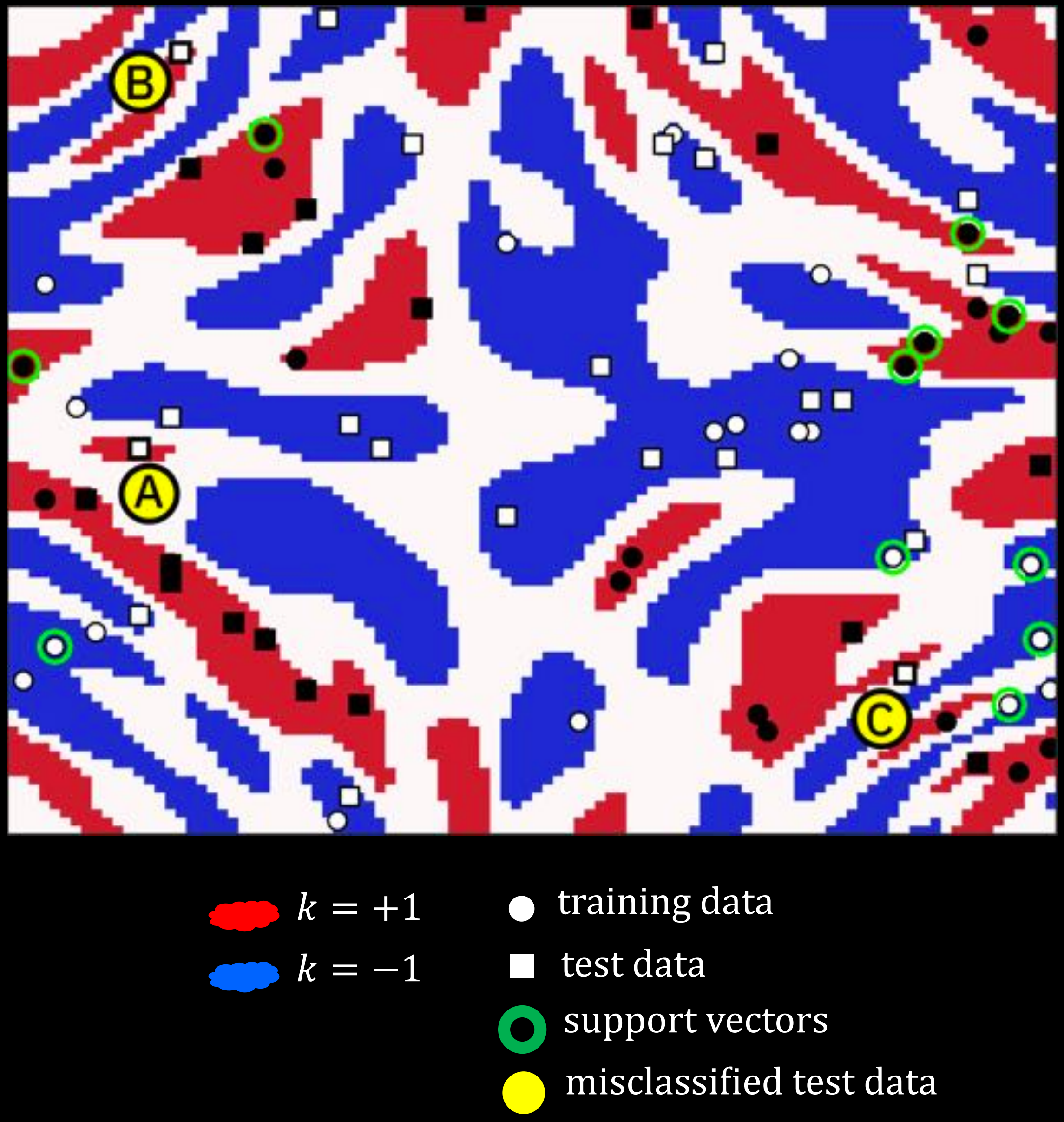
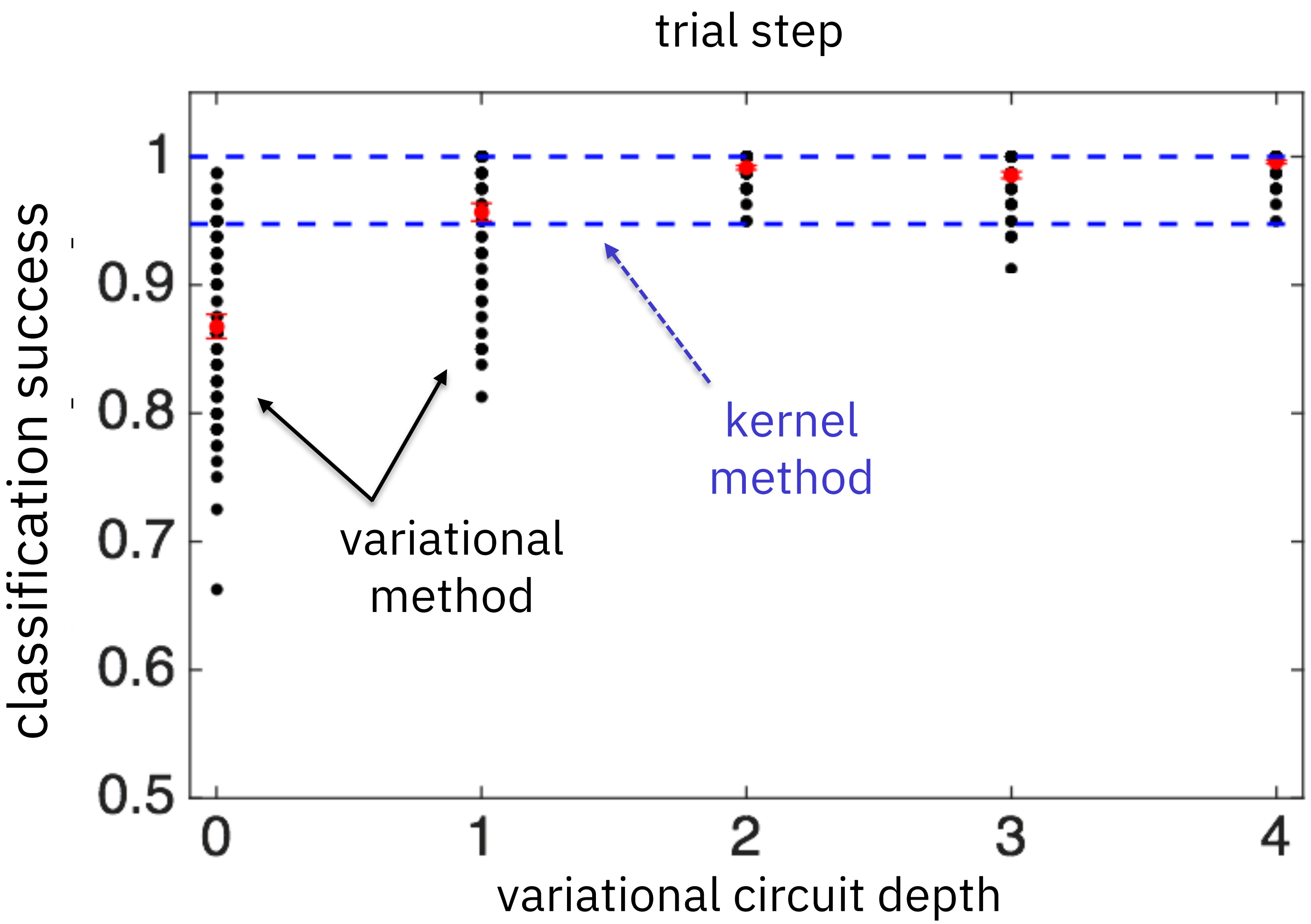
Example training and test set for the Kernel method:



