Present and future quantum computing algorithms

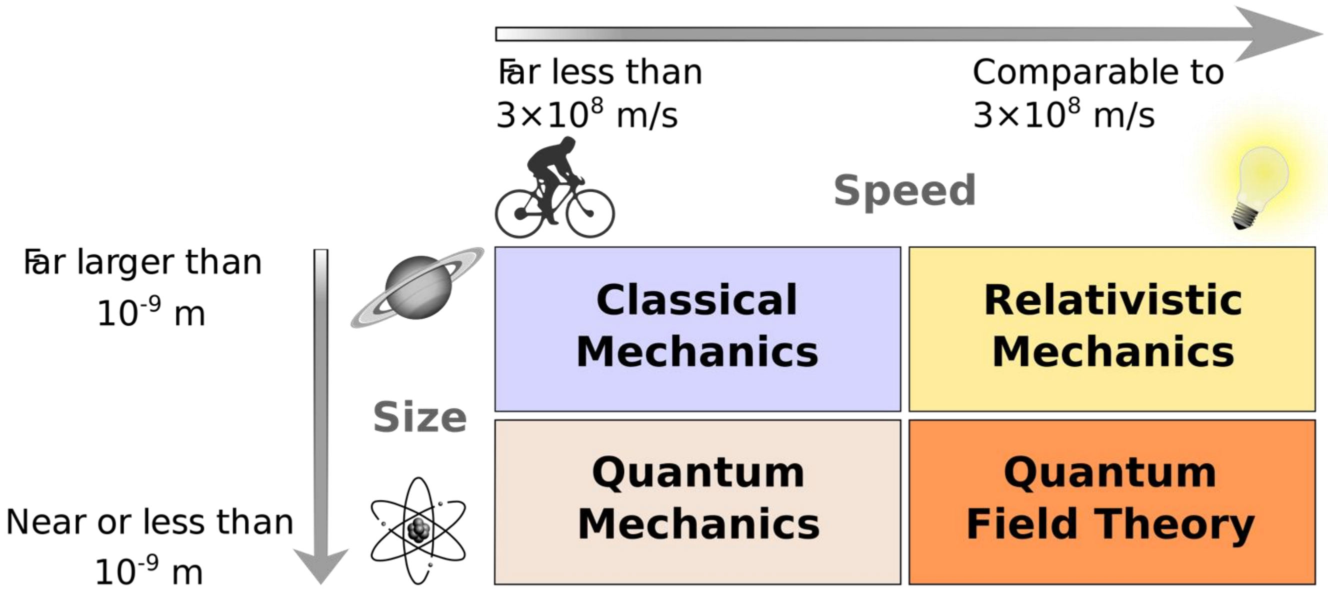
Prof. Dr. Mario Berta

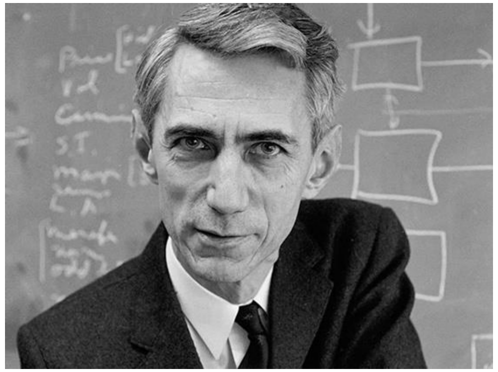
Guest Lecture
Quantum Computing for Engineering
December 18th, 2024

RWTH AACHEN UNIVERSITY

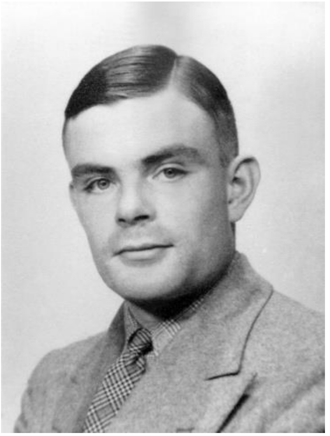
Information science

- Theory of information processing: Mathematical foundations in 1940s
- Abstract theory independent of implementation





Claude Shannon



Alan Turing

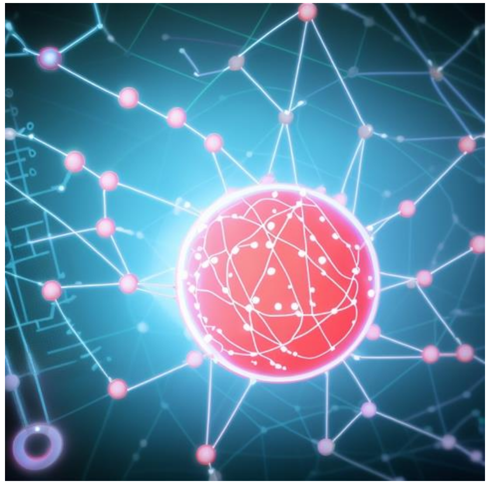
- Question: Also independent of underlying physics?

Quantum information science

- Notion of information for microscopical systems described by quantum mechanics? Quantum information $\neq$ classical information

- Bell’s theorem (1964): Quantum mechanics is incompatible with local hidden-variable theories

John Stewart Bell



- New research area based on quantum technologies: Computing, communication, cryptography, sensing, …

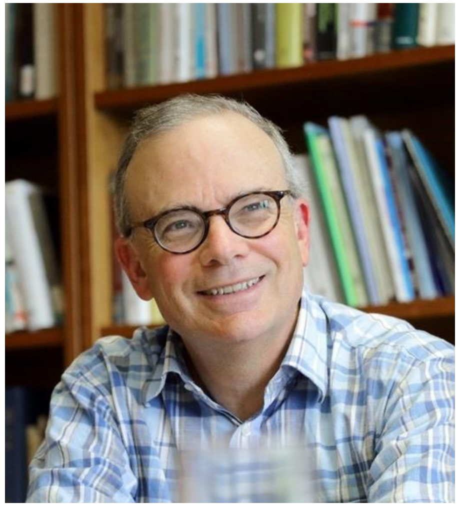
Institute for Quantum Information (IQI)

- In theoretical physics, located at Modulbau Physik II
- Permanent members:

Prof. Dr. Mario Berta

Prof. Dr. Fabian Hassler

Prof. Dr. Markus Müller



Prof. Dr. David DiVincenzo

- Currently around 35 additional members (postdocs, PhD students, MSc students, visitors) + further affiliations @Forschungszentrum Jülich

Group Berta

- Institute for Quantum Information (IQI)
- Theory of quantum information science
- Members:

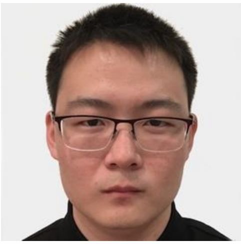

Mario Berta
Professor of Physics


Sreejith Sreekumar
Postdoc


Aditya Nema
Postdoc


Aadil Oufkir
Postdoc


Yongsheng Yao
Postdoc


Michael X. Cao
Postdoc

+ open PhD and postdoc positions, get in contact!


Tobias Rippchen
PhD student


Julius Zeiss
PhD student


Gereon Koßmann
PhD student


Nikolaos Louloudis
PhD student


Richard Meister
Postdoc (Imperial)

+ 5x Master students RWTH Physics / Computer Science

JARA INSTITUTE QUANTUM INFORMATION

AN INITIATIVE OF

RWTH AACHEN UNIVERSITY

JÜLICH Forschungszentrum

Theory of quantum information science

- Our focus areas:
  1. Mathematical foundations of quantum information
  2. Quantum algorithm development
- Cluster of Excellence: Matter and Light for Quantum Computing (ML4Q)
- Visiting Reader at Department of Computing Imperial College London
- Industry ties with Amazon Web Services Center for Quantum Computing

ML4Q MATTER AND LIGHT FOR QUANTUM COMPUTING

erc European Research Council

Imperial College London

EPSRC

aws

Today: Quantum algorithms

PART I: Overview

Origins of quantum computing

- Understanding physics with computers (1981):

"trying to find a computer simulation of physics seems to me to be an excellent program to follow out (...) nature is not classical, dammit, and if you want to make a simulation of nature, you will better make it quantum mechanical, and by golly it is a wonderful problem, because it does not look so easy"


Richard Feynman


Peter Shor

- First query complexity separation results in 1990s
- Breakthrough prime factorization (1994):

n-bit integer factorization in quantum complexity $O(n^2 \log n)$

versus classical complexity $O\left(\exp\left(1.9 \cdot n^{1/3} (\log n)^{2/3}\right)\right)$

Quantum algorithms research

- Steady progress on quantum algorithm development since 1990s, recent flurry of activities and results

