Exponential Volume Scaling in (Constrained) Lattice Gauge Theories

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QUANTUM TECHNOLOGY INITIATIVE

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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

Real-time dynamics, finite-density nuclear matter and non-perturbative properties of chiral gauge theories are 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 carry out exploratory studies of the applicability of this emerging technology

Quantum Simulations of Lattice Gauge Theories

Guiding Principle: Quantum computing is still in its infancy and so we need to think carefully about how best to utilize 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?

Scaling of Gate Count for Simulations of Electromagnetism in 2+1 Dimensions

Main Take-Away Point 1: Naive implementation using only physical states has exponential volume scaling

Main Take-Away Point 2: Scaling can be made polynomial with carefully applied change of operator basis

Gauge Invariance and Gauss' Law

Continuum Theory: Integral over electric and magnetic fields

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

Need to impose
additional constraints

$$\nabla \cdot E = 4\pi\rho \qquad \nabla \cdot B = 0$$

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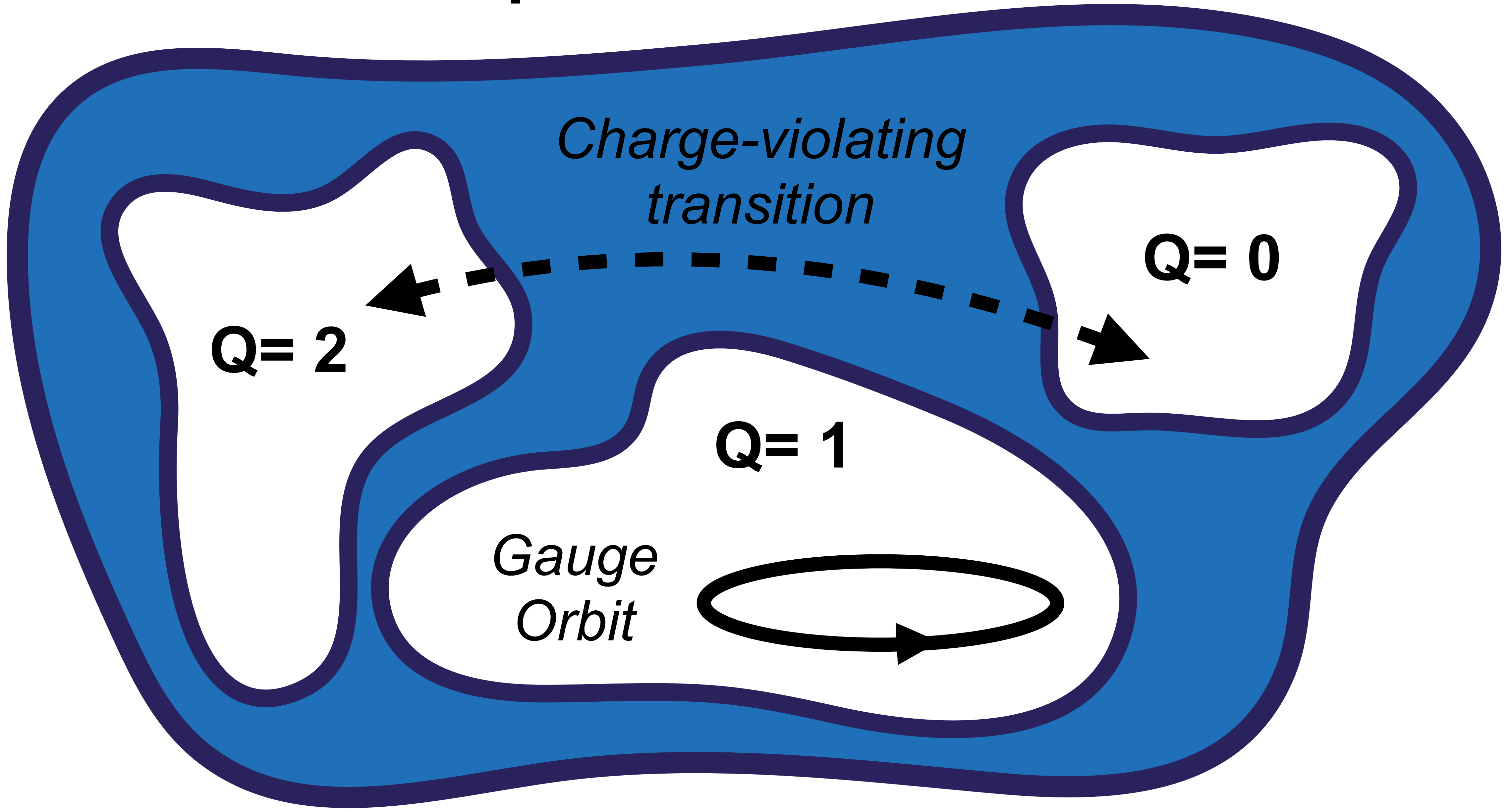
Gauge Invariance and Redundancies

