

Present and future quantum computing algorithms

Prof. Dr. Mario Berta

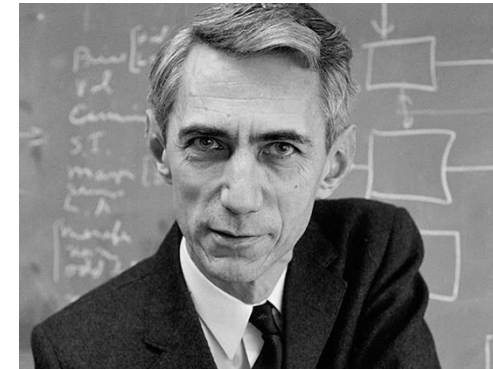
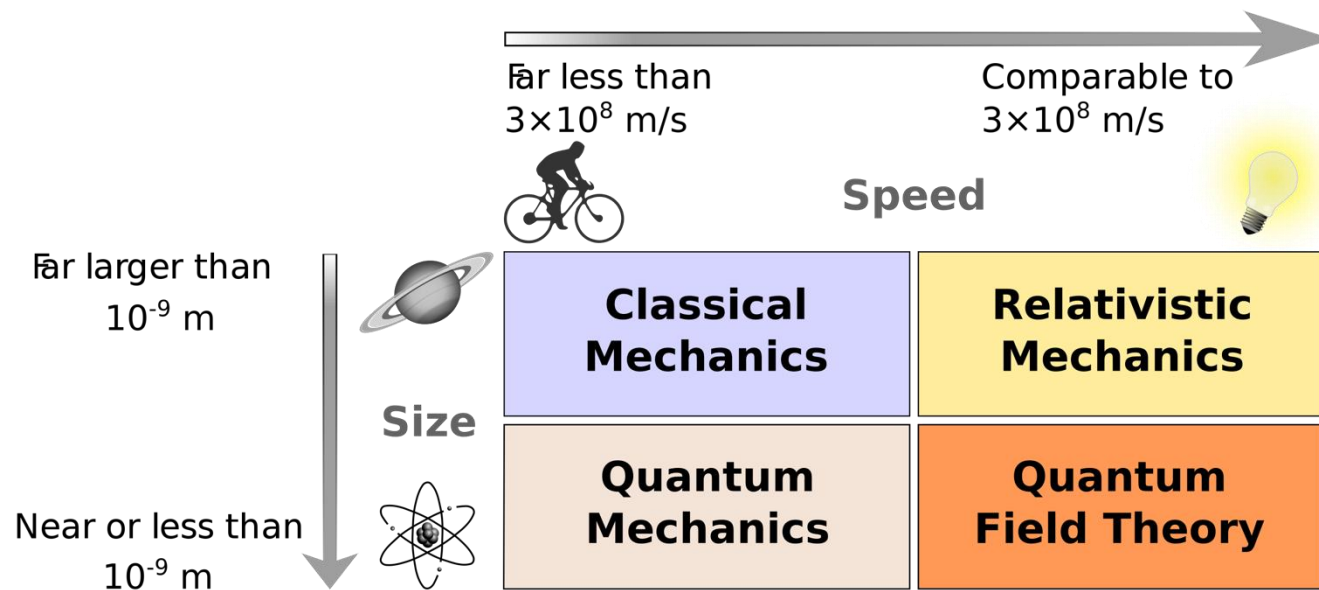
Guest Lecture
Quantum Computing for Engineering
December 18th, 2024

RWTHAACHEN
UNIVERSITY

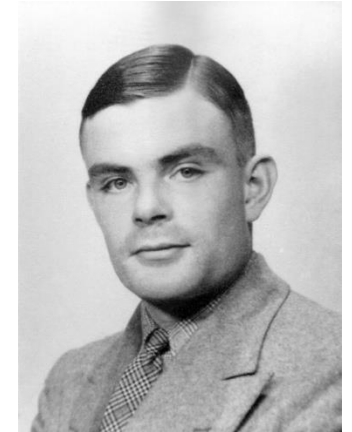


Information science

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



Claude Shannon

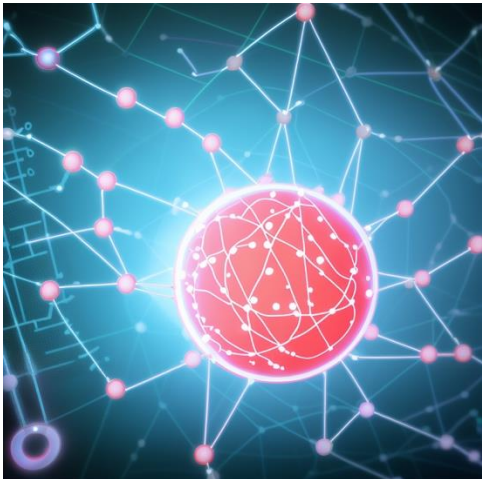


Alan Turing

- 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:

JARA | INSTITUTE
QUANTUM
INFORMATION

AN INITIATIVE OF

RWTHAACHEN
UNIVERSITY

JÜLICH
Forschungszentrum



Mario Berta
Professor of Physics



Sreejith Sreekumar
Postdoc



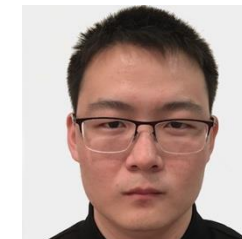
Aditya Nema
Postdoc



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

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



European
Research
Council



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 $O(\exp(1.9 \cdot n^{1/3} (\log n)^{2/3}))$

Quantum algorithms research

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



<quantum|gov>



- Breakthrough prize in physics 2023:
“foundational work in the field of quantum information”



