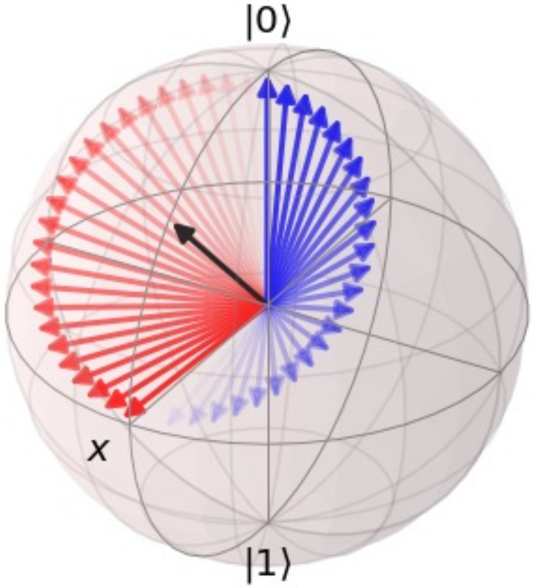

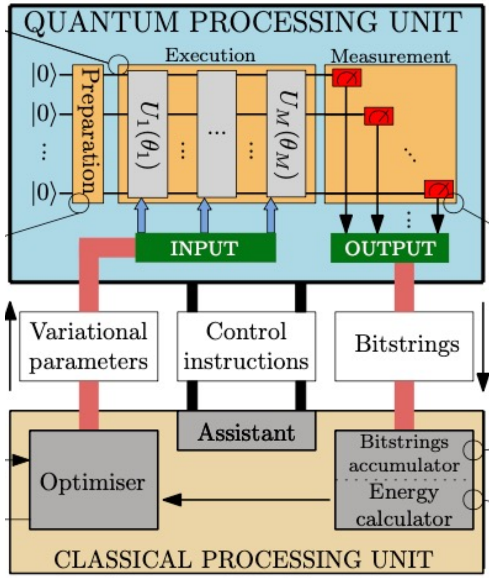

GATE-BASED QUANTUM COMPUTING & VARIATIONAL METHODS

MANPREET JATTANA

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OUTLINE

- A quick recap of quantum computing basics
- Motivation for variational algorithms
- Overview of current algorithms
- Applications and use-cases
- Current challenges in variational algorithms
- Conclusion
- Future roadmap

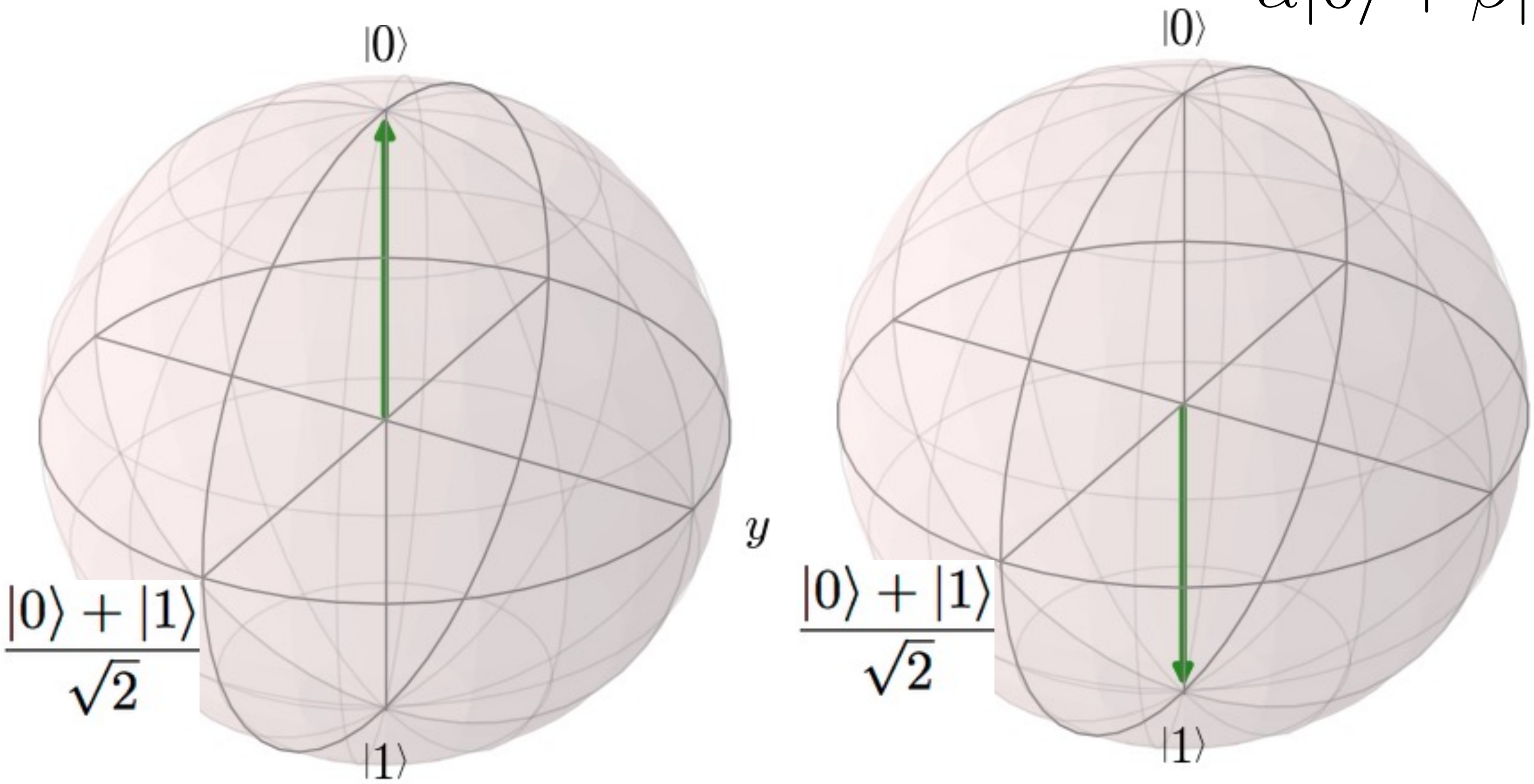
WHAT IS A QUBIT?

Digital Computer:

Binary digIT = BIT

Quantum Computer: QUantum Binary digIT = QUBIT

$$\alpha|0\rangle + \beta|1\rangle$$



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QUANTUM COMPUTERS

Two types

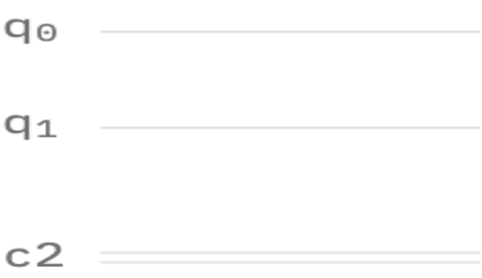
→ **Gate based**

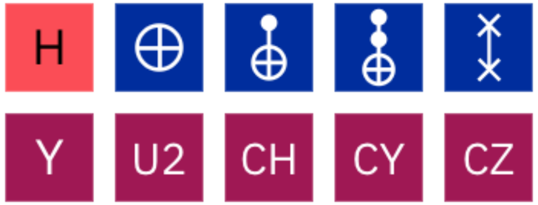
and

Annealers

GATE BASED QUANTUM COMPUTERS

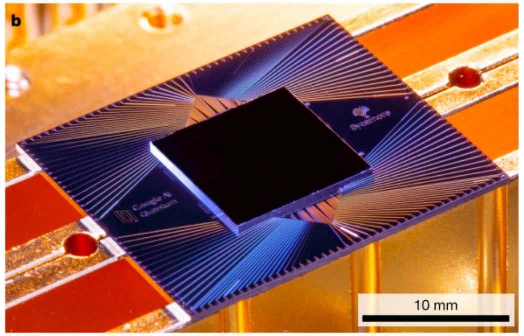
Circuit wires and Gates

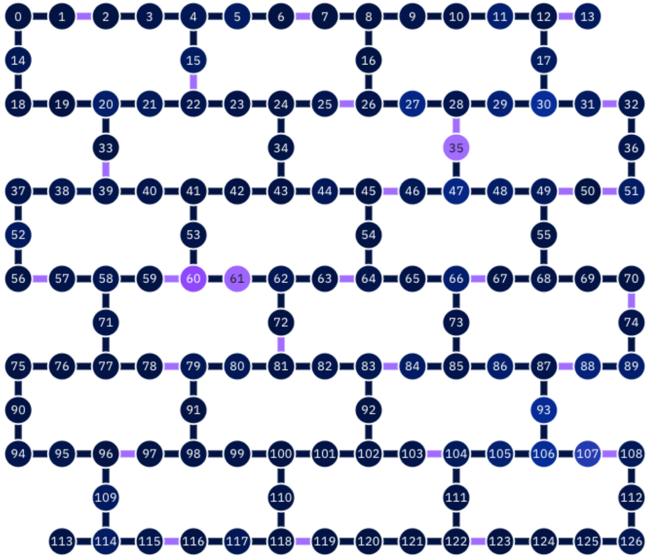




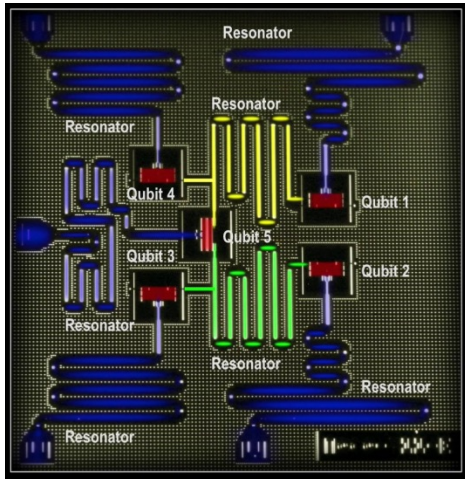
…and many more

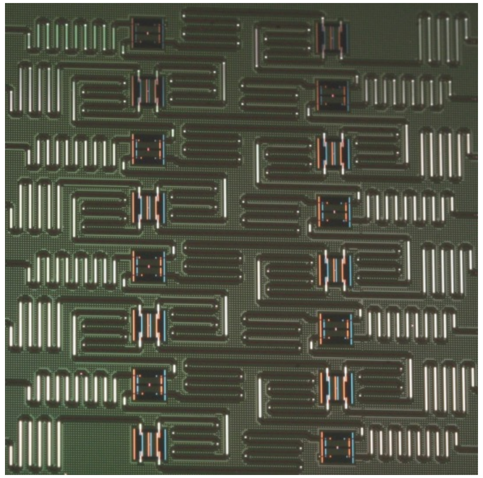
Google: 53, 72 Qubits



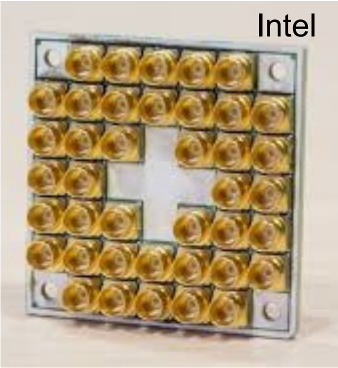


IBM: 1, 5, 7, 16, 27, 127, 433 Qubits





Intel: 17, 49 Qubits



https://quantum-computing.ibm.com/services/resources?tab=systems&limit=50&system=ibm_kyiv

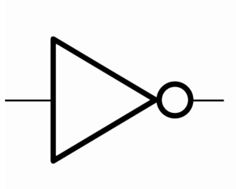
WHAT OPERATIONS CAN WE DO?