QUANTUM FLAGSHIP

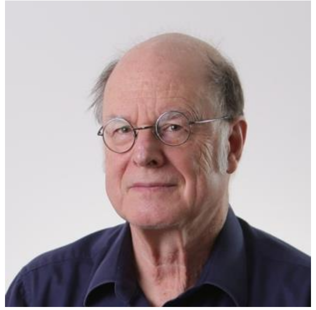
NATIONAL QUANTUM COORDINATION OFFICE

⟨quantum|gov⟩

UK NATIONAL QUANTUM TECHNOLOGIES PROGRAMME

- Breakthrough prize in physics 2023:

  “foundational work in the field of quantum information”


Charles H. Bennett


Gilles Brassard


David Deutsch


Peter Shor

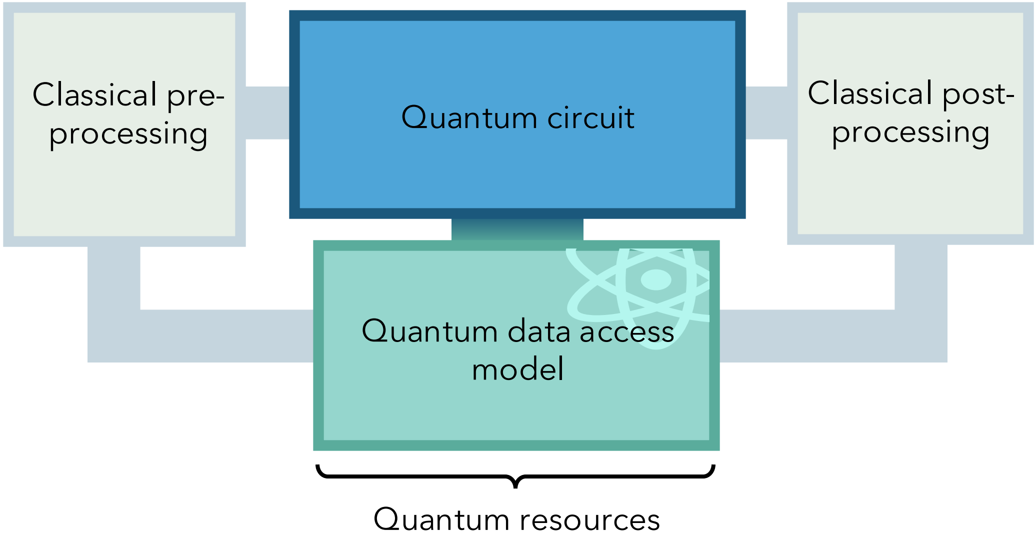
- Ultimate goal: Quantify classical-quantum complexity boundary

Classical versus quantum technologies

- *Do algorithms based on quantum components, including*
  - *quantum processing units (QPU)*
  - *quantum random access memory (QRAM)*

provide computational advantages compared to classical components?

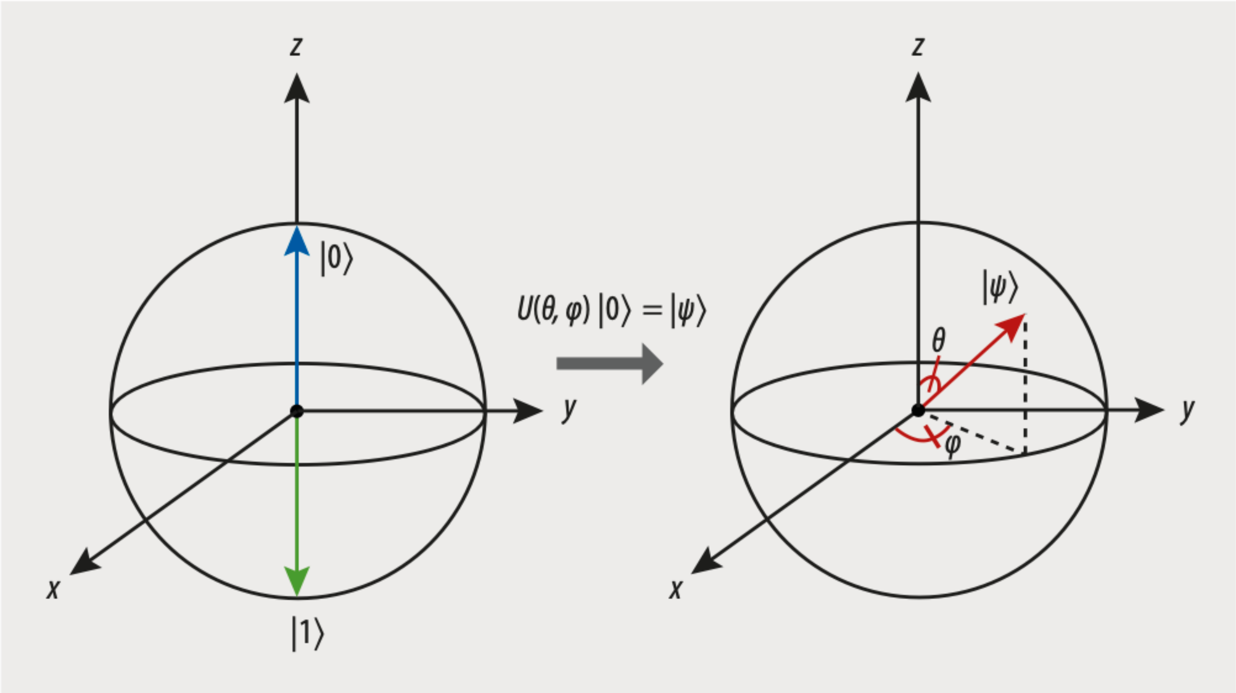
- Goal is to identify use cases / areas of applications with
  - large (super-quadratic) quantum speed-up
  - minimal quantum footprint, i.e., use classical routines whenever possible



Basics: Quantum Circuit Model

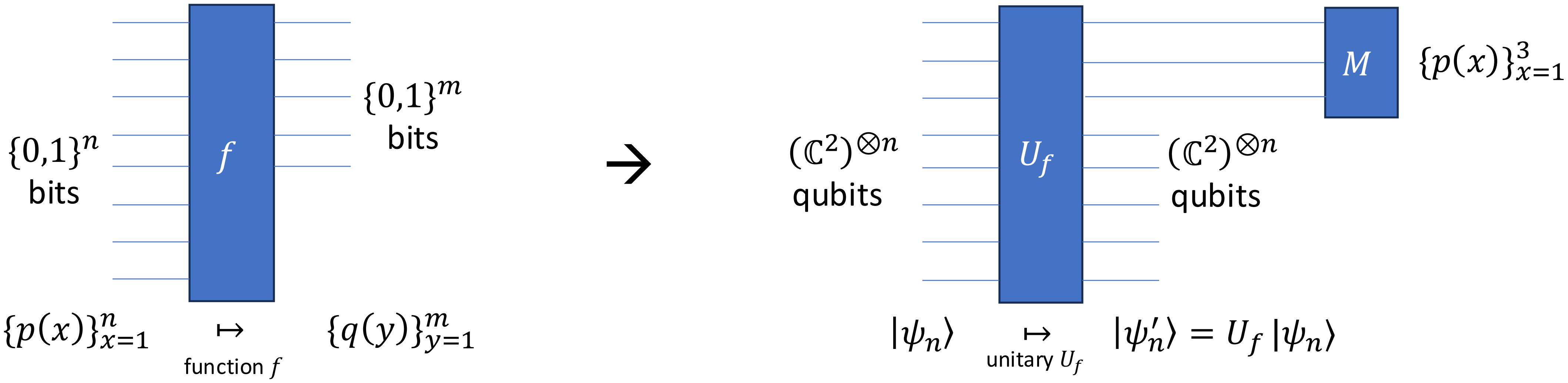
Classical vs quantum model of computation

- What can be realized within abstract model of quantum mechanics?
- Bloch sphere representation of a two-level system – aka quantum bit – aka qubit:



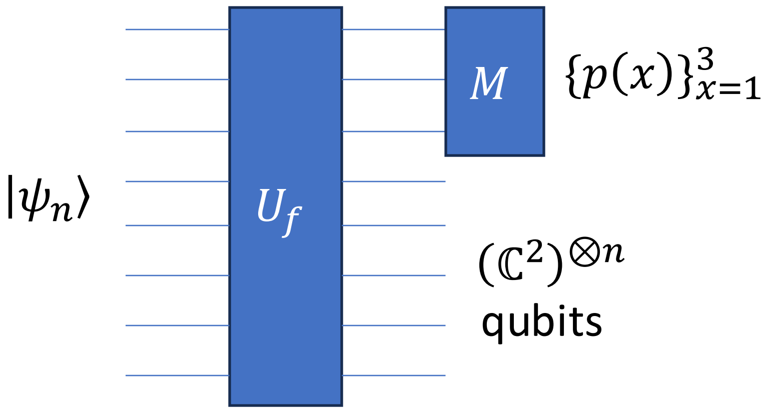
Classical vs quantum model of computation

- What can be realized within abstract model of quantum mechanics?
- Classical versus quantum circuit model:



- Schrödinger time evolution operator $U_f = e^{-iH_f t}$ + measurements

Quantum circuit model



- Where does quantum speed-up come from?

