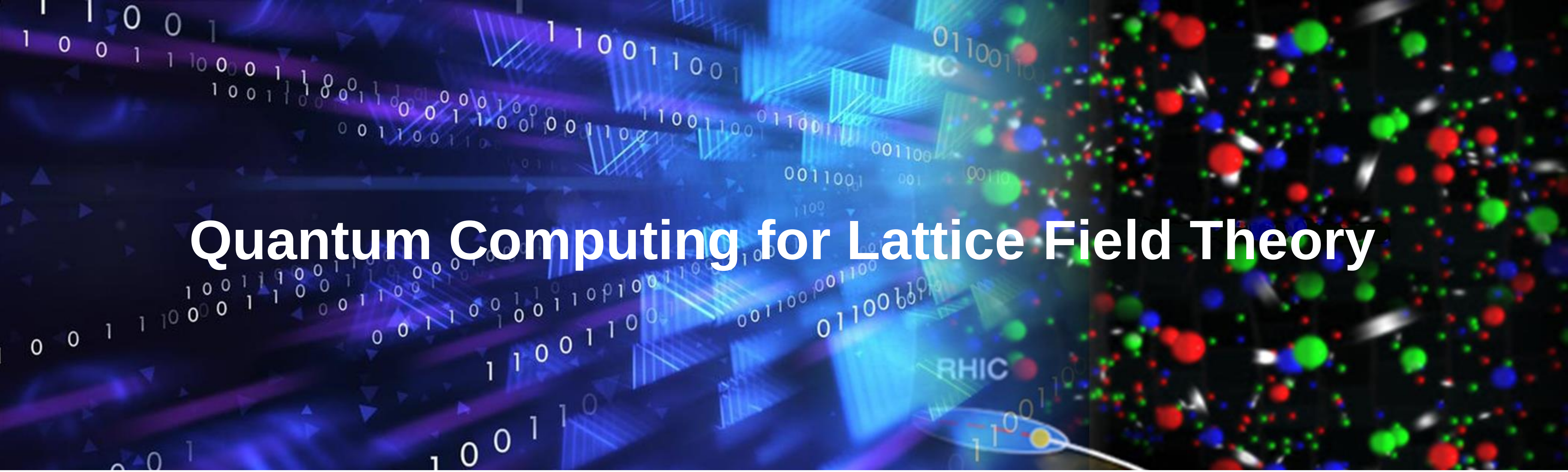
Quantum Computing for Lattice Field Theory



Lena Funcke

UNIVERSITÄT BONN · TRA MATTER, TRANSDISCIPLINARY RESEARCH AREA · HISKP · ML4Q, MATTER AND LIGHT FOR QUANTUM COMPUTING · ⟨NuMeriQS⟩

SIGN25, University of Bern, 23 January 2025

What are the challenges of classical computing?

Classical computational costs

Supercomputer usage for different fields (INCITE 2019)

→ **Lattice QCD: ~ $\mathbf{40\%}$**

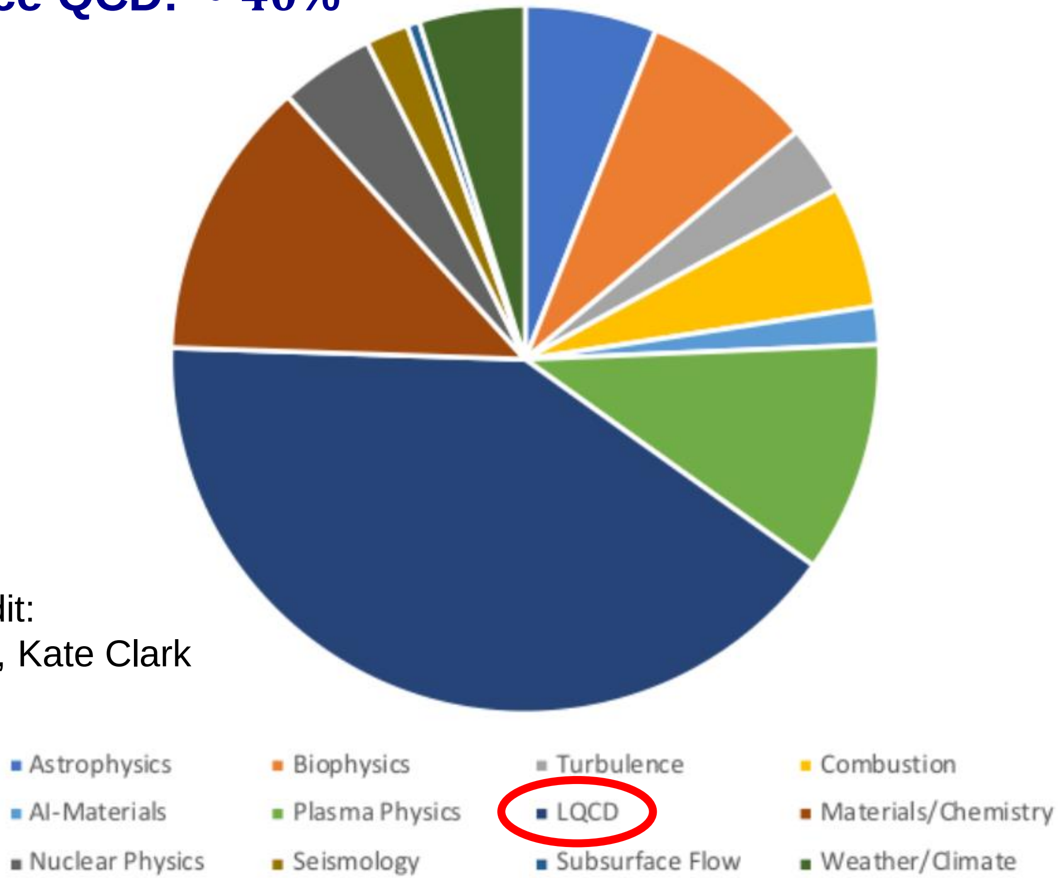
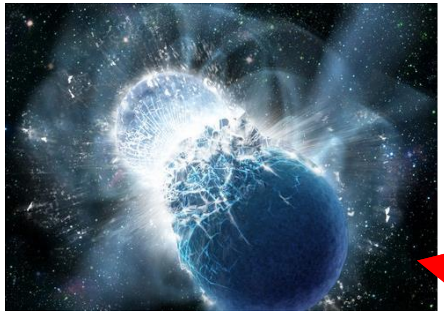


Figure credit:
Jack Wells, Kate Clark

Classical computational limitations

No chemical potentials, θ-terms, real-time evolution, …

→ interior of neutron stars



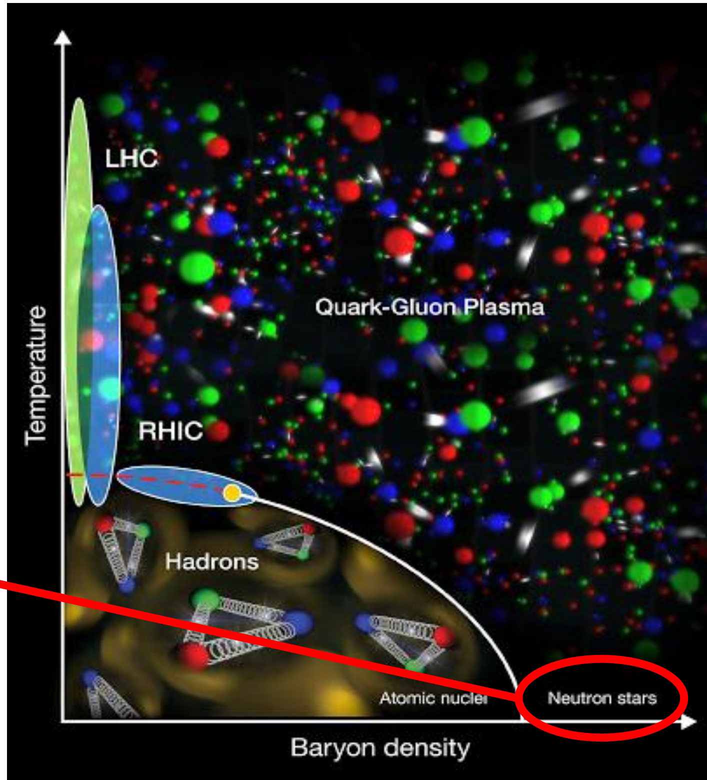


Figure credit:
BNL/RHIC, CfA

What are the challenges of classical computations?

Classical computational costs

Supercomputer usage for different fields (INCITE 2019)

$\rightarrow$ **Lattice QCD: $\sim 40\%$**

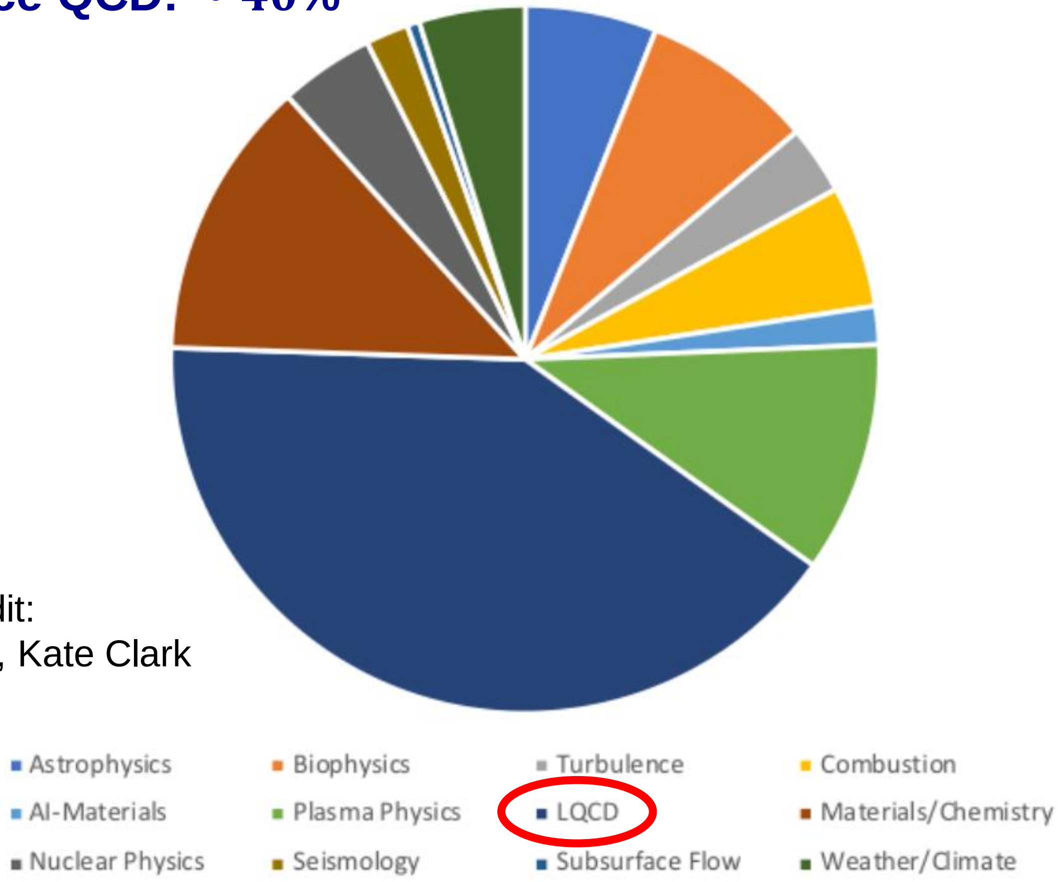


Figure credit:
Jack Wells, Kate Clark

Classical computational limitations

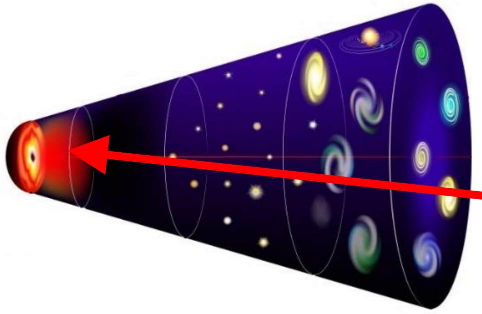
No chemical potentials, θ-terms, real-time evolution, …

$\rightarrow$ interior of neutron stars, heavy-ion collisions, …

$\rightarrow$ out-of-equilibrium phase transitions: early Universe, …

$\rightarrow$ CP violation: $\theta = \pi$, …

$\rightarrow$ …



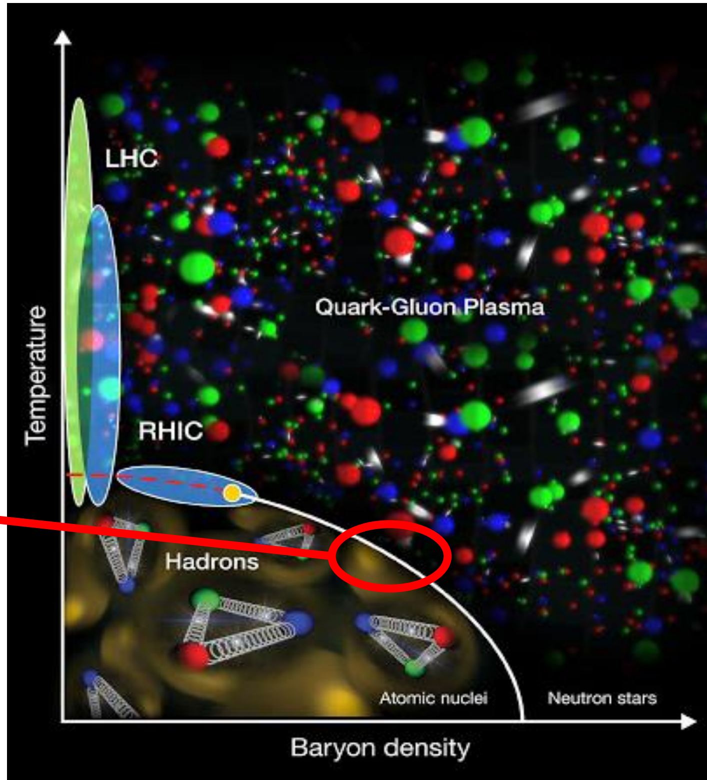


Figure credit:
BNL/RHIC, CfA

What are the challenges of classical computations?