- ***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

Hilbert Space



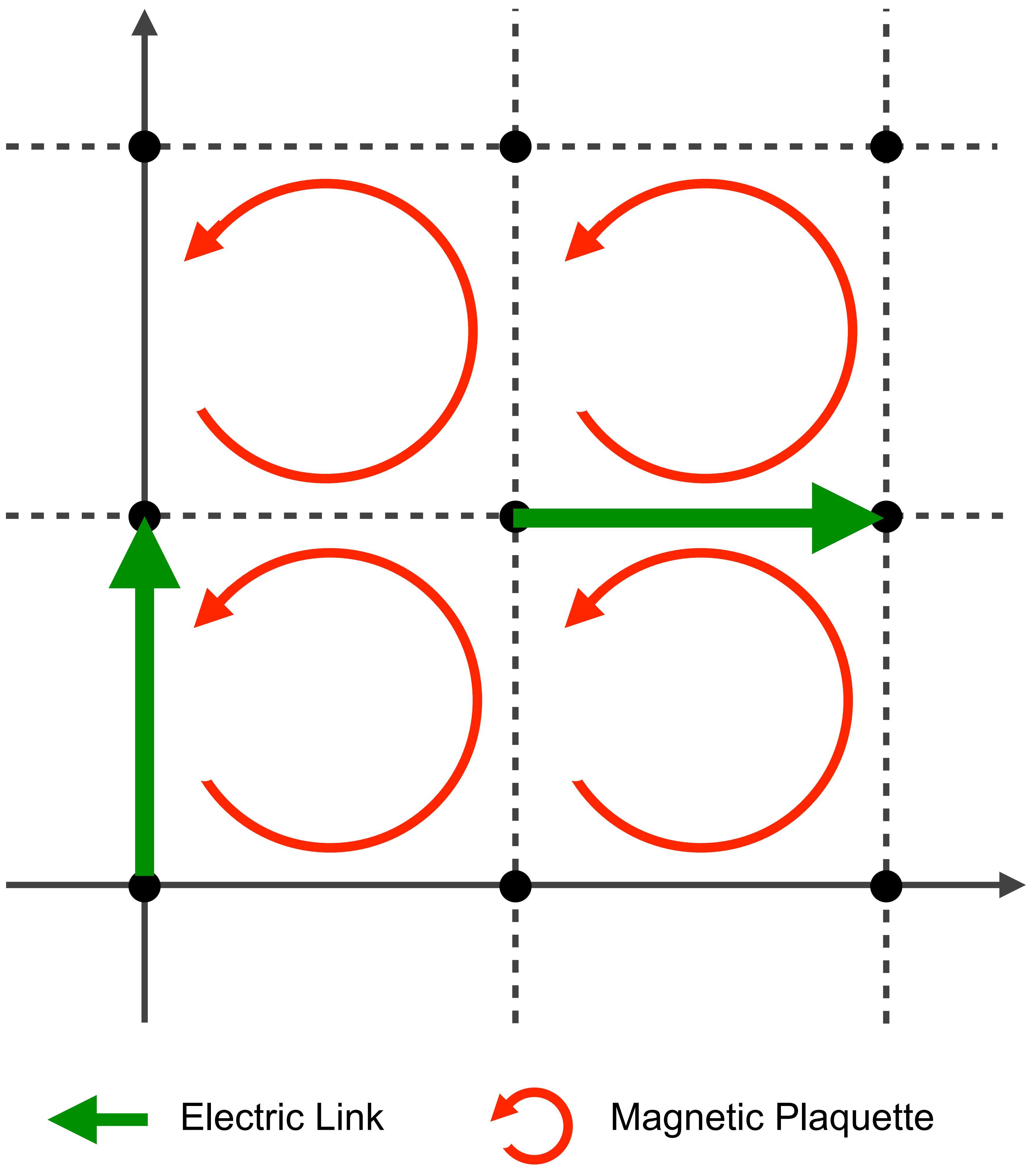
Dual Basis (Rotor) Formulation

General Idea: Work with "gauge-redundancy free" formulation