Charles H. Bennett



Gilles Brassard



David Deutsch

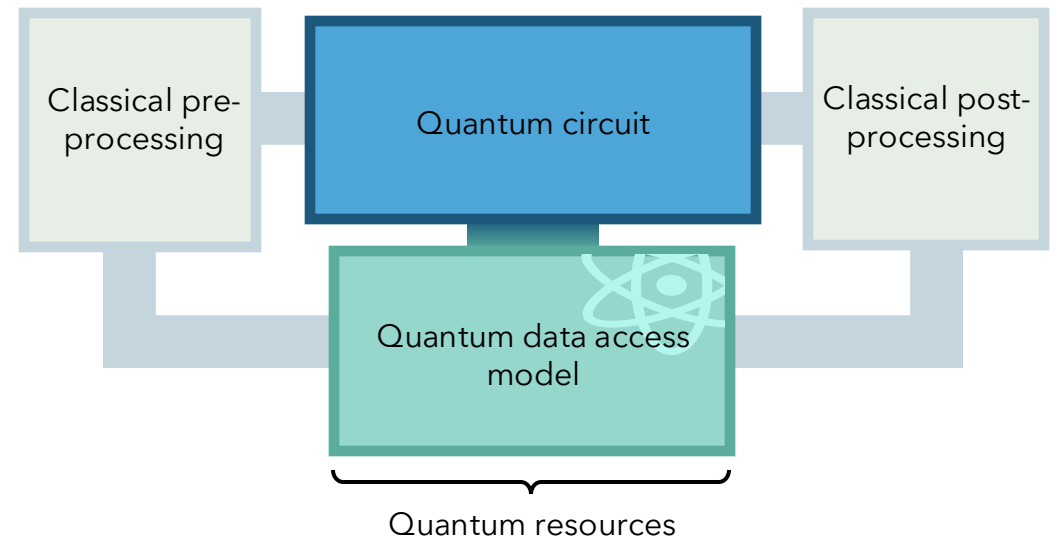


Peter Shor

- Ultimate goal: **Quantify classical-quantum complexity boundary**

Classical versus quantum technologies

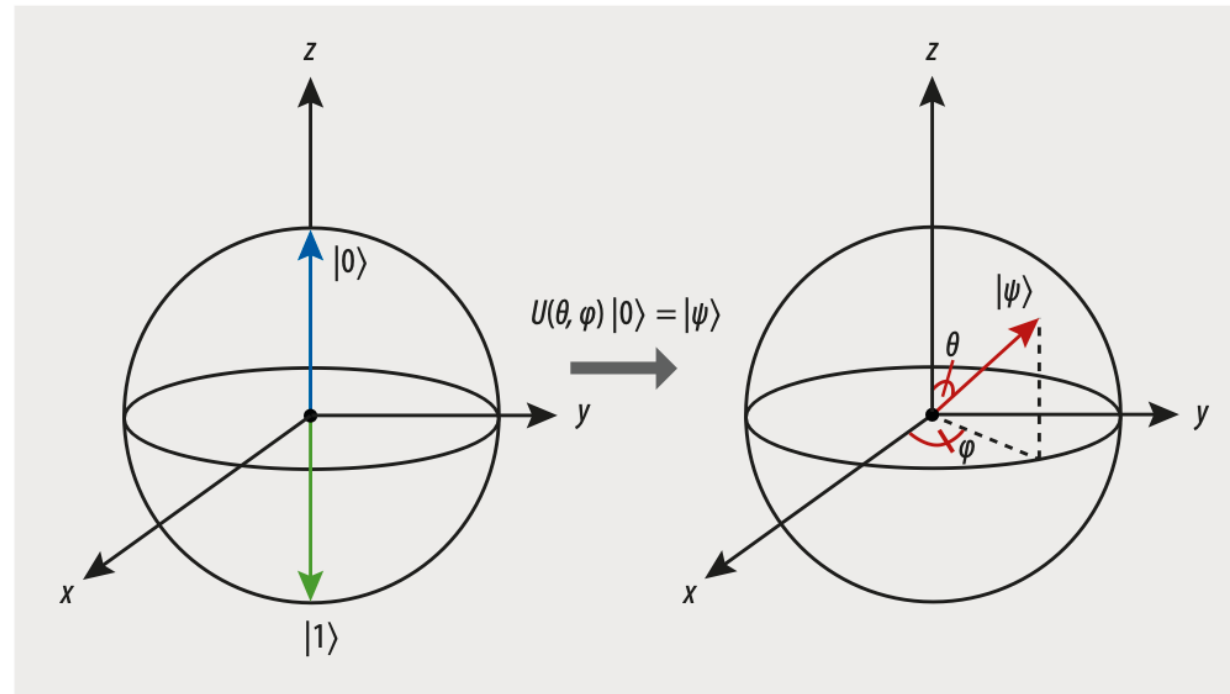
- *Do algorithms based on **quantum components**, including*
 - *quantum processing units (QPU)*
 - *quantum random access memory (QRAM)**provide **computational advantages** compared to classical components?*
- Goal is to identify use cases / areas of applications with
 - large (super-quadratic) quantum speed-up
 - minimal quantum footprint, i.e., use classical routines whenever possible



Basics: Quantum Circuit Model

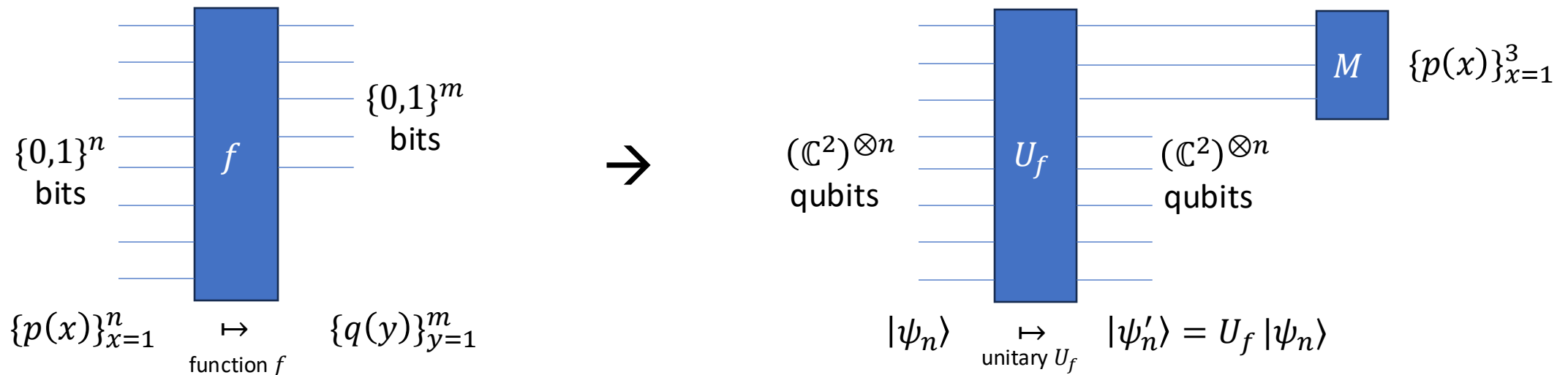
Classical vs quantum model of computation

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



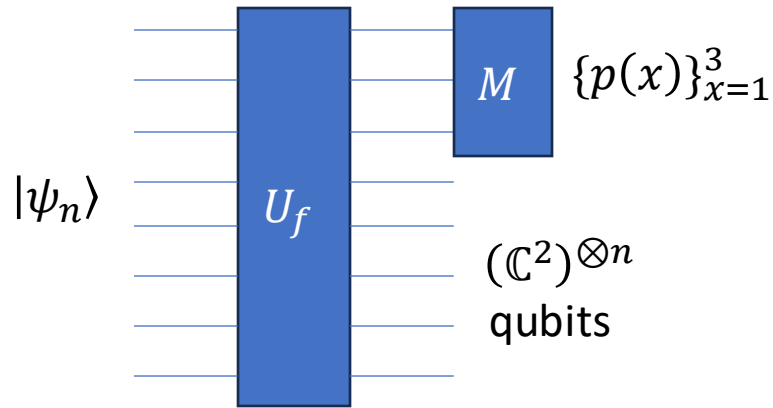
Classical vs quantum model of computation

