# Quantum Computing Methods for Lattice Gauge Theories


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# Motivation

***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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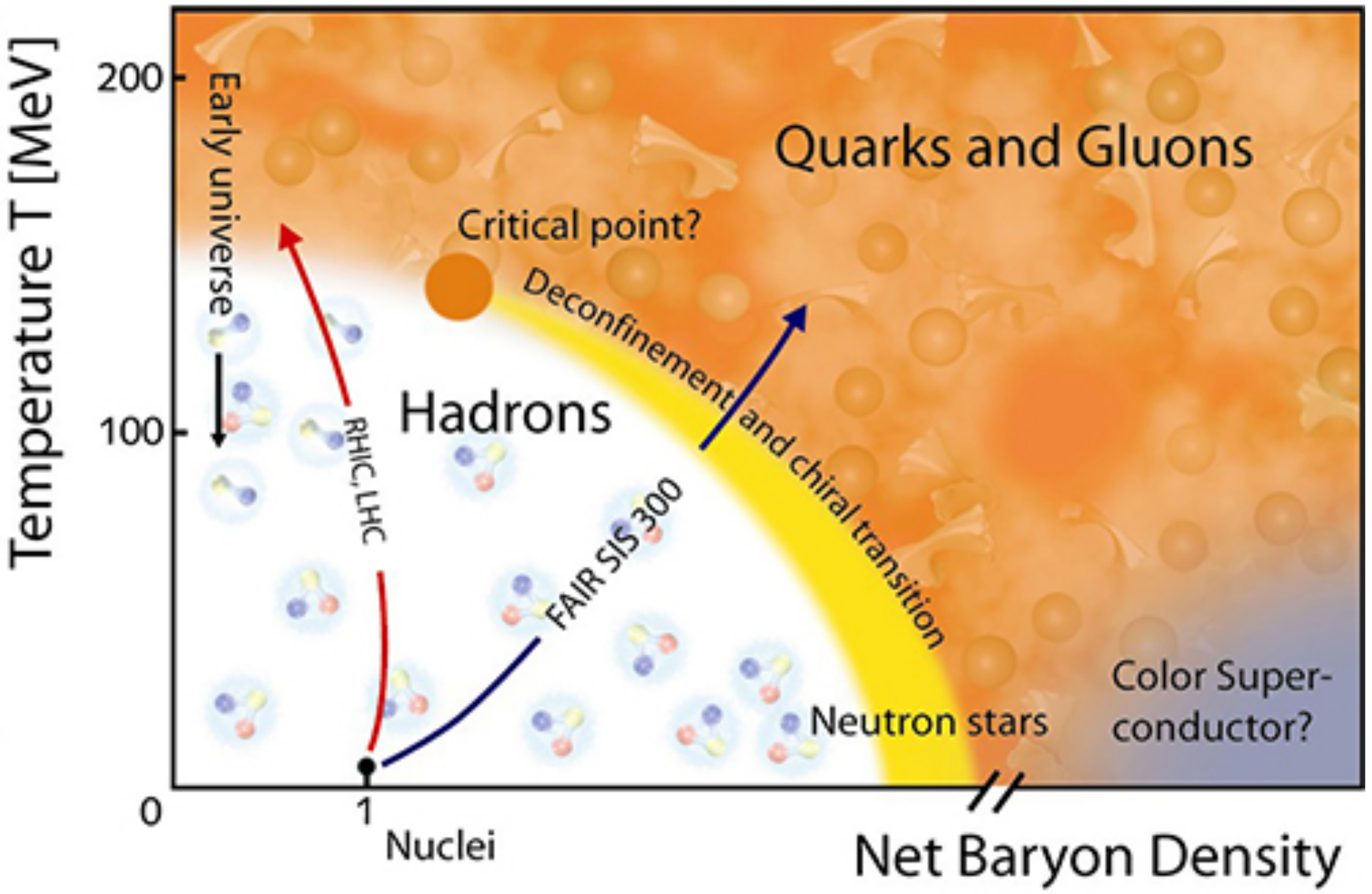
## Quantum Chromodynamics (QCD)

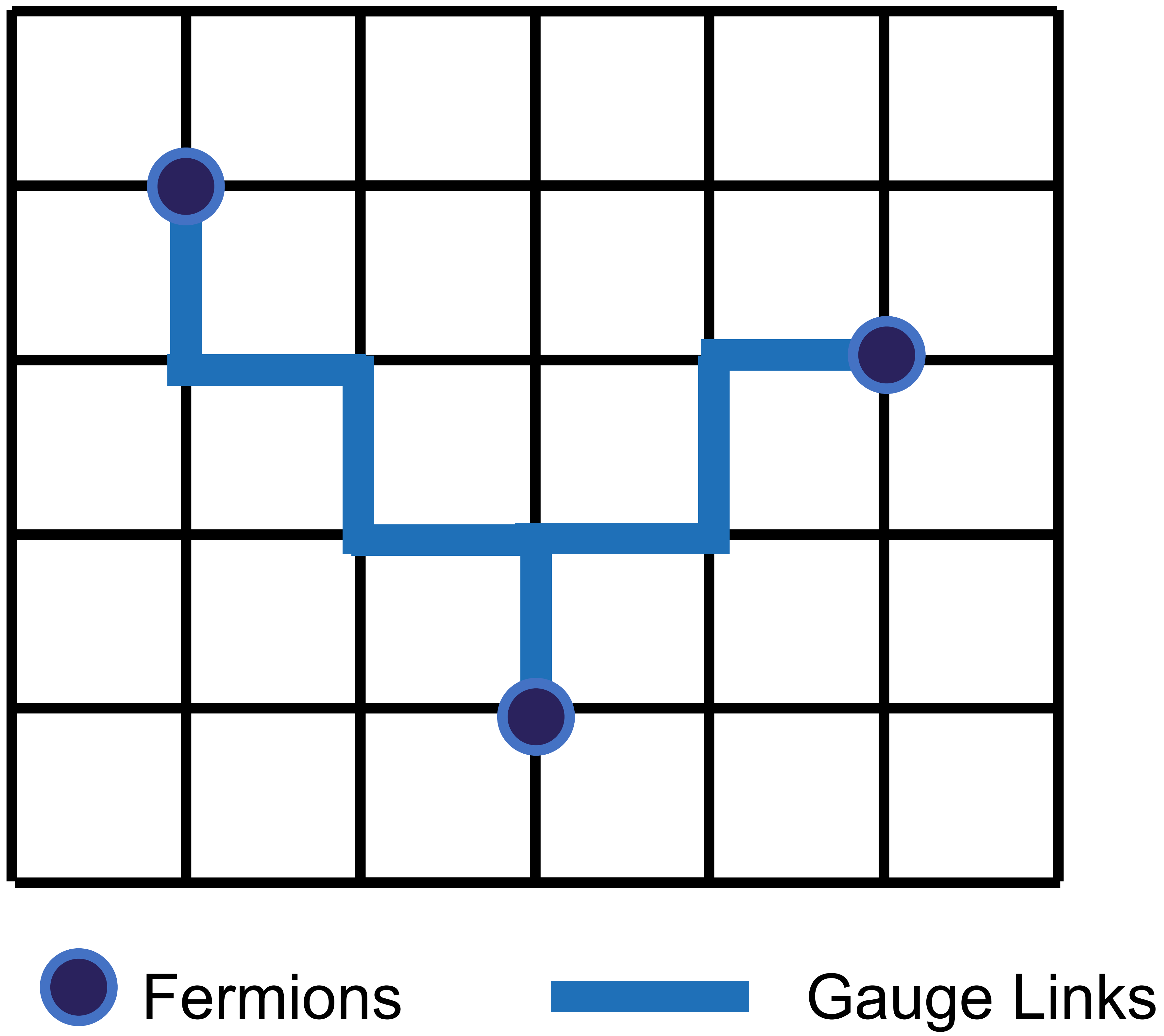
- Provides precise and quantitative description of the strong nuclear force over an broad range of energies
- *Ab-initio* calculations crucial for comparing theoretical predictions of the Standard Model to experimental results
- Gives rise to complex array of emergent phenomena that cannot be identified 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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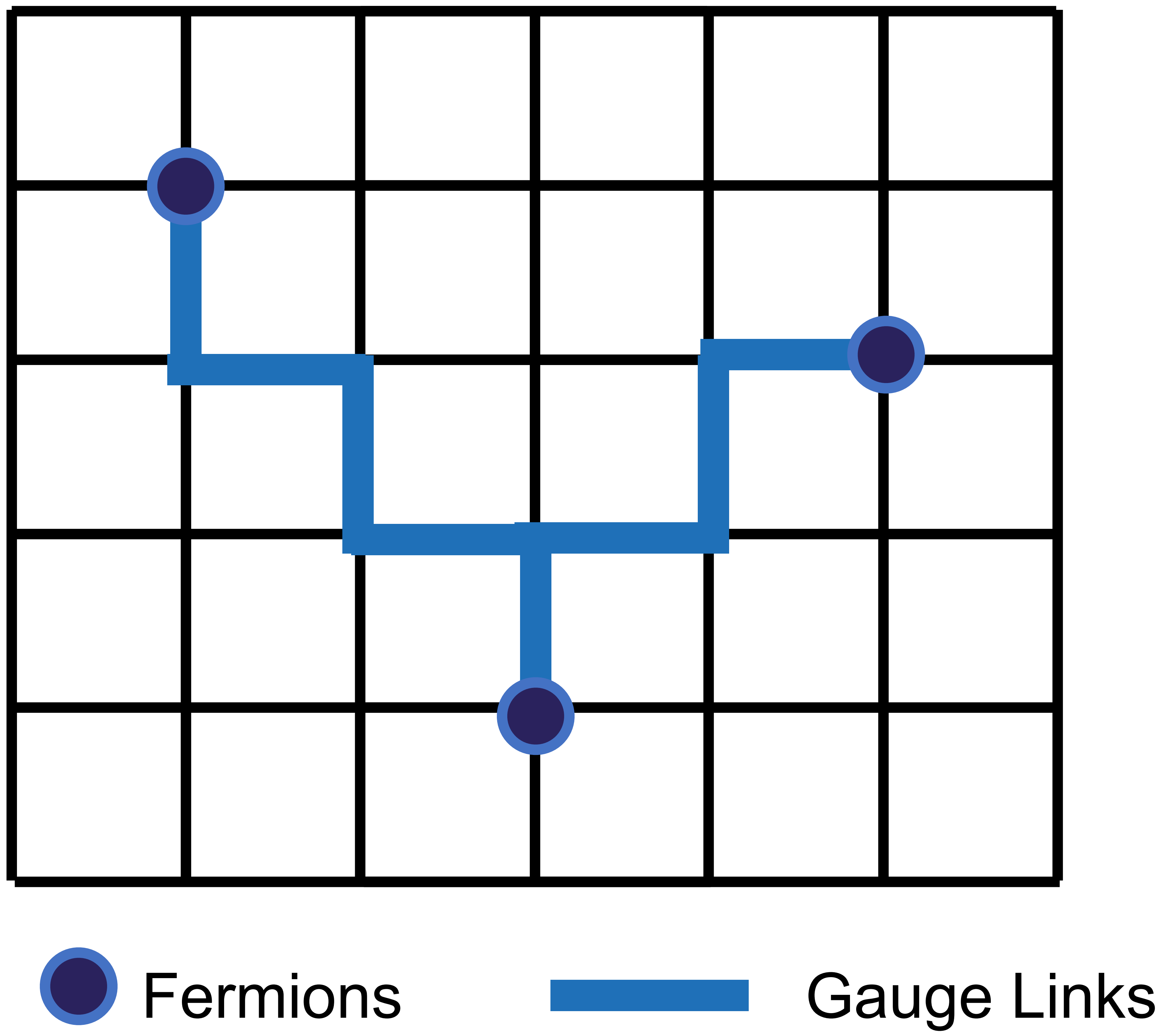
- Sub-percent precision in many single-hadron observables
  - Hadron vacuum polarization for g-2 measurements
  - Hadron spectrum with QED and isospin breaking effects
- Reliable extraction of several two-hadron observables
  - $K \to \pi\pi$ and direct CP violation



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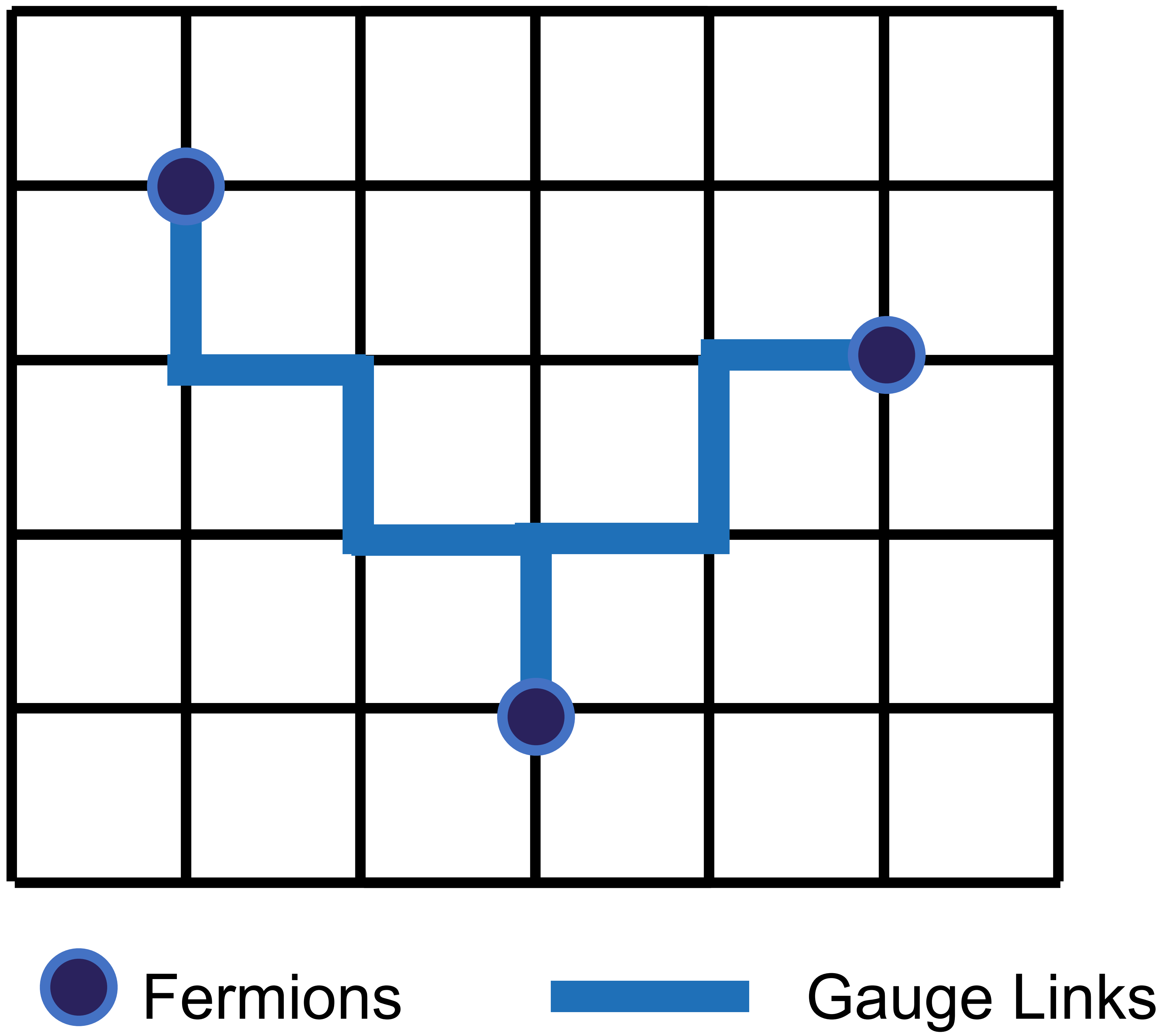


***Only fully-systematic approach to ab-initio computations in the non-perturbative regime***

# Sign Problems in Lattice Gauge Theories

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

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**<u>Real-Time Dynamics</u>**

