Efficient quantum digital simulations of U(1) lattice gauge theories

Dorota Grabowska

InQubator for
Quantum Simulation

@ University of Washington, Seattle

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Motivation

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

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

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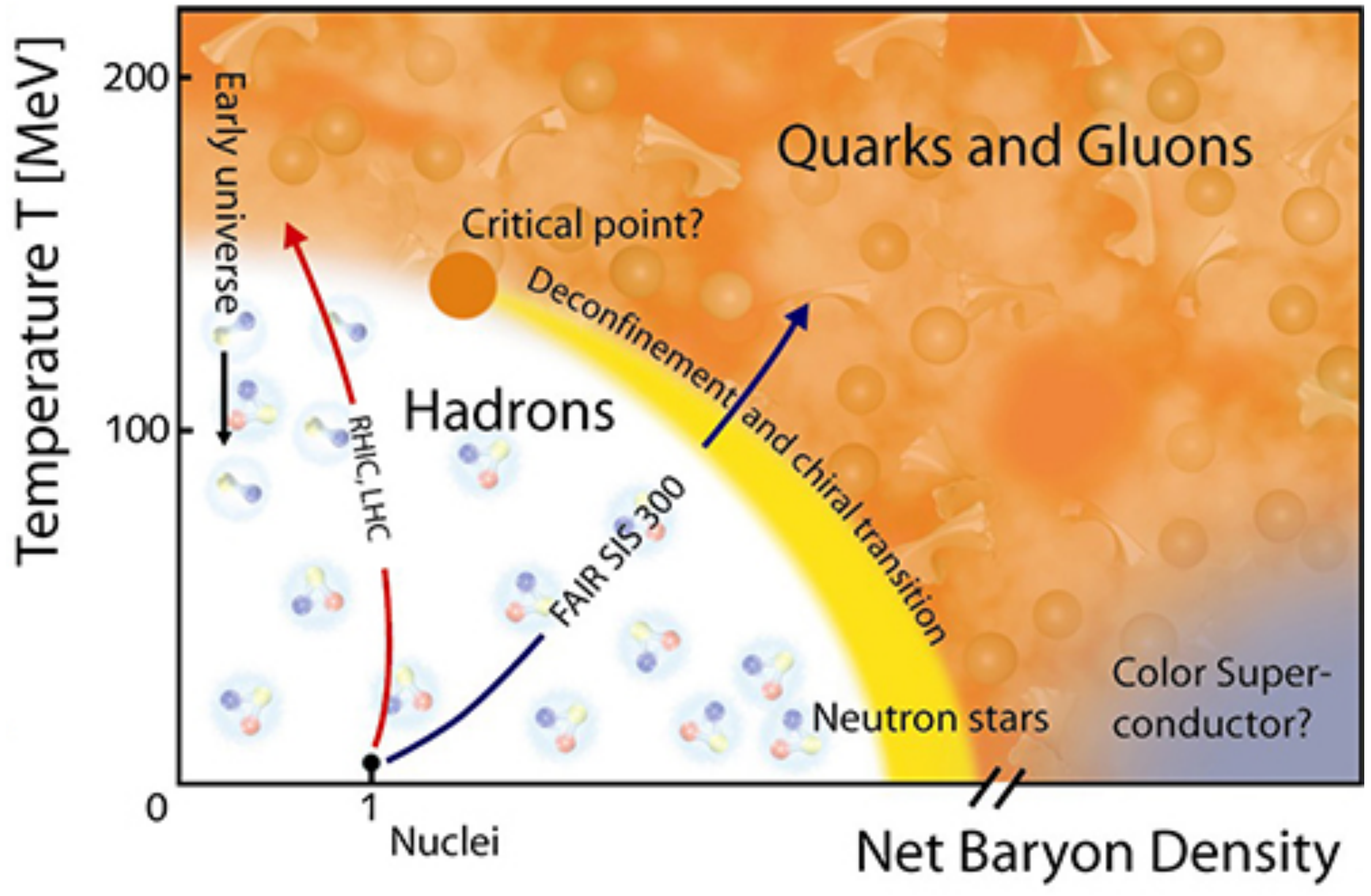
Quantum Chromodynamics (QCD)

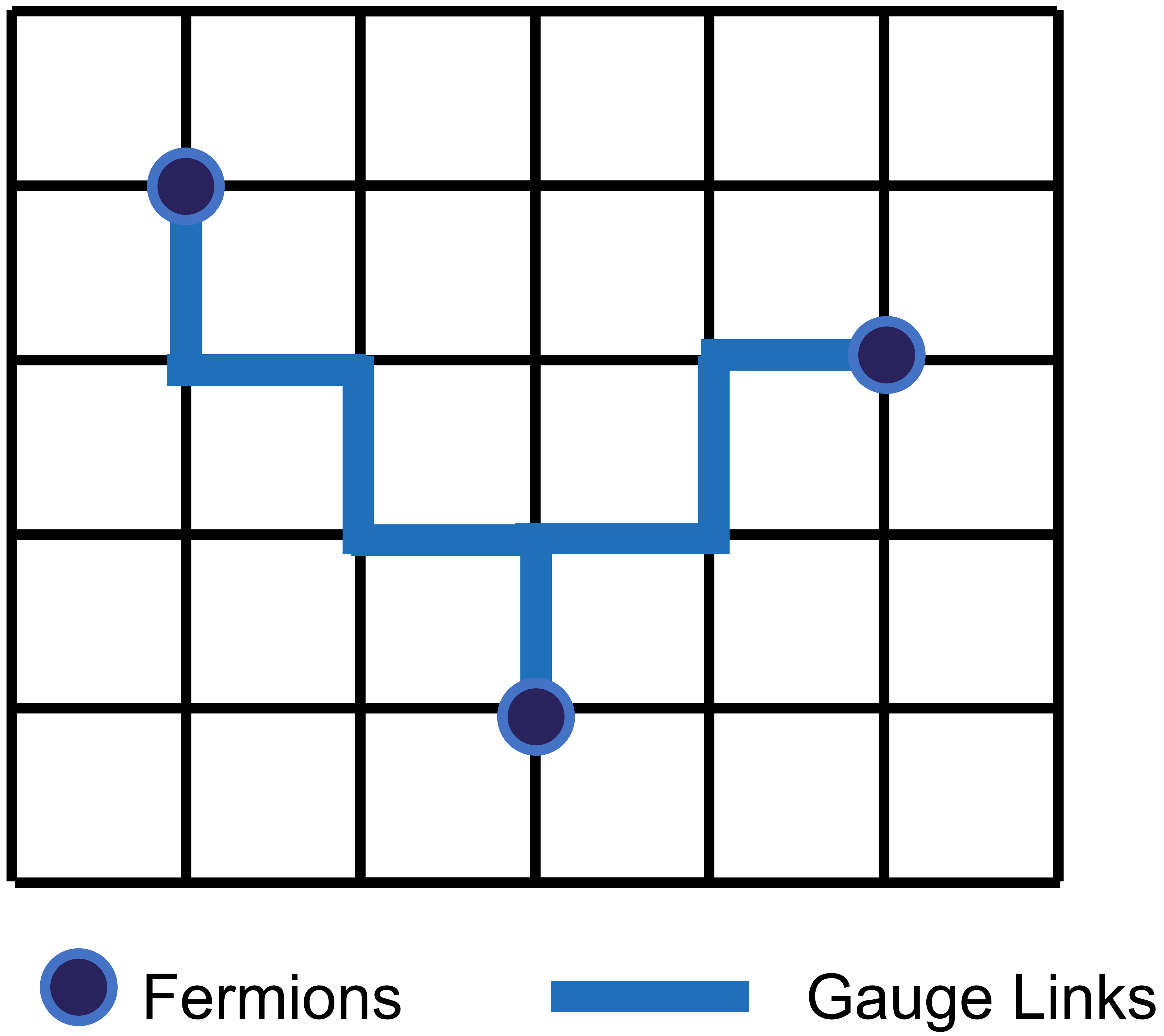
- Provides precise and quantitative description of the strong nuclear force over an broad range of energies
- *Ab-initio* calculations crucial for comparing theoretical predictions of the Standard Model to experimental results
- Gives rise to complex array of emergent phenomena that cannot be identified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



Proposed QCD Phase Diagram

Classical Simulations of Gauge Theories

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



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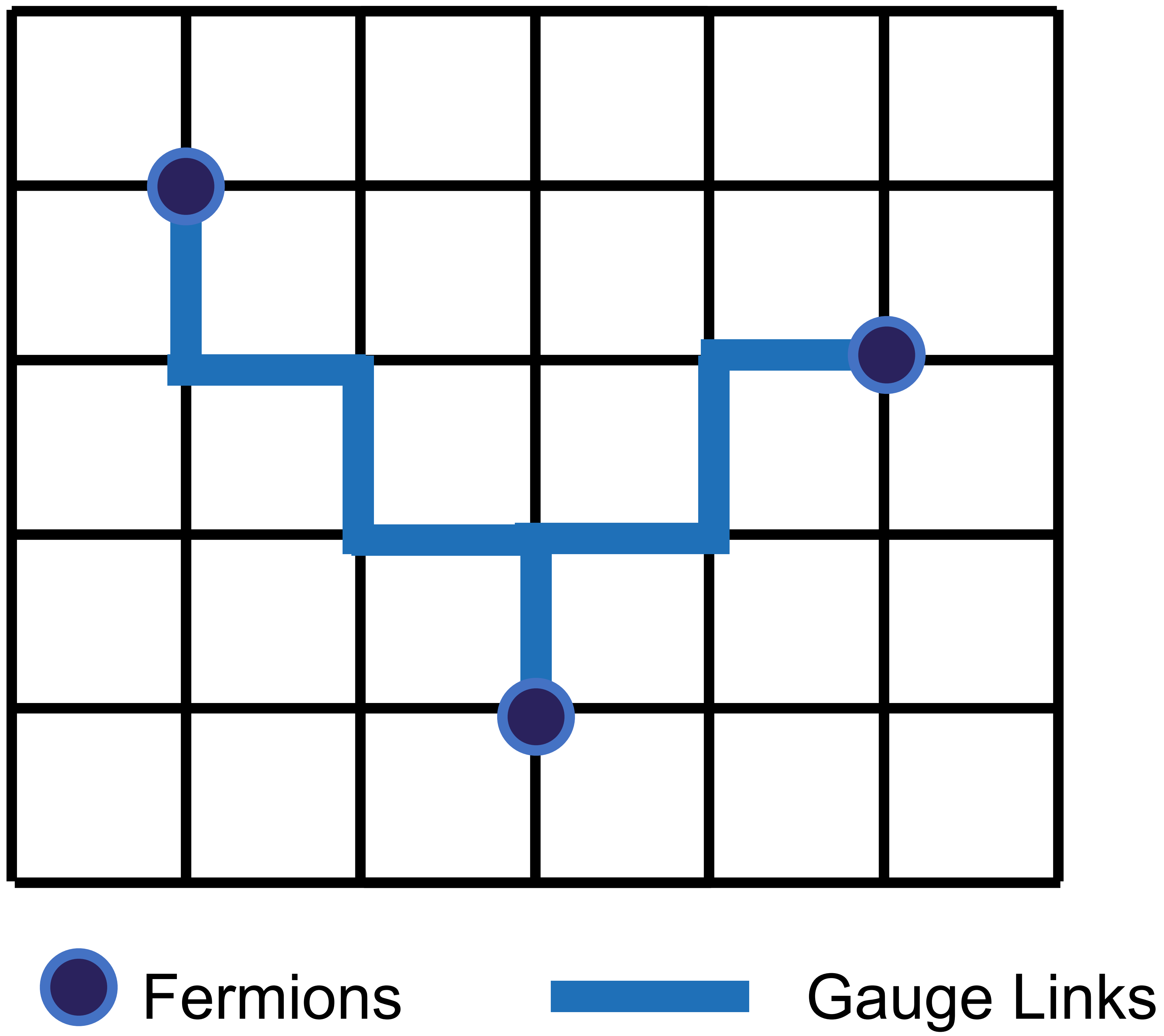
- Due to impressive algorithmic developments, some calculations are now done at physical pion masses
- Sub-percent precision in many single-hadron observables
  - Hadron vacuum polarization for g-2 measurements
  - Hadron spectrum with QED and isospin breaking effects
- Reliable extraction of several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