M. A. Nielsen and I. L. Chuang. Quantum Computation and Quantum Information: 10th Anniversary Edition. Cambridge University Press.

D. P. DiVincenzo. Phys. Rev. A **51**, 1015–1022.

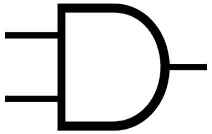
Digital Gates:

1 bit: NOT



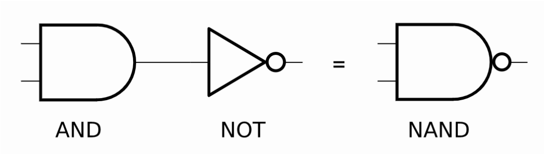
A	NOT A
0	1
1	0

2 bits: AND



A	B	A AND B
0	0	0
0	1	0
1	0	0
1	1	1

…and others.



Quantum Gates:

1 qubit: $\alpha|0\rangle + \beta|1\rangle$

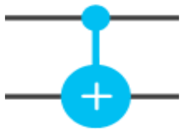
X-Gate (NOT): $|0\rangle$  $|1\rangle$

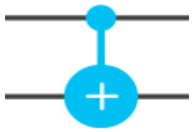
Hadamard (H-Gate): $|0\rangle$  $\frac{|0\rangle + |1\rangle}{\sqrt{2}}$

…and others.

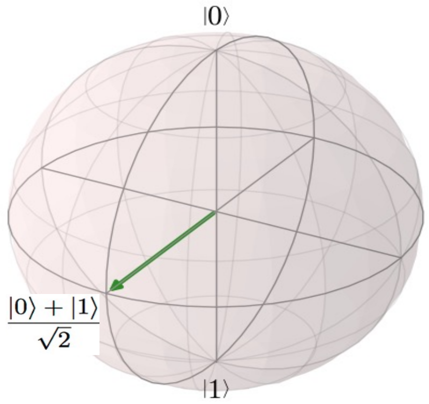
2 qubits: $\alpha|00\rangle + \beta|01\rangle + \gamma|10\rangle + \delta|11\rangle$

CNOT:

$|00\rangle$  $|00\rangle$

$|11\rangle$  $|10\rangle$

…and others.



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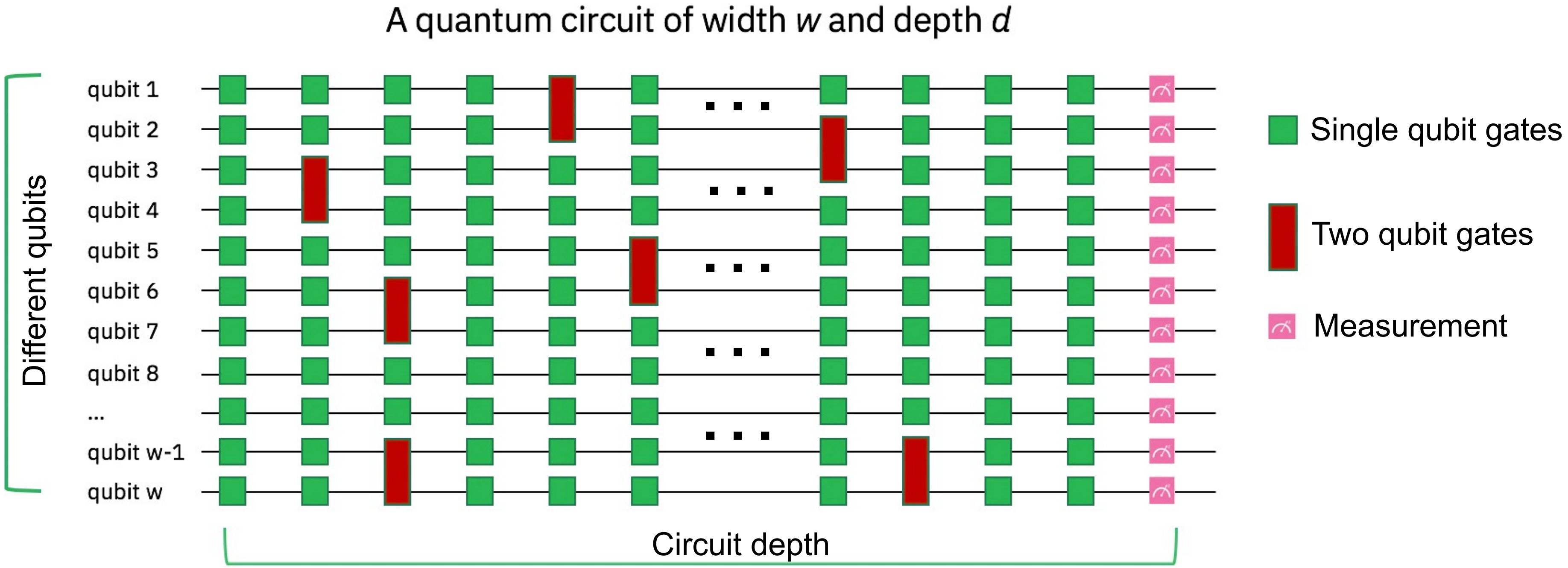
GATE BASED QUANTUM COMPUTERS

Combining gates to execute algorithms



- Circuit is based on the implementation of some algorithm
- Current gate-based quantum hardware can accommodate small depth
- The physical connectivities of the qubits on the device can be relevant

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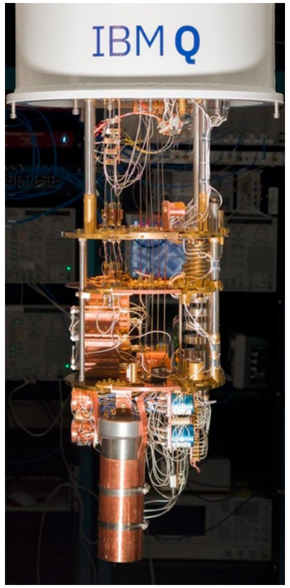
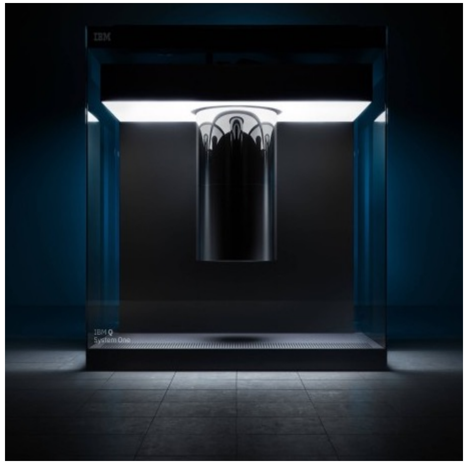
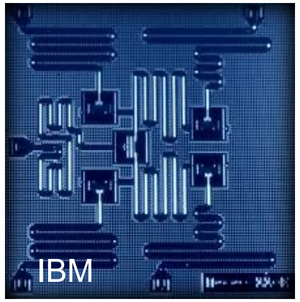
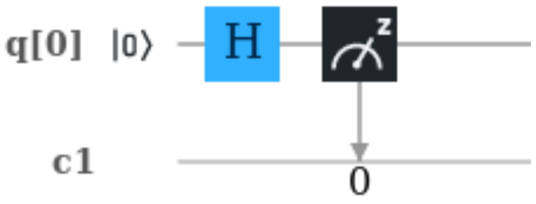
GATE-BASED QC: APPLICATIONS

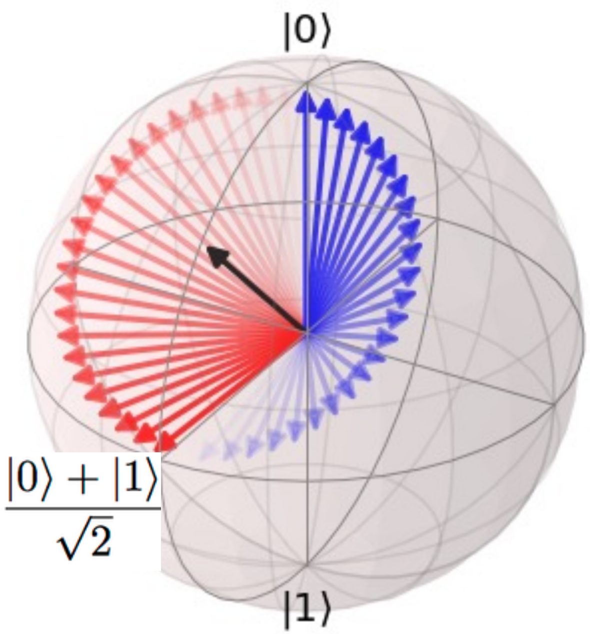
Coin tossing: 1 fair coin



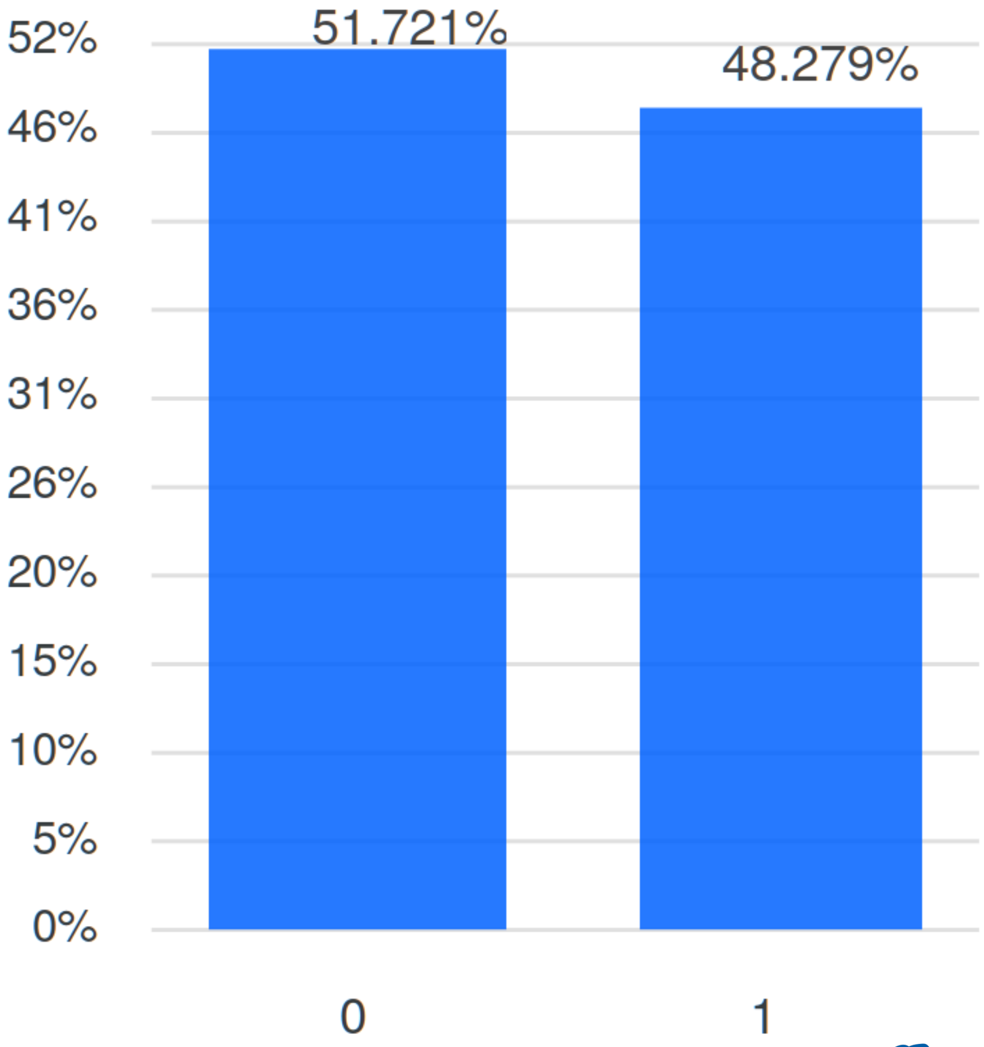








8192 coin tosses:



Error-prone device!