Early Universe Phase Transitions

Requires Minkowski space simulations

**<u>Chiral Gauge Theories</u>**

Fully defined Standard Model

Complex fermion determinant

**<u>Finite-Density Nuclear Matter</u>**

Neutron stars and QCD phase diagram

Complex fermion determinant

***Is this physics more accessible on quantum computers?***

# Digital 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***

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

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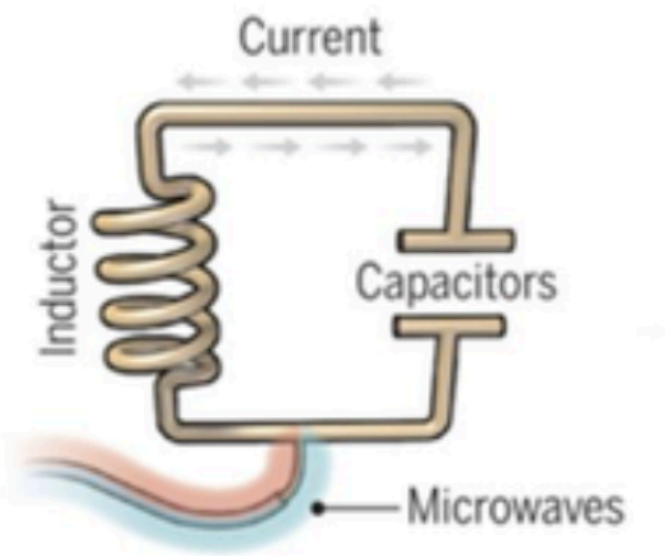
***Can we see a similar improvement for calculations in High Energy Physics?***

# Digital Quantum Computers

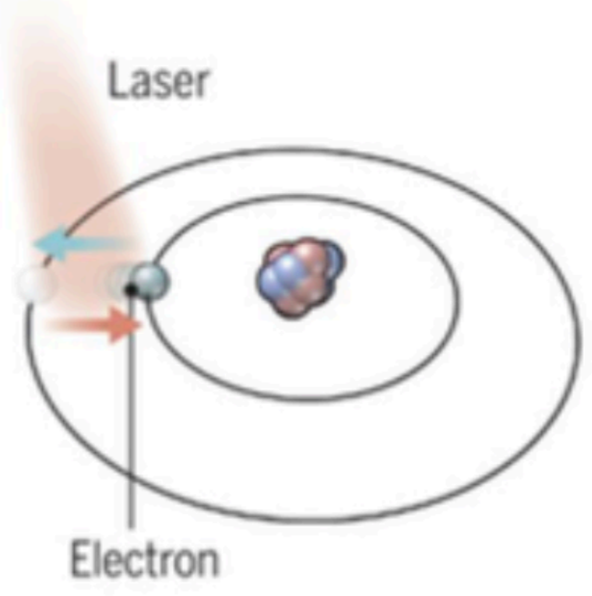
***Computational Strategy:*** Quantum circuit is created by acting on collection of two-state systems (qubits) with reversible unitary transformations (logical gates)

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

- Superconducting loops




- Trapped ions

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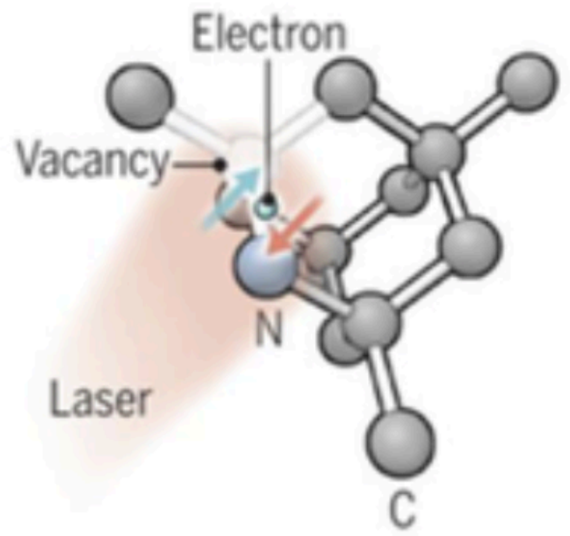


*Graphics by C. Bickle, Science Data by Gabriel Popkin*

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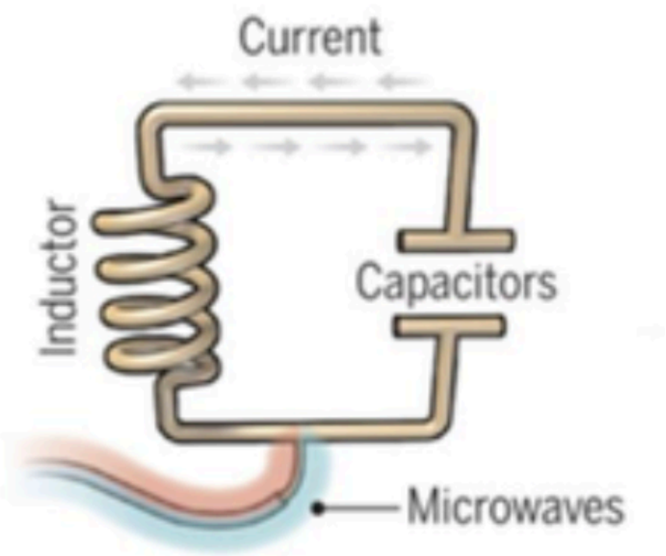


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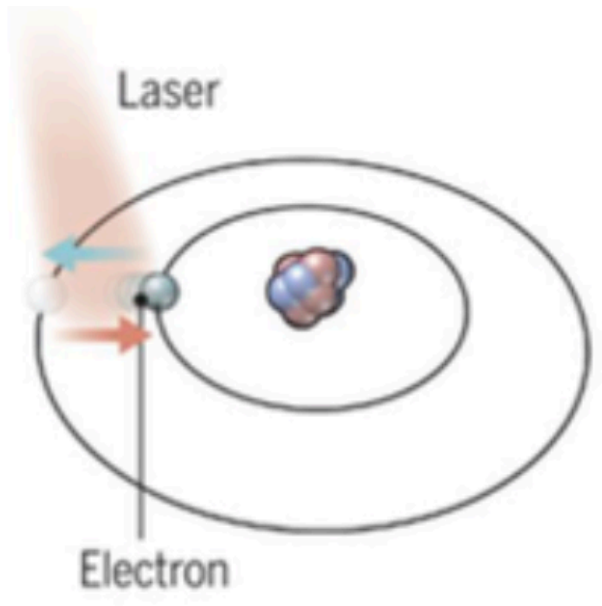


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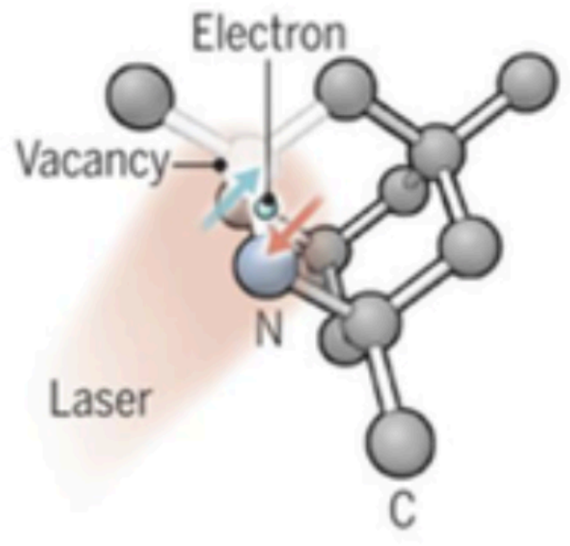


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Currently in ***Noisy Intermediate-Scale Quantum*** (NISQ)-era

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

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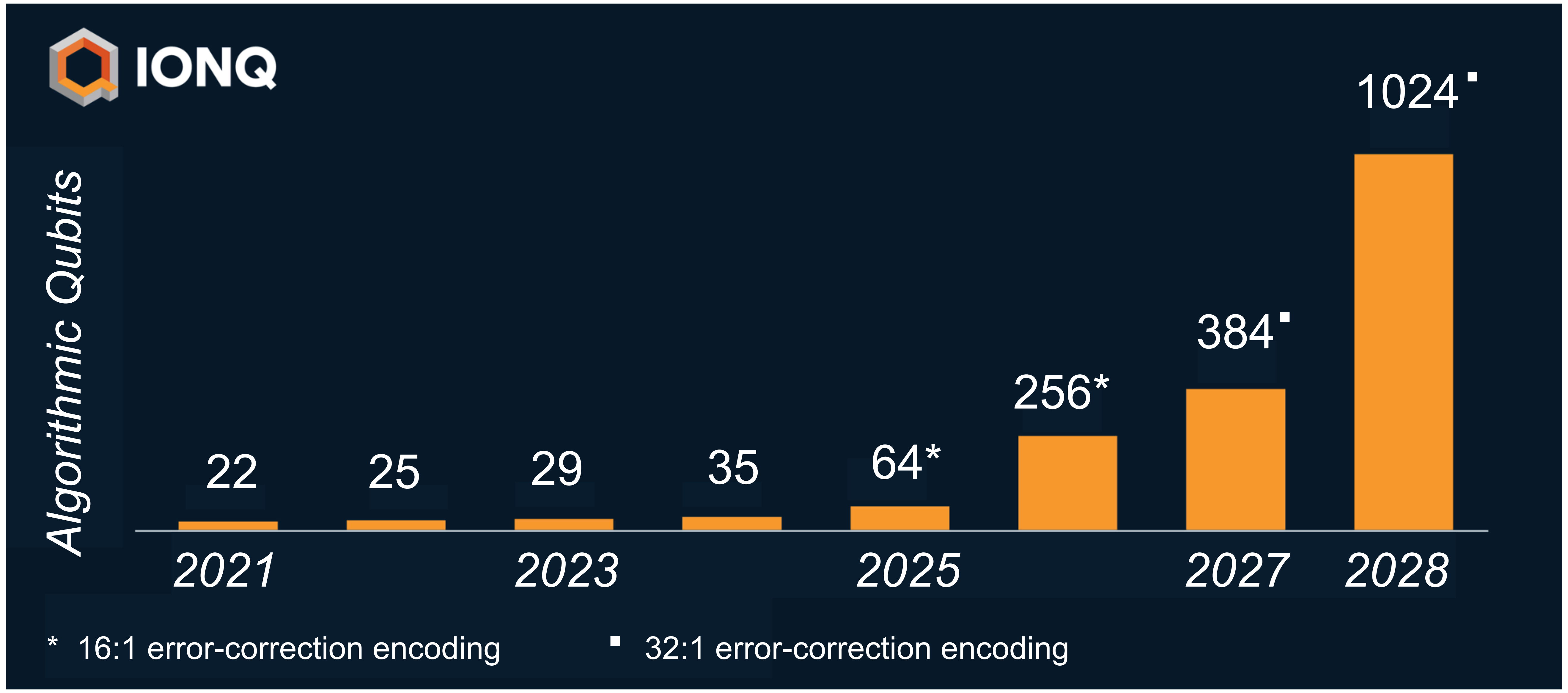


IonQ Roadmap, 2020

*Trapped Ion*

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***Computational Strategy:*** “Tweak” the natural degrees of freedom of experimental setup to mimic behavior of target model

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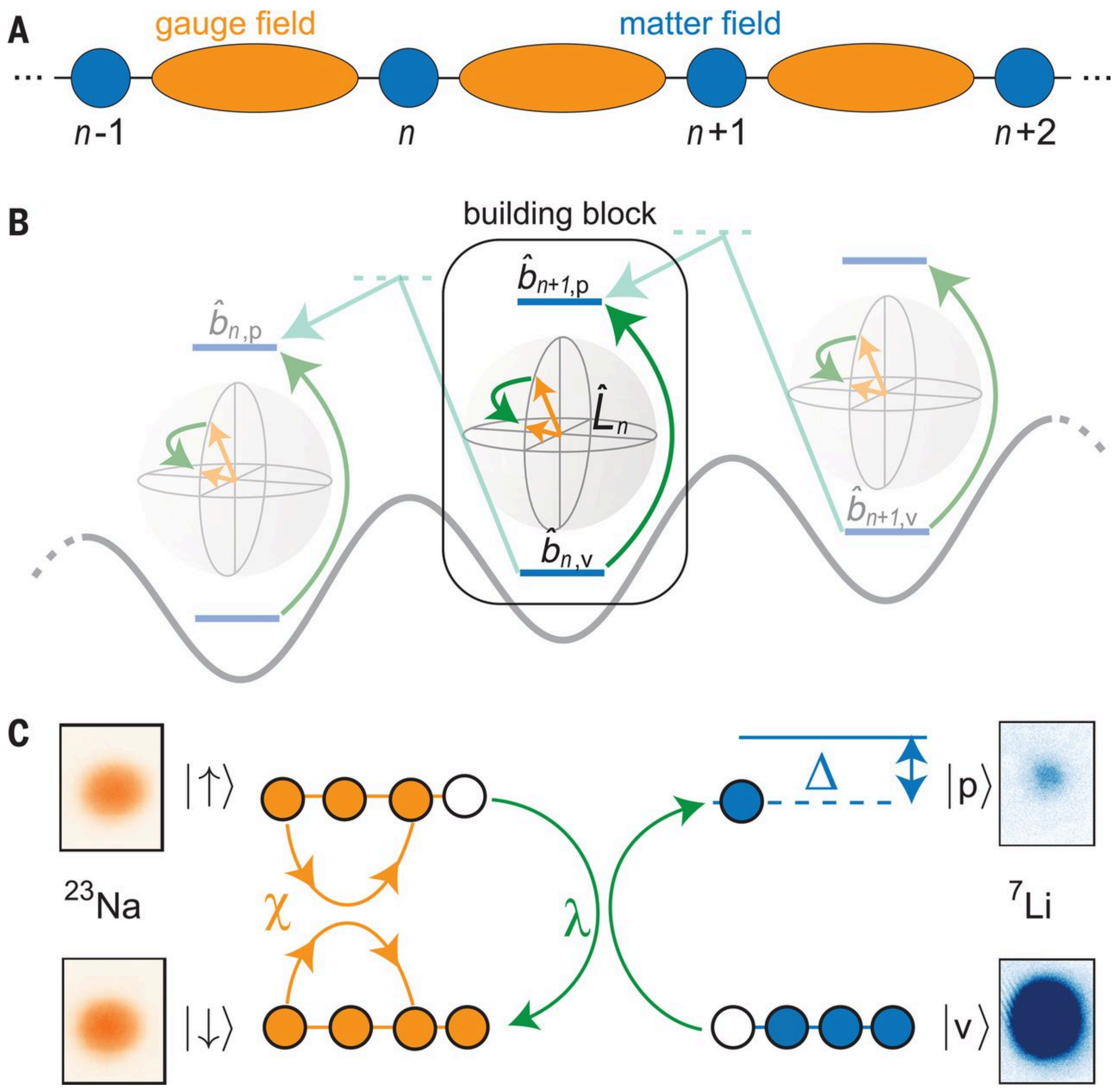
- Interspecies spin-changing collisions mimic gauge-matter interactions




