Towards Quantum Simulations of the Standard Model and Beyond

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QUANTUM
TECHNOLOGY
INITIATIVE

10.06.2022

Quantum Computing and Quantum Simulations

Caveat: I started thinking about quantum computing and quantum simulations of field theories in June 2020, so I am still developing my intuition and learning how to talk about the rapid developments we are seeing in the field

Please feel free to interrupt me with any and all questions!

* Photo + slide credit to Bibhushan Shakya

Non-perturbative Phenomena in Particle + Nuclear Physics

Rich phenomena of non-perturbative quantum field theories is a profitable place to look for new answers to the big questions

Studying the properties of strongly coupled theories from first principles is necessary to fully understand the Standard Model

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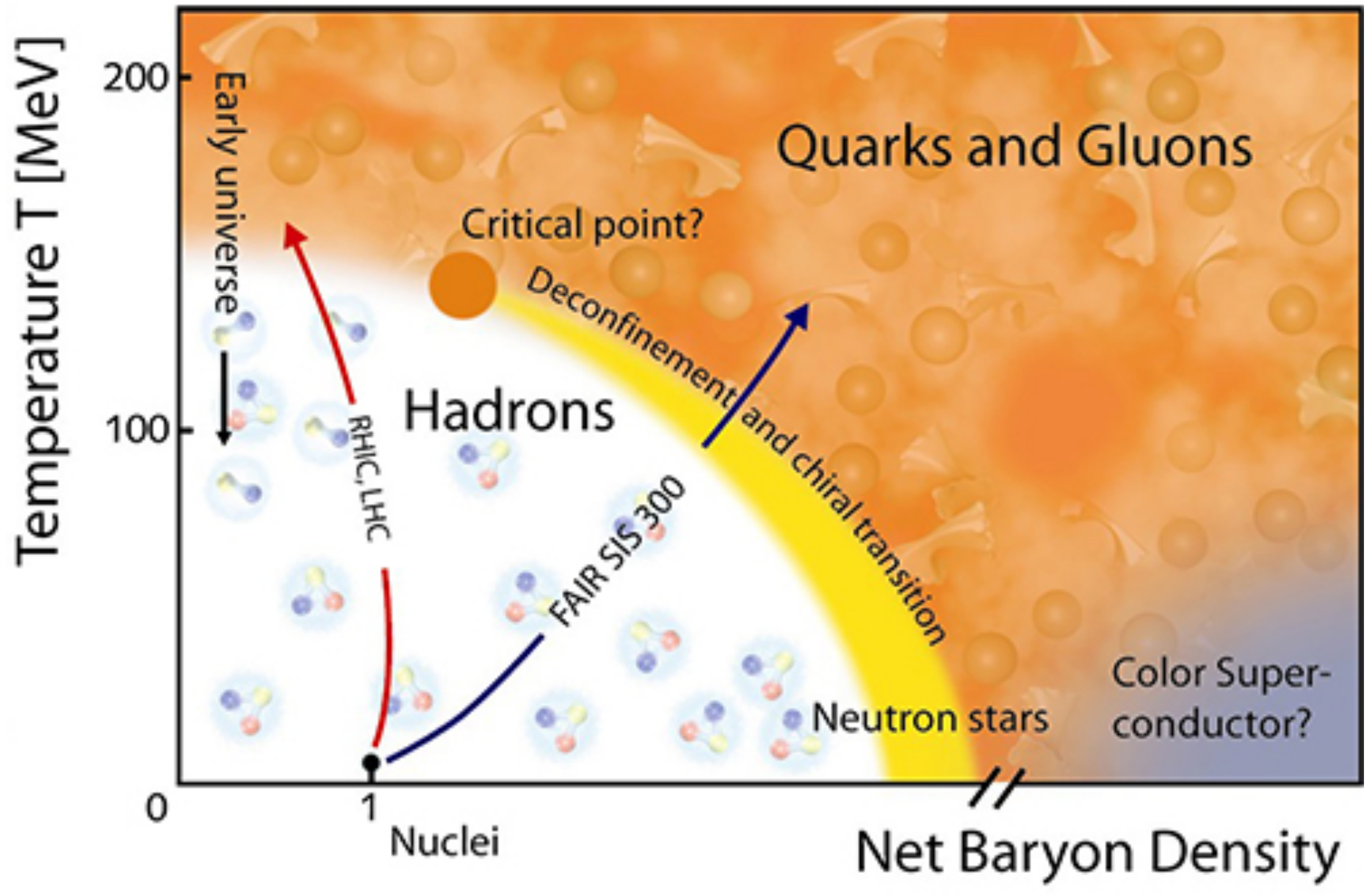
Quantum Chromodynamics (QCD)

- Provides precise and quantitative description of the strong nuclear force over an broad range of energies
- *Ab-initio* calculations crucial for comparing theoretical predictions of the Standard Model to experimental results
- Gives rise to complex array of emergent phenomena that cannot be identified from underlying degrees of freedom



Proposed QCD Phase Diagram

Quantum Simulations of the Standard Model

Quantum computers have a fundamentally different computational strategy and will provide novel probes of fundamental questions in particle and nuclear physics

- The last decade has seen the rapid evolution of real-world quantum computers, with increasing size and decreasing noise
- It is imperative to begin exploratory studies of the applicability of this emerging technology

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Two Complementary Directions

Probe theories that are inaccessible through classical computing techniques

Real-Time Dynamics

Chiral Gauge Theories

Finite-Density Nuclear Matter

Decrease cost for computationally expensive but feasible calculations

Augmentation of Monte Carlo Event Generation via Quantum Machine Learning

Two different approaches with different timescales

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(ask me while hiking if curious)

Two different approaches with different timescales

Quantum Computing

General Idea: Utilize collective properties of quantum states (superposition, interference, entanglement) to perform calculations

Expectation/Hope: Dramatic improvement in run-time scaling for calculations that are exponentially slow with classical methods

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Example

Shor's algorithm: Method for factoring large numbers (backbone of many encryption schemes)

Best Classical Algorithm Run-Time Scaling

$$\mathcal{O}\left(e^{1.9(\log N)^{1/3}(\log\log N)^{2/3}}\right)$$

Quantum Algorithm Run-Time Scaling

$$\mathcal{O}\left((\log N)^2(\log\log N)(\log\log\log N)\right)$$

N: Size of Integer

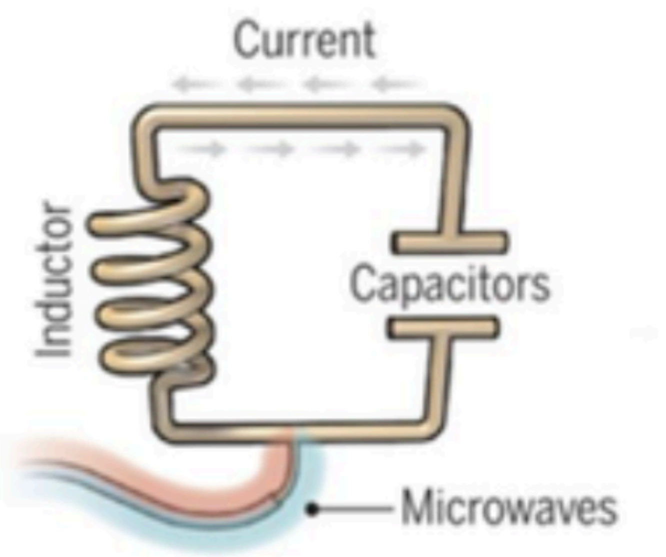
Can we see a similar improvement for calculations in HEP?

Digital Quantum Computing

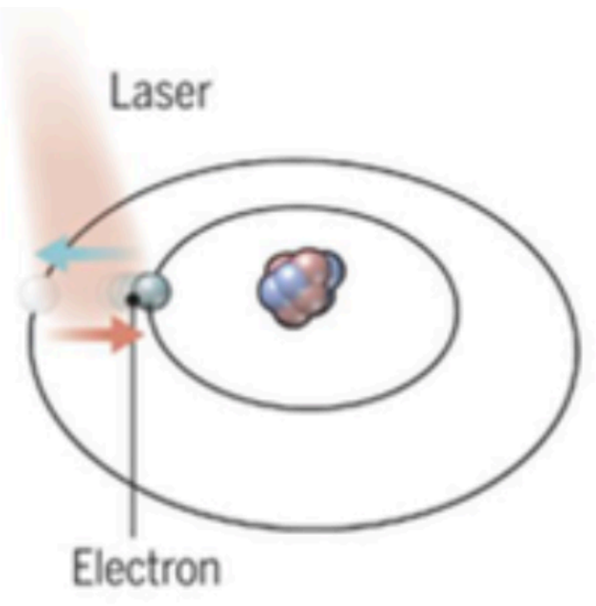
Computational Strategy: Quantum circuits are created by acting on collection of qubits with gates

- Any two-state system can be used as a qubit (in theory)
- Gates are unitary operations that usually act on one or two qubits

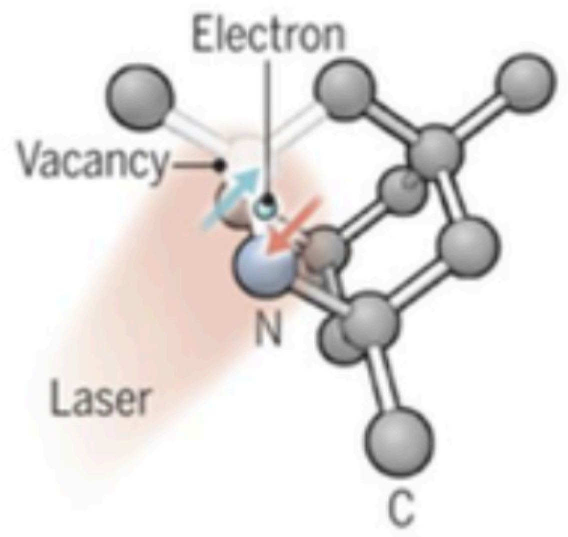
•Superconducting loops



• Trapped ions



• Diamond vacancies



Graphics by C. Bickle, Science Data by Gabriel Popkin

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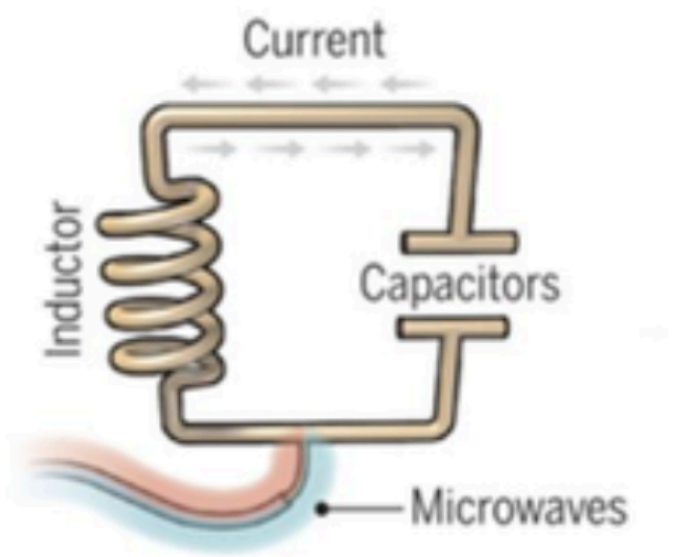

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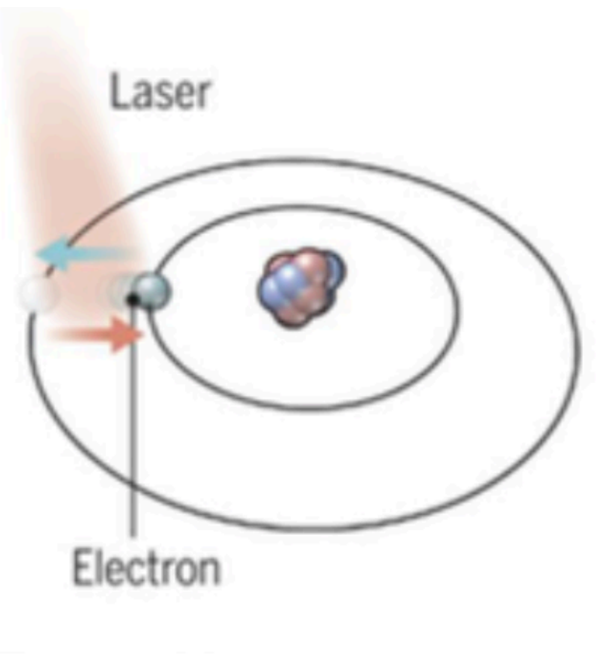

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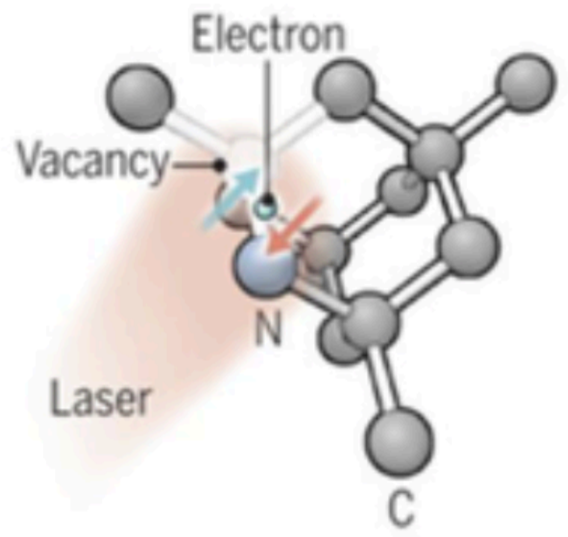