Trained 3 sets of data (20 pts/label) and performed 20 classifications/label per trained set.

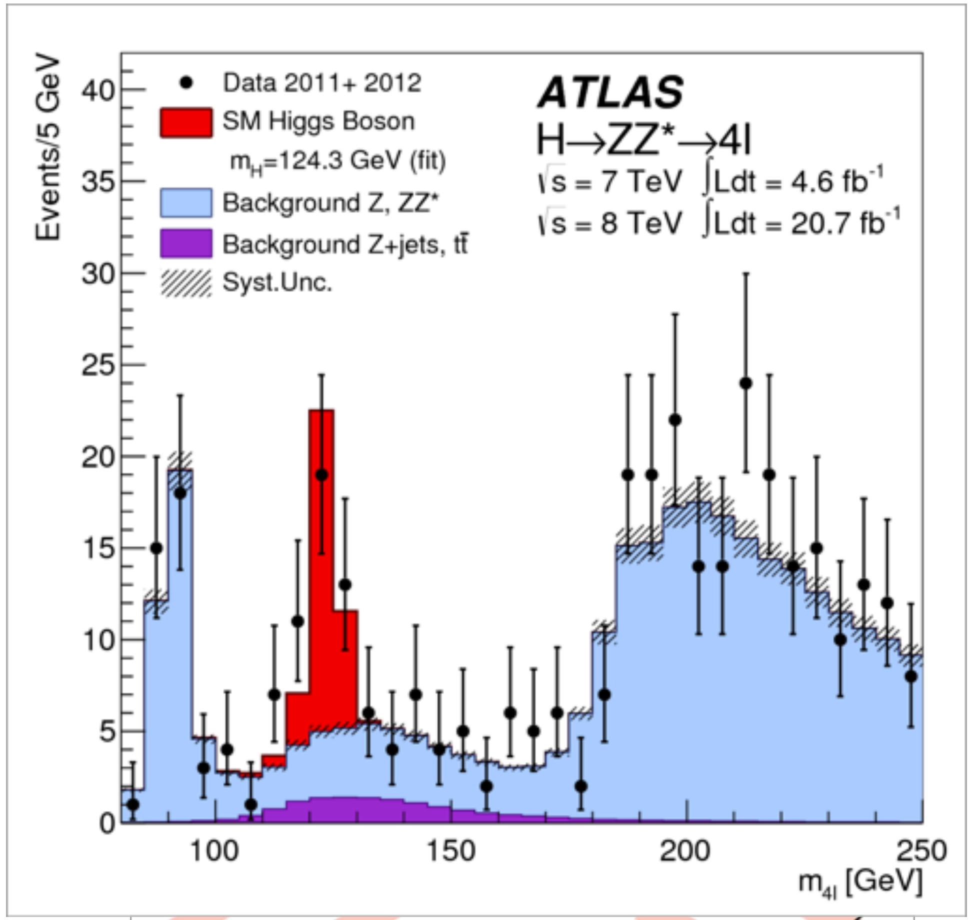


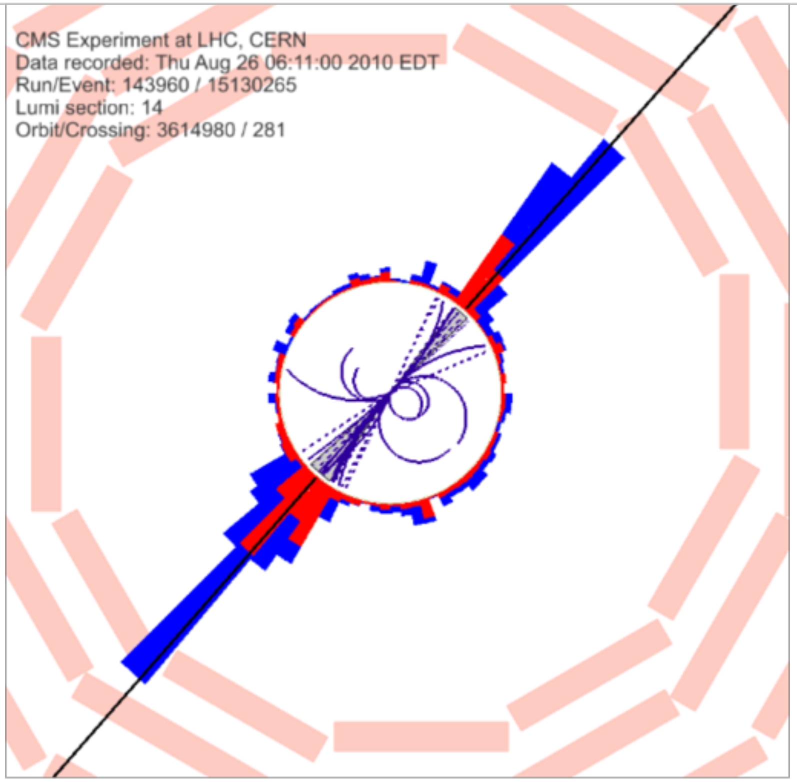
High energy physics

Classification (machine learning and SVM)
Collaboration CERN/IBM Reserach

> Select/identify relevant LHC events

> Reconstruction of tracks – jets tracking





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The Future

... is quantum

Thank you for your attention

Acknowledgements

IBM Q team
(YKT, ZRL, Almaden, Tokyo)