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

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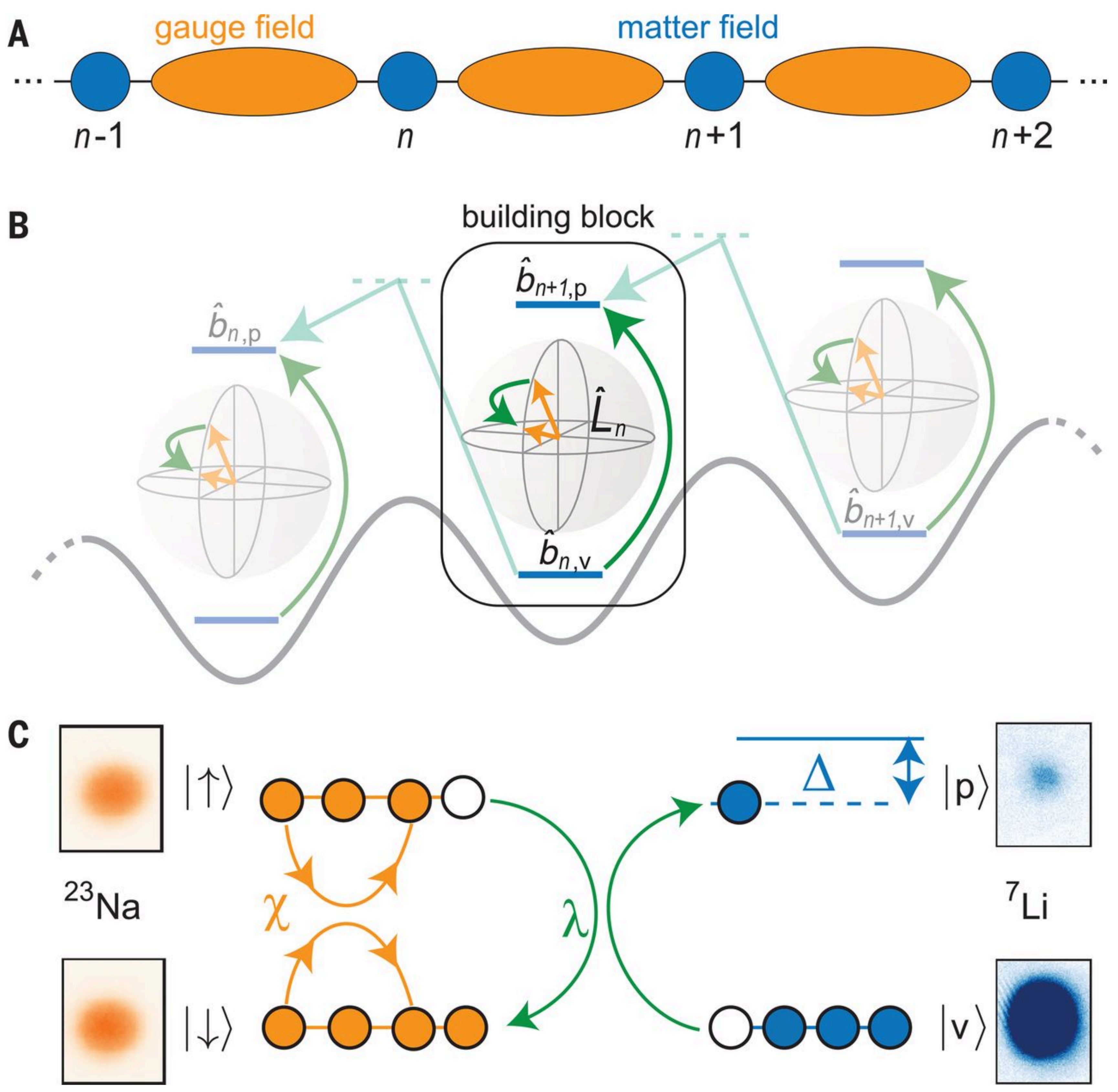
***Analog quantum computation is "effective field theory description made physical"***

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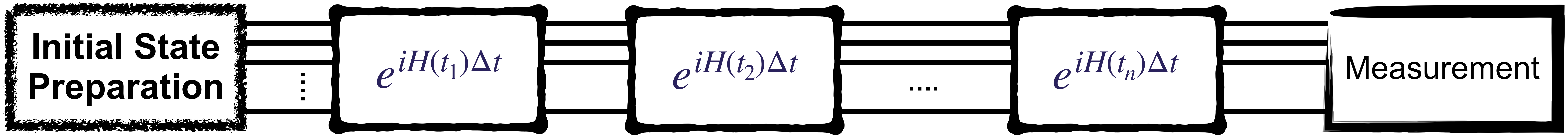
# Quantum Simulations of Gauge Theories

***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

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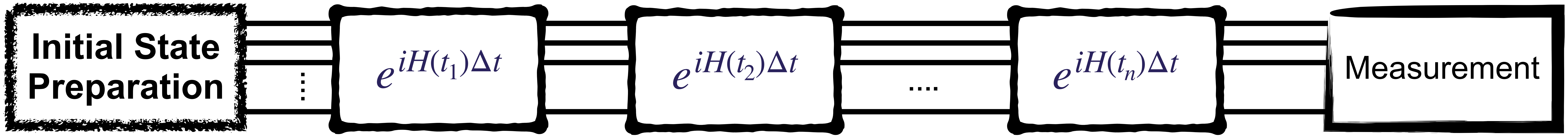


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**Overarching Research Goal**

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

# Quantum Simulations of Gauge Theories

***Guiding Principle 1:*** Important to work on both theoretical developments and algorithmic developments simultaneously

## 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 time?*

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***Guiding Principle 2:*** Resource efficiency and gate + qubit scaling of simulation must always be considered, even when working on smaller machines

***We cannot simply propose "fault-tolerant quantum computers" as the solution to all of our problems***

# Goals of Talk

***I had two goals in preparing this talk***

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**Main Take Away Message**

We are a young vibrant field with many interesting theoretical and algorithmic challenges ahead (and these challenges cannot be put off until the era of fault-tolerant quantum computers!)

# Theoretical Developments

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

*Phys Rev D 11, 395 (1975)*

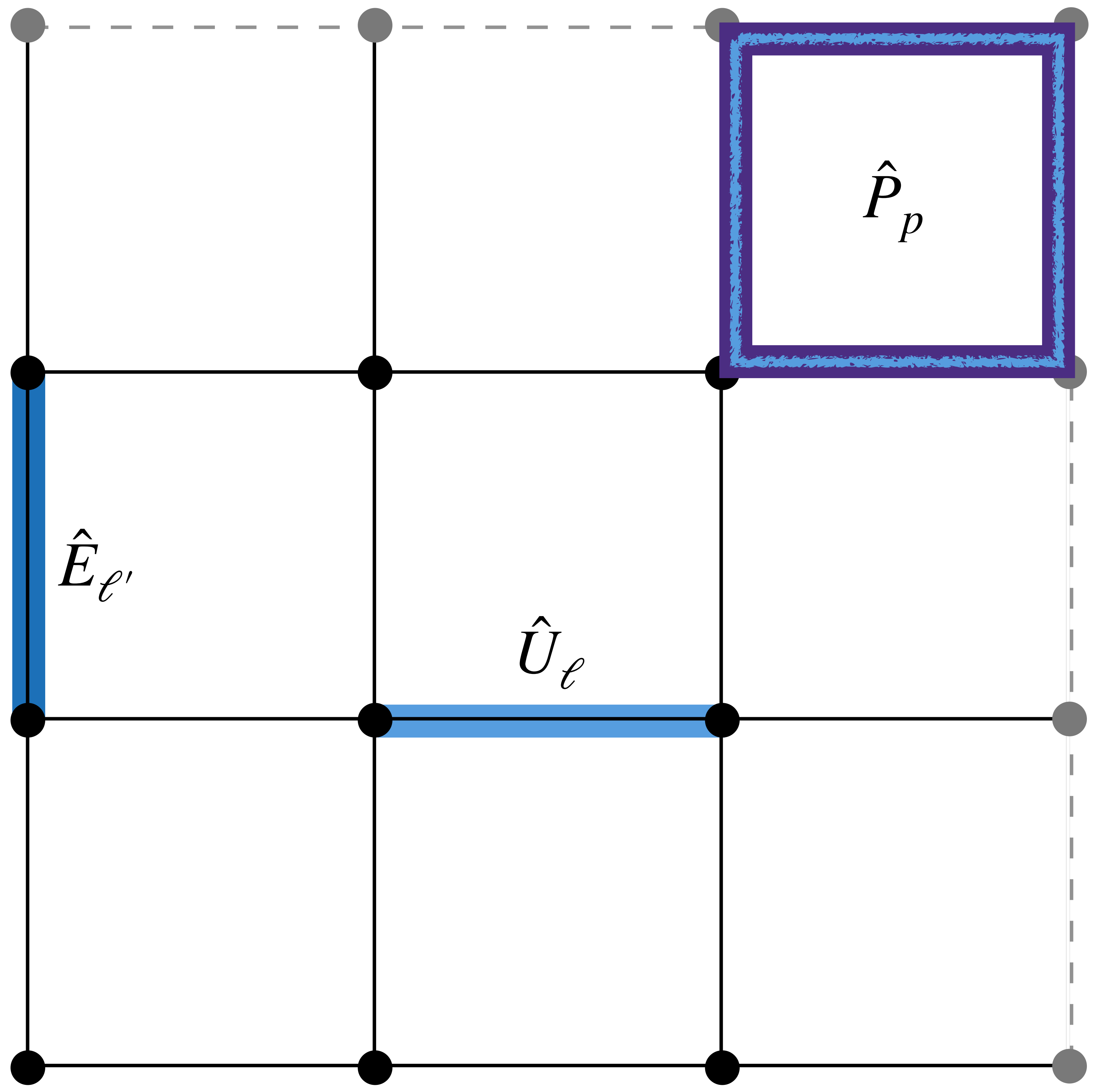
# Hamiltonian Lattice Gauge Theory, Abelian

***Quantum simulations utilize Hamiltonian formulations***

- Continuous time, but discrete space
- Use Weyl Gauge ($A_0 = 0$)

***Kogut-Susskind Hamiltonian***

$$H = \frac{1}{2a}\left[g^2 \sum_{\ell \in links} E_\ell E_\ell + \frac{1}{g^2} \sum_{p \in plaquettes} \mathrm{Tr}\left(2I - P_p - P_p^\dagger\right)\right]$$



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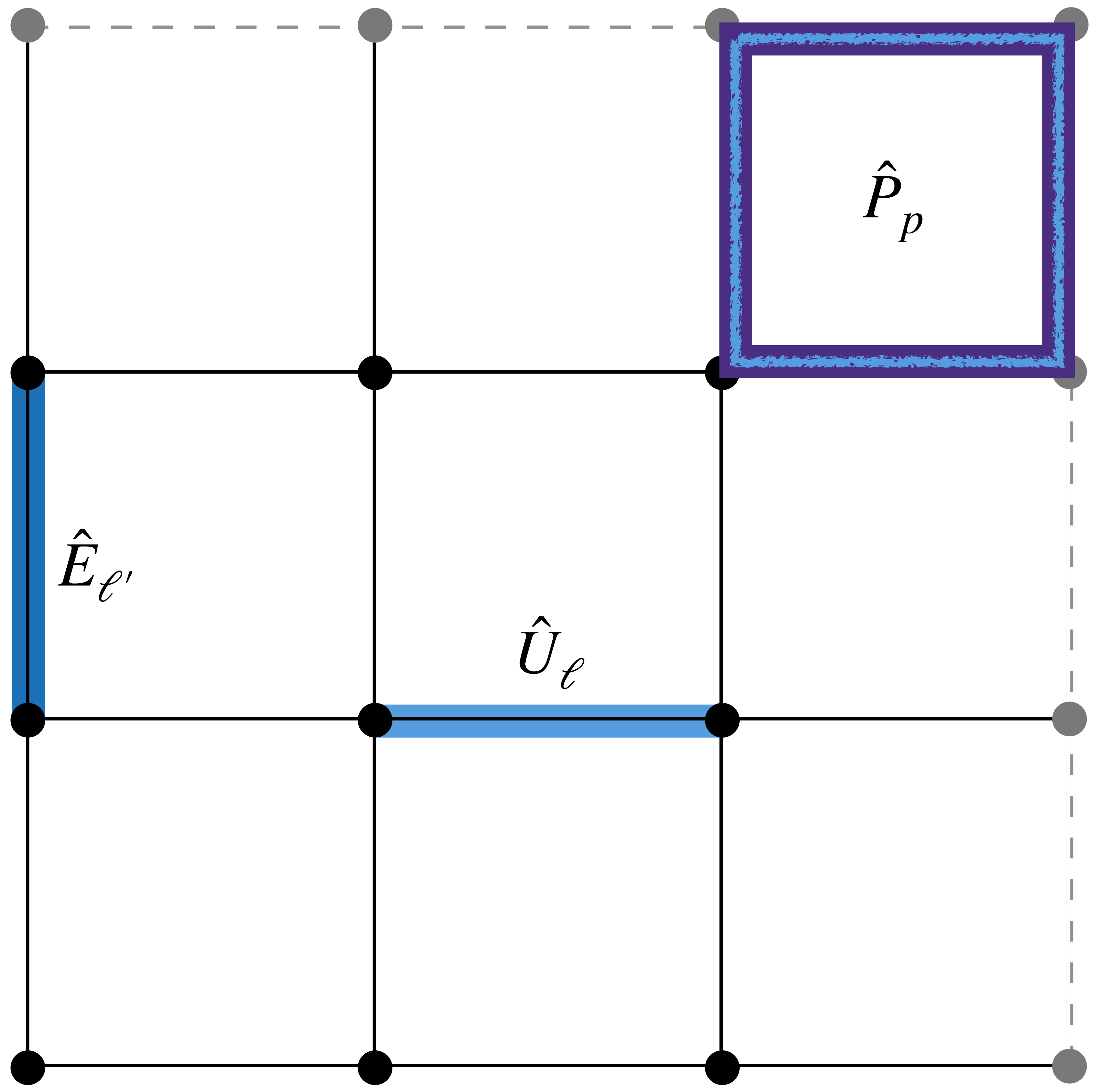

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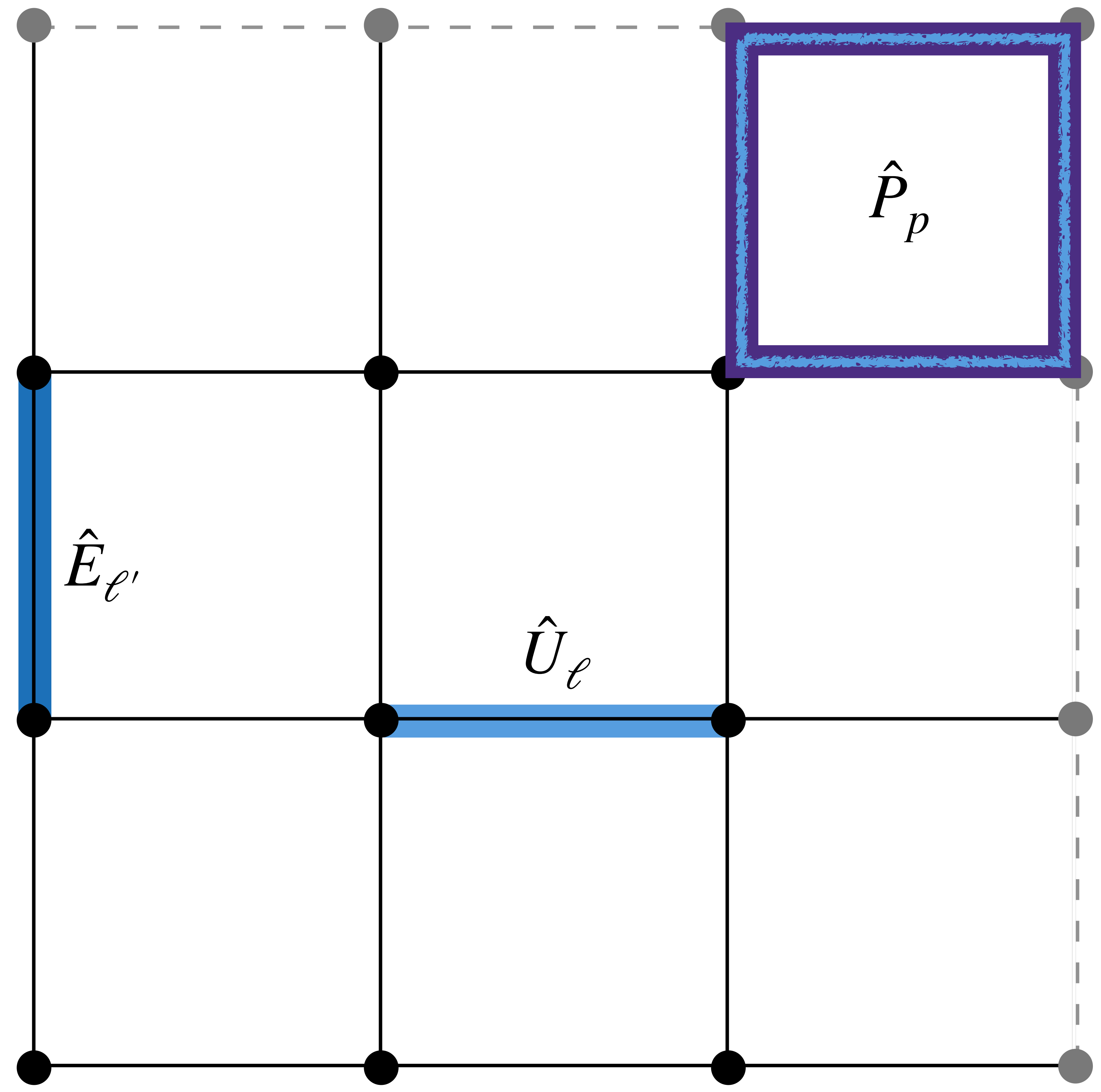