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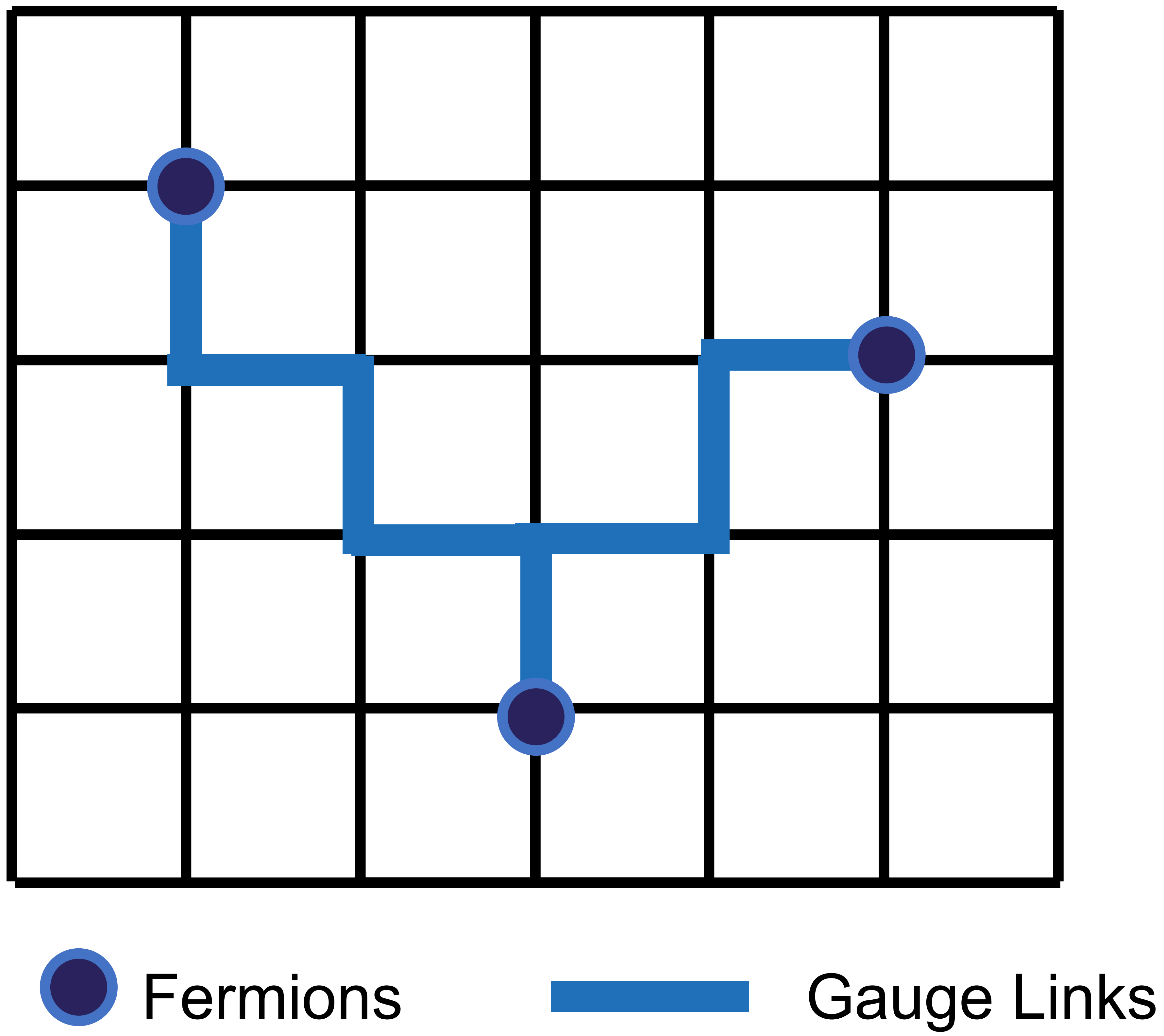

Only fully-systematic approach to ab-initio computations in the non-perturbative regime

Sign Problems in Lattice Gauge Theories

Lattice Simulations: Numerically estimates value of lattice-regulated quantum path integral and correlation functions via Monte Carlo methods

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

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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

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

Simulations of the Standard Model

Lattice QCD: Highly advanced field, utilizing high-performance computing to carry out physical pion mass calculations of light hadron physics

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Real-time dynamics, finite-density nuclear matter and non-perturbative properties of chiral gauge theories seem intractable on classical computers

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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

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

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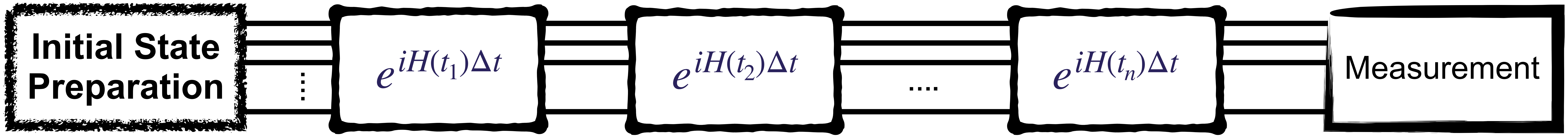
Can we see a similar improvement for calculations in High Energy Physics?

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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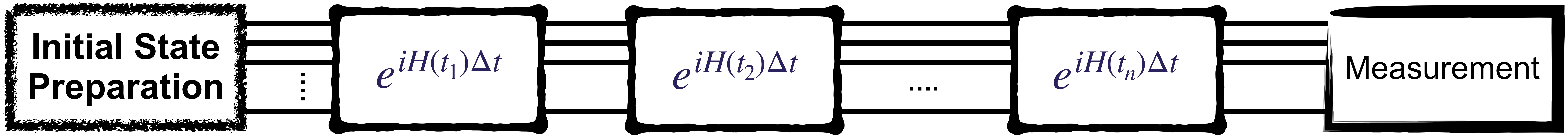

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Overarching Research Goal

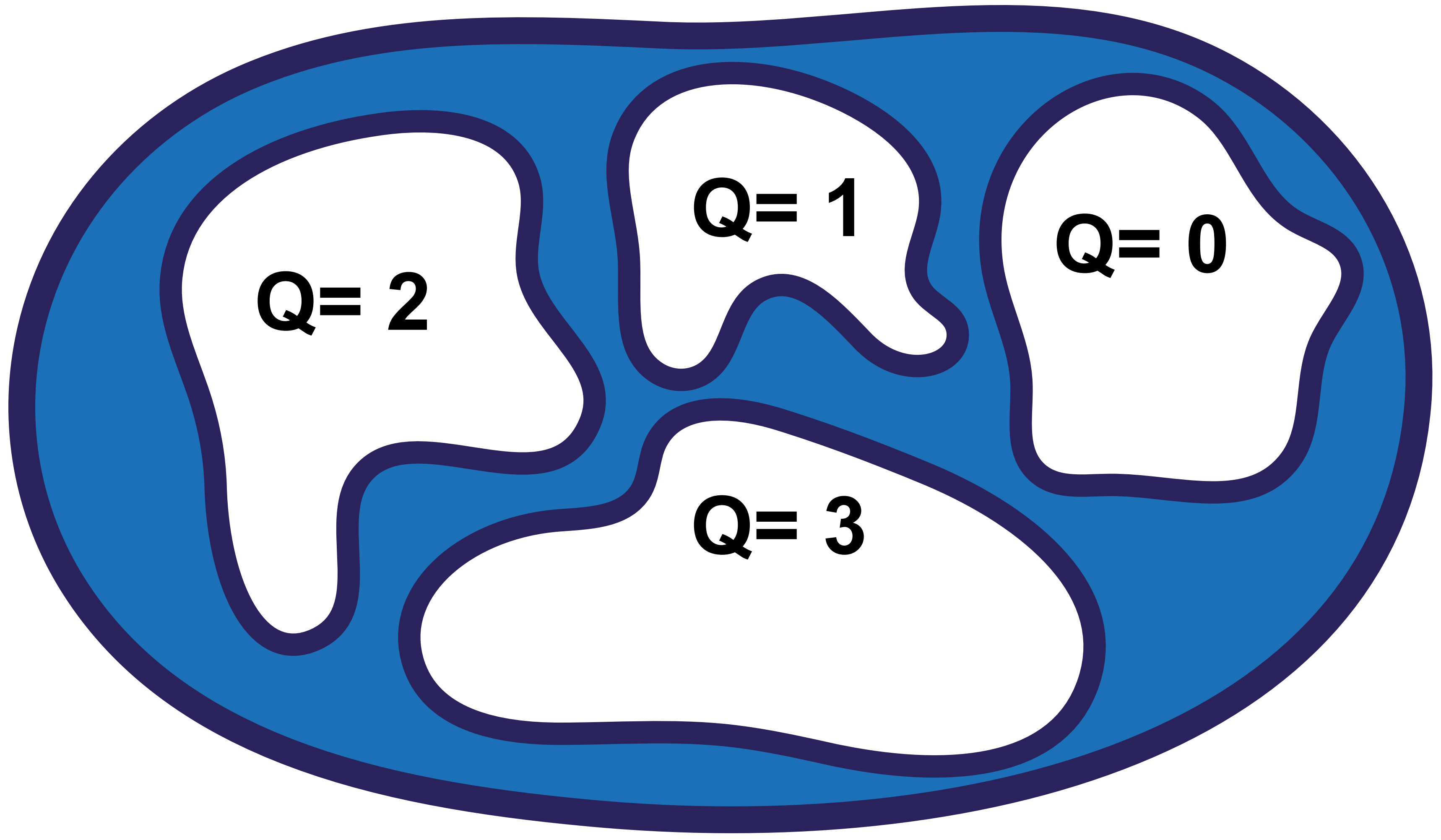
"Re-write" theory into quantum circuit formulation that runs in reasonable amount of time

Challenges of Simulating Hamiltonian Lattice Gauge Theories

Gauge theories have two fundamental properties that must be addressed

Gauss Law is not automatically satisfied

Hilbert Space



Hilbert space is tensor product of different charge sectors

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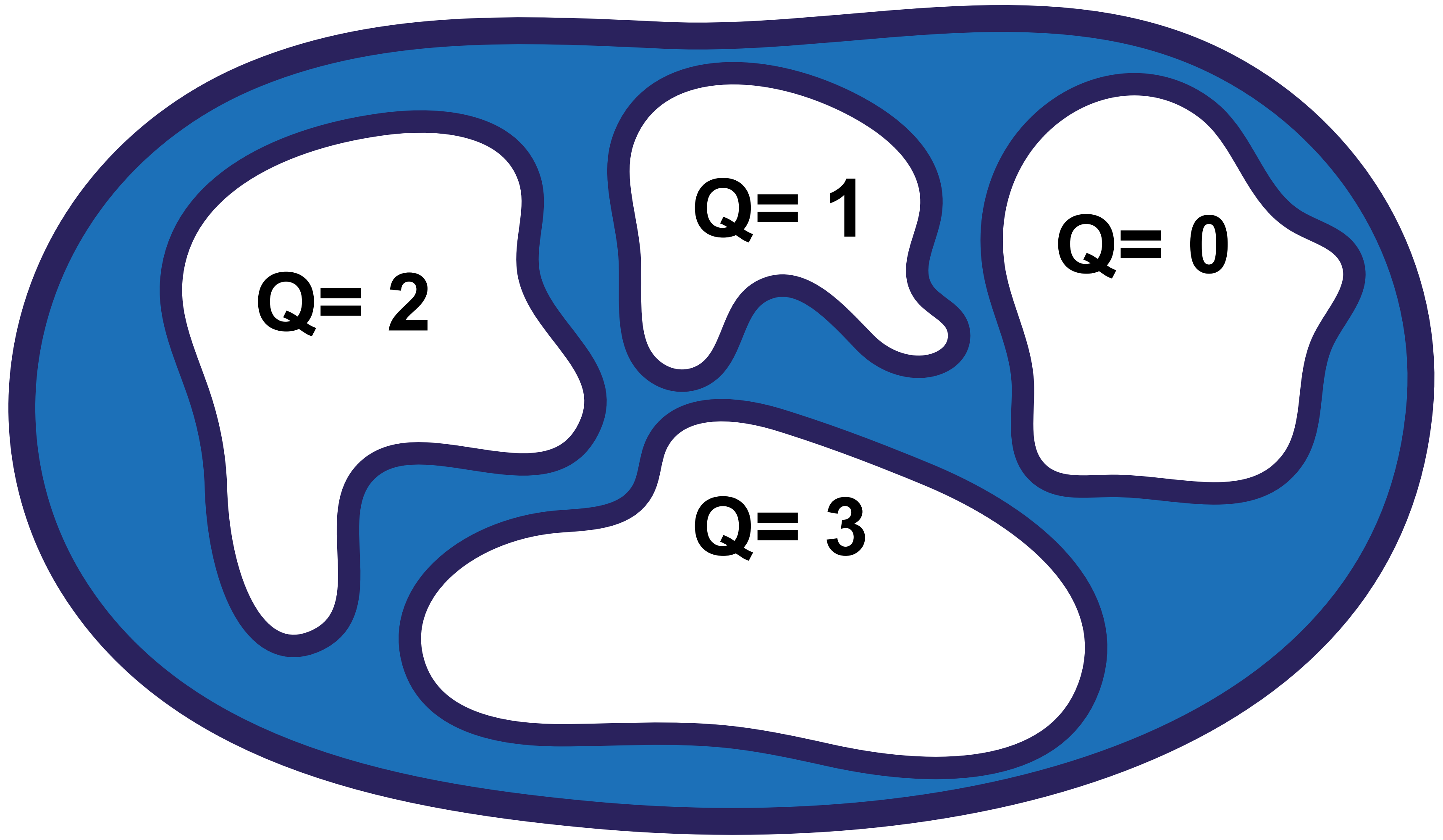