- 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

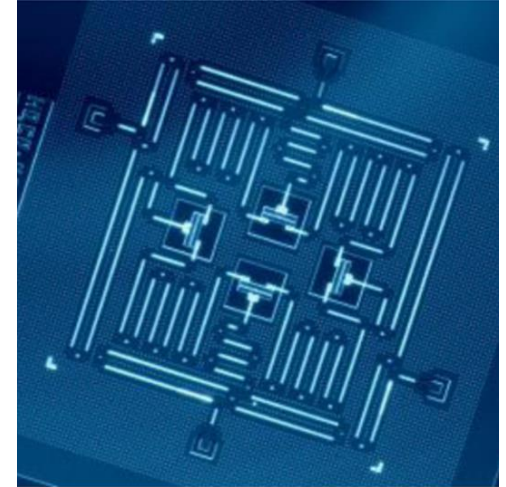


- Where does quantum speed-up come from?
→ precise mathematical reason: complex numbers allow for constructive interference
- Decomposition into set of elementary quantum gates, e.g., single qubit Pauli X , Y , Z and T gates, and two qubit $CNOT$ gate
- Quantum complexity = minimal number of elementary quantum gates
- More precise metric: Quantum depth of non-Clifford gates (i.e., T gates)

Quantum hardware

Quantum hardware

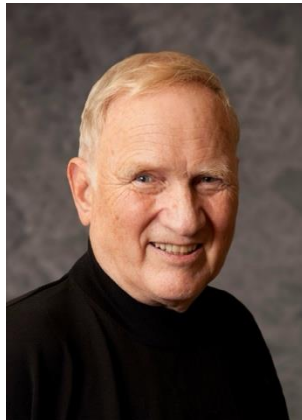
- Different technologies: Superconductors, ion traps, neutral atoms, photonics, etc.
- Groundbreaking physics experiments with **6 orders of magnitude improvements in 30 years+**



4 IBM superconducting qubits



Alain Aspect



John Clauser



Anton Zeilinger

- 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](#)