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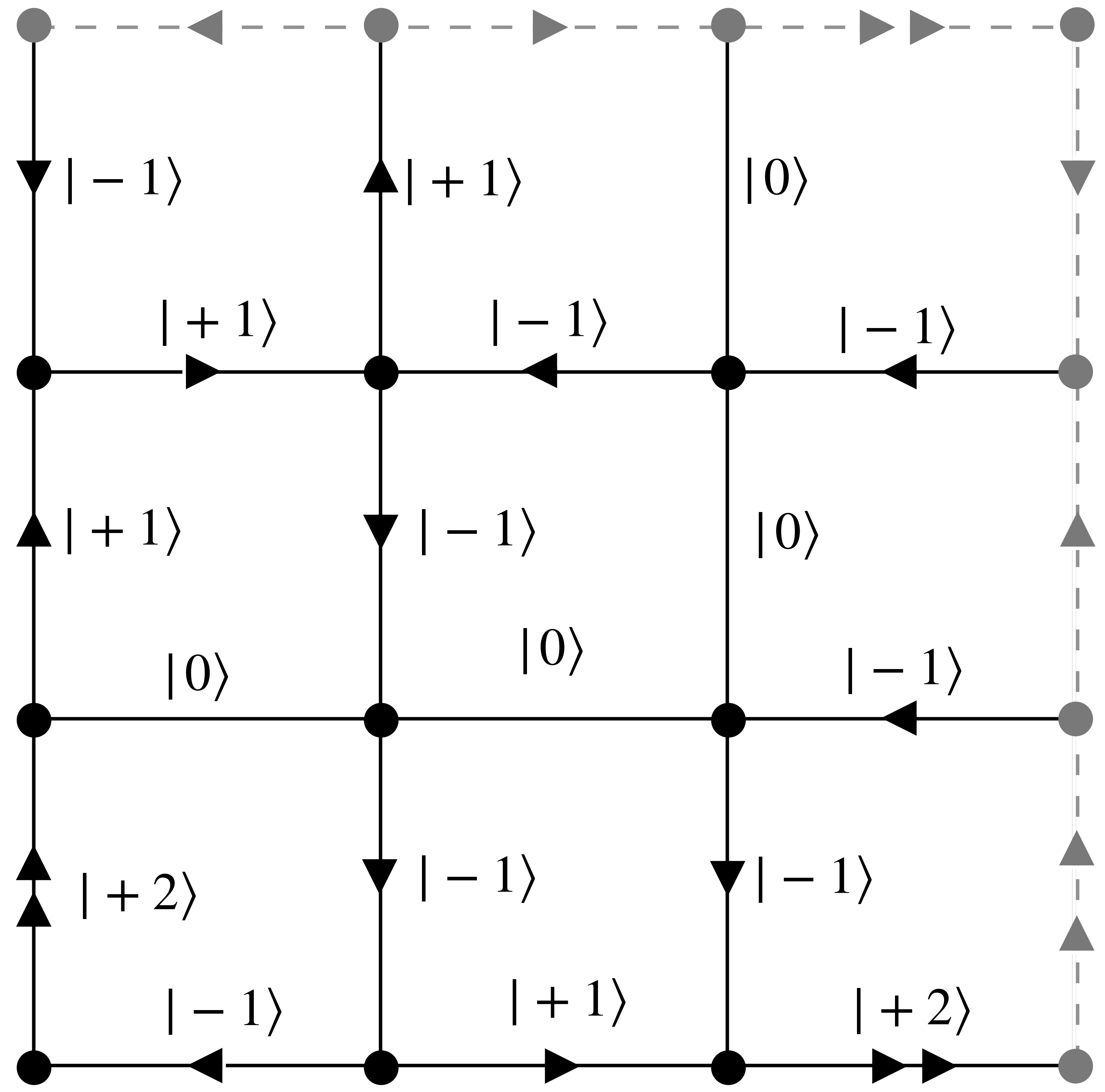

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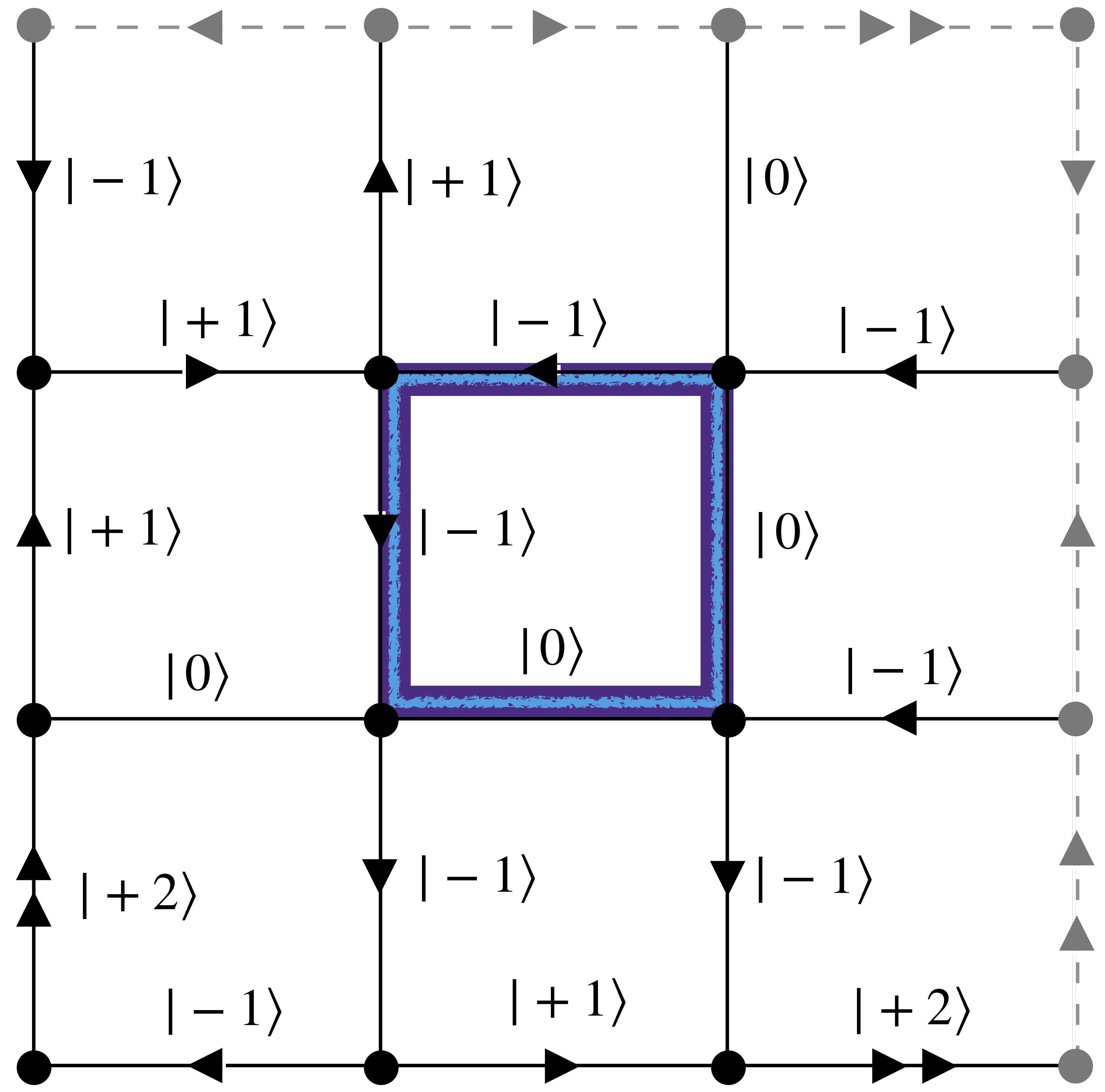

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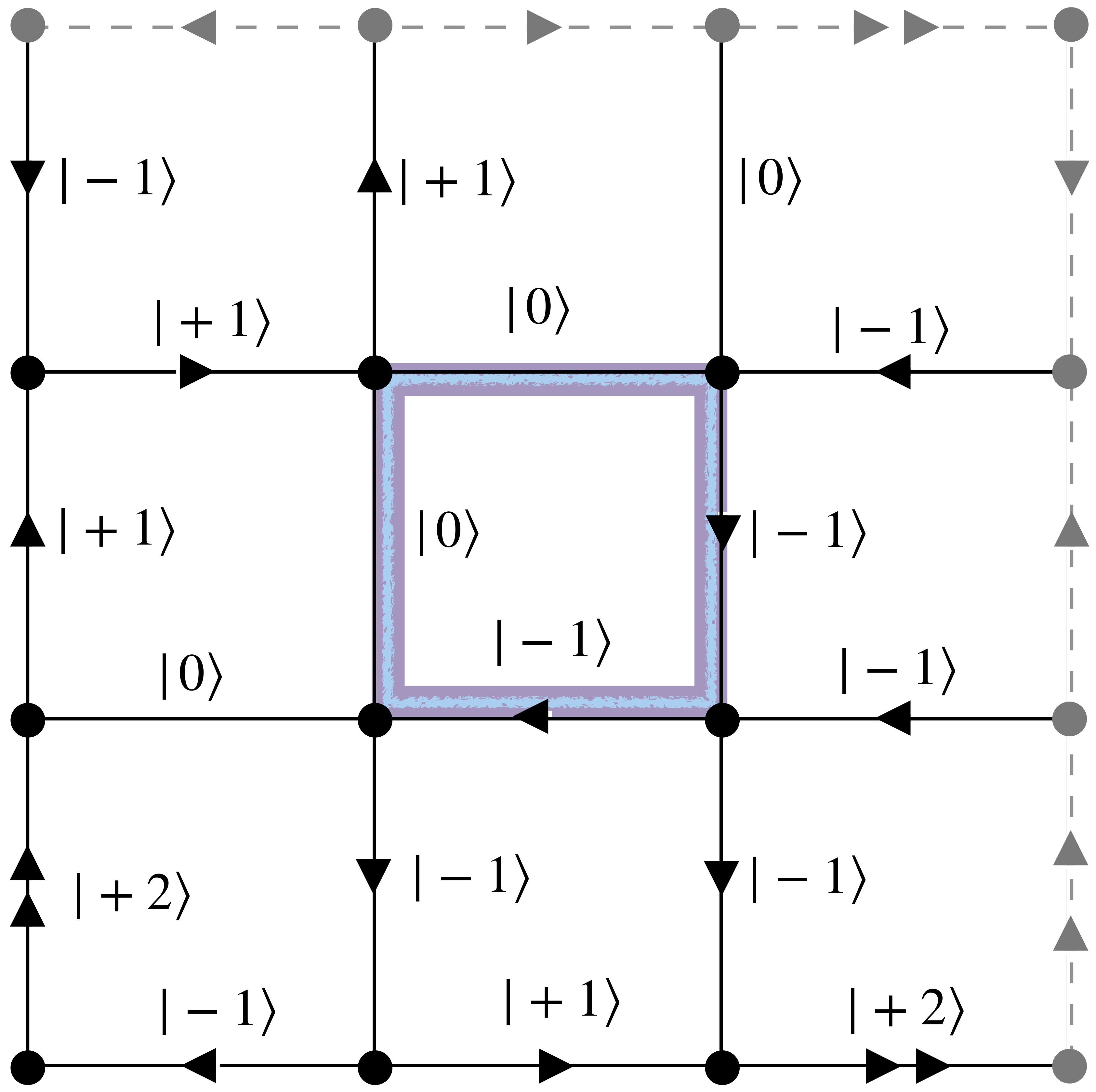

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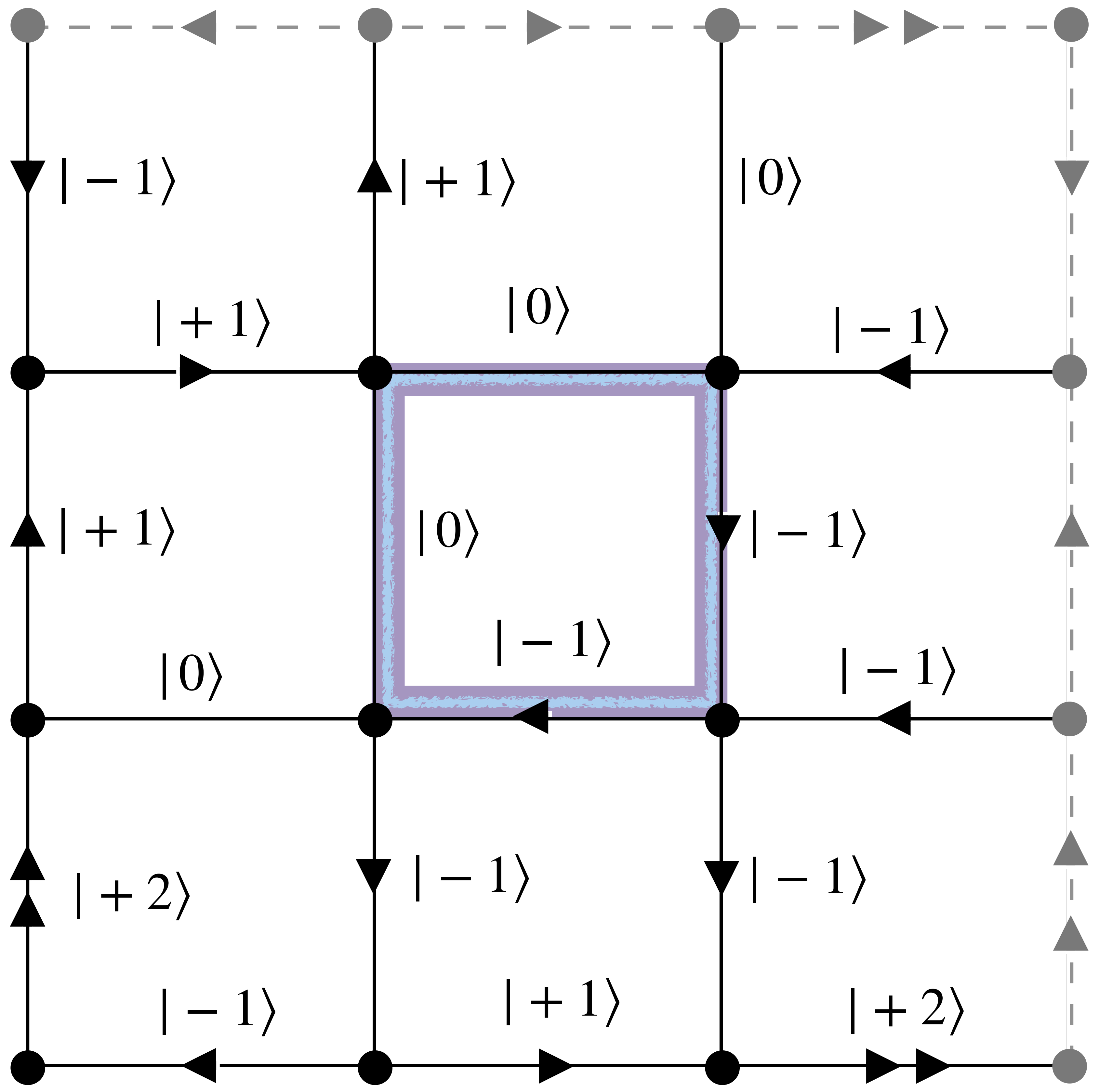


***Is this the end of the story?***

# Theoretical Challenges of Lattice Gauge Theories

***Three fundamental hurdles have to be overcome on the quest for quantum simulation of Hamiltonian lattice field theories***

**_A) Hamiltonians of quantum field theories are infinite-dimensional_**

*Construct finite-dimensional Hermitian matrix that faithfully captures desired physics*

