UNIVERSITY OF Southampton

State Preparation using Quantum Algorithms within Hamiltonian Formulations of Quantum Field Theories

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Quantum Technologies for Fundamental Physics

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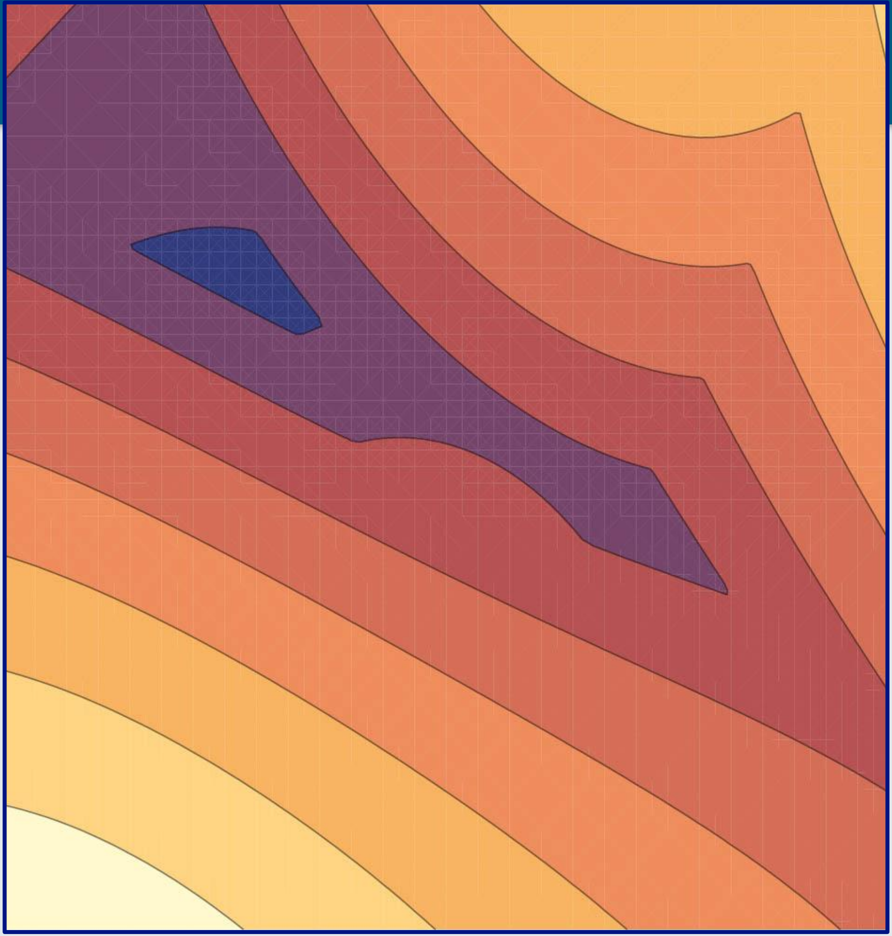

Cambridge-Southampton QA for QFT

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Outline

- **Motivations and Project Structure**
  - Big-picture reasons to consider QAs for QFTs, and our collaboration

- **Quantum State Preparation**
  - Why is quantum state preparation a hard problem?
  - How are variational algorithms effective solutions?
    - The choice of an ansatz

- **Specialising towards Lattice Gauge Theories**
  - Adiabatic Preparation for the Schwinger Model
  - VQE and QAOA for the Schwinger Model
  - Accelerating VQE with equivariant ansatze

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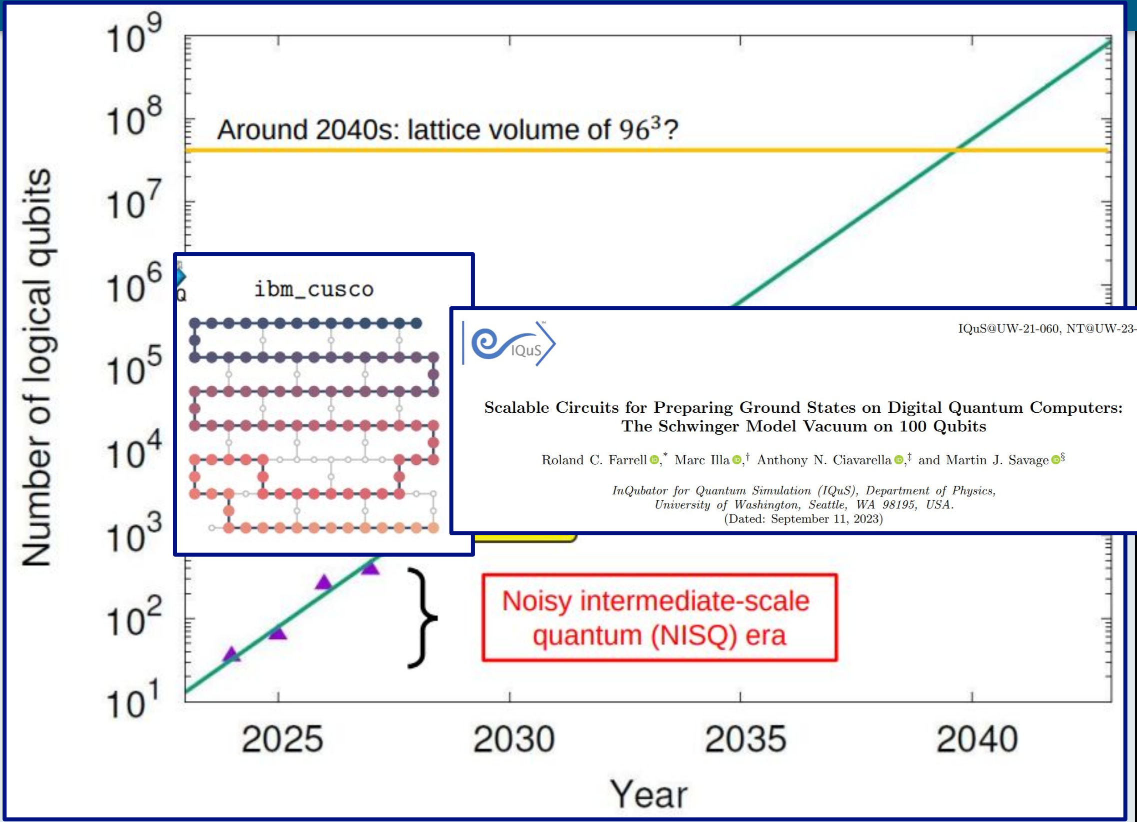
Quantum Scale-up

- All low-qubit, low-depth QAs can be simulated classically.
- Noisy intermediate-scale quantum (NISQ) technology may show **quantum advantage**.
  - 50-100s of qubits
  - 1000s of gate operations before noise dominates.
- Stepping stone towards fault-tolerant QC (2030s)
  - Why wait to do physics?