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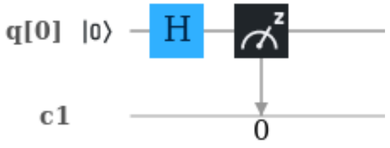
ERROR PRONE COMPUTATION

All kinds of errors destroy the computation



- Error is present even by executing only a single gate
  - In state preparation, gate operation, and measurement

- An algorithm usually consists of hundreds of gates placed over several qubits
  - Expect propagation of error

- *Error correction* techniques require many more qubits than would be available in the near future

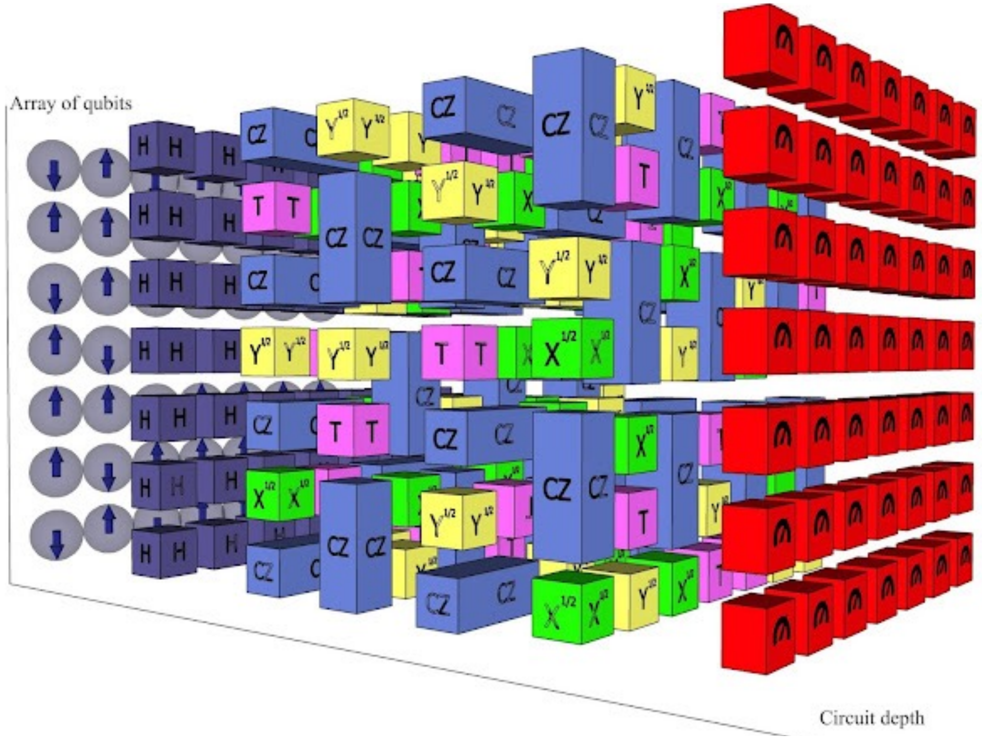
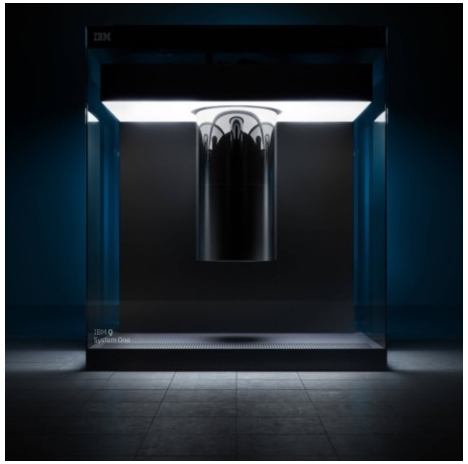


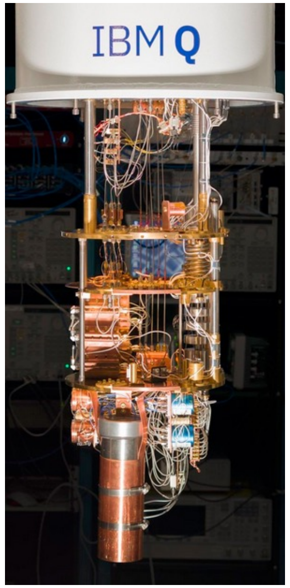
Image from: https://ai.googleblog.com/2018/05/the-question-of-quantum-supremacy.html

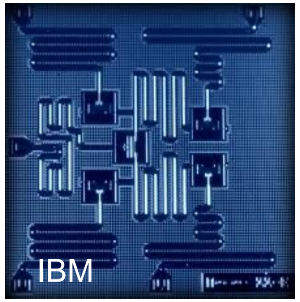
GATE BASED QUANTUM COMPUTERS

SOME OPEN QUESTIONS

- More qubits or better qubits?
- How many ‘better qubits’ are good enough?
- Faster or more stable gate operations?
- Do we agree on what ‘quantum advantage’ is?
- Can we make practical use of noisy hardware?







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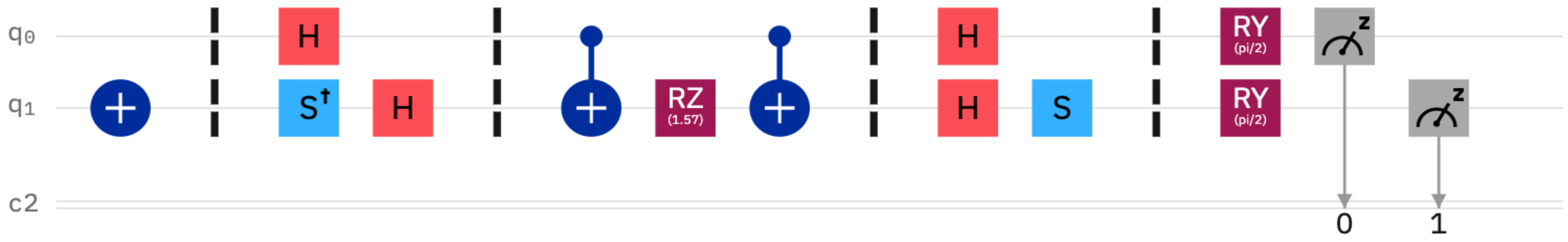
VARIATIONAL METHODS TO THE RESCUE?

Parametrise the circuit

- Design a circuit with suitably placed variational parameters



- For a single parameter we can trace the curve in the range $[0, 2\pi]$

- For multi-parameter circuits of practical interest:
  - Let a classical optimiser navigate the cost function (e.g. energy landscape)
  - Get to a local/global extremum

MOTIVATION FOR VARIATIONAL METHODS

How do we benefit?

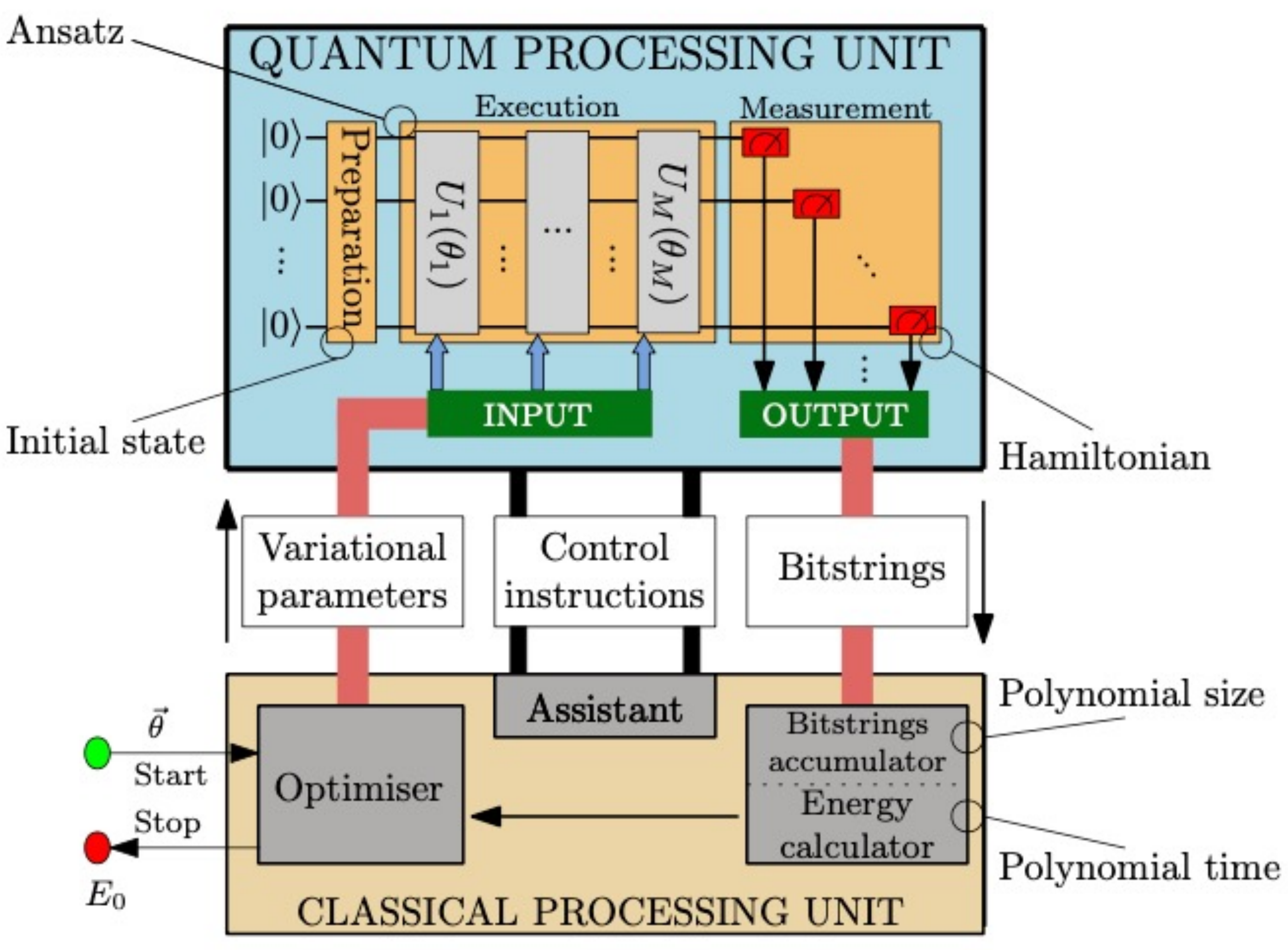
- Smaller circuit depths
  - Small scale prototype applications already demonstrated
    - ✓ G.S.E of molecular Hydrogen — P. J. J. O'Malley et al. Phys. Rev. X **6**, 031007. (2016)
    - ✓ G.S.E of water molecule on an trapped-ion device — Y. Nam, et al. npj Quantum Information **6**, 1. (2020)
    - ✓ G.S.E of a chain of 12 Hydrogen atoms — F. Arute et al.. Science **369**, 1084–1089. (2020)
  - Circuit depths smaller than phase estimation algorithm — D. Wang et al., Phys. Rev. Lett. **122**, 140504. (2019)
- Flexbility of adapting an Ansatz to the actual hardware or problem
  - Hardware efficient Ansatz — A. Kandala et al. Nature **549**, 242–246. (2017)
  - Number preserving Ansatz — C. Cade et al., Phys. Rev. B **102**, 235122. (2020)
  - Variational Hamiltonian Ansatz — D. Wecker et al., Phys. Rev. A **92,** 042303. (2015)
- Fewer number of qubits
  - Compared to phase estimation algorithm