**_B) Phenomenologically-relevant gauge groups are continuous_**

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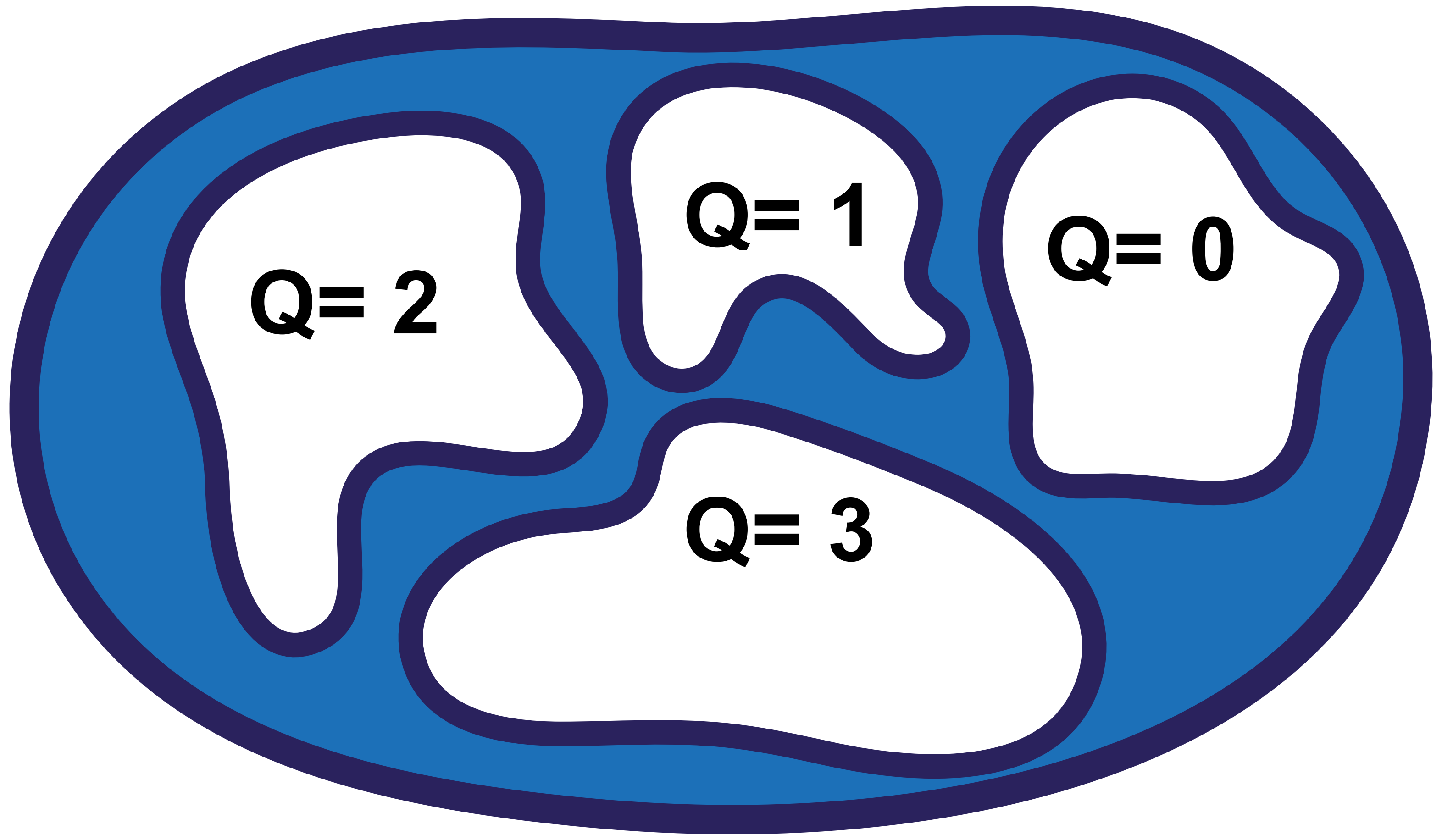
### *C) Gauss Law is not automatically satisfied**

*Develop methods for ensuring unphysical charge-violating transitions do not occur, even in noisy simulations, while being mindful of resource requirements*




*Gauss's law is the constraint associated with the $A_0$ Lagrange multiplier

# Hamiltonian Lattice Gauge Theory, SU(N) Version

***General Idea:*** Similar to Abelian, but electric and gauge link operators carry color indices

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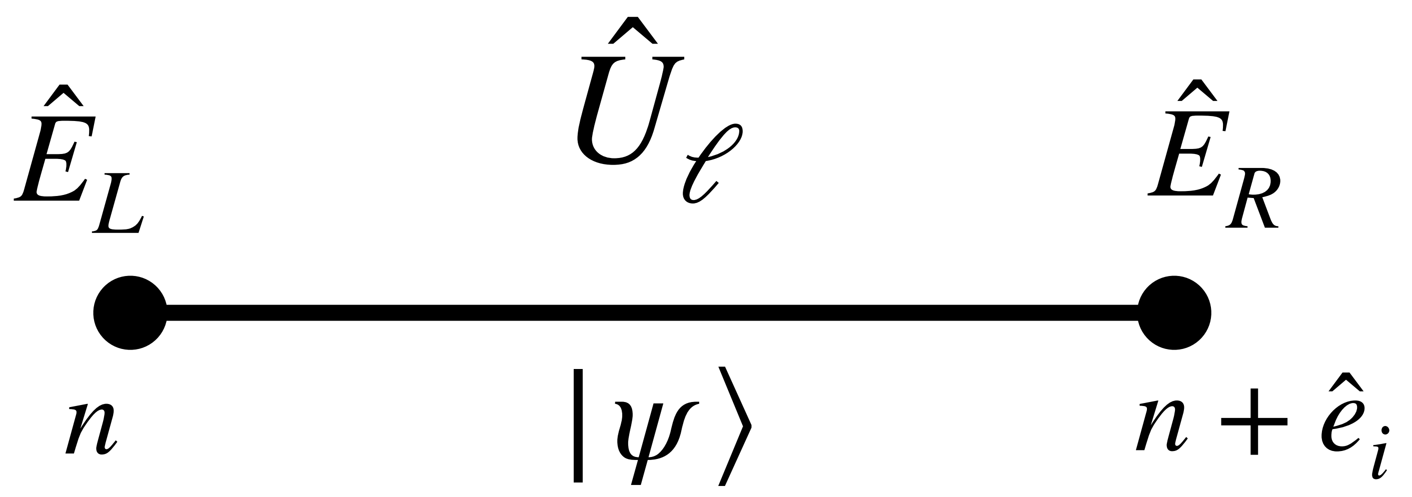
- Theory now contains both left and right electric operators




- Rotations of gauge link from left and right are generated by left and right electric fields

$$\hat{U}(n, e_i) \longmapsto \Omega(n)\, \hat{U}(n, e_i)\, \Omega(n + e_i)^\dagger$$

- Each electric field has their own Lie algebra and commutation relations

$$\left[\hat{E}^a_L, \hat{U}^j_{mn}\right] = T^{ja}_{mm'}\hat{U}^j_{m'n}$$

$$\left[\hat{E}^a_R, \hat{U}^j_{mn}\right] = \hat{U}^j_{mn'}T^{ja}_{n'n}$$

$$\left[\hat{E}^a_L, \hat{E}^b_L\right] = -\,if^{abc}\hat{E}^c_L$$

$$\left[\hat{E}^a_R, \hat{E}^b_R\right] = if^{abc}\hat{E}^c_R$$

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# Gauge Fixing and Gauss Law

***Key Issue:*** Weyl gauge is an incomplete gauge-fixing procedure. Gauge transformations with only spatial dependence still allowed and Gauss law becomes a constraint

SU(N) Gauss Law:

$$D \cdot E^a = 0$$

*Continuum*

$$\hat{G}^a(n) = \sum_{i=1}^{d} \left[ \hat{E}^a_R(n - e_i, e_i) - \hat{E}^a_L(n, e_i) \right]$$

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## Option One: No Additional Gauge Fixing

- Additional "energy penalty" term reduces transitions between charge sectors for noisy simulations
- Most qubits and gate operations are irrelevant to physical process

Halimeh, J.C. and Hauke, P. Phys. Rev. Lett. 125, 030503 (2020)

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$$\hat{G}^a(n) = \sum_{i=1}^{d} \left[ \hat{E}^a_R(n - e_i, e_i) - \hat{E}^a_L(n, e_i) \right]$$

*Lattice*

***Fact:*** Hamiltonian ***does*** commute with Gauss law operators and so charge is conserved

## Option One: No Additional Gauge Fixing

- Additional "energy penalty" term reduces transitions between charge sectors for noisy simulations
- Most qubits and gate operations are irrelevant to physical process

Halimeh, J.C. and Hauke, P. Phys. Rev. Lett. 125, 030503 (2020)

## Option Two: Additional Gauge Fixing

- Expect increase in non-locality due to imposition of Gauss law constraints and therefore longer circuits
- Can be very challenging to write down, especially with the addition of dynamical fermions

*Bauer, C.W. and **DMG**, Phys.Rev.D 107 (2023) 3, L031503*

*Bauer, D'Andrea, Freytsis and **DMG**, arXiv: 2307.11829*

# Gauge Fixing and Gauss Law

Gauss Law ↔ Gauge Invariance

Charge Conservation

**_Key Issue:_** Weyl gauge is an incomplete gauge-fixing procedure. Gauge transformations with only spatial dependence still allowed and Gauss law becomes a constraint

SU(N) Gauss Law:

$$D \cdot E^a = 0$$

*Continuum*

$$\hat{G}^a(n) = \sum_{i=1}^{d} \left[ \hat{E}^a_R(n - e_i, e_i) - \hat{E}^a_L(n, e_i) \right]$$

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# Coupling Strength and Basis Choices

***Starting Point:*** Theory has fundamentally different properties at large and small (bare) gauge coupling

$$H = \frac{1}{2a}\left[g^2 \sum_{\ell \in links} E_\ell^a E_\ell^a + \frac{1}{g^2} \sum_{p \in plaquettes} \mathrm{Tr}\left(2I - P_p - P_p^\dagger\right)\right]$$

## Strong Coupling (Irrep Basis)

*Electric component of Hamiltonian dominates*

*Basis:* $|j, m_L, m_R\rangle$

- States naturally discretized
- Gauss's law is function of electric fields
- Natural UV truncation

GOOD

- Not well-suited for "close to continuum" physics

BAD

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## Weak Coupling (Group Element Basis)

*Magnetic component of Hamiltonian dominates*

*Basis:* $|\mathfrak{g}\rangle$

GOOD

- Gauge links diagonal
- Well-suited for "close to continuum" physics

BAD

- Electric fields are more complicated
- Digitization/truncation of gauge links must be done carefully

# Examples of Abelian & Non-Abelian Formulations + Bases

**Kogut-Susskind formulation**
– Irrep/"angular momentum" basis *Byrnes, Yamamoto, Zohar, Burrello, et al.*
– Group-element basis *Zohar, NuQS collab., et al.*

**Gauge magnets/quantum link models:** *Wiese, Chandrasekharan, et al.*

**Tensor lattice field theory:** *Meurice, Sakai, Unmuth-Yockey, et al.*

**Dual/rotor formulations:** *Kaplan, Stryker, Haase, Dellantonio, et al., Bauer,* **DMG,** *Kane*

**Casimir variables / "local-multiplet basis":** *Klco, Savage, Stryker, Ciavarella*

***Purely fermionic formulations (1+1D & OBC):*** *Muschik, Atas, Zhang, IQuS@UW group, Powell, et al.*

**Prepotential/Schwinger boson formulations:** *Mathur, Anishetty, Raychowdhury, et al.*

**Loop-string-hadron formulation:** *Raychowdhury, Stryker, Davoudi, Shaw, Dasgupta, Kadam*

**Light-front formulation:** *Kreshchuk, Kirby, Love, Yao, et al.*

**Qubit models:** *Chandrasekharan, Singh, et al.*

**q-deformed Kogut-Susskind:** *Zache, González-Cuadra, Zoller*

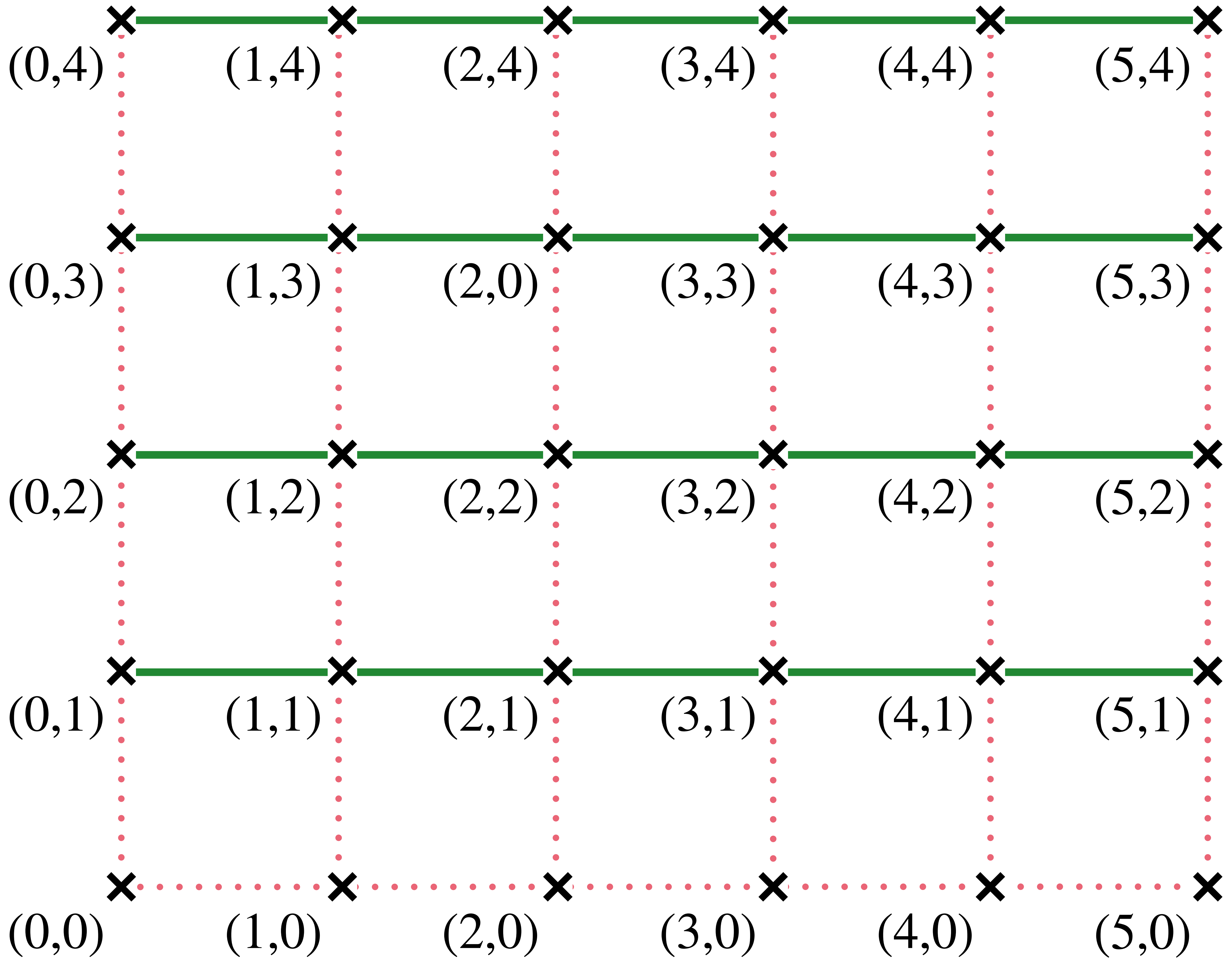
*Slide from J. Stryker, https://indico.ph.tum.de/event/7112/contributions/6917/*

# Mixed-Basis Approach to Digitizing Group Element Basis

***General Idea:*** Gauge fixing allows us to do "importance sampling" on gauge variables

***Step One:*** Gauge fix using maximal-tree gauge fixing procedure

- Gauss's law relates incoming and outgoing links for each lattice site
- Since only some links are physical/independent, gauge transformations can be used to set non-physical tree links to the identity