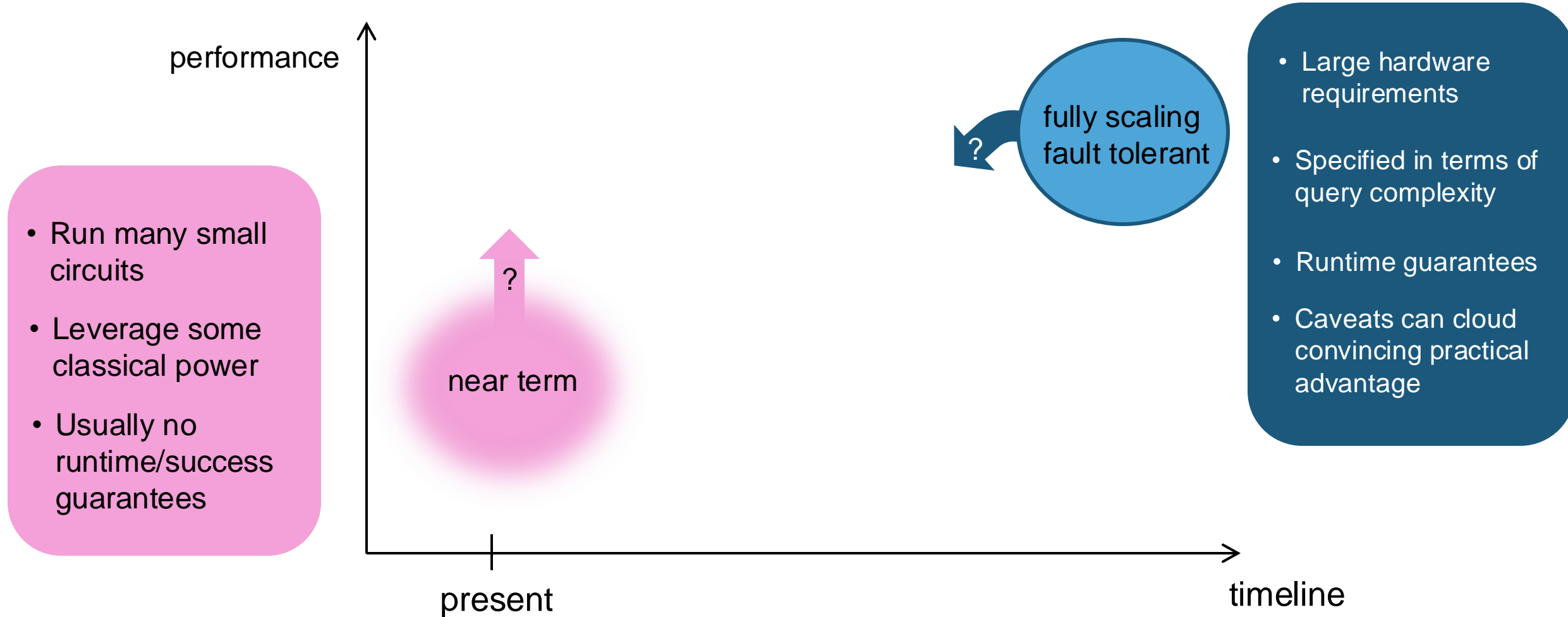
Quantum algorithm design

Regimes for quantum algorithm design

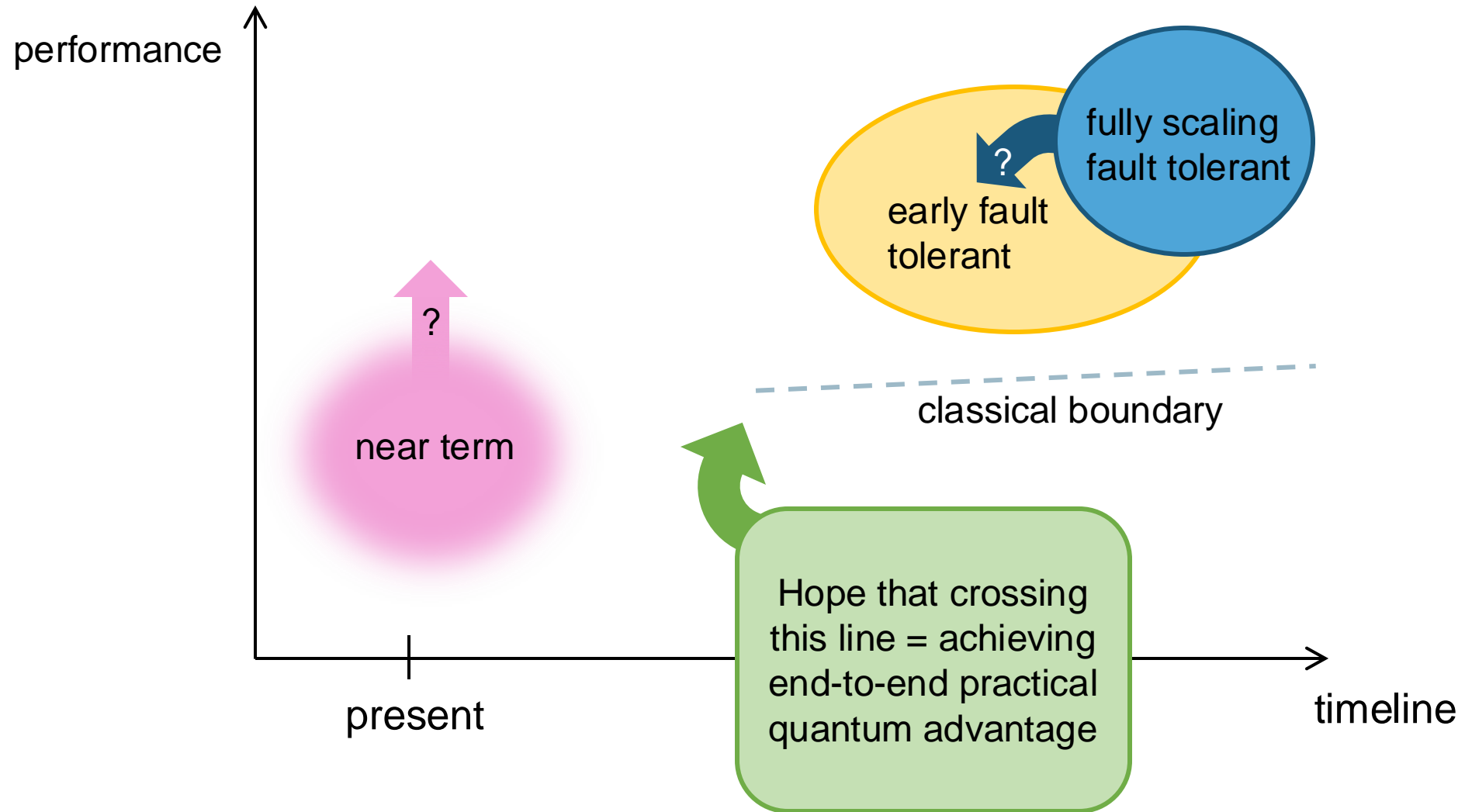
- Nascent state of quantum technologies gives **noisy and intermediate scale quantum (NISQ)** computing, i.e.,
 - Quantum annealers
 - Analogue simulators, not universal, not fully programmable
 - NISQ digital quantum circuits, inbuilt noise resilience, error mitigation, severe scaling limitations, etc.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



Early fault-tolerant regime

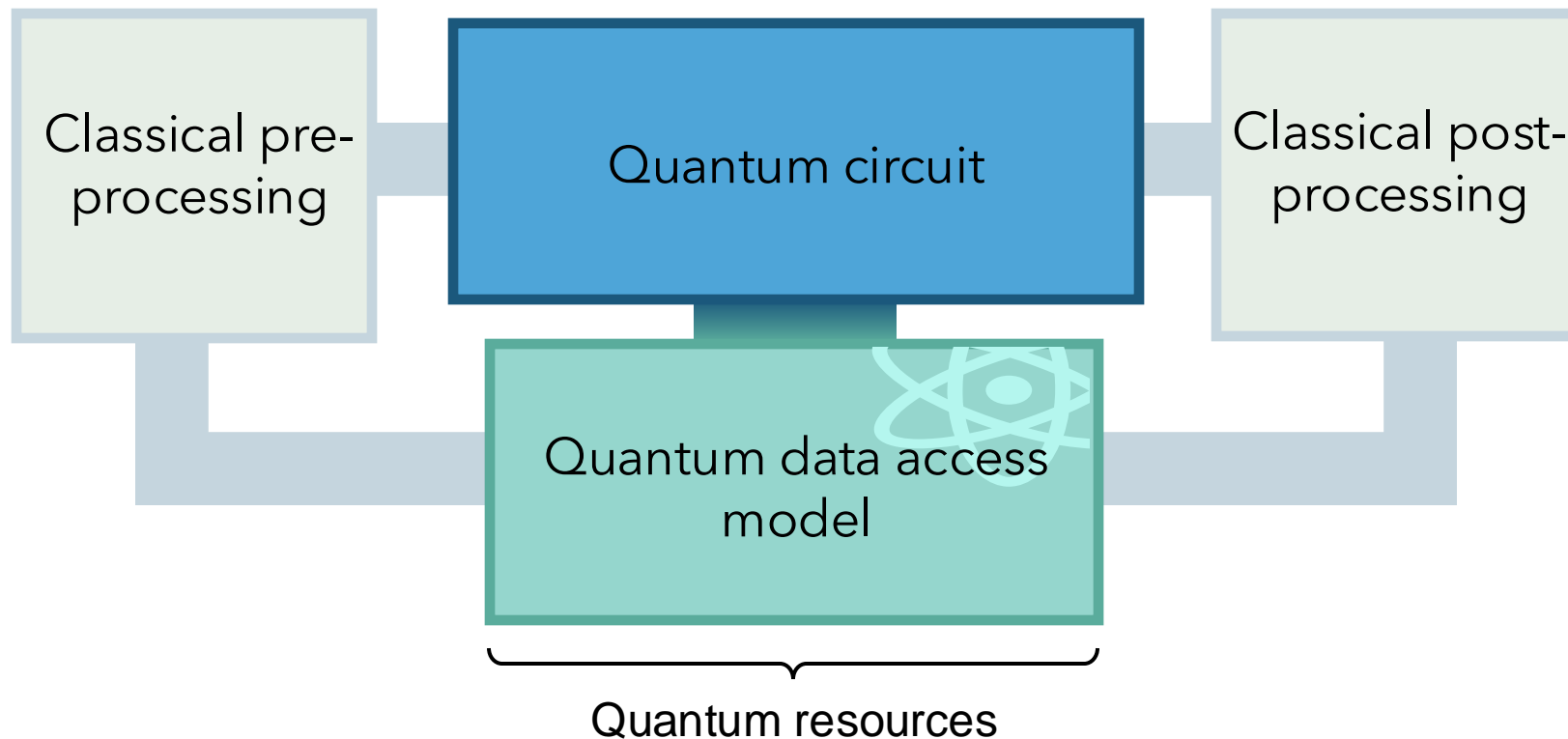


Early fault-tolerance characteristics

- **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:

A survey of applications and end-to-end complexities

Alexander M. Dalzell^{*1}, Sam McArdle^{*1}, Mario Berta^{1,2,3}, Przemyslaw Bienias¹,
Chi-Fang Chen^{1,4}, András Gilyén⁵, Connor T. Hann¹, Michael J. Kastoryano^{1,6},
Emil T. Khabiboulline^{1,7}, Aleksander Kubica¹, Grant Salton^{1,4,8}, Samson Wang^{1,3}
and Fernando G. S. L. Brandão^{1,4}

¹*AWS Center for Quantum Computing, Pasadena, CA, USA*

²*Institute for Quantum Information, RWTH Aachen University, Aachen, Germany*

³*Imperial College London, London, UK*

⁴*Institute for Quantum Information and Matter, Caltech, Pasadena, CA, USA*

⁵*Alfréd Rényi Institute of Mathematics, Budapest, Hungary*

⁶*IT University of Copenhagen, Copenhagen, Denmark*

⁷*Department of Physics, Harvard University, Cambridge, MA, USA*

⁸*Amazon Quantum Solutions Lab, Seattle, WA, USA*

- Cambridge University Press, to appear (available at [arXiv:2310.03011](https://arxiv.org/abs/2310.03011))