THE GENERAL IDEA

Combine quantum and classical computers

The algorithms works as follows

1. Prepare an initial state of the quantum unit and feed (a clever choice of) initial parameters
2. Execute the quantum circuit with those parameters and collect samples by repeating the execution
3. Collect sufficient samples to calculate the cost function to a required accuracy
4. Feed the output to an optimisation algorithm that proposes the next parameters
5. Repeat 2 to 4 until convergence



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P. J. J. O'Malley et al. Phys. Rev. X **6**, 031007. (2016)

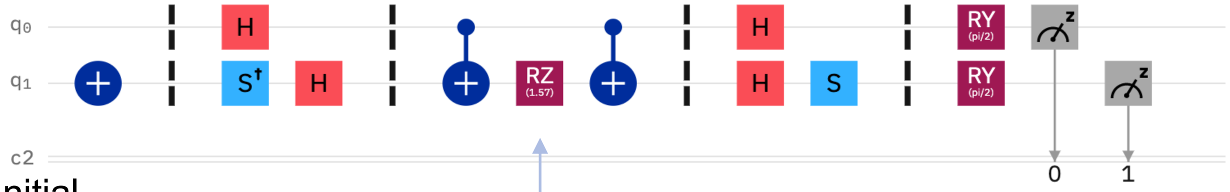
THE GENERAL IDEA

Combine quantum and classical computers

Two-qubit example

quantum

parameterised circuit



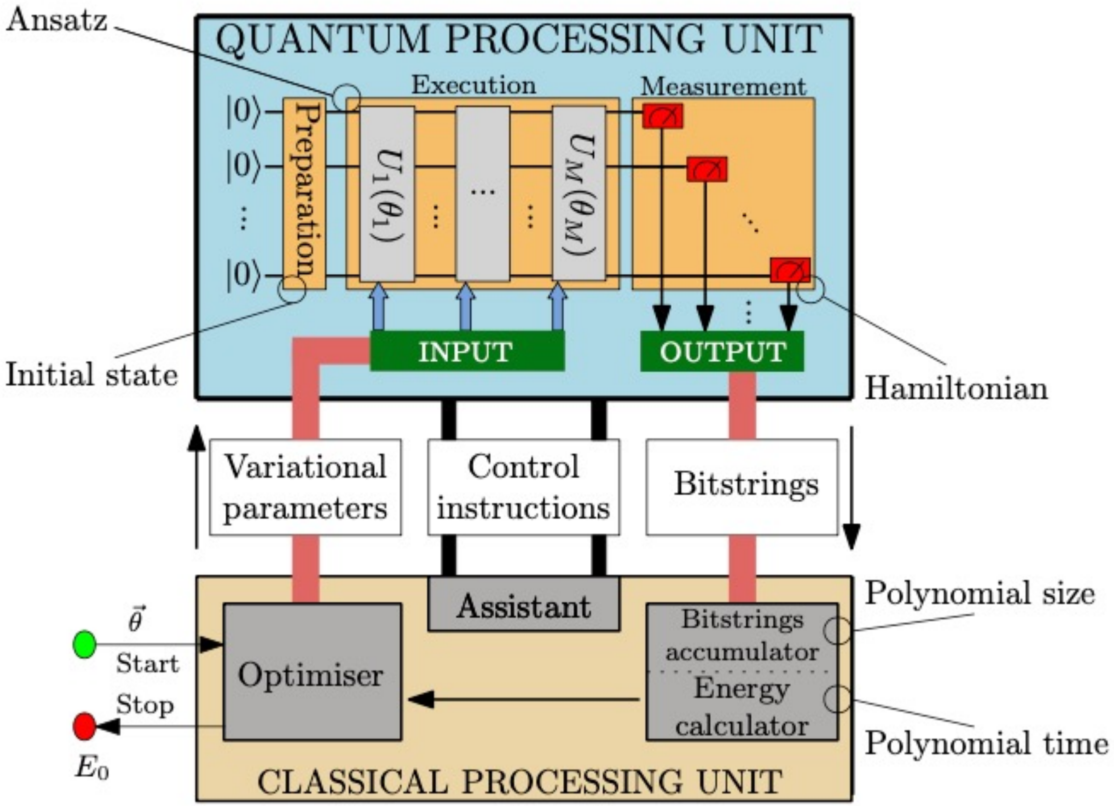
Initial state: 10

Measurement bitstrings

classical

Optimiser suggests new parameters

Calculate energy



- In this example we can scan the parameter space
- In general, we need to rely on some optimisation algorithm

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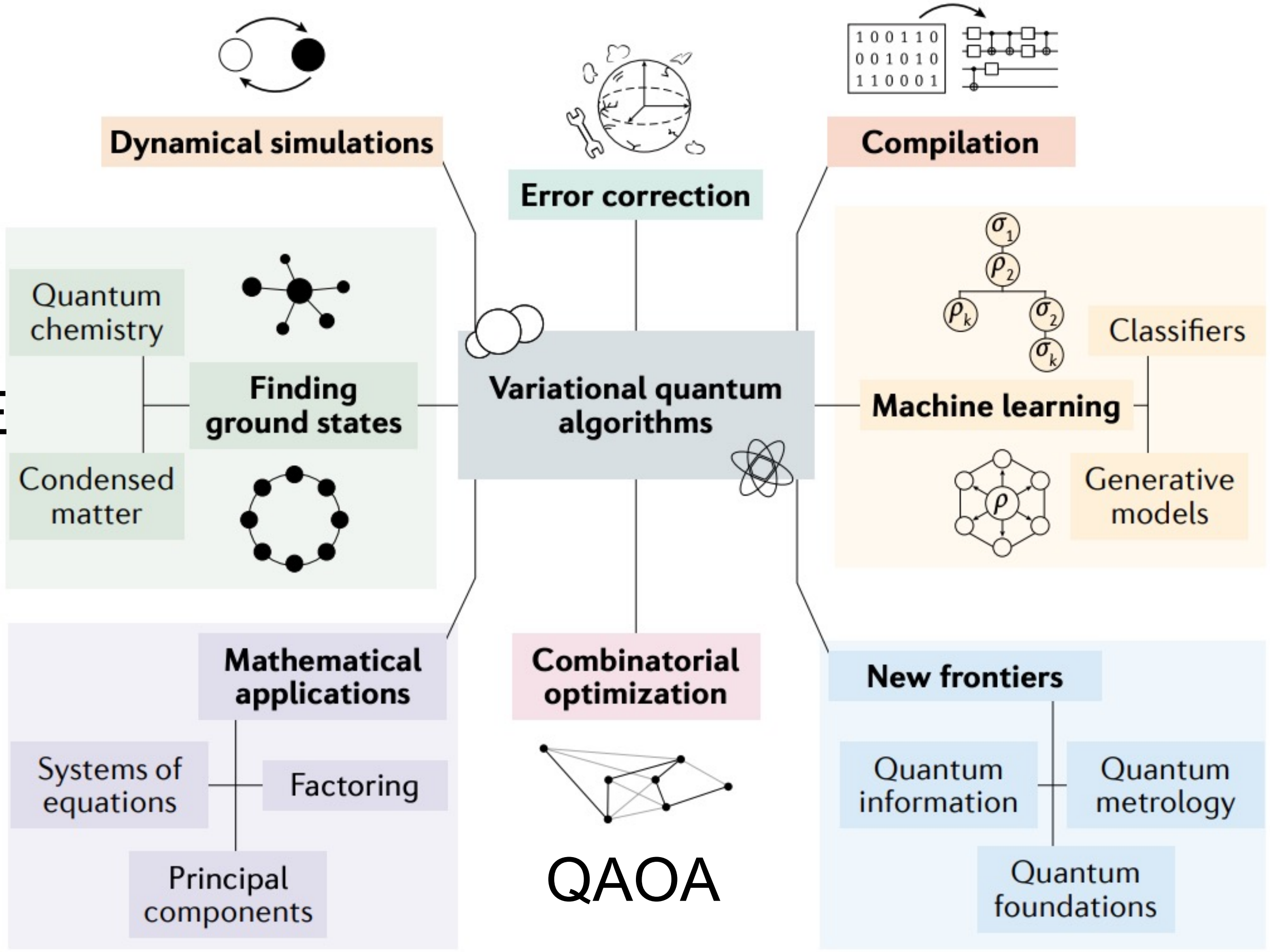
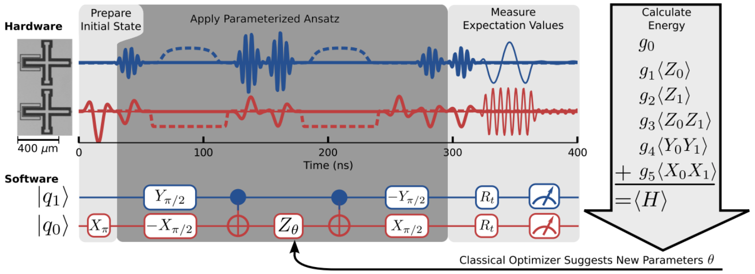
USES OF VARIATIONAL ALGORITHMS

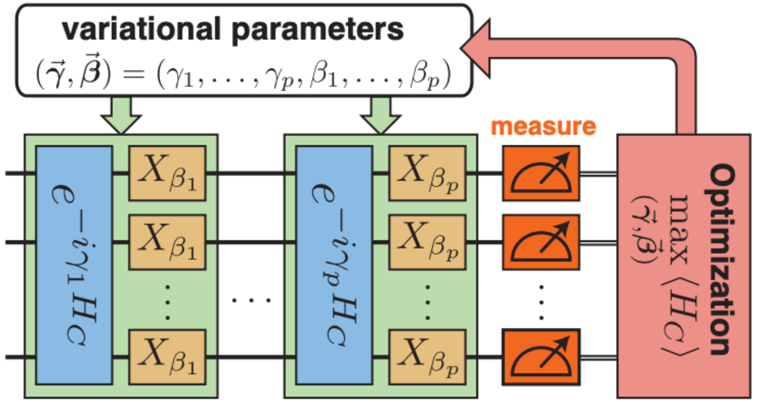
VQE



QAOA

Nature Reviews Physics volume 3, p. 625–644 (2021)