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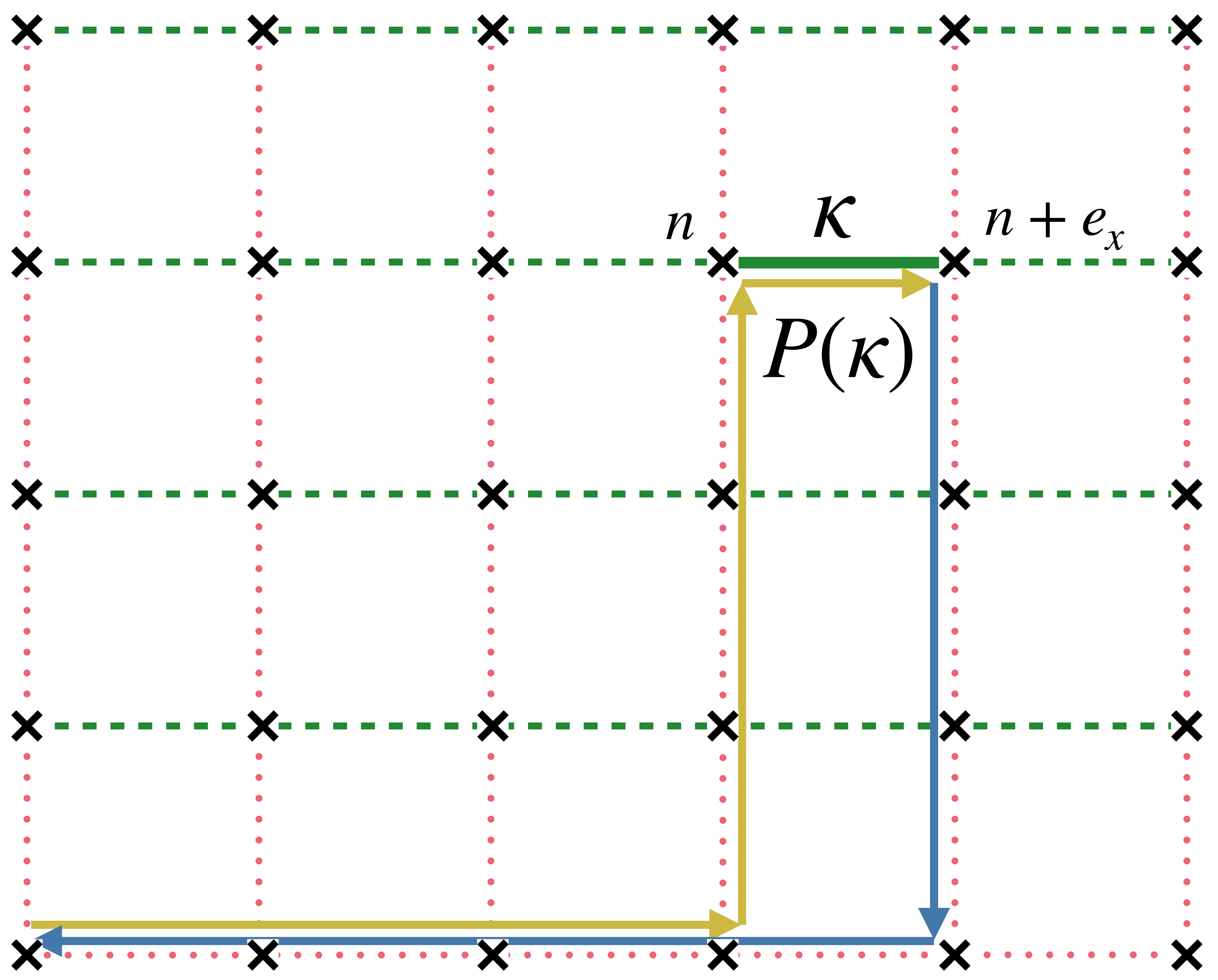
***Step Two:*** Rewrite Hamiltonian in terms of new canonically conjugate variables

- Magnetic Hamiltonian rewritten in terms of Wilson loop operators
- Electric Hamiltonian rewritten in terms of parallel-transported electric link operators



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***Step Two:*** Rewriting Hamiltonian in terms of new canonically conjugate variables

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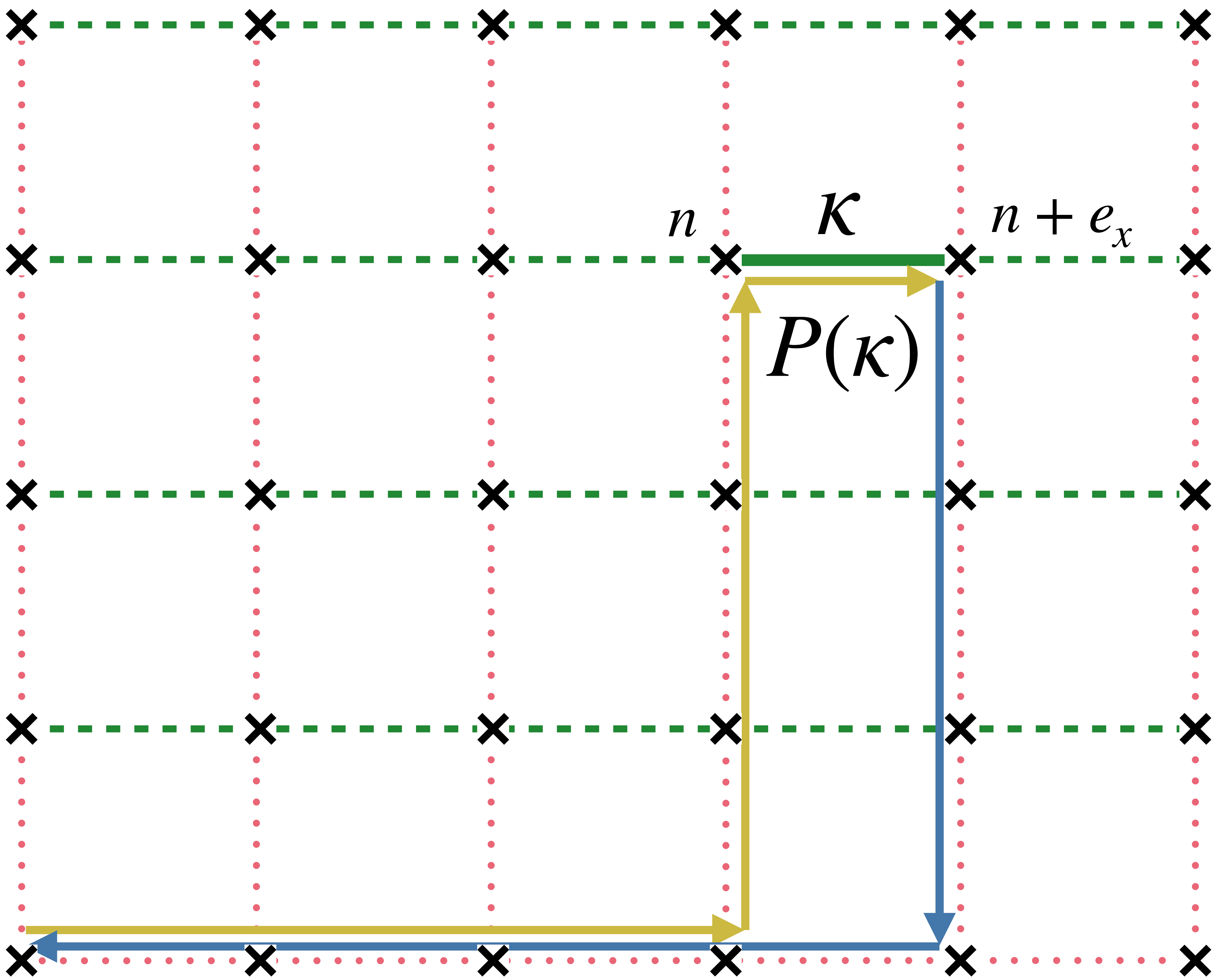
$$H_B = \frac{1}{2g^2 a}\sum_p Tr\left(I - \prod_{\kappa\in p}\hat{X}(\kappa)^{\sigma(\kappa)}\right) + \mathrm{h.c.}$$



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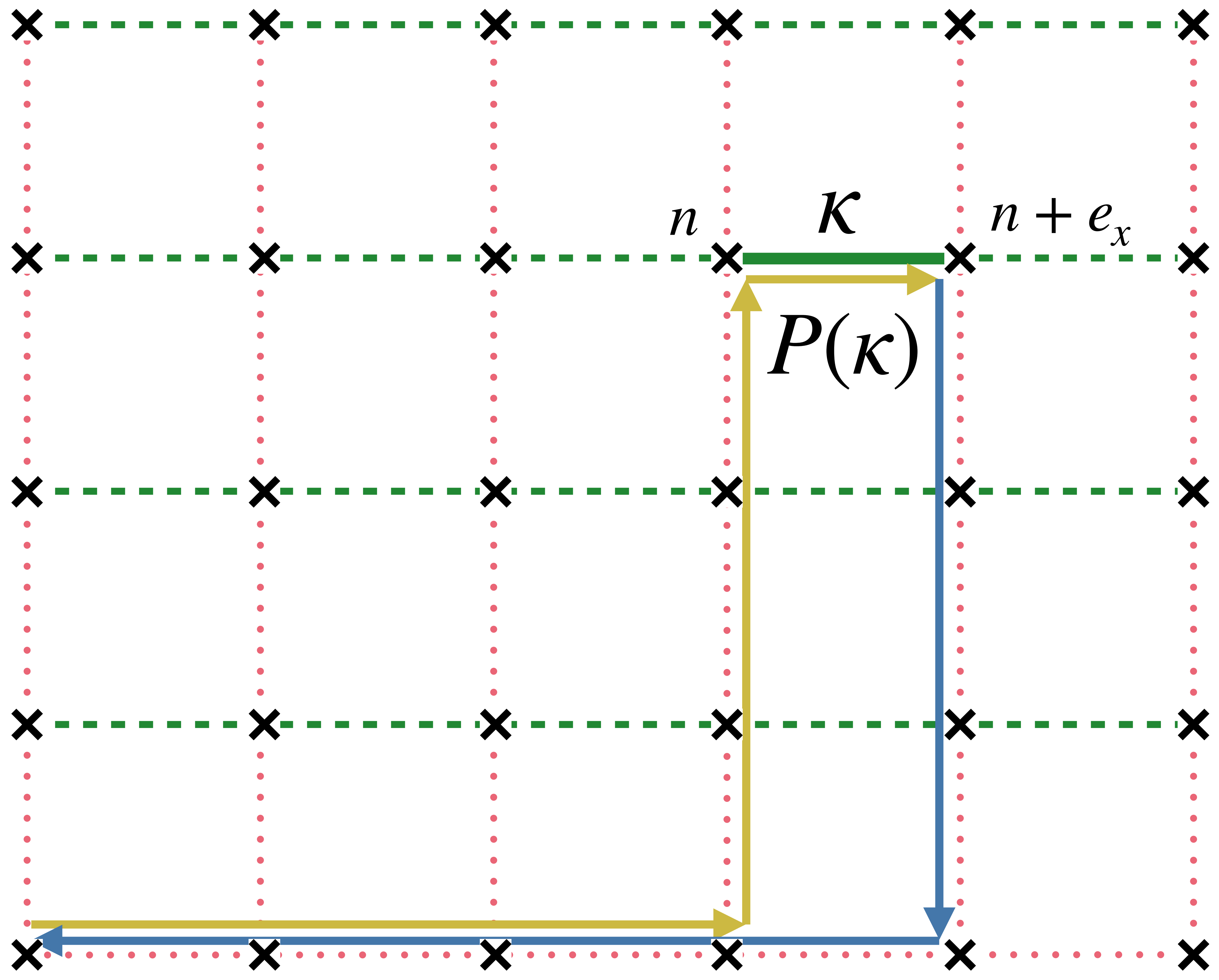
- Electric: *Parallel-transported electric link operators*

$$H_E = \frac{g^2}{2a} \sum_{\ell} \left( \sum_{\kappa \in t_+(\ell)} \hat{\mathscr{E}}^a_{L\kappa} - \sum_{\kappa \in t_-(\ell)} \hat{\mathscr{E}}^a_{R\kappa} \right)^2$$

*Canonical Commutation Relations*

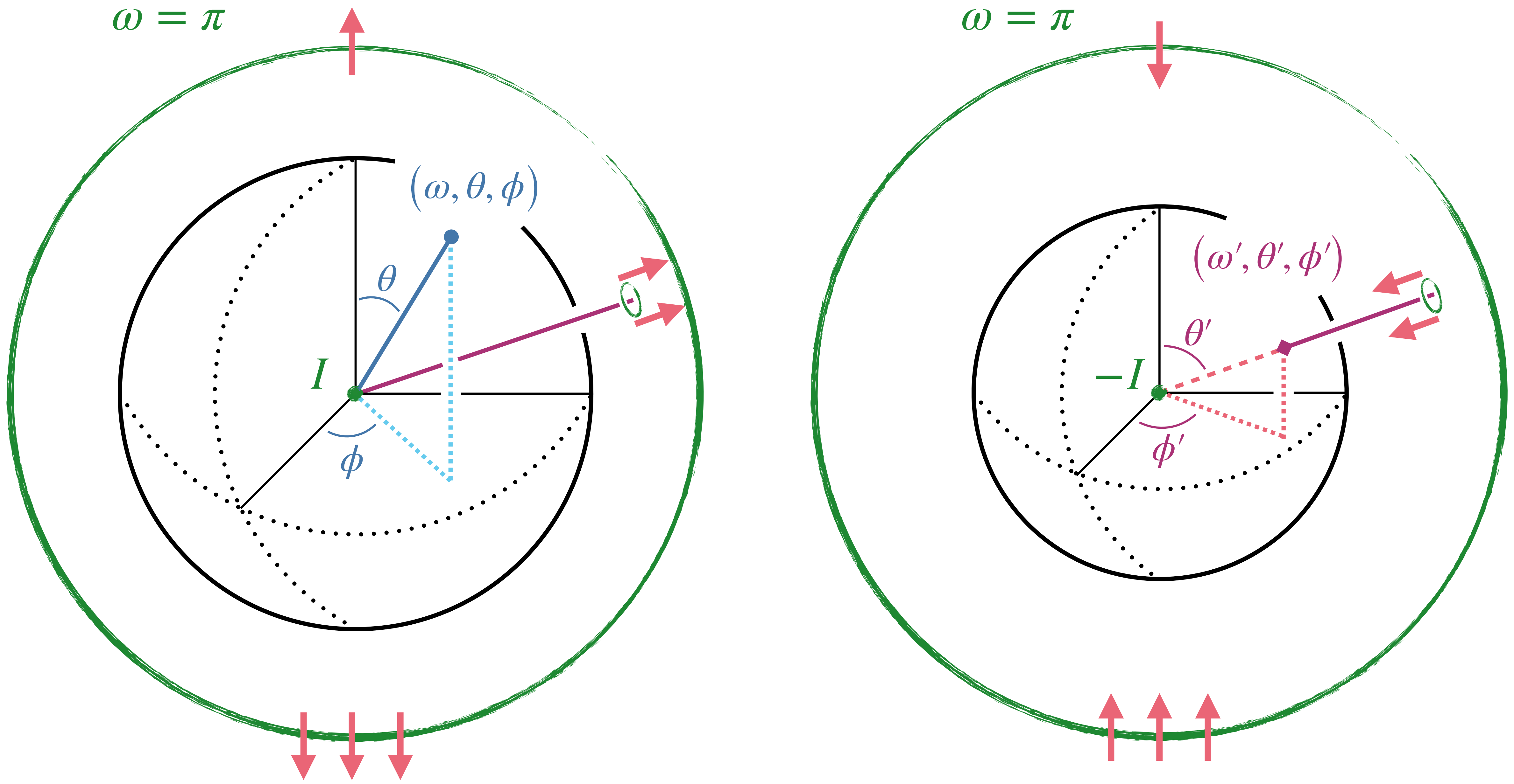
$$[\hat{\mathscr{E}}^a_L(\kappa), \hat{X}(\kappa')] = T^a \hat{X}(\kappa) \delta_{\kappa,\kappa'} \qquad [\hat{\mathscr{E}}^a_R(\kappa), \hat{X}(\kappa')] = \hat{X}(\kappa) T^a \delta_{\kappa,\kappa'}$$



# Mixed-Basis Approach to Digitizing Group Element Basis

***Step Three:*** Utilize axis-angle coordinates to parameterize gauge links and electric links of SU(2)

- Axis-angle coordinates are also hyperspherical coordinates of the double cover of $S^3$