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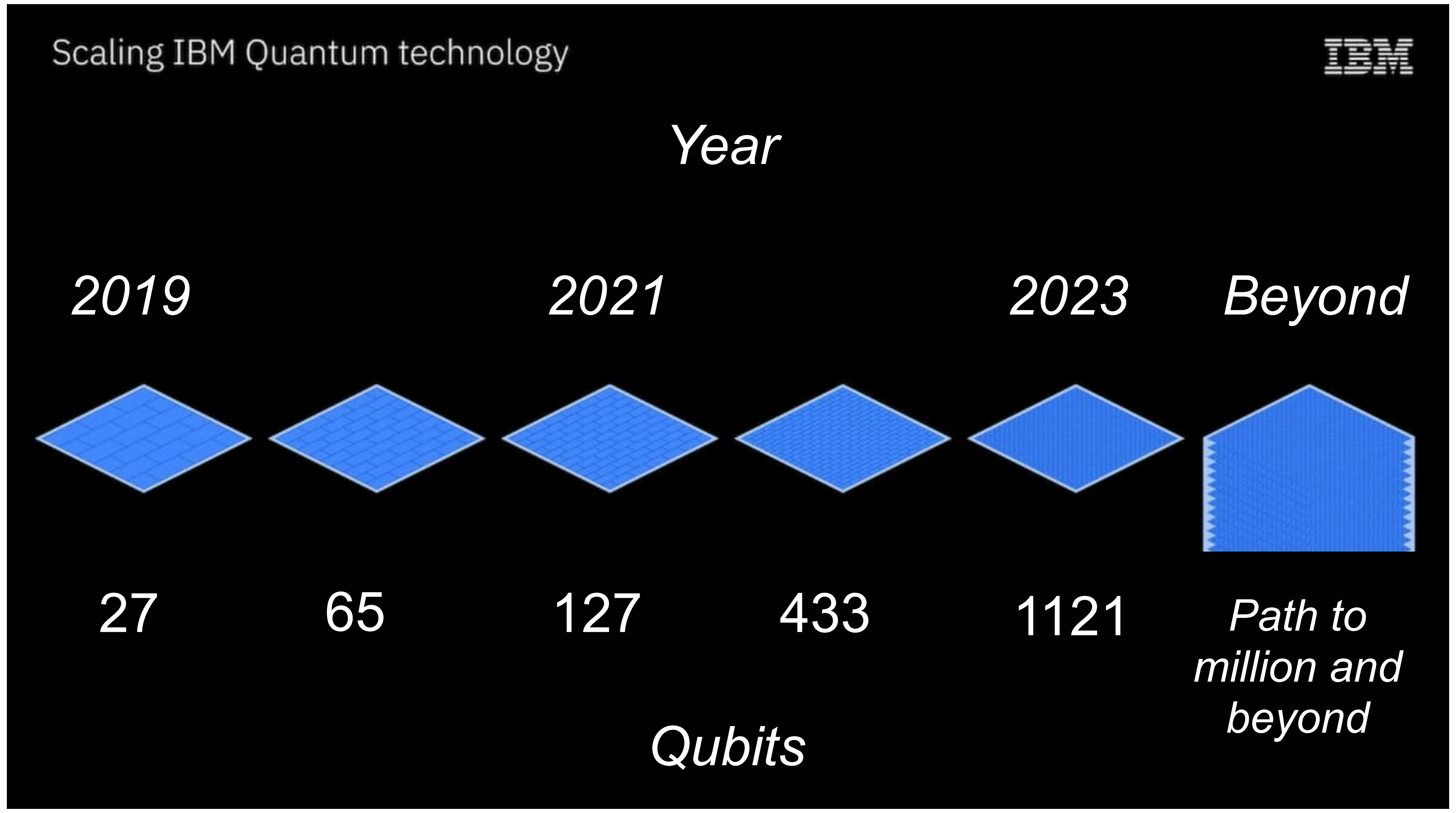
Currently in ***Noisy Intermediate-Scale Quantum*** (NISQ)-era

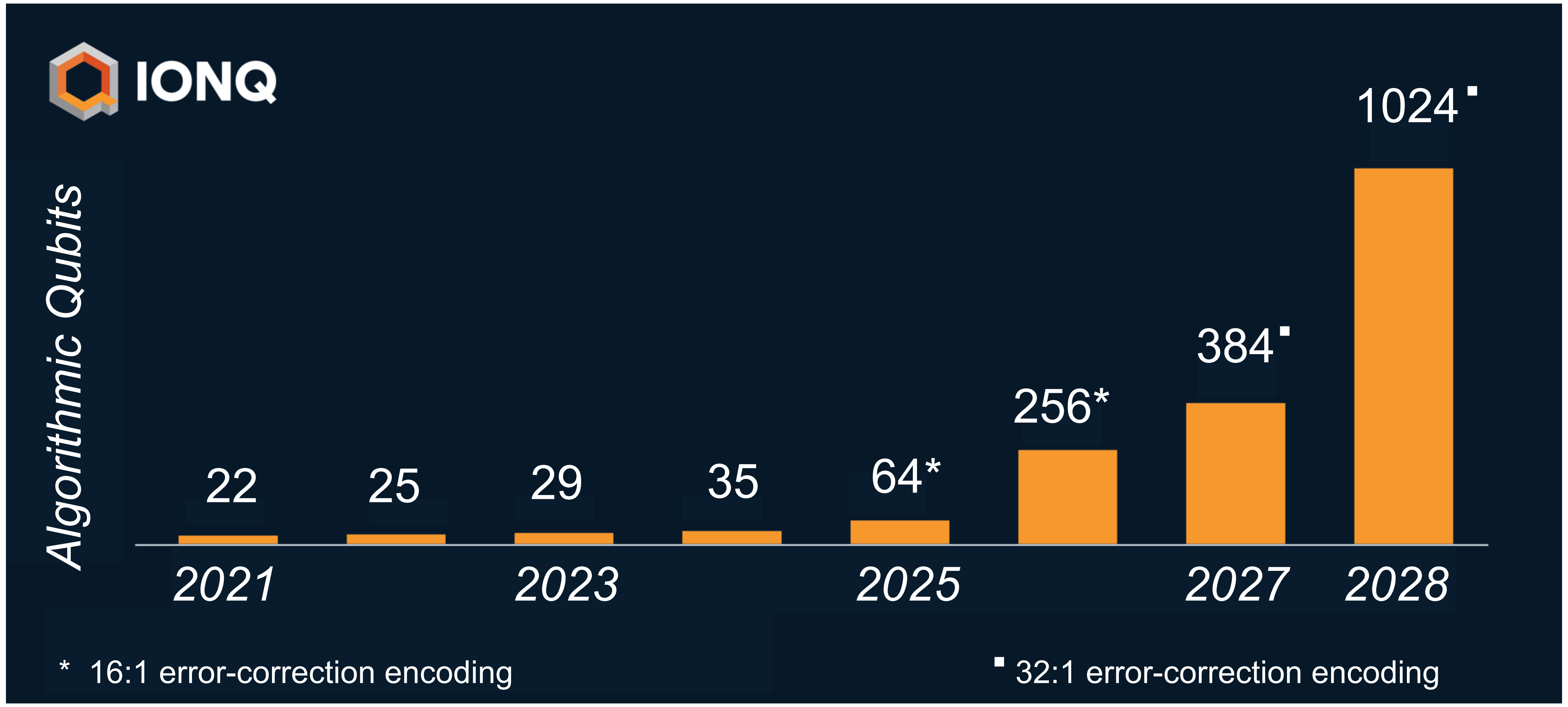
- Machines contain $\mathcal{O}(100)$ noisy qubits without error corrections
- Sensitive to various sources of noise, including decoherence and dephasing

Projection for Near-Future Digital Quantum Computers

Increasing Qubit Count: Many companies projecting 1k+ qubit quantum machines on this timescale



IBM Quantum Roadmap, 2020
Superconducting Qubits



IonQ Roadmap, 2020
Trapped Ion

Gate Noise: Expect decreasing noise which will allow for longer circuits

Quantum Computing for Particle+Nuclear Physics

Guiding Principle: Quantum computing is still in its infancy and so we need to think carefully about what physics problems would be most amenable to this novel computational strategy

Theoretical Developments

How do we formulate field theories in a quantum-computing compatible way?

Algorithmic Developments

How do we map field theories onto quantum circuits that run in reasonable times?

Need to work simultaneously on three interconnected areas

Benchmarking and Optimization

Which quantum hardware is best-suited for specific physics goals?

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Talk will focus on these, applied to simulations of lattice gauge theories

Benchmarking and Optimization

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Simulation of Lattice Gauge Theories

Classical Simulations of Gauge Theories

Lattice QCD: Highly advanced field utilizing high-performance computing to probe non-perturbative properties of QCD from first-principles

- Due to impressive algorithmic developments, some calculations are now done at physical pion masses
- Sub-percent precision in many single-hadron observables
  - Hadron vacuum polarization for g-2 measurements
  - Hadron spectrum with QED and isospin breaking effects
- Reliable extraction of several two-hadron observables
  - $K \to \pi\pi$ and direct CP violation

Only fully-systematic approach to ab-initio computations in the non-perturbative regime

Sign Problems in Lattice Gauge Theories

Lattice Simulations: Numerically estimation of lattice-regulated quantum path integral via Monte Carlo importance sampling requires the existence of a positive probability measure

$$\mathcal{Z} = \int [DU] \det D_F(U)\, e^{-S[U]}$$

Must be real and positive

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"Sign Problem" prohibits first-principles study of phenomenologically-relevant theories

Real-Time Dynamics

Early Universe Phase Transitions

Requires Minkowski space simulations

Chiral Gauge Theories

Fully defined Standard Model

Complex fermion determinant

Finite-Density Nuclear Matter

Neutron stars and QCD phase diagram

Complex fermion determinant

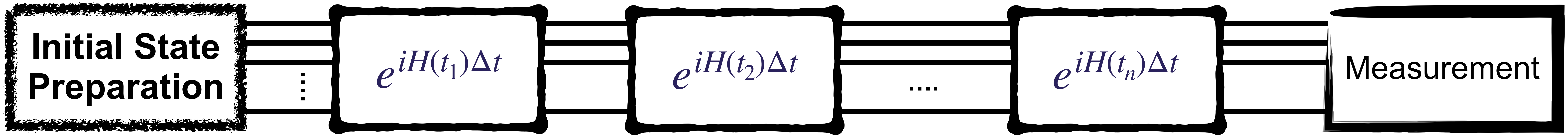
Can quantum computing help?

Quantum Simulations of Gauge Theories

Quantum Lattice: Very young field, utilizing NISQ-era hardware and quantum simulators to carry out exploratory studies on lower-dimensional toy models

General Procedure: Simulation proceeds in three steps

1. Initial State Preparation
2. Evolution via multiple applications of time translation operator
3. Measurement



4. Circuit is re-run multiple times to build up expectation value

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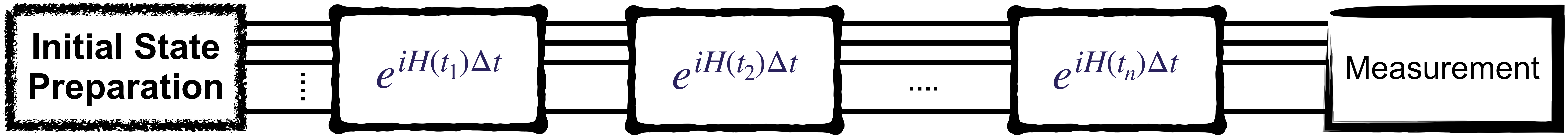

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<u>**Overarching Research Goal**</u>

"Re-write" theory into quantum circuit formulation that runs in reasonable amount of time

Theoretical Development: Time Evolution Operator

Hamiltonian Truncation: Need to map (typically) infinite-dimensional Hamiltonian to finite Hermitian matrix

- Define operators basis and their commutation relations
- Define mapping from state basis to qubit basis
  - How do qubits correspond to the states that span Hilbert space?
- Determine appropriate truncation (UV) and digitation (IR) scale

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Important things to Consider

Gauge and Global Symmetries of the System

Desired Precision of Simulation

Scaling cost with regards to number of qubits and gates

Theoretical Development: Time Evolution Operator

Ex: Quantum Harmonic Oscillator offers various choices

Ladder Operators	***Operator Basis***	Position + Momentum
$[a, a^\dagger] = 1$		$[x, p] = i$
Non-interacting Eigenstates	***State Basis***	Position Eigenstates
$\lvert n \rangle$		$\lvert x \rangle$

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Operator Boundary Conditions	***Finite Matrix Representation***	Momentum Operator Eigenvalues
$a^\dagger \|n_{max}\rangle = \sqrt{n_{max}+1}\,\|0\rangle$, $a\|0\rangle = \sqrt{n_{max}+1}\,\|n_{max}\rangle$ or $a^\dagger\|n_{max}\rangle = 0$, $a\|0\rangle = 0$		$\hat{p}\,\|x\rangle := i\partial_x \|x\rangle$ (Finite difference) or $p_n \sim \frac{n}{N}\frac{2\pi}{\delta x}$

Commutation relations violated in both formulations

Theoretical Developments: Gauge Invariance

Hamiltonian Formulation: Incomplete gauge fixing results in exponentially large Hilbert space, as compared to physical Hilbert space

Key Consideration

Gauge Invariance and Redundancies

- ***Problem:*** Gauss' Law is not automatically satisfied in Hamiltonian formulations
  - Allows for charge-violating transitions
- ***Problem:*** Naive basis of states is over-complete
  - Requires more quantum resources than strictly necessary

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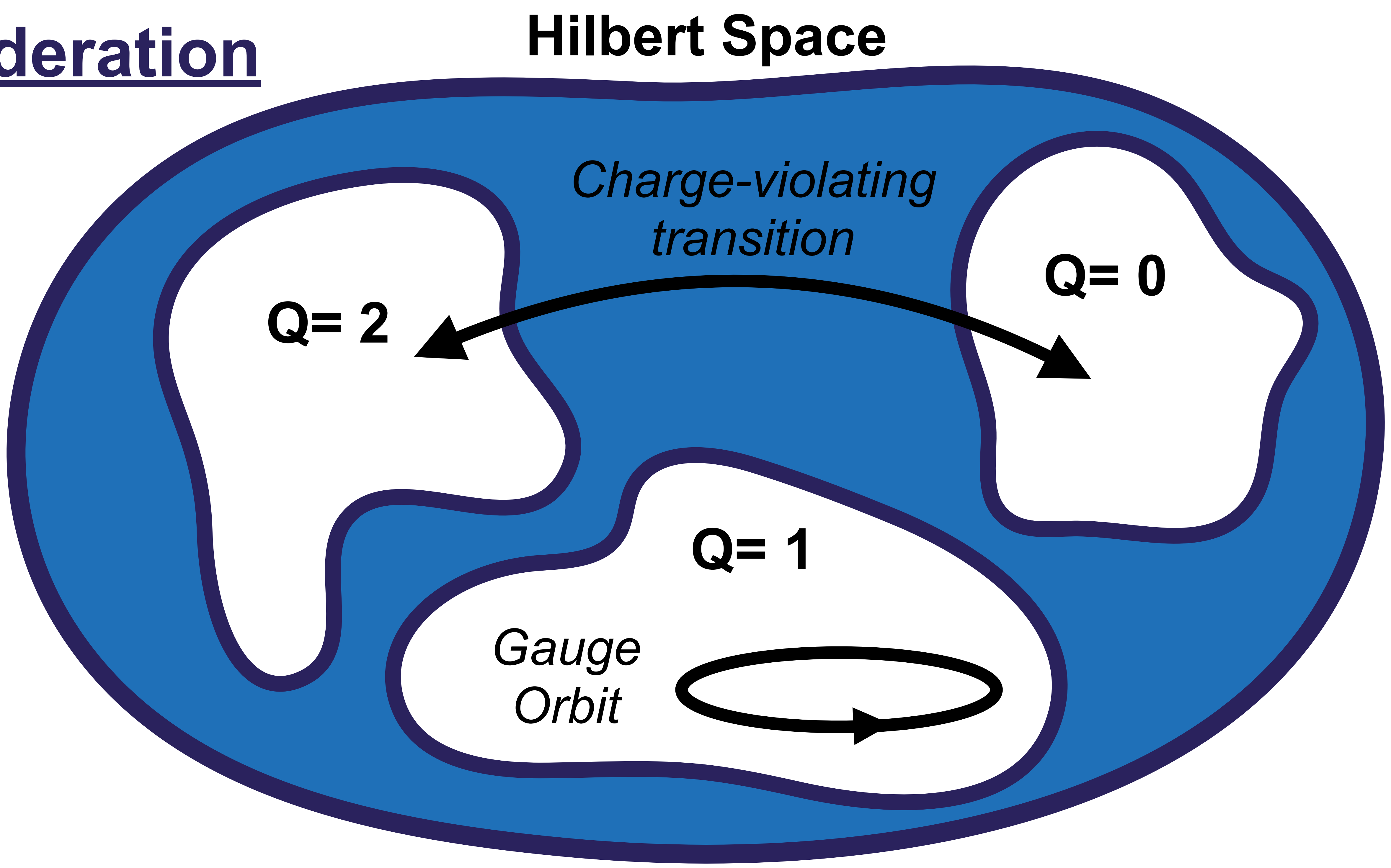