Classical computational costs	Classical computational limitations

Supercomputer usage for different fields (INCITE 2019)

→ **Lattice QCD: ~ 40%**

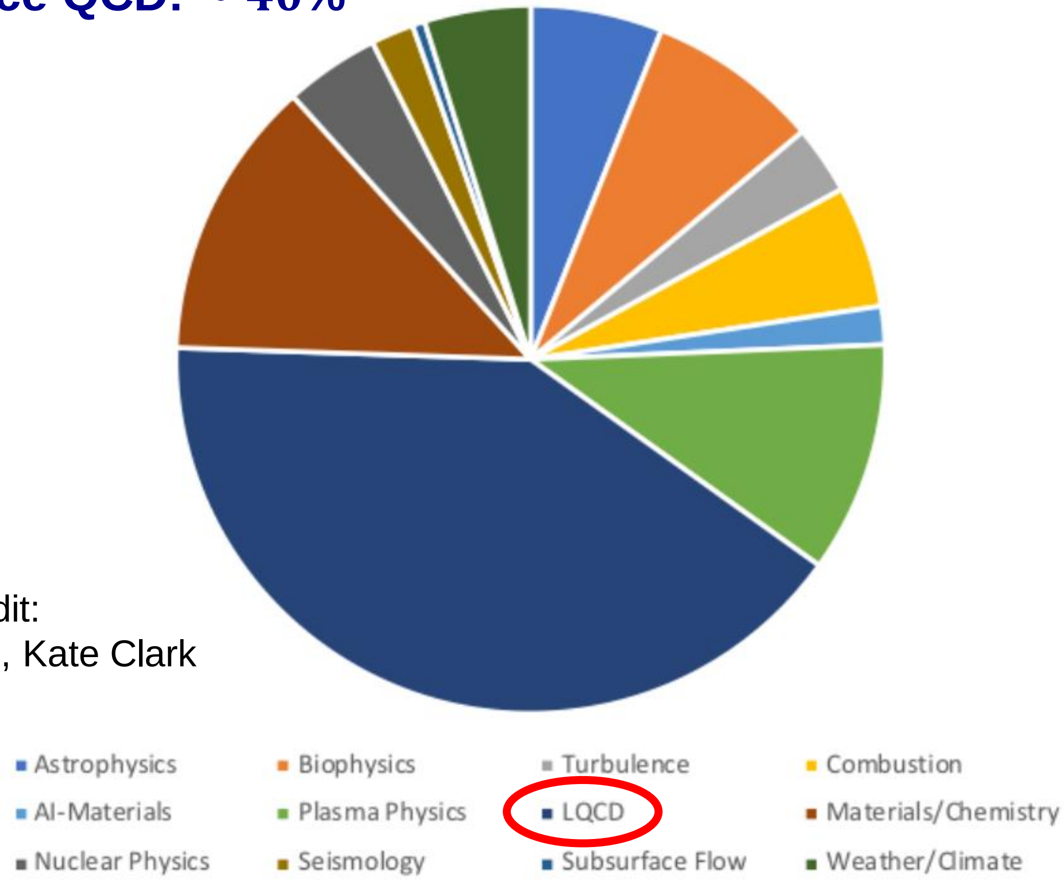


Figure credit:
Jack Wells, Kate Clark

No chemical potentials, θ-terms, real-time evolution, …

→ interior of neutron stars, heavy-ion collisions, …

→ out-of-equilibrium phase transitions: early Universe, …

→ CP violation: $\theta = \pi$, …

→ …

Quantum computing

evades sign problem

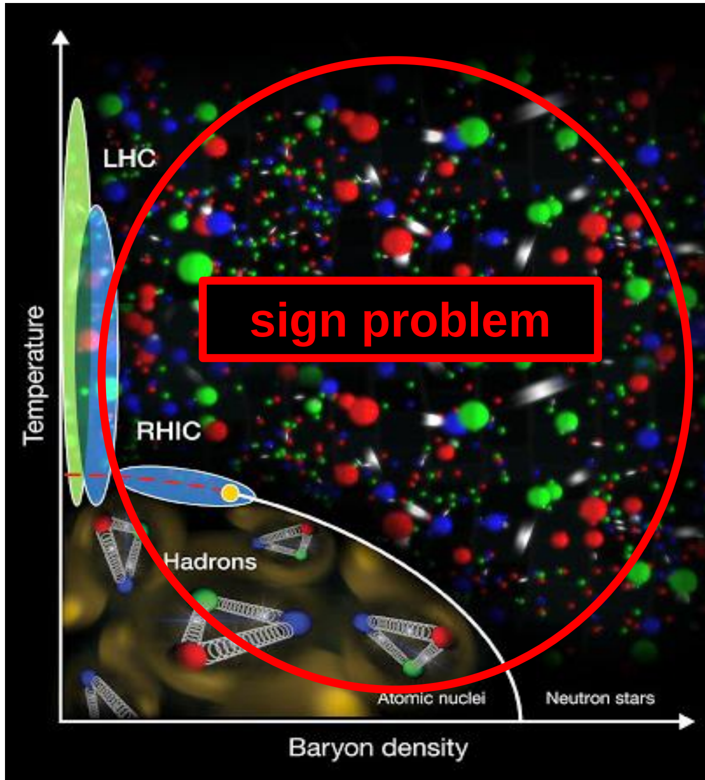


Figure credit:
BNL/RHIC, CfA

What are the challenges of classical computations?

Classical computational costs

Supercomputer usage for different fields (INCITE 2019)

→ **Lattice QCD: $\sim 40\%$**

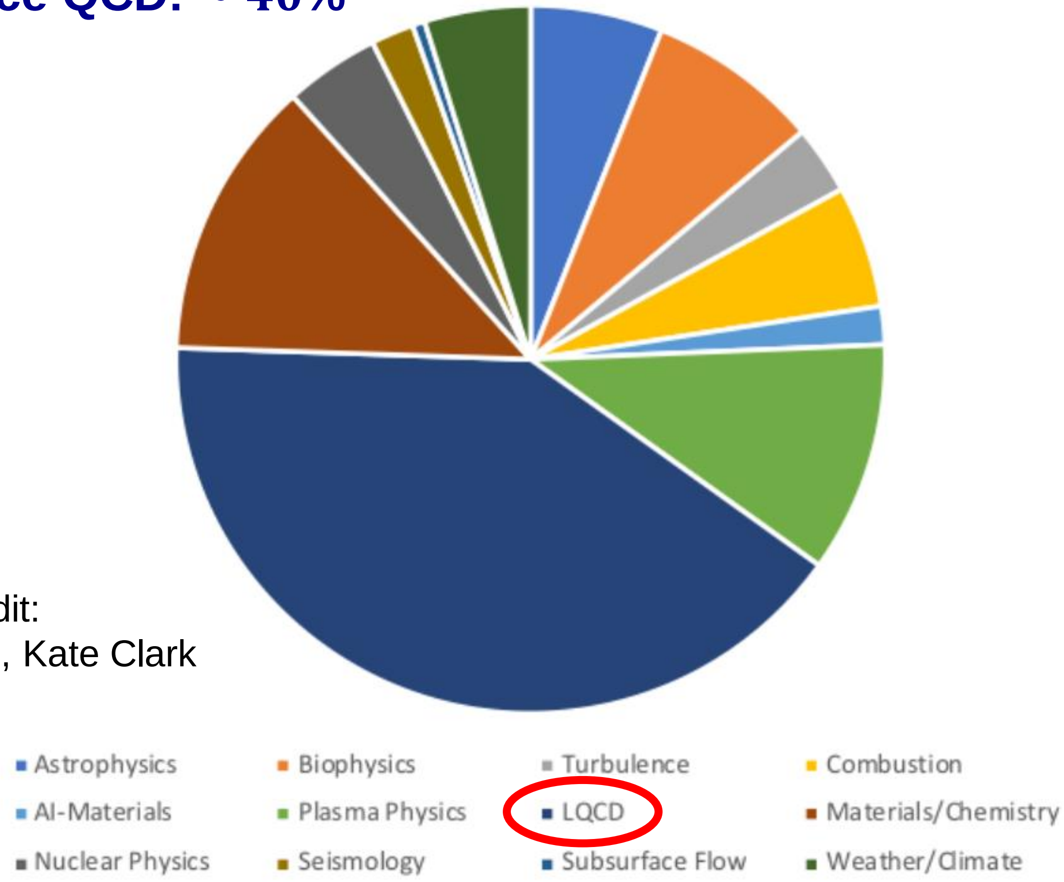


Figure credit:
Jack Wells, Kate Clark

Classical computational limitations

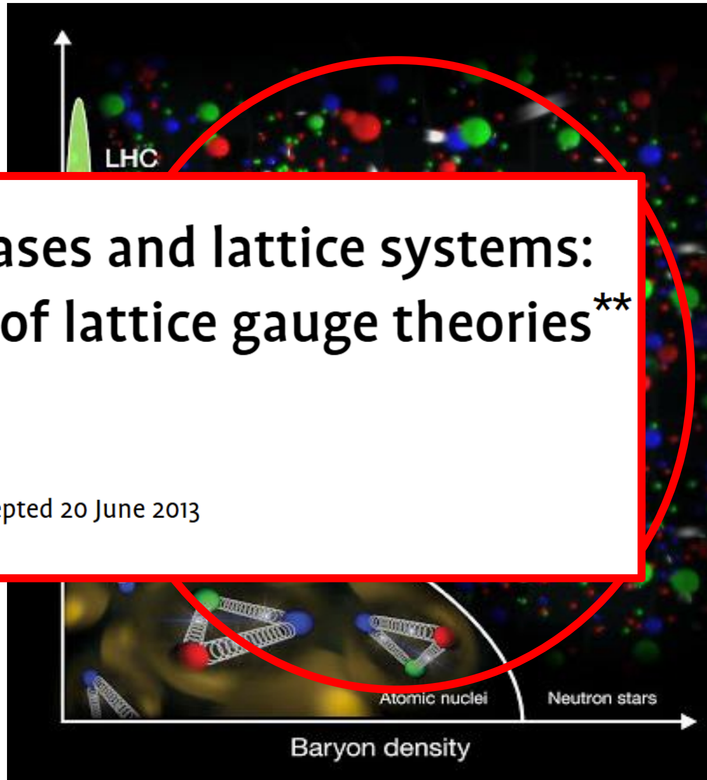
No chemical potentials, θ-terms, real-time evolution, …

→ interior of neutron stars, heavy-ion collisions, …

→ out-of-equilibrium phase transitions: early Universe, …

→ CP violation: $\theta = \pi$, …

→ …



Ultracold quantum gases and lattice systems: quantum simulation of lattice gauge theories**

Uwe-Jens Wiese[1,2,*]

Received 6 May 2013, revised 11 June 2013, accepted 20 June 2013
Published online 24 July 2013

Figure credit:
BNL/RHIC, CfA

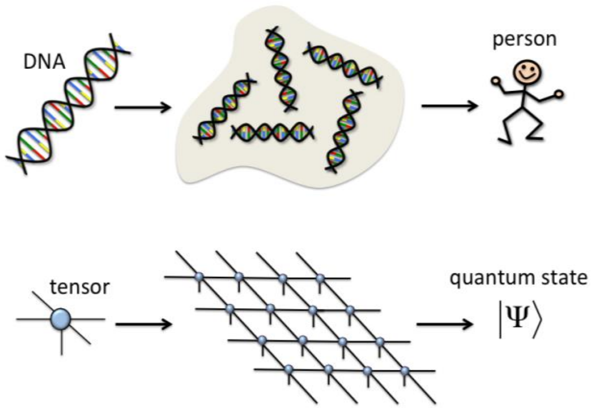
Do we really need quantum computing?

Classical approaches to tackle the sign problem	Why is(n't) classical computing enough?

Tensor network states

Compute observables: $\langle O \rangle = \langle \psi | O | \psi \rangle$, approximate $|\psi\rangle$

→ e.g. $|\psi\rangle = \sum c_{i_1 \cdots i_n} |i_1\rangle \cdots |i_n\rangle \approx \sum A^1_{i_1} \cdots A^n_{i_n} |i_1\rangle \cdots |i_n\rangle$



Orus (2014)

Other approaches

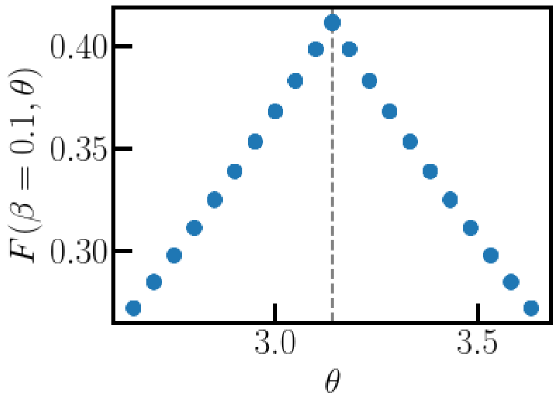
Complex Langevin, Lefschetz thimbles, ...

