Accurate Quantum Computing in the Utility Era

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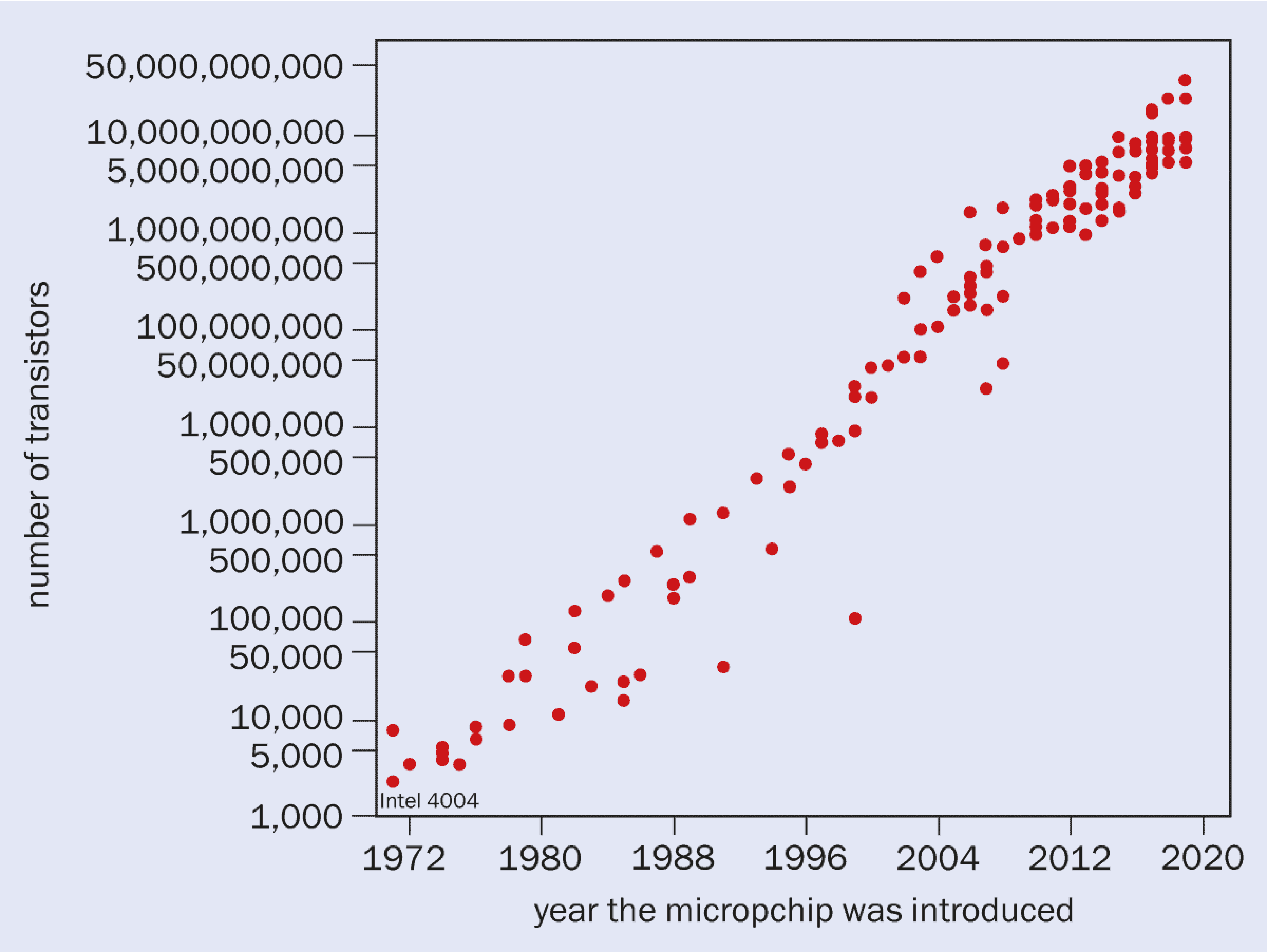
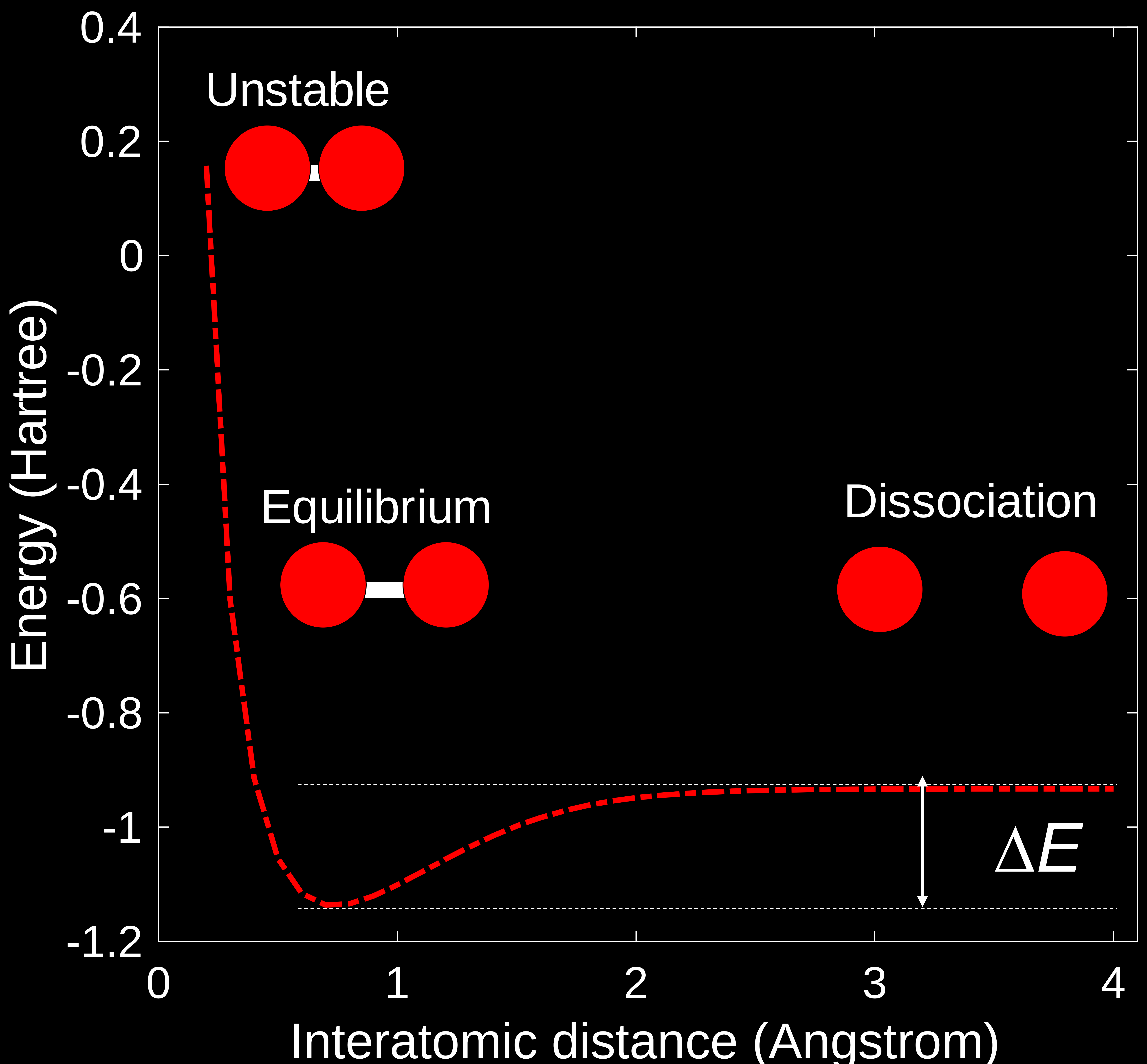
Principal Research Scientist

Do we need faster computers?



Wikipedia

Potential energy curve of a molecule



Rate ∝ Exp($-\Delta E/kT$)

The Electronic Structure Problem

Interacting fermionic problems: A core challenge in modern computational physics and High-performance computing

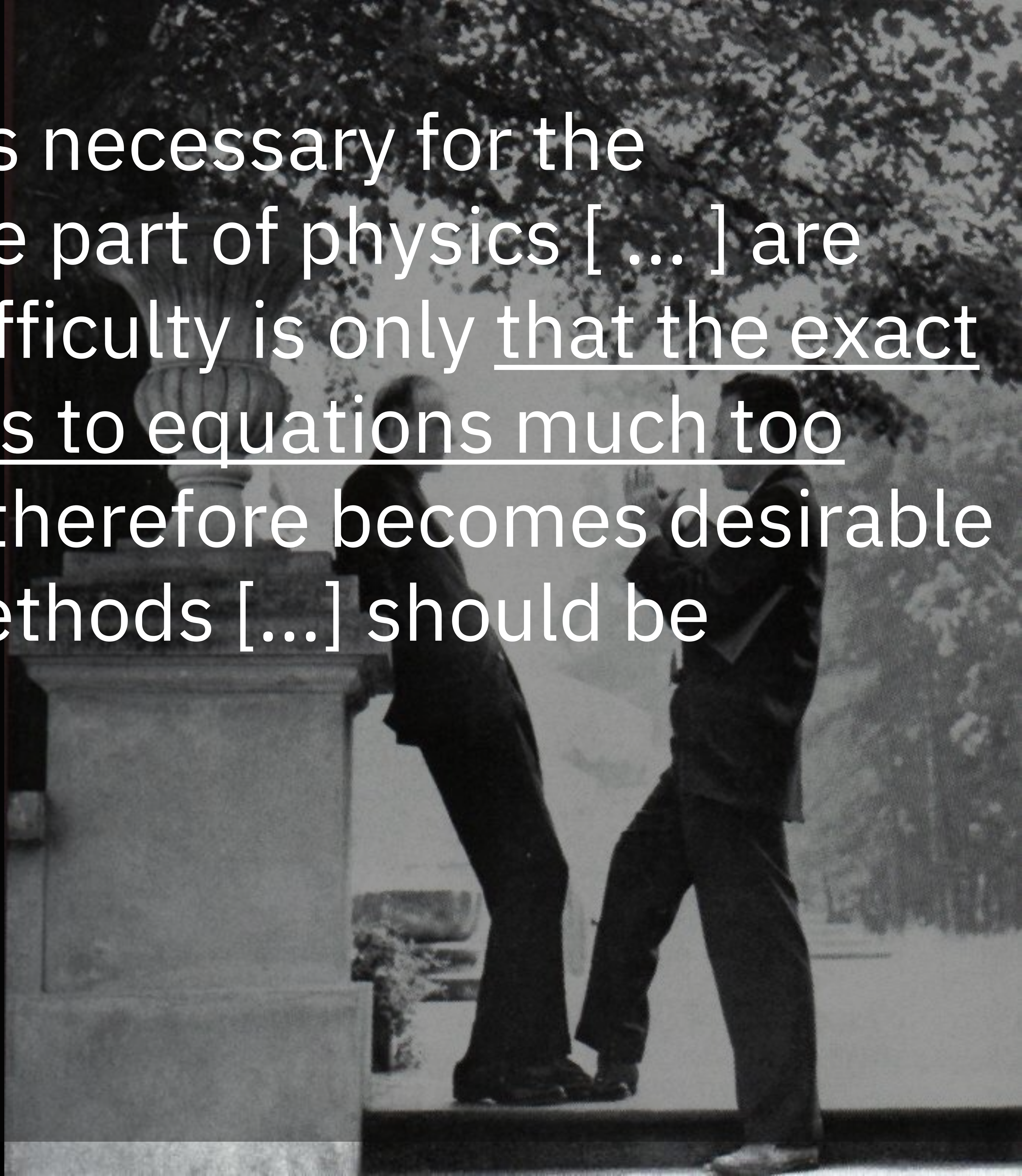
$$H|\psi_G\rangle = E_G|\psi_G\rangle$$

$$\begin{bmatrix} & & \\ & H_{x,y} & \\ & & \end{bmatrix} \begin{bmatrix} \\ \\ \\ \end{bmatrix} = E_G \begin{bmatrix} \\ \\ \\ \end{bmatrix}$$

Brute force solution: For *N* spin orbitals, will entail diagonalizing a matrix of size 2^N x 2^N

“ The underlying physical laws necessary for the mathematical theory of a large part of physics […] are completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. It therefore becomes desirable that approximate practical methods […] should be developed… “

Paul Dirac (1929)