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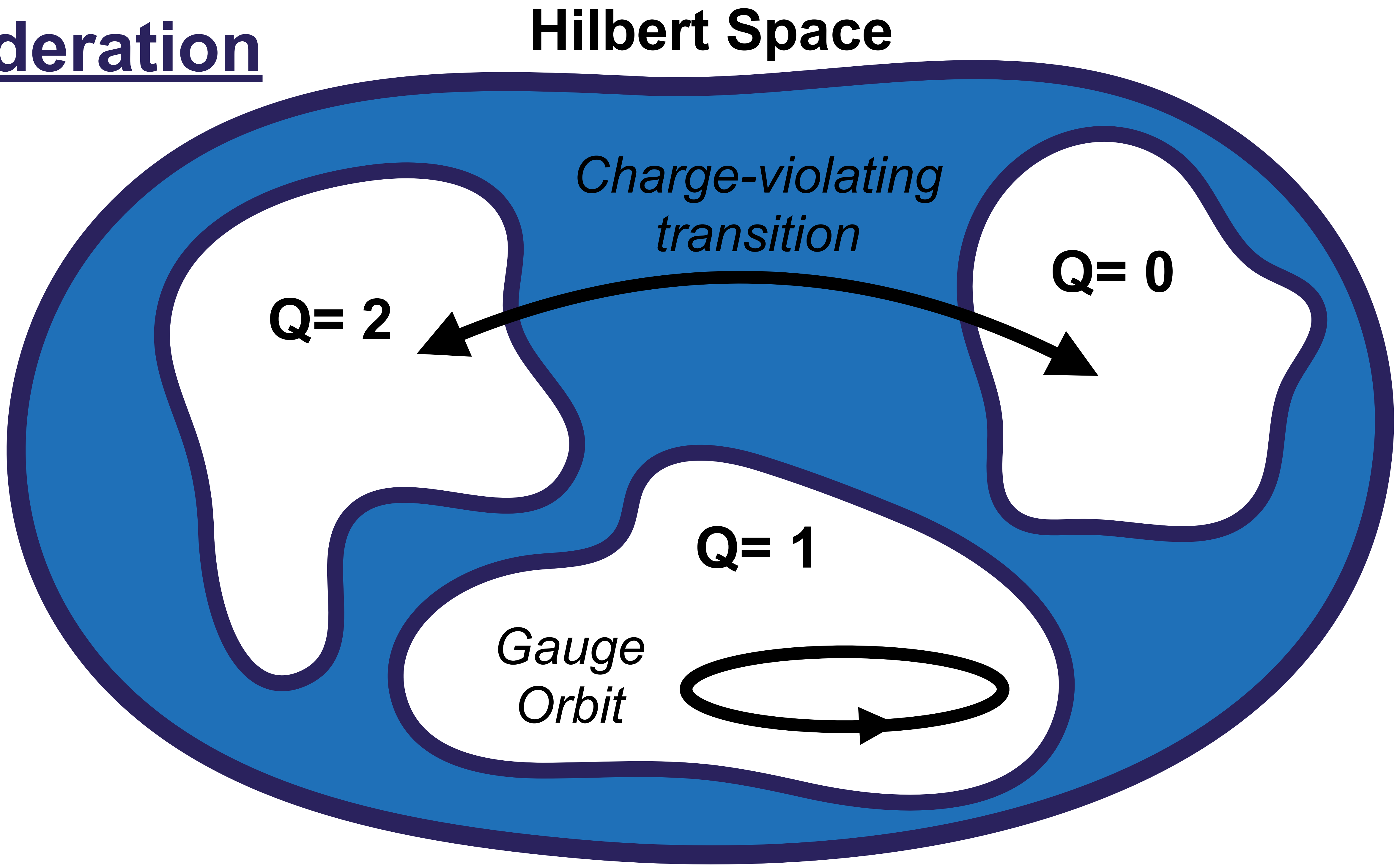

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Continuum Theory: Integral over electric and magnetic fields

$$H = \int d^2x \left(E^2 + B^2\right)$$

Nothing prohibits Gauss law violating fields!

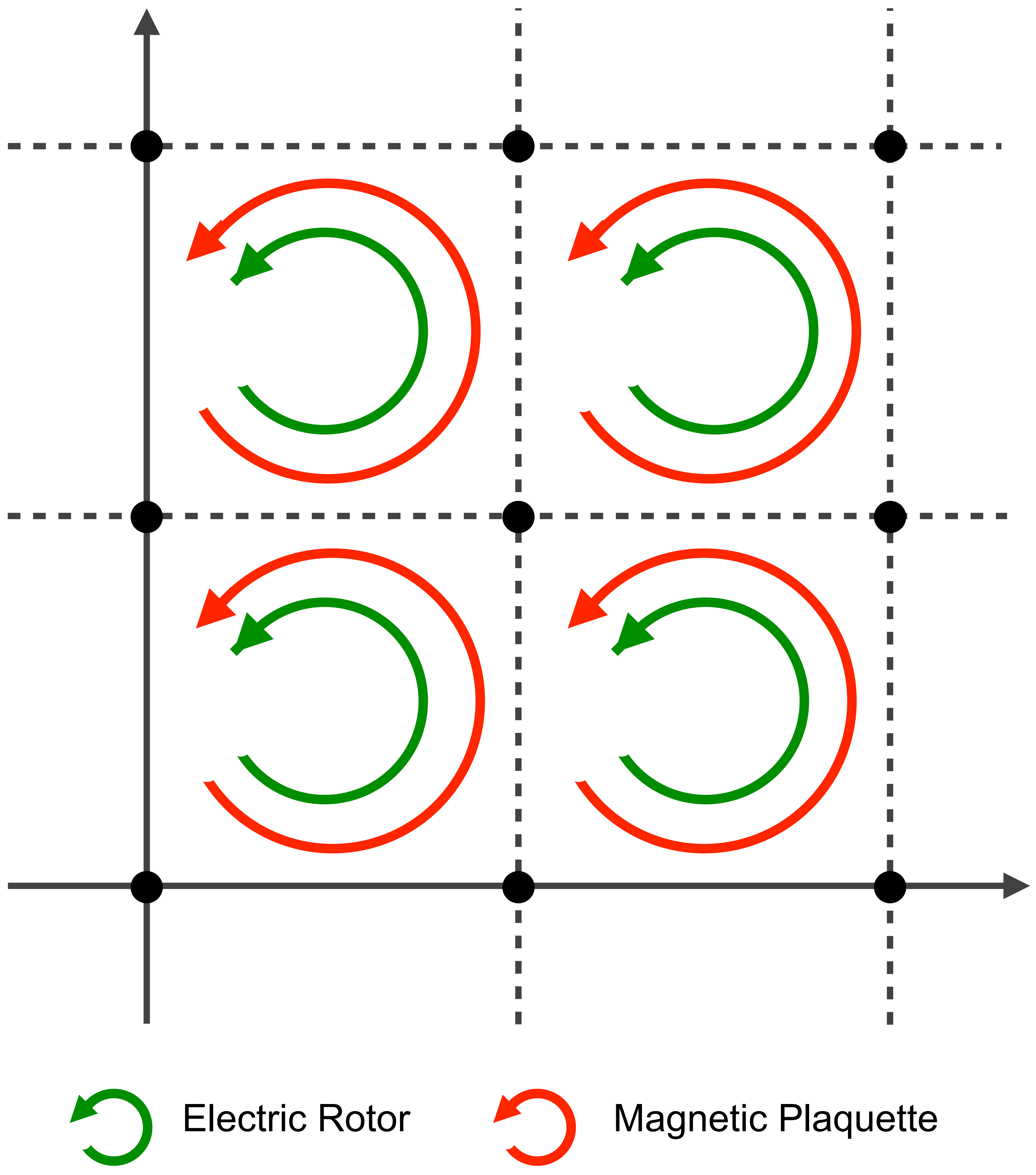
Electromagnetism in Two Spatial Dimensions

General Idea: Work with "gauge-redundancy free" formulation, which is a dual basis formulation

- Hamiltonian defined in terms of plaquette variables: electric rotors and magnetic plaquettes

$$[B_p, R_{p'}] = i\delta_{pp'}$$

- Gauss' law automatically satisfied
- No redundant degrees of freedom
- Formulations works for all values of the gauge coupling



Bauer, C.W. and Grabowska, D.M. arXiv: 2111.08015

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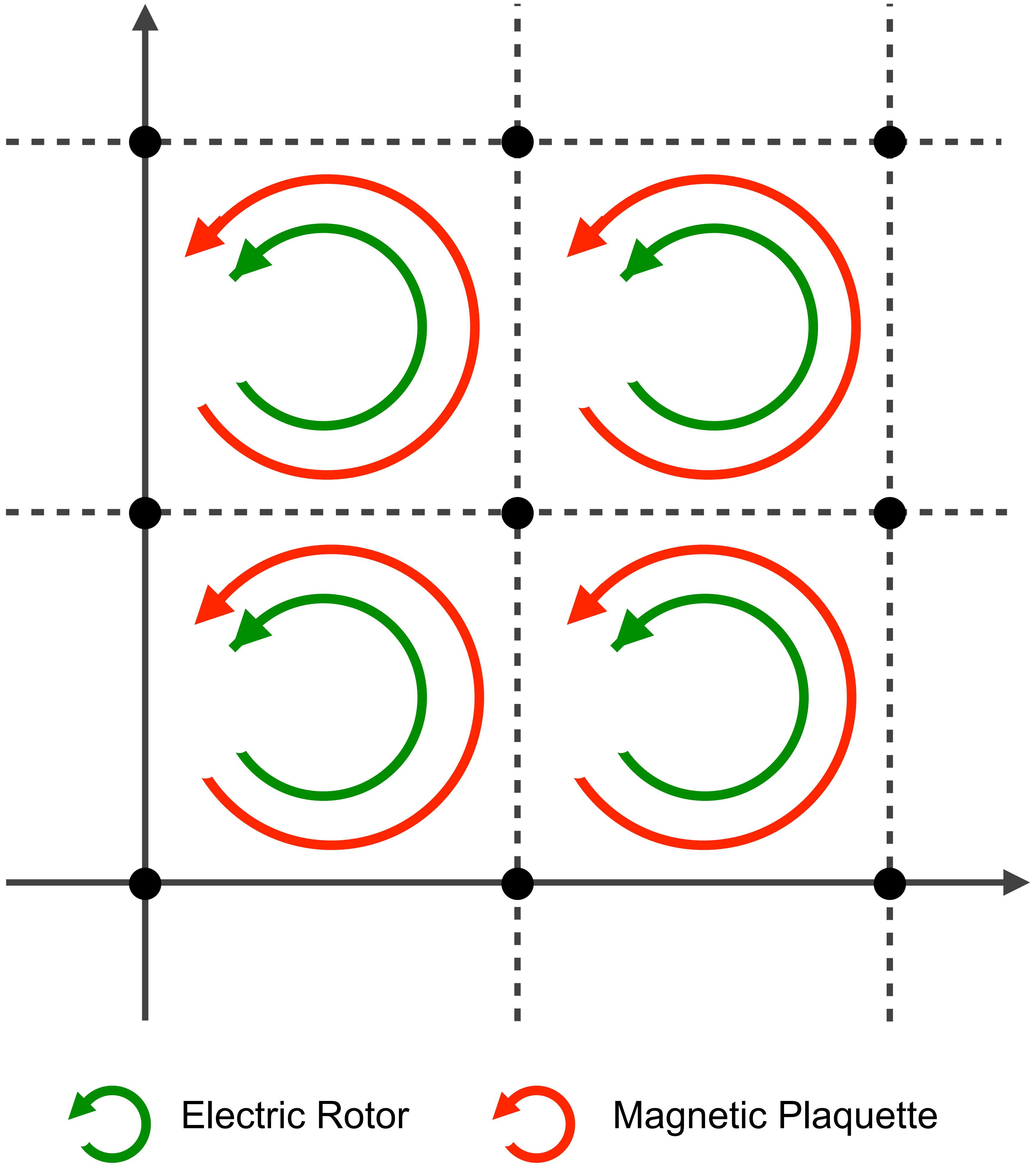

$$H = \frac{1}{2a}\left[g^2 \sum_p \left(\nabla_L \times R_p\right)^2 + \frac{1}{g^2} \begin{cases} \sum_p B_p^2 + \left(\sum_p B_p\right)^2 & \text{non compact} \\ -2\sum_p \cos B_p - 2\cos\left(\sum_p B_p\right) & \text{compact} \end{cases} \right]$$

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Electromagnetism in Two Spatial Dimensions

General Idea: Combine "gauge-redundancy free" dual representation with digitization method that strives to minimize violation of commutation relations

- Truncation scale and digitization scale are not independent and there is an optimal choice
- Canonical commutation relations are minimally violated for that optimal choice