→ see other talks this week

Example of tensor networks

Simulate chemical potential, θ-term, real-time dynamics [1]

→ focus on 1+1D, first ansätze in 2+1D & 3+1D [2]



Nakayama, LF, et al. (2022)

Challenges

Approximation inefficient for highly entangled states

→ real-time evolution: tensor size can grow exponentially

[1] Byrnes et al. (2002), Pichler et al. (2016), Banuls et al. (2017), Schneider et al. (2021), …
LF, et al. (2020), LF, et al. (2023), Angelides, LF, et al. (2023), …, [2] Kuramashi et al. (2018), Felser et al. (2020), Magnifico et al. (2021), ...

Quantum computing: where do we stand?

Quantum hardware

Achievements

Quantum advantage: outperformed classical computers [1]

Exponential speedup of specific classical computations

Challenges

$\mathcal{O}(10 - 1000)$ qubits with $V_Q \leq 2^{21}$ → increase size

Noise → need quantum error mitigation / correction

Quantum algorithms

Future applications

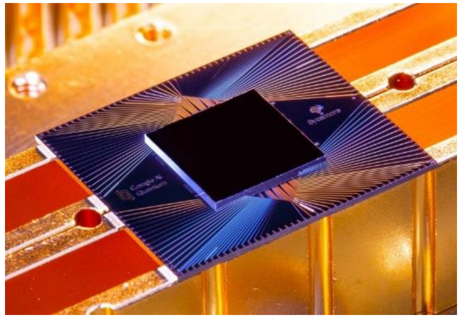
Cryptography, quantum chemistry, …

Particle / nuclear / condensed matter physics, …

Challenges

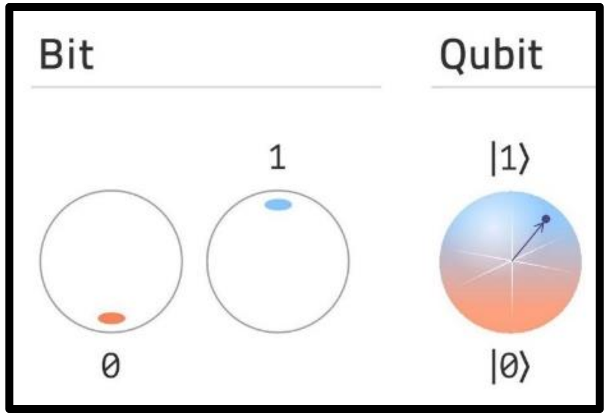
New technology → need fundamentally new algorithms

Competition → classical algorithms quickly advance

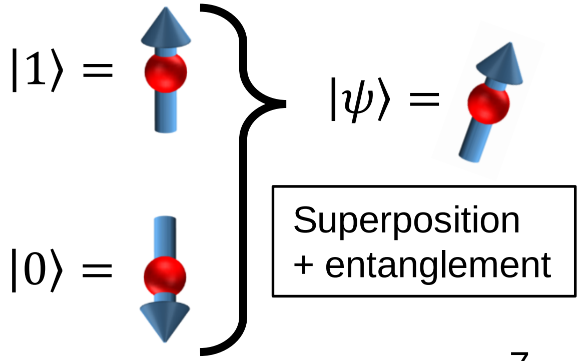


Arute et al. (2019)

Zhong et al. (2020)



Astibuag (2022)



[1] Morvan et al. (2024), earlier claims by e.g. Arute et al. (2019), Zhong et al. (2020), Madsen et al. (2022) refuted by e.g. Liu et al. (2021), Oh et al. (2024)

How can we reduce the noise?

Error mitigation versus error correction

Problem

Error rates $\mathcal{O}(0.1\% - 1\%)$ for gates and measurement

Near-term solution

Error mitigation: reduce errors, e.g., by post-processing

Long-term solution

Quantum error correction (QEC): fault-tolerant devices

Bit-flip code,[1] Shor code,[2] surface code,[3] GKP code,[4] …

Quantum threshold theorem

For QEC, need extra qubits and errors below threshold [5]

E.g. surface code needs > 1000 extra qubits for $p < 0.1\%$

Progress in quantum error correction

Many recent advances, including:

Quantum error correction below the surface code threshold

Google Quantum AI and Collaborators
(Dated: November 27, 2024)

Quantum error correction [1–4] provides a path to reach practical quantum computing by combining multiple physical qubits into a logical qubit, where the logical error rate is suppressed exponentially as more qubits are added. However, this exponential suppression only occurs if the physical error rate is below a critical threshold. Here, we present two below-threshold surface code memories on our newest generation of superconducting processors, Willow: a distance-7 code, and a distance-5 code integrated with a real-time decoder. The logical error rate of our larger quantum memory is suppressed by a factor of $\Lambda = 2.14 \pm 0.02$ when increasing the code distance by two, …

Analogy: Curing (correcting) sickness (errors)

Current: less sick (less errors) after medication (“QEC”)

Future: cured (fault-tolerant) after medication (QEC)

[1] Peres (1985), [2] Shor (1995), [3] Kitaev (1997), [4] Gottesmann et al. (2001), ...
[5] Shor (1996), Knill et al. (1998), Kitaev (2003), Aharonov et al. (2008)

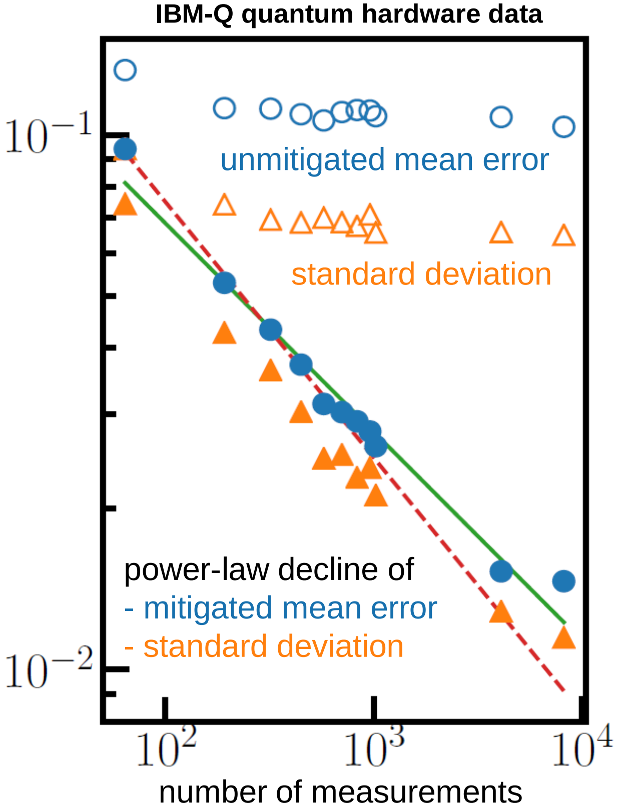
How can we reduce the noise?

Example: measurement error mitigation

Operator rescaling method[1]

Benchmark: Z and $Z_1 Z_2$ operators on IBM-Q hardware

Result: measurement error reduced by factor 10



LF et al. (2020)

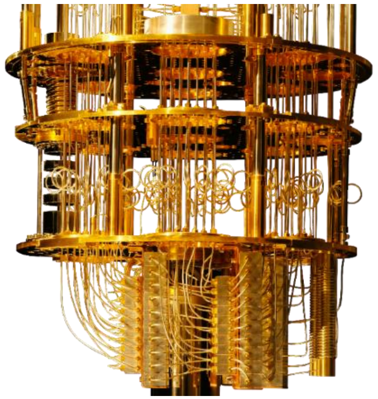


Figure credit: Graham Carlow

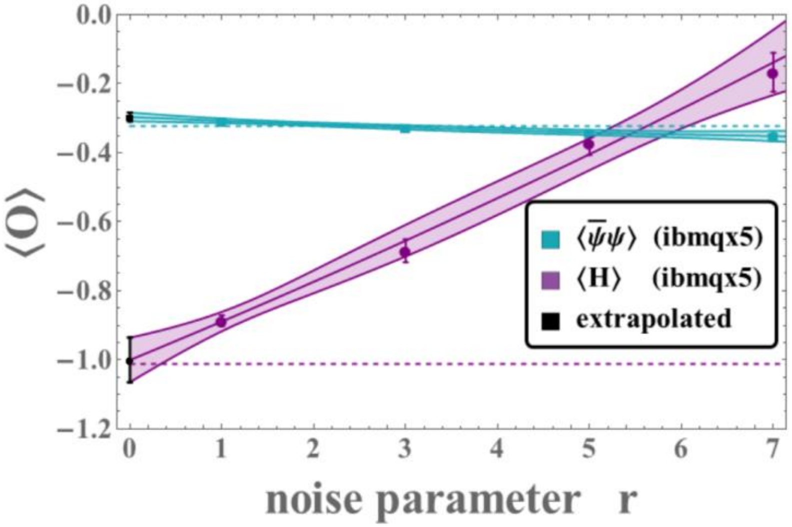
Example: gate error mitigation

Other mitigation techniques

Zero-noise extrapolation,[2] randomized compiling,[3] quasi-probability decomposition,[4] … (see other talks)

Lattice field theory applications

E.g. zero-noise extrapolation for lattice Schwinger model:



Klco et al. (2018)

[1] Kandala et al. (2017), Yeter-Aydeniz et al. (2019), LF et al. (2020), ...,
[2] Temme et al. (2017), Li et al. (2017), ..., [4] Temme et al. (2017), ...

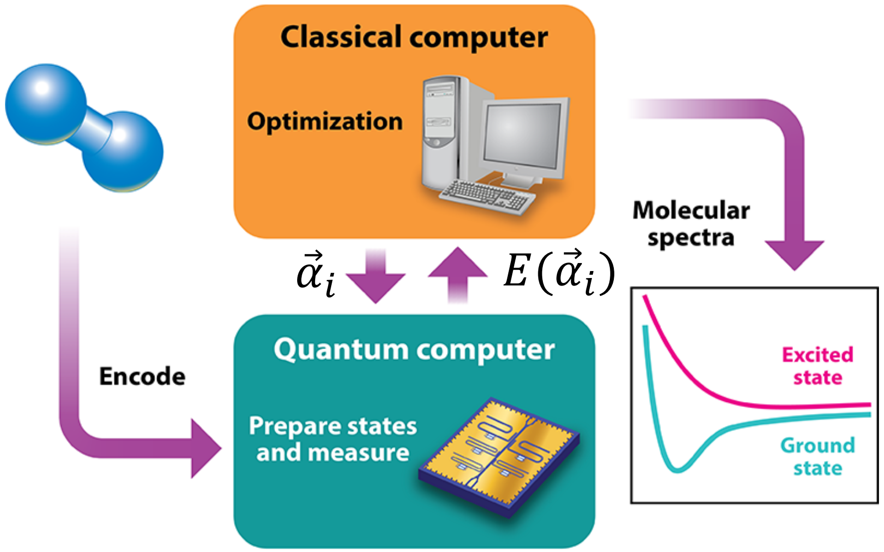
Which quantum algorithms does one currently use?

Example: hybrid quantum-classical algorithms

Key concept

Classical computer: main computation

Quantum computer: classically hard/intractable part



Sim et al. (2018)

[1] Peruzzo et al. (2014);
[2] Nicoli, Anders, LF, et al. (2023), Anders, et int., LF, et al. (2024)

Variational Quantum Eigensolver (VQE) [1]

Goal

Find ground state of problem Hamiltonian $\mathcal{H}$

Variational approach

Minimize $E(\vec{\alpha}) = \langle\psi(\vec{\alpha})|\mathcal{H}|\psi(\vec{\alpha})\rangle$ w.r.t. parameters $\vec{\alpha}$

Quantum computer

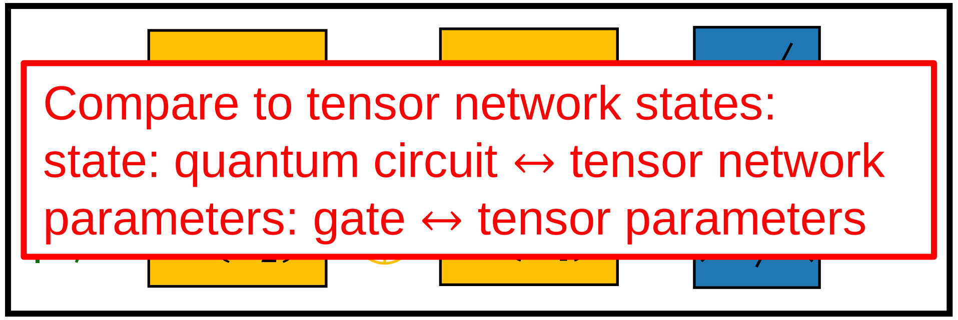
Given $\vec{\alpha}_i$, prepare $|\psi(\vec{\alpha})\rangle$ and measure $E(\vec{\alpha}_i)$

Classical computer

Given $E(\vec{\alpha}_i)$, find optimized parameters $\vec{\alpha}_{i+1}$

→ optimization using machine learning [2]

$|\psi(\vec{\alpha})\rangle =$



Compare to tensor network states:
state: quantum circuit ↔ tensor network
parameters: gate ↔ tensor parameters

Quantum Computing for High-Energy Physics
State of the Art and Challenges
Summary of the QC4HEP Working Group