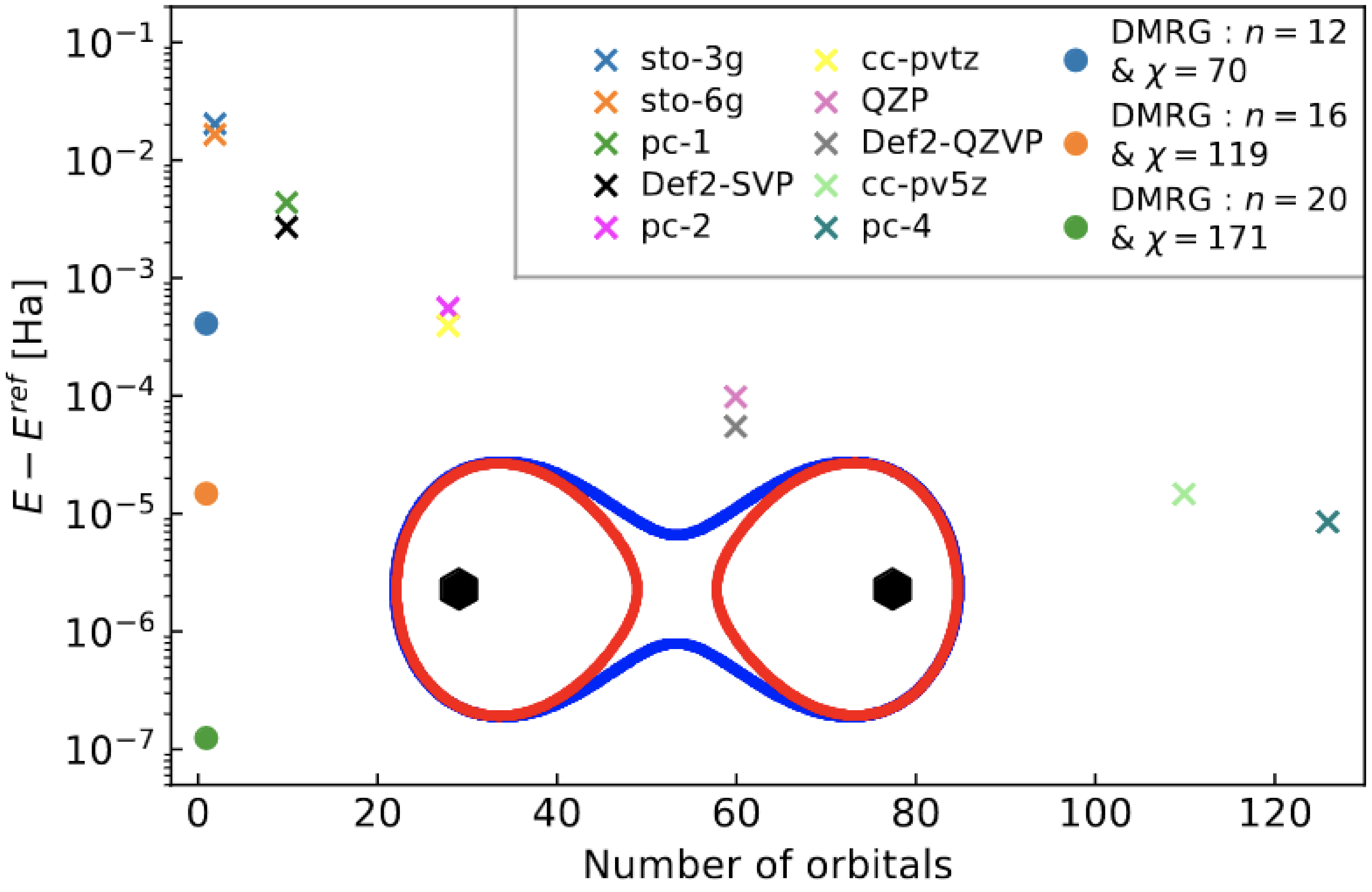
Computing beyond brute-force diagonalization:

The classical simulation playbook

1. Benchmark method where exact diagonalization is accessible/analytical solutions are known at “special points”

2. Compare method to other well-controlled classical approximations

3. Systematically increase computational resource (say, bond dimension) and check for convergence.



Jolly et al, Tensorized orbitals for computational chemistry, arXiv: 2308.03508

Can we now play this game with a quantum computer?

1. Need devices at scales beyond brute-force classical simulation

2. Need the device to produce trust-worthy solutions

Probability of hardware error

Transistor in a
Classical Computer

$$p \sim 10^{-27}$$

VS

Qubit in a
Quantum Computer

$$p \sim 10^{-3}$$

The only known long-term solution to this is quantum error correction

P. Shivakumar, M. Kistler, S. W. Keckler, D. Burger, L. Alvisi, *Proceedings of the 2002 International Conference on Dependable Systems and Networks* (2002); R. Baumann, *IEEE Design & Test of Computers*, 22 (3), 2005.

Can we now play this game with a quantum computer?

1. Need devices at scales beyond brute-force classical simulation

2. Can current devices already produce trust-worthy solutions?

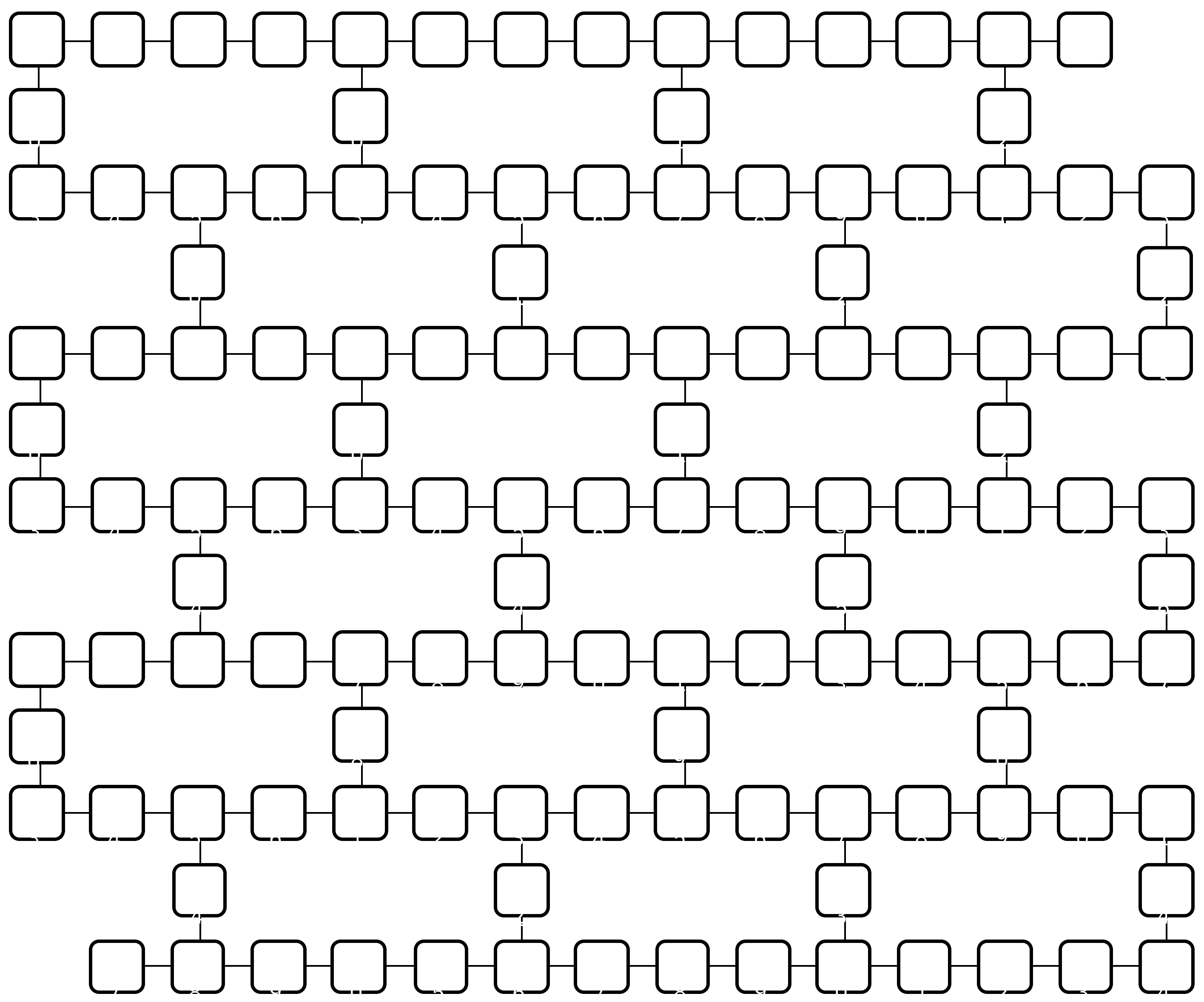
What can one do before fault tolerance?

Qubits: 100

Number of total two qubit gates: $N \sim 10{,}000$

Two-qubit gate fidelity: $f \sim 0.999$

Estimated state fidelity f^N < **5e-4**



$$|\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow \ldots \uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\rangle$$

Magnetization : $M = 1$

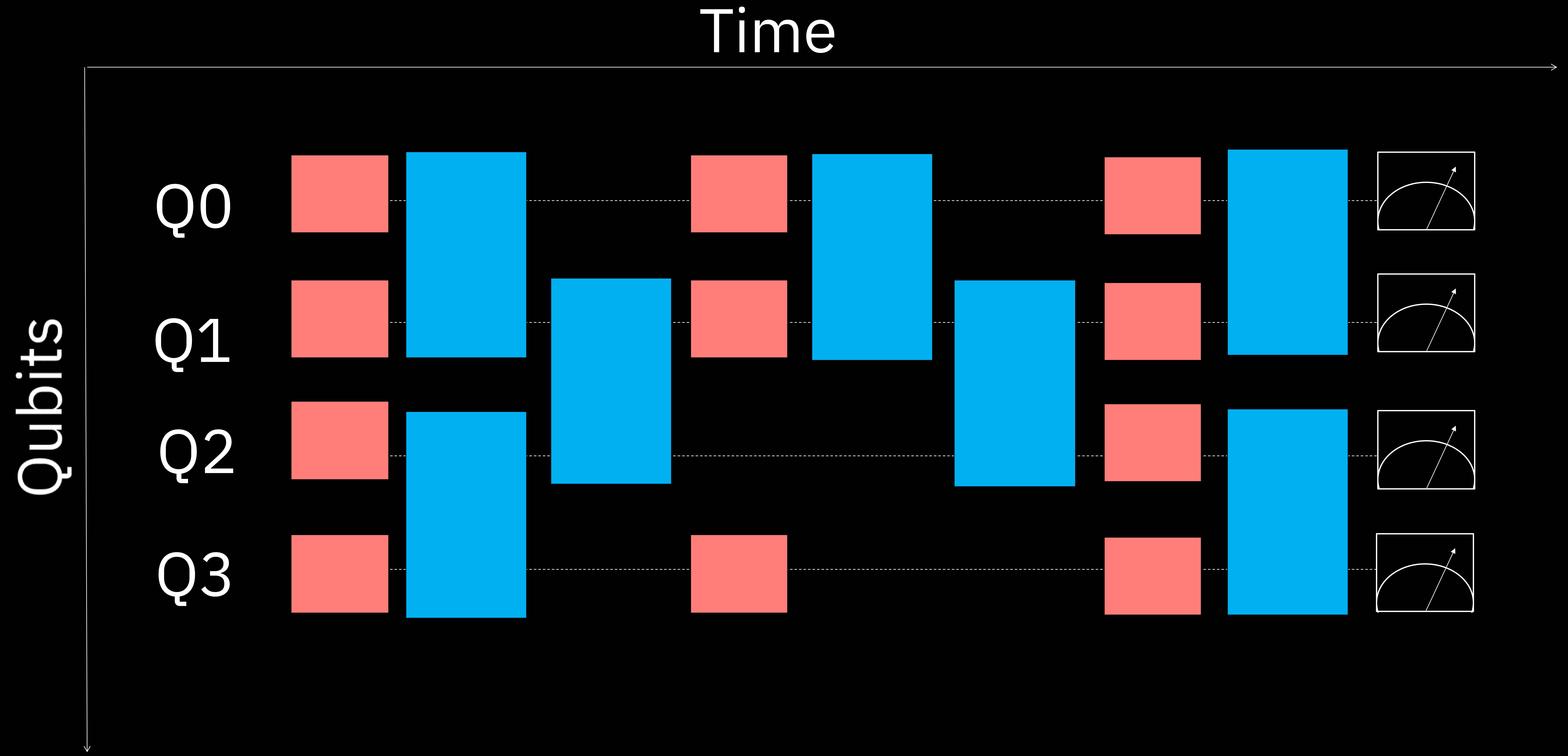
Fidelity : $F = 1$

$$|\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow \ldots \uparrow\uparrow\downarrow\uparrow\uparrow\uparrow\rangle$$