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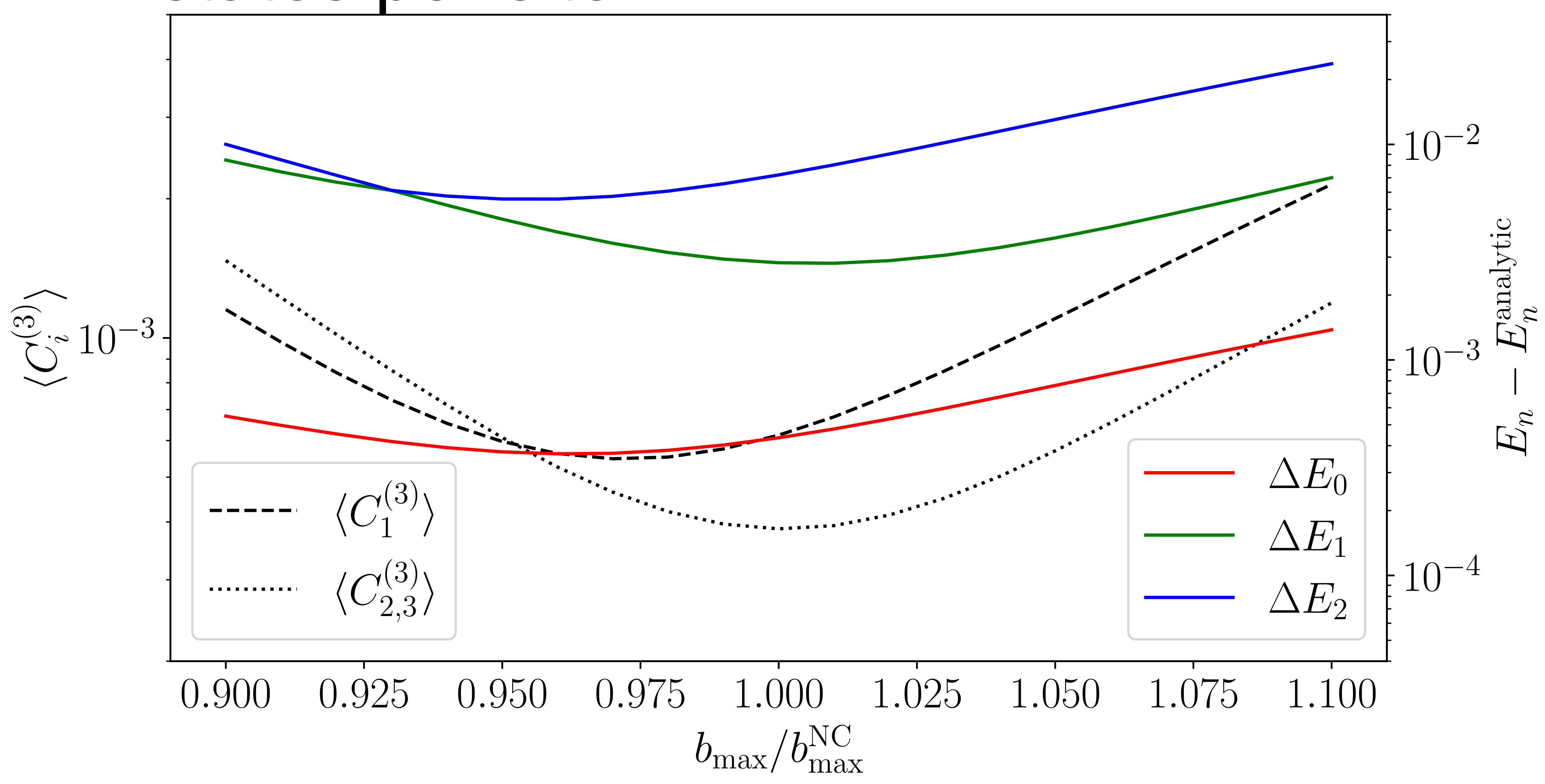
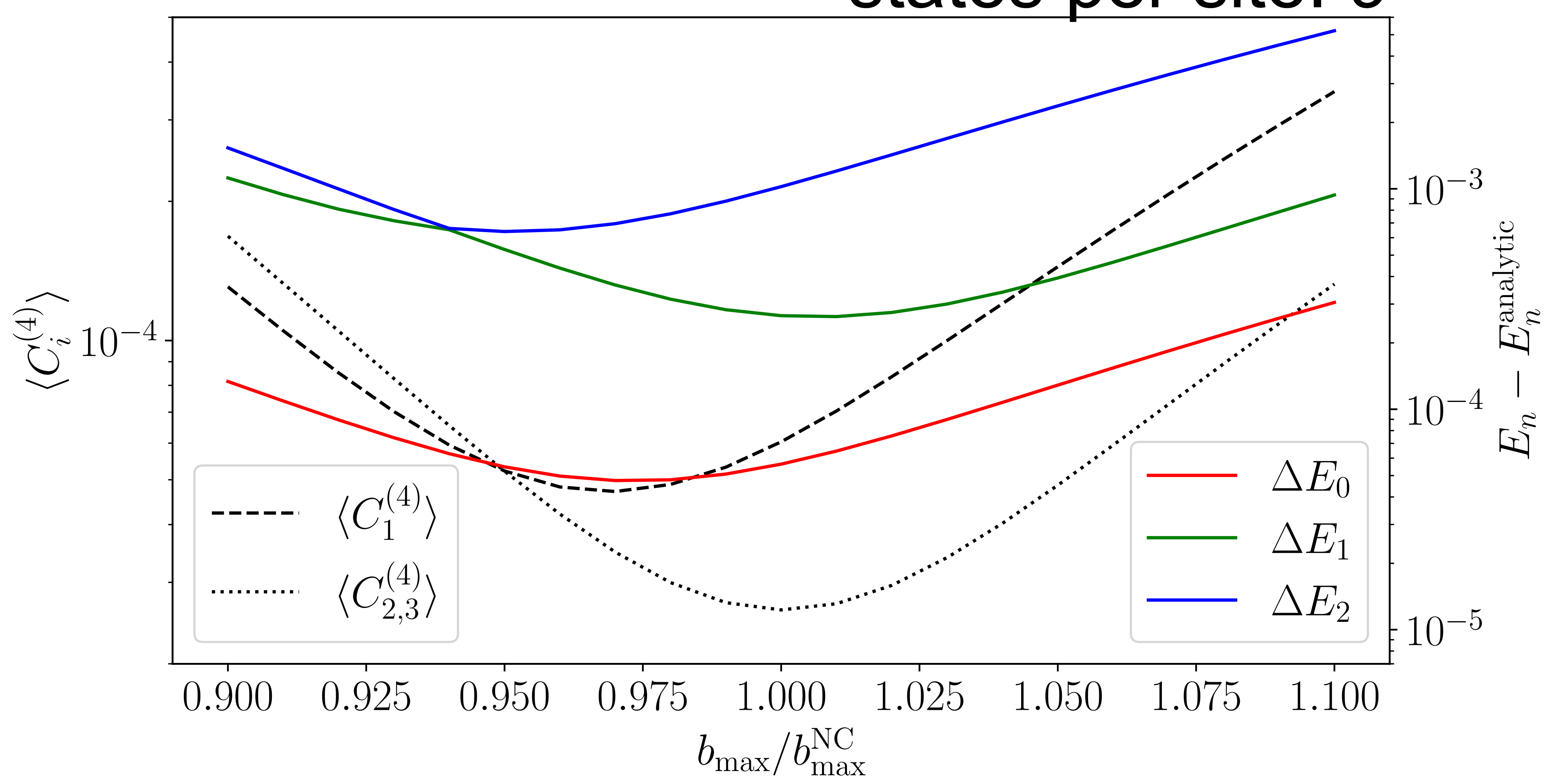
Comparison to exact solution

Violation of Commutation Relations

states per site: 7



states per site: 9



Precision in Low-Lying Energy Eigenvalue

Scanning through truncation scale, compared to optimal truncation scale

Bauer, C.W. and Grabowska, D.M. arXiv: 2111.08015

Algorithmic Development: Exponential Volume Scaling

General Idea: Imposing magnetic Gauss' law without any gauge redundancy requires quantum circuit whose length scales exponentially with volume (for compact theory)

Issue: Total magnetic flux conservation results in maximally non-local term

$$H_B \propto \sum_{p=1}^{N_P} \cos\left(B_p\right) + \cos\left(\sum_{p=1}^{N_P} B_p\right)$$

$2^{n_q} \times 2^{n_q}$ matrix

$2^{n_q N_p} \times 2^{n_q N_p}$ matrix

$N_P \sim$ Number of Plaquettes (volume)

$2^{n_q} \sim$ number of states per plaquette

Grabowska et all, to appear shortly

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Time Evolution: Implementing a single time step requires $\mathcal{O}\left(2^{n_q N_p}\right)$ gates

Example: Small 8 x 8 lattice with two qubits (four states) per plaquette requires

10^{38} quantum gates 10^{14} years on a exo-scale classical computer to create circuit

Grabowska et all, to appear shortly

Algorithmic Development: Polynomial Scaling

General Idea: Carry out field operator change of basis to reduce non-locality

$$B_p \to \mathscr{W}_{pp'} B_{p'} \qquad\qquad R_p \to \mathscr{W}_{pp'} R_{p'}$$

$\mathscr{W}$ is a block diagonal rotation matrix with N_S sub-blocks of dimension d_i

$$\cos\left[\sum_{i=1}^{N_p} B_p\right] \to \cos\left[\sum_{i=1}^{N_s} \sqrt{d_{(i)}} B_{D_{(i)}}\right] \qquad\qquad \cos\left[B_i\right] \to \sum_{k=1}^{d_{(i)}} \cos\left[\sum_{j=1}^{d_{(i)}} \Omega_{kj}^{(i)} B_{D_{(i)}+j-1}\right]$$

Non-local term becomes more local   *Local terms becomes more non-local*

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Local terms becomes more non-local

Time Evolution: Implementing a single time step requires $\mathcal{O}\left(N_p^{n_q}\right)$ gates

Example: Small 8 x 8 lattice with two qubits (four states) per plaquette requires

10^4 quantum gates $\qquad$ 10^5 classical FLOPs to create circuit

Grabowska et all, to appear shortly

Generalizations and Applications

Next Steps: Generalize formulation to more physically-relevant theories

Standard Model

3+1 dimensional gauge theory

$SU(3) \times SU(2)_L \times U(1)_Y$

Higher Dimensions

Imposing Gauss' law in 3+1 dimensions is more complicated

Fermions

Introduce fermions with good chiral symmetry

Non-Abelian Groups

Self-interaction of gauge fields introduces additional complications

Concluding Remarks

Conclusions

Rich phenomena of non-perturbative quantum field theories is a profitable place to look for new answers to the big questions

Quantum computers have a fundamentally different computational strategy and will provide novel probes of fundamental questions in particle and nuclear physics

Quantum computing is still in its infancy and so need to think carefully about what physics problems would be most amenable to this novel computational strategy

<u>Theoretical Developments</u>

How do we formulate field theories in a quantum-computing compatible way?

<u>Algorithmic Developments</u>

How do we map field theories onto quantum circuits that run in reasonable times?

Back Up Slides

Analog Quantum Computer

Computational Strategy: Use controllable quantum system to simulate the behavior of another

- Generally built from cold atoms on an optical lattice
- Non-universal: needs to be tuned to reflect the desired physics
- Continuous time evolution

Analog quantum computer are like an effective field theory for a more fundamental quantum field theory, but made physical

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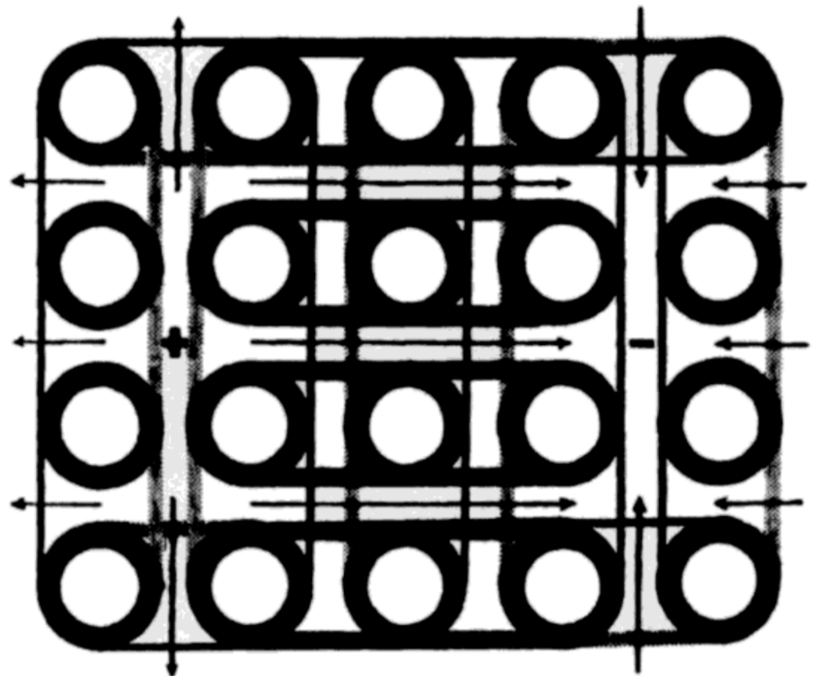
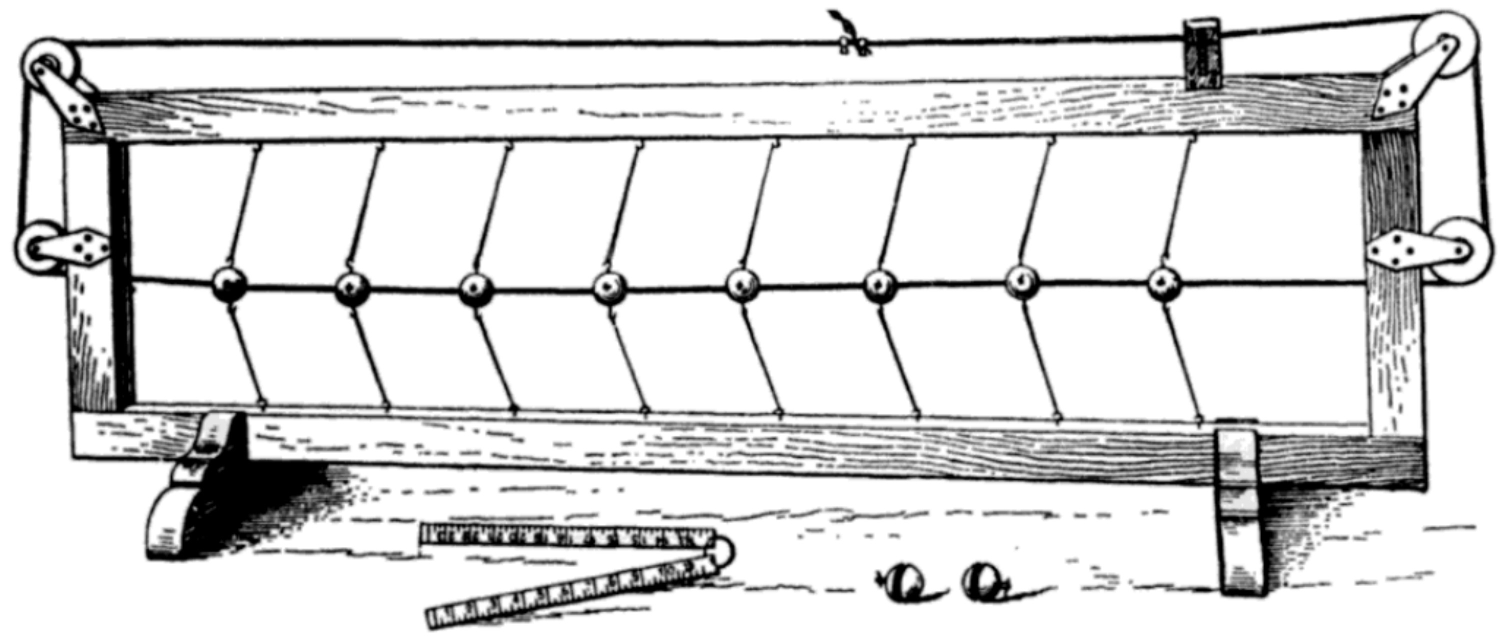
Method of using physical toy models to understand more complicated system has a long history in physics

Ex: Physical systems made of rollers, bands and string used to understand Maxwell's law and the Luminiferous Aether