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

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

Kogut-Susskind



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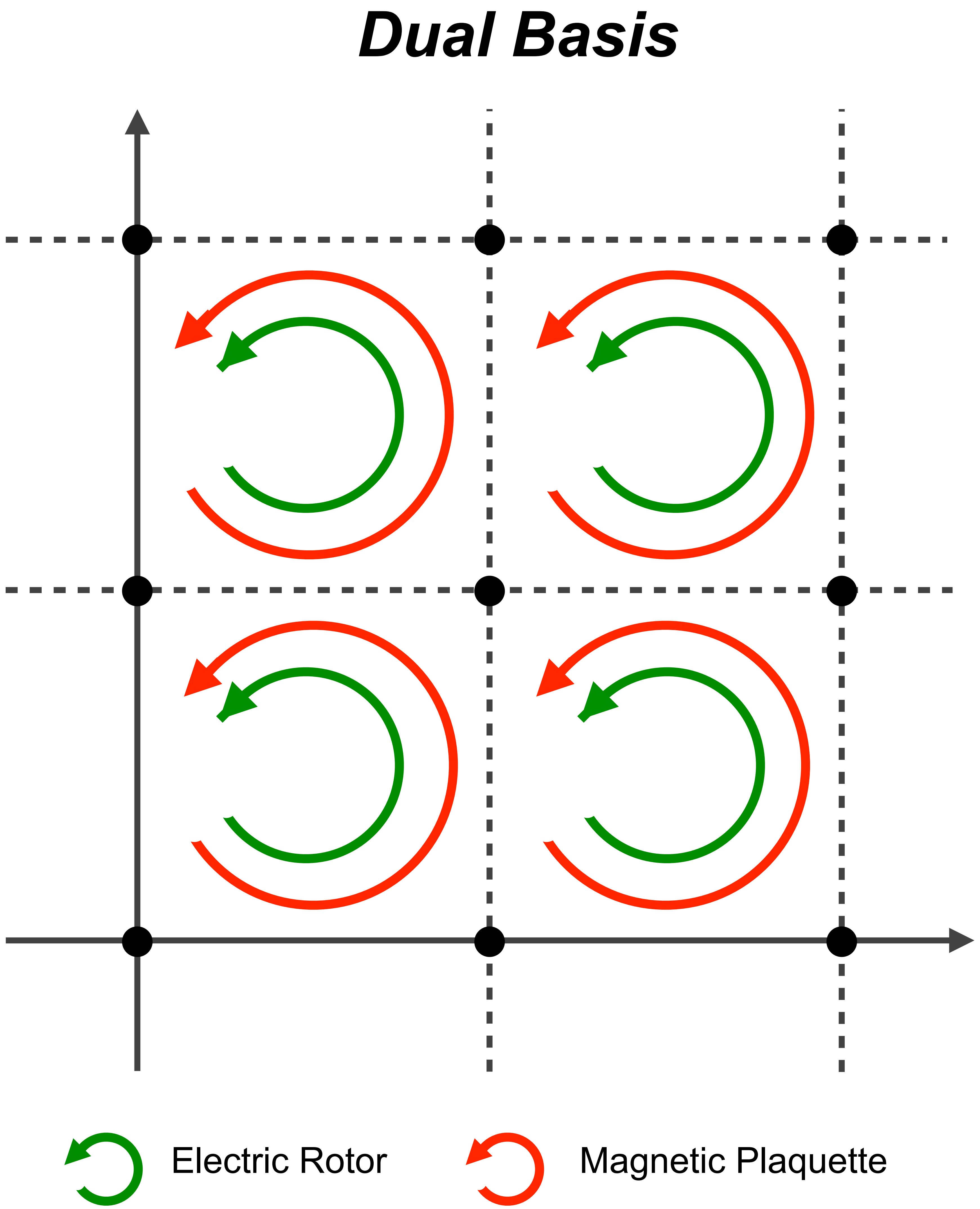