Magnetization : $M = 0.998$

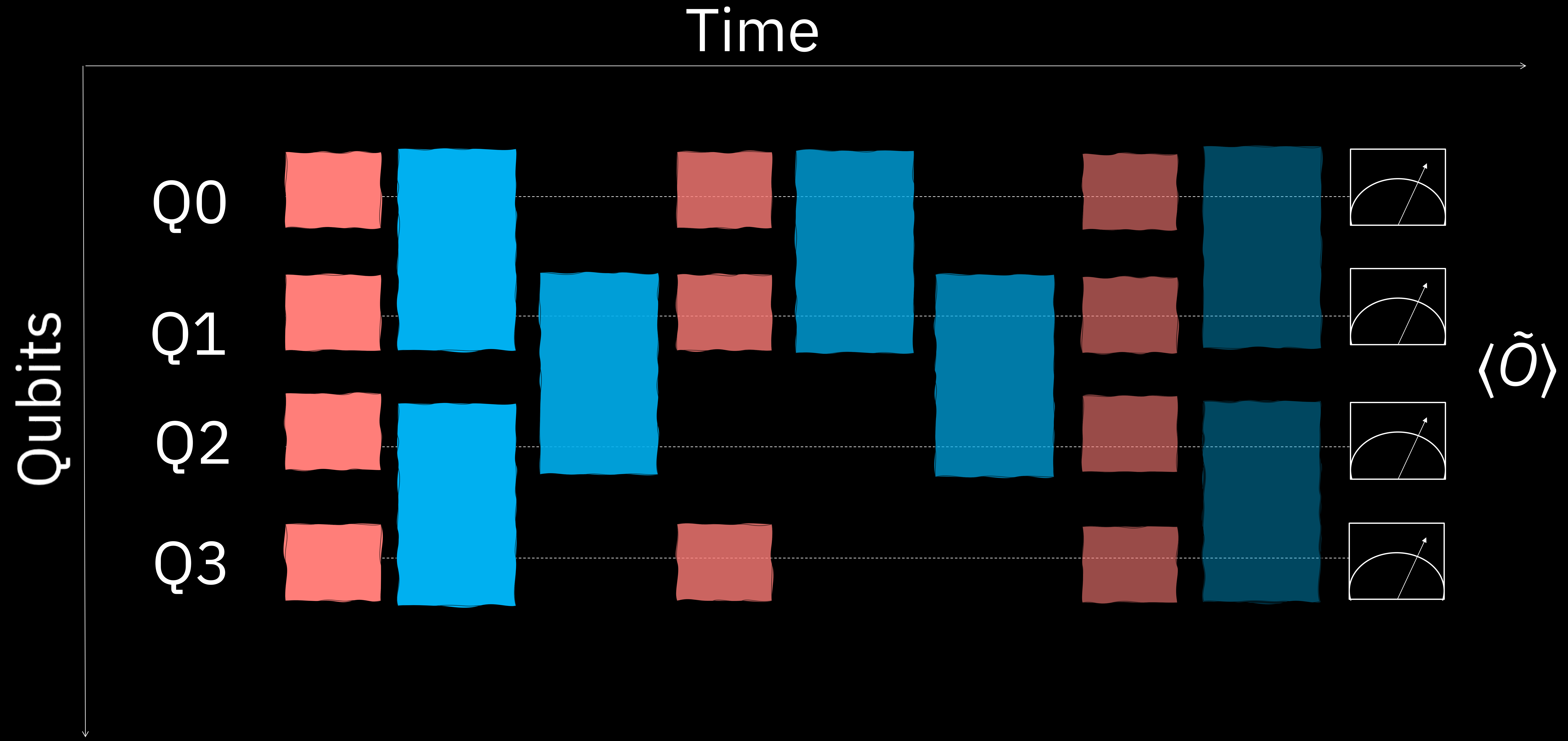
Fidelity : $F = 0$

Quantum circuits

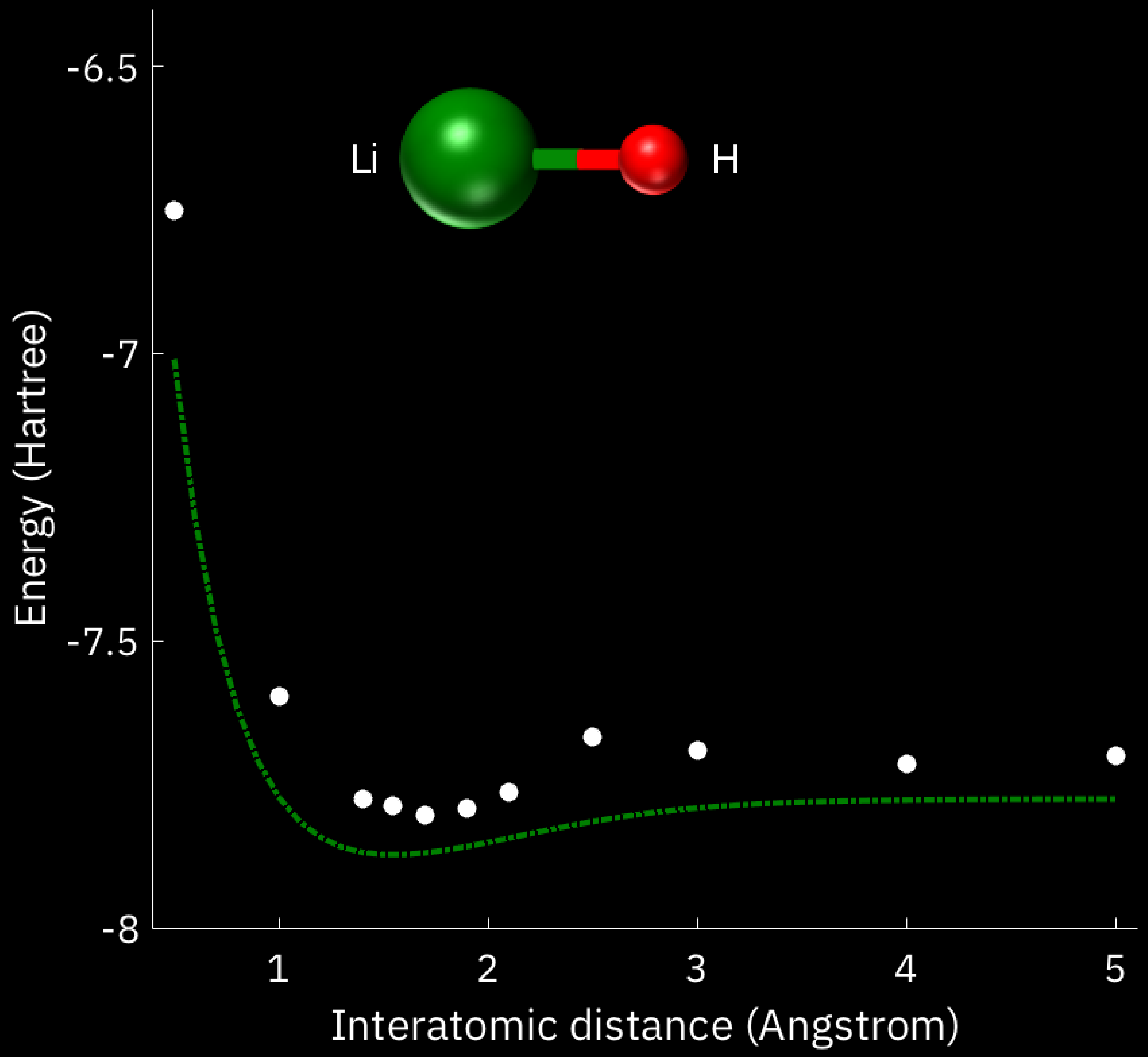


Short-depth Quantum circuits

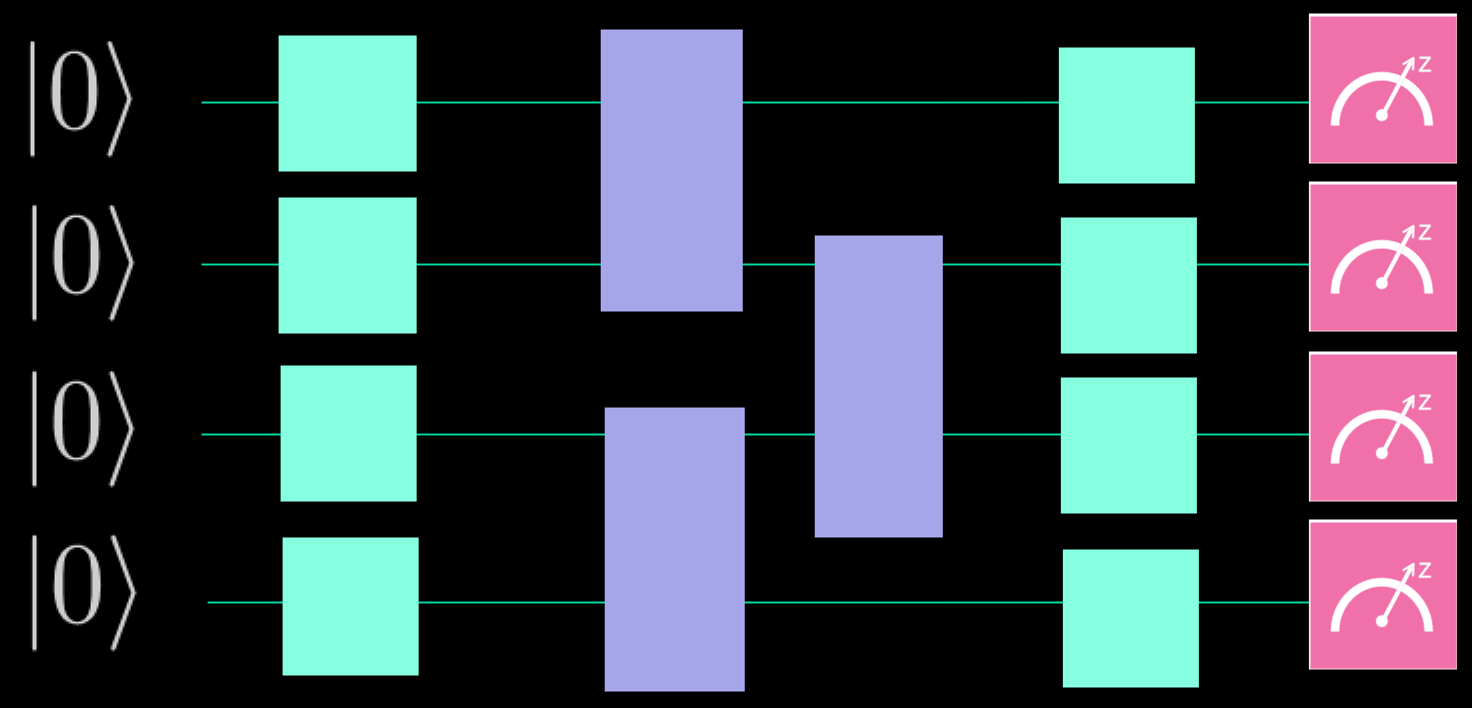
IBM **Quantum**



Molecular simulation with short depth circuits



2017: 4 qubits, Depth 2



Kandala et al, Nature **549**, 242-246 (2017)