4.3. FitzGerald's wheel-and-band model (strained and locked).



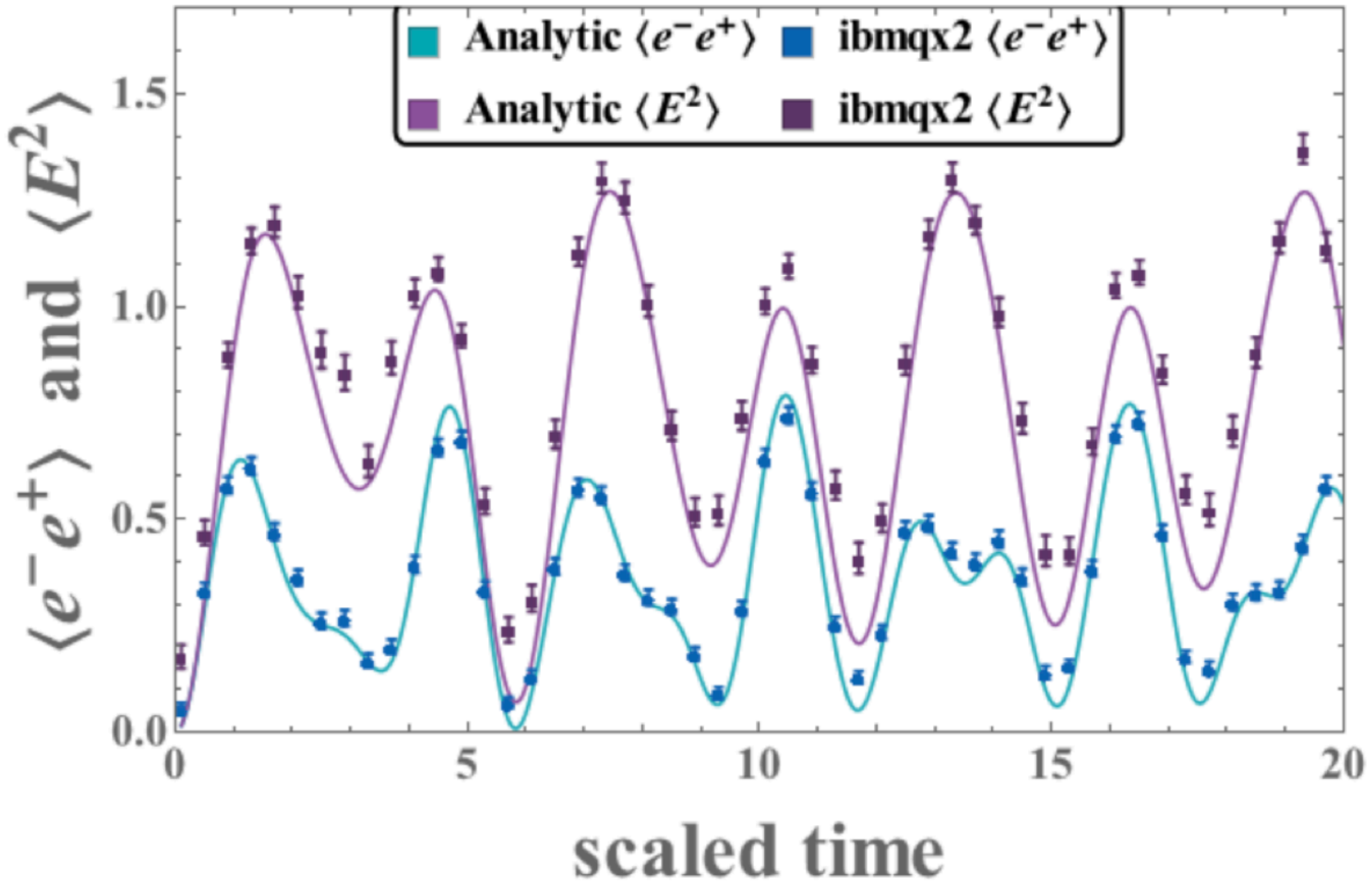
4.4. Lodge's string-and-button model of an electric circuit. The string runs through slots in the buttons, which are attached by rubber bands to the wooden frame. By tightening or loosening the screws holding the buttons to the string, the model can be made to represent either a dielectric or a conducting circuit.

"The Maxwellians", Bruce J. Hunt, Cornell University Press (1991)

Simulation of Lattice Schwinger Model

Key Observation*:* Time-dependent pair production

Digital: Realized via qantum circuit utilizing superconducting qubits



Klco, N. et al (Phys. Rev. A **98**, 032331 (2018)

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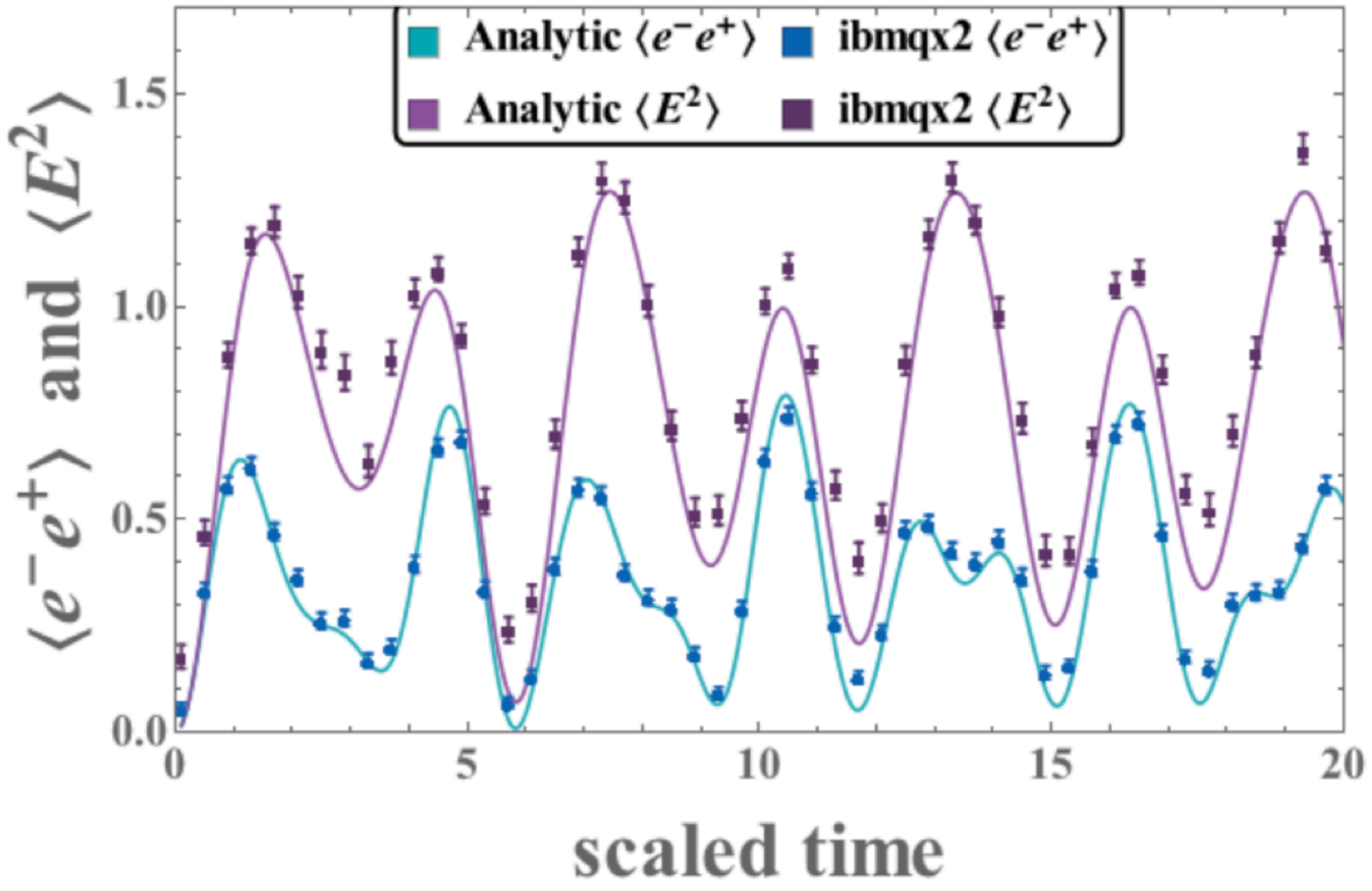

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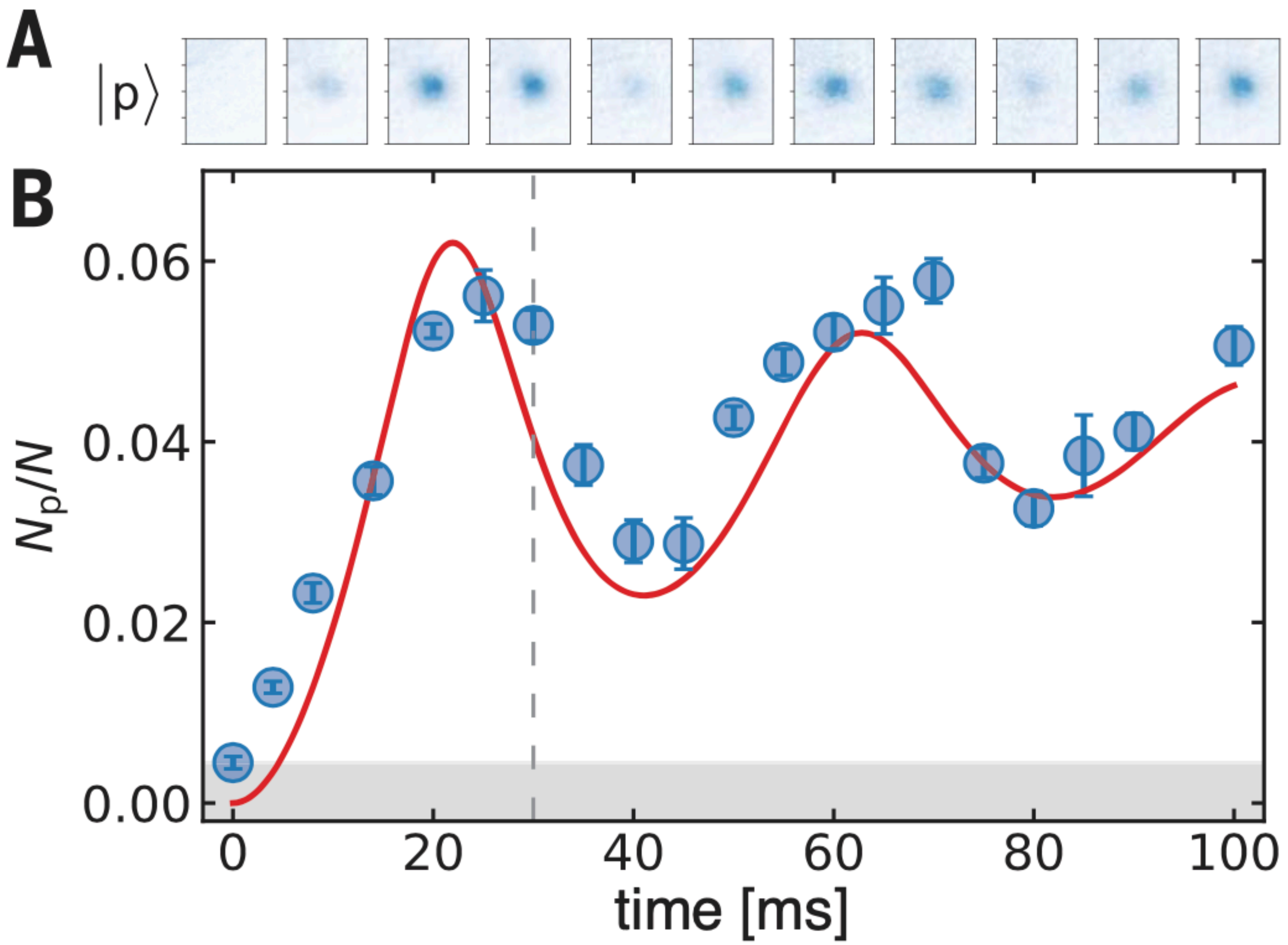
Analog: Realized via cold atoms in a trapping potential



Mil A. et al., Science 367:1128-1130 (2020)

Digitization Example: Quantum Harmonic Oscillator

This simple toy model clearly demonstrates the pitfalls of unwise digitisation choices

Goal: Using only $2L+1$ states, how well can we replicate the low-lying states of the QHO?

$$H = \frac{1}{2}X^2 + \frac{1}{2}P^2$$

1) Working in the X basis, it is trivial to digitize X

$$X_k = -X_{\text{max}} + k\delta X \qquad \delta X = \frac{X_{\text{max}}}{L}$$

X_{max} is a free parameter

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2) Question: How to digitizing P, as it is not diagonal in this basis

Option One: Use finite difference version

$$P^2 = \frac{1}{\delta X^2}\begin{pmatrix} 2 & -1 & 0 & 0 & -1 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ -1 & 0 & 0 & -1 & 2 \end{pmatrix}$$

Digitization Example: Quantum Harmonic Oscillator

This simple toy model clearly demonstrates the pitfalls of unwise digitisation choices

Goal: Using only $2L+1$ states, how well can we replicate the low-lying states of the QHO?

$$H = \frac{1}{2}X^2 + \frac{1}{2}P^2$$

1) Working in the X basis, it is trivial to digitize X

$$X_k = -X_{\text{max}} + k\delta X \qquad \delta X = \frac{X_{\text{max}}}{L}$$

X_{max} is a free parameter

2) Question: How to digitizing P, as it is not diagonal in this basis

Option One: Use finite difference version

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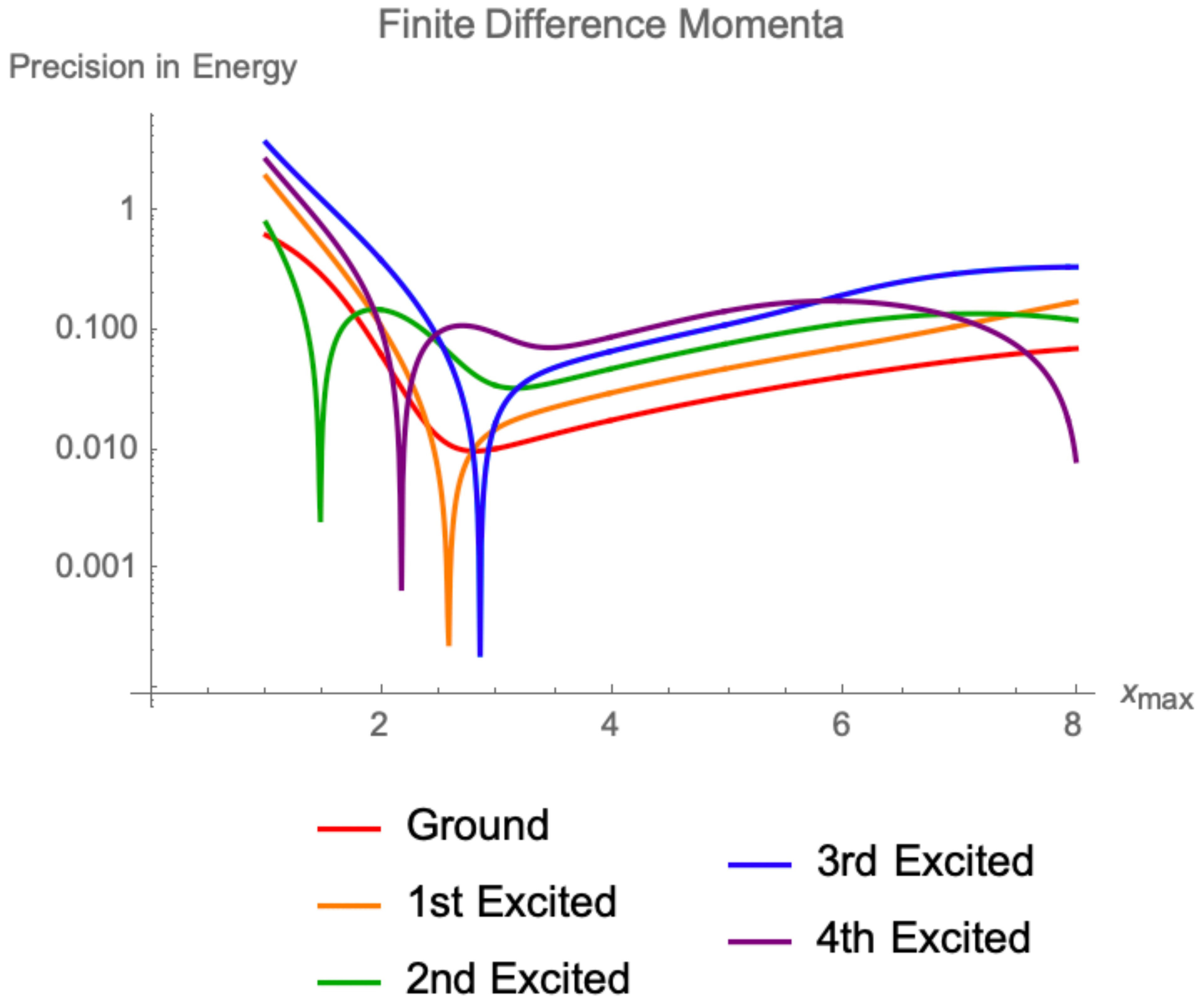