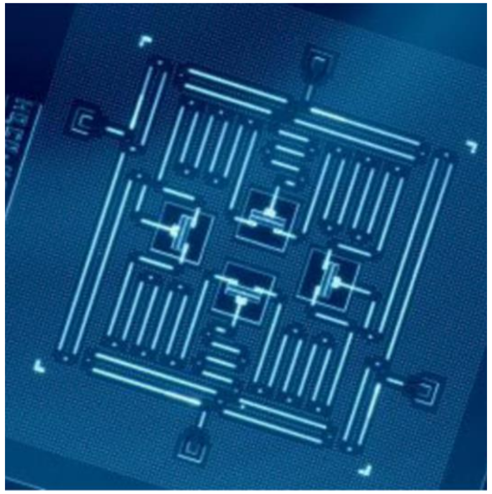
  → precise mathematical reason: complex numbers allow for constructive interference

- Decomposition into set of elementary quantum gates, e.g., single qubit Pauli X, Y, Z and T gates, and two qubit $CNOT$ gate
- Quantum complexity $=$ minimal number of elementary quantum gates
- More precise metric: Quantum depth of non-Clifford gates (i.e., T gates)

Quantum hardware

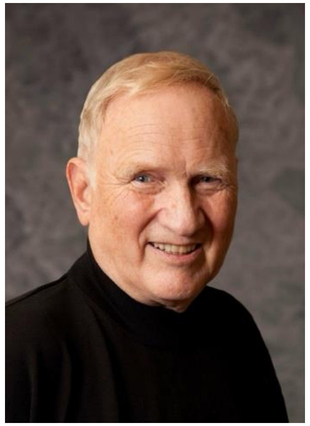
Quantum hardware

- Different technologies: Superconductors, ion traps, neutral atoms, photonics, etc.
- Groundbreaking physics experiments with 6 orders of magnitude improvements in 30 years+



4 IBM superconducting qubits

Alain Aspect



John Clauser

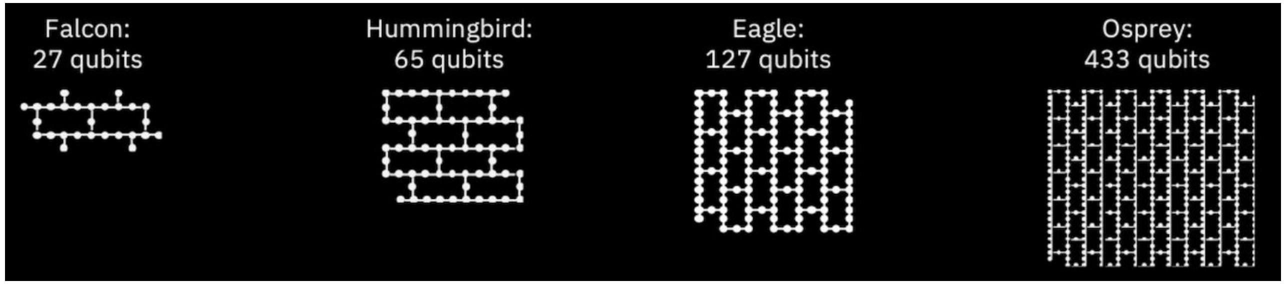
Anton Zeillinger

- Nobel prize in physics 2022:

  “experiments with entangled photons, establishing the violation of Bell inequalities and pioneering quantum information science”

Current quantum technologies

- Led by quantum industry (hundreds of billion dollars scale), e.g., IBM Quantum (up to 433 qubits) or Google Quantum AI (105 qubits)



IBM Quantum Processing Units

- Severe restrictions: Qubit count, connectivity, one qubit Pauli gates, two qubit CNOT gates, read-out measurement errors, clock speed, etc.
- Quantum error correction:

Quantum Computing Inches Closer to Reality After Another Google Breakthrough

The New York Times

Article | Published: 09 December 2024

Quantum error correction below the surface code threshold

Google Quantum AI and Collaborators

Nature (2024) | Cite this article

Quantum algorithm design

Regimes for quantum algorithm design

- Nascent state of quantum technologies gives noisy and intermediate scale quantum (NISQ) computing, i.e.,
  - Quantum annealers
  - Analogue simulators, not universal, not fully programmable
  - NISQ digital quantum circuits, inbuilt noise resilience, error mitigation, severe scaling limitations, etc.
- Versus what one really wants long-term:

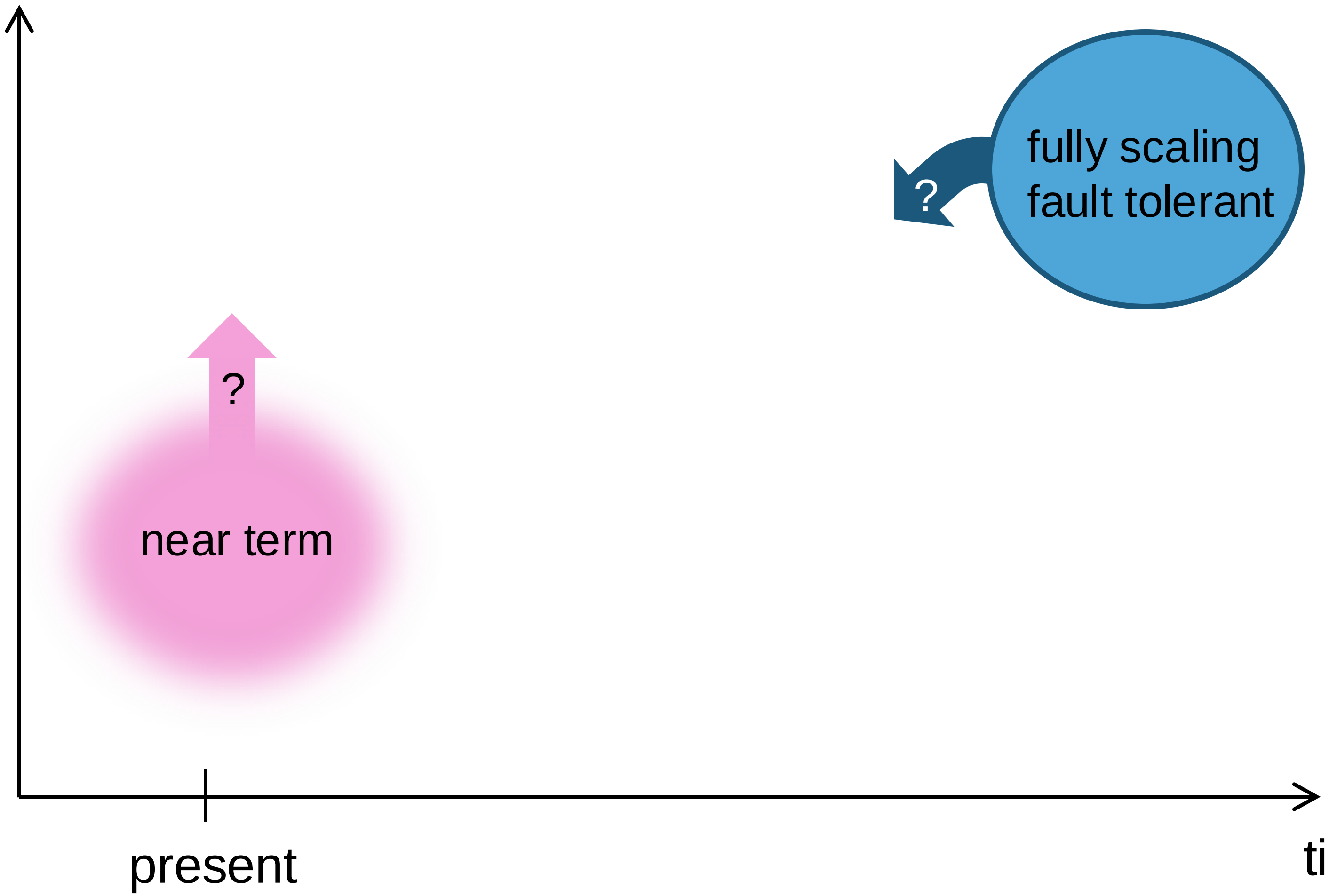
Quantum error-corrected and scaling quantum computer

(roughly two orders of magnitude away)

- Intermediate regimes of interest?