PRL 119, 180509 (2017) PHYSICAL REVIEW LETTERS week ending 3 NOVEMBER 2017

Error Mitigation for Short-Depth Quantum Circuits

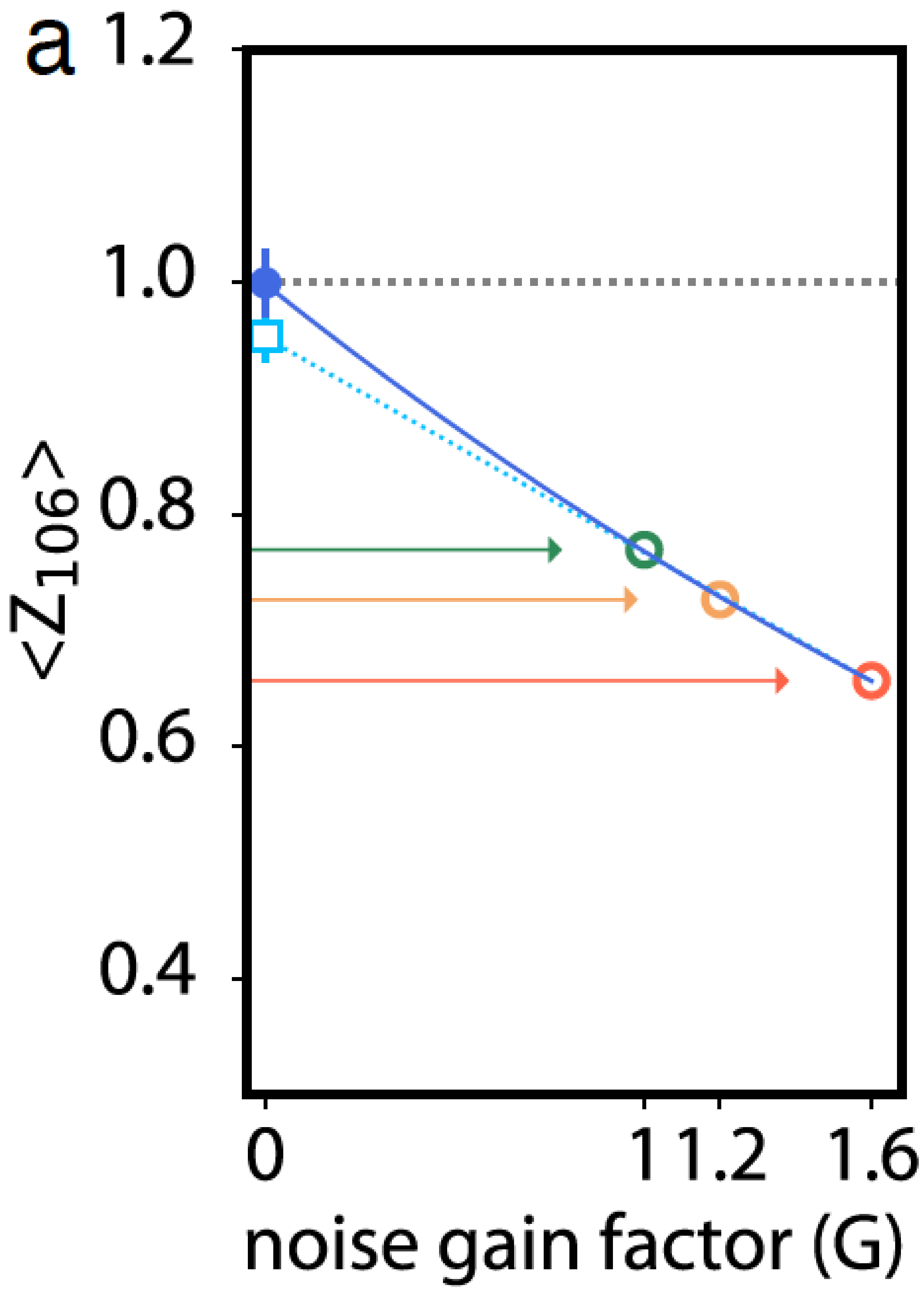
Kristan Temme, Sergey Bravyi, and Jay M. Gambetta
IBM T. J. Watson Research Center, Yorktown Heights, New York 10598, USA
(Received 21 July 2017; published 3 November 2017)

Two schemes are presented that mitigate the effect of errors and decoherence in short-depth quantum circuits. The size of the circuits for which these techniques can be applied is limited by the rate at which the errors in the computation are introduced. Near-term applications of early quantum devices, such as quantum simulations, rely on accurate estimates of expectation values to become relevant. Decoherence and gate errors lead to wrong estimates of the expectation values of observables used to evaluate the noisy circuit. The two schemes we discuss are deliberately simple and do not require additional qubit resources, so to be as practically relevant in current experiments as possible. The first method, extrapolation to the zero noise limit, subsequently cancels powers of the noise perturbations by an application of Richardson's deferred approach to the limit. The second method cancels errors by resampling randomized circuits according to a quasiprobability distribution.

Also: Li and Benjamin, Phys. Rev. X 7, 021050 (2017)

1. Characterize noise
2. Manipulate noise
3. Undo its effect

Undoing the effect of noise: Zero noise extrapolation

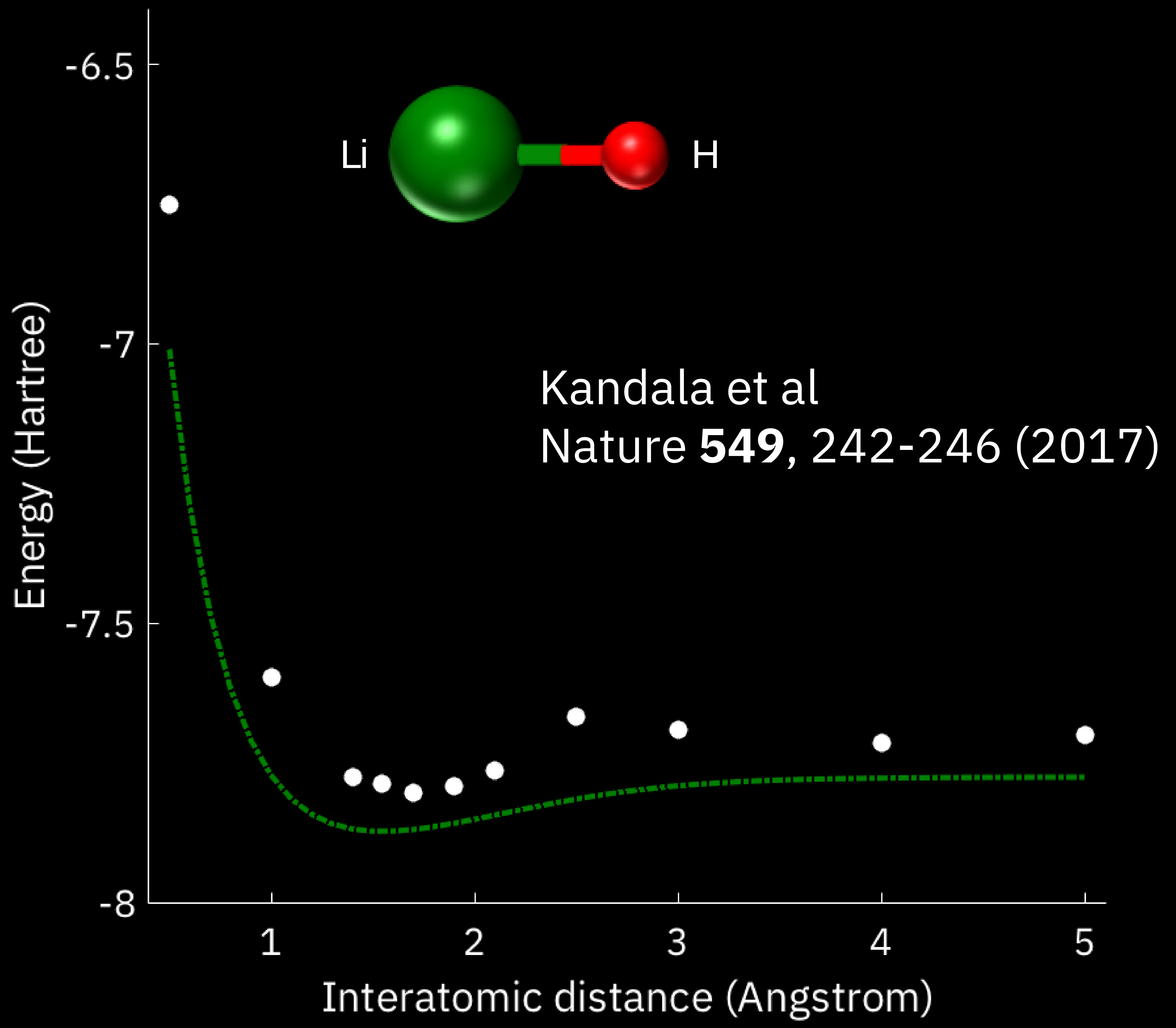


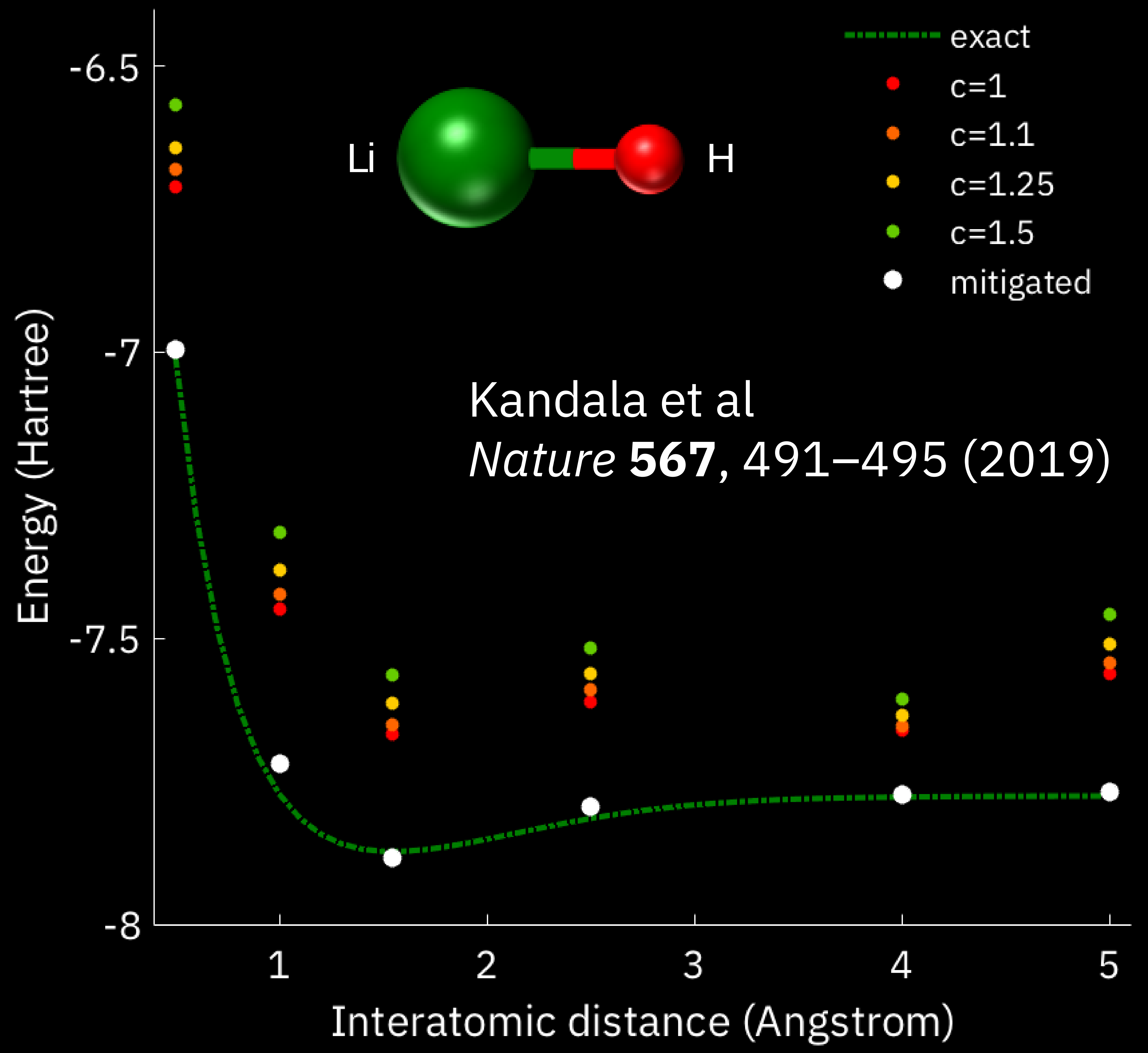
Exponential extrapolation:

1. Endo et al PRX 8, 031027 (2018).
2. Z. Cai, npj Quantum Information 7, 80 (2021)

IBM **Quantum**

Molecular simulation with short depth circuits



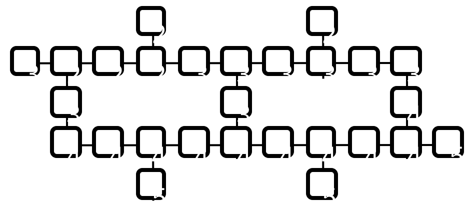


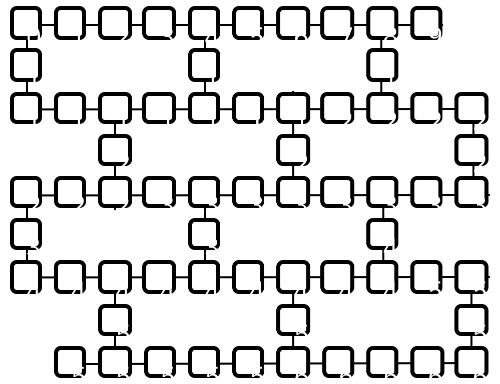
What criteria do we need to satisfy for a quantum computer to have utility?