PART I AREAS OF APPLICATION

Condensed matter physics

- 1.1 Fermi–Hubbard model
- 1.2 Spin models
- 1.3 SYK model

Quantum chemistry

- 2.1 Simulating electrons in molecules and materials
- 2.2 Simulating vibrations in molecules and materials

Nuclear and particle physics

- 3.1 Quantum field theories
- 3.2 Nuclear physics

Combinatorial optimization

- 4.1 Search algorithms à la Grover
- 4.2 Beyond quadratic speedups in exact combinatorial optimization

Continuous optimization

- 5.1 Zero-sum games: Computing Nash equilibria
- 5.2 Conic programming: Solving LPs, SOCPs, and SDPs
- 5.3 General convex optimization
- 5.4 Nonconvex optimization: Escaping saddle points and finding local minima

Cryptanalysis

- 6.1 Breaking cryptosystems
- 6.2 Weakening cryptosystems

Solving differential equations

Finance

- 8.1 Portfolio optimization
- 8.2 Monte Carlo methods: Option pricing

Machine learning with classical data

- 9.1 Quantum machine learning via quantum linear algebra
- 9.2 Quantum machine learning via energy-based models
- 9.3 Tensor PCA
- 9.4 Topological data analysis
- 9.5 Quantum neural networks and quantum kernel methods

PART II QUANTUM ALGORITHMIC PRIMITIVES

Quantum linear algebra

- 10.1 Block-encodings
- 10.2 Manipulating block-encodings
- 10.3 Quantum signal processing
- 10.4 Qubitization
- 10.5 Quantum singular value transformation

Hamiltonian simulation

- 11.1 Product formulas
- 11.2 qDRIFT
- 11.3 Taylor and Dyson series (linear combination of unitaries)
- 11.4 Quantum signal processing / quantum singular value transformation

Quantum Fourier transform

Quantum phase estimation

Amplitude amplification and estimation

- 14.1 Amplitude amplification
- 14.2 Amplitude estimation

Gibbs sampling

Quantum adiabatic algorithm

Loading classical data

- 17.1 Quantum random access memory
- 17.2 Preparing quantum states from classical data
- 17.3 Block-encoding dense matrices of classical data

Quantum linear system solvers

Quantum gradient estimation

Variational quantum algorithms

Quantum tomography

Quantum interior point methods

Multiplicative weights update method

Approximate tensor network contraction

Quantum Algorithms Wiki

PART III FAULT-TOLERANT QUANTUM COMPUTING

Basics of fault tolerance

Quantum error correction with the surface code

Logical gates with the surface code

<i>Appendix</i>	Background, conventions, and notation
A.1	Quantum systems and bra-ket notation
A.2	The quantum circuit model
A.3	Noise in quantum gates and the NISQ era
A.4	Big- \mathcal{O} notation
A.5	Complexity theory background

References

Index

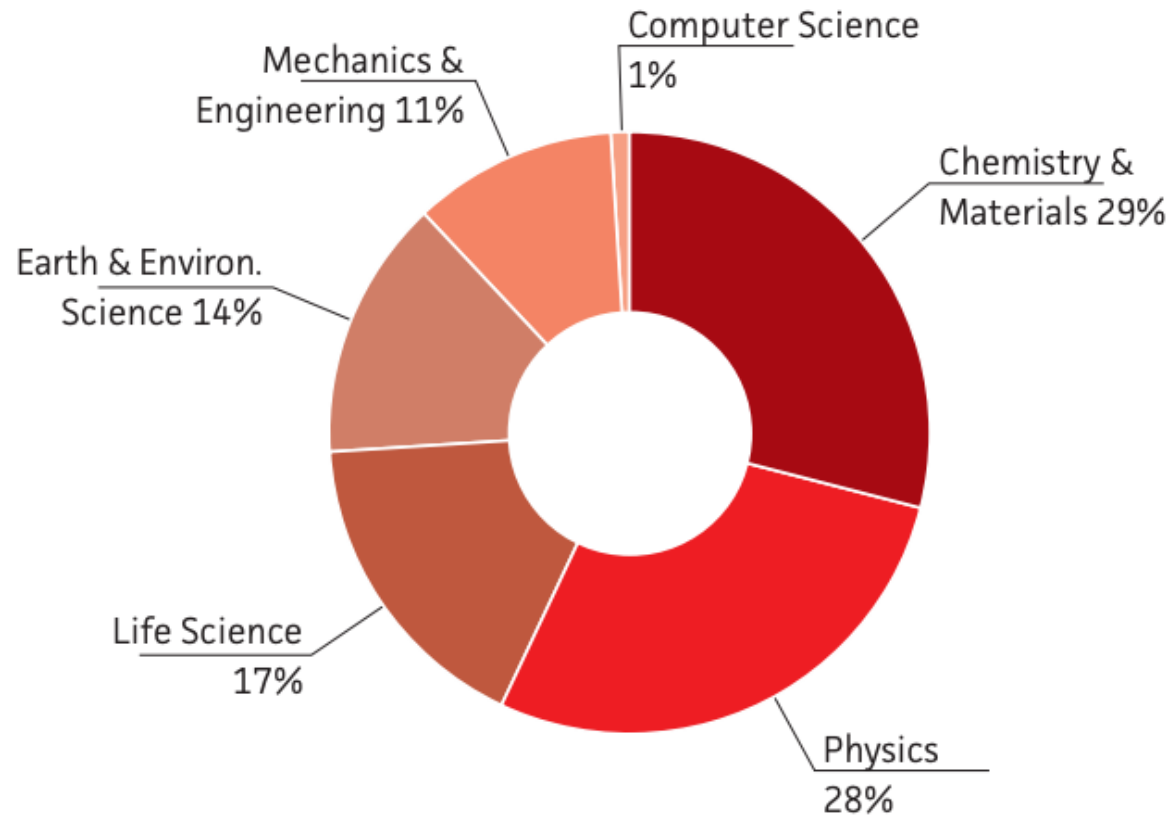
Quantum Algorithms: Lecture Notes

- 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!)