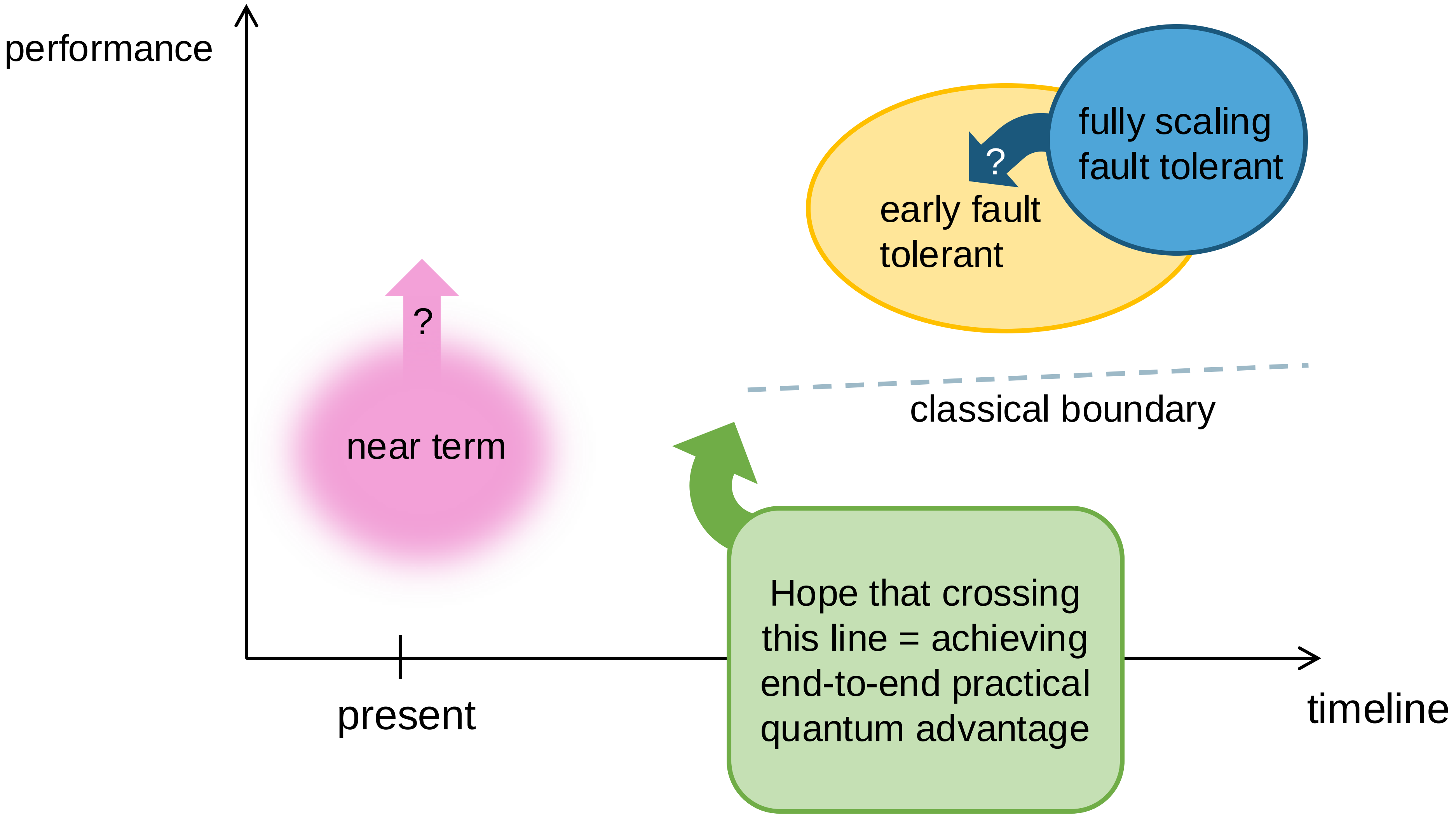
Early fault-tolerant regime

- Run many small circuits
- Leverage some classical power
- Usually no runtime/success guarantees



- Large hardware requirements
- Specified in terms of query complexity
- Runtime guarantees
- Caveats can cloud convincing practical advantage

Early fault-tolerant regime

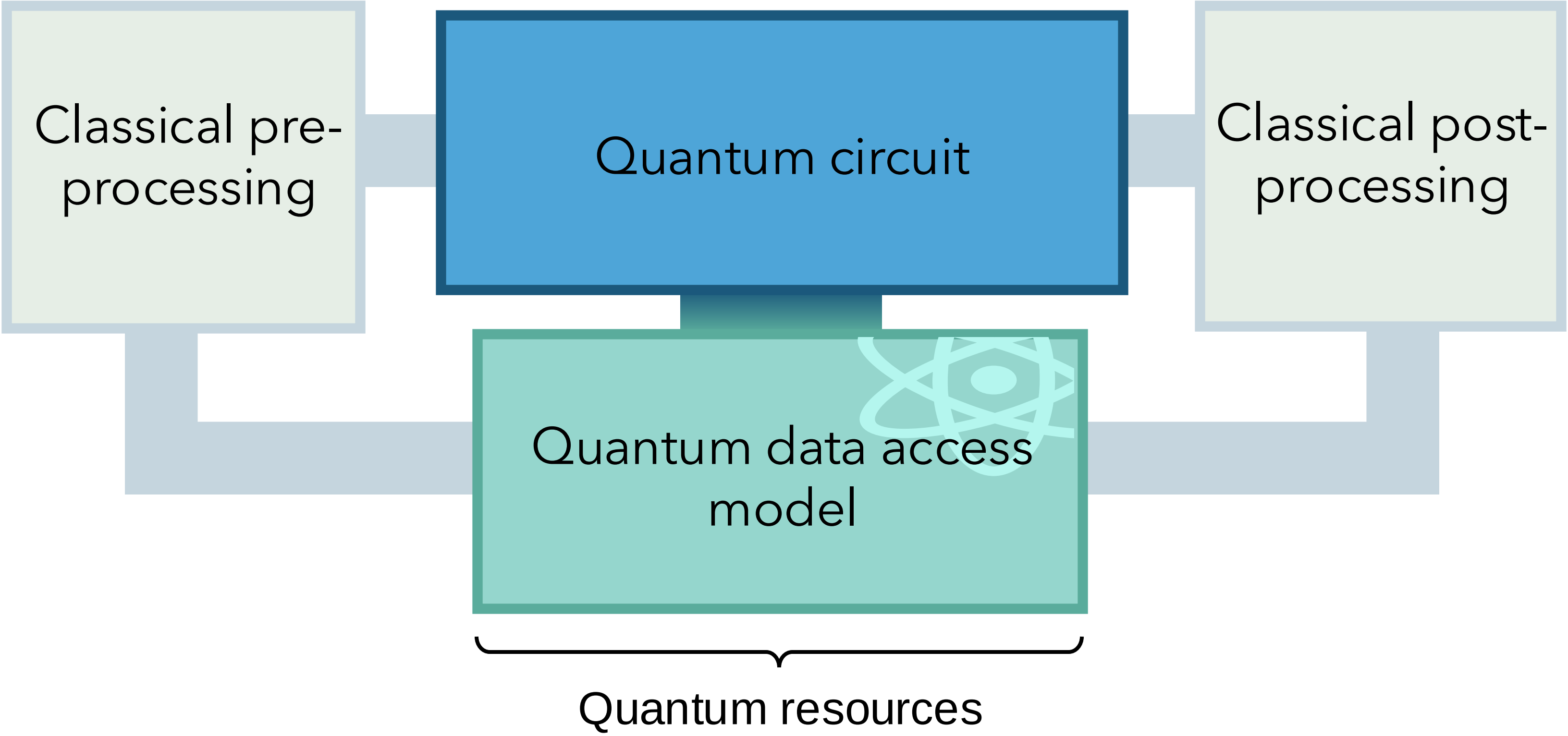


Early fault-tolerance characteristics

- Limited number of logical qubits, with limited quantum clock speed from error correction overhead
- Price of resources from most expensive to cheap:
  1. Number of qubits
  2. Depth of quantum circuits
  3. Sample complexity
  4. Classical pre- and post-processing
- Goal is flexible trade-off between different resources
- Stay with provable worst-case guarantees + add strong heuristic about average case performances