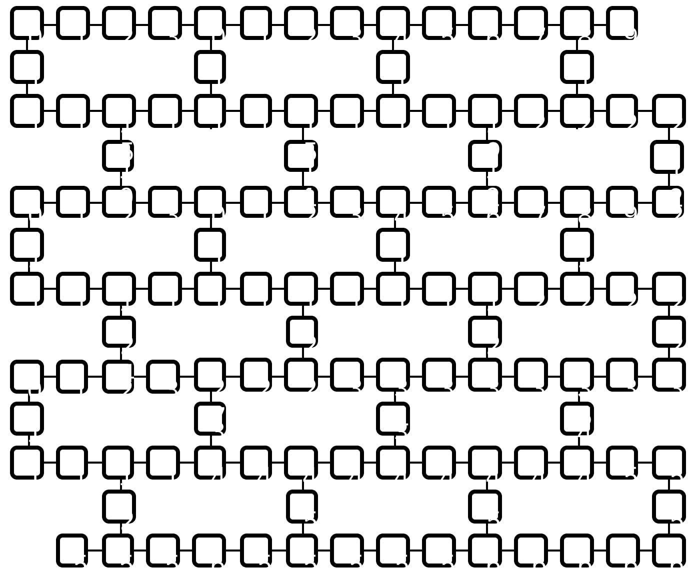
1. Need qubit counts at scales beyond brute-force classical simulation. Else, just use a classical computer.

2. Even at this scale, need the QC to produce trust-worthy solutions. Then we can begin to play the game that computational scientists have played for decades.

IBM quantum processors







2019
Falcon
27 Qubits
Flipchip

2020
Hummingbird
65 Qubits
Multiplexing

2021
Eagle
127 Qubits
TSV and MLW

2022
Osprey
433 Qubits
IO Scaling

2023
Condor
1121 Qubits
Yield

What criteria do we need to satisfy for a quantum computer to have utility?

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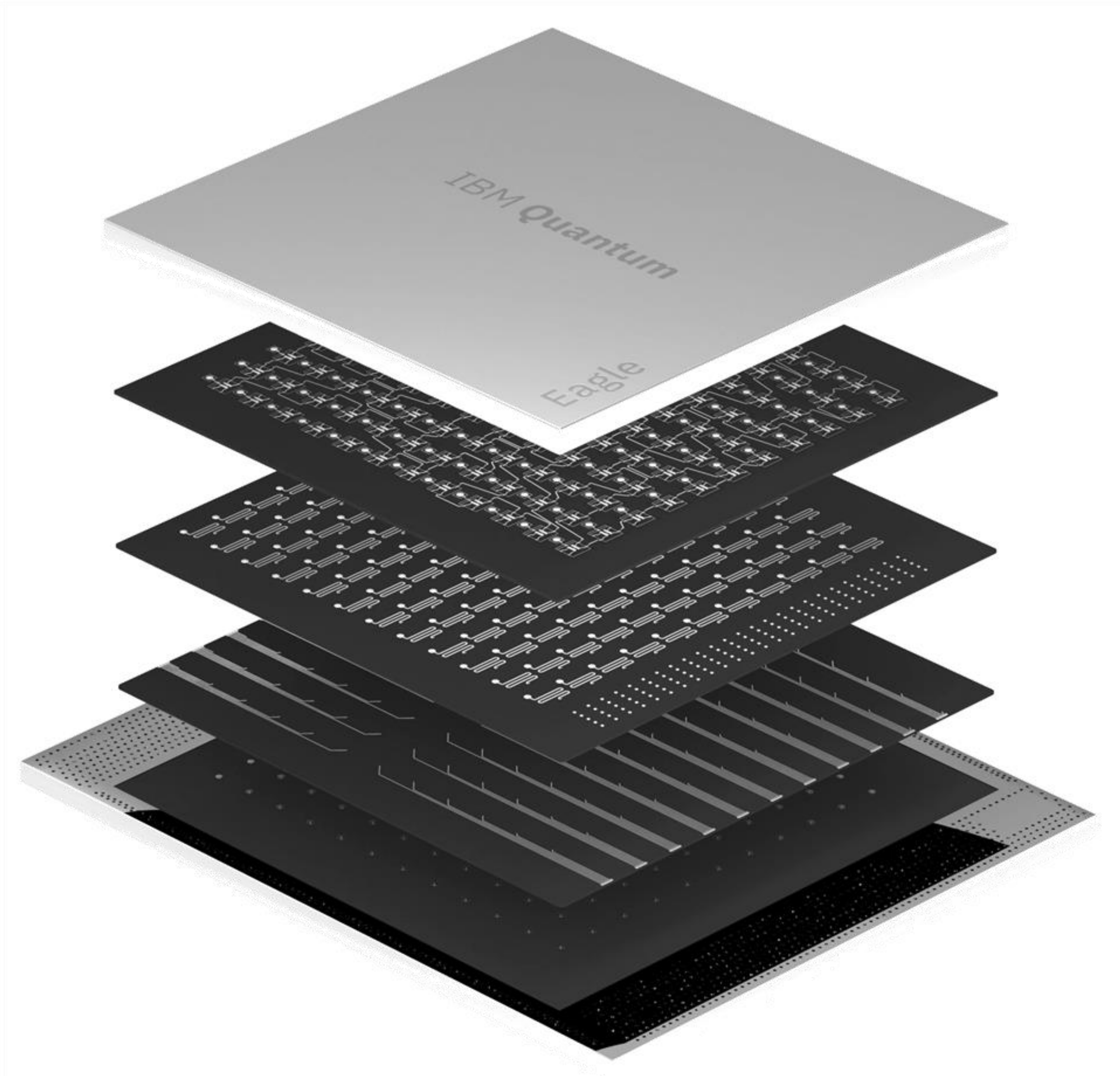
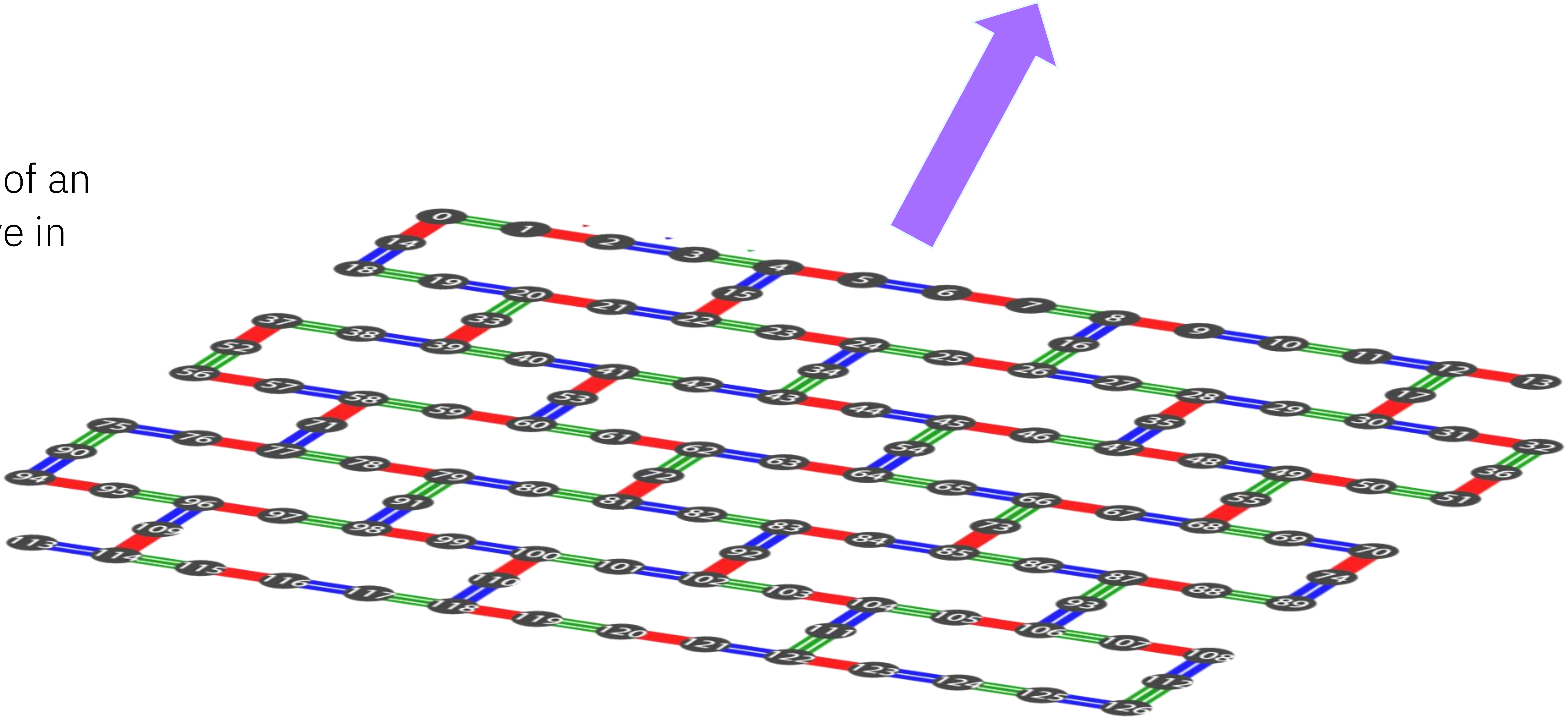
The “quantum utility” experiment



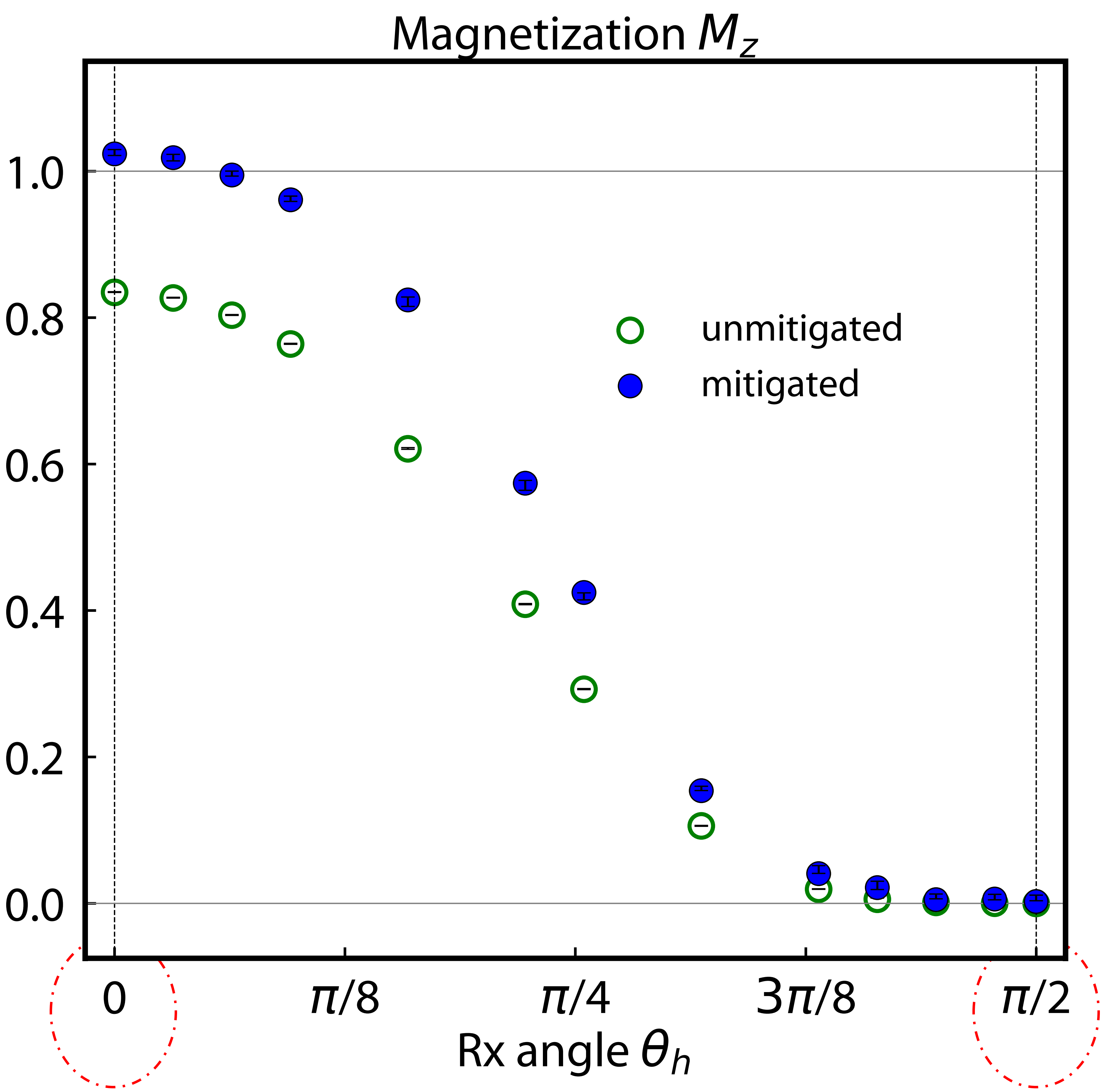
127 qubits

The “quantum utility” experiment

How does the magnetization of an interacting spin system evolve in the presence of an external magnetic field “kick”?