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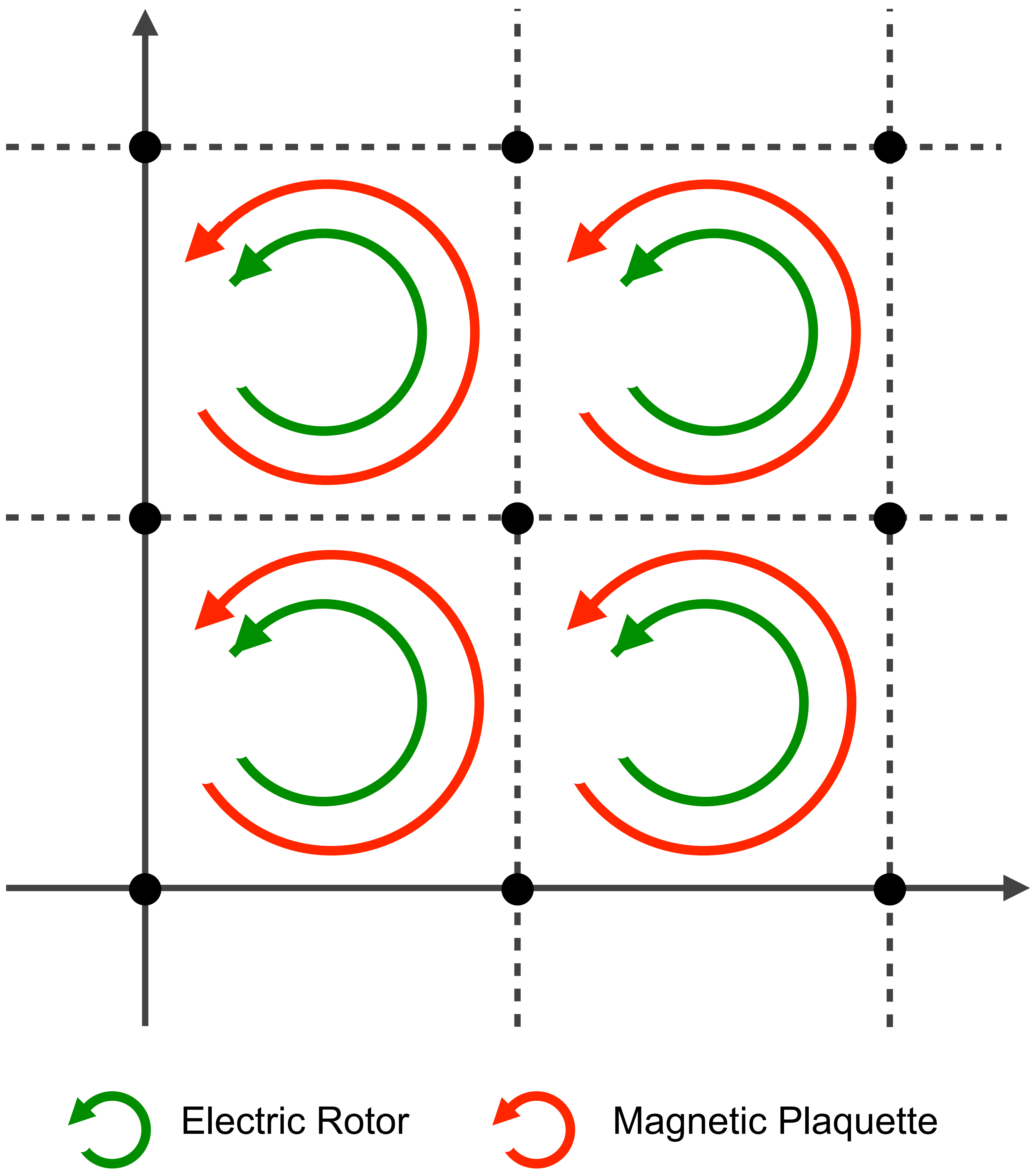
$$[B_p, R_{p'}] = i\delta_{pp'}$$

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

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

$N_p =$ **Number of Plaquettes**

Dual Basis



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Global Constraints in Rotor Formulation

General Idea: Locally imposed constraints 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

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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 magnetic Gauss' law leads to highly non-local term

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

Grabowska et al, to appear

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Hilbert space: dim 2^{n_q}

Hilbert space dim: $2^{N_p n_q}$

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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!