[Figure by Funcke (Lattice2022)]

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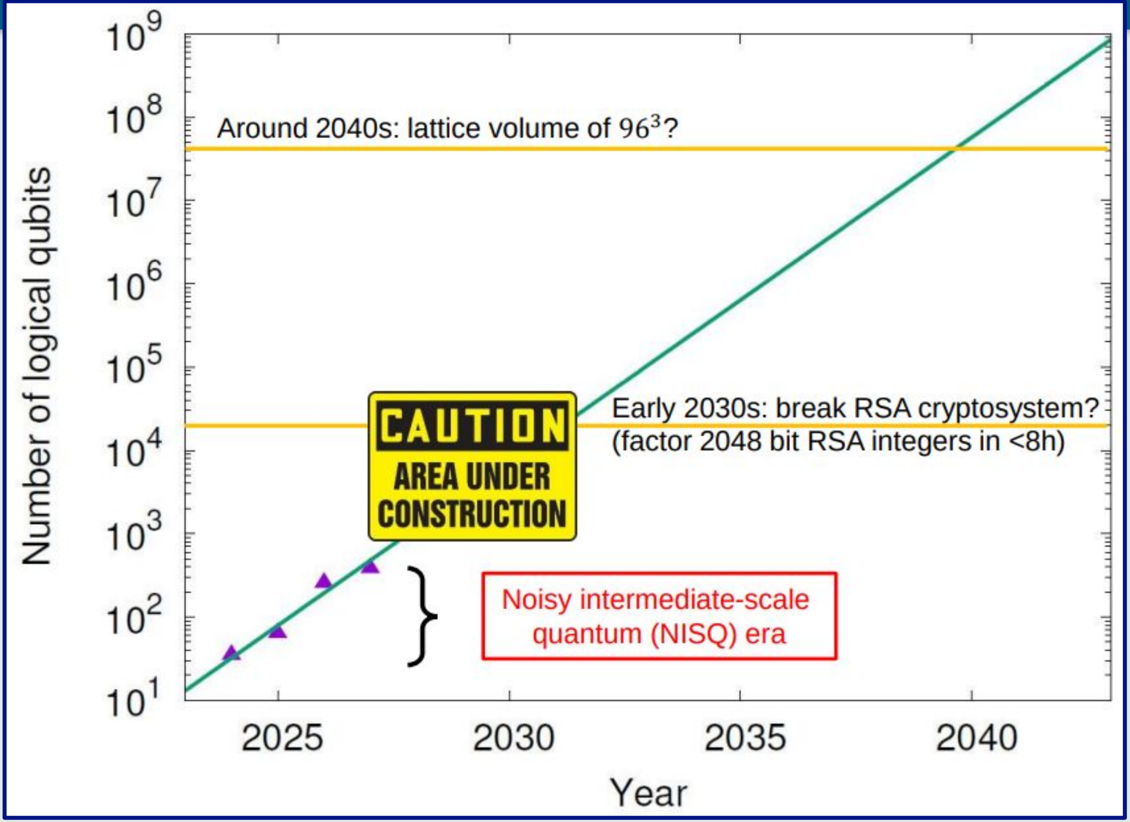
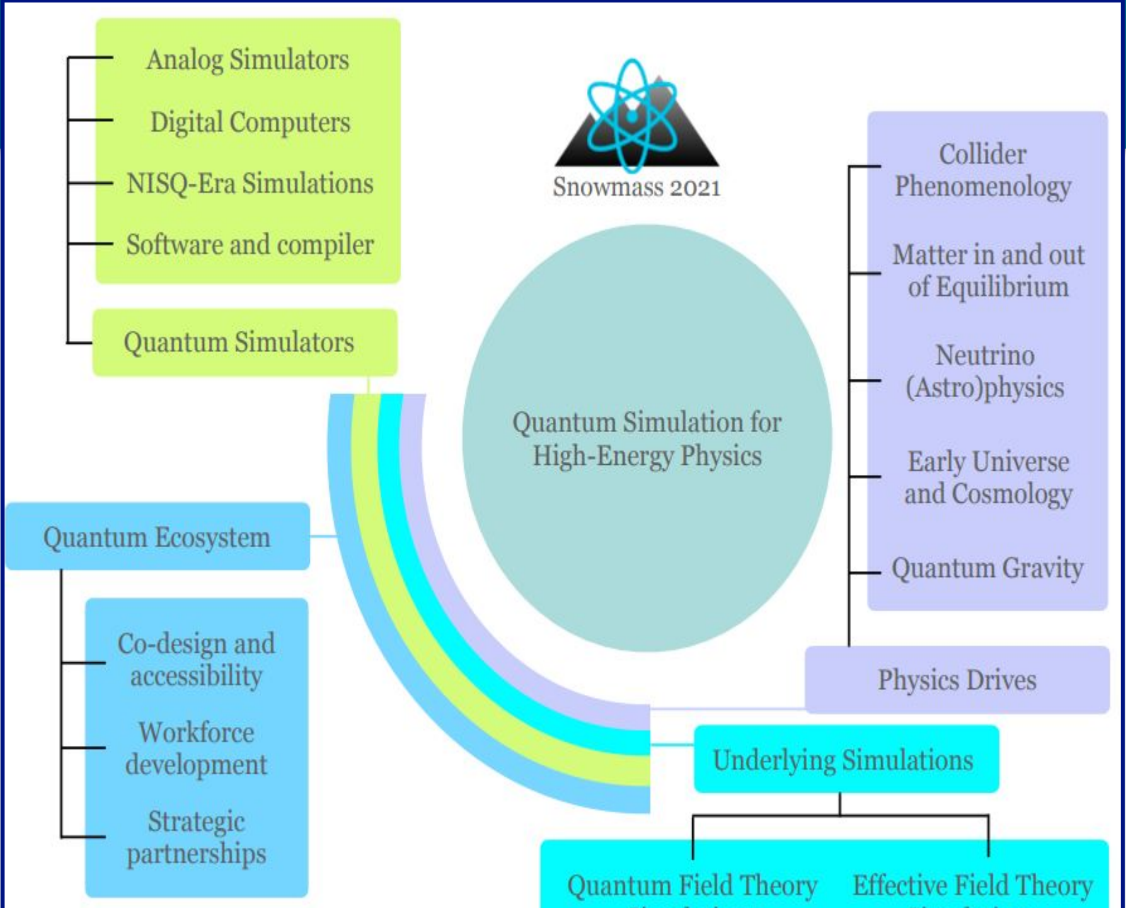


[Figure by Funcke (Lattice2022)]