Hilbert space is tensor product of different charge sectors

Gauge groups are continuous*

Ex: U(1)

** At least ones that are phenomenologically relevant to nuclear and particle physics*

Gauss' Law and Hilbert Space Dimensionality

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Continuum Theory: Integral over electric and magnetic fields

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

Need to impose additional constraints

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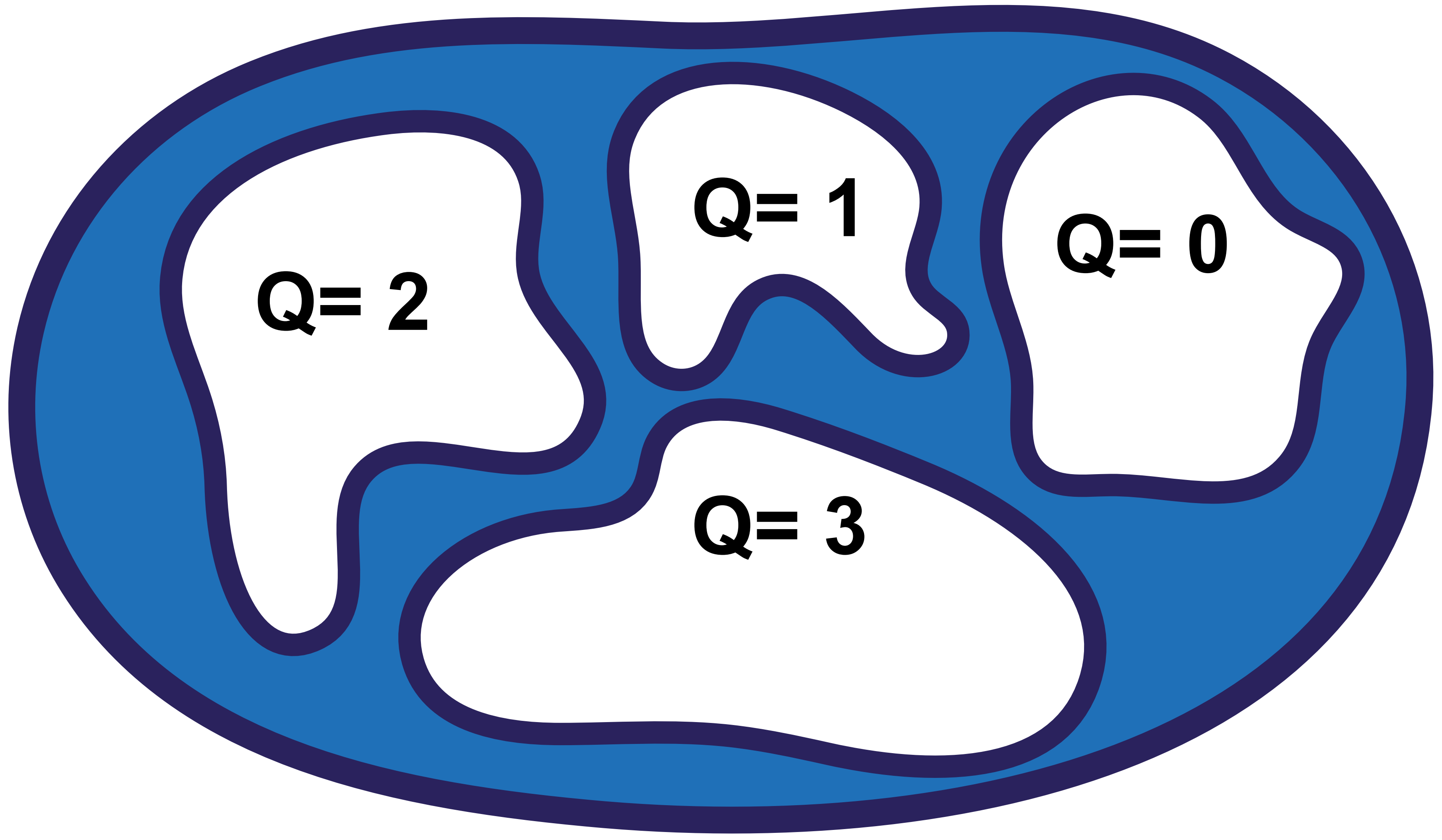


Hilbert space is tensor product of different charge sectors

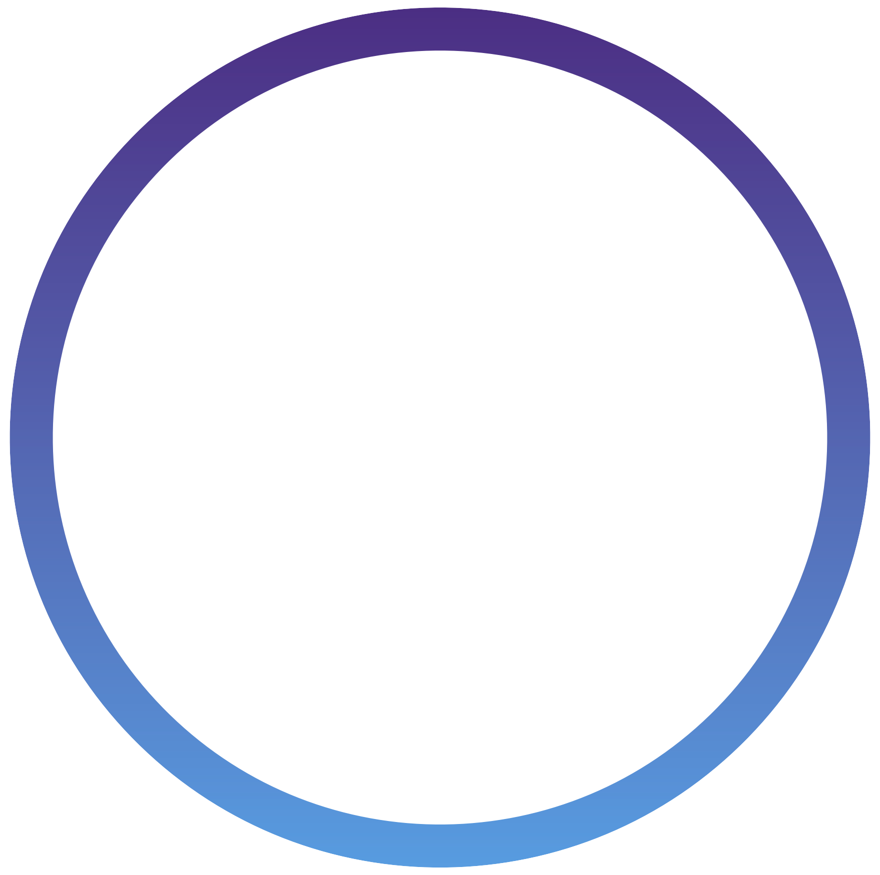
- Need to decide if and how to reduce from full Hilbert space to physical Hilbert space
- Decision has dramatic ramifications on
  - number of qubits
  - circuit depth
  - sensitivity to noise

Digitizing Gauge Manifolds and “Good” Samplings

Standard Model gauge groups are continuous

Digital Quantum Computer: Needs to sample gauge fields and map values to computational basis

Ex: Compact U(1)



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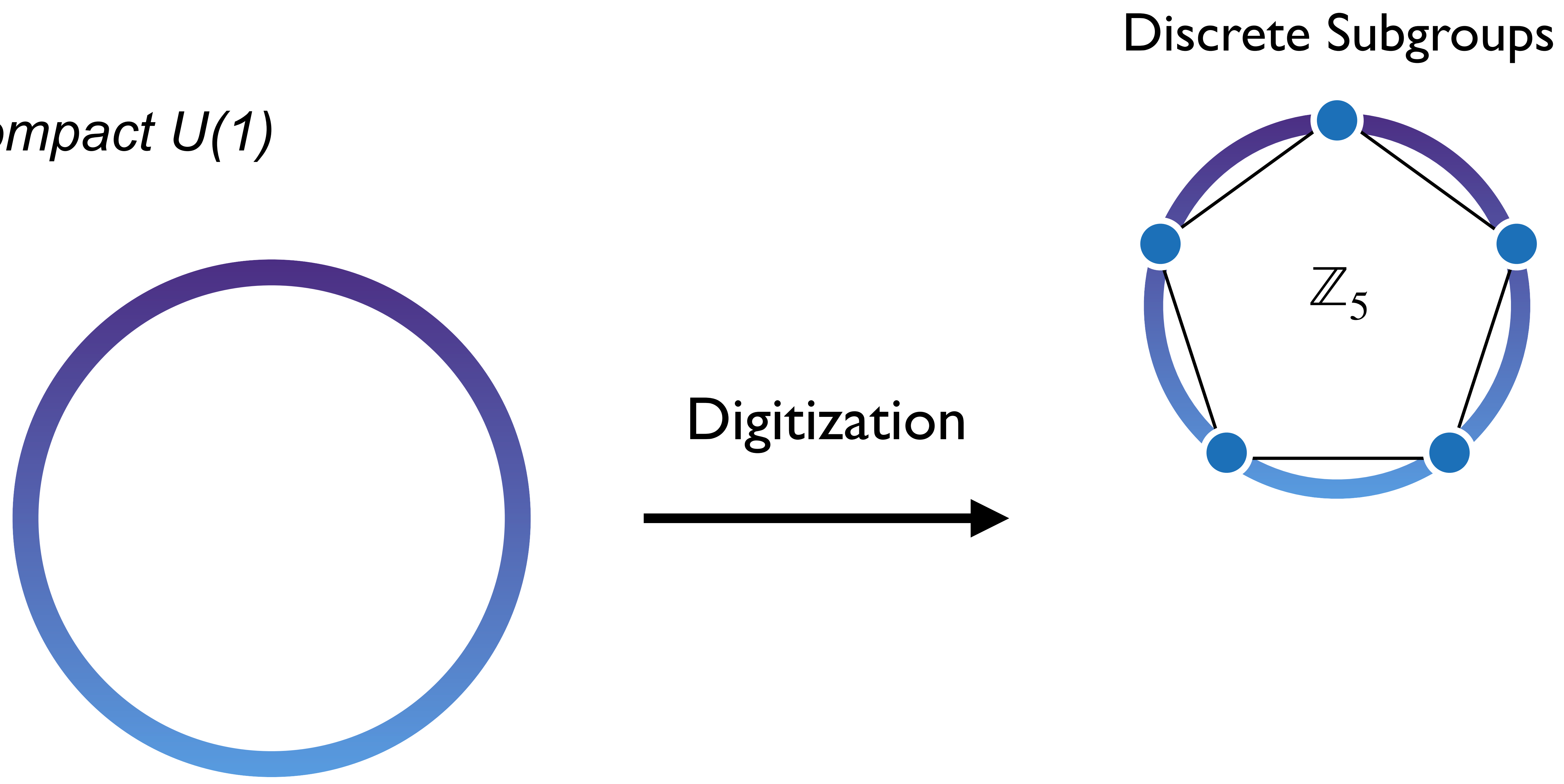