1 Overview	
1.1 Introduction	
1.2 Organization	7
1.3 Classical circuit model	
1.4 Computational complexity theory	
2 Quantum circuit model	
2.1 Quantum systems	
2.2 Quantum bits and quantum gates	
2.3 Quantum measurements	
2.4 Remarks on quantum error correction	
3 Quantum query complexity	
3.1 Setting	
3.2 Deutsch's problem	
3.3 Deutsch-Josza problem	
3.4 Simon's problem	
3.5 Other oracle based quantum algorithms	
4 Quantum Fourier transform	
4.1 Discrete Fourier transform	
4.2 Quantum circuit	
4.3 Remarks on period finding and Shor's algorithm	
5 Quantum phase estimation	←
5.1 Problem setting	
5.2 Quantum circuit	
5.3 Variations and caveats	
6 Hamiltonian simulation	←
6.1 Task	
6.2 Commuting case	
6.3 Trotter based methods	
6.4 Linear combination of unitary based methods	
6.5 State-of-the-art methods and caveats	
7 Ground state energy estimation	←
7.1 Task	
7.2 Mapping to qubit form	
7.3 Quantum phase estimation	
7.4 Quantum state preparation and other bottlenecks	
8 Quantum linear system solver (QLSS)	
8.1 Task and classical landscape	
8.2 Quantum task	
8.3 Quantum data access	
8.4 Basic quantum linear system solver	
8.5 State-of-the-art methods and caveats	
9 Quantum random access memory (QRAM)	
9.1 Motivation	
9.2 Quantum state preparation: Basic ideas	
9.3 Quantum state preparation: Circuits	
9.4 Quantum read only memory (QROM)	
9.5 Fanout QRAM	
9.6 Bucket-brigade QRAM	
9.7 Extensions and caveats	
10 Quantum singular value transform (QSVT)	
10.1 Motivation	
10.2 Block encoding data access	
10.3 Transformation of block encodings	
10.4 Example polynomials	
Bibliography	

PART II: Example Application

Quantum simulation for scientific computing

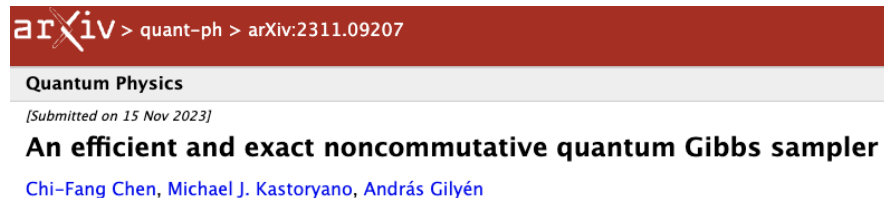


Swiss National Supercomputing Centre Annual Report 2022

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:



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

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

i.e., $P_l^n = P_1 \otimes \cdots \otimes P_n$ 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

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

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

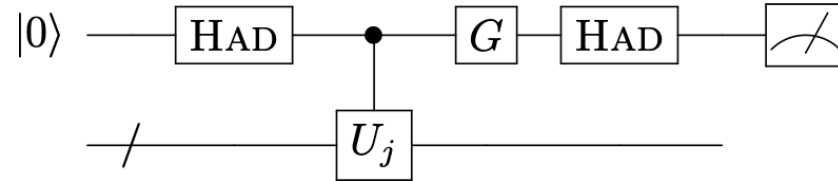
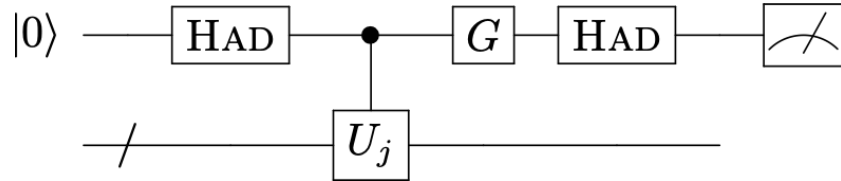
$$\langle \phi_0 | \psi \rangle \geq \eta > 0$$

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

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

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

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

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:

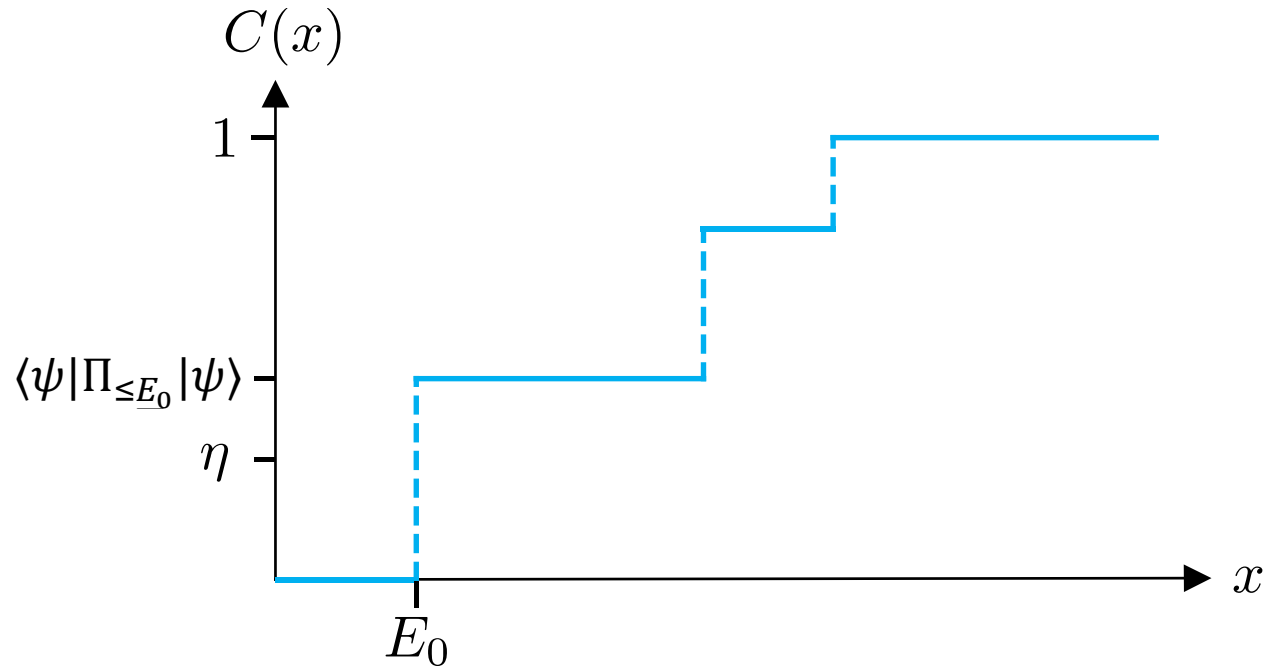
Gate complexity $\tilde{O}(\sqrt{L}\lambda\Delta^{-1})$ for $\tilde{O}(\sqrt{L})$ qubits \rightarrow total $\tilde{O}(L\lambda\Delta^{-1})$

Basic idea

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

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

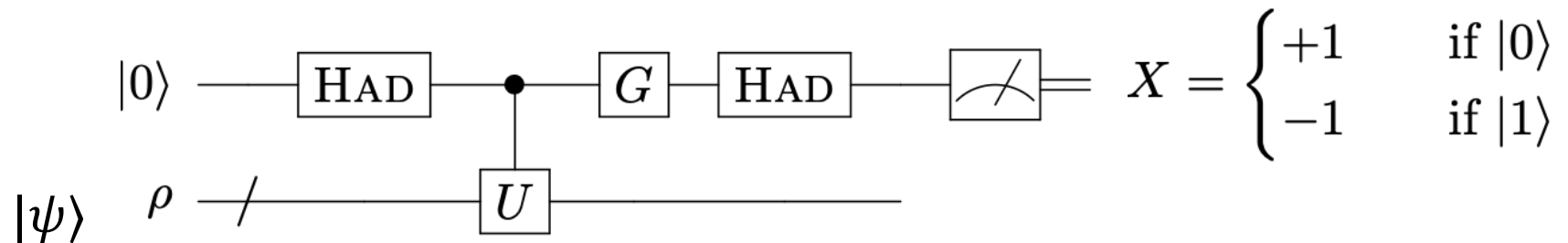
- Evaluate $C(x)$ via quantum?
- Two algorithmic ingredients:
 - (A) Hadamard test
 - (B) Importance sampling