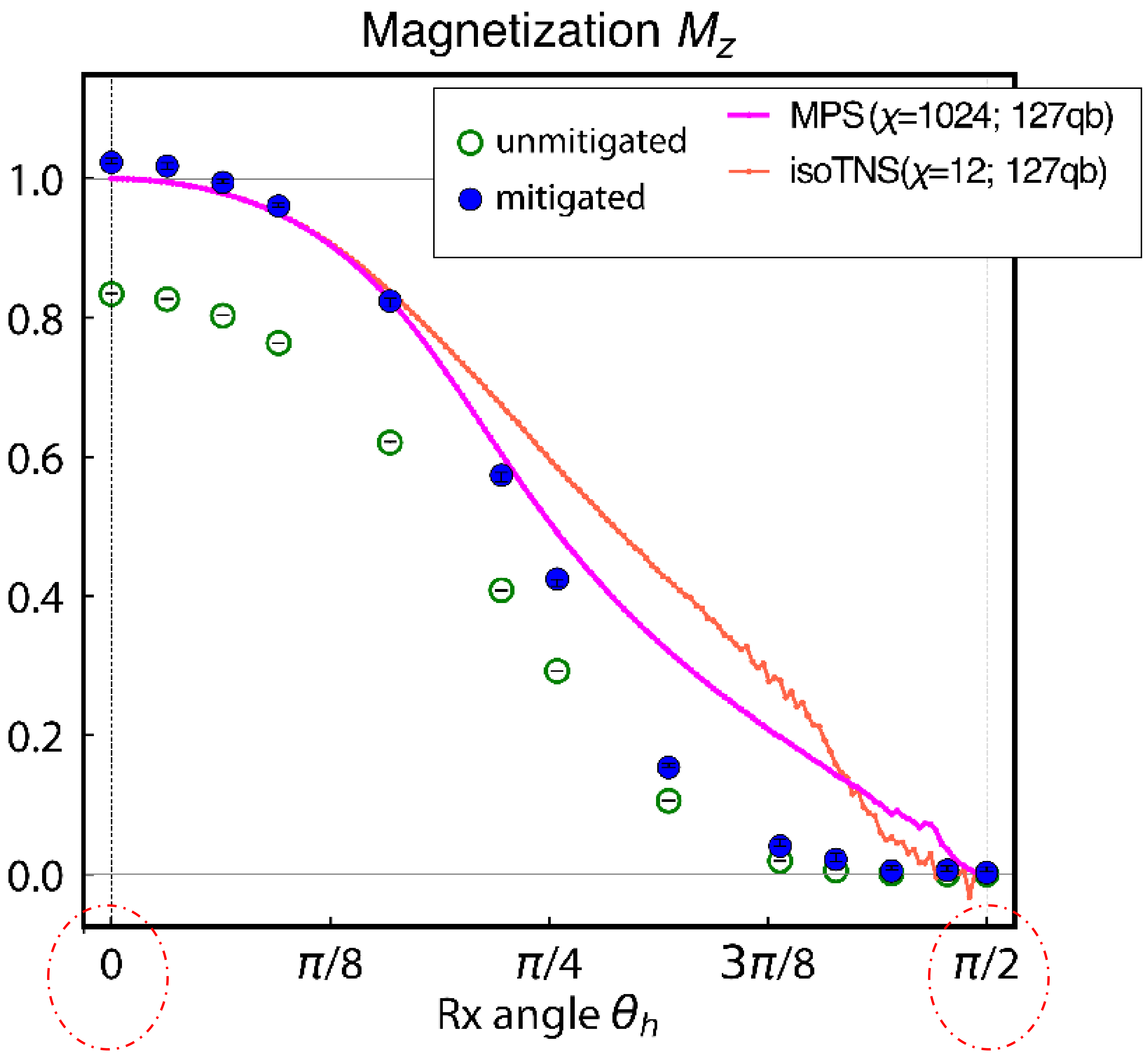
127 qubit x 15 entangling layers



Sajant Anand

Prof. Mike Zaletel

127 qubit x 15 entangling layers



Sajant Anand

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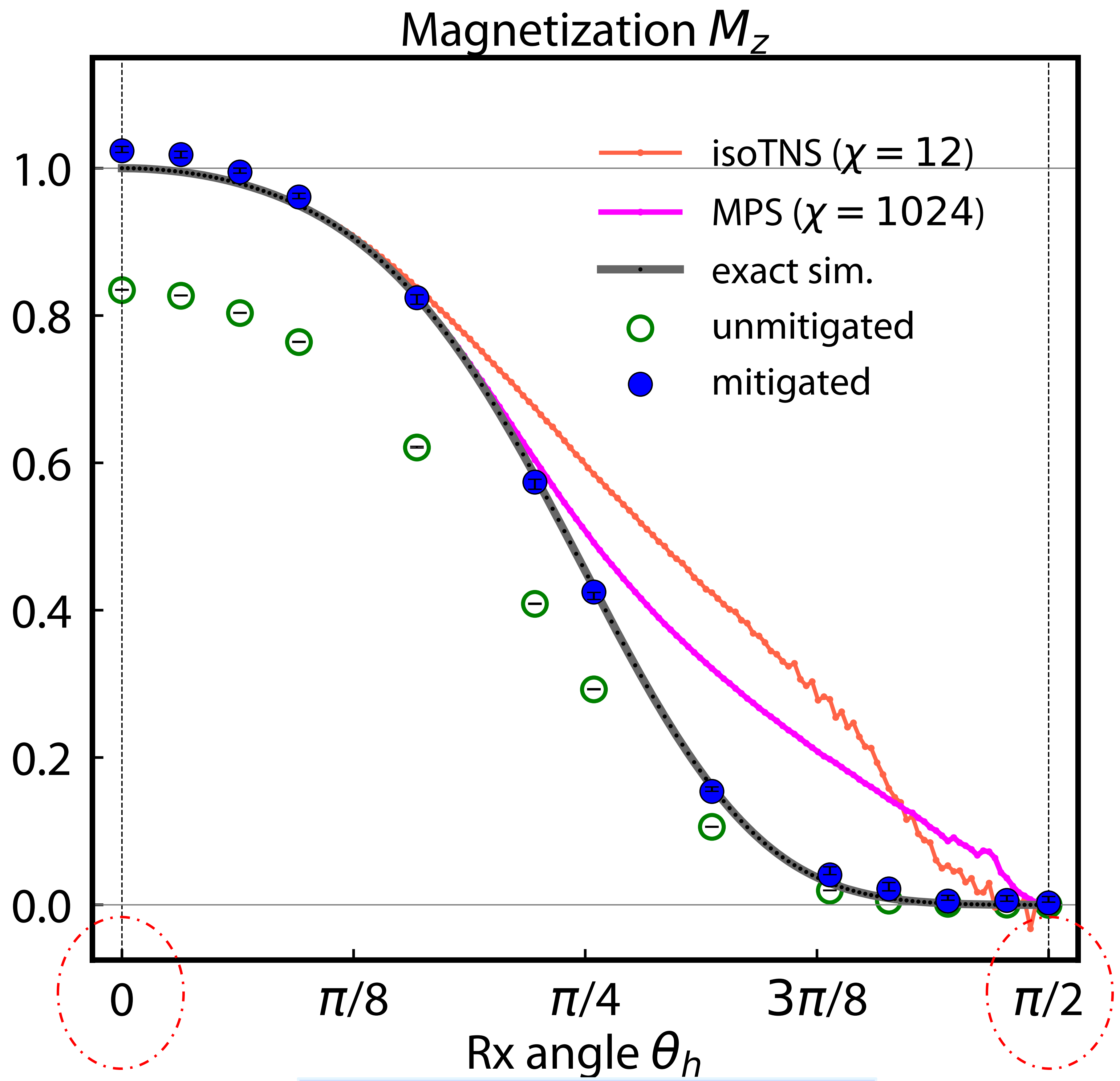
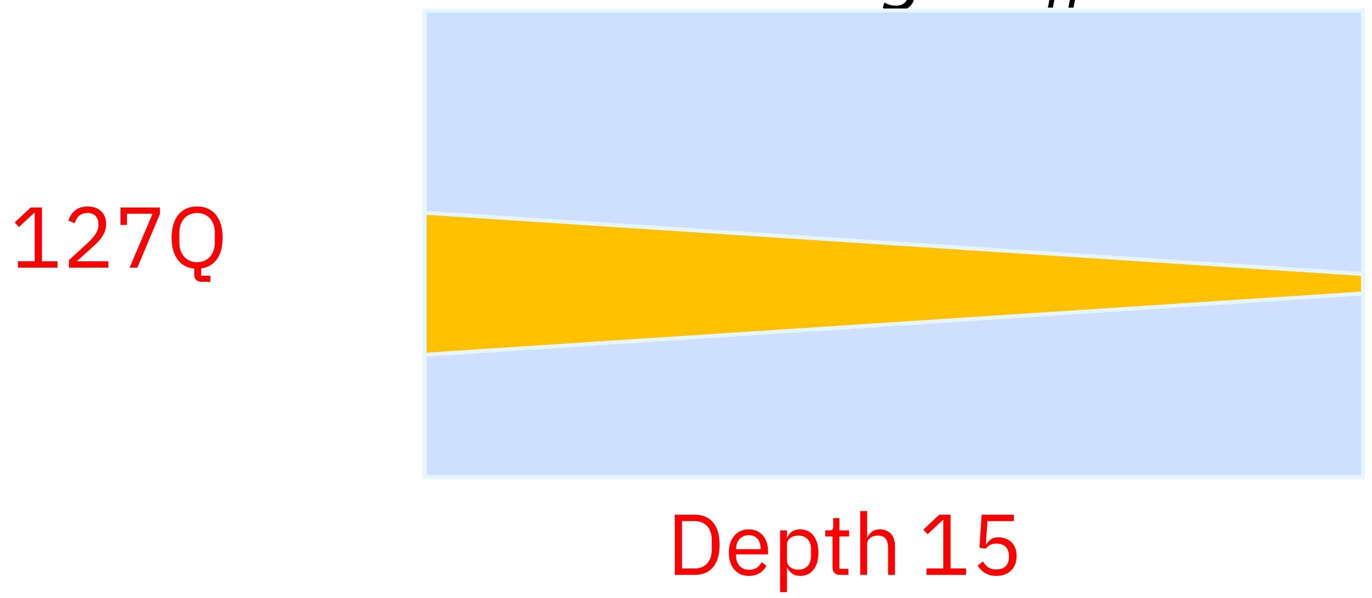
127 qubit x 15 entangling layers: Building trust