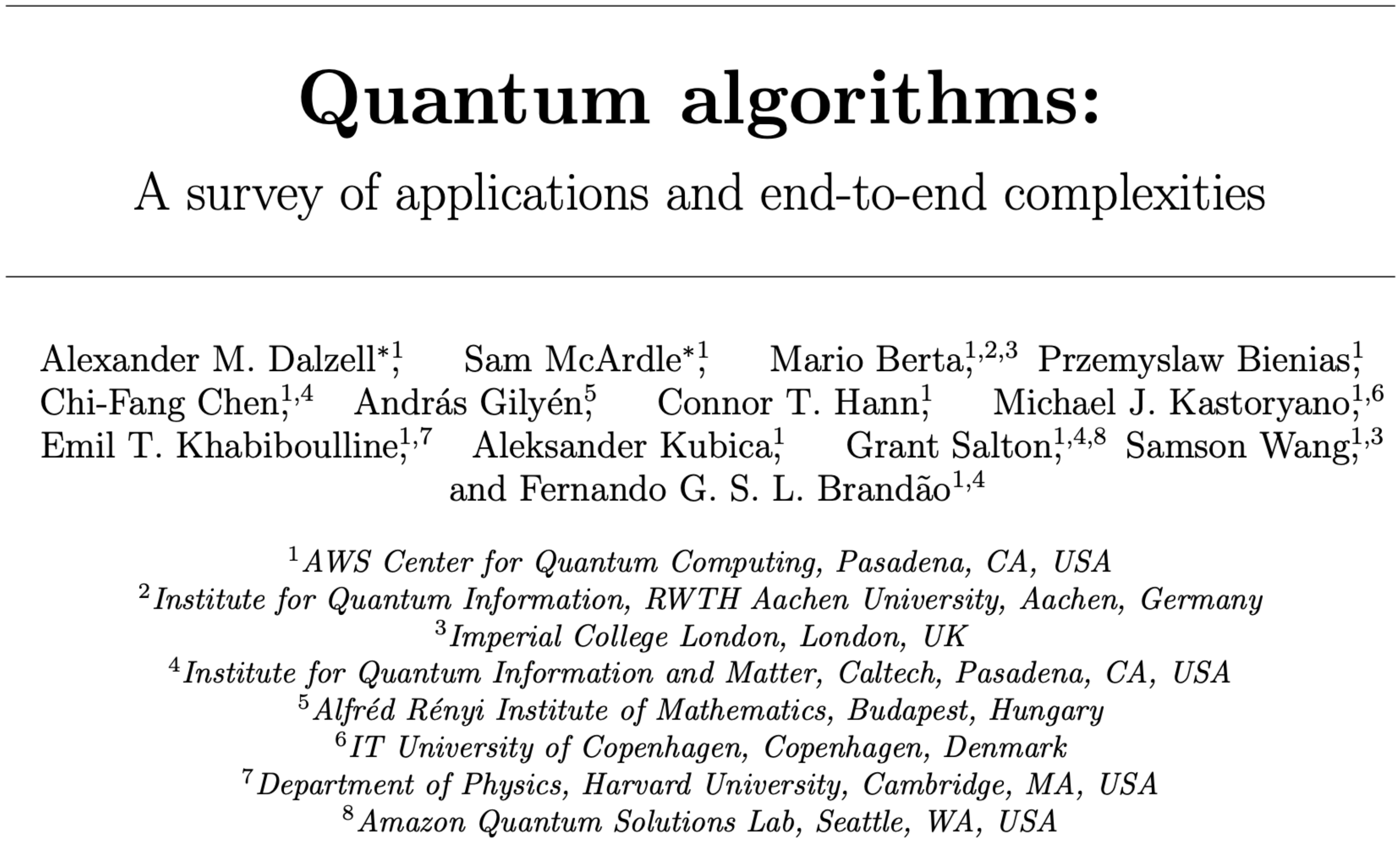
Our work on early fault-tolerance

- Hybrid classical-quantum schemes with end-to-end complexity analysis



- Resource estimates for comparison with state-of-the-art classical methods

Quantum Algorithms Wiki



- Cambridge University Press, to appear (available at arXiv:2310.03011)

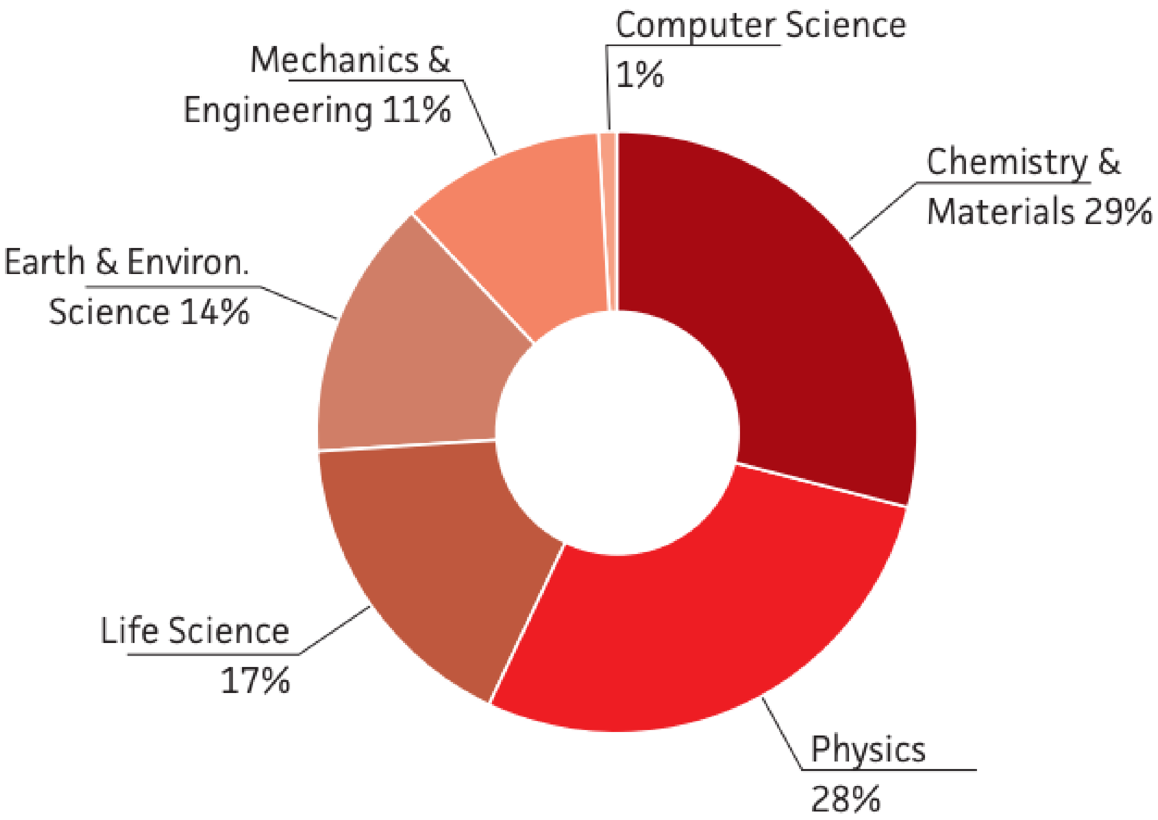
Quantum Algorithms Wiki

Quantum Algorithms: Lecture Notes

- Focus on end-to-end complexities
- Focus on scientific computing with promise of large quantum advantages
- Available at marioberta.info
- Lecture SS25: Department of Physics (open to all!)

PART II: Example Application

Quantum simulation for scientific computing



Swiss National Supercomputing Centre Annual Report 2022

Quantum algorithms for quantum simulation

- Resolve properties of quantum many body systems
- Temperature $T = 0$ physics, e.g., estimate ground state energy: Quantum phase estimation (quantum Fourier transform)
- Non-zero temperature $T > 0$ physics, e.g., create quantum Gibbs state: Quantum Gibbs samplers (simulated Lindbladian thermalization)

Recent breakthrough result:

arXiv > quant-ph > arXiv:2311.09207

Quantum Physics

[Submitted on 15 Nov 2023]

An efficient and exact noncommutative quantum Gibbs sampler

Chi-Fang Chen, Michael J. Kastoryano, András Gilyén

To appear soon:

Polynomial Time Quantum Gibbs Sampling for Fermi-Hubbard Model at any Temperature

(Smid, Meister, B., Bondesan)

Early fault-tolerant algorithm: Ground state energy estimation

Randomized quantum algorithm for statistical phase estimation

Physical Review Letters (2022) with Campbell and Wan
Quantum Information Processing (QIP) 2022

Quantum many body systems

- Consider n-qubit Hamiltonian

$$\mathrm{H} = \sum_{l=1}^{L} \alpha_l P_l^n \text{ with } P_l^n \; n\text{-qubit Pauli operator},$$

i.e., $\mathrm{P}_l^n = \mathrm{P}_1 \otimes \cdots \otimes P_n$ with $P_i \in \{X, Y, Z, 1\}$