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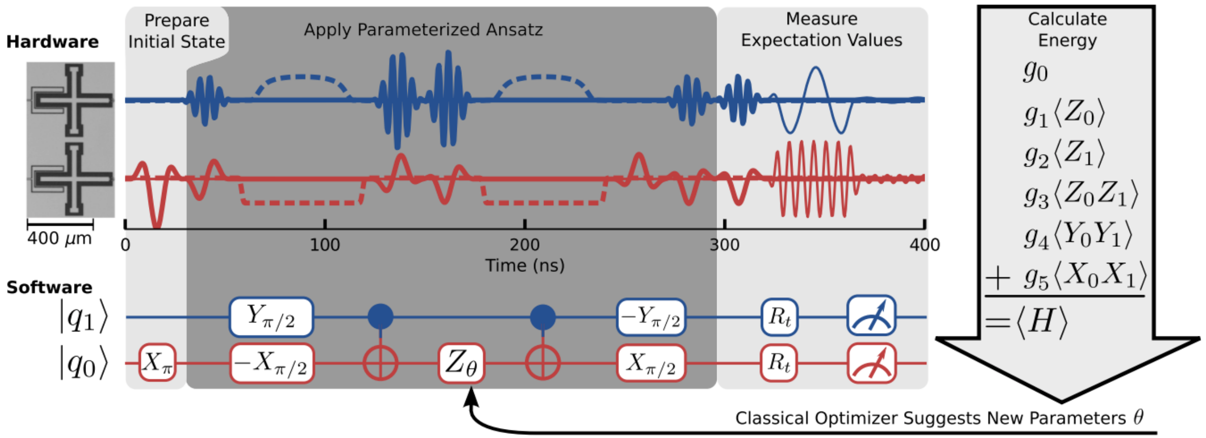
Phys. Rev. X **6**, 031007, 2016
Nat. Commun. 5, 4213, 2014
Science 369 (6507), 1084-1089, 2020
Phys. Rev. Lett. 127, 110503
Quantum Sci. Technol. 4 043001

VARIATIONAL QUANTUM EIGENSOLVER (VQE)

Recent uses

- Originally used for Chemical Hamiltonians
- Proof-of-principle demonstration for H_2 on a real device
- Since then has been used for
  - ❖ Chains of 12 atoms: $H - H - H - \cdots$
  - ❖ Eigenvalues of general sparse Hamiltonians
  - ❖ Hubbard model
  - ❖ Heisenberg model
  - ❖ Many others…



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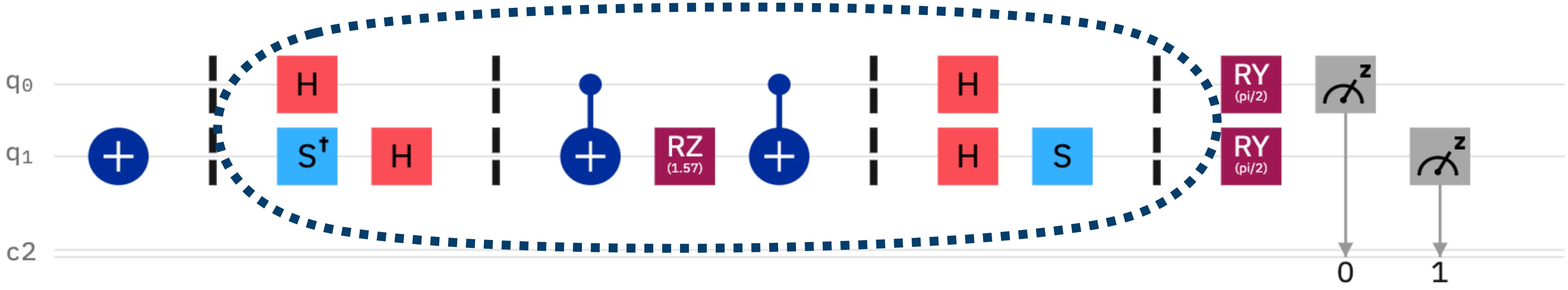
Nature Communications 10, 3007, 2019
Nature volume 549, p. 242–246, 2017
Quantum Sci. Technol. 4 014008, 2018

VARIATIONAL QUANTUM EIGENSOLVER (VQE)

What are the possibilities to explore?

- How to build a proper ansatz?



- The variational principle allows any possible circuit _but_ not all are equally good!
- One solution is to build step by step: an *adaptive method* (ADAPT-VQE)
- Another solution is to rely on extensions of classical theories (e.g. UCC ansatz)
- Limited connectivity in actual hardware: *Hardware efficient ansatz*
- Low depth for near-term devices to tolerate errors to some extent

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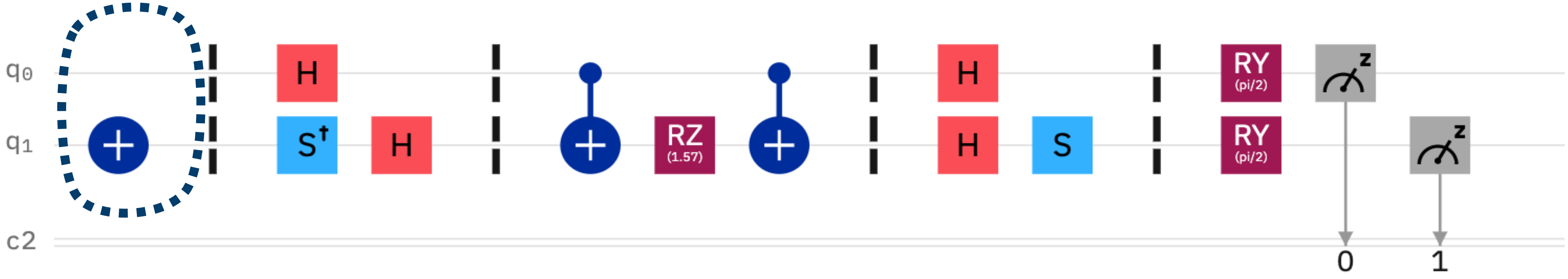
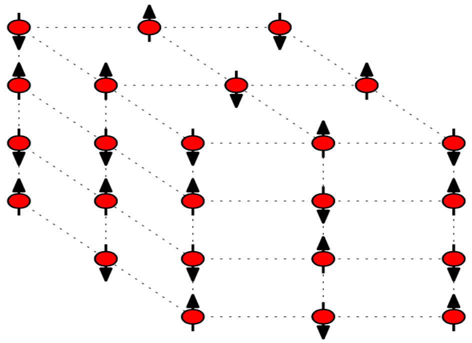
VARIATIONAL QUANTUM EIGENSOLVER (VQE)

What are the possibilities to explore?

- How to build a proper initial state?



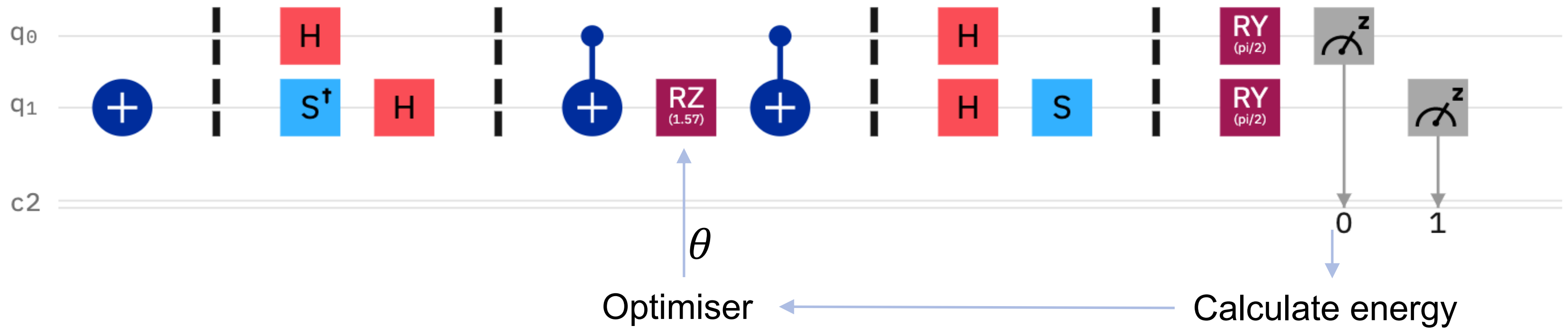
- Easy for the coin tossing experiment but difficult in general
- Rely on available theories/information
  - Example 1: Neél state for the Heisenberg model
  - Example 2: Hartree-Fock state for the Chemical problems
  - Example 3: Ground state for unperturbed Hamiltonians



VARIATIONAL QUANTUM EIGENSOLVER (VQE)

What are the possibilities to explore?

- Which optimiser to use?



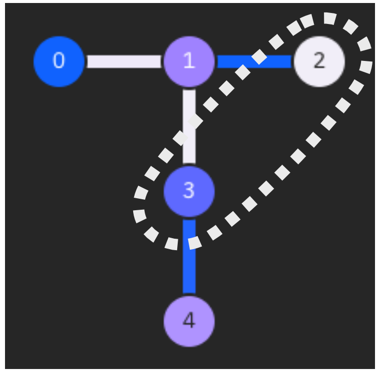
- Gradient-based
  - Advantage: Converge faster (in multidimensions), may require fewer energy evaluations
  - Disadvantage: Do not work with noise, may trap in local minima
- Gradient-free
  - Advantage: Often work with noise, may find global minima
  - Disadvantage: Converge slower, require more energy evaluations

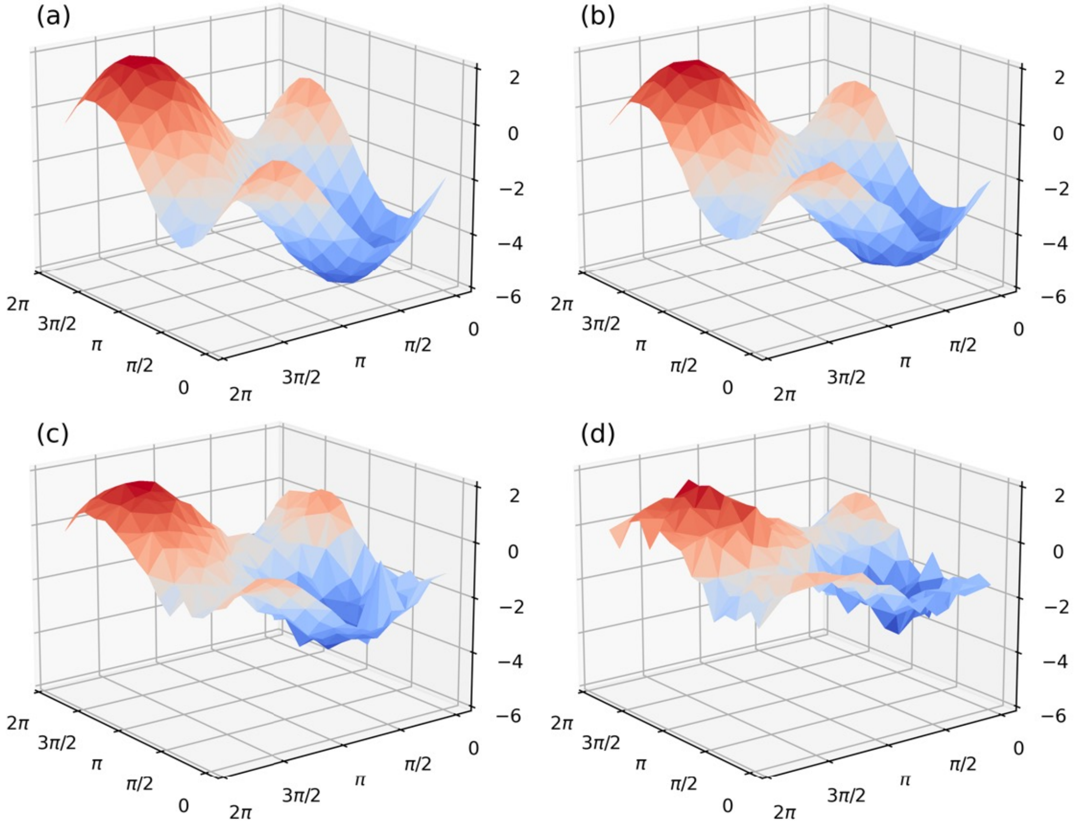
BENCHMARKING USING VQE

On IBM Q devices

- Using a 5-qubit device, we plot the energy landscape for a 2-parameter ansatz
- Problem is the *mean-field* model which is analytically solved