Physics drives

- Collider phenomenology
  - Parton showers, S-matrices
- Strongly-interacting systems
  - Lattice QCD, hadronisation
- Neutrino (astro)physics
  - Oscillations, mean-field
- Early-universe cosmology
  - Inflation, CP-violation
- Gauge-gravity duality
  - QEC, SYK / matrix models



[Bauer et al., Snowmass 2021]

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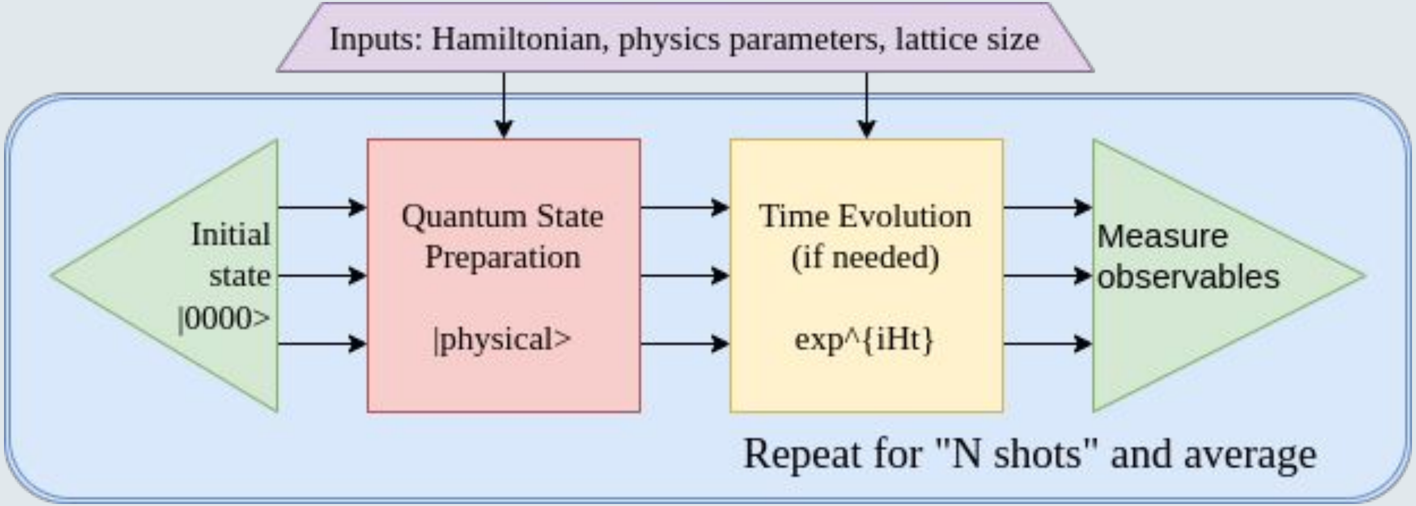
Quantum Simulation Protocols

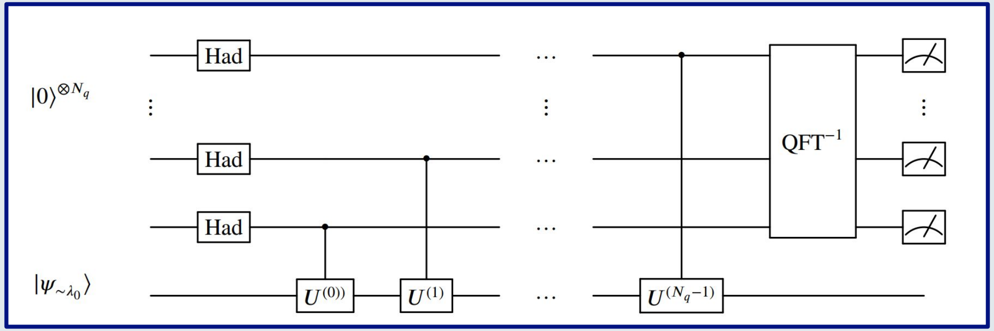


- Circuit depth O(2^n / n) needed to prepare generic n-qubit state
  - Can be reduced to O(n) with O(2^n) ancilla qubits

- We want eigenstates of given Hamiltonians, physicality/symmetry advantages

Quantum Phase Estimation (QPE) vs Variational Quantum Algorithms

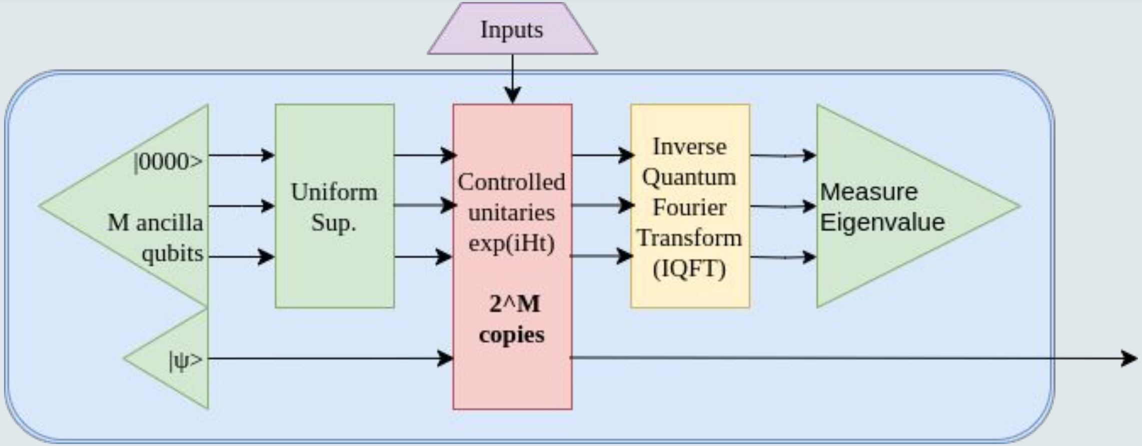
QPE:



- Purely quantum algorithm, O(1) shots needed but O(1/ε) depth to achieve precision ε.
  - M = 1/log2(ε) ancilla qubits needed

Quantum Phase Estimation (QPE) vs Variational Quantum Algorithms

QPE:

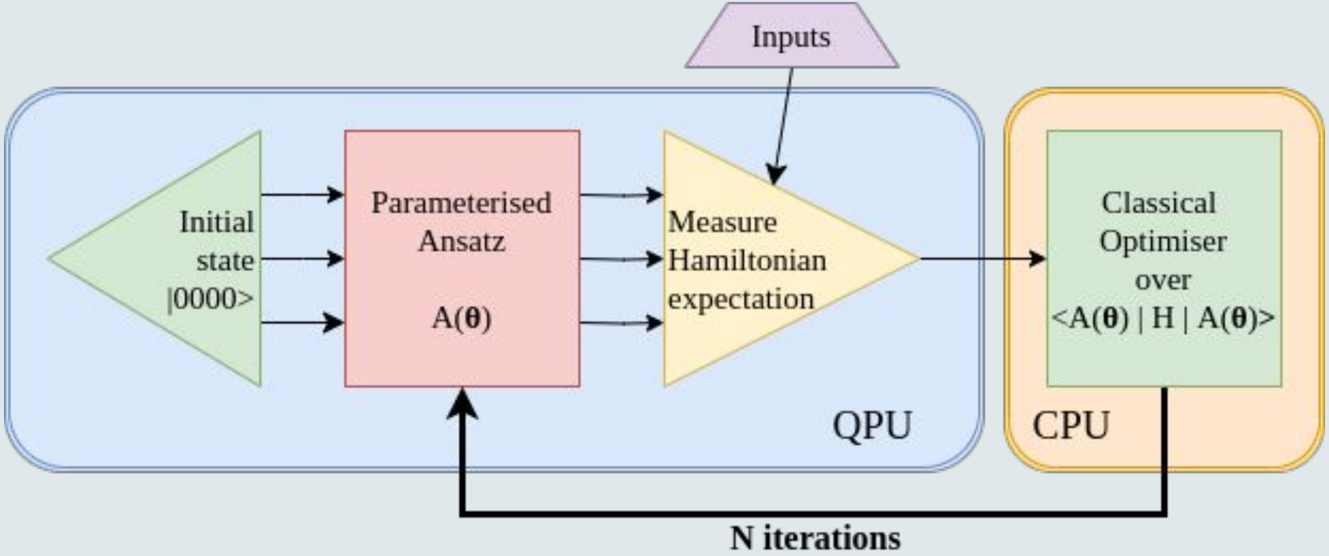


- Purely quantum algorithm, O(1) shots needed but O(1/ε) depth to achieve precision ε.
  - M = 1/log2(ε) ancilla qubits needed

- Iterative quantum state preparation with a classical optimiser
  - O(1/ε^2) shots needed but only O(1) depth, ideal for NISQ.

Quantum Phase Estimation (QPE) vs Variational Quantum Eigensolver

VQE:

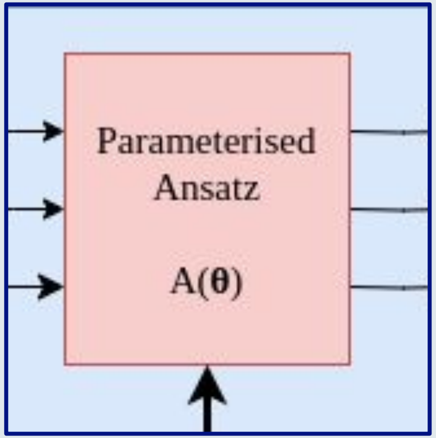


- Iterative quantum state preparation with a classical optimiser – a "hybrid" algorithm.
  - $O(1/\varepsilon^2)$ shots needed but only O(1) depth,
  - Although QPE has better asymptotics, VQE ideal for NISQ

Ansatz Selection

- Desirable qualities:
  - Low circuit depth
  - Minimally contain physical spectrum
  - Avoid barren plateaus for larger # qubits

- Heuristic approaches: k-local gatesets
- Adaptive approaches: ADAPT-VQE, Generative VQE
- Model-driven approaches:
  - Coupled-cluster
  - Quantum Approximate Optimisation (QAOA)
  - Efficient symmetry-preservation (ESP)



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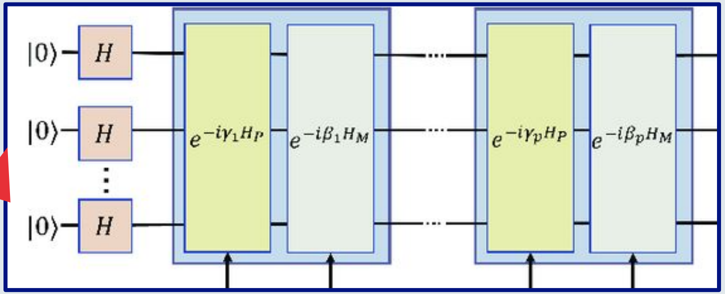
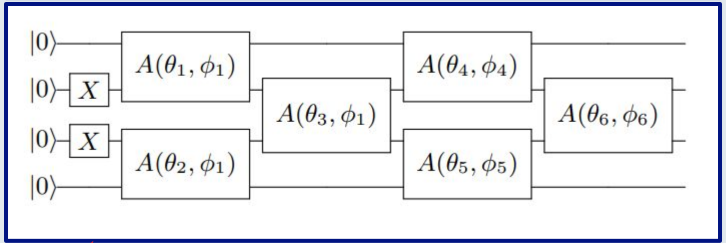
[Huang et al., 2022]





$$A(\theta, \phi) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\theta & e^{i\phi}\sin\theta & 0 \\ 0 & e^{-i\phi}\sin\theta & -\cos\theta & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

[Gard et al., 2020]

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(1+1)d Kogut-Susskind Hamiltonian

- Lattice gauge theory with group G, staggered fermion:

$$H = w\sum_{n=1}^{N}\left(\phi_n^\dagger U_n^j \phi_{n+1} + h.c.\right) + m\sum_{n+1}^{N}(-1)^n \phi_n^\dagger \phi_n + J\sum_{n=1}^{N} \vec{L}_n^2$$

$$\hat{Q}_n^a = \sum_{r,s} \hat{\phi}_n^{r,\dagger}\left[\hat{T}_j^a\right]_{rs}\hat{\phi}_n^s,$$

$$\hat{R}_n^a = \sum_b 2\mathrm{Tr}\left[\hat{U}_n \hat{T}_j^a \hat{U}_n^\dagger \hat{T}_j^b\right]\hat{L}_n^b,$$

$$\hat{G}_n^a = \hat{L}_n^a - \hat{Q}_n^a - \hat{R}_n^a = 0$$

- In (1+1)d, gauge redundancy given boundary conditions
  - Solve Gauss's Law to "fermionise" the Hamiltonian
  - For d > (1+1), we will have to be clever.

- Map fermions to qubits, e.g. Jordan-Wigner, Bravyi-Kitaev
  - For G = SU(n) or U(n), one fermion ⇒ n qubits.

$$\phi^\dagger U \phi \mapsto X \otimes X + Y \otimes Y,$$

$$\phi^\dagger \phi \mapsto Z,$$

$$L^2 \mapsto \sum_{1\leq l\leq n} Z_l$$

Adiabatic State Prep, Schwinger Model

- Take G = U(1) with theta term. [Chakraborty et al., PRD 105.9 (2022)]
- Evolve from H[m=0,w=0,th=0] vacuum to vacuum of interest.