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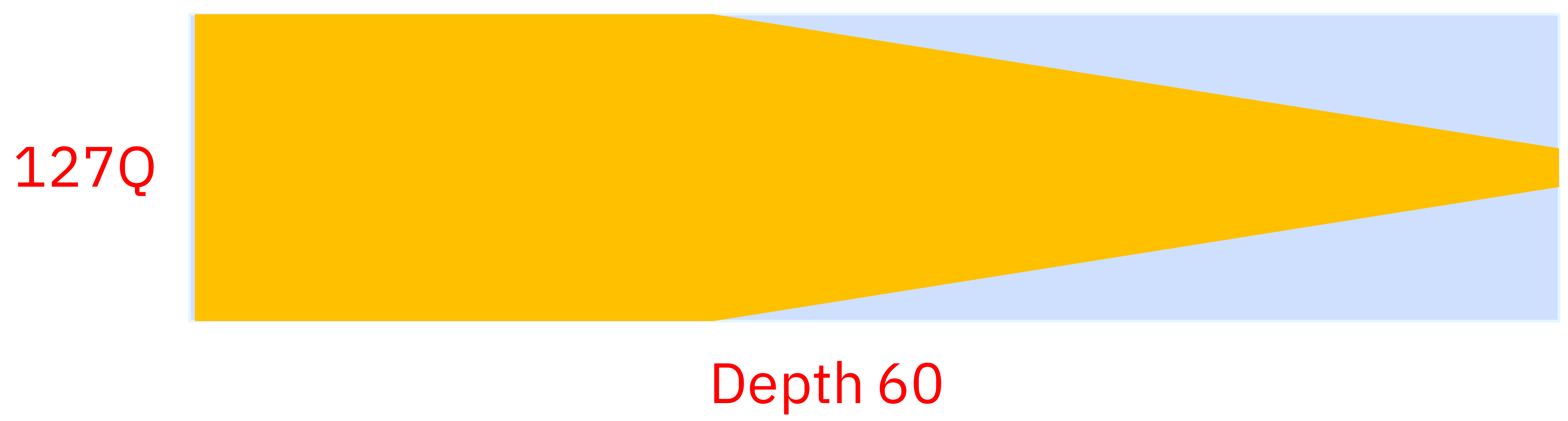
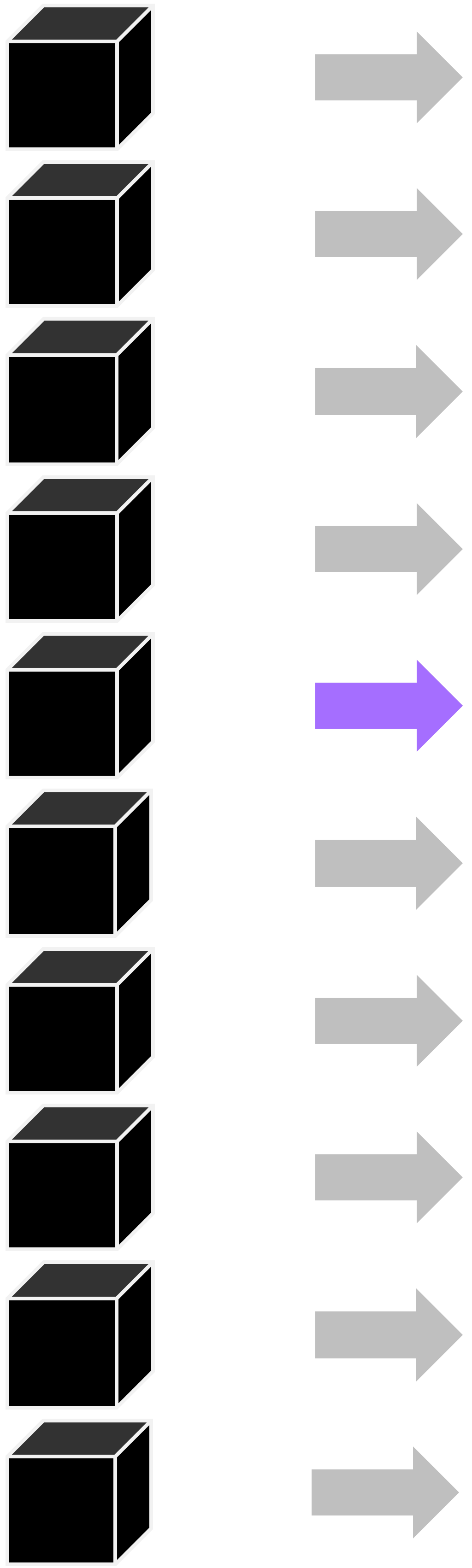
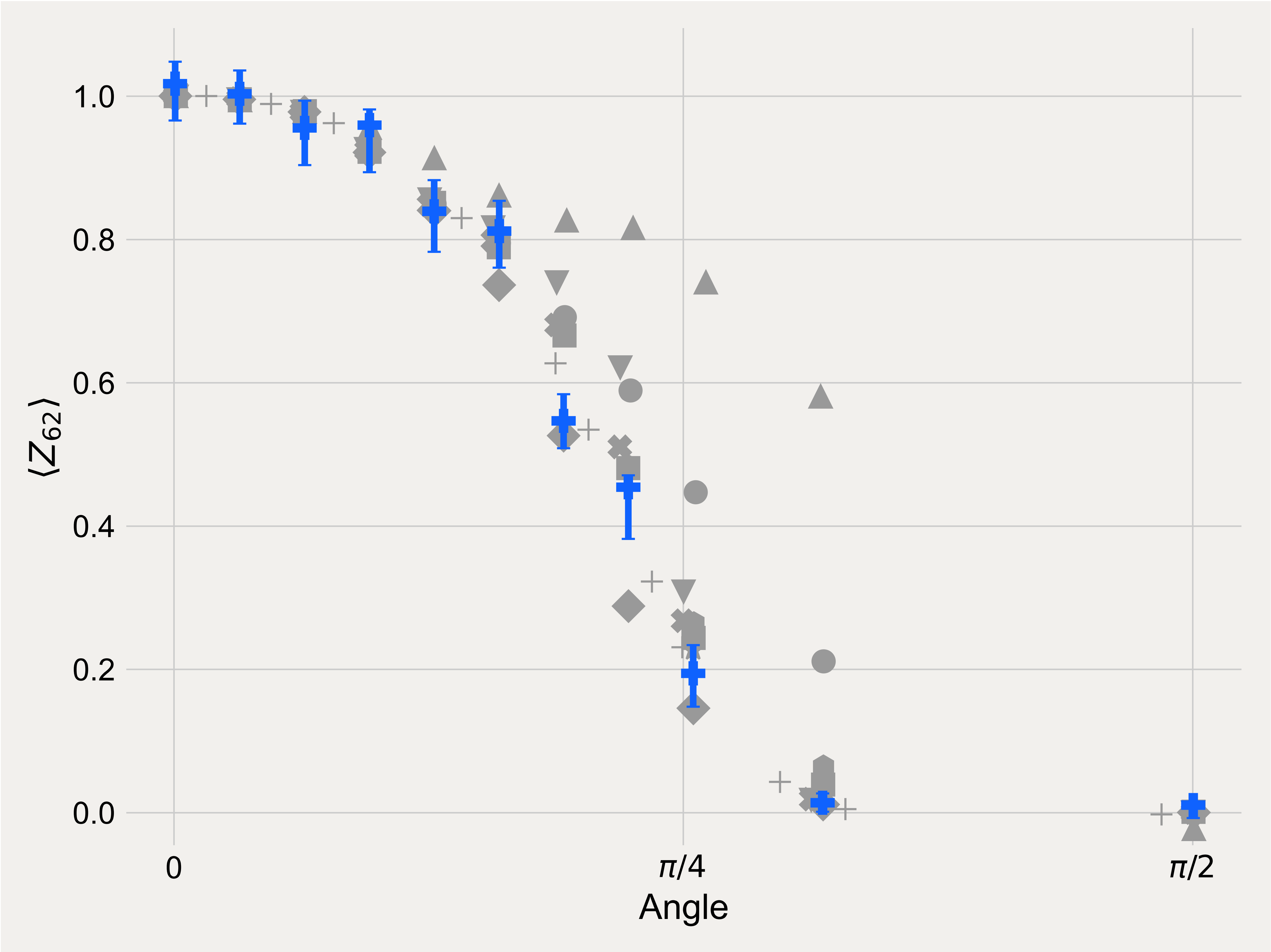
Beyond exact verification

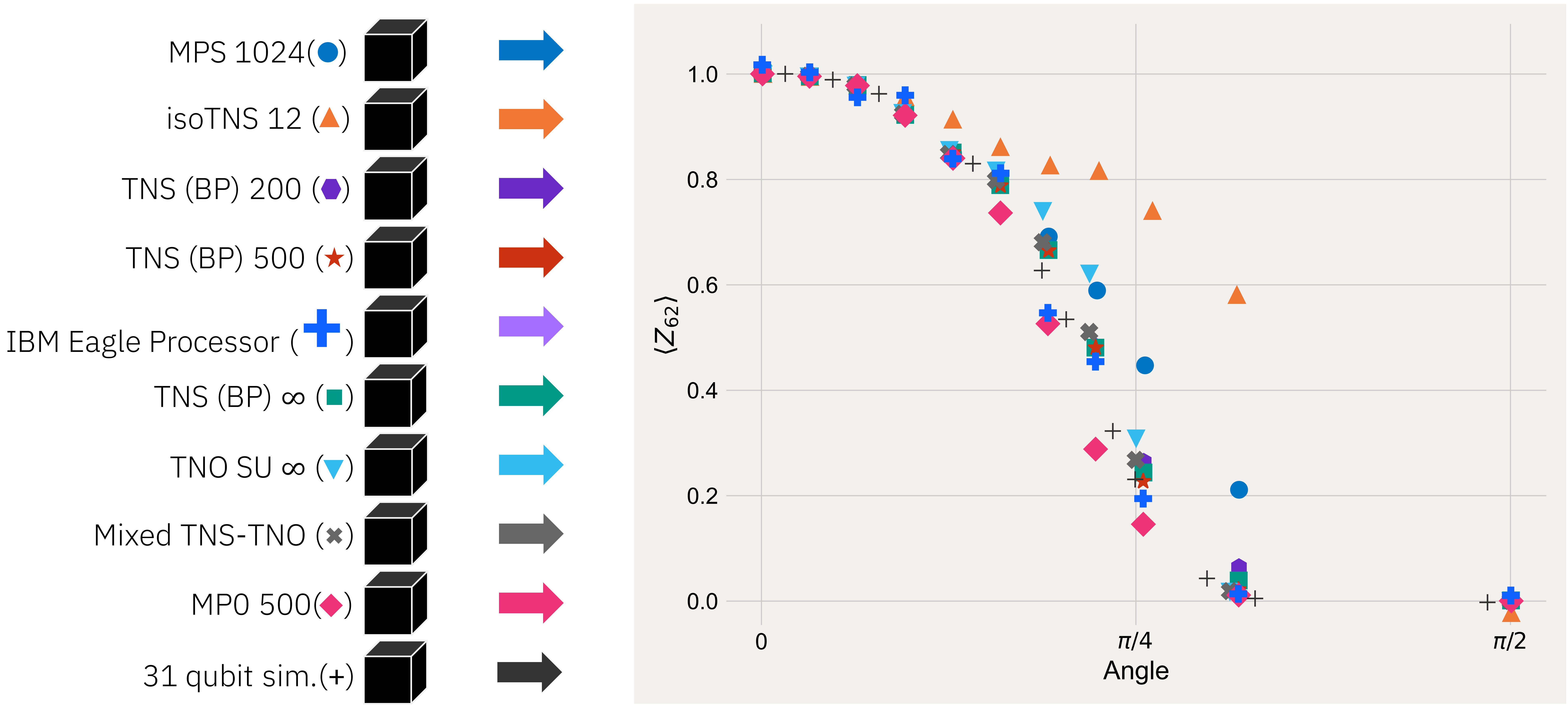


IBM Eagle Processor (✚)





Adapted from PRX Quantum **5**, 010308 (2024)



Adapted from PRX Quantum **5**, 010308 (2024)

Pre-fault tolerant quantum computers can already produce trust-worthy computations at scales that are beyond brute-force classical simulation.