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Option One: Use finite difference version
Option Two: Use exact form and Fourier transform to change basis

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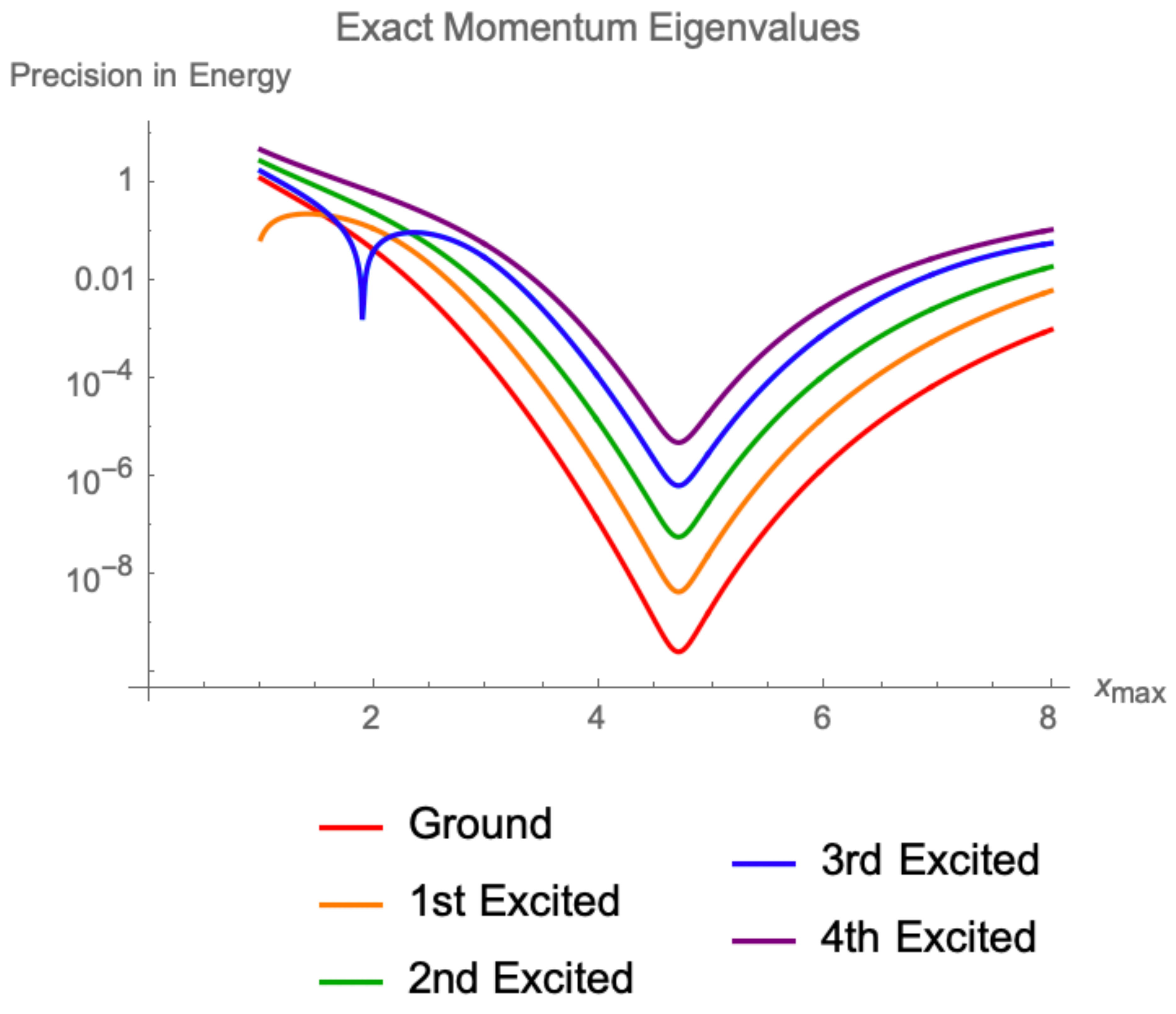

Digitization Example: Quantum Harmonic Oscillator

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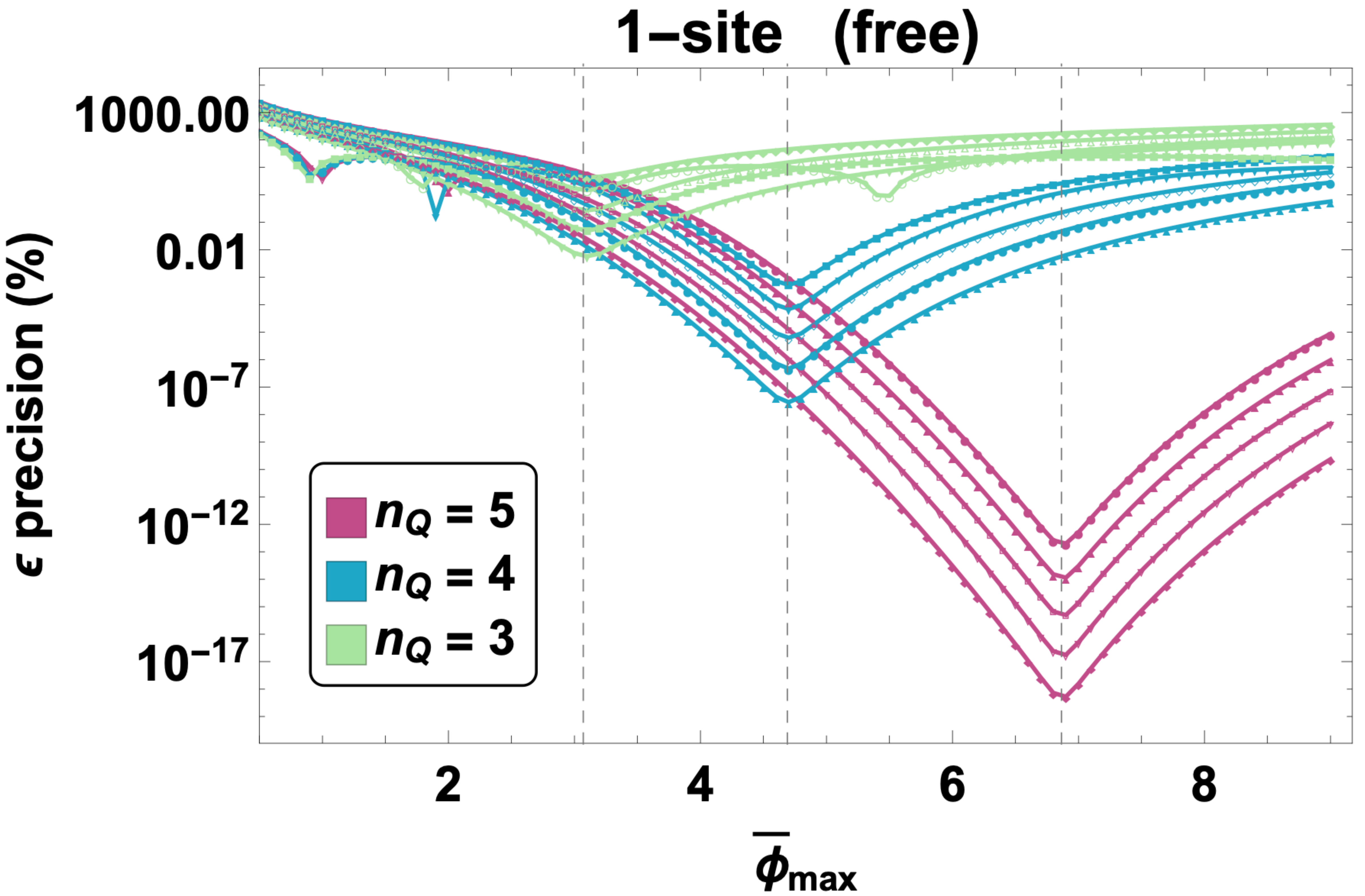
Optimal value can be calculated exactly

$$x_{\text{max}} = L\sqrt{\frac{2\pi}{2L+1}}$$

Intuitive Understanding: *Eigenstate has the same width in both position and momentum space and so* $\delta x = \delta p$



(Plot done with qubit encoding so different number of states per site)

Klco, N. and Savage, M.J.: Phys. Rev. A 99, 052335 (2019) [arXiv: 1808.10378]

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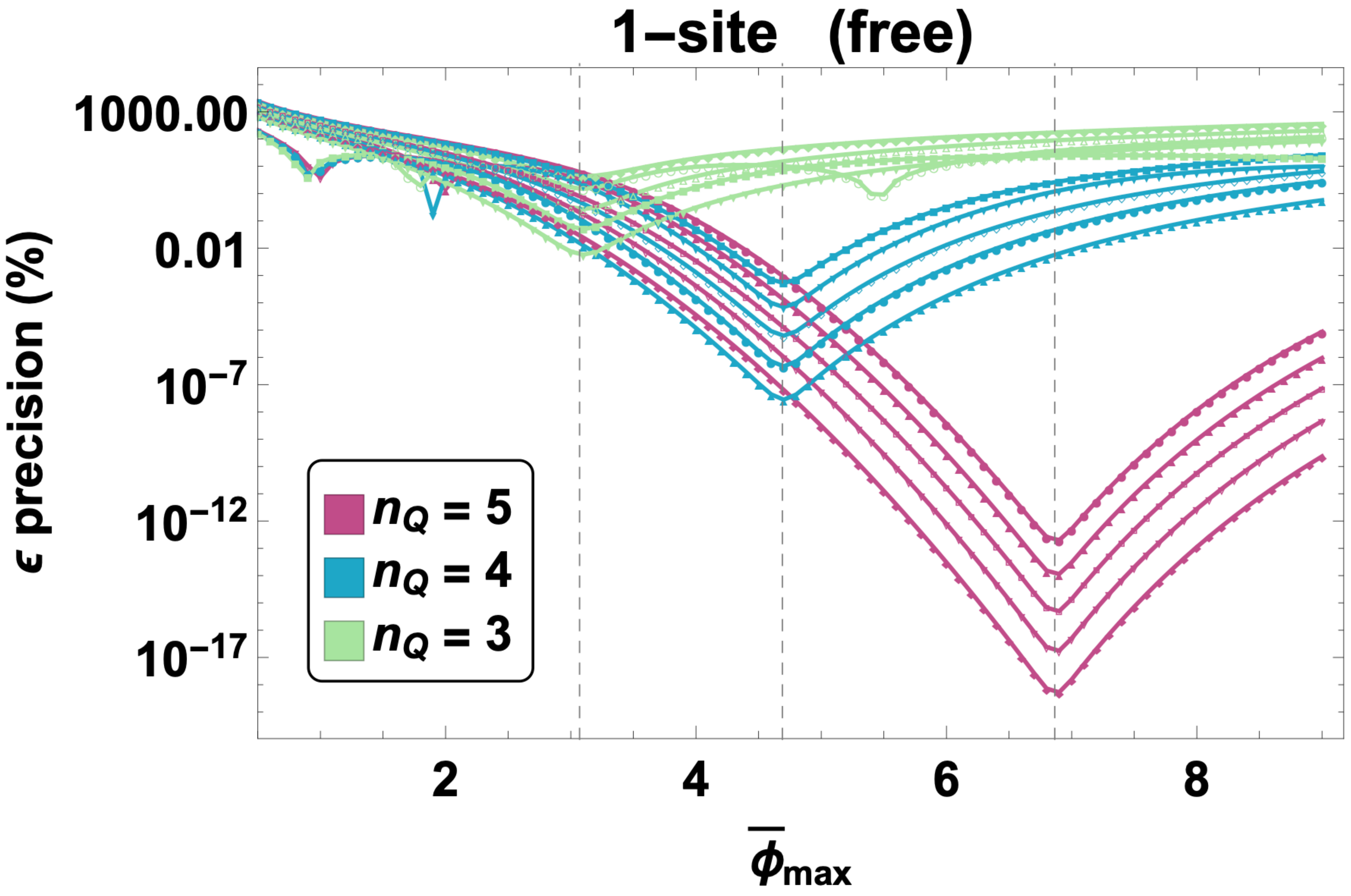
Value for optimal X_{max} can also be related to Nyquist–Shannon sampling theorem

Macridin, A.,Spentzouris, P., Amundson, J., and Harnik, R: Phys. Rev. Lett. 121, 110504 (2018) and Phys. Rev. A 98, 042312 (2018)



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Digitizing the Dual Formulation in the Magnetic Basis

General Idea: Combine "gauge-redundancy free" dual representations with digitization method motived by quantum harmonic oscillator example [Bauer, C.W. and **DMG** arXiv: 2111.08015]

- Magnetic basis and rotor basis related by Fourier transform
- Use exact continuum eigenvalues for digitization

Step One: Digitize rotor and magnetic fields

$$b_p^{(k)} = -\, b_{\max} + k\,\delta b \qquad \delta b = \frac{b_{\max}}{\ell} \qquad r_p^{(k)} = -\, r_{\max} + \left(k + \frac{1}{2}\right)\delta r \qquad \delta r = \frac{2\pi}{\delta b(2\ell + 1)} \qquad r_{\max} = \frac{\pi}{\delta b}$$

- Variable k labels the eigenvalues
- Number of eigenvalues: $2\ell + 1$

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Step Two: Define digitized rotor and magnetic operators

$$\langle b_p^{(k)} | B_p | b_{p'}^{(k')} \rangle = b_p^{(k)} \delta_{kk'} \delta_{pp'} \qquad \langle b_p^{(k)} | R_p | b_{p'}^{(k')} \rangle = \sum_{n=0}^{2\ell} r_p^{(n)} (\mathrm{FT})^{-1}_{kn} (\mathrm{FT})_{nk'} \delta_{pp'}$$