Alberto Di Meglio,[1,*] Karl Jansen,[2,3,†] Ivano Tavernelli,[4,‡] Constantia Alexandrou,[5,3] Srinivasan Arunachalam,[6] Christian W. Bauer,[7] Kerstin Borras,[8,9] Stefano Carrazza,[10,1] Arianna Crippa,[2,11] Vincent Croft,[12] Roland de Putter,[6] Andrea Delgado,[13] Vedran Dunjko,[12] Daniel J. Egger,[4] Elias Fernández-Combarro,[14] Elina Fuchs,[1,15,16] Lena Funcke,[17] Daniel González-Cuadra,[18,19] Michele Grossi,[1] Jad C. Halimeh,[20,21] Zoë Holmes,[22] Stefan Kühn,[2] Denis Lacroix,[23] Randy Lewis,[24] Donatella Lucchesi,[25,26,1] Miriam Lucio Martinez,[27,28] Federico Meloni,[8] Antonio Mezzacapo,[6] Simone Montangero,[25,26] Lento Nagano,[29] Voica Radescu,[30] Enrique Rico Ortega,[31,32,33,34] Alessandro Roggero,[35,36] Julian Schuhmacher,[4] Joao Seixas,[37,38,39] Pietro Silvi,[25,26] Panagiotis Spentzouris,[40] Francesco Tacchino,[4] Kristan Temme,[6] Koji Terashi,[29] Jordi Tura,[12,41] Cenk Tüysüz,[2,11] Sofia Vallecorsa,[1] Uwe-Jens Wiese,[42] Shinjae Yoo,[43] and Jinglei Zhang[44,45]

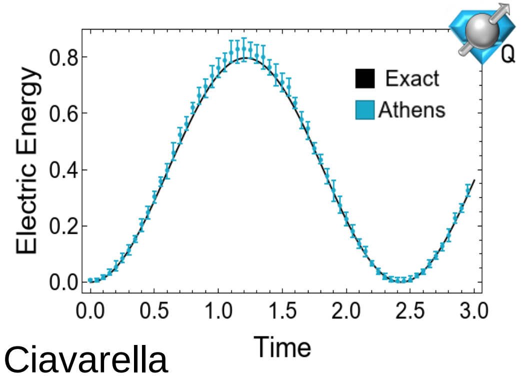
Quantum computers offer an intriguing path for a paradigmatic change of computing in the natural sciences and beyond, with the potential for achieving a so-called quantum advantage—namely, a significant (in some cases exponential) speedup of numerical simulations. The rapid development of hardware devices with various realizations of qubits enables the execution of small-scale but representative applications on quantum computers. In particular, the high-energy physics community plays a pivotal role in accessing the power of quantum computing, since the field is a driving source for challenging computational problems. This concerns, on the theoretical side, the exploration of models that are very hard or even impossible to address with classical techniques and, on the experimental side, the enormous data challenge of newly emerging experiments, such as the upgrade of the Large Hadron Collider. In this Roadmap paper, led by CERN, DESY, and IBM, we provide the status of high-energy physics quantum computations and give examples of theoretical and experimental target benchmark applications, which can be addressed in the near future. Having in mind hardware with about 100 qubits capable of executing several thousand two-qubit gates, where possible, we also provide resource estimates for the examples given using error-mitigated quantum computing. The ultimate declared goal of this task force is therefore to trigger further research in the high-energy physics community to develop interesting use cases for demonstrations on near-term quantum computers.

Which field theories have already been simulated?

Experimental results on “public” QC

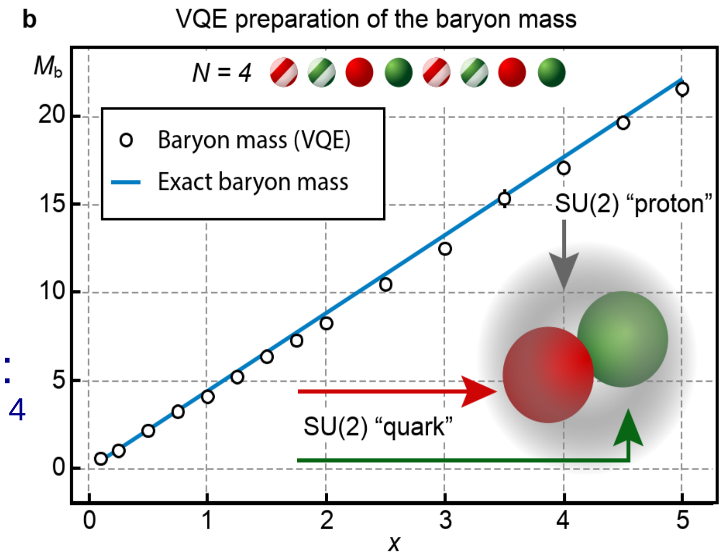
Superconducting qubits

Real-time evolution: Schwinger model,[1] SU(2),[2] SU(3),[3] ...



Ciavarella et al. (2019)

Variational computation: SU(2) “hadron” masses [4]



Experimental results on “private” QC

Trapped ions

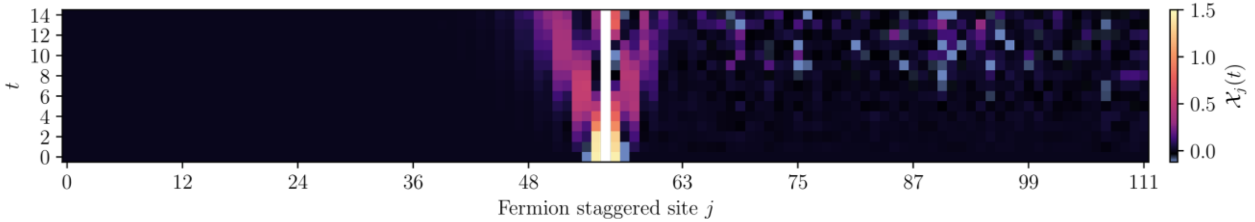
Real-time evolution: Schwinger model, [5]…

Cold atoms

Real-time evolution: Schwinger model,[6] Bose-Hubbard,[7] ...

Superconducting qubits

Hadron dynamics: Schwinger model with > 100 qubits,[8] …



[1] Klco et al. (2018), de Jong et al. (2021), …, [2] Klco et al. (2019), …, [3] Ciavarella et al. (2019), …, [4] Atas et al. (2021), …,
[5] Martinez et al. (2016), Nguyen et al. (2021), …, [6] Yang et al. (2020), Mil et al. (2020), ..., [7] Bloch et al. (2012), …, [8] Farrell et al. (2024), …

How to address the sign problem in 1+1D and 2+1D?

Sign-problem-afflicted regimes	Lattice fermions

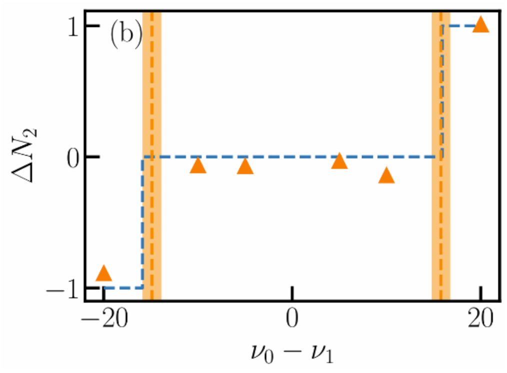
Topological terms

1+1D Abelian gauge theories with θ-term [1]

2+1D U(1) gauge theory with Chern-Simons term [2]

Chemical potentials

1+1D U(1) gauge theory with chemical potentials ν_f [3]



→ extension to 2+1D: [4] see talk by Emil Rosanowski

Staggered fermions

“Hamiltonian community” focuses on staggered fermions

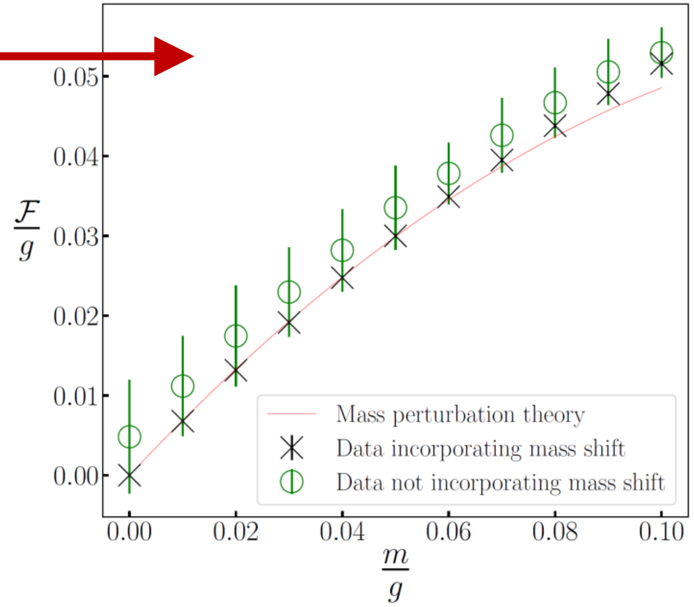
→ however, no rooting trick → need Wilson fermions…?

Wilson fermions

1+1D implementation [5]

→ extension to 2+1D [4]

→ relevant for hybrid MCMC-quantum computations [6]



[1] Angelides et al. (2023), Crane, et int., LF, et al. (2024); … [2] Peng, Diamantini, LF, et al., (2024); [3] Schuster, Kühn, LF, et al. (2023); [4] ongoing work with Rosanowski et al.; [5] Angelides, LF, et al. (2023); [6] Crippa, Romiti, LF, et al. (2024); Avkhadiev, LF, et al. (2024); …

Outlook: how to address the sign problem in 3+1D?

Example: U(1) lattice gauge theory with θ-term

Goal

Study phase transition at $\theta = \pi$ and large $g = \beta^{-1/2}$

Theoretical requirements

Derive 3+1D θ-term in Hamiltonian lattice formulation [1]

Develop Hamiltonian algorithms for 1+1D,[2] 2+1D,[3] 3+1D

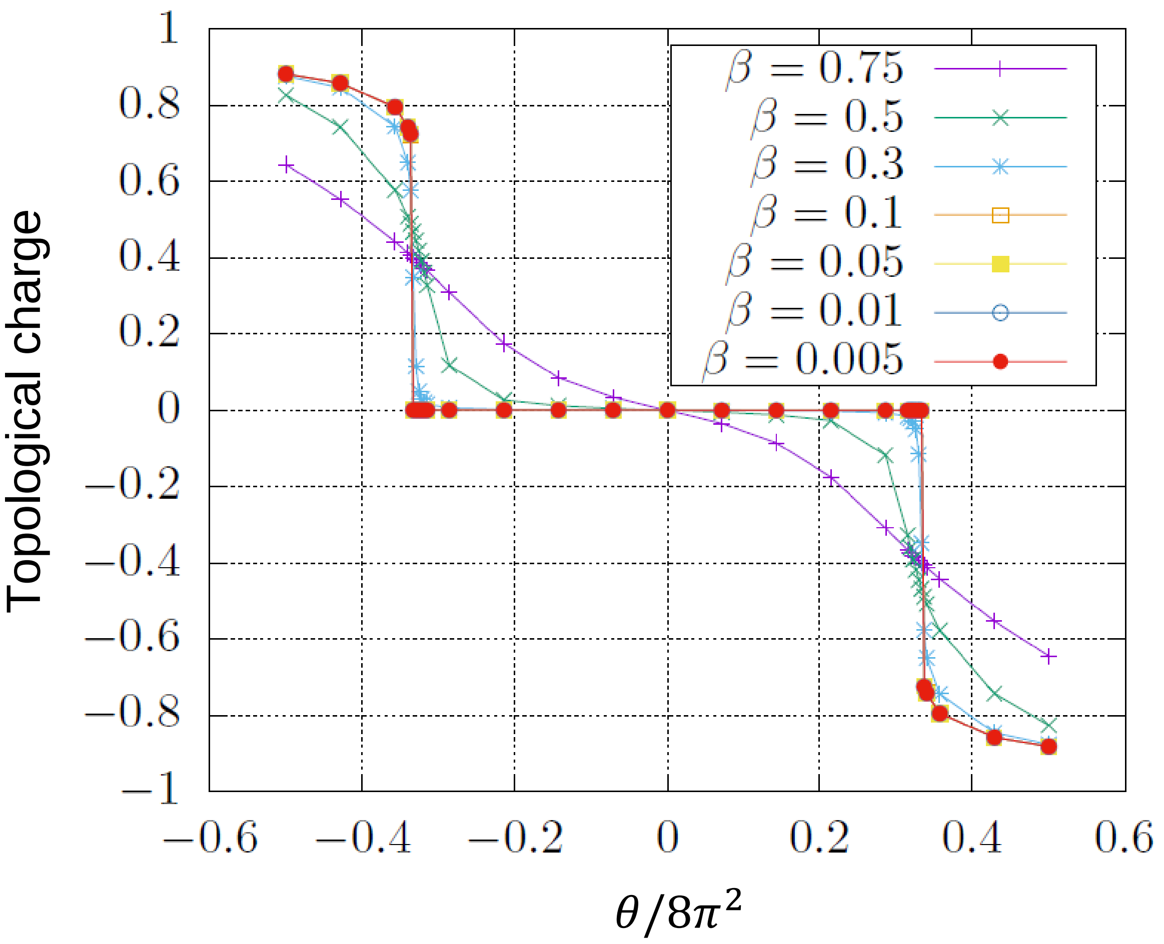
First classical computations

Study phase transition with exact diagonalization [1]

Future work

Larger volumes: tensor network & quantum computations

First classical results for a single cube



[1] Kan, LF, Kühn, Zhang, Haase, Muschik, Jansen (2021)
[2] Many papers by various groups…; Schuster, Kühn, LF, et al. (2023); …
[3] Crippa, Romiti, LF, et al. (2024); Crane, et int., LF, et al. (2024); …
Reviews: LF, et al., (2023); …

Summary: where do we stand, where will we go?