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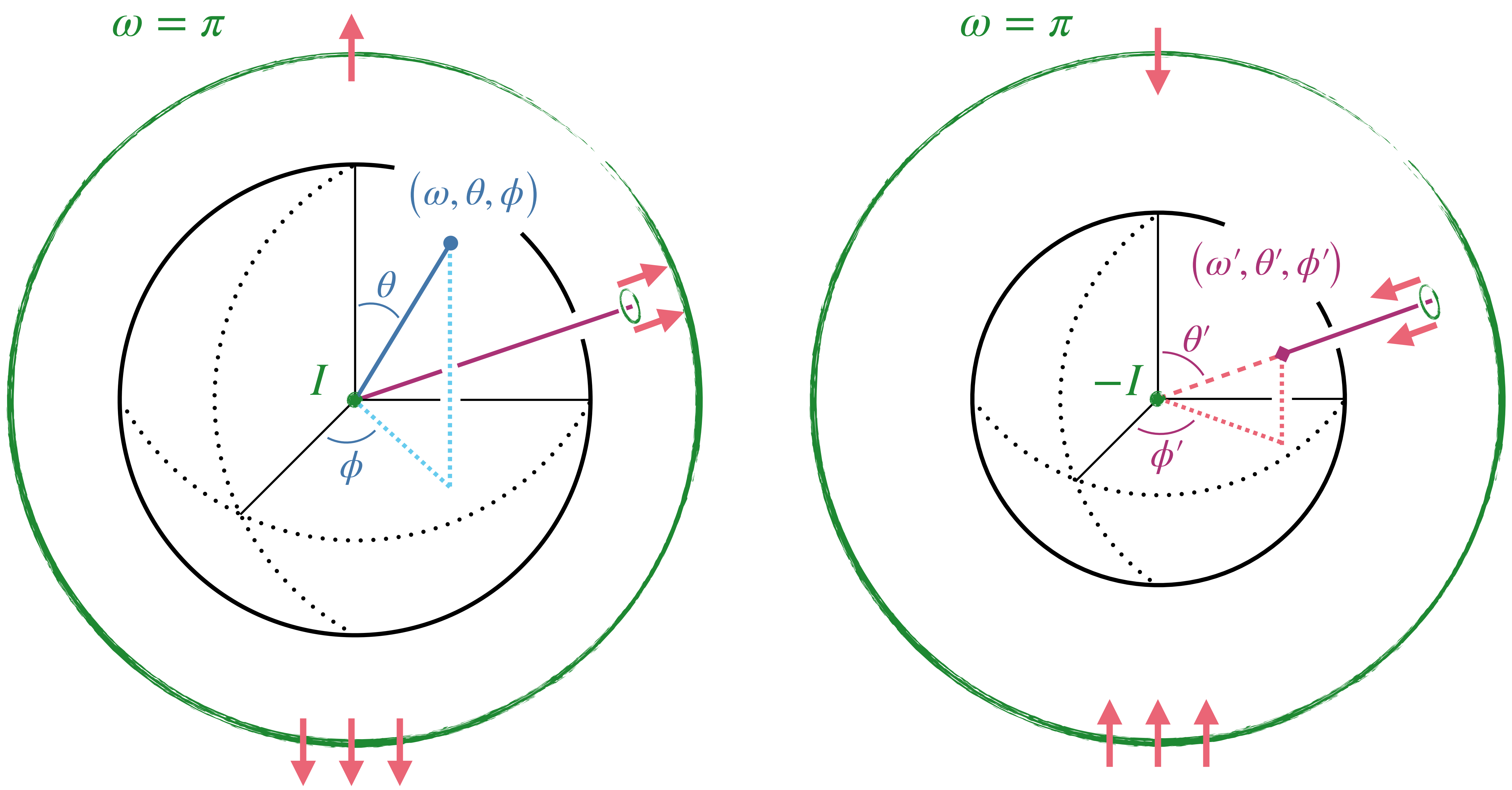
$$X = \begin{pmatrix} \cos\frac{\omega}{2} - i\sin\frac{\omega}{2}\cos\theta & -i\sin\frac{\omega}{2}\sin\theta e^{-i\phi} \\ -i\sin\frac{\omega}{2}\sin\theta e^{i\phi} & \cos\frac{\omega}{2} + i\sin\frac{\omega}{2}\cos\theta \end{pmatrix}$$

- Electric operators are differential operators of $\omega, \theta, \phi$



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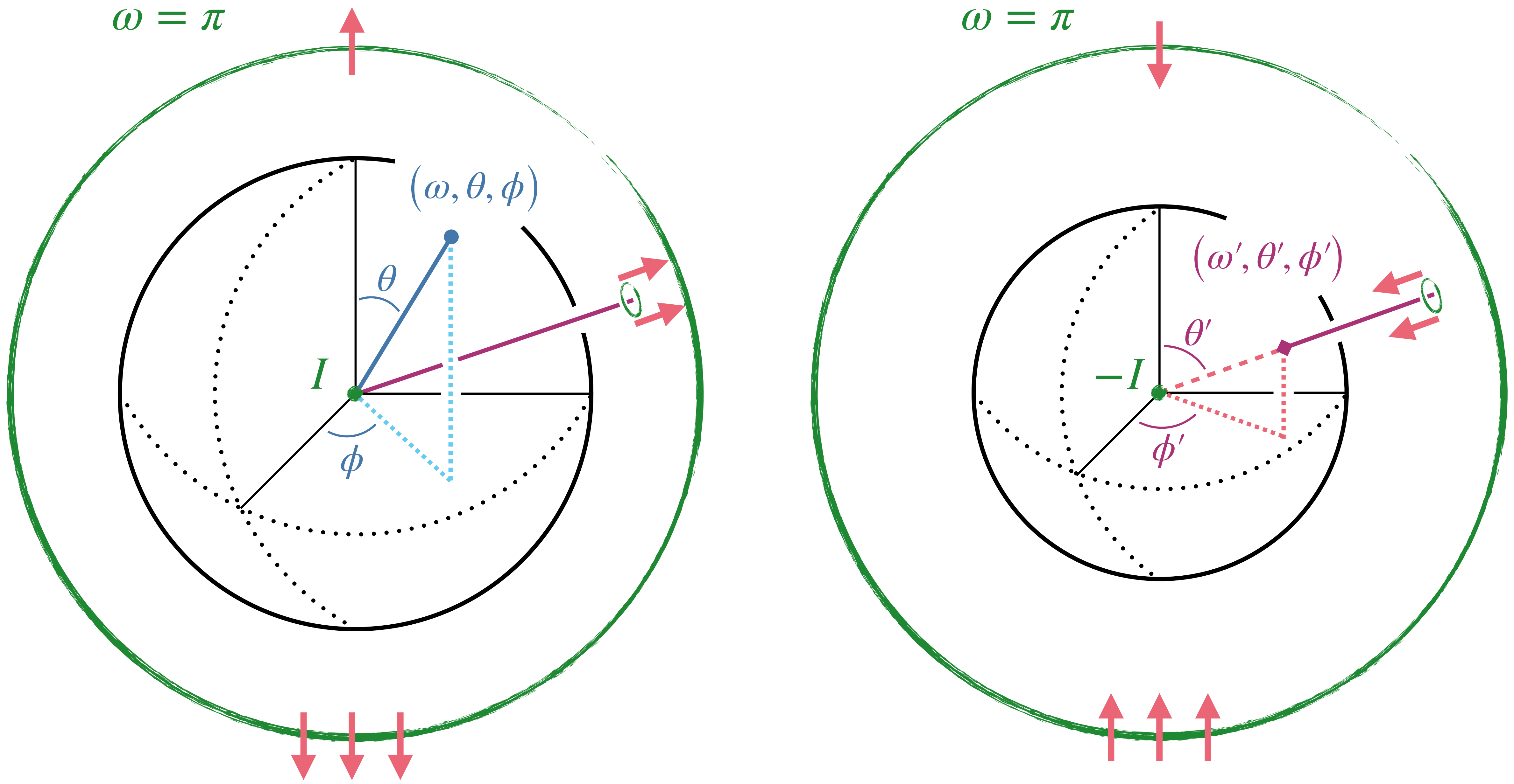


***Step Four:*** Continuous angular variables $|\theta, \phi\rangle$ can be converted to discrete angular momentum quantum numbers $|\ell, m\rangle$

***Since all* gauge redundancy has been removed, Hamiltonian can be truncated/digitized without worry***

# Mixed-Basis Approach to Digitizing Group Element Basis

***Step Five:*** Digitize in $(\omega_i, \theta_i, \phi_i) \rightarrow (\omega_i, \ell_i, m_i)$

- Variable $\omega_i$ acts like a radial coordinate and can be easily digitized using previously developed methods*
- Variables $(\theta_i, \phi_i)$ are angular coordinates and can be digitized via truncations on spherical harmonics
- Utilize discrete fourier transformation to move between electric and magnetic basis

** Bauer, C.W. and **DMG**, Phys.Rev.D 107 (2023) 3, L031503*

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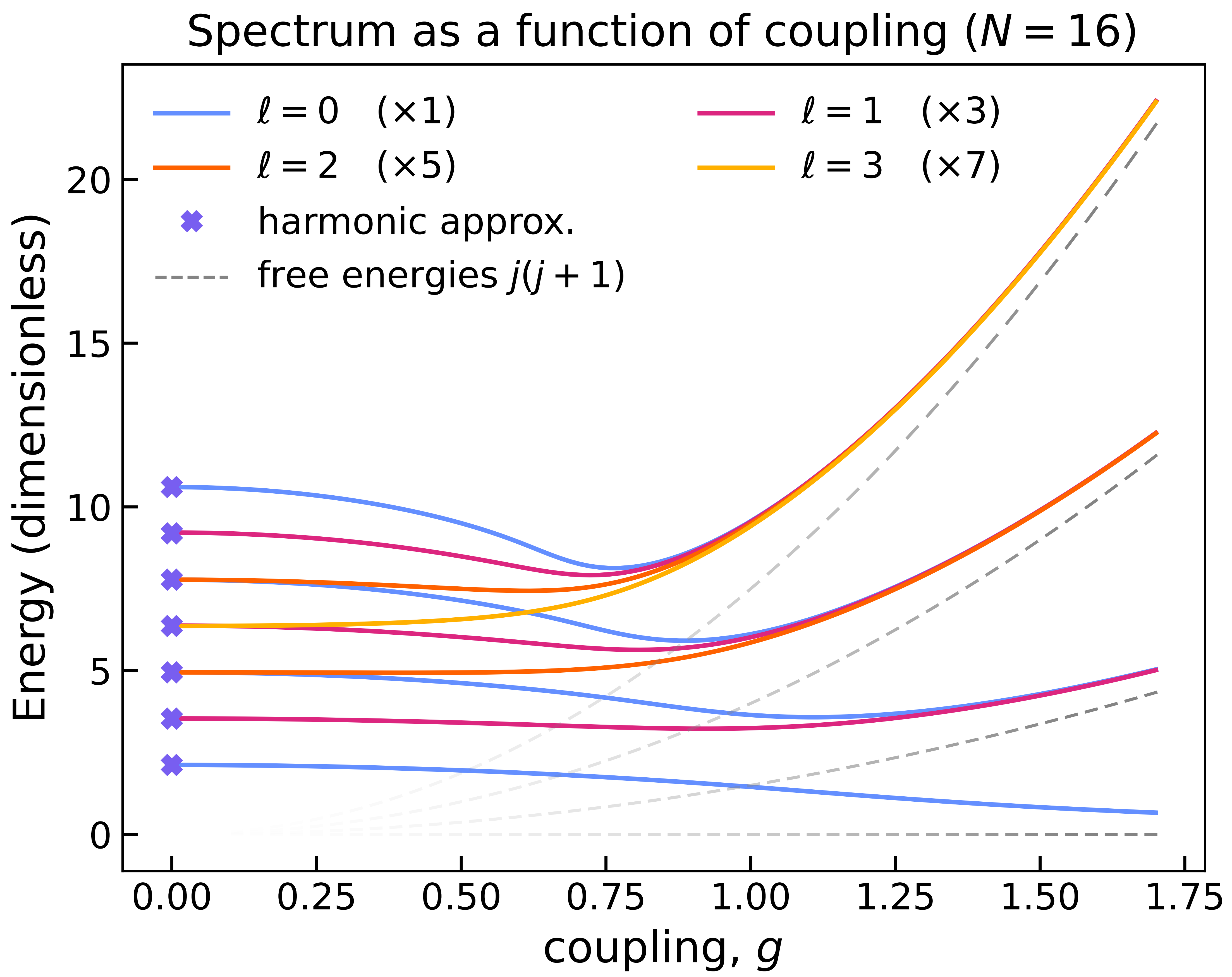
***Example:*** One plaquette, open boundary conditions

$$H_{[1]} = \frac{2g^2}{a}\frac{\hat{L}^2}{4\sin^2\frac{\omega}{2}} - \frac{\partial^2}{\partial^2\omega} - \cot\frac{\omega}{2}\frac{\partial}{\partial\omega} + \frac{2}{g^2 a}\left(1 - \cos\frac{\omega}{2}\right)$$

*total charge zero sector*

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# Algorithmic Developments

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

# Global Conservation Laws

***General Idea:*** Fully gauged-fixed Hamiltonian is thought to be highly non-local and thus expensive to implement on any machine

***Toy Model:*** Imagine laying down a pattern with playing cards whose two sides are different

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*Global Charge: Number of purple cards - Number of blue cards*

***Intuitive Idea:*** If each cards is allowed to be flipped, but the global charge must stay the same, then a component of the algorithm must “look” at the full system, not just small local patches

# 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*

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

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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**

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

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

$W_d$ : "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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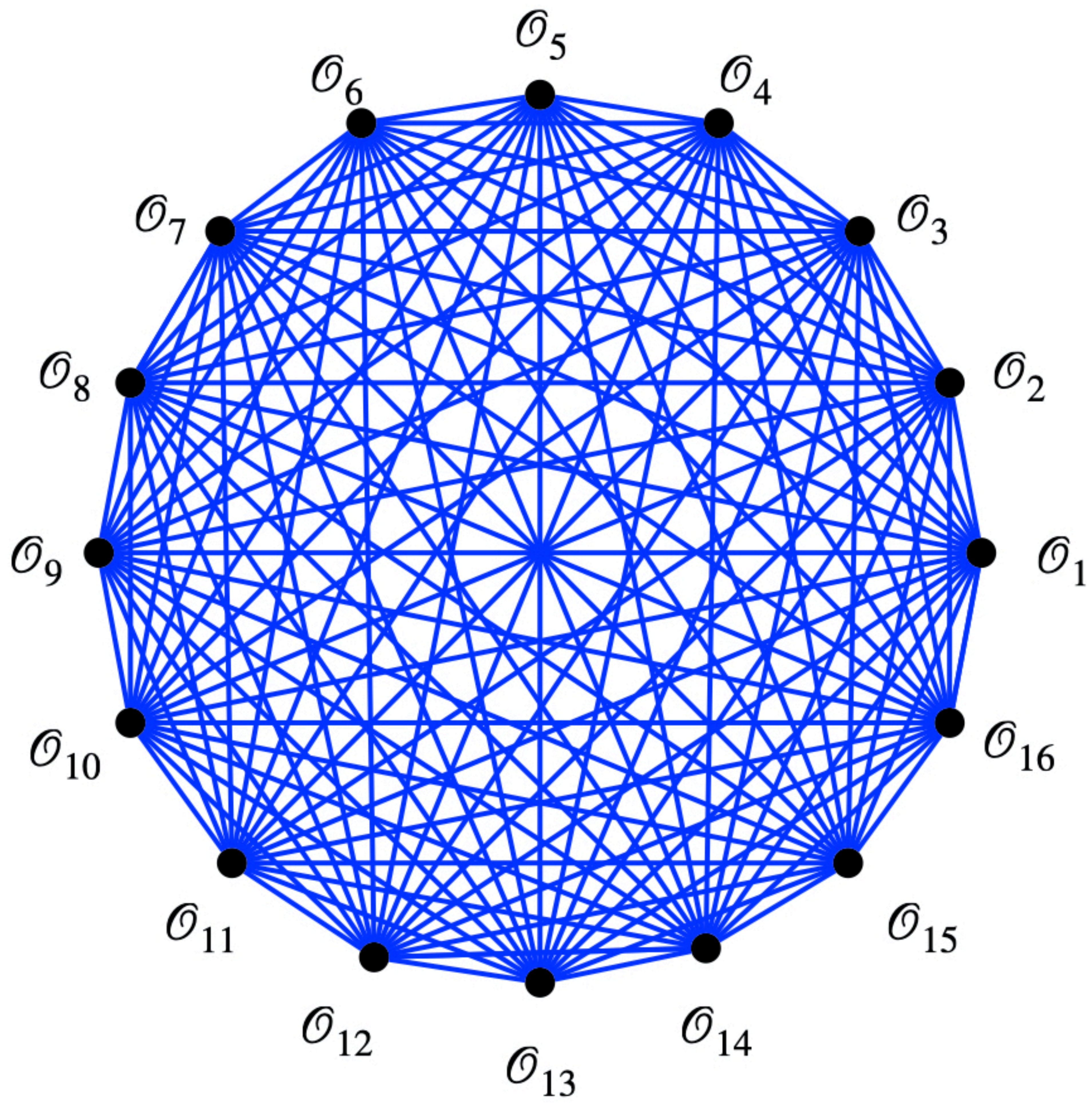
**Note about Classical Computational Cost**