Grabowska et al, to appear

Reducing (Operator) Non-Locality

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 $\mathcal{W}$ and W_d

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

- 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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Implementing new “Weaved” Hamiltonian requires $\mathcal{O}(N_p^{\log_2 N_L})$ gates!

(Recall N_L is volume independent)

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Note about Classical Computational Cost

- Carrying out change of basis for 192 x 192 lattice takes few second on laptop
- Scaling is slightly worse than linear in lattice volume ($\sim N_p^{1.25}$)

Grabowska et al, to appear

Conclusions

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Back Up Slides

Examples of Weaved Matrices

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

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

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

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

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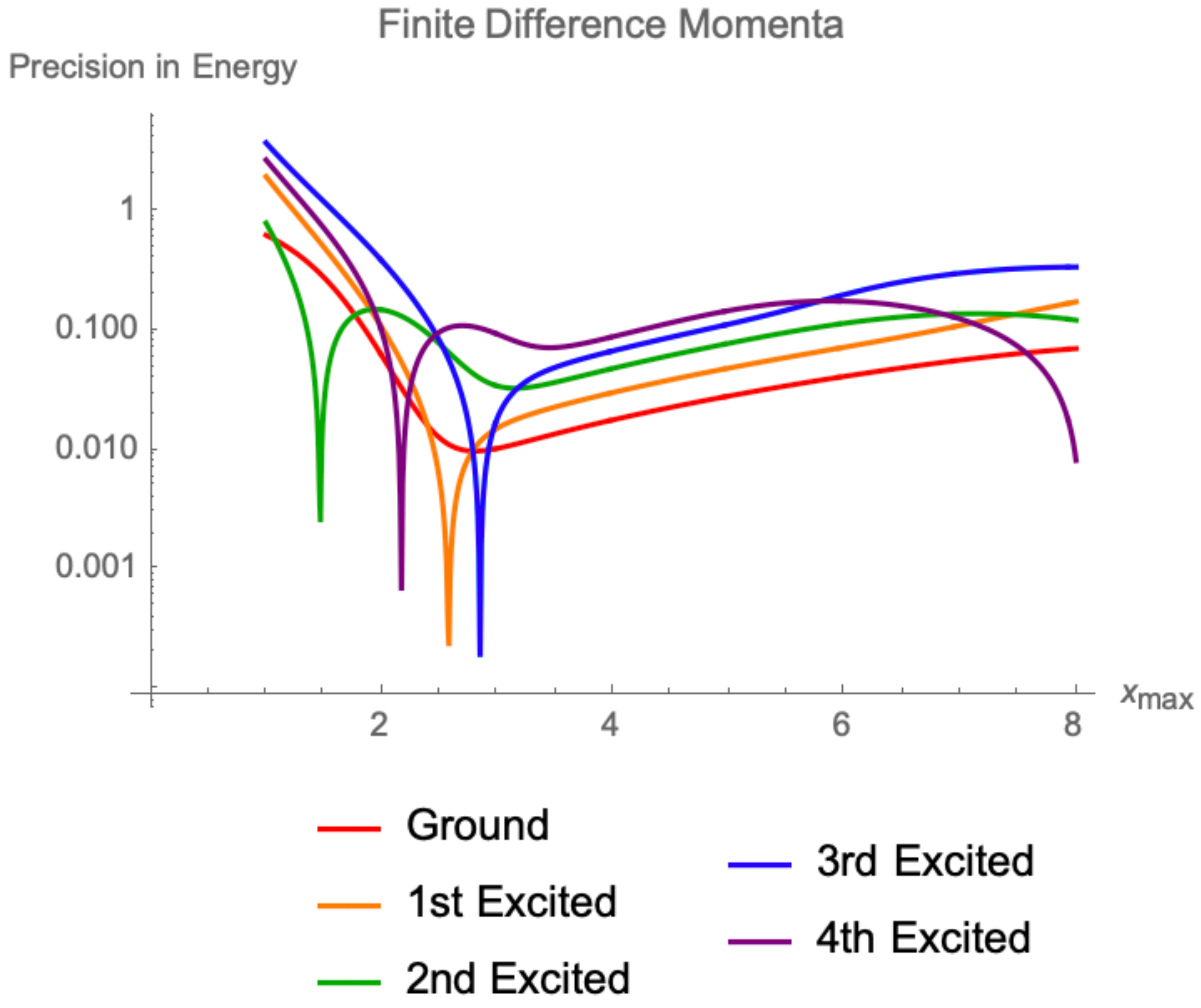