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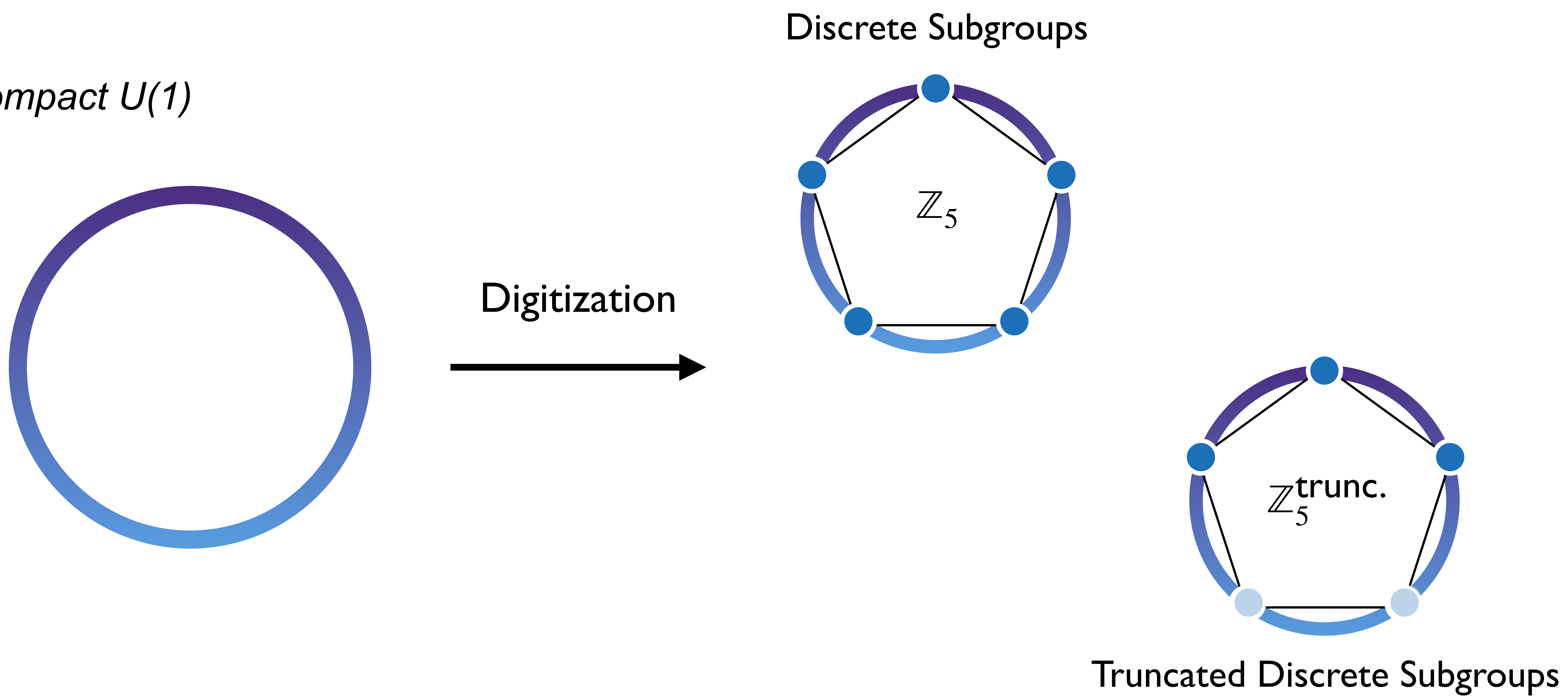

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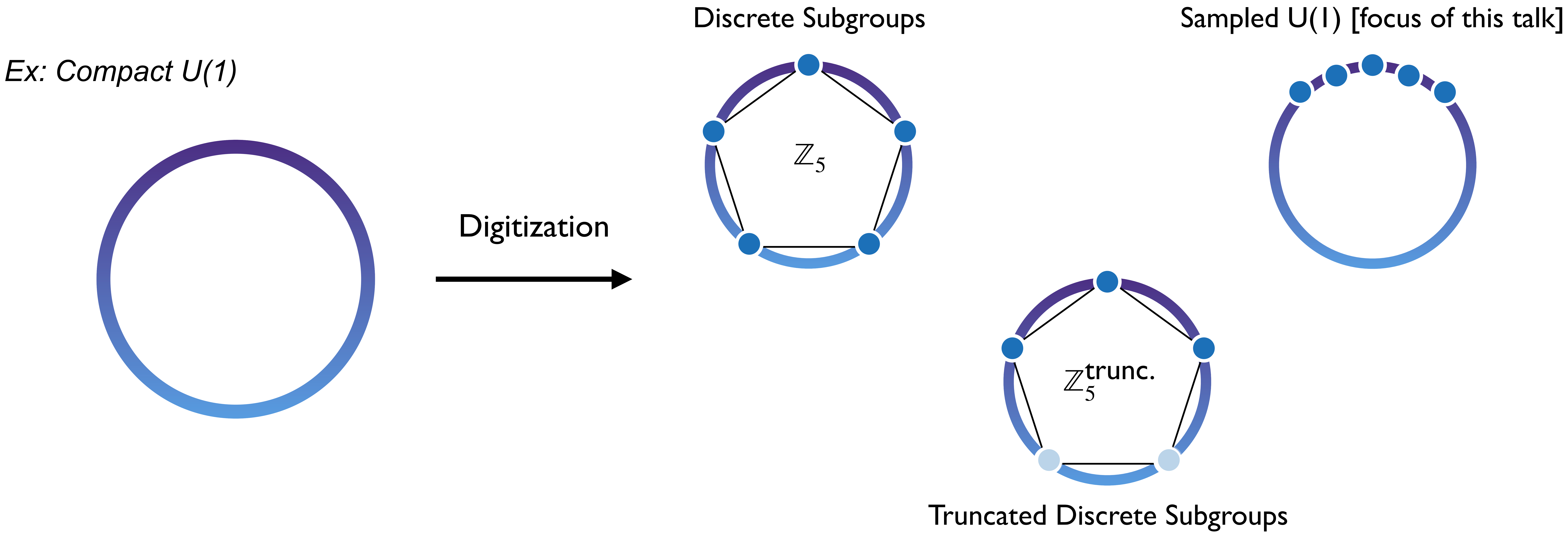

Digital Quantum Simulation

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

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

Gauge Theories: Due to gauge symmetries, there is not a clear "best approach" for the Hamiltonian truncation and each decision carries an associated cost

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Gauge Theories: Due to gauge symmetries, there is not a clear “best approach” for the Hamiltonian truncation and each decision carries an associated cost

It is imperative to consider the scaling of quantum computing resources for simulating gauge theories on both near-term and far-future (fault-tolerant) quantum computers

Resource Efficiency in a Quantum World

"Non-trivial" Toy Model: Working towards implementing just the gauge sector in this (sometimes exactly solvable) model illustrates a lot of the complications we will face

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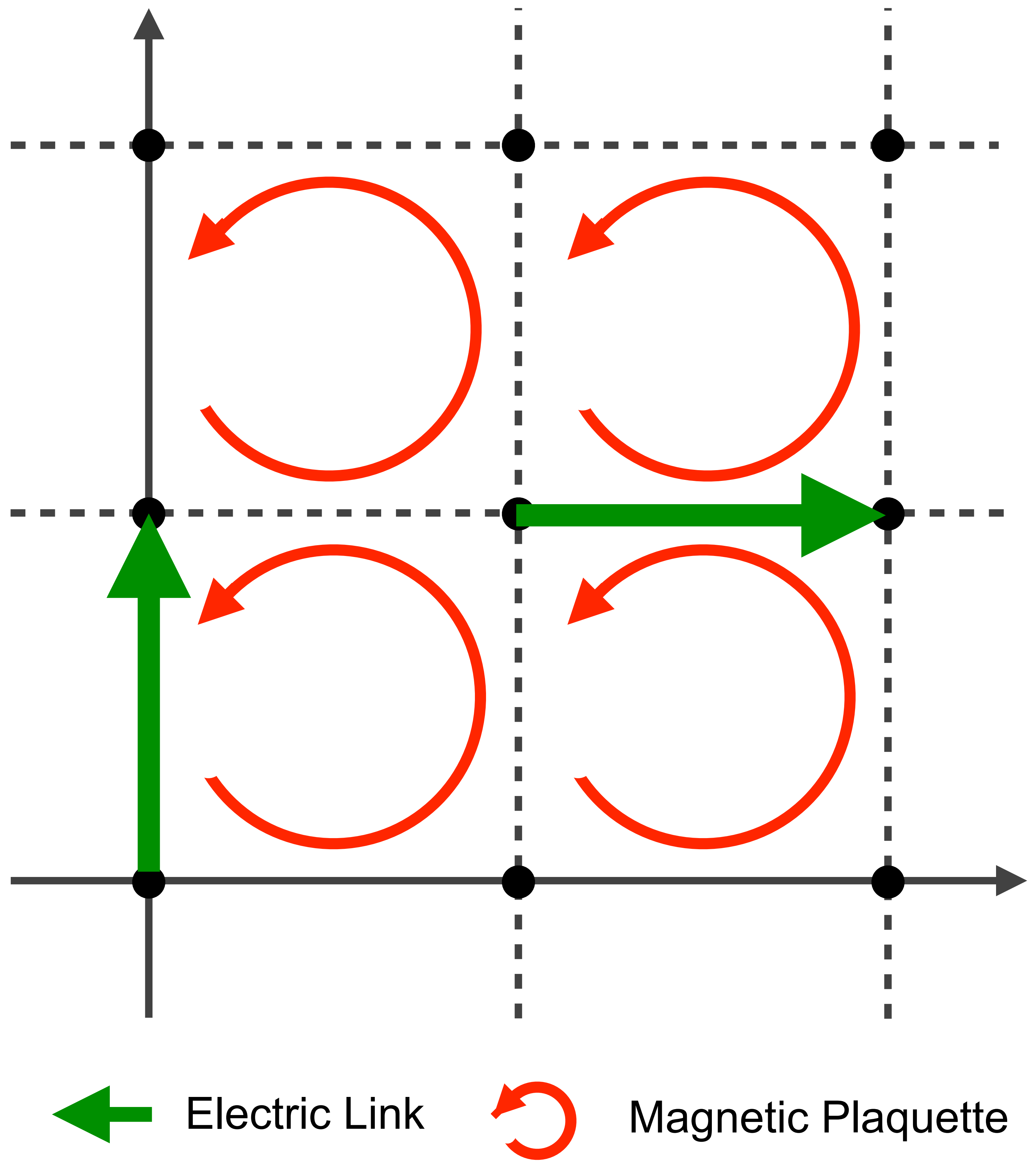
Remainder of talk will focus on:

- Derivation of Hamiltonian that spans only physical Hilbert space
  - Makes use of "dual basis" formulation
- Digitization of said Hamiltonian that works well for all values of gauge coupling
  - Weak coupling limit is also the continuum limit
- Period boundary conditions create an additional constraint/super-selection rule
  - Naive gate count for time evolution is exponential in volume, but can be made polynomial

*Bauer, C.W. and **DMG** Phys.Rev.D 107 (2023) 3, L031503*
***DMG**, C. Kane, B. Nachman and C.W. Bauer arXiv: 2208.03333*
*C. Kane, **DMG**, B. Nachman and C.W. Bauer arXiv: 2211.10497*