- Native example: Ising model on two-dimensional square lattice

$$H_{Ising} = C \cdot \sum_{j \in J} Z_{i,j} \otimes Z_{i+1,j} + Z_{i,j} \otimes Z_{i,j+1}$$

- General fermionic or bosonic systems from condensed matter physics and computational chemistry can be mapped efficiently to qubits

Problem: Ground state energy estimation

- Given n-qubit Hamiltonian

$$\mathrm{H} := \sum_{l=1}^{L} \alpha_l P_l \text{ with } P_l \text{ } n\text{-qubit Paulis}$$

and one-norm $\lambda := \sum_{l=1}^{L} |\alpha_l|$, together with efficiently preparable n-qubit ansatz state $|\psi\rangle$ with overlap

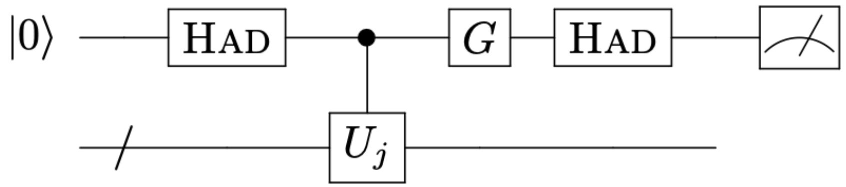
$$\langle \phi_0 | \psi \rangle \geq \eta > 0$$

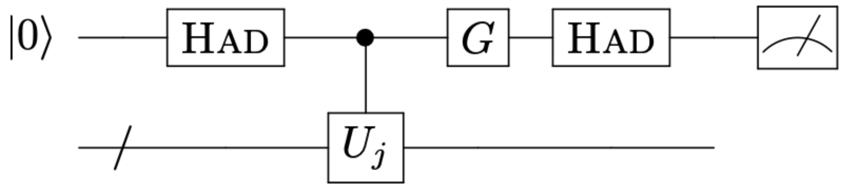
for true ground state $|\phi_0\rangle$ with energy E_0

- Goal: Compute estimate $\tilde{E}_0$ with precision $|\tilde{E}_0 - E_0| \leq \Delta$

Early fault-tolerance approach

1. Minimize number of qubits needed – one ancilla with Hadamard test:





2. Trade-off gate versus sample complexity
3. Decrease error by solely taking more samples
4. Independent of the number L of Pauli terms in H

Algorithmic result: Quantum phase estimation

- Output $\tilde{E}_0$ with $\left|\tilde{E}_0 - E_0\right| \leq \Delta$ with probability $1 - \xi$ by employing

$$C_{sample} = \tilde{O}(\eta^{-2}) \quad \left[= O\left(\eta^{-2}\log^2(\lambda\Delta^{-1}\log(\eta^{-1}))\log(\xi^{-1}\log(\lambda\Delta^{-1}))\right)\right]$$

quantum circuits on $n + 1$ qubits, each using one copy of $|\psi\rangle$ and

$$C_{gate} = \tilde{O}(\lambda^2\Delta^{-2}) \quad \left[= O(\lambda^2\Delta^{-2}\log^2(\eta^{-1}))\right]$$

single-qubit Pauli rotations $\exp(i\theta P_l)$

- Note: Ansatz state η-overlap bottleneck vs classical methods

Complexity ground state energy estimation

- n qubit Hamiltonian, $n+1$ qubits with quantum complexities independent of L:

$$C_{gate} = \tilde{O}(\lambda^2 \Delta^{-2}) \text{ for } C_{sample} = \tilde{O}(\eta^{-2})$$

- Randomized algorithm with classical pre- and post-processing
- Comparison state-of-the-art qubitization based approach:

Gate complexity $\tilde{O}\left(\sqrt{L}\lambda\Delta^{-1}\right)$ for $\tilde{O}\left(\sqrt{L}\right)$ qubits → total $\tilde{O}(L\lambda\Delta^{-1})$

[Lee et al., PRX Quantum (2021)]

Basic idea

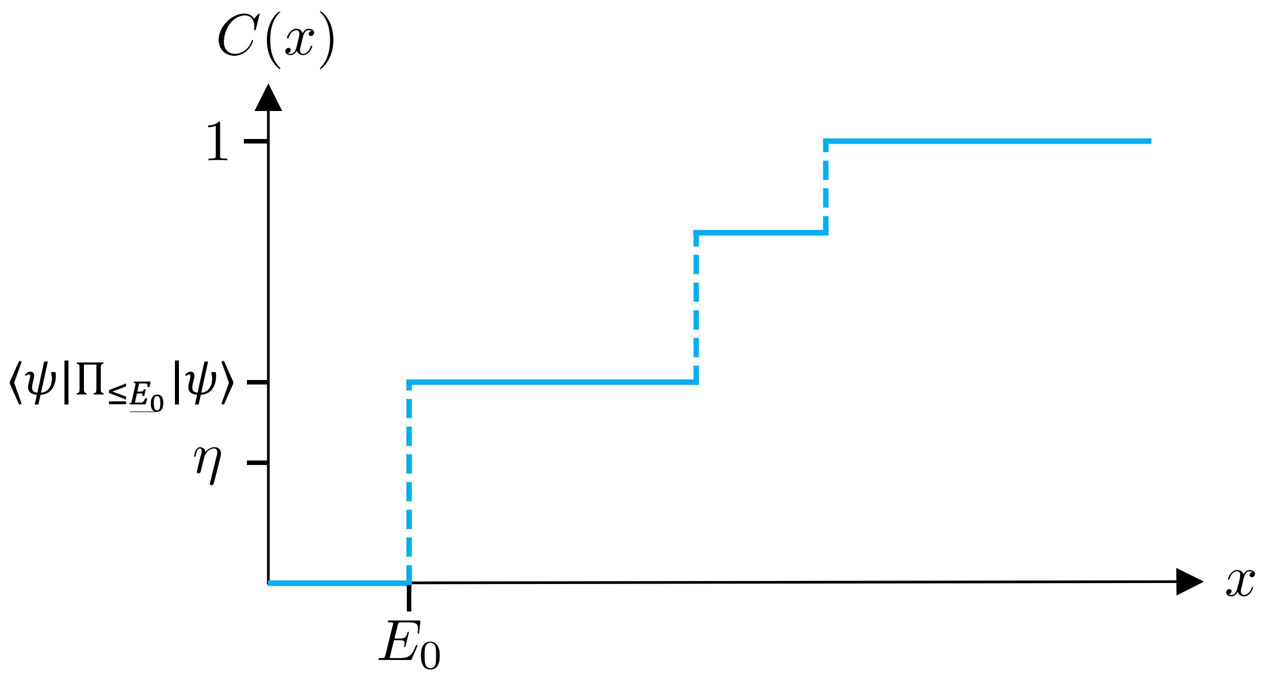
- Cumulative distribution function (CDF) relative to $|\psi\rangle$ is

$$C(x) \coloneqq \langle\psi|\Pi_{\leq x}|\psi\rangle$$

- Evaluate $C(x)$ via quantum?

- Two algorithmic ingredients:

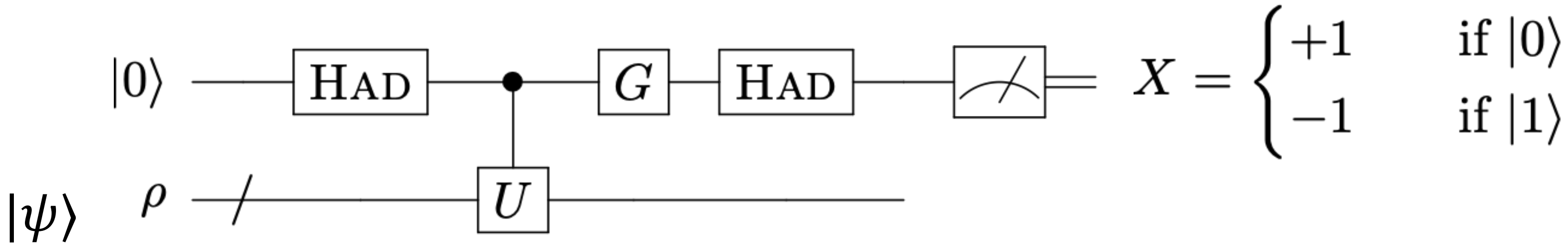
  (A) Hadamard test
  (B) Importance sampling



Quantum routine to evaluate CDF

Workhorse A: Hadamard test

- Input: n-qubit state $|\psi\rangle$ together with n-qubit unitary U
- Quantum circuit:



- Output is unbiased estimate of $\langle\psi|U|\psi\rangle$ from

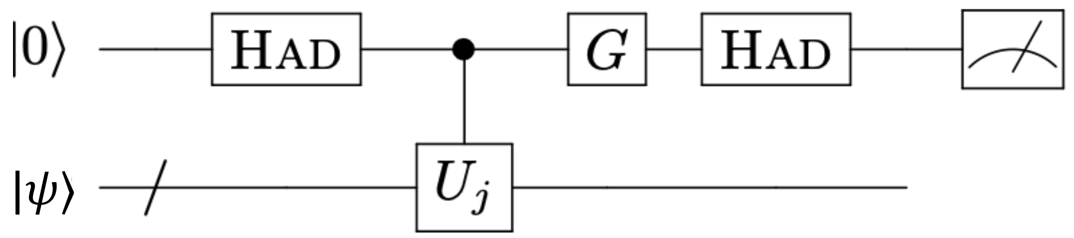
$$G = 1 \;\Rightarrow\; \mathbb{E}[X] = Re(\langle\psi|U|\psi\rangle)$$
$$G = S^* \;\Rightarrow\; \mathbb{E}[X] = Im(\langle\psi|U|\psi\rangle)$$

Workhorse B: Importance sampling

- Estimate linear combination:

  $\sum_j a_j \langle\psi|U_j|\psi\rangle$ for unitaries U_j with $a_j > 0$ and normalization $A := \sum_j a_j$

- Sample j with probability $a_j \cdot A^{-1}$ and perform Hadamard test on $(|\psi\rangle, U_j)$:

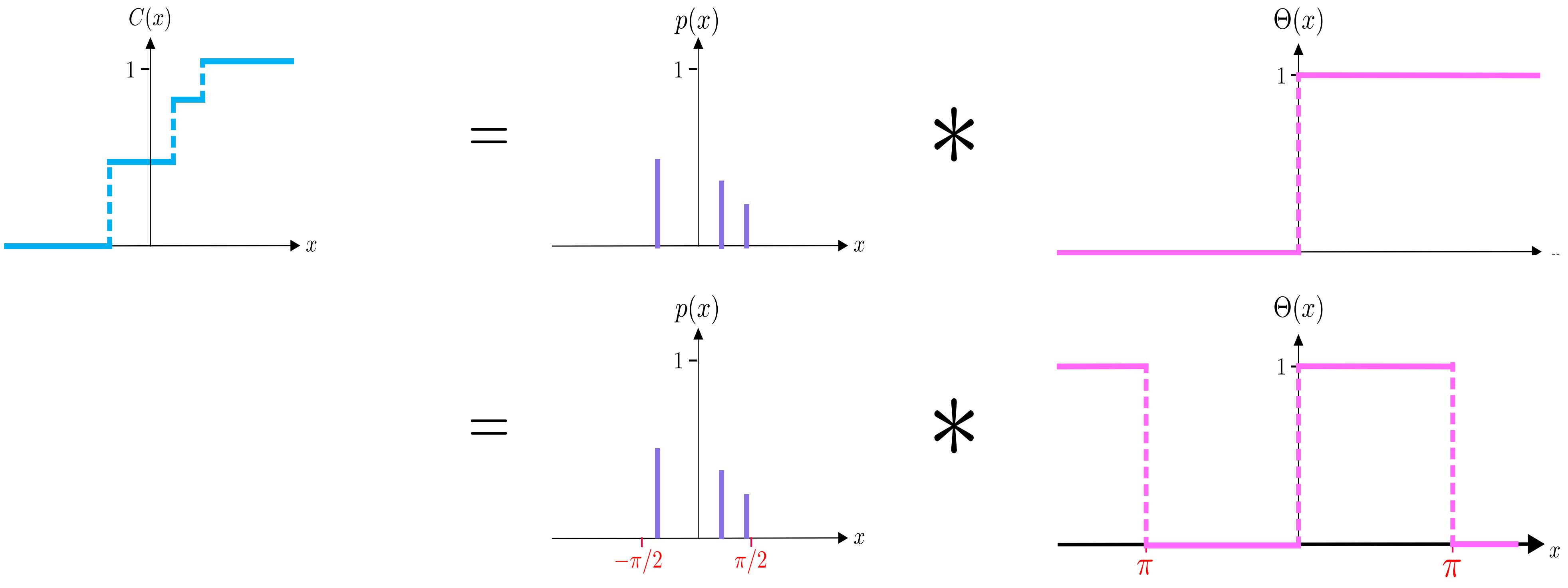


$\Rightarrow$ estimate $\langle\psi|U_j|\psi\rangle$

- Take average of samples, number required is $\lceil A^2\sigma^{-2}\rceil$ for variance $\sigma > 0$
- Expected gate complexity becomes $A^{-1} \cdot \sum_j a_j COST(C - U_j)$

Towards quantum implementation of CDF

- Normalize Hamiltonian with c $\cdot \, ||H||_\infty \leq c \cdot \lambda$ to put spectrum in $\left[-\frac{\pi}{2}, +\frac{\pi}{2}\right]$
- CDF $C(x) \equiv \langle\psi|\Pi_{\leq x}|\psi\rangle = (\Theta * p)(x)$ from convolution with Heaviside $\Theta(x)$:



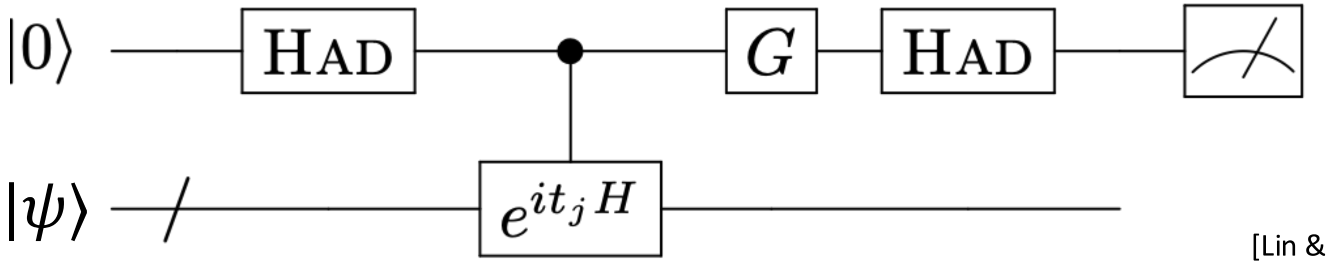
CDF via Fourier series

- Replace Heaviside $\Theta(x)$ by finite Fourier series $F(x) := \sum_{j\in S} \hat{F}_j e^{ijx}$
- Approximate CDF:

$$C(x) \approx (p * F)(x) = \sum_{j\in S} \hat{F}_j e^{ijx} \cdot \langle\psi|e^{it_jH}|\psi\rangle$$

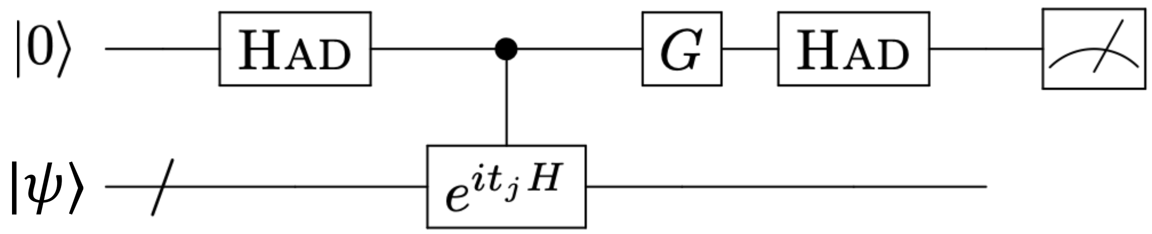
with runtimes $t_j = j \times$ normalization

- Hadamard test + importance sampling + Hamiltonian simulation:



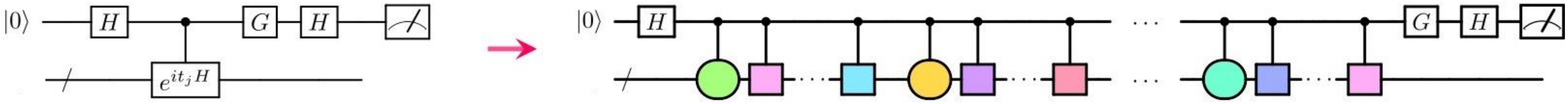
[Lin & Tong, PRX Quantum (2022)]

Hadamard test on Fourier series



$$C(x) \approx \sum_{j \in S} \hat{F}_j e^{ijx} \cdot \langle \psi | e^{it_j H} | \psi \rangle$$