The path to go…	A rough sketch…

State of the art

First quantum simulations of 1+1D & 2+1D lattice theories

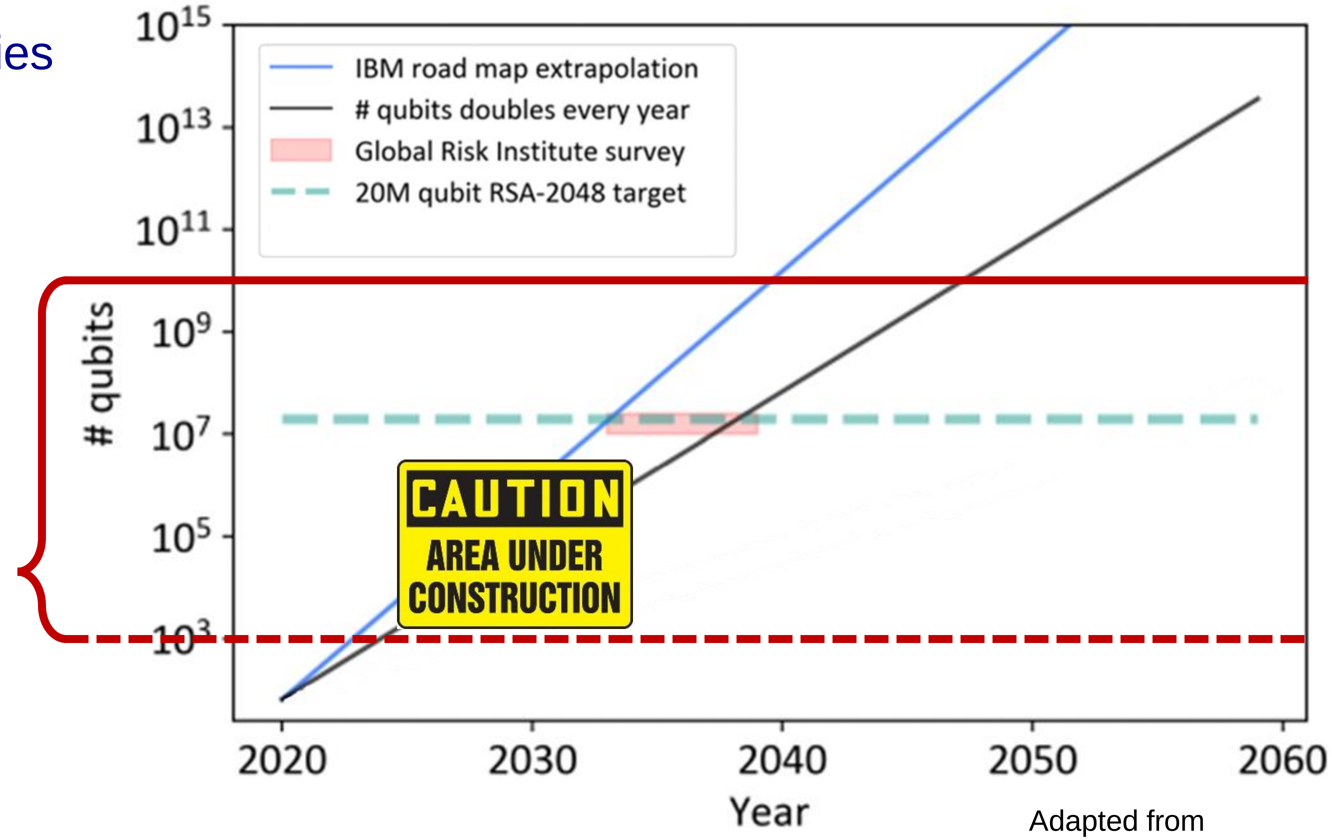
Noise mitigation, circuit optimization, new algorithms

Future goals

Quantum simulations for 2+1D & 3+1D theories

To evade sign problem, … of Lattice QCD and beyond

Analogous to Lattice QCD from 1980s to 2020s?



Adapted from Groenland (2024)

Thanks to my collaborators and my group

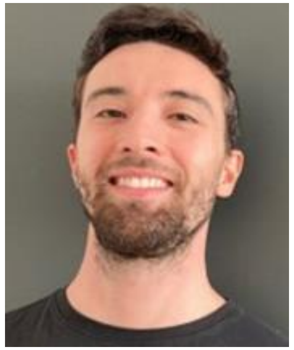
Karl Jansen
(DESY)

Stefan Kühn
(DESY)

Carsten Urbach
(Bonn U.)

Christine Muschik
(Waterloo U.)

Arianna Crippa
(DESY)



Simone Romiti
(Bern U.)

Di Luo
(UCLA)

Eleanor Crane
(MIT)

and more…

Thanks to you for listening! Questions?

Backup: examples of quantum advantage

Early claims of quantum advantage	Current status of quantum advantage

Classical simulations of circuit [1] / boson [2] sampling

Closing the "Quantum Supremacy" Gap: Achieving Real-Time Simulation of a Random Quantum Circuit Using a New Sunway Supercomputer

a new milestone for classical simulation of quantum circuits; and reduces the simulation sampling time of Google Sycamore to 304 seconds, from the previously claimed 10,000 years.

Classical algorithm for simulating experimental Gaussian boson sampling

modest computational resources. We exhibit evidence that our classical sampler can simulate the ideal distribution better than the experiment can, which calls into question the claims of experimental quantum advantage.

Quantum-classical race

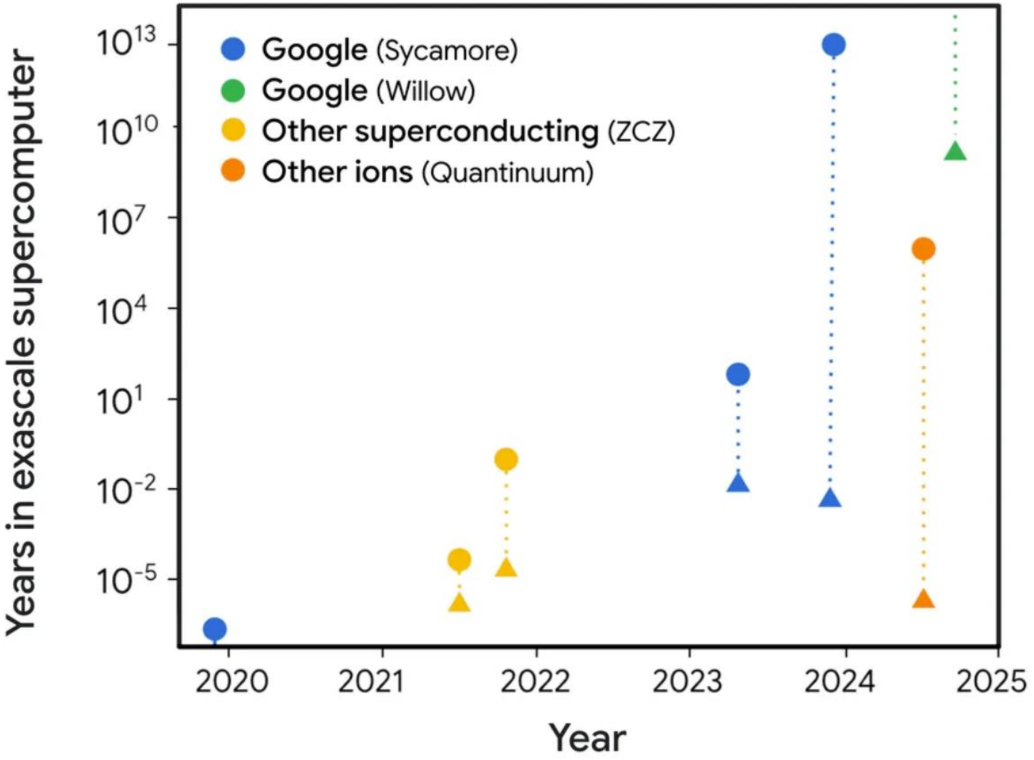
Algorithms and hardware quickly advance on both sides

For exponentially hard problems

Small quantum step ↔ giant classical leap

[1] Liu et al. (2021), [2] Oh et al. (2024), [3] Neven (2024)

Benchmark of random circuit sampling [3]



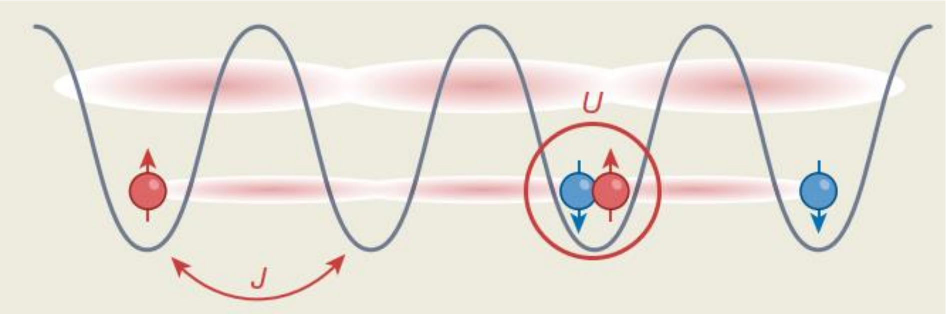
Computational costs are heavily influenced by available memory. Our estimates therefore consider a range of scenarios, from an ideal situation with unlimited memory (▲) to a more practical, embarrassingly parallelizable implementation on GPUs (●).

Backup: do we really need quantum computing?

Example: 1+1D Bose-Hubbard model

Hamiltonian

$$\mathcal{H} = \sum_j -J\left(\hat{a}_j^\dagger \hat{a}_{j+1} + h.c.\right) + \frac{U}{2}\hat{n}_j(\hat{n}_j - 1)$$



Real-time simulation [1]

Analog quantum simulator: ultracold atoms

Classical benchmark: tensor networks (MPS)

Experimental results

“the controlled [quantum] dynamics runs for longer times than present classical algorithms can keep track of” [1]

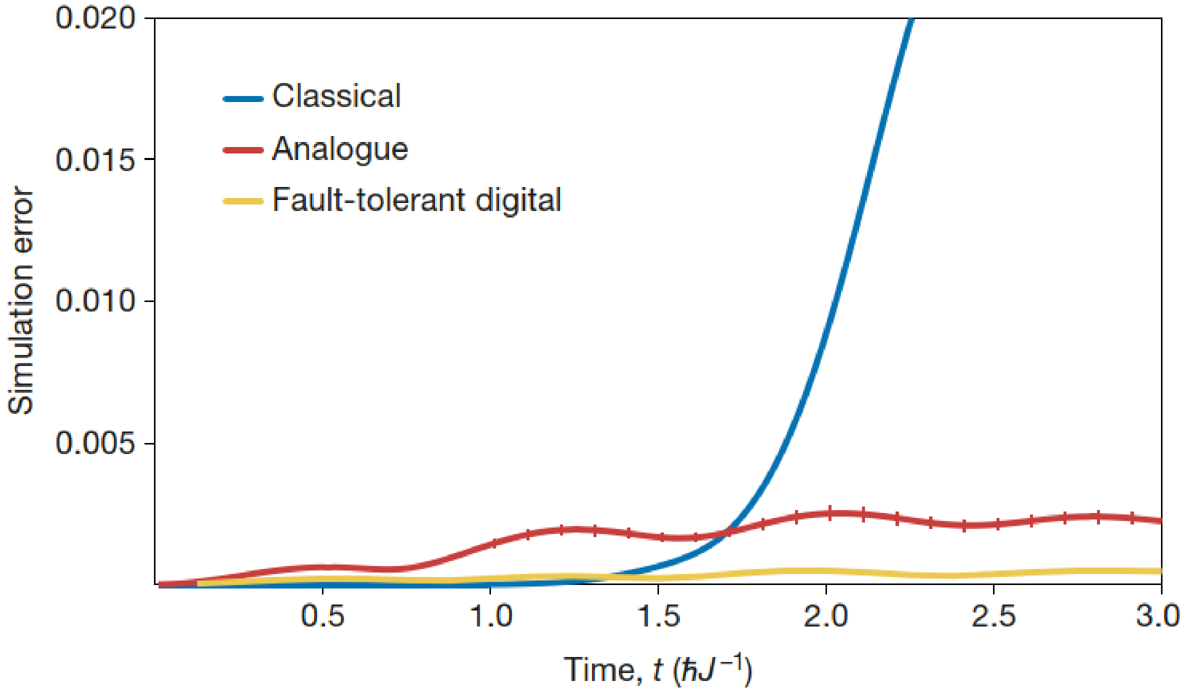
[1] Trotzky et al. (2012)

Why is(n’t) classical computing enough?