- (a) Ideal simulator
- (b) IBM Q Santiago (no swaps)
- (c) IBM Q Belem (no swaps)
- (d) IBM Q Belem (one swap)





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BENCHMARKING USING VQE - EVEN LARGER DEVICES

- The problem is the mean-field model whose result is analytically known
- The Hamiltonian is given as

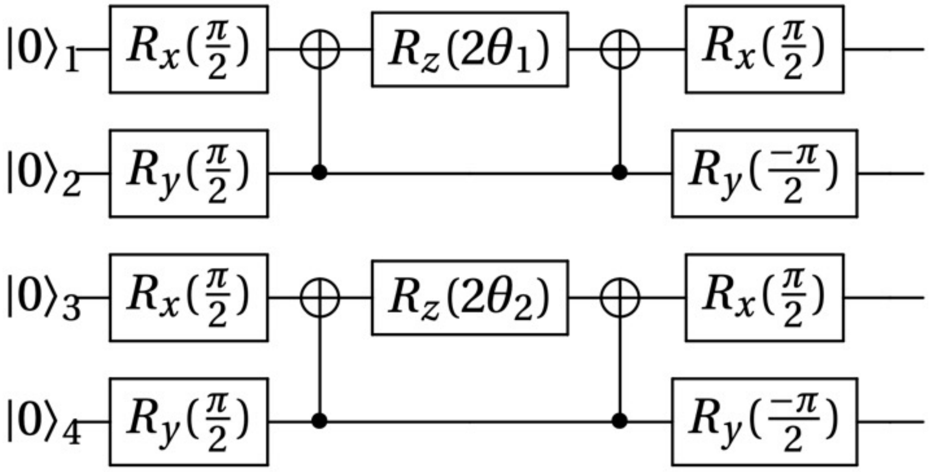
$$H = \sum_{<i,j>} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y + \sigma_i^z \sigma_j^z)$$

- The solution (ground state energy) is given by the expression 3(a - N)/2 where a=1 for odd N and a=0 for even N.
- We will try a case of N=4 and a=0, giving the ground state energy equal to -6
- We will also need suitable ansatz that represents the problem!

BENCHMARKING USING VQE - EVEN LARGER DEVICES

On IBM Q devices

- Using a 127-qubit device, we plot the energy landscape for a 2-parameter ansatz
- We use only 4 qubits
- Problem is the *mean-field* model which is analytically solved
- Done in June 2024



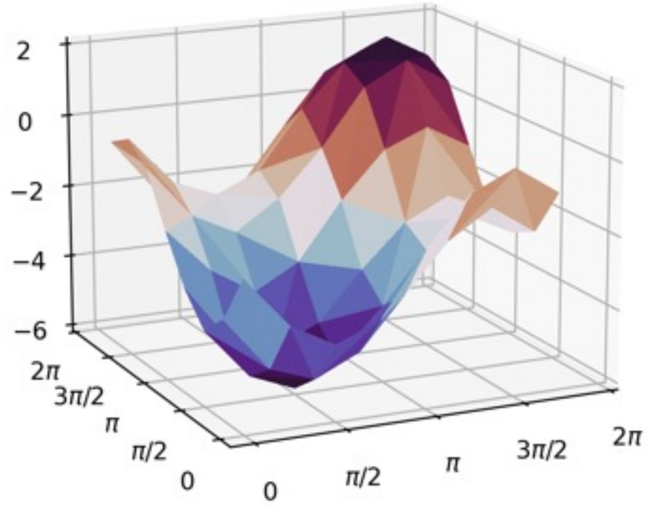
- (a) Ideal simulator
- (b) IBM Q Osaka
- 8 x 8 grid
- ~ 8 minutes of compute time

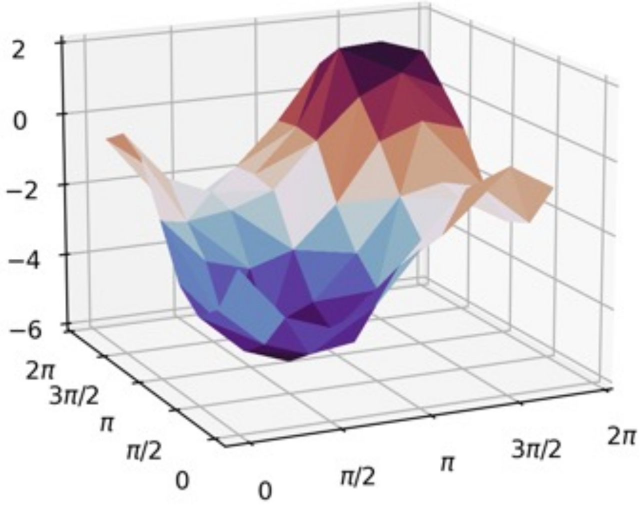
BENCHMARKING USING VQE - EVEN LARGER DEVICES

On IBM Q devices

- Using a 127-qubit device, we plot the energy landscape for a 2-parameter ansatz
- We use only 4 qubits
- Problem is the *mean-field* model which is analytically solved
- Done in June 2024

- Lowest IBMQ value is – 5.28
- True lowest value is – 6.00



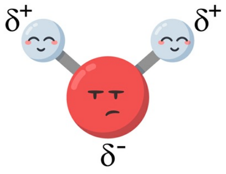


M.S. Jattana, et. al, Phys. Rev. Applied **19**, 024047. (2023)

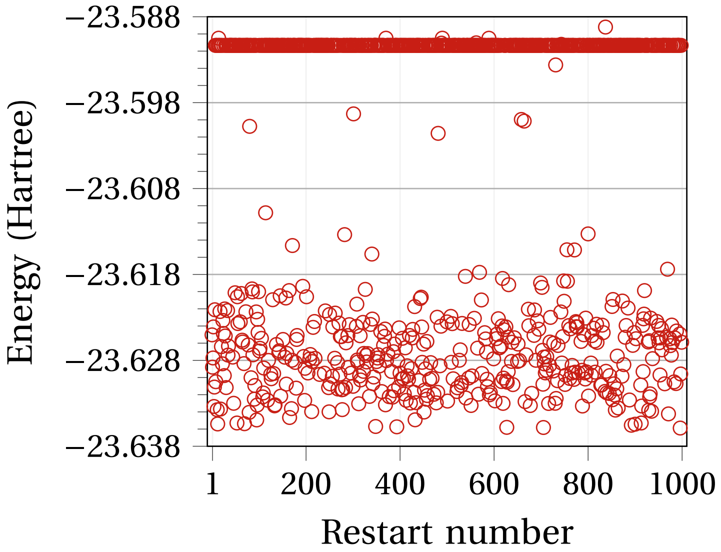
TWO PROBLEMS FACED BY VARIATIONAL METHODS

Local minima and barren plateaus

- The optimisation algorithm is unable to find the global minimum of the energy landscape



- Problem: 8 qubits water molecule
  Ansatz: 30 parameters
  Plotted is final energy after random restarts



- The energy obtained from initial parameters lies in a flat neighbourhood away from the global minimum

- 3 x 3 x 3 isotropic Heisenberg lattice
  702 parameters
  G.S.E. = -73.452 ; **N.S.E.** = -54.000
  Plotted is random initial parameters energy

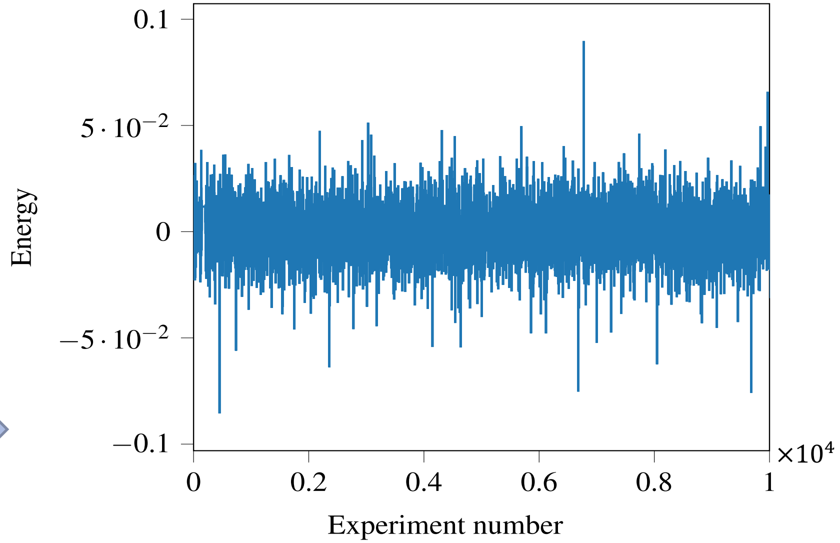


Image source: https://theory.labster.com/welcome_h2o/

J. R. R. McClean et al., Nature Communications **9**, 1–6. 2018.
E. Grant et al., Quantum **3**, 214. 2019.
T. L. Patti et al., Phys. Rev. Research **3**, 033090. 2021.