PHYSICAL REVIEW D 105, 094503 (2022)

Classically emulated digital quantum simulation of the Schwinger model with a topological term via adiabatic state preparation

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We designed a protocol for digital quantum computation of a gauge theory with a topological term in Minkowski spacetime, which is practically inaccessible by standard lattice Monte Carlo simulations. We focus on 1 + 1 dimensional quantum electrodynamics with the θ term known as the Schwinger model and test our protocol for this on an IBM simulator. We construct the true vacuum state of a lattice Schwinger model using adiabatic state preparation which, in turn, allows us to compute an expectation value of the fermion mass operator with respect to the vacuum. Upon taking a continuum limit we find that our result in the massless case agrees with the known exact result. In the massive case, we find an agreement with mass perturbation theory in the small-mass regime and deviations in the large-mass regime. We estimate computational costs required to take a reasonable continuum limit. Our results imply that digital quantum simulation appears a promising tool to explore nonperturbative aspects of gauge theories with real time and topological terms.

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I. INTRODUCTION

Gauge theory plays a central role in understanding our universe as all the known fundamental forces are described in the framework of gauge theory. Quantum chromodynamics (QCD) is the gauge theory describing the strong interaction among quarks and gluons. Since QCD is asymptotically free, we need a nonperturbative treatment at low energy to interpolate perturbative picture of quarks/gluons and physics of hadrons. The only successful first-principle approach to handle this is lattice QCD in which we conventionally consider QCD on 4D Euclidean spacetime and discretize the spacetime by lattice to make the path integral finite dimensional. Evaluating the regularized path integral numerically and taking a continuum limit carefully, one can study nonperturbative phenomena such as confinement and chiral symmetry breaking, and reproduce the correct hadron spectrum [1–4]. Numerical integration of the path integral in lattice-field theory is usually done by the Markov Chain Monte Carlo method which regards Boltzmann weight as a probability. Therefore, it encounters a problem when the integrand is nonreal positive and highly oscillating so that sampling becomes much less efficient. This problem, known as the sign problem physically happens, e.g., when we have topological terms [5], chemical potentials [6], or real time [7]. All of the above cases are crucial to understand our universe and therefore, an efficient way to explore the above situations is highly demanded [3–7].

There are various approaches to challenge the sign problem within the framework of the path integral formalism [6]; however, there is limited success as the sign problem gets stronger. One may wonder if it is possible to attack gauge theories with the sign problem by switching to the Hamiltonian formalism where the sign problem is absent from the beginning. Instead, we have to regularize infinite-dimensional Hilbert space and play with huge vector space whose dimension is typically more than exponential of spatial volume in the unit of UV cutoff. It seems beyond the capacity of current/near-future supercomputers when spacetime dimension is not low. However, it is reasonable to expect that *quantum computers* do this job in the not so distant future. Anticipating growth of quantum computational resources, it is worth to develop methods to analyze gauge theories suitable for quantum computers to prepare for the coming era of quantum supremacy [8,9]. It is particularly

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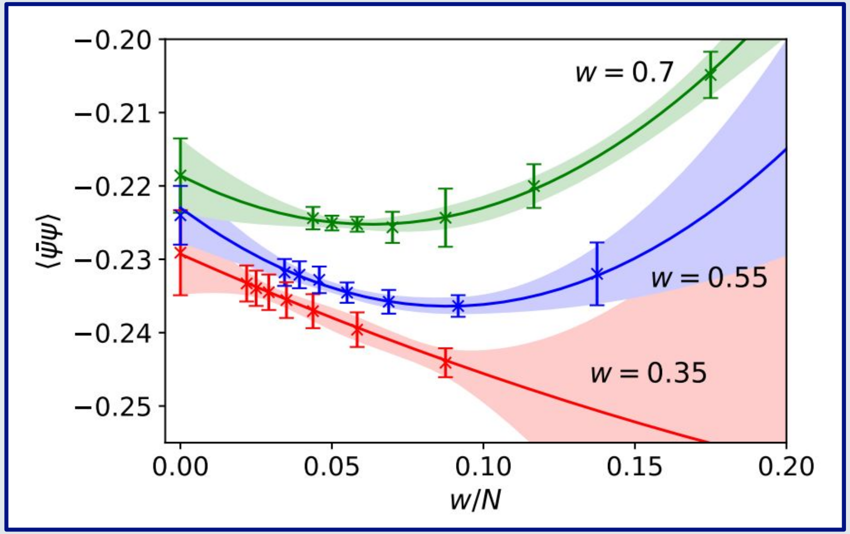
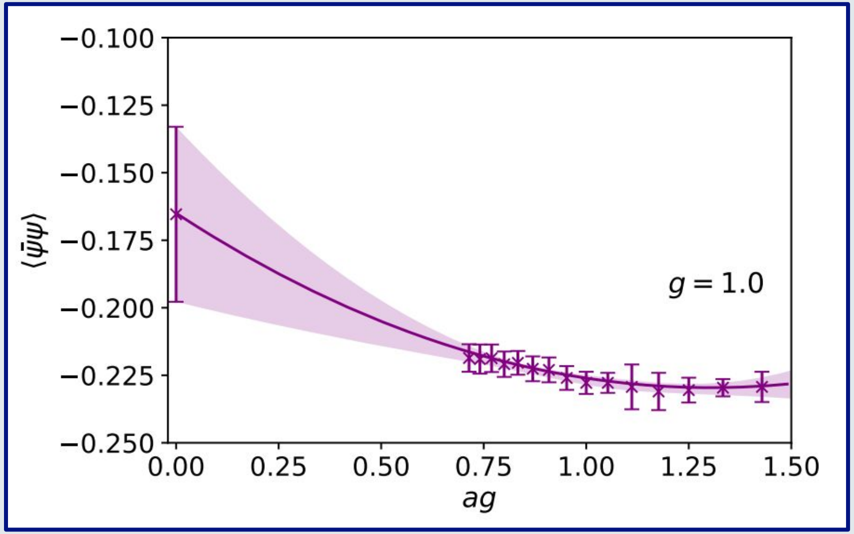
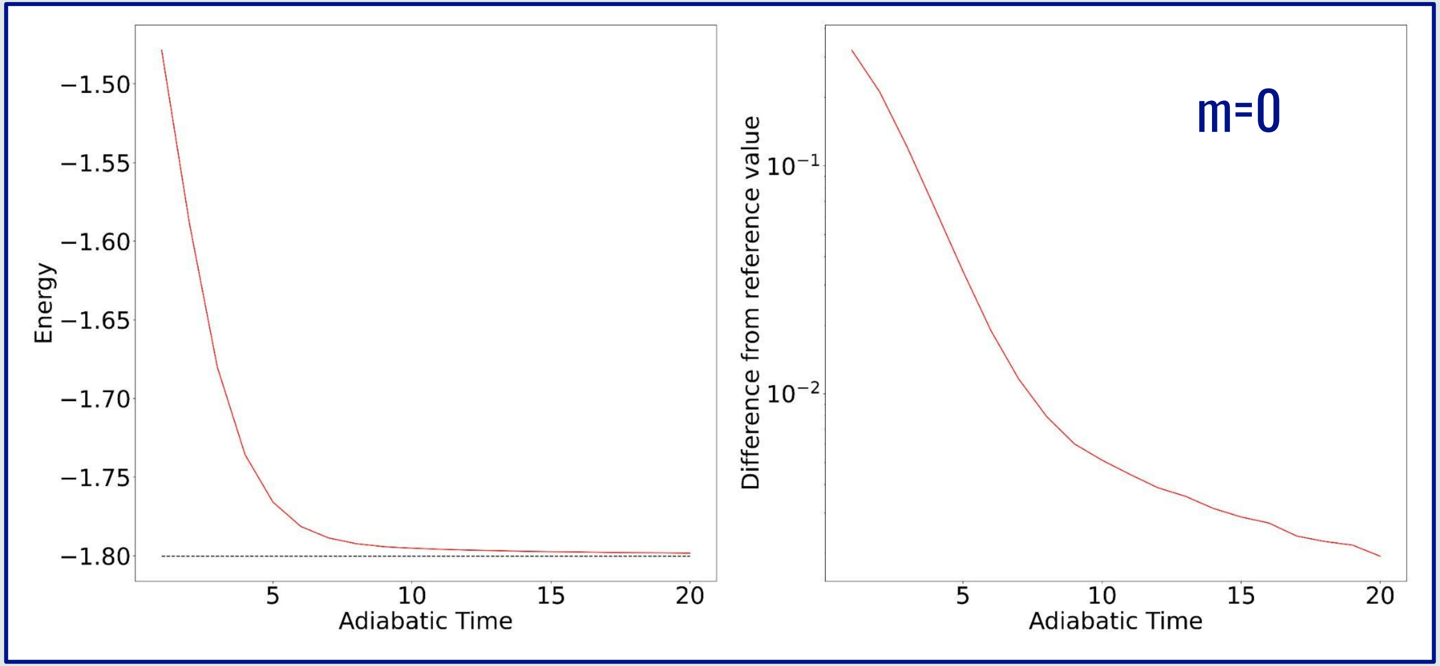