Free parameter $b_{\max}$ needs to be determined

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Step Three: Choose an optimal value for b_{max}

Non-Compact Theory

- Simply a complicated coupled harmonic oscillator at all values of the coupling
- Optimal value can be calculated analytically

$$b_{\text{max}}^{\text{NC}}(g,\ell) = g\ell\sqrt{\frac{\sqrt{8\pi}}{2\ell+1}}$$

Intuition: *Rescaled eigenstate has same width in both rotor and magnetic space and so* $\delta b = \delta r$

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Compact Theory

- Reduces to a complicated coupled harmonic oscillator at weak coupling
- Equivalent to Kogut-Susskind Hamiltonian

$$b_{\text{max}}^{\text{C}}(g,\ell) = \min\left[b_{\text{max}}^{\text{NC}}, \frac{2\pi\ell}{2\ell+1}\right]$$

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Intuition: *Smooth interpolation between strong and weak coupling regime*

Formulation works well for all values of the gauge coupling

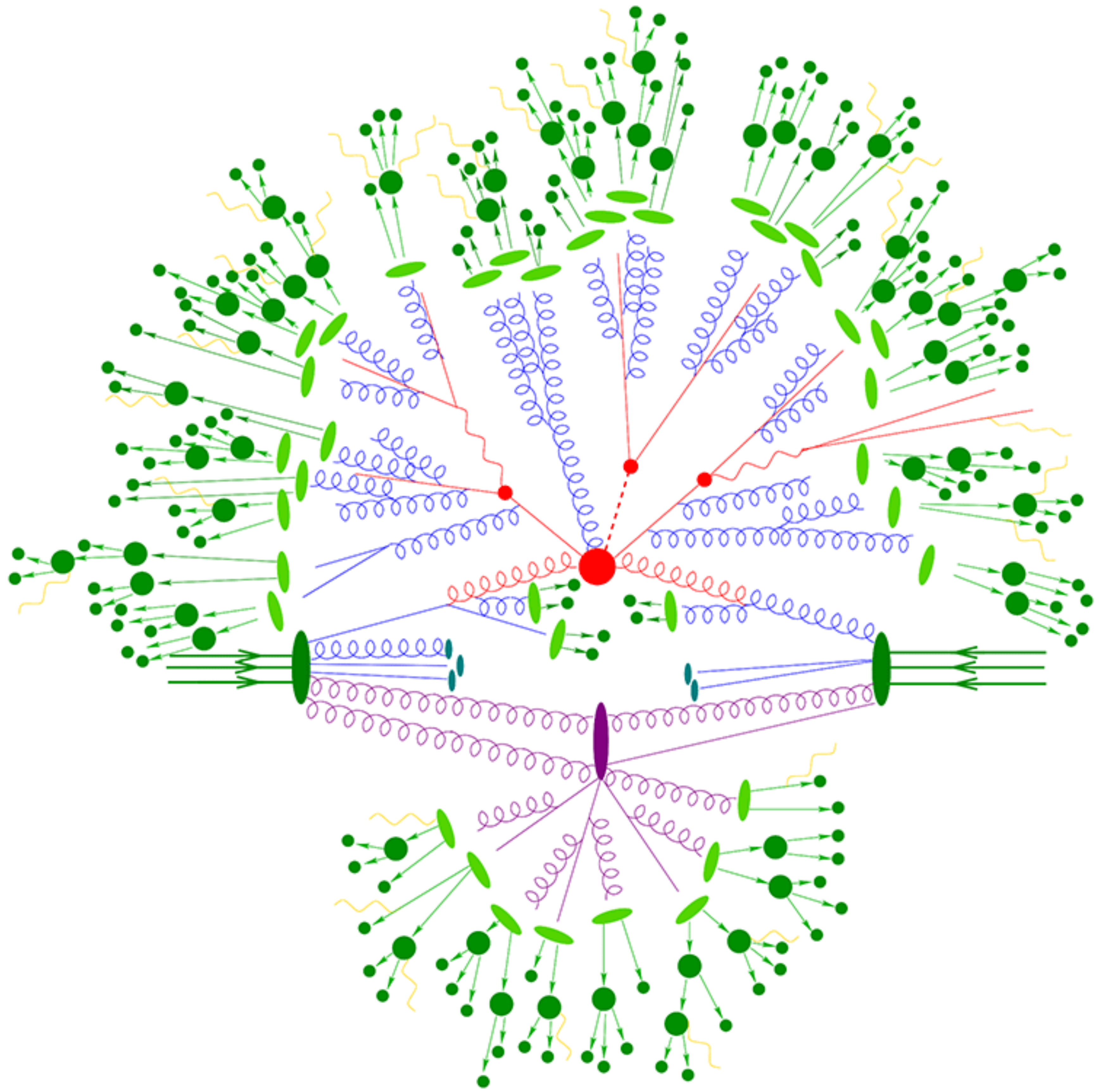
Quantum Machine Learning* For Monte Carlo Event Generation

*QML

High-Energy Collisions at the Large Hadron Collider

LHC Collisions: Extremely complex events that span many different energy scales, further complicated by detector construction and experimental configuration

- No simple one-to-one mapping between Standard Model parameters and experimental measurements
- Monte Carlo event generation is necessary to compare theoretical expectation to experimental reality



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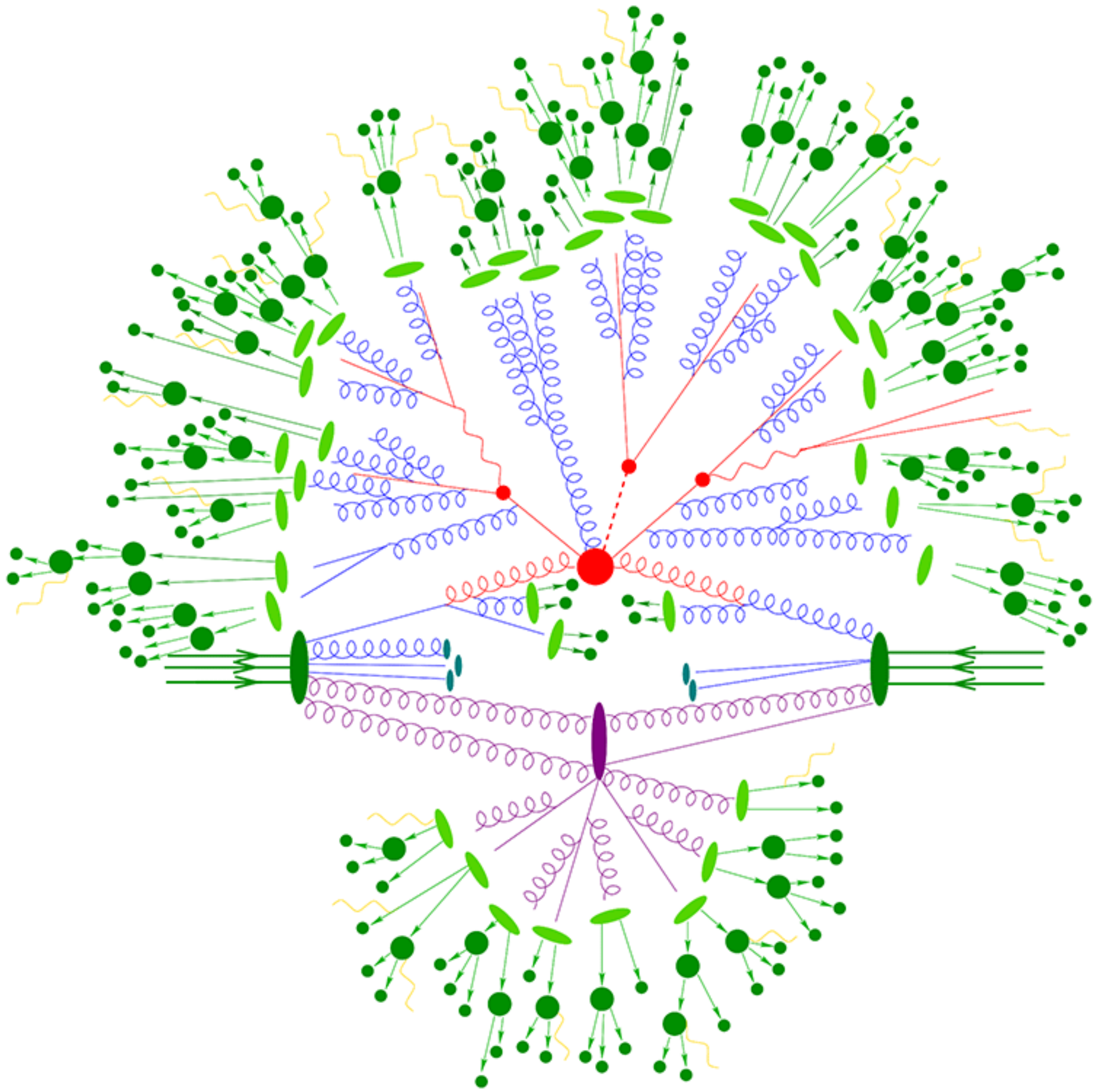


Monte Carlo Event Generation: Pipeline that transforms Standard Model parameters into event distributions

- Feasible on classical machines, but computationally expensive

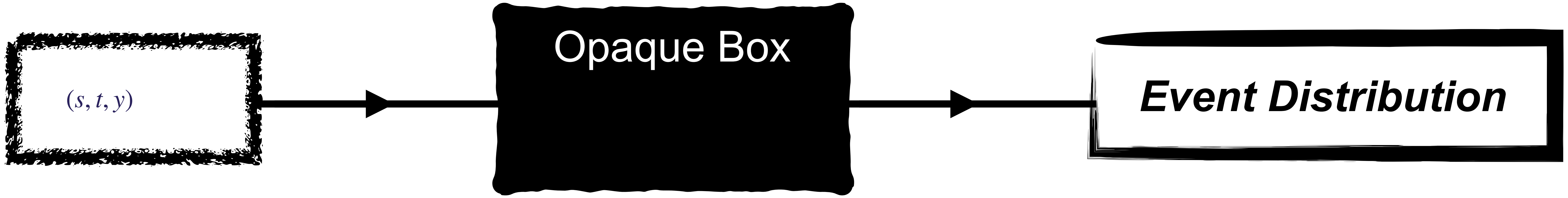
Can quantum machine learning help?

(Quantum) Machine Learning

Machine Learning: Computer algorithm that improves automatically through experience and use of data

Intuitive Definition: Algorithm creates improvable opaque box that transforms input variables to output distributions

Ex: Transform set of Mandelstam variables plus rapidity into underlying event distribution of these variables



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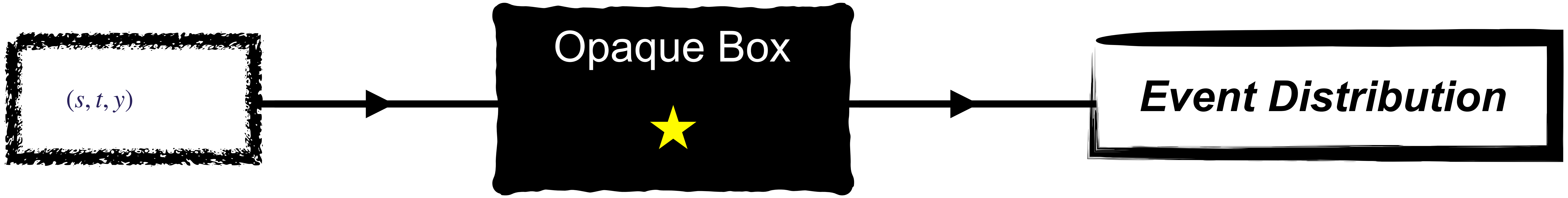

Training improves how well the opaque box replicates the underlying distribution

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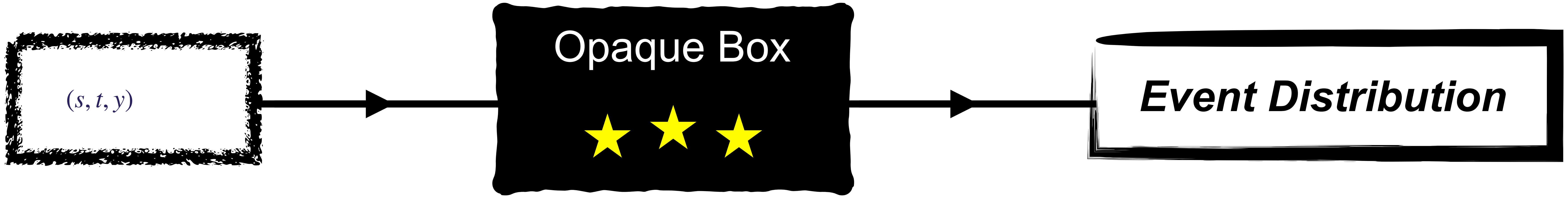


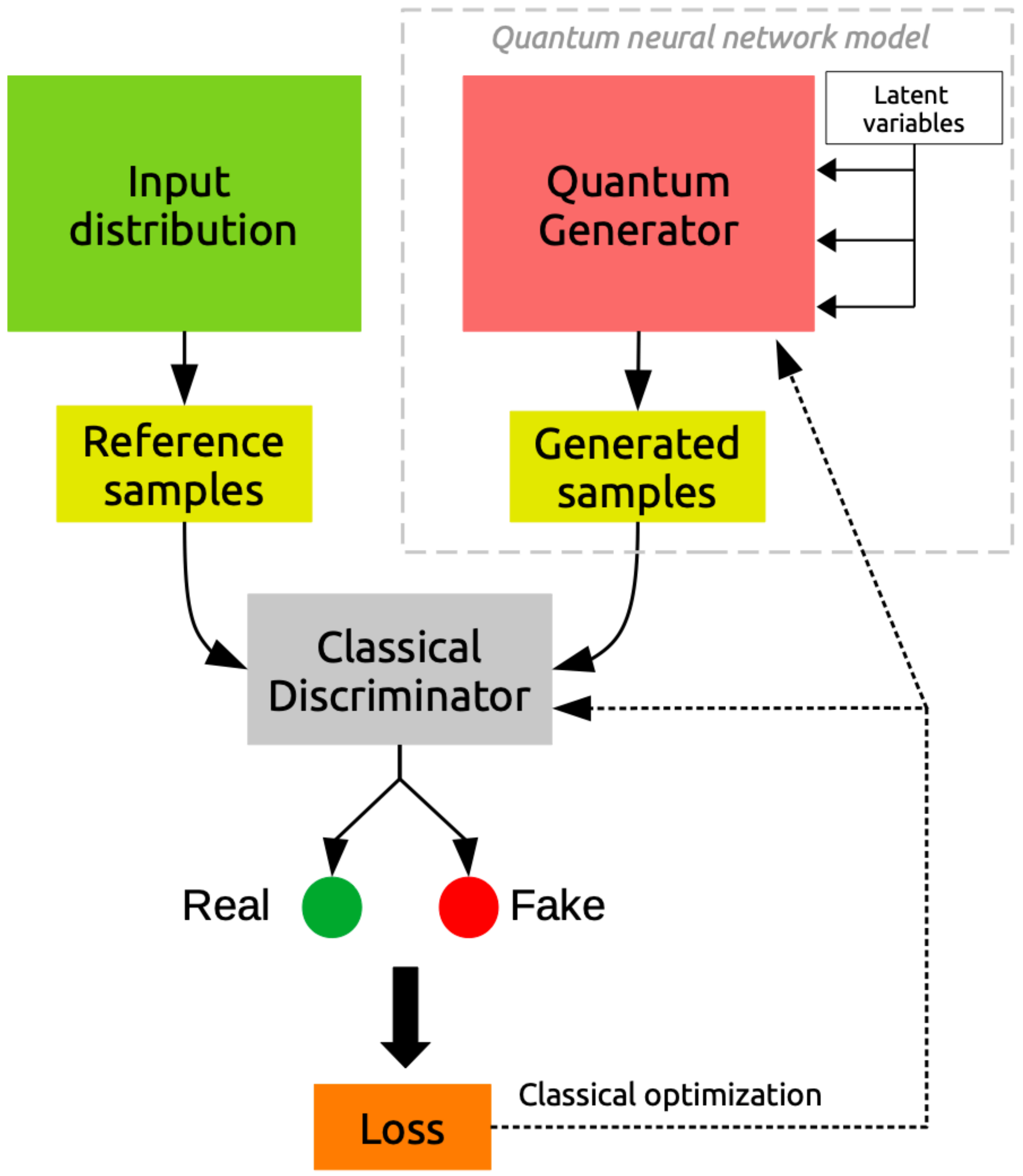
Training improves how well the opaque box replicates the underlying distribution