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TWO PROBLEMS FACED BY VARIATIONAL METHODS

Local minima and barren plateaus

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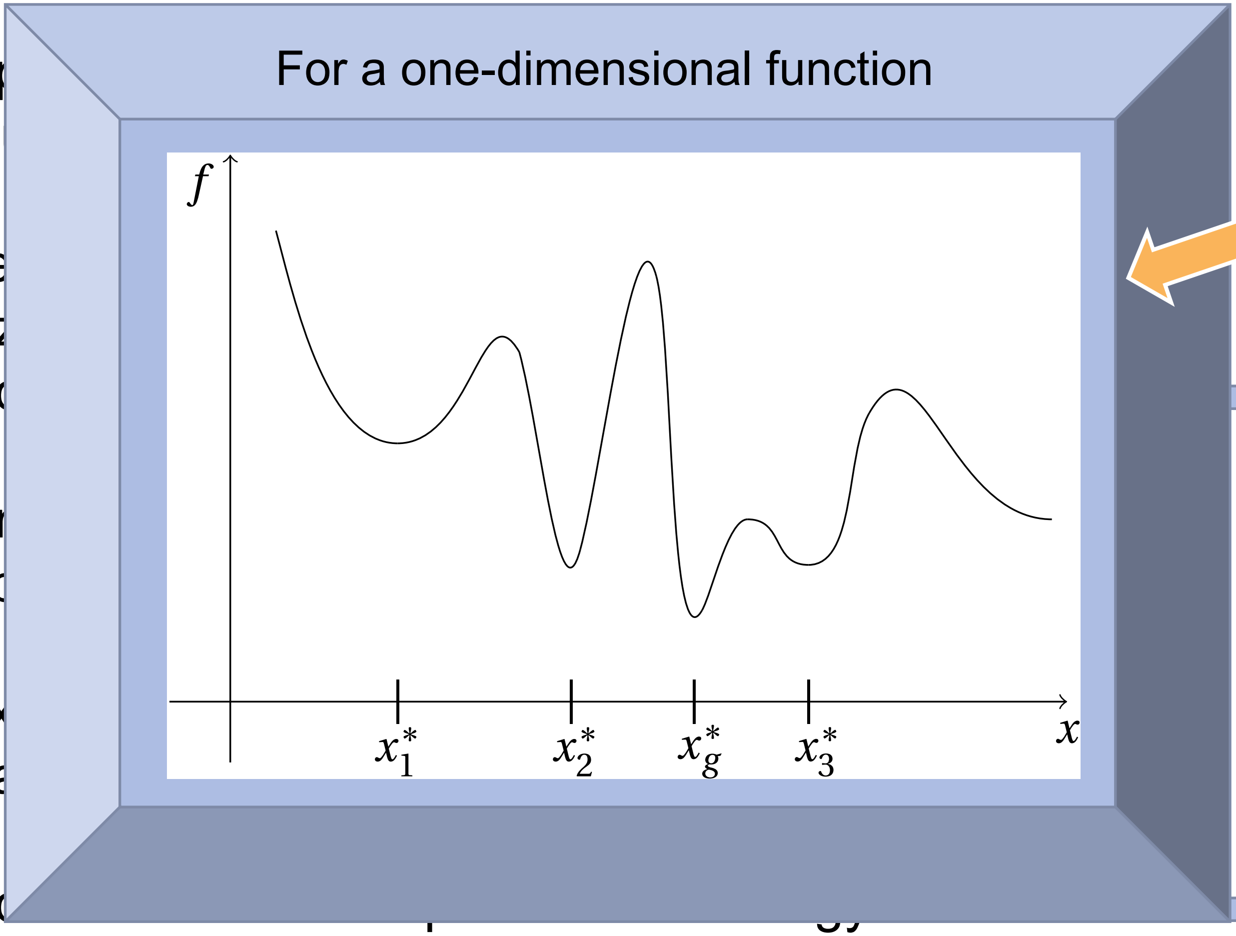
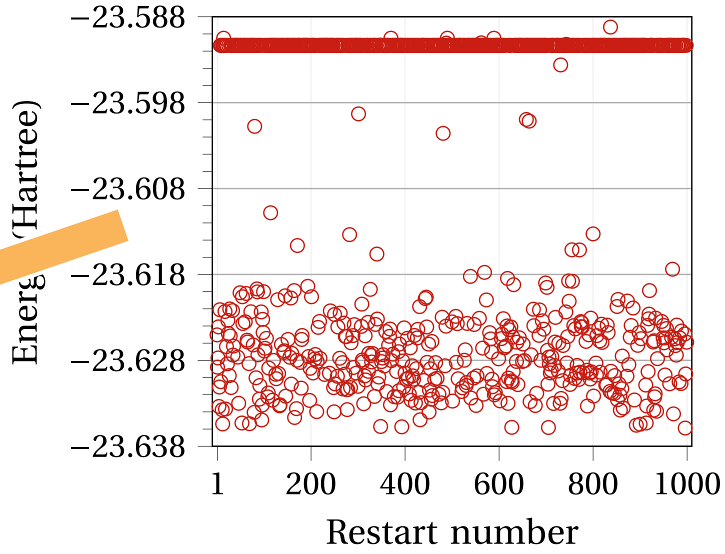
  Plotted





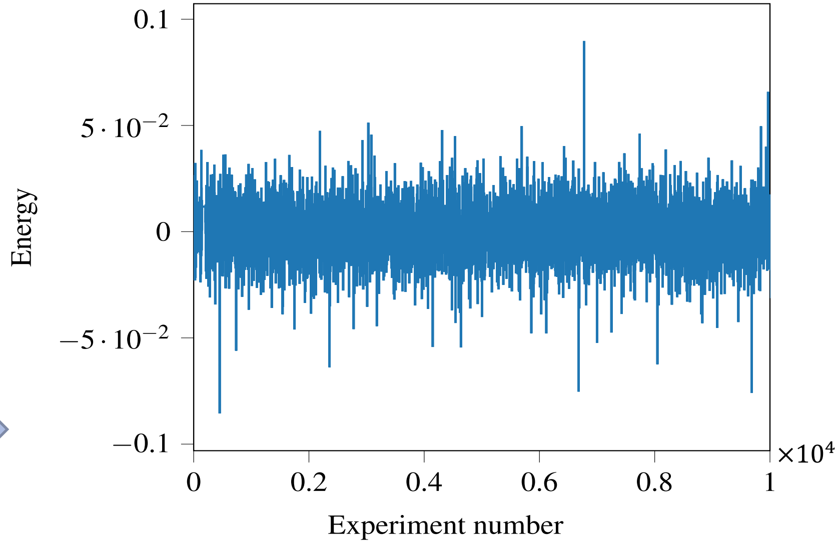


Image source: https://theory.labster.com/welcome_h2o/

J. R. R. McClean et al., Nature Communications **9**, 1–6. 2018.
E. Grant et al., Quantum **3**, 214. 2019.
T. L. Patti et al., Phys. Rev. Research **3**, 033090. 2021.

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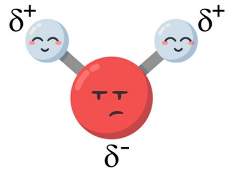
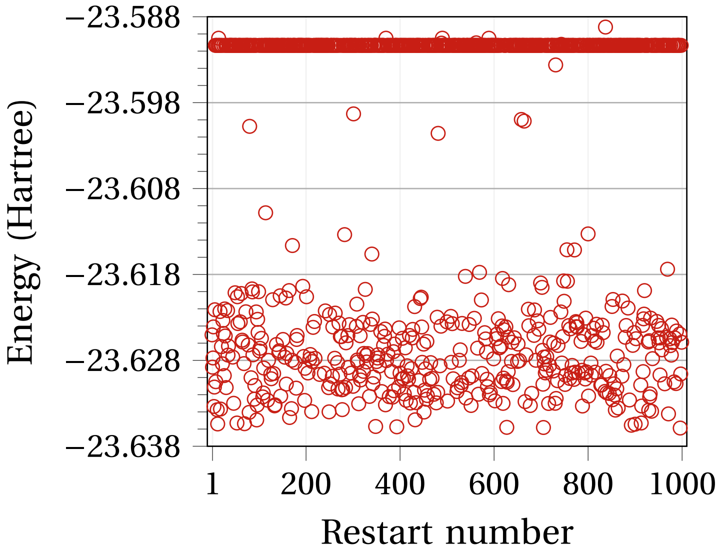
Local minima and barren plateaus

- The optimisation algorithm is unable to find the global minimum of the energy landscape

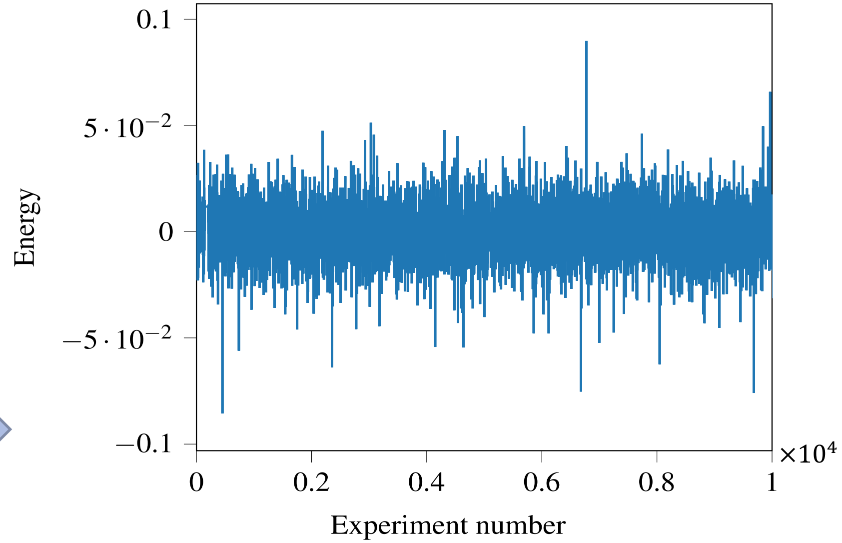


- Problem: 8 qubits water molecule
  Ansatz: 30 parameters
  Plotted is final energy after random restarts



- The energy obtained from initial parameters lies in a flat neighbourhood away from the global minimum

- 3 x 3 x 3 isotropic Heisenberg lattice
  702 parameters
  G.S.E. = -73.452 ; **N.S.E.** = -54.000
  Plotted is random initial parameters energy



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Local minima and barren plateaus