Y. Kim, A. Eddins, et al, Nature. 618, 500–505 (2023)

Article

Evidence for the utility of quantum computing before fault tolerance

https://doi.org/10.1038/s41586-023-06096-3

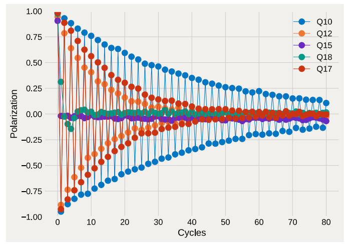
Received: 24 February 2023

Accepted: 18 April 2023

Youngseok Kim[1,6]✉, Andrew Eddins[2,6]✉, Sajant Anand[3], Ken Xuan Wei[1], Ewout van den Berg[1], Sami Rosenblatt[1], Hasan Nayfeh[1], Yantao Wu[3,4], Michael Zaletel[3,5], Kristan Temme[1] & Abhinav Kandala[1]✉

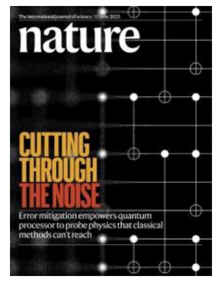
Post-utility

If you build it, they will come…



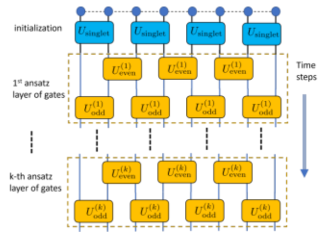
Characterizing quantum processors using discrete time crystals
arXiv:2301.07625
80 qubits / 7900 CX gates

simulation



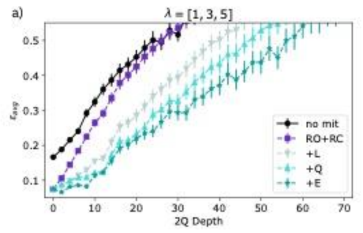
Evidence for the utility of quantum computing before fault tolerance
Nature, 618, 500 (2023)
127 qubits / 2880 CX gates

simulation



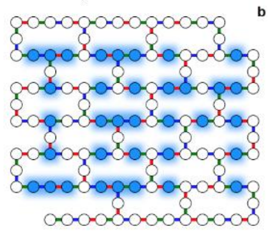
Simulating large-size quantum spin chains on cloud-based superconducting quantum computers
Phys. Rev. Research 5, 013183 (2023)
102 qubits / 3186 CX gates

simulation



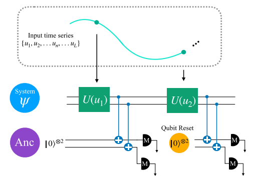
Best practices for quantum error mitigation with digital zero-noise extrapolation
arXiv:2307.05203
104 qubits / 3605 ECR gates

tools



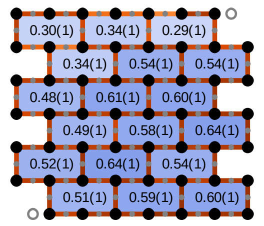
Uncovering Local Integrability in Quantum Many-Body Dynamics
arXiv:2307.07552
124 qubits / 2641 CX gates

simulation



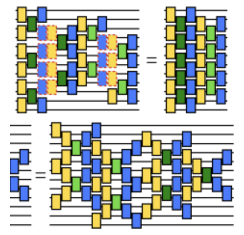
Quantum reservoir computing with repeated Measurements on superconducting devices
arXiv:2310.06706
120 qubits / 49470 gates + meas.

simulation



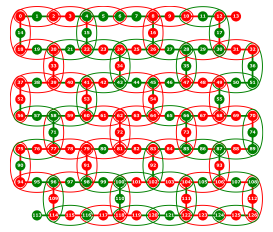
Realizing the Nishimori transition across the error threshold for constant-depth quantum circuits
arXiv:2309.02863
125 qubits / 429 gates + meas.

simulation



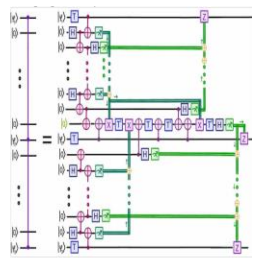
Scalable Circuits for Preparing Ground States on Digital Quantum Computers: The Schwinger Model Vacuum on 100 Qubits
PRX Quantum 5, 020315 (2024)
100 qubits / 788 CX gates

simulation



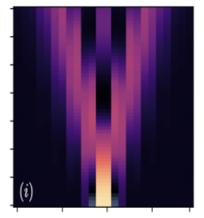
Scaling Whole-Chip QAOA for Higher-Order Ising Spin Glass Models on Heavy-Hex Graphs
arXiv:2312.00997
127 qubits / 420 CX gates

optimization



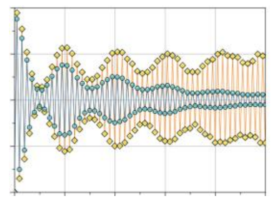
Efficient Long-Range Entanglement using Dynamic Circuits
arXiv:2308.13065
101 qubits / 504 gates + meas

tools



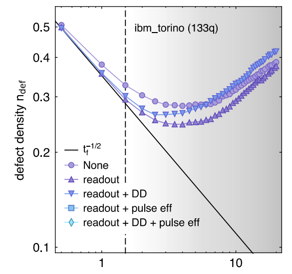
Quantum Simulations of Hadron Dynamics in the Schwinger Model using 112 Qubits
arXiv:2401.08044
112 qubits / 13,858 gates

simulation



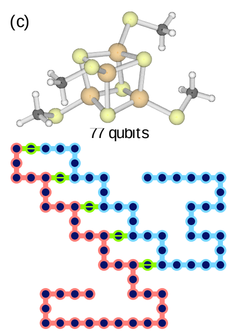
Unveiling clean two-dimensional discrete time quasicrystals on a digital quantum computer
arXiv:2403.16718
133 qubits / 15,000 CZ gates

simulation



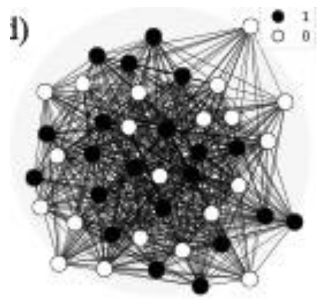
Benchmarking digital quantum simulations and optimization above hundreds of qubits using quantum critical dynamics
arXiv:2404.08053
133 qubits / 1440 CX gates

simulation



Chemistry Beyond Exact Solutions on a Quantum-Centric Supercomputer
arXiv:2405.05068
77 qubits / 3590 CZ gates

simulation



Towards a universal QAOA protocol: Evidence of quantum advantage in solving combinatorial optimization problems
arXiv:2405.09169
109 qubits / 21,200 gates

optimization

Post-utility

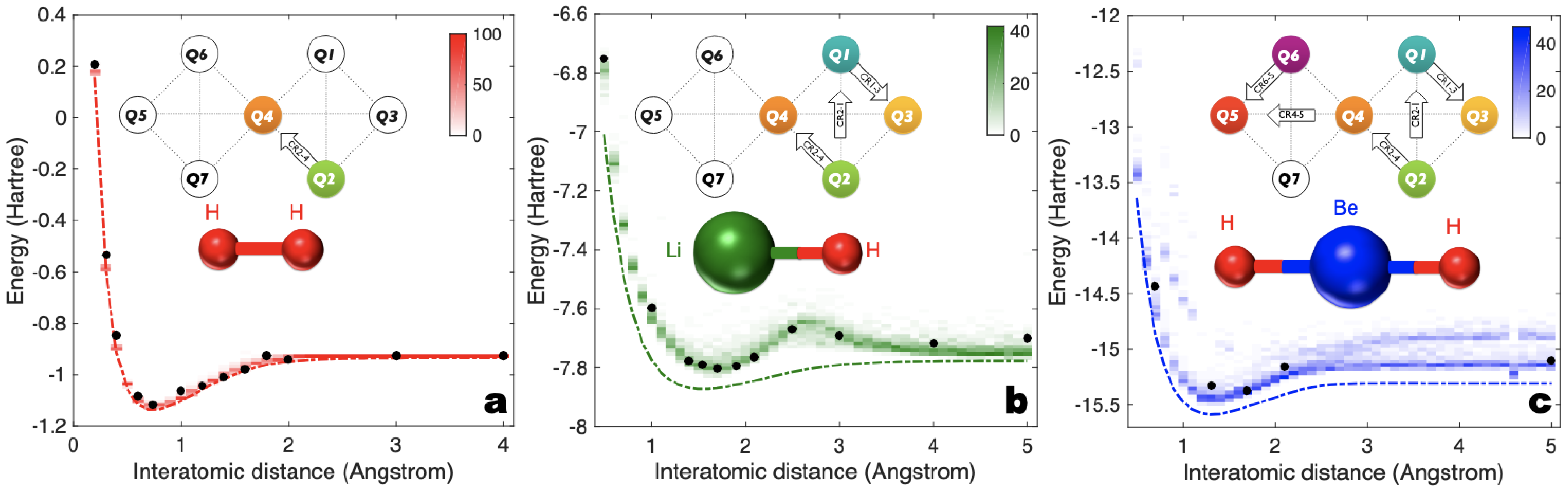
- Many more utility-scale demonstrations

- More reliable, faster software tools (75x speed-up in Utility expt.)

- Hardware improvements
  - Improved error rates (5x improvement in 2Q error rates)
  - Noise stabilization (arXiv:2407.02467)

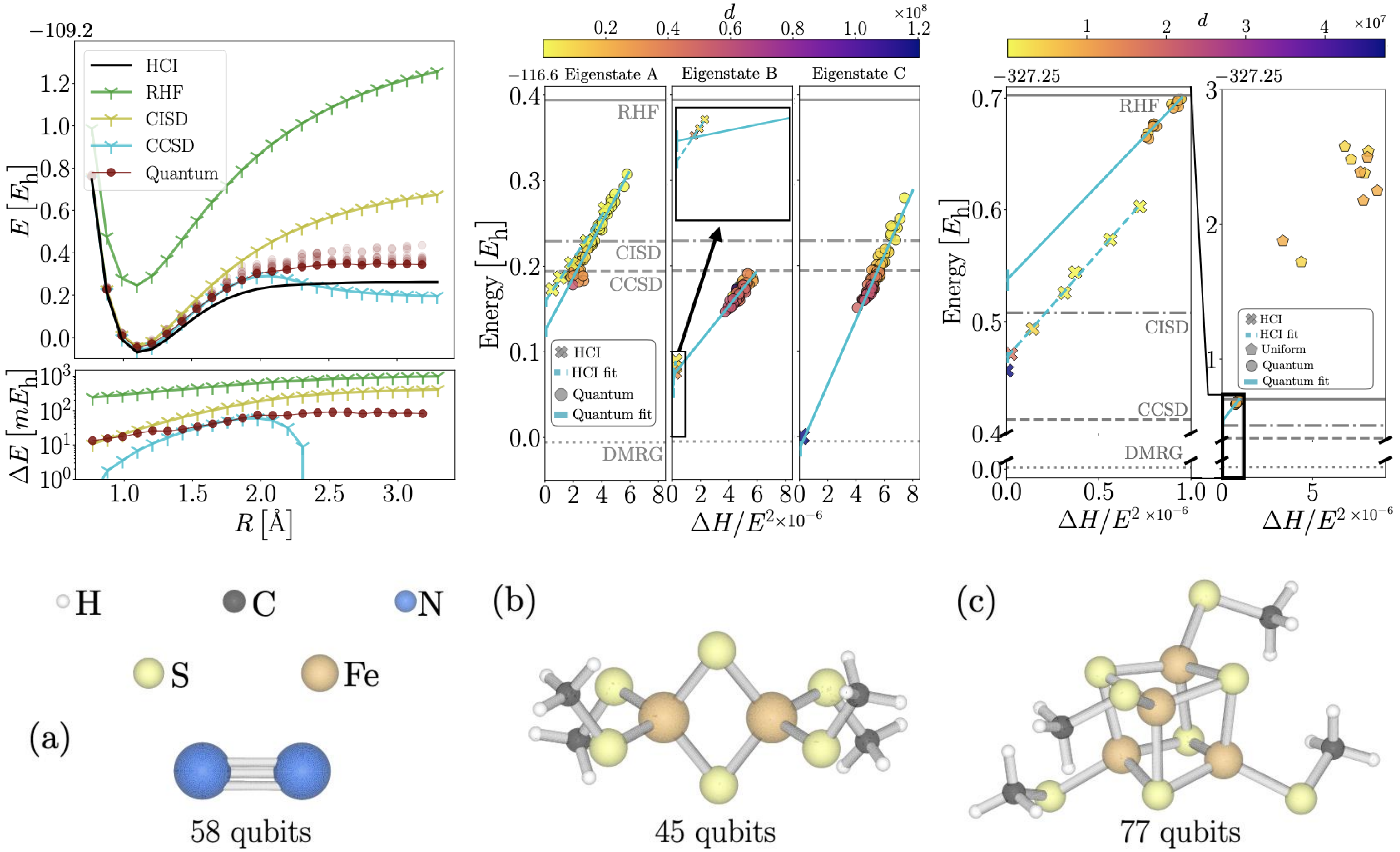
- Advances in error mitigation, error detection (2409.04401, 2411.00765, 2504.15725)

- Quantum + Classical (Quantum-centric supercomputing)
  - Novel algorithms (2405.05068, 2407.17405, 2502.01897)
  - Lower overhead error mitigation (2409.04401, 2411.00765)



Quantum chemistry on QC, 2017: 6 Qubits

Nature (2017)



Quantum chemistry on QC, 2024: 77 Qubits

arXiv:2405.05068

A new paradigm: Quantum + Classical HPC

Take home messages

- Noisy quantum computers today can perform accurate computations at non-trivial scales.

- Improvements in speed and quality of quantum systems, and integration with classical HPC will take us from utility to advantage