Challenges

No efficient parametrization of highly entangled states

In real-time evolution, tensor size can grow exponentially



Daley et al. (2022)

Backup: dealing with gauge fields

Infinite Hilbert space	**Gauge invariance**

Infinite Hilbert space

Problem

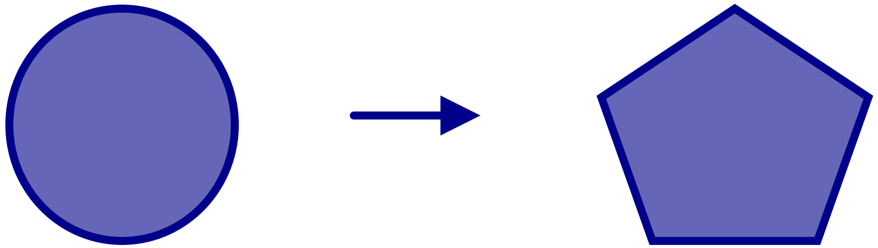
Continuous gauge theory requires ∞-dim. Hilbert space

First approach

Integrate out gauge field: only possible in 1+1D

Second approach

Approximate gauge group:[1] e.g. $U(1) \rightarrow \mathbb{Z}_n$



Third approach

Truncate irreps:[2] e.g. for $F_j|l\rangle = |l\rangle$, use finite $|l| < L$

Many more approaches…

Gauge invariance

Problem

Gauge invariance requires imposing local constraints

First approach

Penalize unphysical states,[3] e.g. $\mathcal{H}_{\text{penalty}} = \lambda\left(\sum_{j=1}^{N} Q_j\right)^2$

Second approach

Analytically solve Gauß law at every site [4]

Third approach

Gauge-invariant formulation, e.g. loop-string-hadron [5]

Many more approaches…

[1] Zohar et al. (2013), ..., [2] Horn (1981), ..., [3] Banerjee et al. (2012), ..., [4] Klco et al. (2018), ..., [5] Raychowdhury, Stryker (2020)

Backup: measuring the energy on a quantum computer

Example: massless Schwinger model

Original Hamiltonian

$$\mathcal{H} = -\frac{i}{2a}\sum_{n=0}^{N-2}\left(\phi_n^\dagger e^{i\theta_n}\phi_{n+1} - \text{h.c.}\right) + \frac{ag^2}{2}\sum_{n=0}^{N-2} F_n^2$$

with $\theta_n = -aqA_n^1,\ gF_n = E_n,\ [\theta_n, L_m] = i\delta_{nm},\ \theta_n \in [0,2\pi]$

Eliminate θ_n

$\phi_n^\dagger e^{i\theta_n}\phi_{n+1} \rightarrow \phi_n^\dagger \phi_{n+1}$ from gauge transformation:

$\phi_n \rightarrow \left(\prod_{k=0}^{n-1} e^{-i\theta_n}\right)\phi_n$ and $\phi_n^\dagger \rightarrow \phi_n^\dagger\left(\prod_{k=0}^{n-1} e^{i\theta_{n-k}}\right)$

Eliminate F_n

$F_n = \sum_{k=0}^{n} Q_k$ from solving Gauß law (for OBC):

$F_n - F_{n-1} = Q_n\ \forall n$, where $Q_n = \phi_n^\dagger\phi_n - \frac{1}{2}[1-(-1)^n]$

[1] Banks et al. (1976), Hamer et al. (1997)

Mapping the model to qubits

Dimensionless spin Hamiltonian [1]

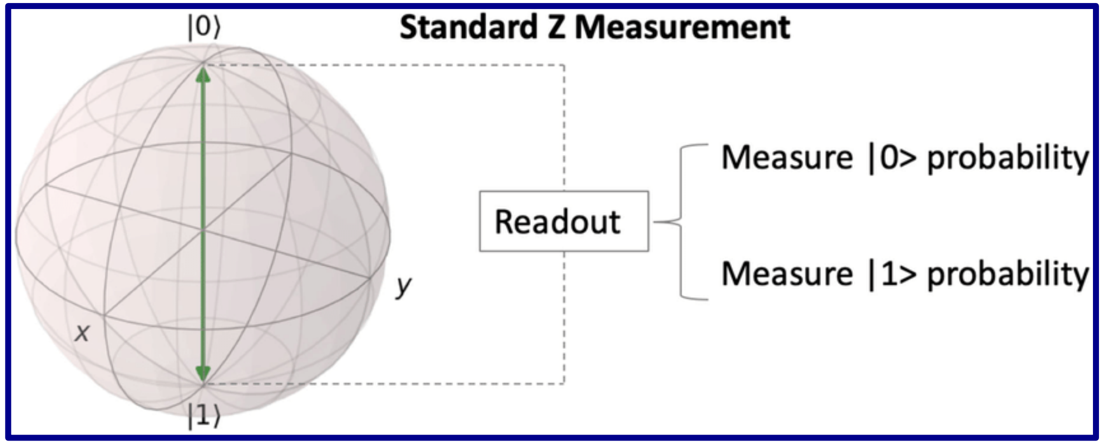
$$\mathcal{H} = x\sum_{n=0}^{N-2}\left(\sigma_n^+\sigma_{n+1}^- + \sigma_n^-\sigma_{n+1}^+\right) + \frac{1}{2}\sum_{n=0}^{N-2}\left\{\sum_{k=0}^{n}[(-1)^k + \sigma_k^z]\right\}^2$$

from mapping $\phi_n^\dagger\phi_{n+1} \rightarrow \sigma_n^+\sigma_{n+1}^-$ and $\phi_n^\dagger\phi_n \rightarrow \frac{1}{2}(\sigma_n^z + \mathbb{I})$

Quantum computer

Measurement of $\langle\psi|\boldsymbol{O}|\psi\rangle$ with $\boldsymbol{O} \in \{\mathbb{I}, \sigma^z\}^{\otimes N}$

$\mathcal{H} = \sum_k h_k U_k^* \boldsymbol{O}_k U_k$ with $U_k^*\boldsymbol{O}_k U_k \in \{\mathbb{I}, \sigma^x, \sigma^y, \sigma^z\}^{\otimes N}$

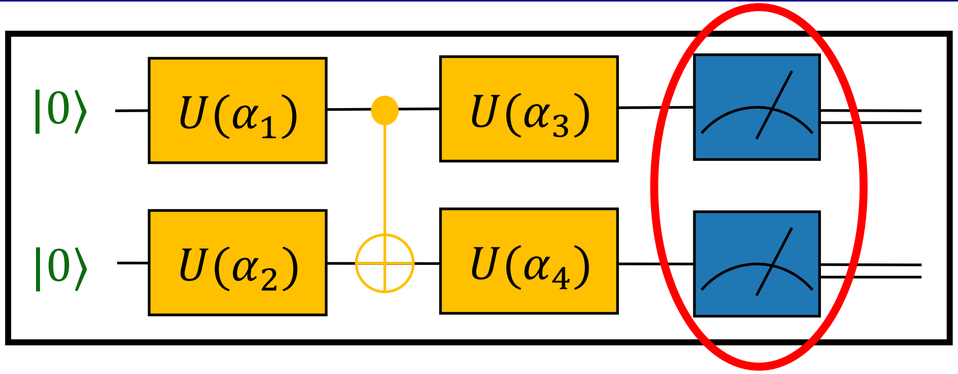


Gokhale et al. (2020)

Backup: how can we mitigate the quantum errors?

Example: measurement error mitigation

$|\psi(\vec{\alpha})\rangle =$



Operator rescaling method[1]

Goal

mitigate bit-flip errors during readout: $0 \xrightarrow{p_0} 1$ or $1 \xrightarrow{p_1} 0$

Method

replace operators by noisy operators: $\langle\tilde{\psi}|\boldsymbol{O}|\tilde{\psi}\rangle \to \langle\psi|\tilde{O}|\psi\rangle$

Readout	Bit Flips	Probability	Noisy Operator
correct	$0 \to 0,\ 1 \to 1$	$(1-p_0)(1-p_1)$	$\tilde{O} = \boldsymbol{Z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
incorrect … for both outcomes	$0 \to 1,\ 1 \to 0$	$p_0 p_1$	$\tilde{O} = -Z = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$
… for outcome 0	$0 \to 1,\ 1 \to 1$	$p_0(1-p_1)$	$\tilde{O} = -\mathbb{I} = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$
… for outcome 1	$0 \to 0,\ 1 \to 0$	$(1-p_0)p_1$	$\tilde{O} = \mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

Total noisy operator: $\tilde{O}$

$$= (1-p_0)(1-p_1)\boldsymbol{Z} + p_0 p_1(-Z) + p_0(1-p_1)(-\mathbb{I}) + (1-p_0)p_1\mathbb{I}$$

Rescaled (zero-noise) operator:

$$\to \boldsymbol{Z} = \frac{1}{1-p_0-p_1}\tilde{O} - \frac{p_1-p_0}{1-p_0-p_1}\mathbb{I}$$

[1] Single Z operator: Kandala et al. (2017), strings of Z operators: Yeter-Aydeniz et al. (2019), generalizations: LF, Hartung, Jansen, Kühn, Stornati, Wang (2020), (2021); Alexandrou, LF, et al. (2021a), (2021b)

Backup: quantum volume

Concept	Timeline

Motivation

Number of noisy qubits: no good performance measure

New performance measure

Measure capabilities and error rates of quantum device

IBM's definition

$$\log_2 V_Q = \arg\max_{n \leq N} \{\min[n, d(n)]\}$$

Example

Successfully run circuit of depth $d = 8$ on $n = 8$ qubits: quantum volume is $V_Q = 2^8 = 256 \rightarrow$ size of state space

"Success"

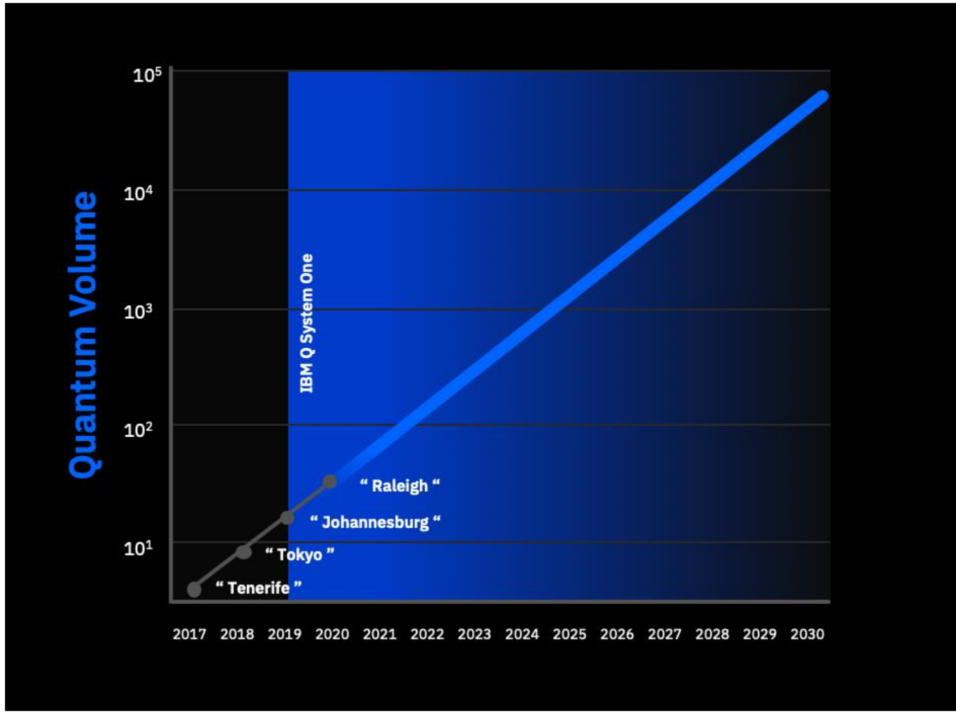
Most likely outputs of the circuit are computed correctly 67% of the time with a 2σ confidence interval

Last three years

Early 2020: $V_Q = 32$ (IBM) for $d = 5$, $n = 5$

Early 2021: $V_Q = 512$ (Honeywell) for $d = 9$, $n = 9$

Early 2022: $V_Q = 4096$ (Quantinuum) for $d = 12$, $n = 12$



Chow, Gambetta (2020)

Backup: TRG results for free energy of CP(1) model

Free energy

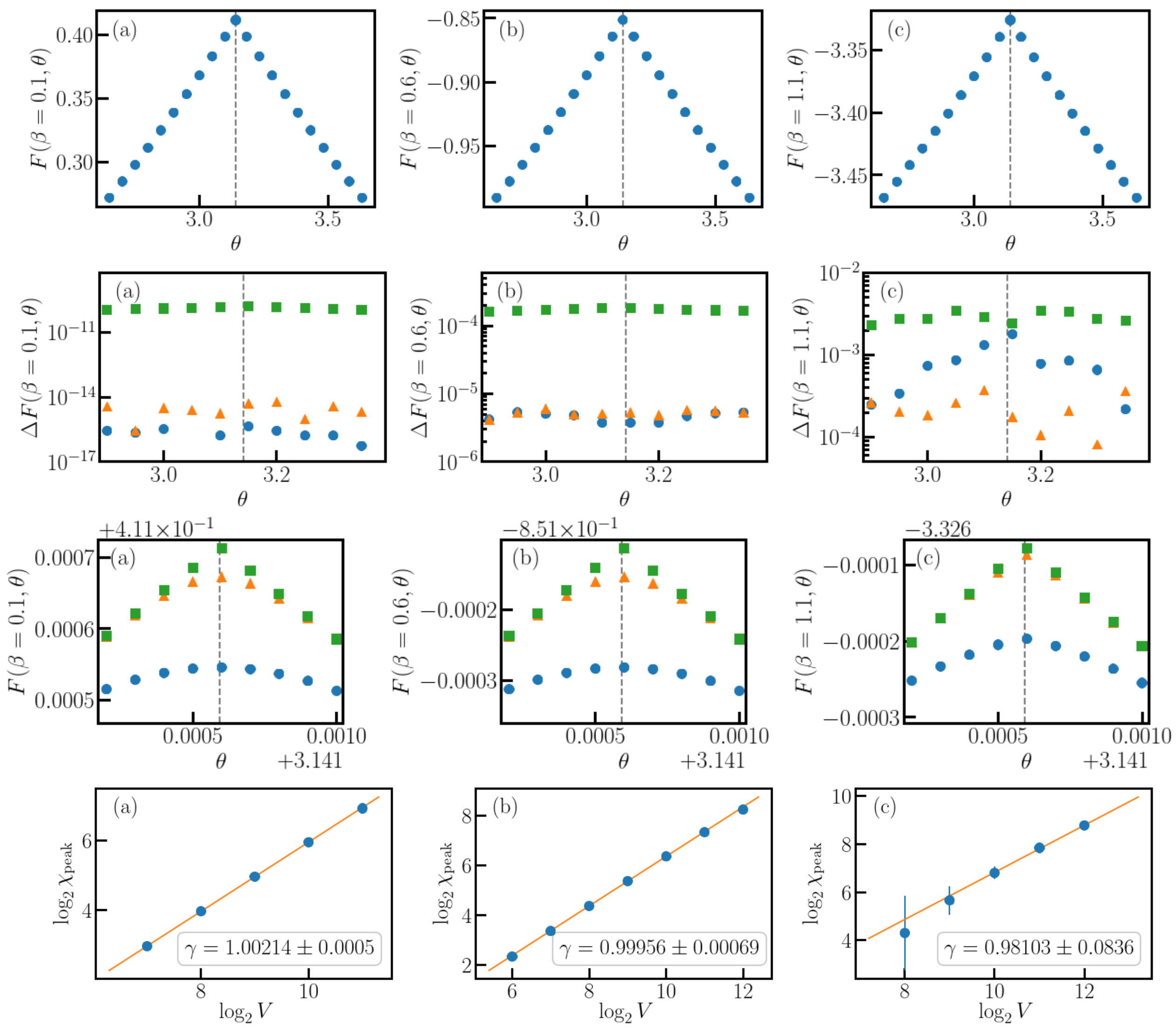
- $F(\beta,\theta) = -\frac{1}{\beta V}\log \mathcal{Z}_\theta$
- $V = 2^{24}$, $D = 80$, $\beta = 0.1, 0.6, 1.1$