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

$$G = 1 \Rightarrow \mathbb{E}[X] = \text{Re}(\langle\psi|U|\psi\rangle)$$

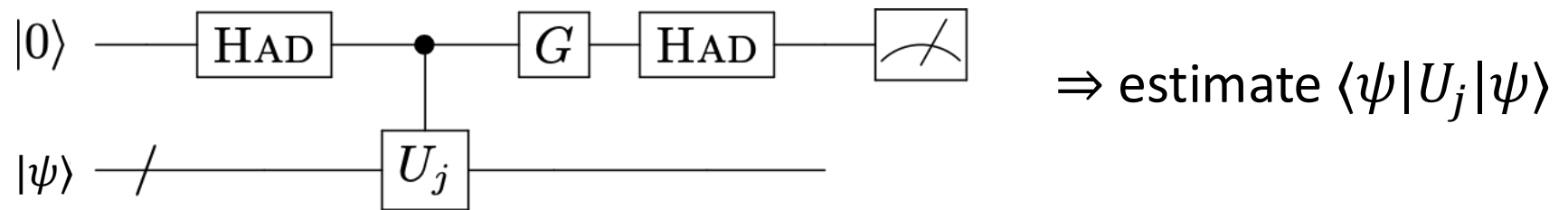
$$G = S^* \Rightarrow \mathbb{E}[X] = \text{Im}(\langle\psi|U|\psi\rangle)$$

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 $A := \sum_j a_j$

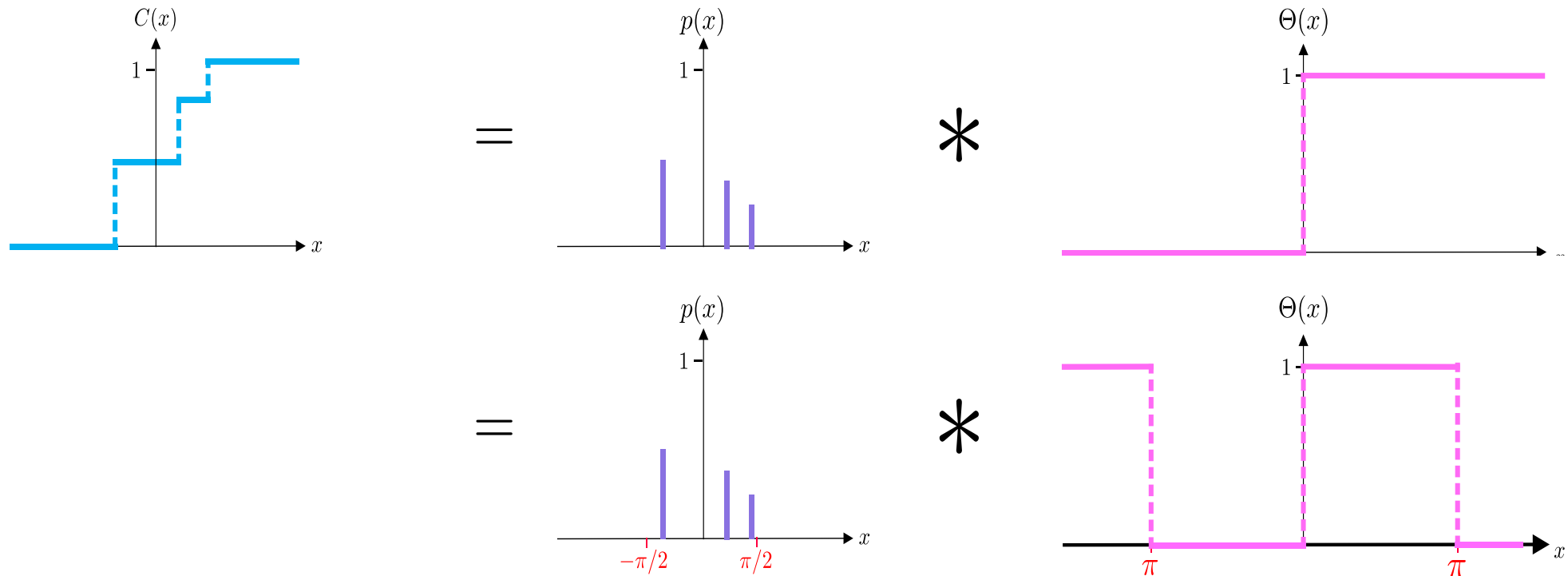
- Sample j with probability $a_j \cdot A^{-1}$ and perform Hadamard test on $(|\psi\rangle, U_j)$:



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

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 $\Theta(x)$:



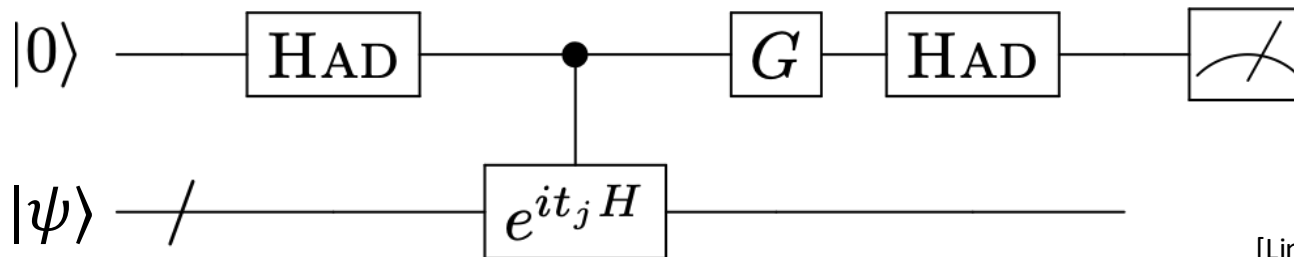
CDF via Fourier series

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

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

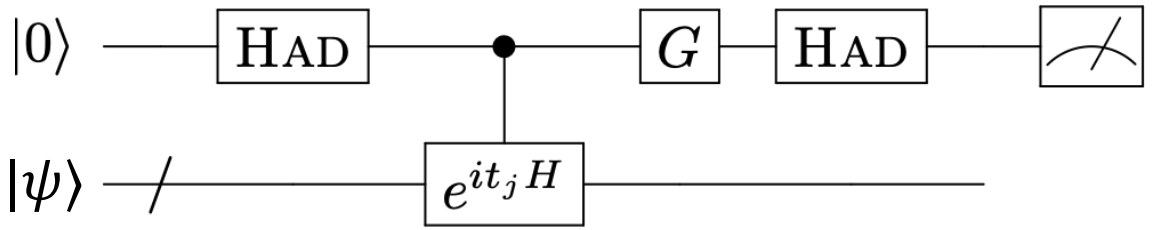
with runtimes $t_j = j \times \text{normalization}$