U(1) Lattice Gauge Theory

Kogut-Susskind



Hilbert space contains ***all*** charge sectors

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pure gauge sector for now

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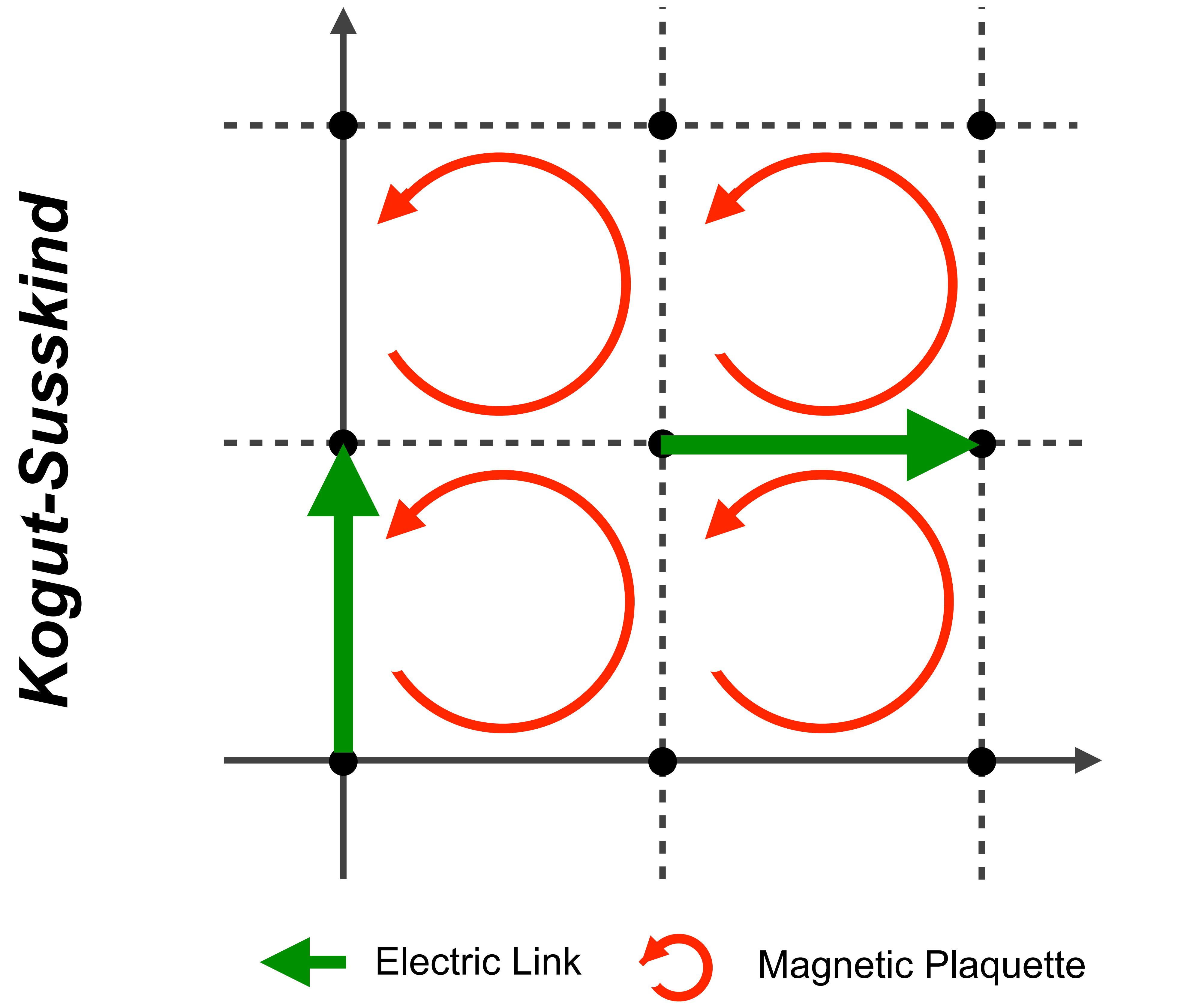

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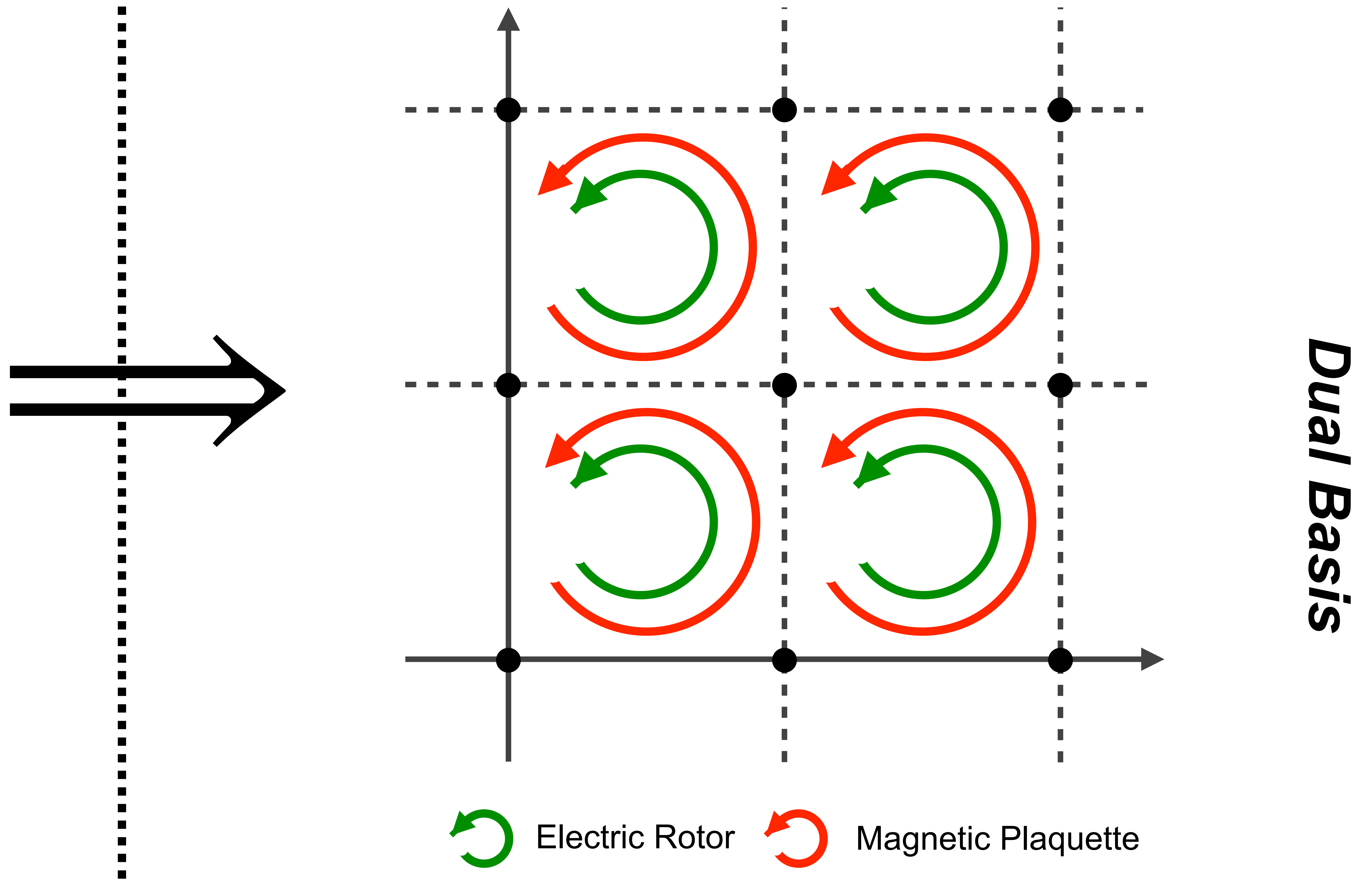

Hilbert space contains ***only one*** charge sector

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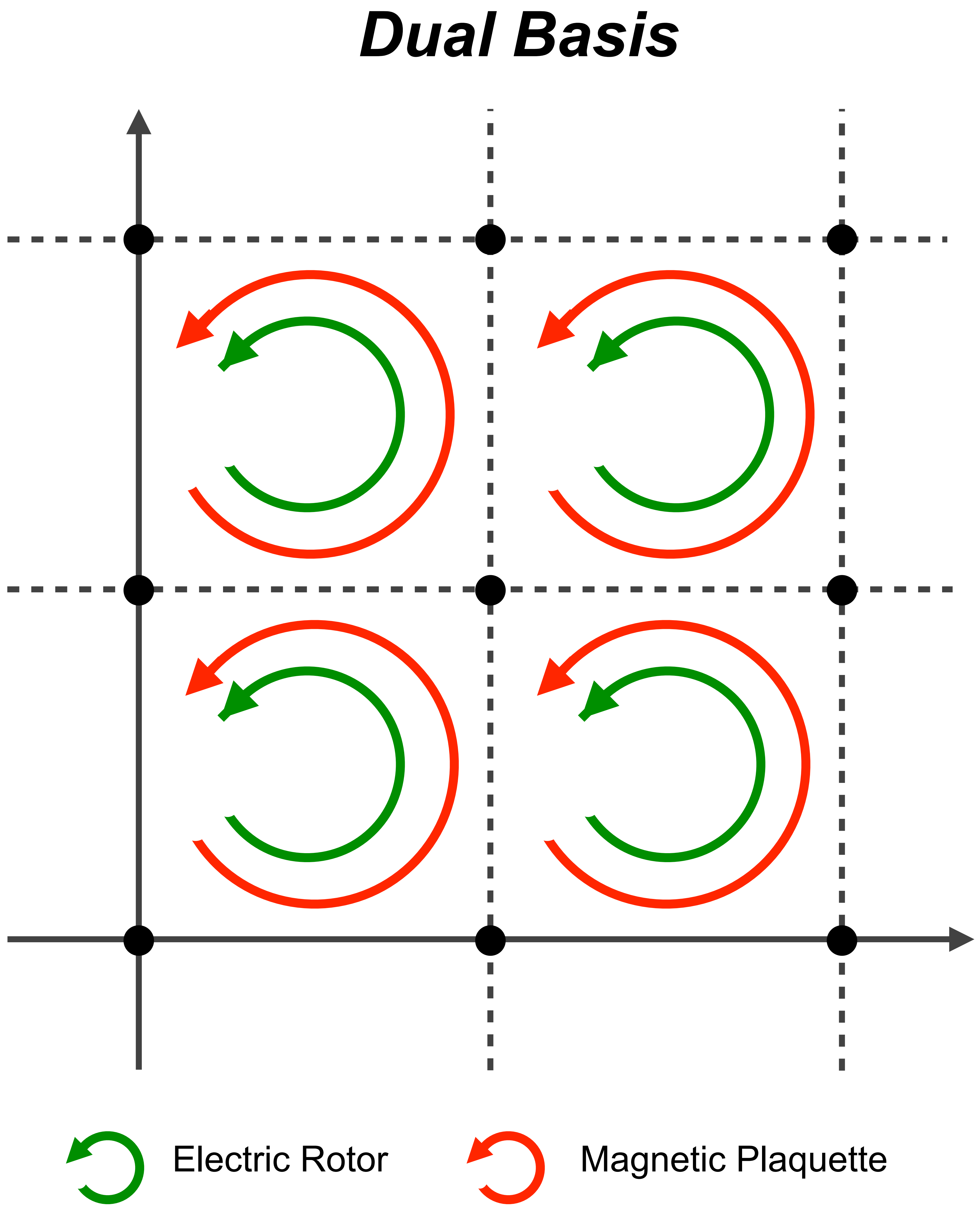
Dual Basis (Rotor) Formulation

General Idea: Work with "gauge-redundancy free" 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