ASP for the Schwinger Model

- Example for 4 qubits, lattice spacing a = 1.43 , masses m = 0,1
  - Deterministic evolution to true vacuum



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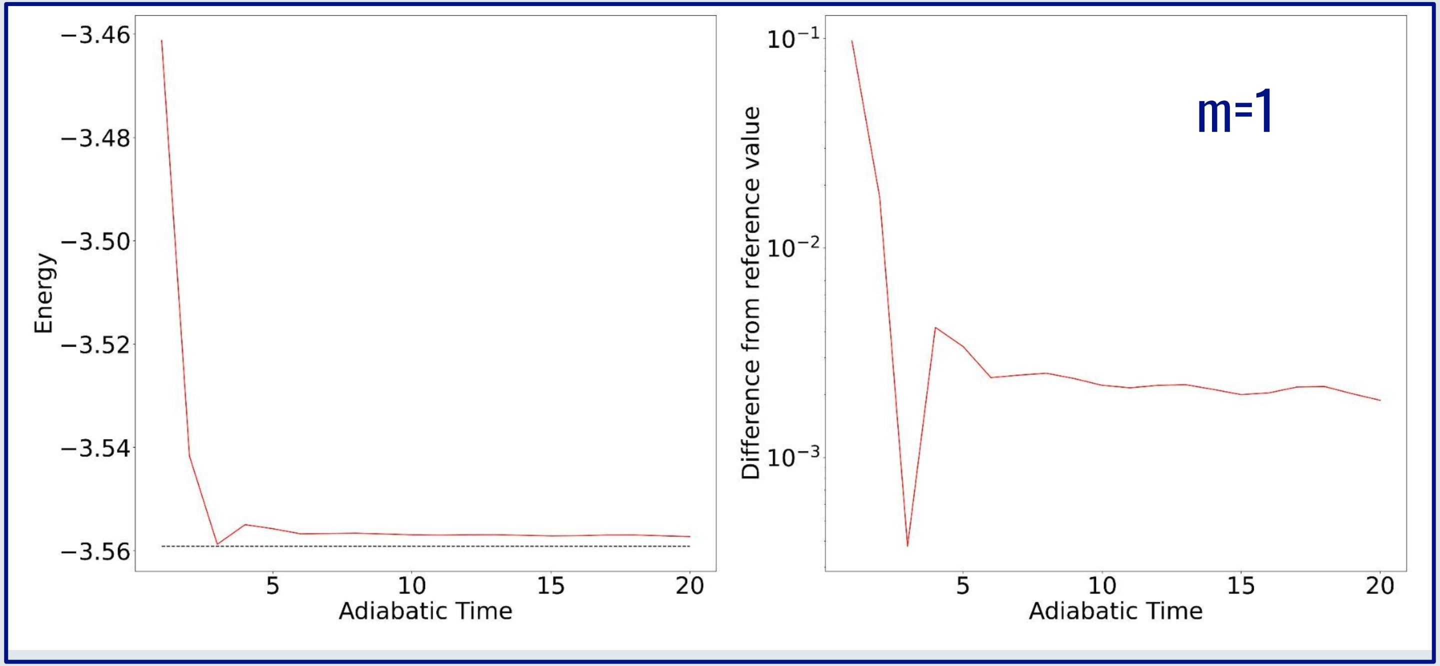
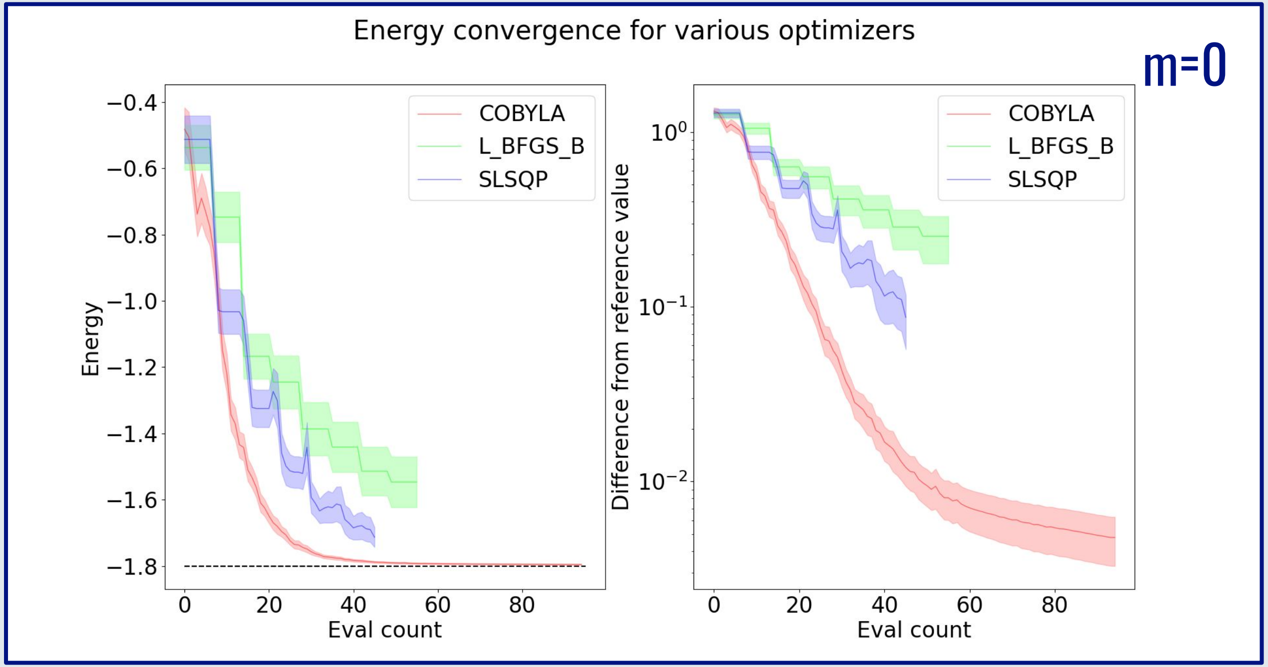