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Option One: Use finite difference version

Option Two: Use exact form and Fourier transform to change basis

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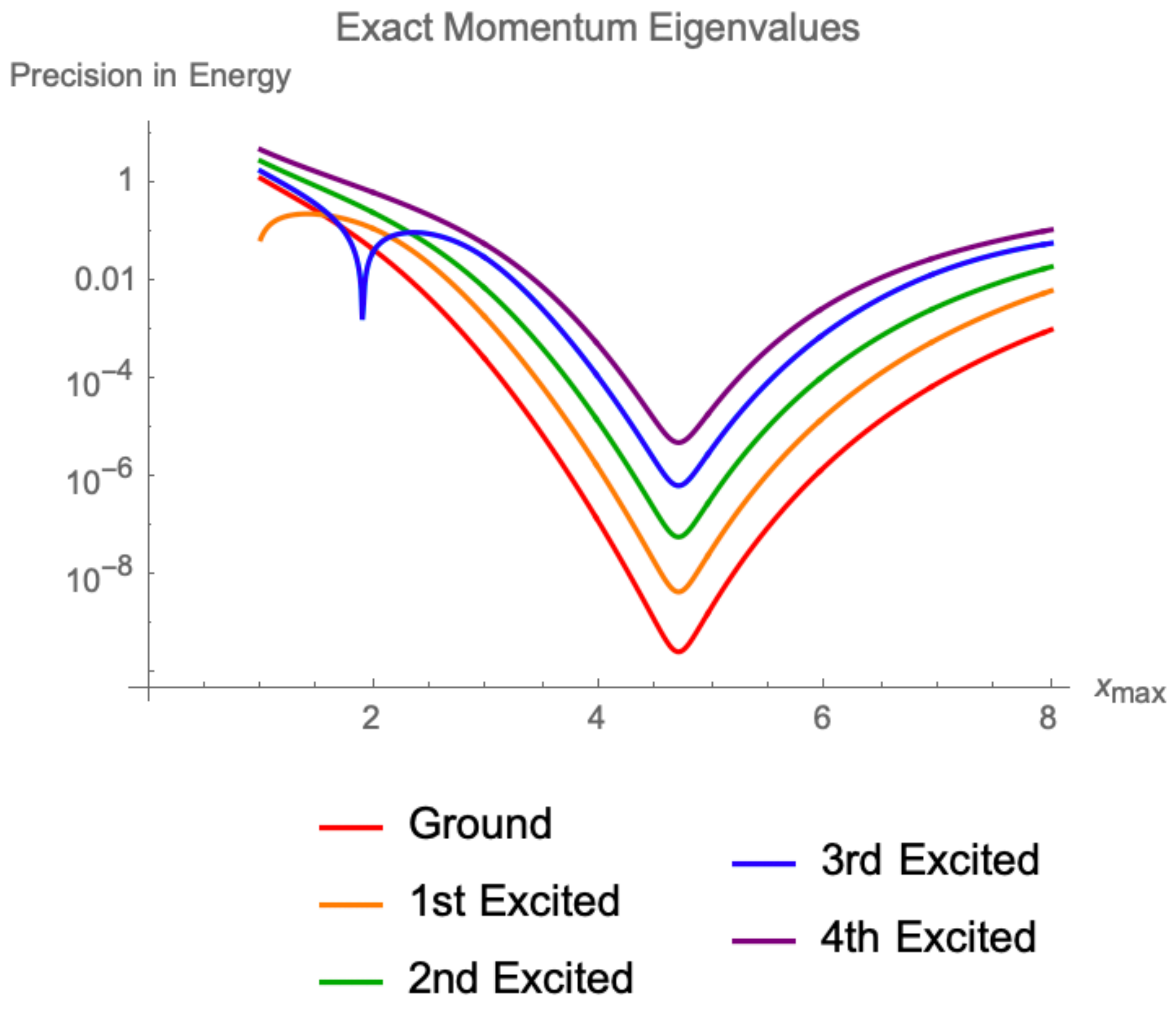