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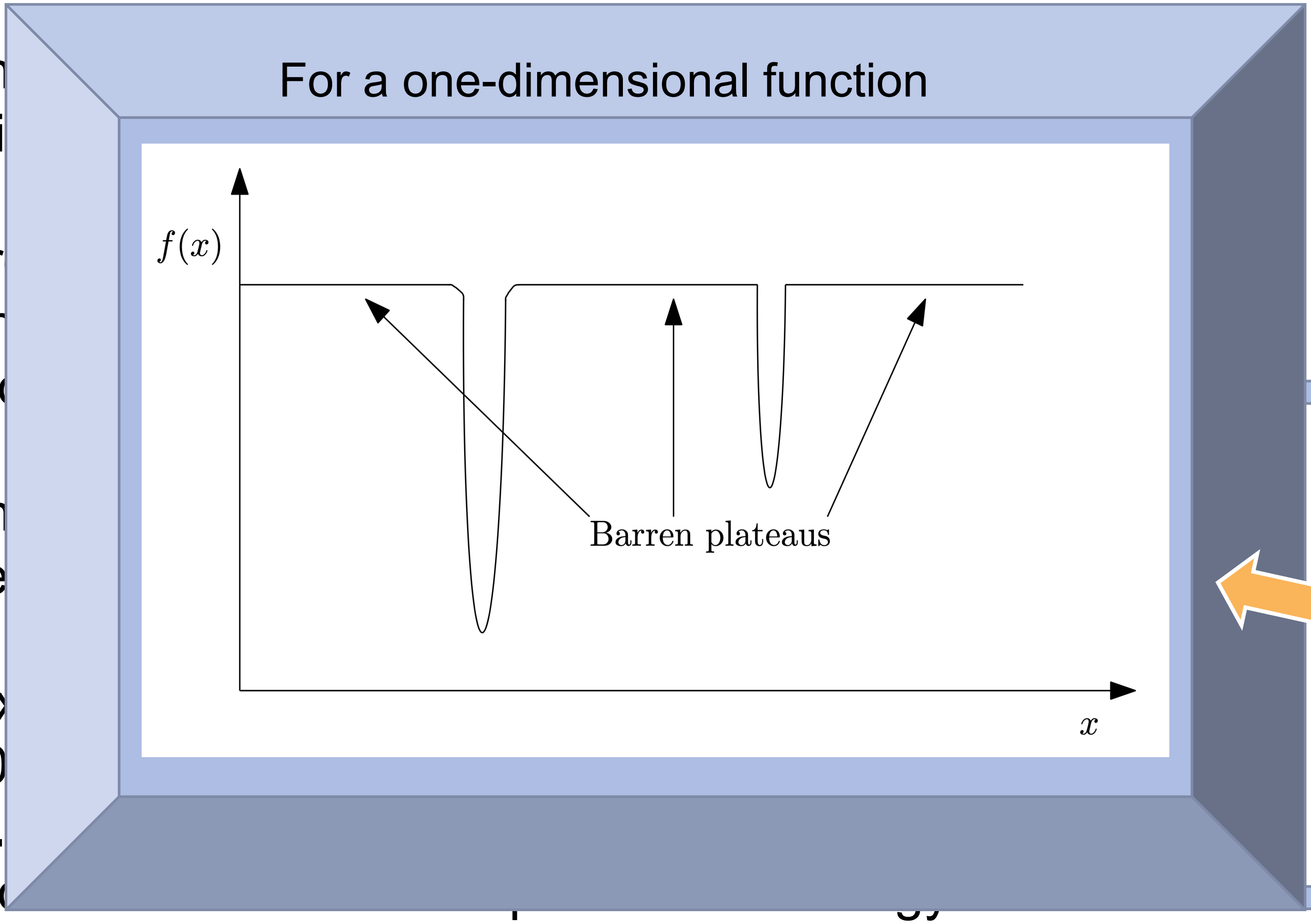

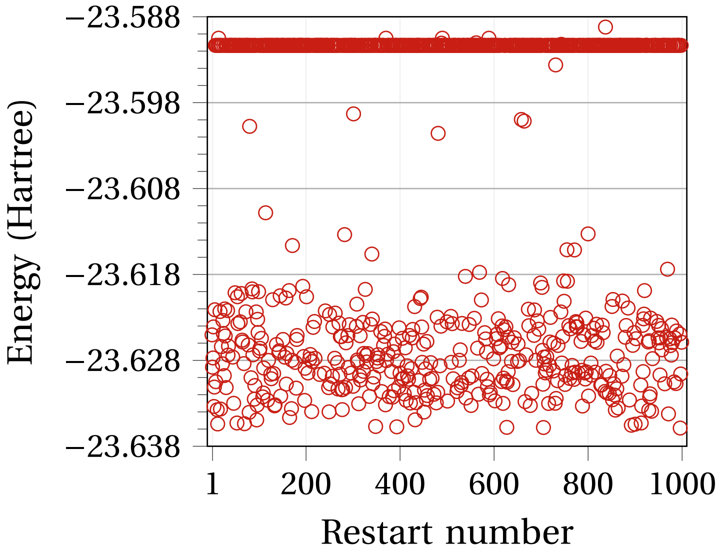

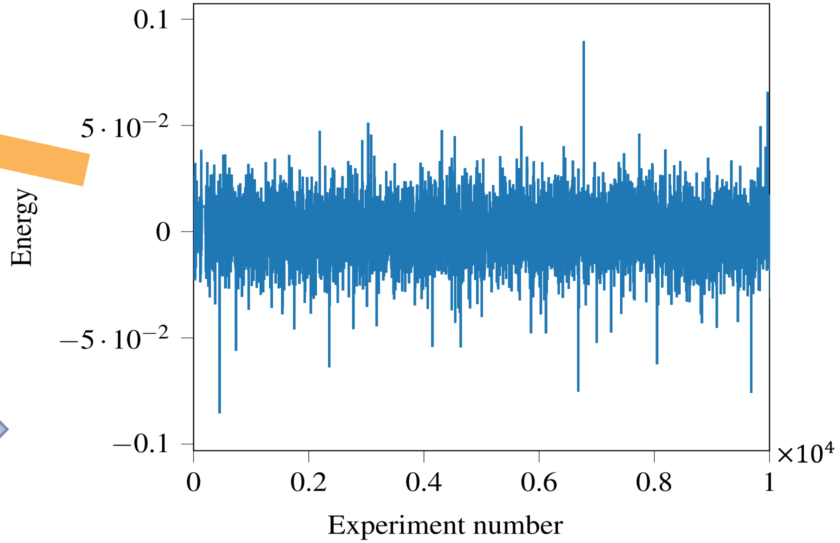

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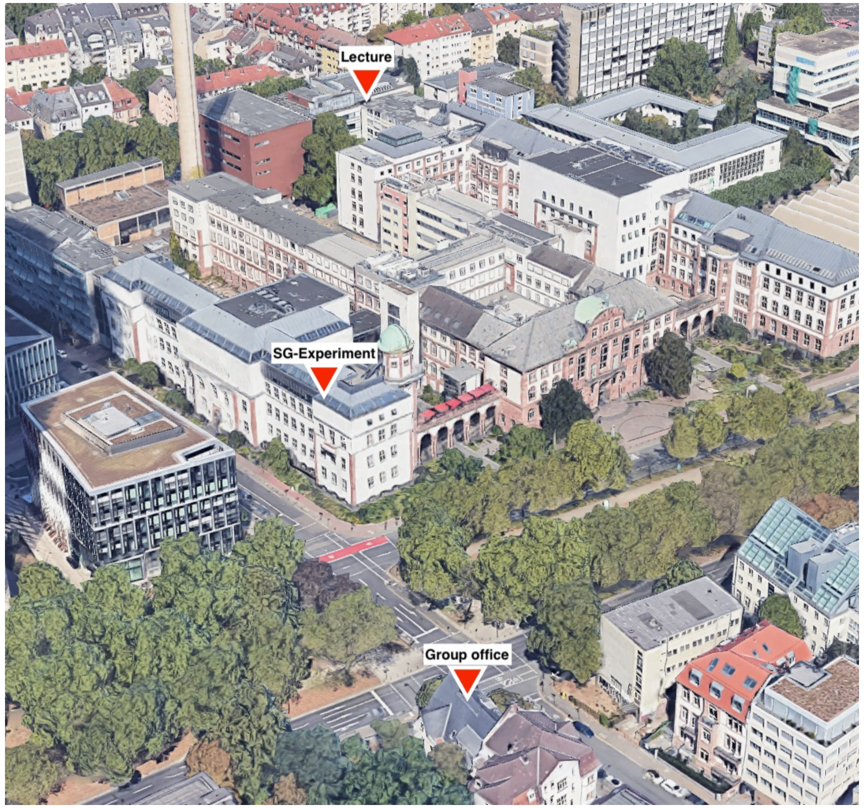
QUANTUM COMPUTING AT GOETHE UNIVERSITY

A little bit about current and future plans…

QUANTUM COMPUTING AT GOETHE UNIVERSITY

A peek into the past

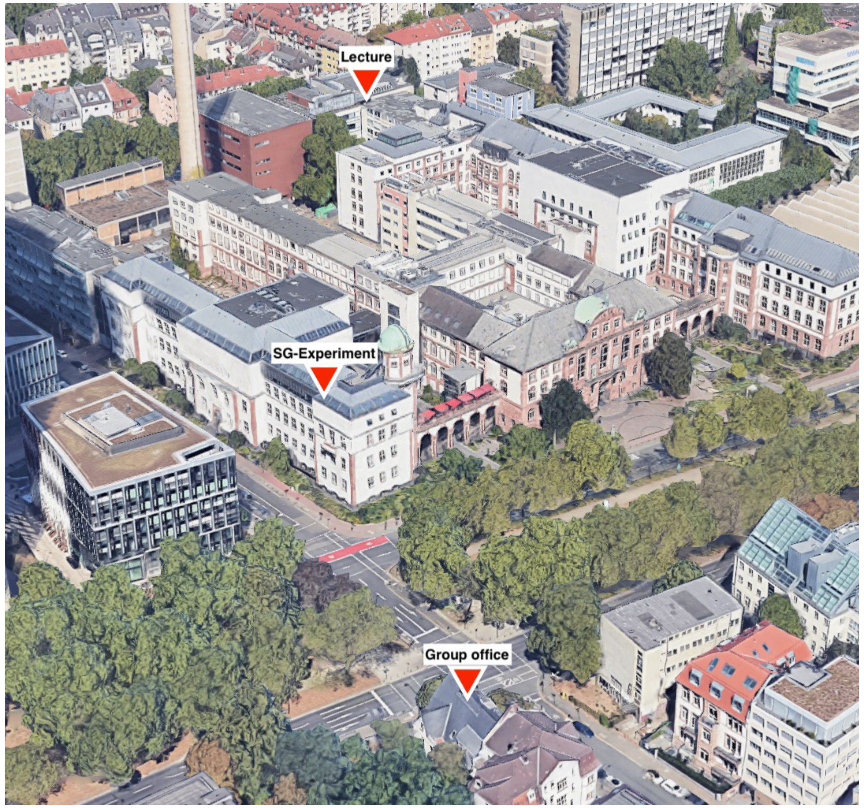
- The historic Stern-Gerlach experiment
- Lots of quantum computing vibes!



QUANTUM COMPUTING AT GOETHE UNIVERSITY

A peek into the future

- The historic Stern-Gerlach experiment
- Lots of quantum computing vibes!



Device Specifications:

Name: *Baby Diamond* ™
Qubits: *5*
Topology: *all-to-one*
Type: *Diamond NV-center*
Location: Kettenhofweg 139
Temperature: room temp.
Tours: Late summer

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SUMMARY

- Simple applications of quantum computers – coin tossing
- Variational quantum algorithms: VQE and QAOA
- Two problems with variatiational methods
- Directions of work for improving VQE
- A heuristic as potential solution with results
- Used VQE for benchmarking quantum devices
- Quantum computing at Frankfurt (in collaboration with NHR)

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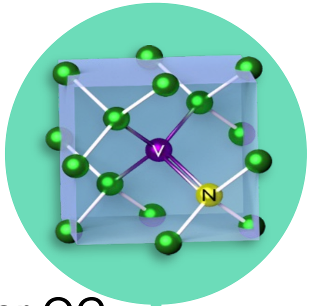
FRANKFURT ROADMAP

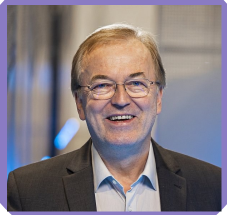


Potential upgrade to more qubits

NV-Center QC Procurement 5-qubits (Baby Diamond)
XeedQ GmbH

2020 | 2021 | 2022 | 2023 | 2024 | … | 2029

Group created

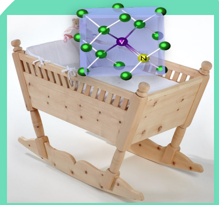


Market research for potential QCs

I joined

Delivery and Operation

Access via NHR



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