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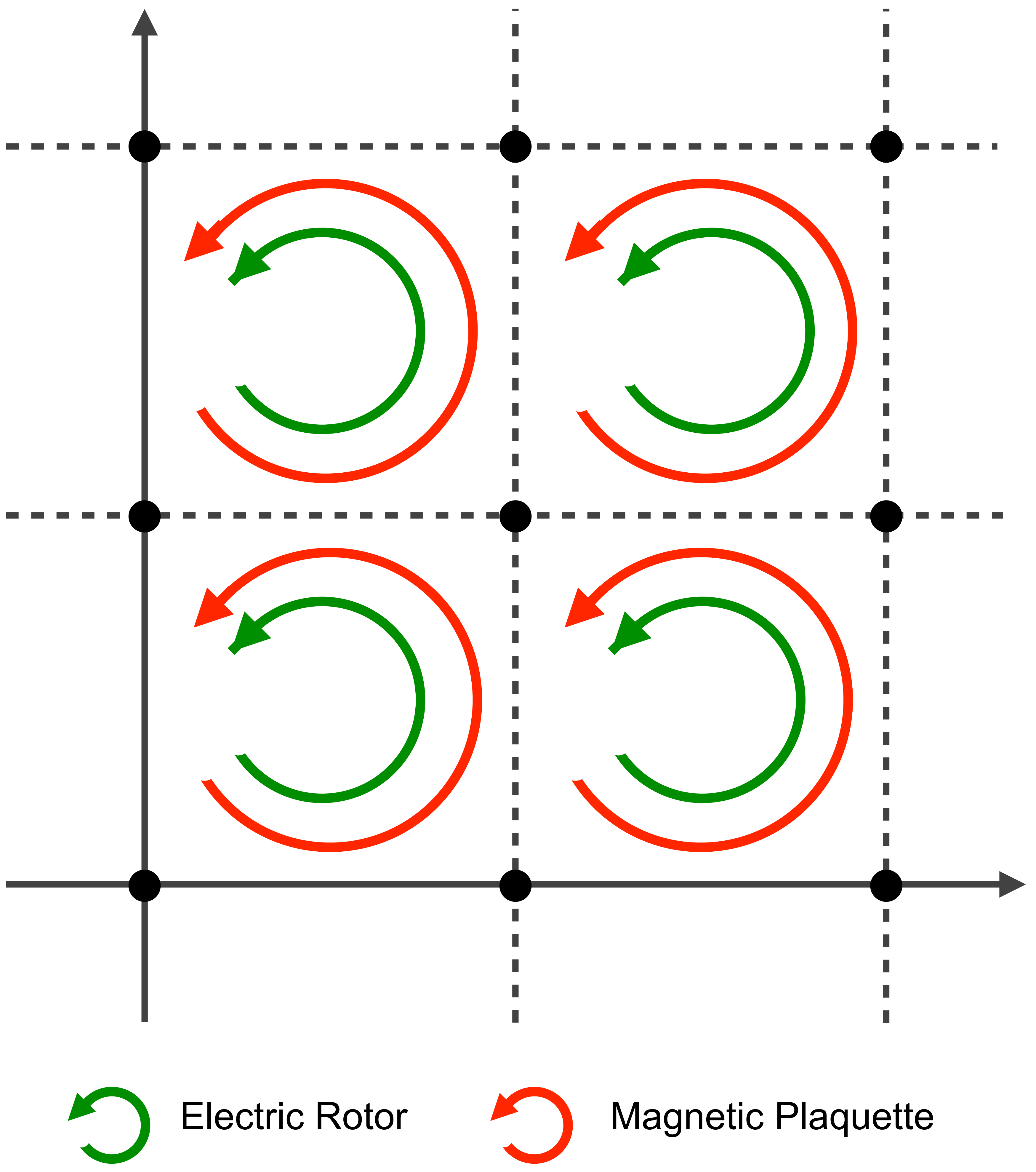
$$H = \frac{1}{2a}\left[g^2 \sum_p \left(\nabla_L \times R_p \right)^2 - \frac{2}{g^2} \begin{Bmatrix} \sum_p \cos B_p & \text{compact} \\ -\frac{1}{2}\sum_p B_p^2 & \text{non compact} \end{Bmatrix} \right]$$

$E_T = \nabla \times R$ $\qquad$ $N_p =$ **Number of Plaquettes**

Dual Basis



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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 weak-coupling eigenstate localization*

Guiding Principle

At weak coupling, eigenstates are exponentially localized around $B_p = 0$

$$H_{NC} = \frac{1}{2a}\left[g^2 \sum_{pp'} a_{pp'} R_p R_{p'} + \frac{1}{g^2}\sum_p B_p^2\right]$$

$$H_C = \frac{1}{2a}\left[g^2 \sum_{pp'} a_{pp'} R_p R_{p'} - \frac{2}{g^2}\sum_p \cos B_p\right]$$

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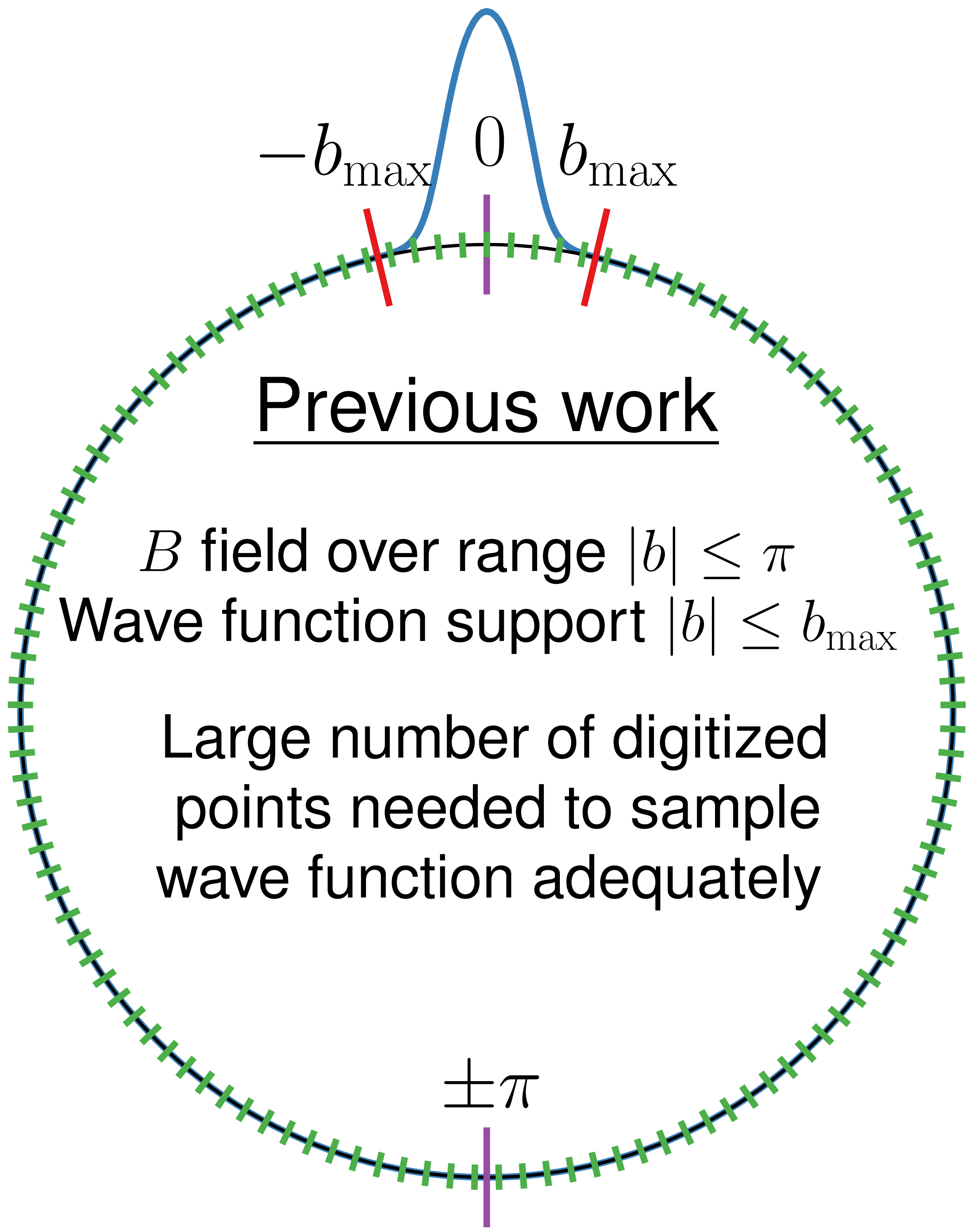

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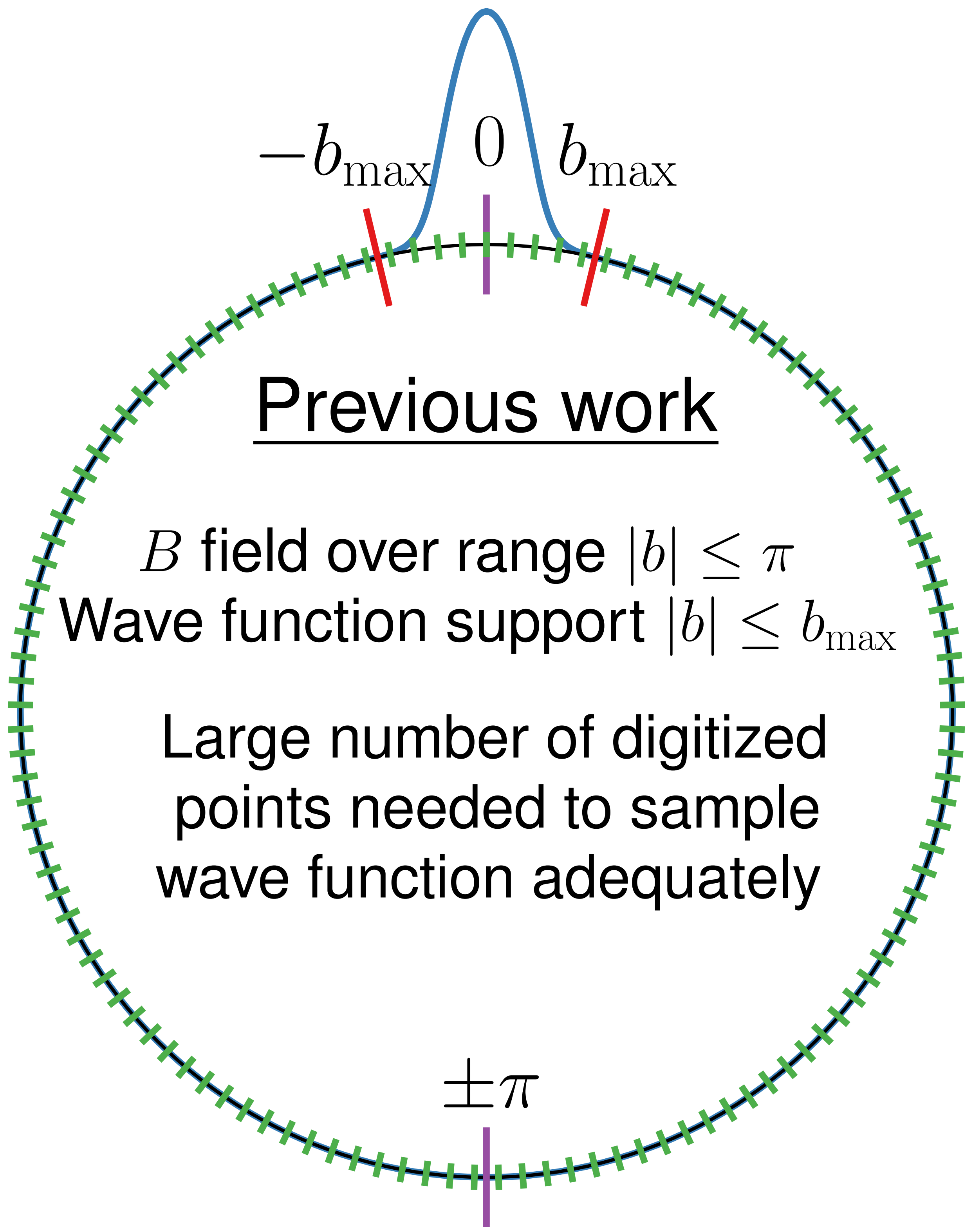