- Hadamard test + importance sampling + Hamiltonian simulation:



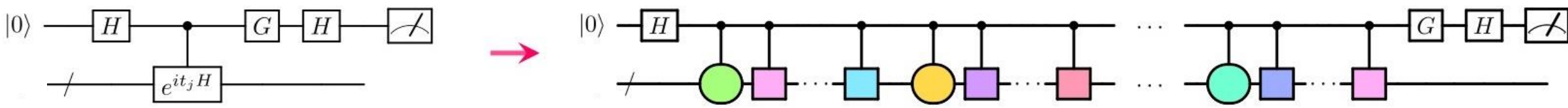
[Lin & Tong, PRX Quantum (2022)]

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



novel **random compiler lemma** (Hamiltonian simulation)

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

Example systems

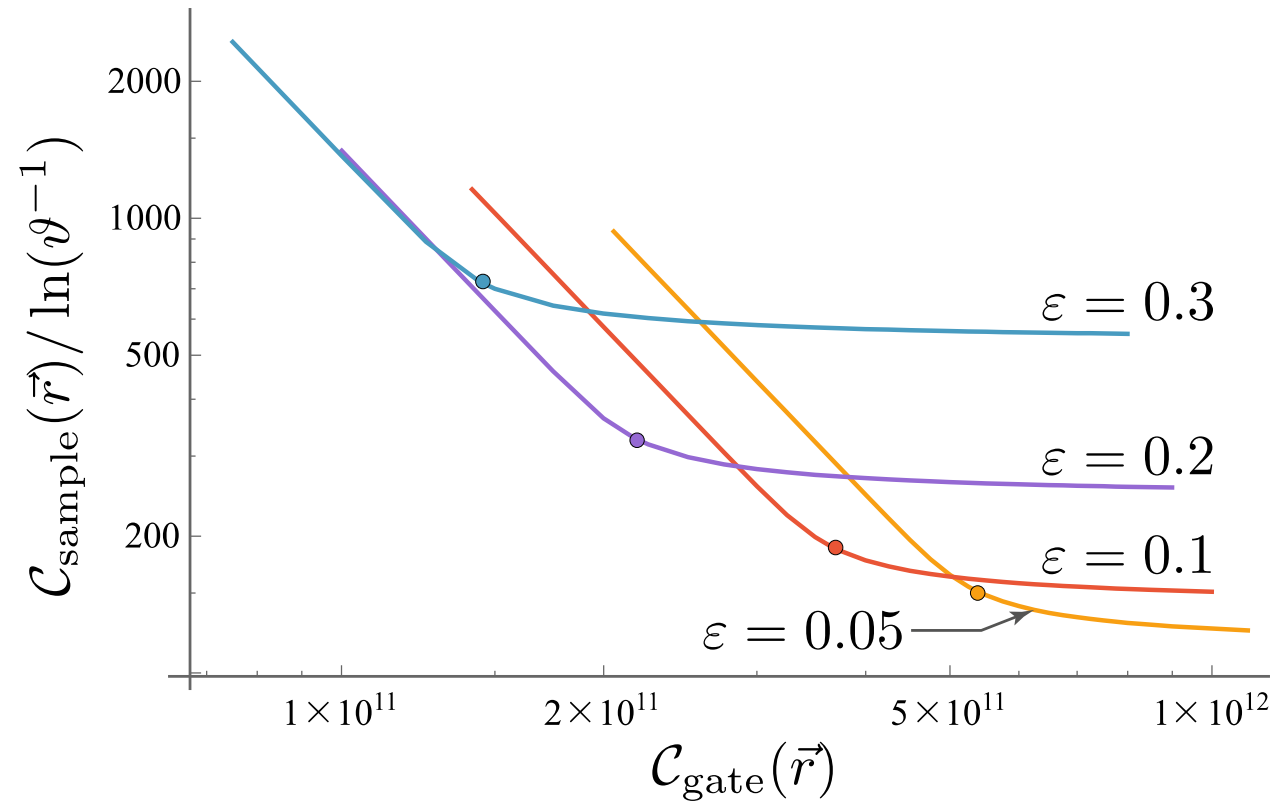
FeMoco benchmark – resource trade-offs

- 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: $C_{gate} = \tilde{O}(N^{0.68})$

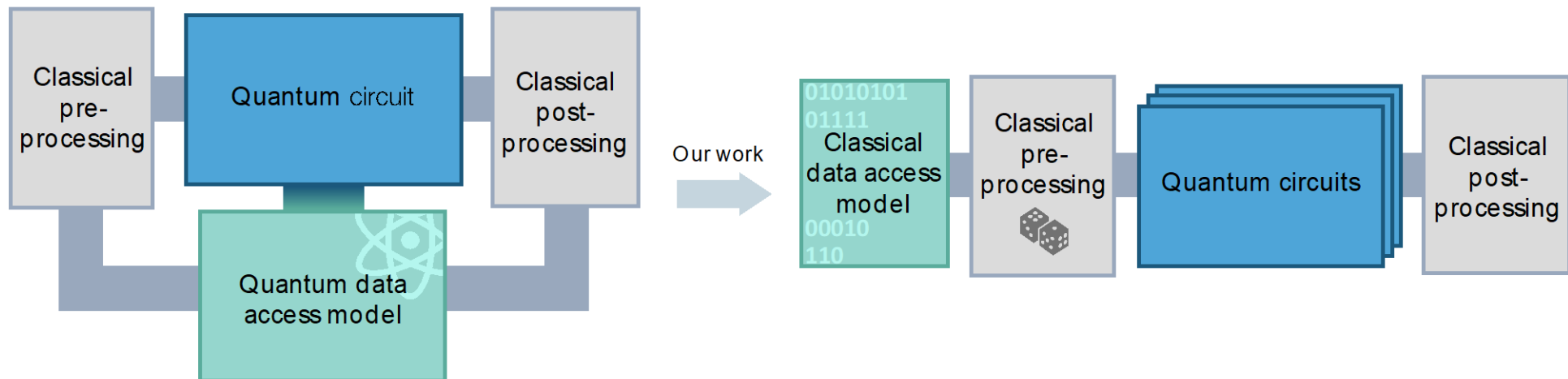
Conclusion

Recap main result

- Given: n -qubit Hamiltonian $H = \sum_{l=1}^L \alpha_l P_l$ with $\lambda = \sum_{l=1}^L |\alpha_l|$, 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 $|\tilde{E}_0 - E_0| \leq \Delta$
- 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?
- 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

SCHWERPUNKT

QUANTENCOMPUTING

Algorithmen für neue Hardware

Quantenalgorithmen lösen nur bestimmte Rechenprobleme signifikant effizienter als klassische Algorithmen.

Mario Berta