Opaque box is reproducible and can generate same distributions in the future

Quantum Machine Learning Strategy

General Idea: Use a trained neural network to augment data produced by classical Monte Carlo event generation

- Data augmentation decreases classical computational cost due to "filling in" the distribution without having to rerun entire pipeline
- Quantum approach may be beneficial due to small number of highly correlated input variables



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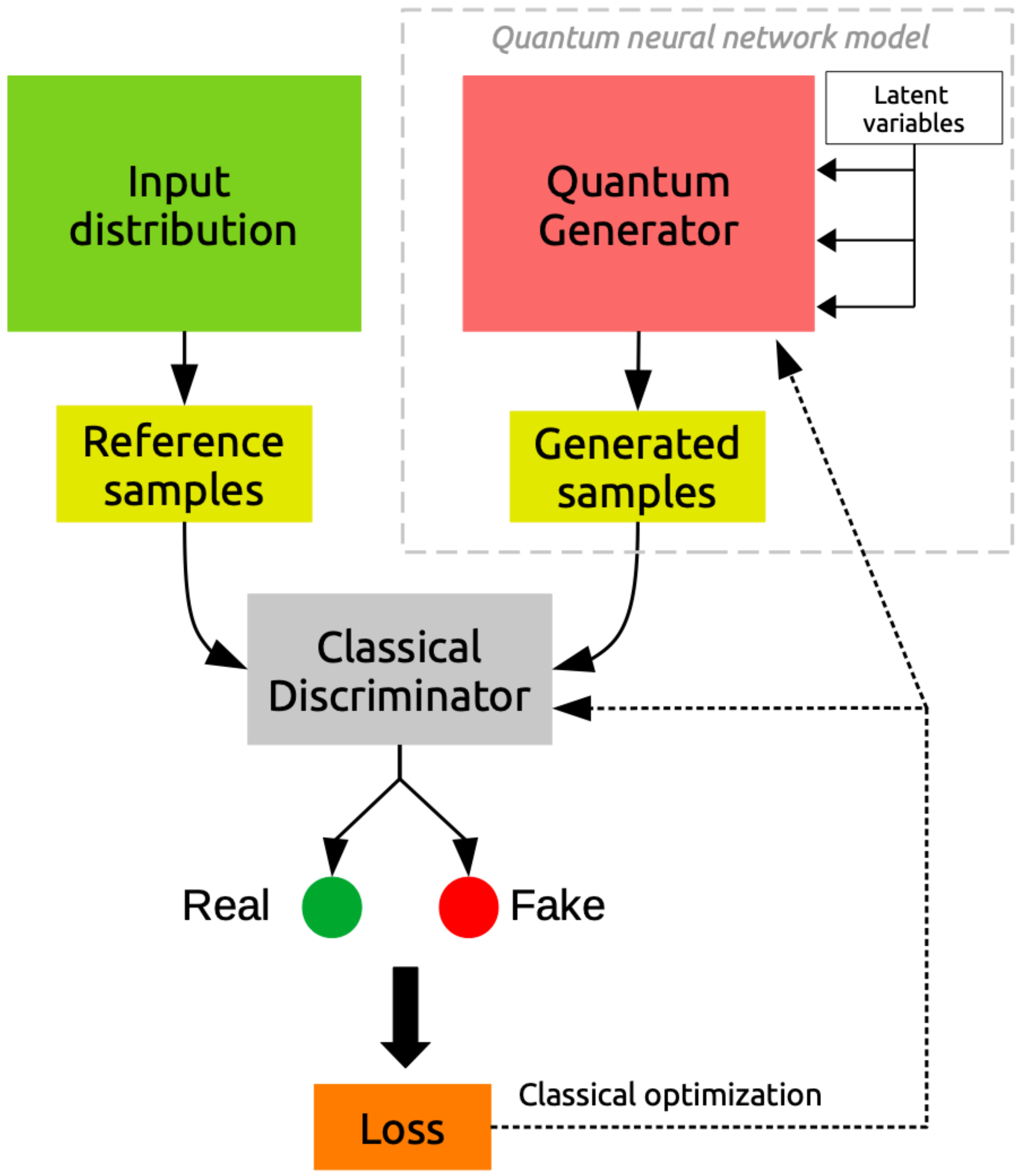
Generative Adversarial Network (GAN): Two networks compete against one another and through this competition, one network learns the underlying distribution

- Hybrid approach as no viable quantum training algorithm



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Real Quantum Machine, Real Monte Carlo Data

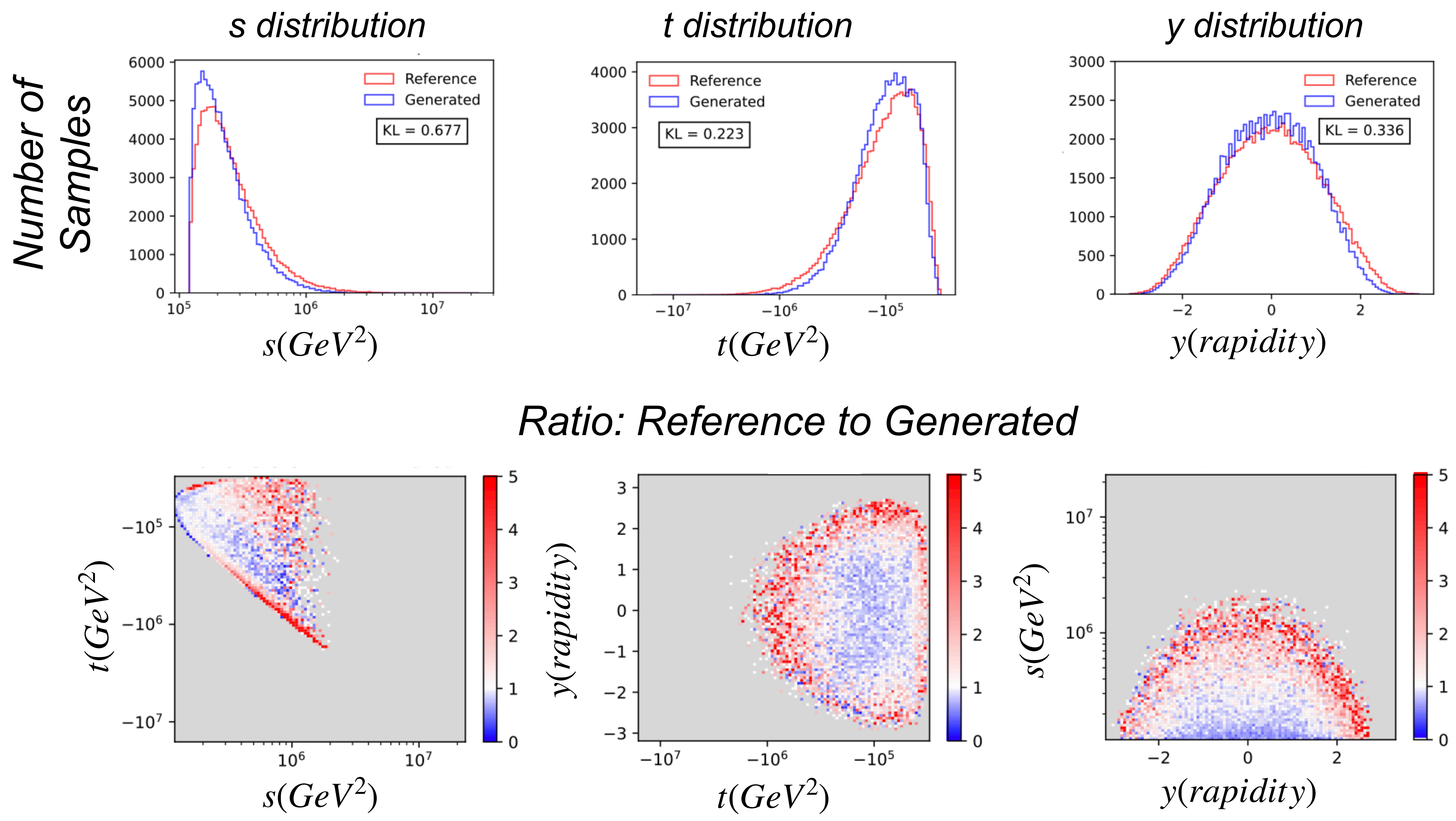
General Idea: Create new qGAN architecture that can learn the underlying distribution for a process that occurs that the LHC

Key Result: See successful data augmentation on noisy machine

- Non-trivial proof-of-principles as data is non-gaussian and highly correlated
- Significantly simpler algorithm than corresponding classical neural network
- See similar results on different classes of quantum hardware

$pp \rightarrow t\bar{t}$

Distributions: 10^5 *samples*



ibmq_santiago

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Benchmarking, Transfer Learning and Future Directions

Recall: For calculations that are feasible but expensive on classical hardware, performing comparison studies is imperative

Does QML data augmentation improve total run-time?

Are there other ways that QML can improve run-time?

How does QML compare to ML, especially in number of hidden parameters?

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Transfer Learning

Can we recycle neural net trained on one scattering process and use it for other processes

$pp \rightarrow t\bar{t}$ — *partial re-training* → $pp \rightarrow WW$

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Fully Quantum Approach

Can we create a fully quantum approach to machine learning that benefits from quantum speed-up?

MAJOR ROADBLOCK

No good quantum training algorithms

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Results on running style-qGAN on $pp \rightarrow t\bar{t}$ Data

Comparison between (superconducting) transmon and trapped ion machines

Transmon

ibmq_santiago

Trapped Ion

IonQ

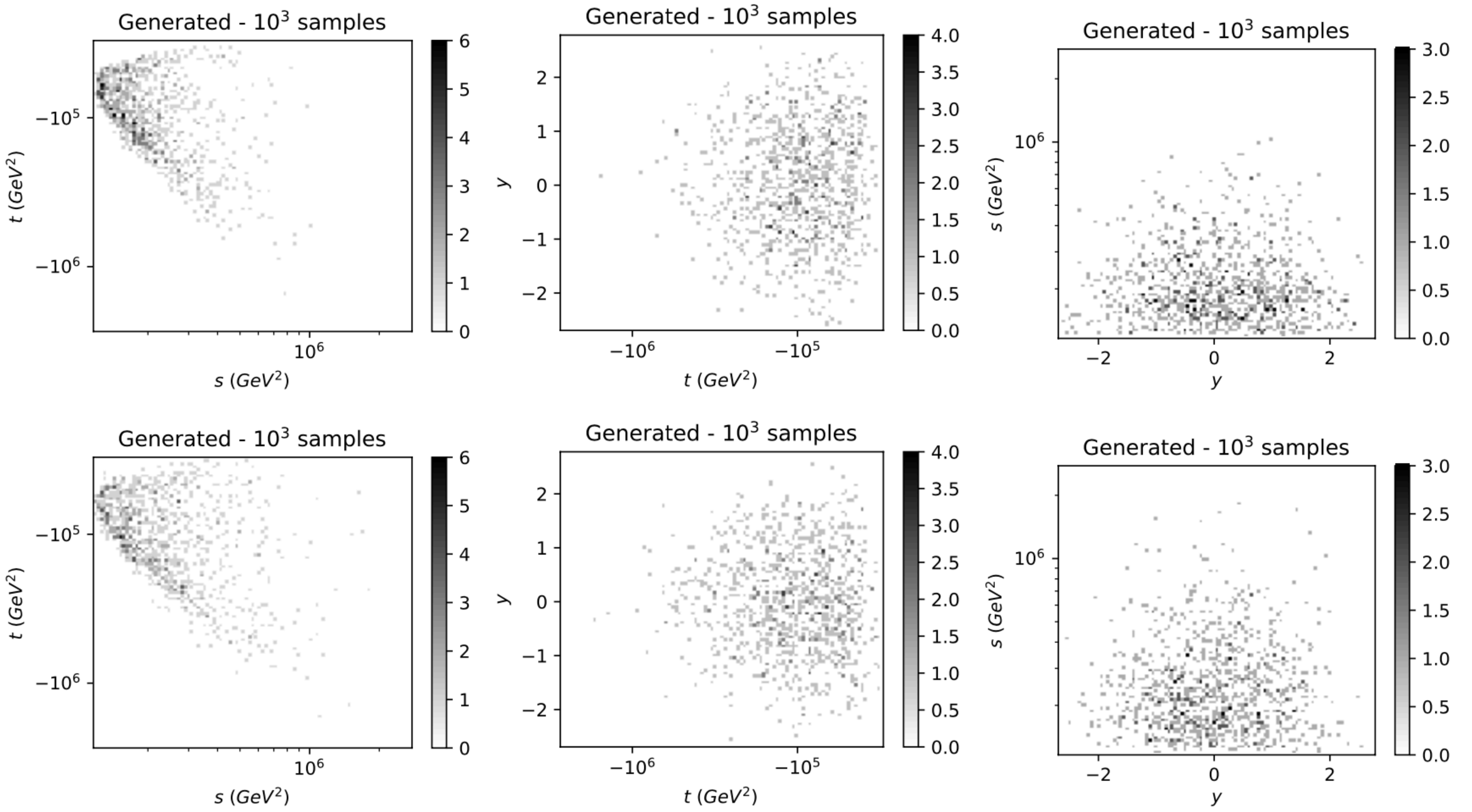

FIG. 8. Example of two-dimensional sampling projections for $pp \rightarrow t\bar{t}$ production using the style-qGAN generator model on `ibmq_santiago` (top row) and IonQ (bottom row) trained with 10^4 samples.

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