Errors ΔF

- Blue: $D = 112$, $k_{\mathrm{max}} = 2$, $\chi_\theta = 2$ (truncate CE)
- Orange: $D = 112$, $k_{\mathrm{max}} = 3$, $\chi_\theta = 2$
- Green: $D = 112$, $k_{\mathrm{max}} = 2$, $\chi_\theta = 4$

Volumes

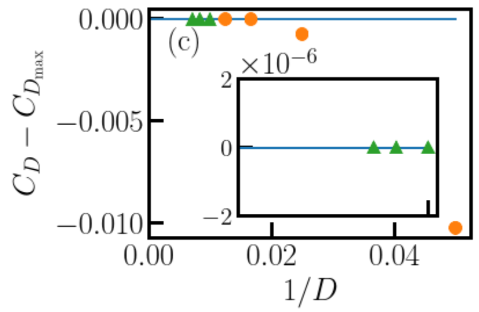
- Blue: $V = 2^{12}$, Orange: $V = 2^{14}$, Green: $V = 2^{24}$
- Susceptibility: $\chi(\beta,\theta) = -\beta \frac{\partial^2 F(\beta,\theta)}{\partial \theta^2}$ at $\theta = \pi$
- $\chi_{\mathrm{peak}} \propto V^\gamma$ with $\gamma = 1$ for first-order transition



Backup: MPS extrapolation procedure

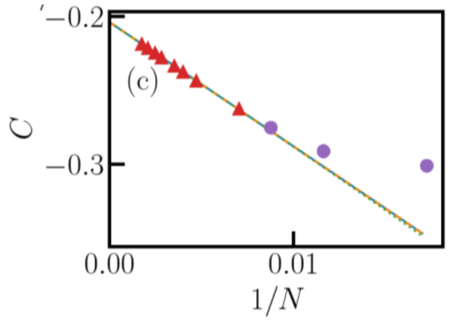
Bond dim.

- Extrapolation: to infinite bond dimension, $1/D \to 0$
- Errors: $\delta O = \sqrt{\left(\left|O_{D_{\max}} - O_{D=\infty}\right|/2\right)^2 + \left(\sqrt{\eta} O_{D_{\max}}\right)^2}$, where $\eta = 10^{-10}$



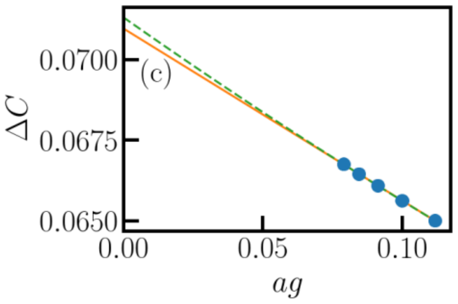
Inf. volume

- Extrapolation: to infinite-volume limit, $1/N \to 0$
- Errors: from fitting coefficient and from comparing to next-order polynomial



Continuum

- Extrapolation: to the continuum, $ag \to 0$
- Errors: from fitting coefficient and from comparing to next-order polynomial
- Total error: around 1% for UV-finite chiral condensate ΔC



Plots: $x = 160$, $m/g = 0.07$, $N = 354$, $\theta = 0.2$

Backup: why are topological terms in 2+1D interesting?

3+1D: Topological θ-Term	2+1D: Topological Chern-Simons Term
Relevance Strong CP problem, Grand Unified Theories, …	**Relevance** Quantum Hall effect, fermion/boson dualities, …
Parameter Continuous angle $\theta \in [0,2\pi)$	**Parameter** [1] Quantized Chern-Simons coupling $k \in \mathbb{Z}$, called “level”
Degeneracy Ground state has no θ-dependent degeneracy	**Degeneracy** [2] Ground state has k-fold degeneracy on a torus
Mass generation No mass from θ-term, only from QCD and Higgs	**Mass generation** [3] Photon mass from Chern-Simons term: $m_\gamma = ke^2/2\pi$ → “Maxwell-Chern-Simons (MCS) theory”

[1] Pisarski (1986)
[2] Eliezer, Semenoff (1992)
[3] Deser, Jackiw, Templeton (1982)

Backup: how to formulate MCS theory on the lattice?

Problem	State-of-the-Art

Continuum: 2+1D Chern-Simons term

$$S_{CS}(A) = -\frac{ik}{4\pi}\int d^3x \epsilon^{\mu\nu\rho} A_\mu \partial_\nu A_\rho$$

Naïve lattice discretization:

$$S_{CS}(A) = -\frac{ik}{4\pi} a^2 d\tau \sum_{x\in \text{sites}} \epsilon^{\mu\nu\rho} A_{x;\mu}\Delta_\nu A_{x+\hat{\mu};\rho}$$

Problem: compact gauge fields → monopoles
→ Chern-Simons term violates gauge invariance! [1]

[1] Pisarski (1986), Affleck et al. (1989)

Lattice formulation of non-compact MCS Hamiltonian [2]
However, non-compact gauge field → no simulations

Lattice formulation of compact CS Hamiltonian [3]
Villain approach, monopoles eliminated → gauge invariant
However, non-commuting geometry → no simulations

Our goal: Derive compact MCS lattice Hamiltonian
Paves the way for simulations on (quantum) computers

[2] Lüscher (1989), …
[3] Jacobson, Sulejmanpasic (2024)

Backup: compact MCS Lattice Hamiltonian

2+1D Maxwell Lattice Hamiltonian + Extension

Magnetic field term: similar to QED (without monopoles)
Electric field term: modified by Chern-Simons term

Compact Gauge Fields

Gauge configurations: can take values in $(-\infty, +\infty)$
Compactness: ensured by constraints on Hilbert space

$$\hat{H} = \frac{e^2}{2a^2} \sum_{\text{plaquettes}} \left[\left(\hat{p}_1 - \left(\frac{ka^2}{4\pi}\right) \hat{A}_2 \right)^2 + \left(\hat{p}_2 + \left(\frac{ka^2}{4\pi}\right) \hat{A}_1 \right)^2 \right]$$

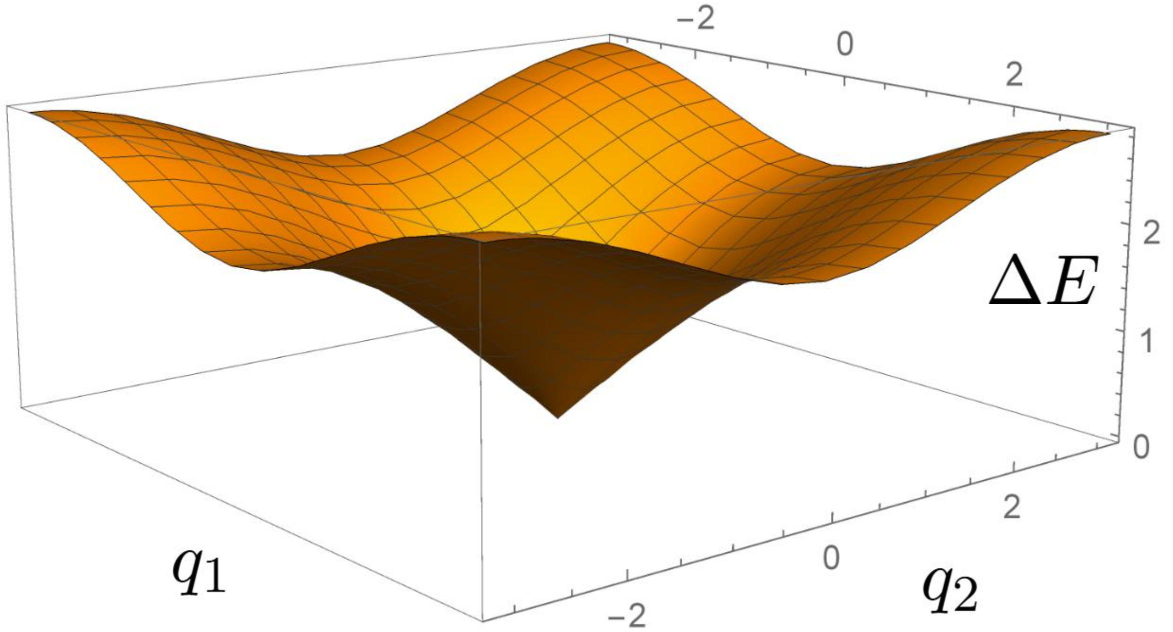
$$+ \frac{1}{2e^2} \sum_{\text{plaquettes}} \left(-\hat{A}_1 \; -\hat{A}_2 \; \hat{A}_2 \; \hat{A}_1 \right)^2$$

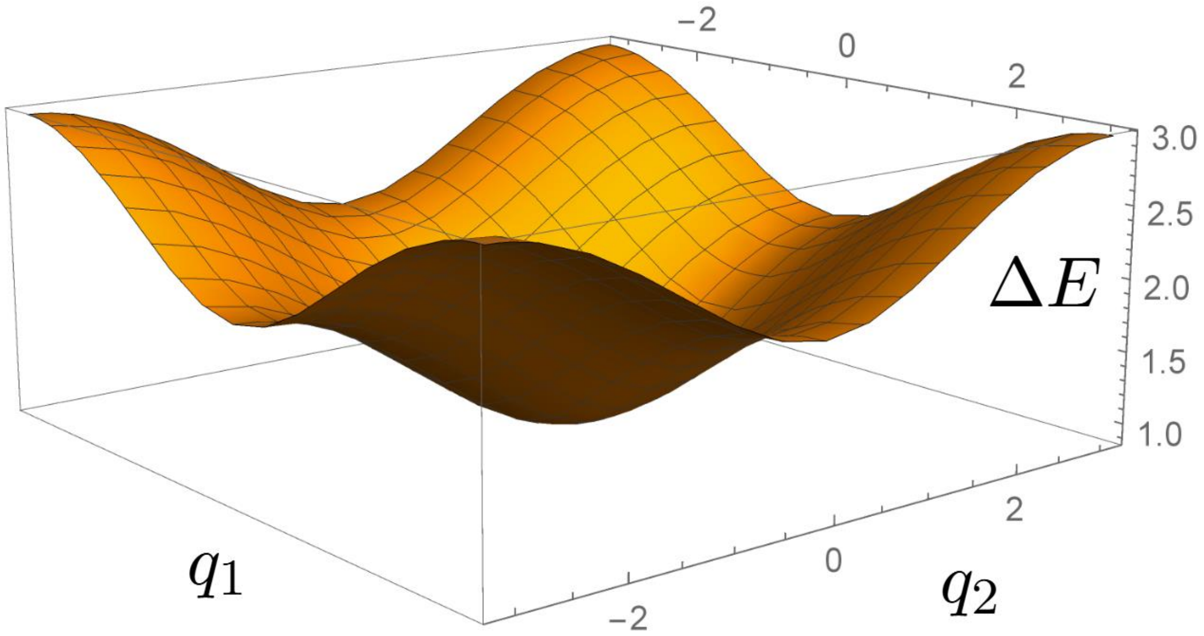
Commutation relations: $[\hat{A}_x, \hat{p}_y] = i\delta_{x,y}$

Quadratic Hamiltonian: can be solved analytically!

Backup: exact Solution of Lattice Hamiltonian

Pure Maxwell Theory	Maxwell-Chern-Simons Theory
No gap: Linear dispersion relation of gapless photon	**Gap:** Chern-Simons term gives mass to photon





Plot of dispersion relation: $\Delta E = \omega = \sqrt{\frac{1}{a^2}\left[2(1-\cos q_1) + 2(1-\cos q_2)\right] + \left(\frac{ke^2}{4\pi}\right)^2 \left[2 + 2\cos(q_1+q_2)\right]}$

Backup: can we reproduce all topological properties?