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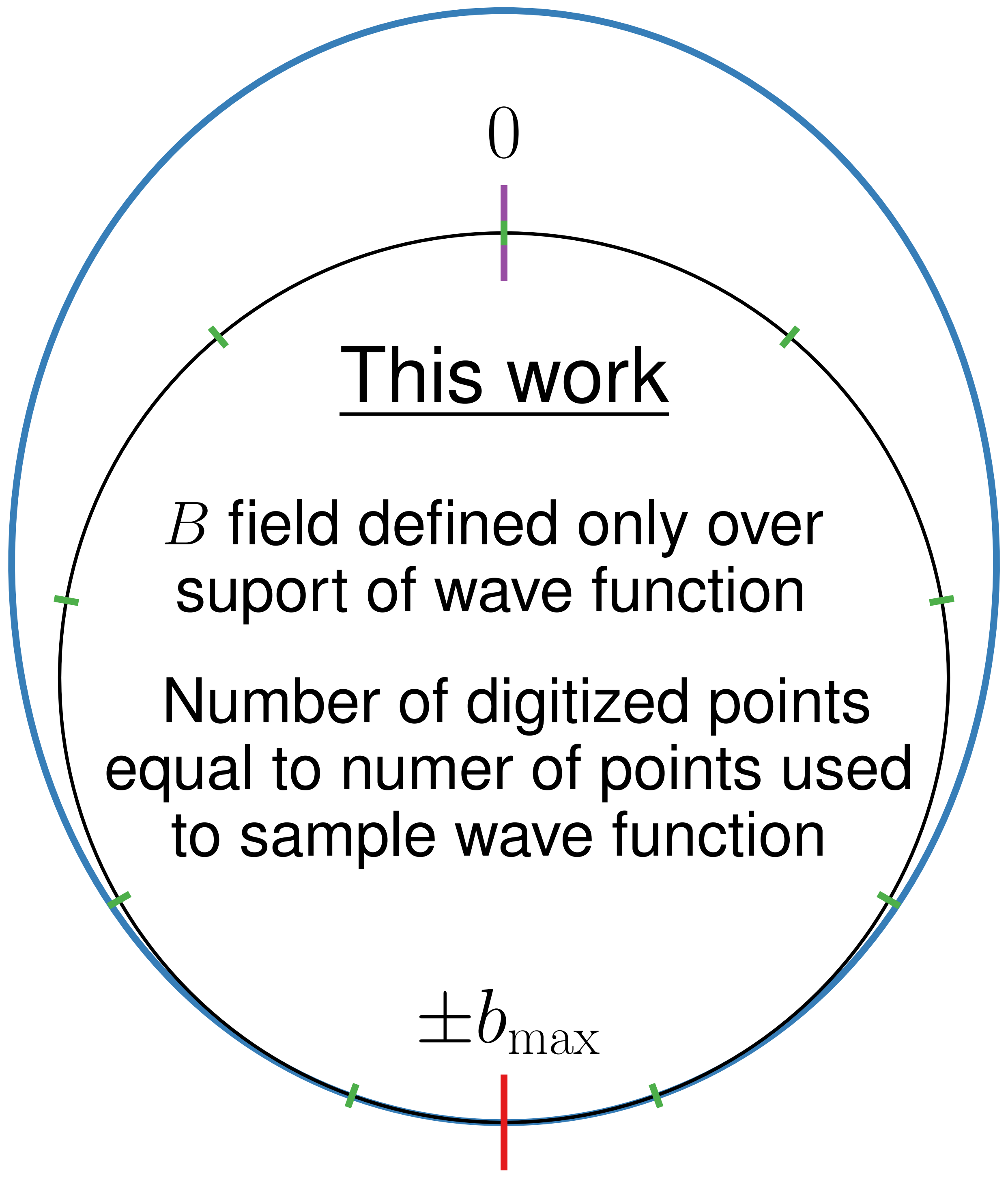

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Step One: Digitize rotor and magnetic fields

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

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

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Step Two: Define digitized rotor and magnetic operators

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

Free parameter b_{max} needs to be determined

Digitizing the Dual Formulation in the Magnetic Basis

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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 at strong coupling

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

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

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- Equivalent to Kogut-Susskind Hamiltonian at strong coupling

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

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

Formulation works well for all values of the gauge coupling

Global Constraints in Rotor Formulation

General Idea: Locally imposed constraints are automatically satisfied, but not global

Different ways to see remaining global constraint:

- Rewrite rotors in terms of electric links: too many links if Gauss' law and electric winding is fixed*
- Solve non-compact case exactly and find decoupled quantum harmonic oscillators + 'CoM movement'

**D. B. Kaplan and J. R. Stryker, Phys. Rev. D 102, 094515*

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Example: 2 x 2 Lattice, periodic boundary conditions

$$H = \frac{1}{a}\left[2g^2\left(R_0^2 + R_1^2 + R_2^2 + R_3^2 - (R_0 + R_1)(R_2 + R_3)\right) + \frac{1}{2g^2}\left(B_0^2 + B_1^2 + B_2^2 + B_3^2\right)\right]$$

Orthogonal Change of Basis

$$H = \frac{1}{a}\left[2g^2\left(4\tilde{R}_1^2 + 2\tilde{R}_2^2 + 2\tilde{R}_3^2\right) + \frac{1}{g^2}\left(\tilde{B}_0^2 + \tilde{B}_1^2 + \tilde{B}_2^2 + \tilde{B}_3^2\right)\right]$$

"Plane wave solution" for $\tilde{B}_0$

**D. B. Kaplan and J. R. Stryker, Phys. Rev. D 102, 094515*

Non-local Constraint (Magnetic “Gauss Law”)

Magnetic “Gauss Law”: Zeroth plaquette is equal to sum of all others: $\sum_{p=1}^{N_P} B_p = -B_0$

Constrained Hamiltonian: Imposing this constraint leads to highly non-local term

Compact formulation

$$H_B = \frac{1}{ag^2} \sum_p \cos B_p + \cos\left(\sum_p B_p \right)$$

DMG, C. Kane, B. Nachman and C.W. Bauer: arXiv: 2208.03333

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Exponential Volume Scaling: If it takes $\mathcal{O}(N_L)$ gates to implement single plaquette term, it will take $\mathcal{O}(N_L^{N_P})$ gates to implement the non-local term!

This makes even the smallest lattices require thousands of gates for a single time step!

***DMG**, C. Kane, B. Nachman and C.W. Bauer: arXiv: 2208.03333*

Reducing Degree of (Operator) Connectivity

Requirement: Carry out orthonormal basis change such that no single term in the Hamiltonian spans a Hilbert space larger than than $\mathcal{O}(2^{n_q \log_2 N_p})$

Basis Change

$$B_p \rightarrow \mathscr{W}_{pp'} B_{p'}$$

$$\mathscr{W} = \begin{pmatrix} W_{d_{(1)}} & 0 & 0 & 0 \\ 0 & W_{d_{(2)}} & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & W_{d_{(N_S)}} \end{pmatrix}$$

W_d : "Weaved" matrix of dimension d

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Properties of $\mathscr{W}$ and W_d

- $\mathscr{W}$ is block diagonal with $N_s \sim \log_2 N_p$ sub-blocks
  - Each sub-block W_d has dimension $d \sim N_p / \log_2 N_p$
- First column of any W_d has all entries equal to $1/\sqrt{d}$

→ ***Maximally non-local term now spans Hilbert space of dimension $N_p^{n_q}$***

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- Every row of W_d has no more than $\lceil \log_2 d \rceil + 1$ non-zero entries

→ ***Previously local terms spans Hilbert space of dimension $(N_p / \log_2 N_p)^{n_q}$***

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Requirement: Carry out orthonormal basis change such that no single term in the Hamiltonian spans a Hilbert space larger than than $\mathcal{O}(2^{n_q \log_2 N_p})$

Example of Basis Change

$\mathscr{W}_{16} = \text{Diagonal Matrix}[W_4, W_4, W_4, W_4]$

$$W_4 = \begin{pmatrix} \frac{1}{2} & -\frac{1}{\sqrt{2}} & -\frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{\sqrt{2}} & -\frac{1}{2} & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & -\frac{1}{\sqrt{2}} \\ \frac{1}{2} & 0 & \frac{1}{2} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

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Implementing new "Weaved" Hamiltonian requires $\mathcal{O}(N_p^{n_q})$ gates!

3 x 3 lattice with two qubits per plaquette requires $\mathcal{O}(10^2)$ gates instead of $\mathcal{O}(10^5)$ gates!

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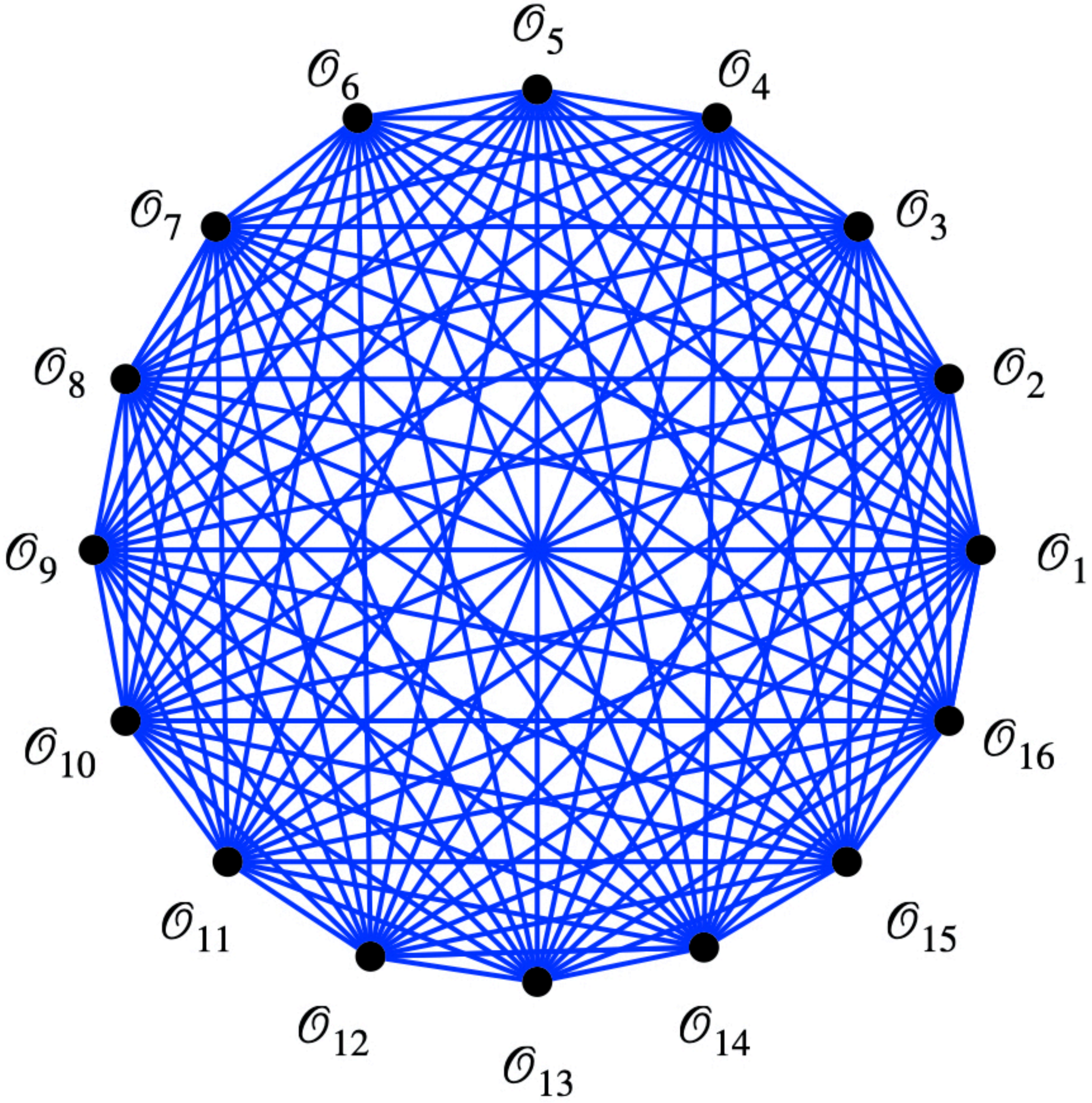
<u>Note about Classical Computational Cost</u>

- Creation of W_N scales as $\mathcal{O}(N \log_2 N)$
- Coefficient is 10^{-5} sec. on old laptop using Mathematica