VQE for the Schwinger Model

- VQE guarantees exact convergence for good ansatz
  - Six-parameter ESP ansatz which spans charge-subspace (adjustable)



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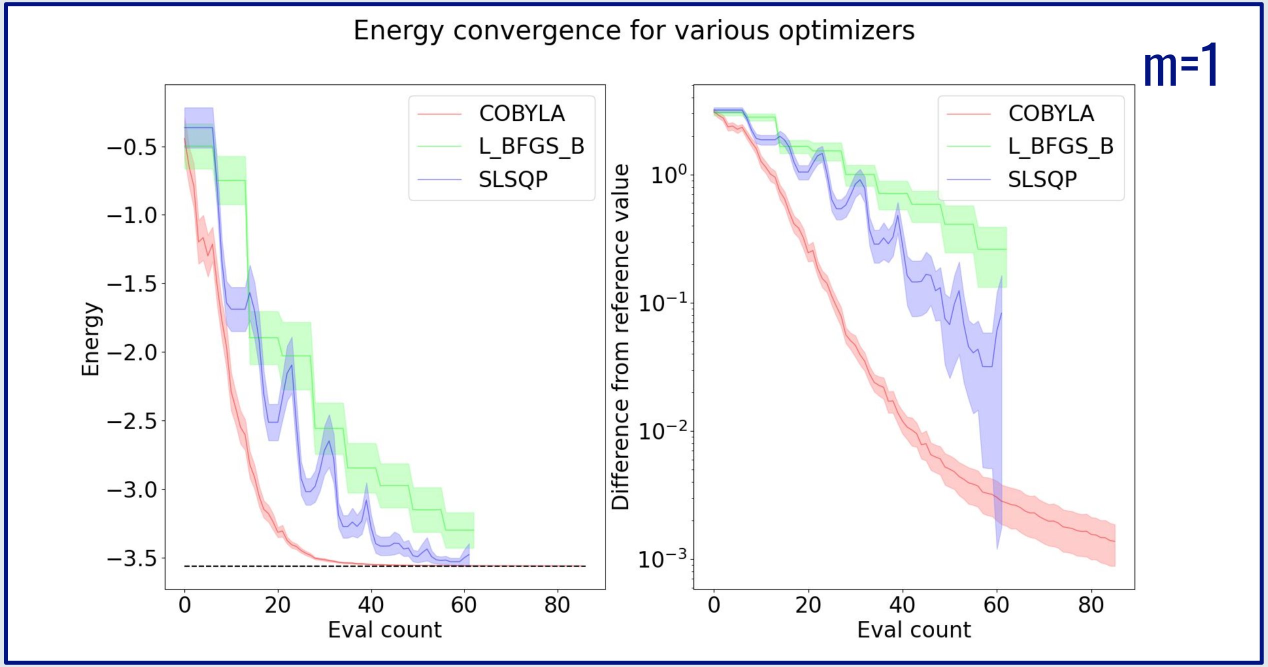
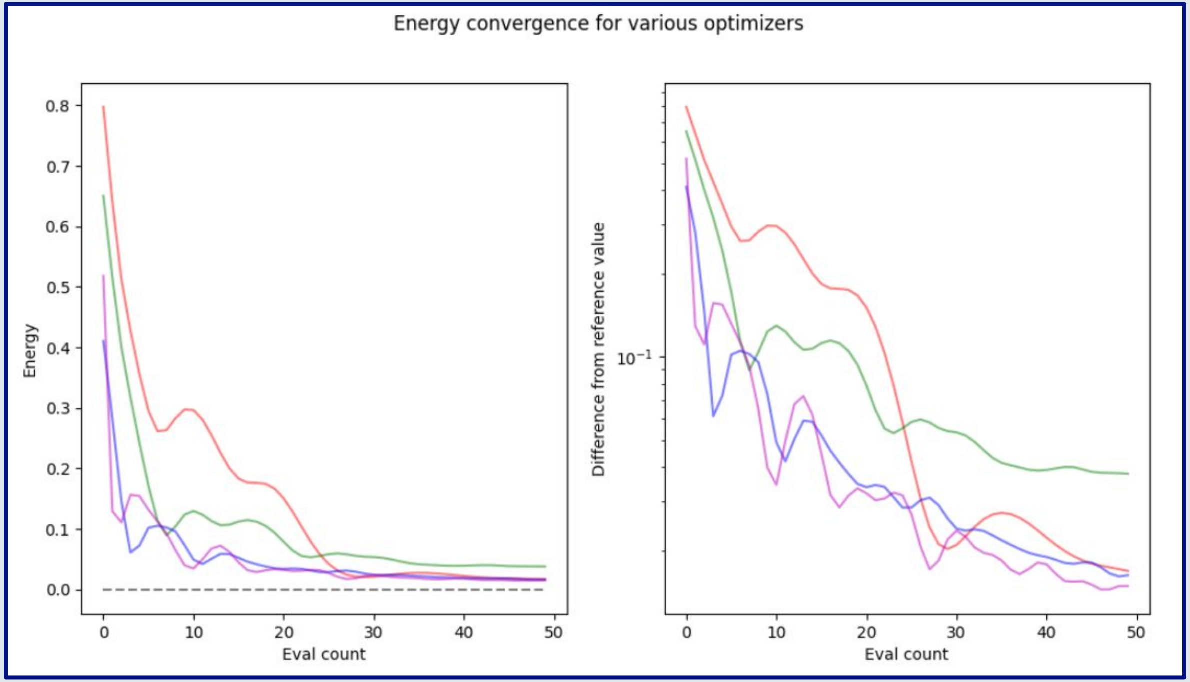