Photon Mass & Quantized Coupling

Continuum limit of dispersion relation

Correctly reproduces photon mass in continuum: [1]

$$\omega^2 \to |\tilde{q}|^2 + \left(\frac{ke^2}{2\pi}\right)^2$$

Quantization of Chern-Simons level

Constraint from large gauge transformations:

$$e^{2\pi i \hat{L}_1} e^{2\pi i \hat{L}_2} = e^{2\pi i k} e^{2\pi i \hat{L}_2} e^{2\pi i \hat{L}_1}$$

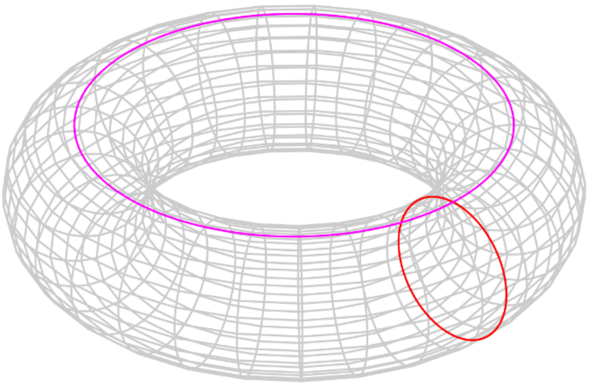
Correctly reproduces quantization property: [2]

$$e^{2\pi i k} = 1 \qquad \Longrightarrow \quad k \in \mathbb{Z}$$

Ground-State Degeneracy

Degeneracy for torus

Torus: periodic boundary conditions → non-trivial topology



Correctly reproduce k-fold degeneracy of ground state [3]

→ good cross-check / benchmark for numerical methods!

[1] Deser, Jackiw, Templeton (1982)
[2] Pisarski (1986)
[3] Eliezer, Semenoff (1992)
Image credit: https://commons.wikimedia.org/w/index.php?curid=32176358

Backup: Monopole Problem of Compact MCS Theory

1+1D Lattice Theories	Modified Villain Approach

Compact Maxwell Theory
Existence of quantized magnetic fluxes:

$$\int_\Sigma dA \in 2\pi\mathbb{Z}$$

If closed surface is contractible, **monopole** inside

Compact MCS Theory
Monopole configuration: large gauge transformation → changes Chern-Simons action → boundary terms at spatial infinity → action **violates gauge invariance**

Conventional Villain Approach
Add discrete plaquette variables n, encode magnetic flux
Interpret n as discrete gauge fields for shift symmetry:

$$A_0 \to A_0 + \frac{2\pi}{d\tau}, \quad A_i \to A_i + \frac{2\pi}{a}, \quad i = 1, 2$$

Gauge the discrete shifts → study compact gauge theory:

$$U(1) = \mathbb{R}/2\pi\mathbb{Z}$$

Modified Villain Approach
Eliminate monopoles with Lagrange multiplier

Backup: 2+1D QED With(out) Monopoles

Lagrangian Formalism	Hamiltonian Formalism

Compact variables
For compact θ_i, action contains terms $\cos(\sum_i c_i\theta_i)$

Conventional Villain approach
Replace cosine terms by periodic Gaussian potential:

$$e^{\beta\cos(\theta)} \approx \sum_{n=-\infty}^{\infty} e^{-\frac{\tilde{\beta}}{2}(\theta+2\pi n)^2}$$

→ discrete gauge fields n can take values in $(-\infty, +\infty)$
→ compactness ensured by constraints on Hilbert space

Modified Villain approach
Eliminate monopoles with Lagrange multiplier → flat n

2+1D Compact QED …

… including monopoles / instantons

$$H = \frac{e^2}{2a^2}\sum_{\text{links}} E_i^2 + \frac{1}{e^2a^2}\sum_{\text{plaquettes}}\left(1-\cos a^2B\right)$$

… with monopoles / instantons removed

$$H = \frac{e^2}{2a^2}\sum_{\text{links}} E_i^2 + \frac{a^2}{2e^2}\sum_{\text{plaquettes}} B^2$$

Backup: Constraints on Hilbert Space

Local Gauge Transformations	Large Gauge Transformations

Gauss' law

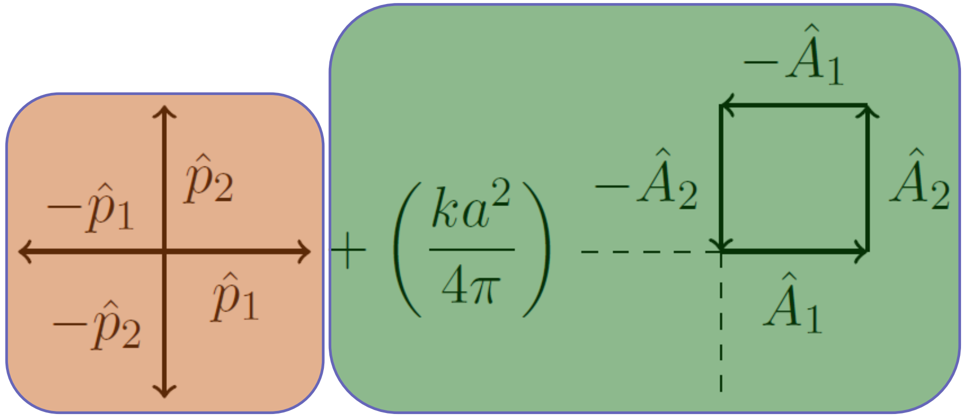
Constraints on physical states in Hilbert space:

$$e^{i\lambda\hat{G}}|\psi\rangle = |\psi\rangle, \quad \forall\lambda\in\mathbb{R}, \qquad [\hat{H},\hat{G}]=0$$

Generator for local gauge transformations

Similar as for QED, but modified by Chern-Simons term:

$\hat{G} =$



Two additional constraints

$$e^{2\pi i\hat{L}_1}|\psi\rangle = e^{i\theta_1}|\psi\rangle, \quad e^{2\pi i\hat{L}_2}|\psi\rangle = e^{i\theta_2}|\psi\rangle$$

→ compactify gauge field configurations
→ similar as for QED (without monopoles)

Generators for large gauge transformations

Similar as for QED, but modified by Chern-Simons term
→ enforce quantized Chern-Simons coupling

Backup: Compactification Through Constraints

Large Gauge Transformations

Constraints on Hilbert space …

$$e^{2\pi i \hat{L}_i}|\psi\rangle = e^{i\theta_i}|\psi\rangle$$

… allow only certain gauge field configurations

$$\hat{L}_i|\psi\rangle = \left(\frac{\theta_i}{2\pi} + m_i\right)|\psi\rangle, \; m_i \in \mathbb{Z}, \; i = 1, 2$$

Different topological sectors of theory

Transformation $|\psi\rangle \to e^{2\pi i \hat{L}_j}|\psi\rangle$

… changes sector $m_i \to m_i + k\,\epsilon_{ij}$

… due to non-zero commutator $[\hat{L}_1, \hat{L}_2] = -\frac{k}{2\pi} i$

Invariance of Partition Function

Partition function
Sum over all sectors / values of m_i with equal weights
→ stays invariant under large gauge transformations

Similarity to Villain approximation:

$$e^{\beta \cos(\theta)} \approx \sum_{n=-\infty}^{\infty} e^{-\frac{\tilde{\beta}}{2}(\theta + 2\pi n)^2}$$

→ obtain periodic function (i.e., compact gauge field) by summing over multiple non-periodic functions

Numerical simulation
Truncation of infinite sum, neglect terms with large n

Backup: Large Gauge Transformation Constraint #1

2+1D Compact QED … | **… With Chern-Simons Term**

Constraint on Hilbert space

$$e^{2\pi i \hat{L}_1}|\psi\rangle = e^{i\theta_1}|\psi\rangle$$

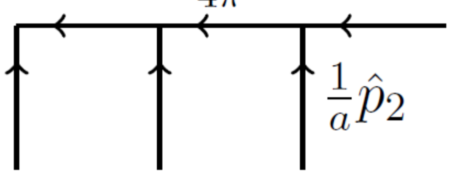
Generator for large gauge transformation

$$\hat{L}_1 = \cdots$$

$$= \frac{1}{a}\sum_{x_1=0}^{N_1-1} \hat{p}_{(x_1,N_2-1);2}$$

Modified generator for large gauge transformation

$$\hat{L}_1 = \cdots$$



$$= \sum_{x_1\in\{0,1,\ldots,N_1-1\}} \left(\frac{1}{a}\hat{p}_{(x_1,x_2);2} - \frac{ka}{4\pi}\hat{A}_{(x_1,x_2+1);1}\right)$$

Backup: Large Gauge Transformation Constraint #2

2+1D Compact QED …

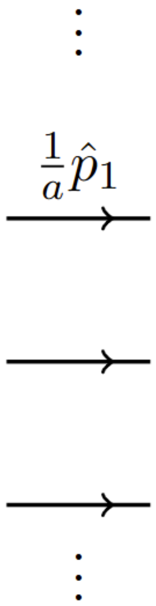
… With Chern-Simons Term

Constraint on Hilbert space

$$e^{2\pi i \hat{L}_2}|\psi\rangle = e^{i\theta_2}|\psi\rangle$$

Generator for large gauge transformation

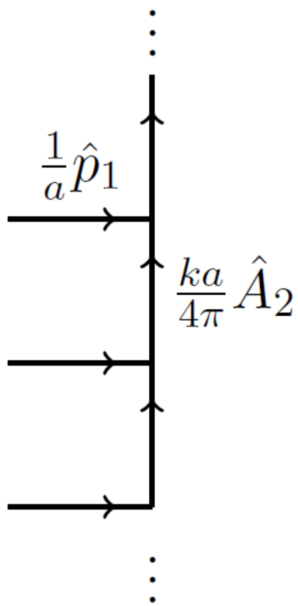
$\hat{L}_2 =$



$$= \frac{1}{a}\sum_{x_2=0}^{N_2-1} \hat{p}_{(N_1-1,x_2);1}$$

Modified generator for large gauge transformation

$\hat{L}_2 =$



$$= \sum_{x_2\in\{0,1,\dots,N_2-1\}} \left(\frac{1}{a}\hat{p}_{(x_1,x_2);1} + \frac{ka}{4\pi}\hat{A}_{(x_1+1,x_2);2}\right)$$

Backup: Compatibility of Constraints

Commutators

Constraints need to commute with Hamiltonian

$$[\hat{H}, \hat{G}] = 0$$

$$[\hat{H}, \hat{L}_i] = 0, \quad i = 1, 2$$

Constraints need to commute with Gauss' law

$$[\hat{G}, \hat{L}_i] = 0, \quad i = 1, 2$$

But: constraints do not commute with each other!

$$[\hat{L}_1, \hat{L}_2] = -\frac{k}{2\pi} i$$

Quantization of Chern-Simons Level

Non-zero commutator yields quantization condition!

Constraint from large gauge transformations:

$$e^{2\pi i \hat{L}_1} e^{2\pi i \hat{L}_2} = e^{2\pi i k} e^{2\pi i \hat{L}_2} e^{2\pi i \hat{L}_1}$$

Correctly reproduces quantization property: [1]

$$e^{2\pi i k} = 1 \qquad \Longrightarrow \quad k \in \mathbb{Z}$$

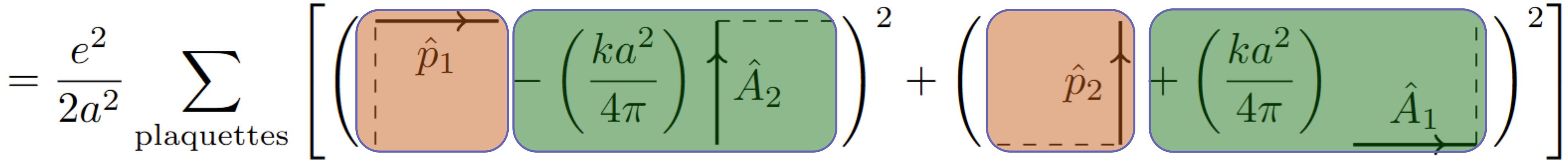
[1] Pisarski (1986)

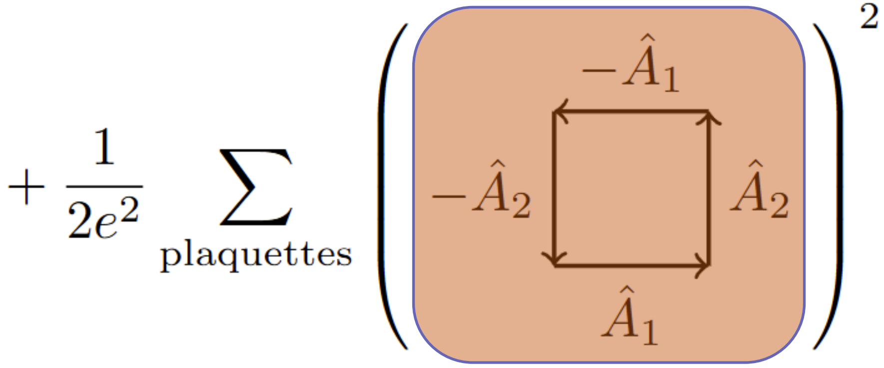
Backup: Plaquette Visualization of Lattice Hamiltonian

Compact MCS Hamiltonian

Magnetic field term: similar to QED (without monopoles)
Electric field term: modified by Chern-Simons term

$$\hat{H} = \sum_{x \in \text{sites}} \frac{e^2}{2a^2} \left[\left(\hat{p}_{x;1} - \frac{ka^2}{4\pi} \hat{A}_{x-\hat{2};2} \right)^2 + \left(\hat{p}_{x;2} + \frac{ka^2}{4\pi} \hat{A}_{x-\hat{1};1} \right)^2 \right] + \frac{1}{2e^2} \left(\Box \hat{A}_{x;1,2} \right)^2$$





Plaquette operator:

$$\Box \hat{A}_{x;1,2} \equiv \hat{A}_{x;1} + \hat{A}_{x+\hat{1};2} - \hat{A}_{x+\hat{2};1} - \hat{A}_{x;2}$$