See manuscript for explicit proofs

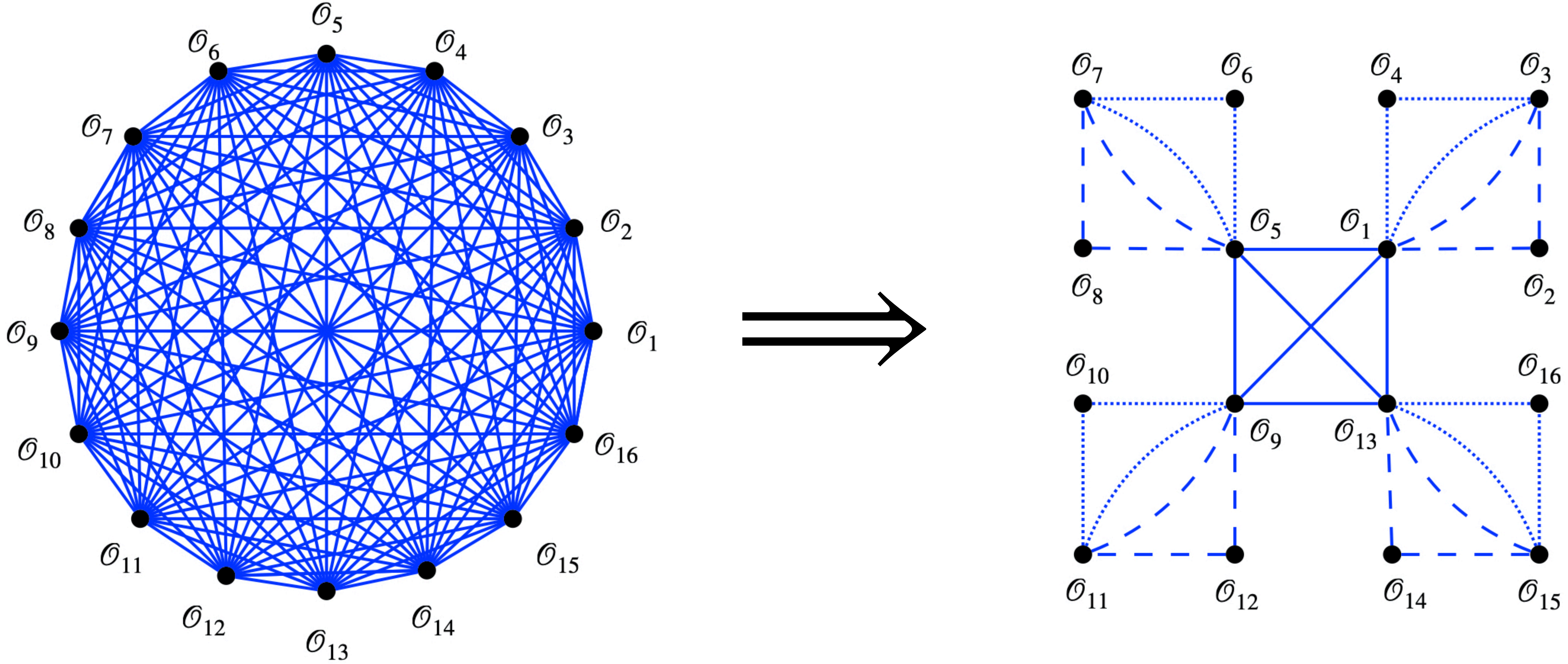
Reducing Degree of (Operator) Connectivity



16 Operator Constrained Hamiltonian

***DMG**, C. Kane, B. Nachman and C.W. Bauer: arXiv: 2208.03333*

Reducing Degree of (Operator) Connectivity



16 Operator Constrained Hamiltonian

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Conclusions

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

It is important to carefully consider the scaling of quantum computing resources for simulating gauge theories on far-future fault tolerant quantum computers

Main Take-Away Point 1: We have a method for constructing a resource-efficient Hamiltonian that only spans the physical subspace of 2 +1 U(1) lattice gauge theory

Main Take-Away Point 2: It is imperative to carefully explore the resource cost of constrained Hamiltonians due to their inherent non-locality.

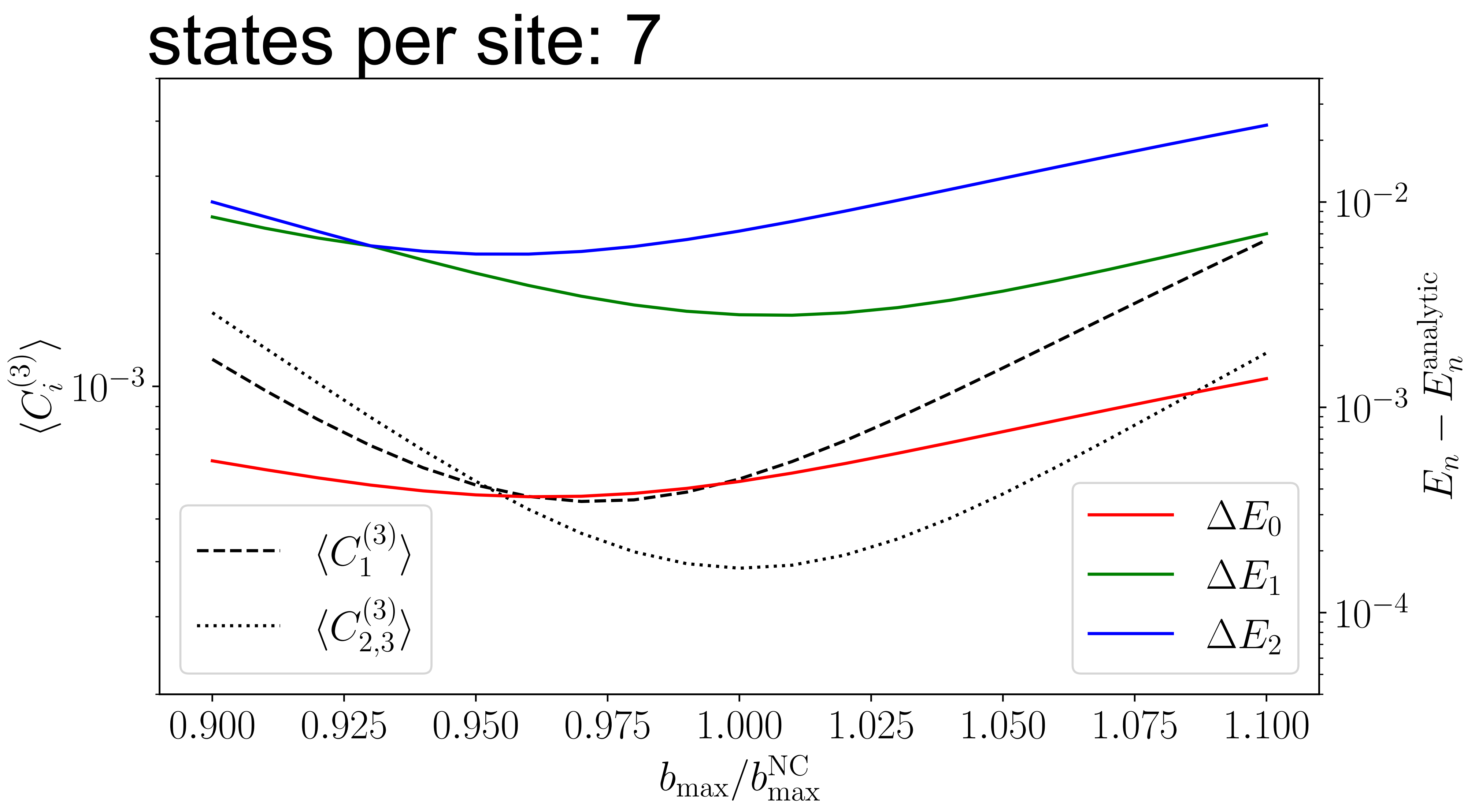
Back Up Slides

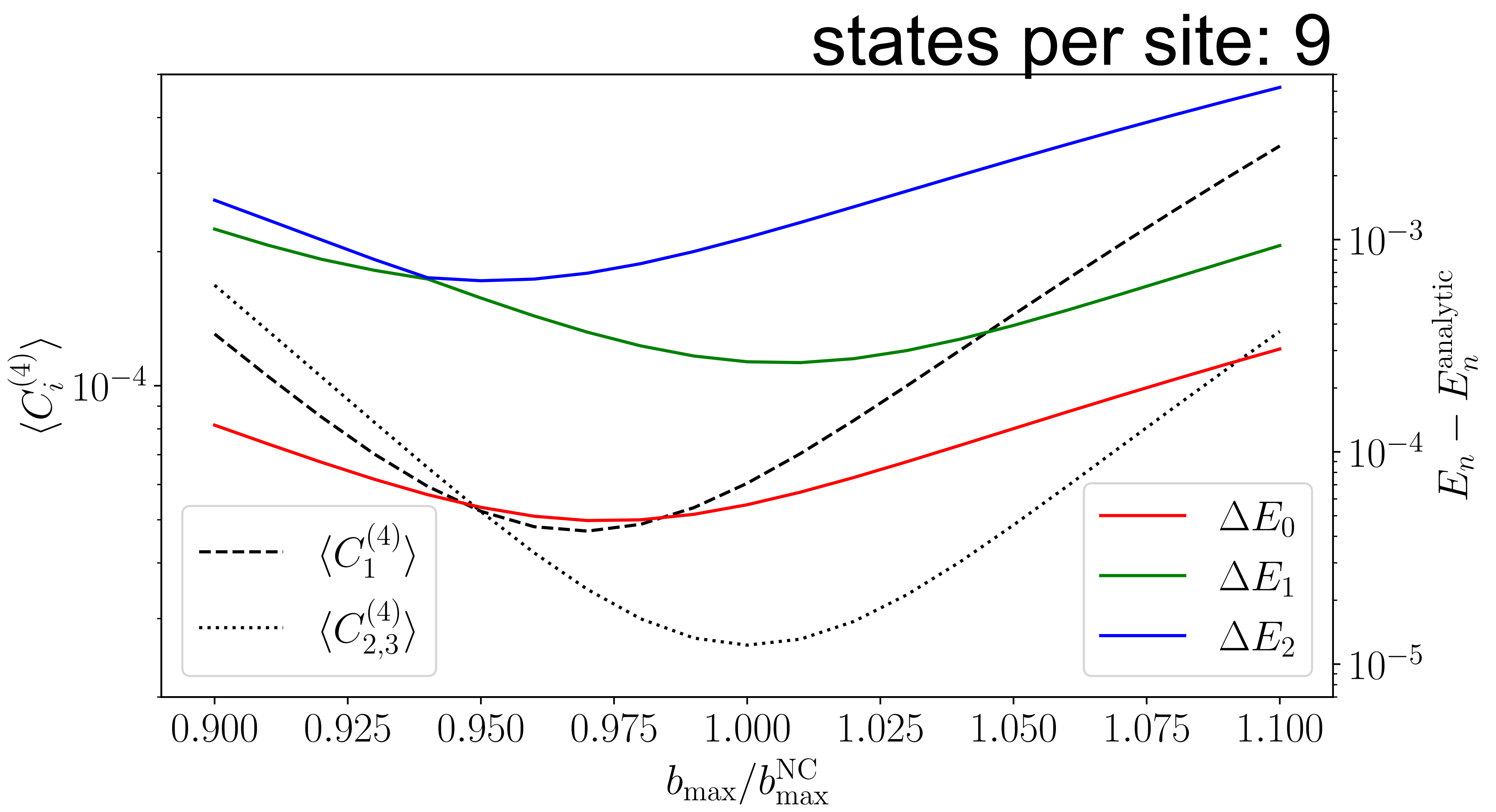
Digitizing the Dual Formulation in the Magnetic Basis

General Idea: Combine "gauge-redundancy free" dual representations with digitization method motived by weak-coupling eigenstate localization*

Comparison to exact solution

Violation of Commutation Relations





Precision in Low-Lying Energy Eigenvalue

Scanning through truncation scale, compared to optimal truncation scale

Examples of Weaved Matrices

$$W_4 = \begin{pmatrix} \frac{1}{2} & -\frac{1}{\sqrt{2}} & -\frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{\sqrt{2}} & -\frac{1}{2} & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & -\frac{1}{\sqrt{2}} \\ \frac{1}{2} & 0 & \frac{1}{2} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

$$W_{11} = \begin{pmatrix}
\frac{1}{\sqrt{11}} & -\sqrt{\frac{2}{3}} & 0 & -2\sqrt{\frac{2}{33}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{\sqrt{11}} & \frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{2}} & -2\sqrt{\frac{2}{33}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{\sqrt{11}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} & -2\sqrt{\frac{2}{33}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{\sqrt{11}} & 0 & 0 & \frac{\sqrt{\frac{3}{22}}}{2} & -\frac{1}{\sqrt{2}} & -\frac{1}{2} & 0 & -\frac{1}{2\sqrt{2}} & 0 & 0 & 0 \\
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\end{pmatrix}$$