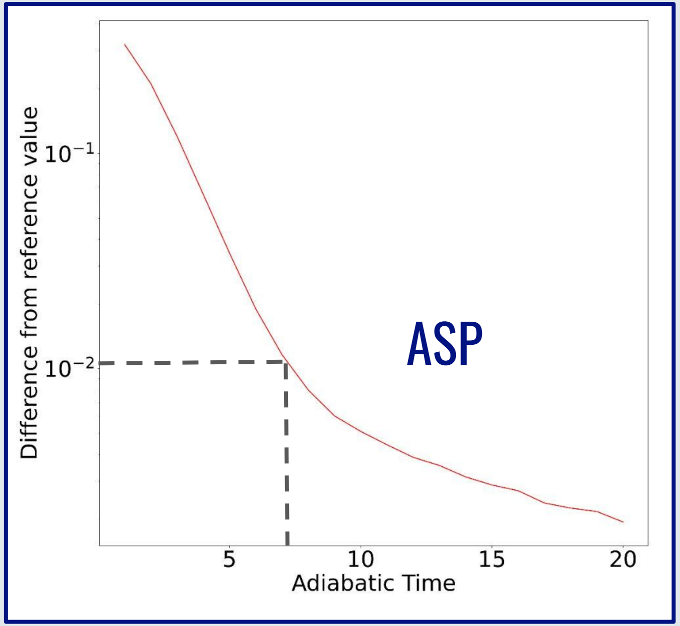
QAOA for the Schwinger Model

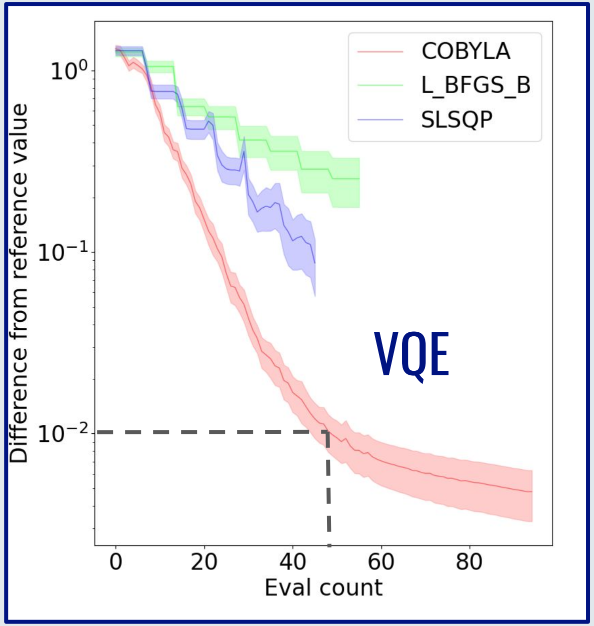
- QAOA sacrifices exactness for ease of construction
  - Ansatz determined by Hamiltonian, plus flexible choice of “mixer”

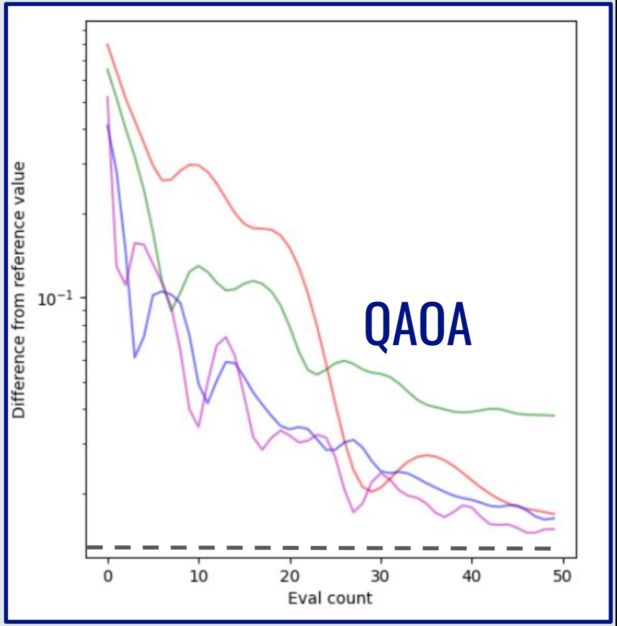


Efficiency Comparison

- Total “runtime” = evaluation count * circuit depth





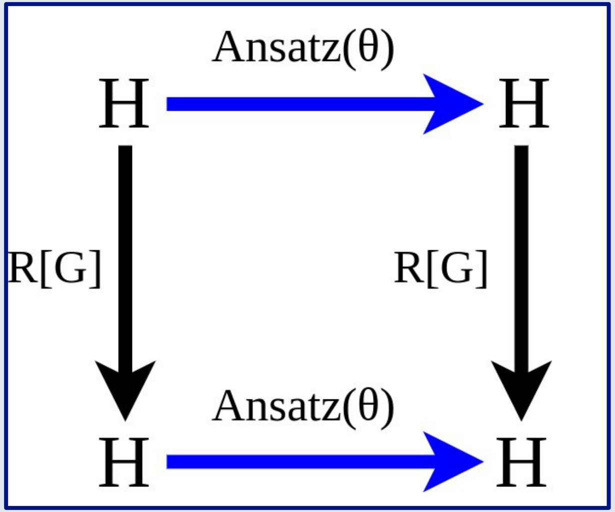


Per eval: 18 CNOT + 13 R | 7 CNOT + 7 R | 14 CNOT + 10 R

Equivariance and Expressivity

- Geometric ML:
  - Predictions invariant to symmetries of data.
- Geometric VQE:
  - Observables invariant to symmetries of Hamiltonian.

- Equivariant embeddings restrict to a symmetry sector
  - Also provides desirable parameter-dependence
  - Must sacrifice some expressivity of the ansatz



- In simple (1+1)d cases, equivariance reproduces ESP, better explanatory power
  - In general, will provide a (very) competitive toolbox for ansatz design

Summary

- State preparation is a crucial bottleneck for near-term quantum simulations.
- Variational algorithms are a leading contender for low-depth QAs for physics.
- Continued developments of ansatze required if we are to:
  - Take maximal advantage of the hardware frontier as it moves.
  - Extend QAs to otherwise inaccessible LGTs, etc.

- Next step: (2+1)d

THANK YOU FOR LISTENING!

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Thank you to UKLFT, and our hosts here in Plymouth!

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