- 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*

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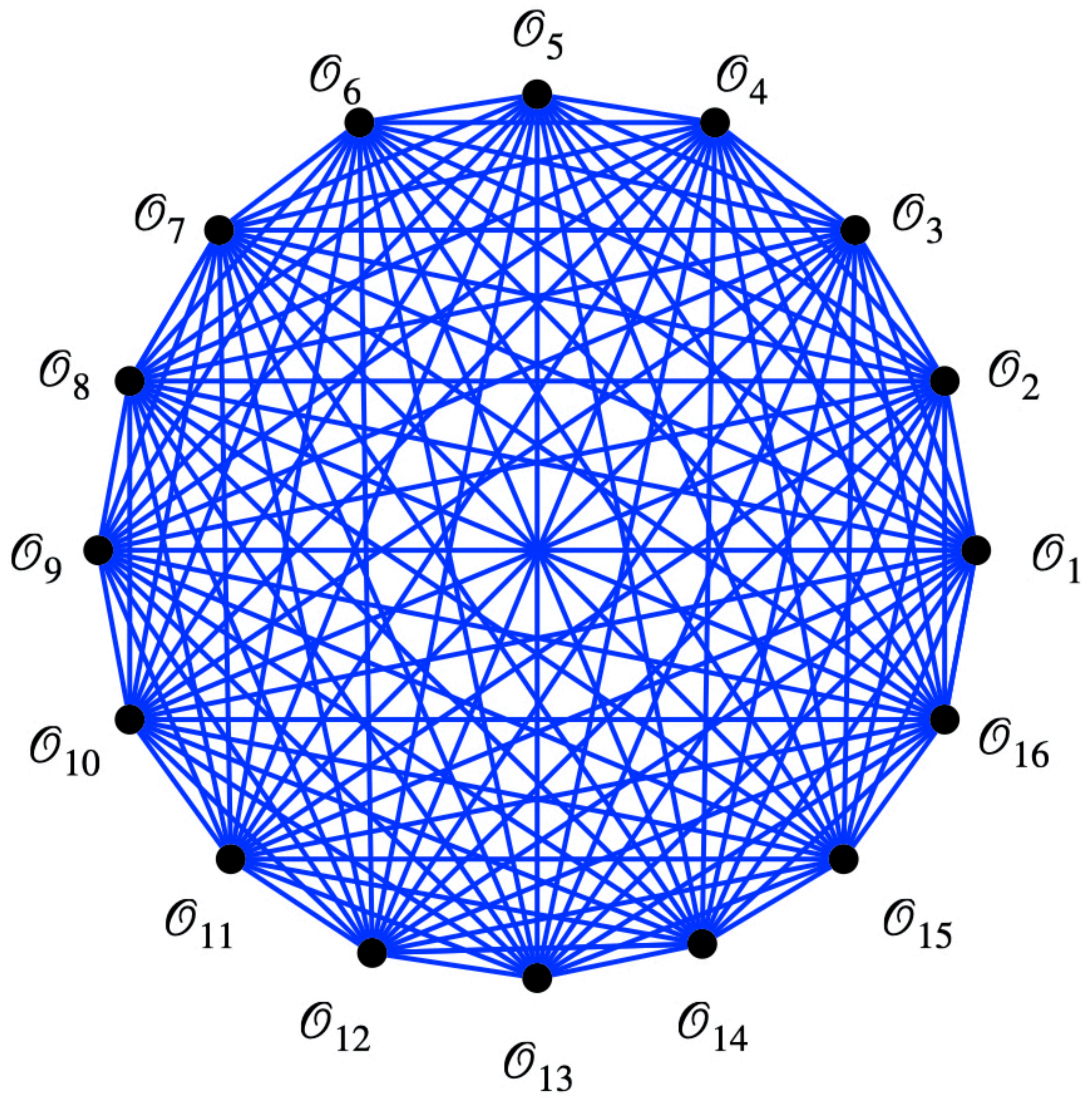
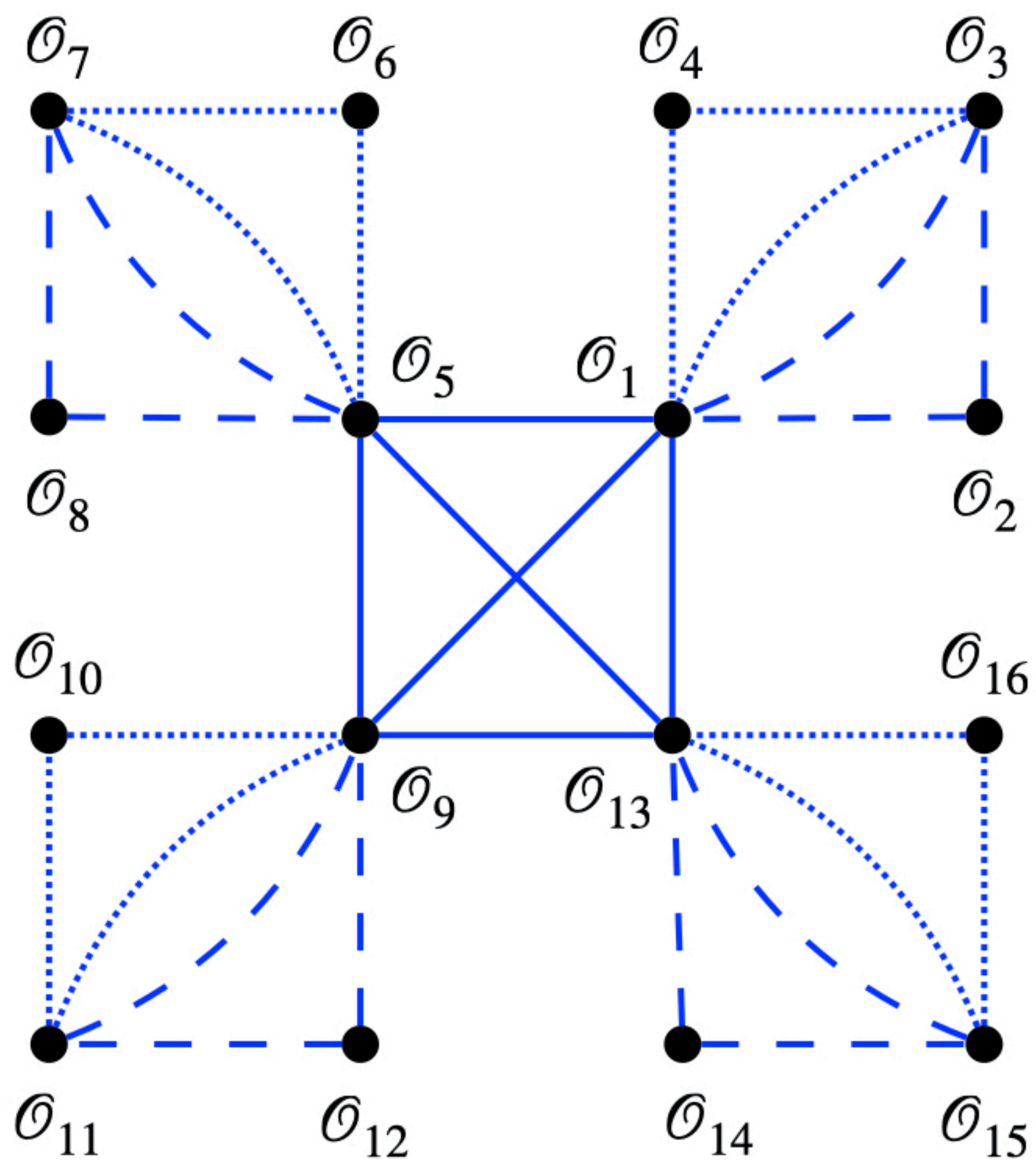



$\Longrightarrow$

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***Question 1:*** Is it possible to write down Hamiltonian with fixed global charge?

**DMG,** *Bauer, Kane; work in progress*

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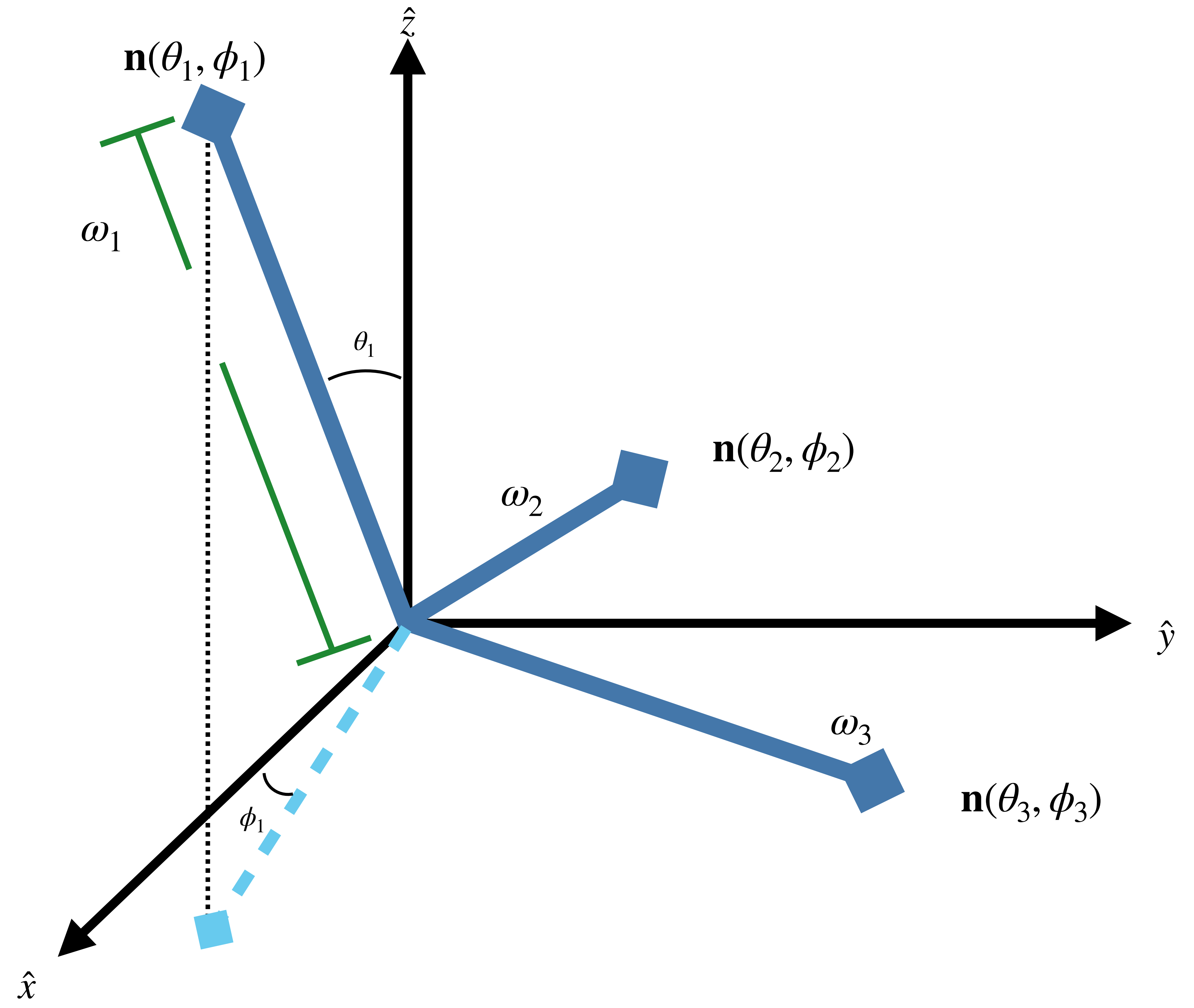


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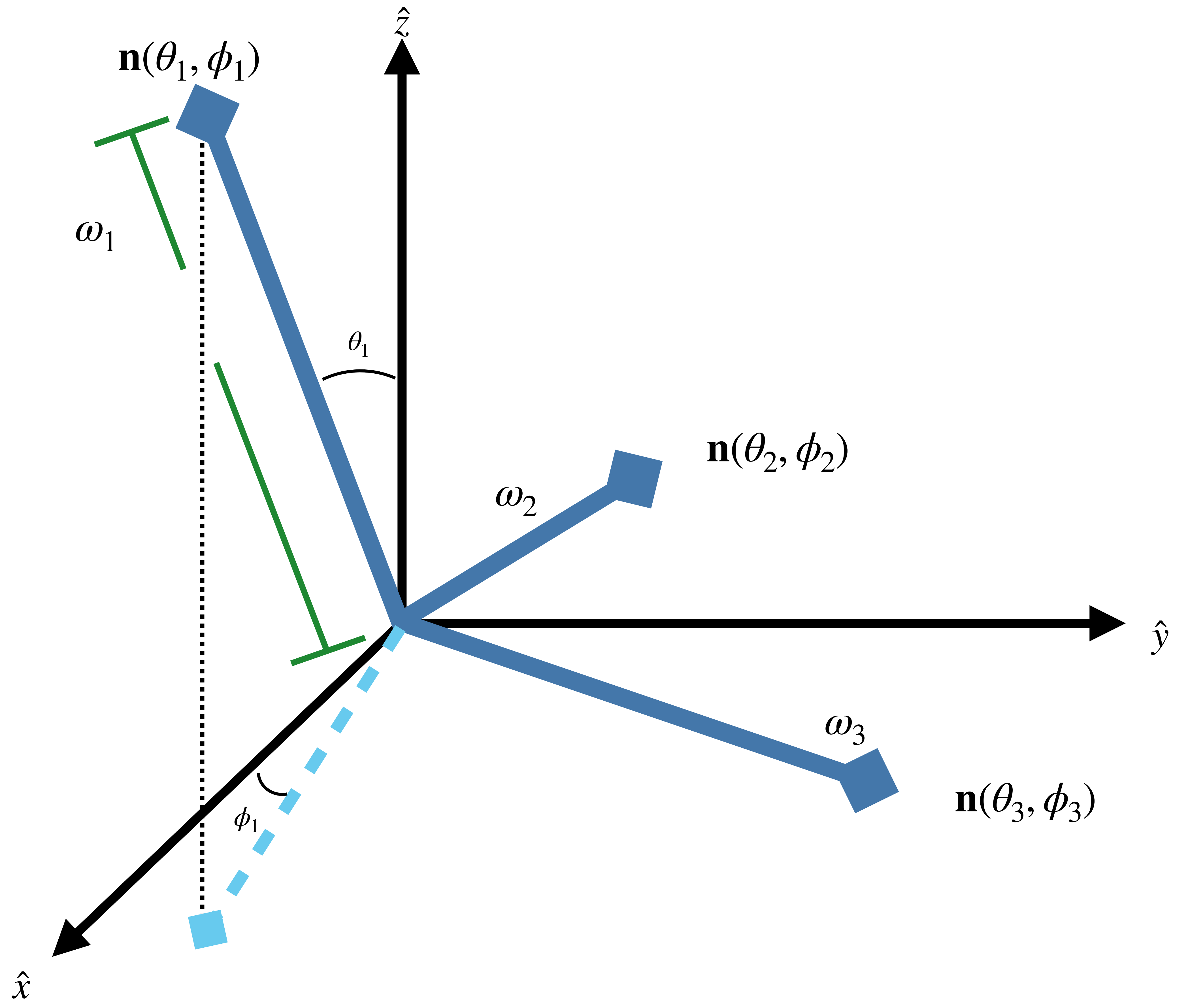
***Question 2:*** How non-local is the Hamiltonian and the resultant quantum circuit?

***Answer:*** Much more local than expected and resultant circuit does not seem horrendous

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# Conclusions

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

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

***Main Take-Away Point 1:*** We are still in the early days of utilizing quantum computers to address open problems in particle physics. There is much still to do, both in theoretical and algorithmic developements, while we wait for the fault-tolerant era

***Main Take-Away Point 2:*** It is important to carefully consider scaling of quantum computing resources for simulating gauge theories on far-future fault-tolerant machines

# Back Up Slides

# Examples of Weaved Matrices

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

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