- Implement Hamiltonian simulation unitary $\mathrm{U_j} = e^{it_j H}$ for $\mathrm{H} = \sum_{l=1}^{L} \alpha_l P_l$
- Independent of L? Technical contribution II:



novel random compiler lemma (Hamiltonian simulation)

Versus previous random compiler:
[Campbell, PRL (2019)]

Example systems

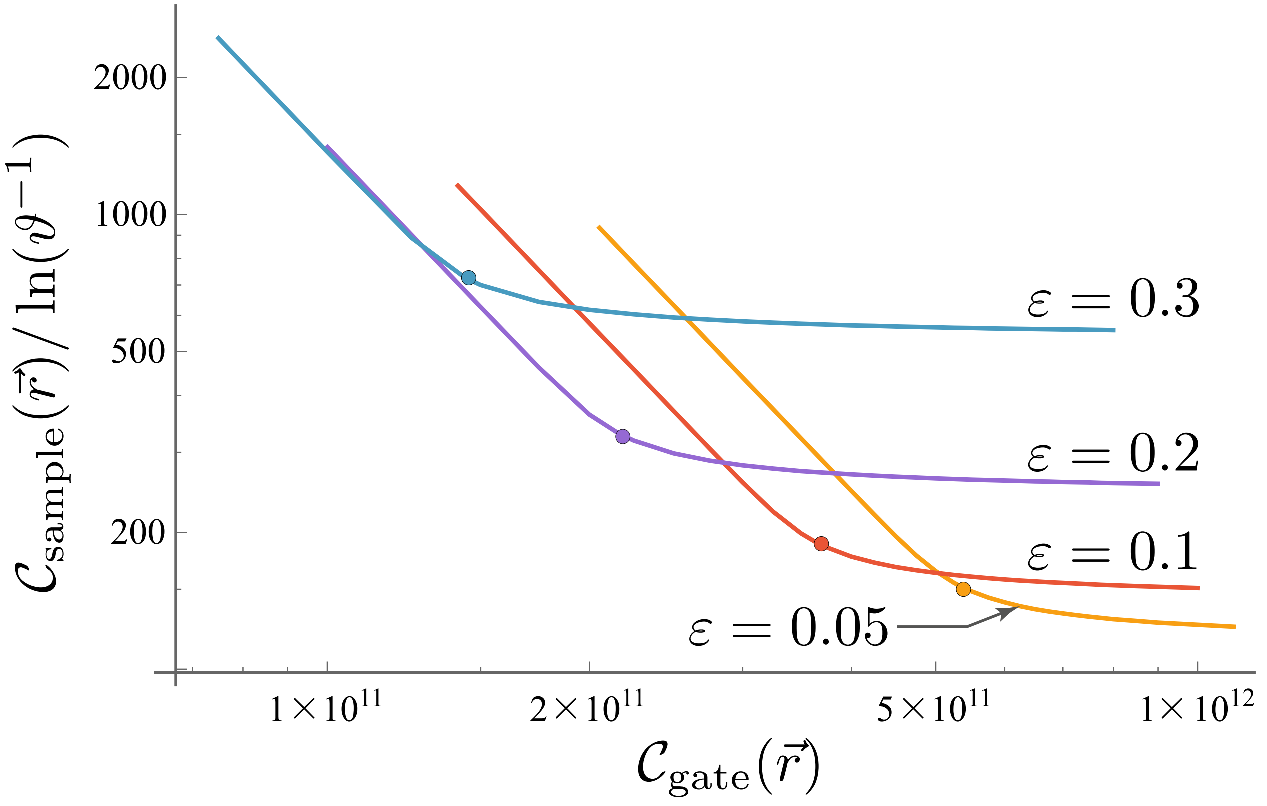
FeMoco benchmark – resource trade-offs

- Li et al. FeMoco Hamiltonian with 152 spin orbitals: 152+1=153 qubits
- Chemical accuracy $\Delta = 0.0016$ Hartree, one-norm $\lambda = 1511$
- State-of-the-art qubitization

$$C_{gate} = 3.2 \cdot 10^{10} \text{ on 2196 qubits}$$

[Lee et al., PRX Quantum (2021)]

- Ansatz state η-overlap bottleneck + classical methods scale polynomial!



Hydrogen chains benchmark

- For length N chain, one-norm estimate $\lambda \approx O(N^{1.34})$ [Koridon et al., PRR (2021)]
- Our work: $C_{gate} = \tilde{O}(N^{2.68}\Delta^{-2})$
- Qubitization based approaches:
  A. rigorous $C_{gate} = \tilde{O}(N^{3.34}\Delta^{-1})$
  B. sparse method $C_{gate} = \tilde{O}(N^{2.3}\Delta^{-1})$ [Berry et al., Quantum (2019)]
  C. tensor hypercontraction method $C_{gate} = \tilde{O}(N^{2.1}\Delta^{-1})$ [Lee et al., PRX Quantum (2021)]
- Extensive properties $\Delta \propto N$ interesting for our methods: $C_{gate} = \tilde{O}(N^{0.68})$

Conclusion

Recap main result

- Given: n-qubit Hamiltonian $\mathrm{H} = \sum_{\mathrm{l}=1}^{\mathrm{L}} \alpha_{\mathrm{l}} \mathrm{P}_{\mathrm{l}}$ with $\lambda = \sum_{\mathrm{l}=1}^{\mathrm{L}} |\alpha_{\mathrm{l}}|$, plus ansatz state ρ with ground state overlap $\langle \phi_0 | \rho | \phi_0 \rangle \geq \eta > 0$
- Output: ground state energy estimate $\tilde{E}_0$ with $\left|\tilde{E}_0 - E_0\right| \leq \Delta$
- Result: $n + 1$ qubits, $C_{gate} = \tilde{O}(\lambda^2 \Delta^{-2})$, $C_{sample} = \tilde{O}(\eta^{-2})$
- Advantages:

I. rigorous estimates

II. only depends on $\lambda \leq L$

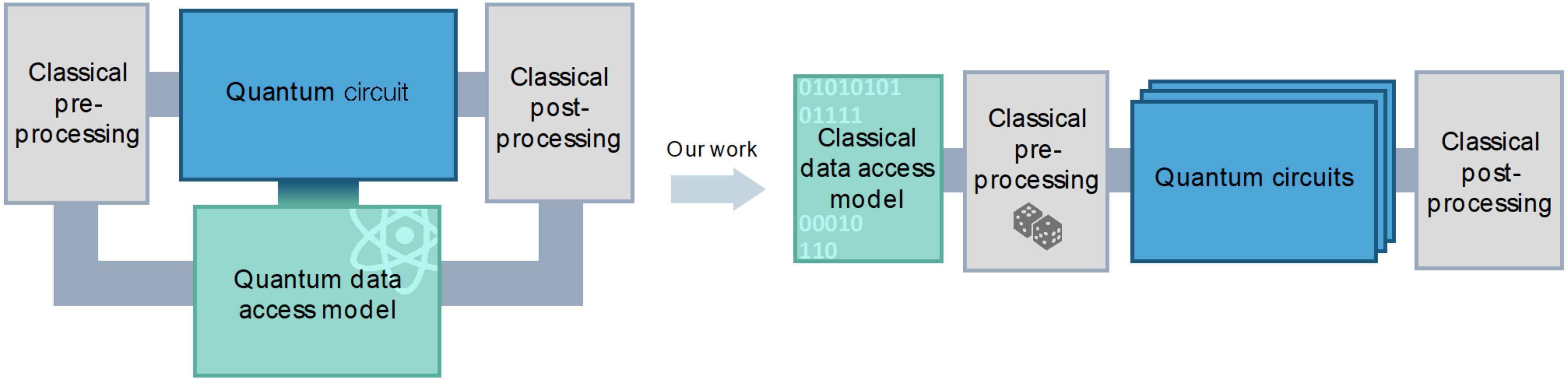
III. only uses one ancilla

IV. flexible trade-off gate versus sample complexity

V. decrease error by solely taking more samples → still state preparation bottleneck!

Quantum algorithms for early fault-tolerance

- Use as few qubits and quantum routines as possible, use classical methods whenever sufficient
- Early fault-tolerant methods can even be competitive with state-of-the-art (non-qubit aware) schemes in terms of asymptotic complexities



Outlook

- Quantum resource counts for applications featuring end-to-end complexity analyses with quantum speed-up?

SCHWERPUNKT

QUANTENCOMPUTING

Algorithmen für neue Hardware

Quantenalgorithmen lösen nur bestimmte Rechenprobleme signifikant effizienter als klassische Algorithmen.

Mario Berta

- Guiding questions:
  - What quantum algorithms do we eventually want to run?
  - For what applications is the quantum footprint the smallest to become competitive with classical methods?
- 50-100 error corrected qubits could allow for truly insightful experiments