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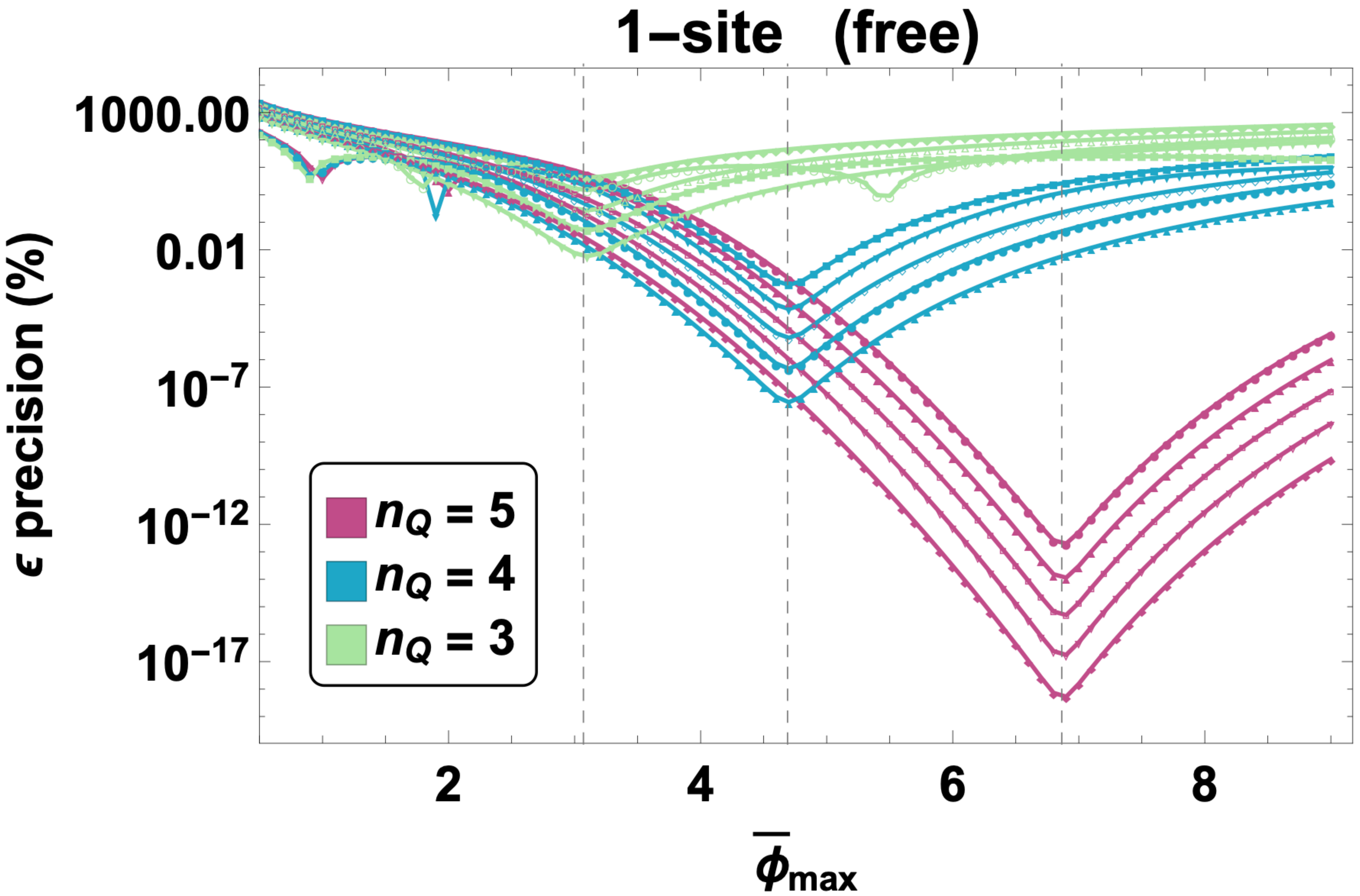
Intuitive Understanding: *Eigenstate has the same width in both position and momentum space and so* $\delta x = \delta p$



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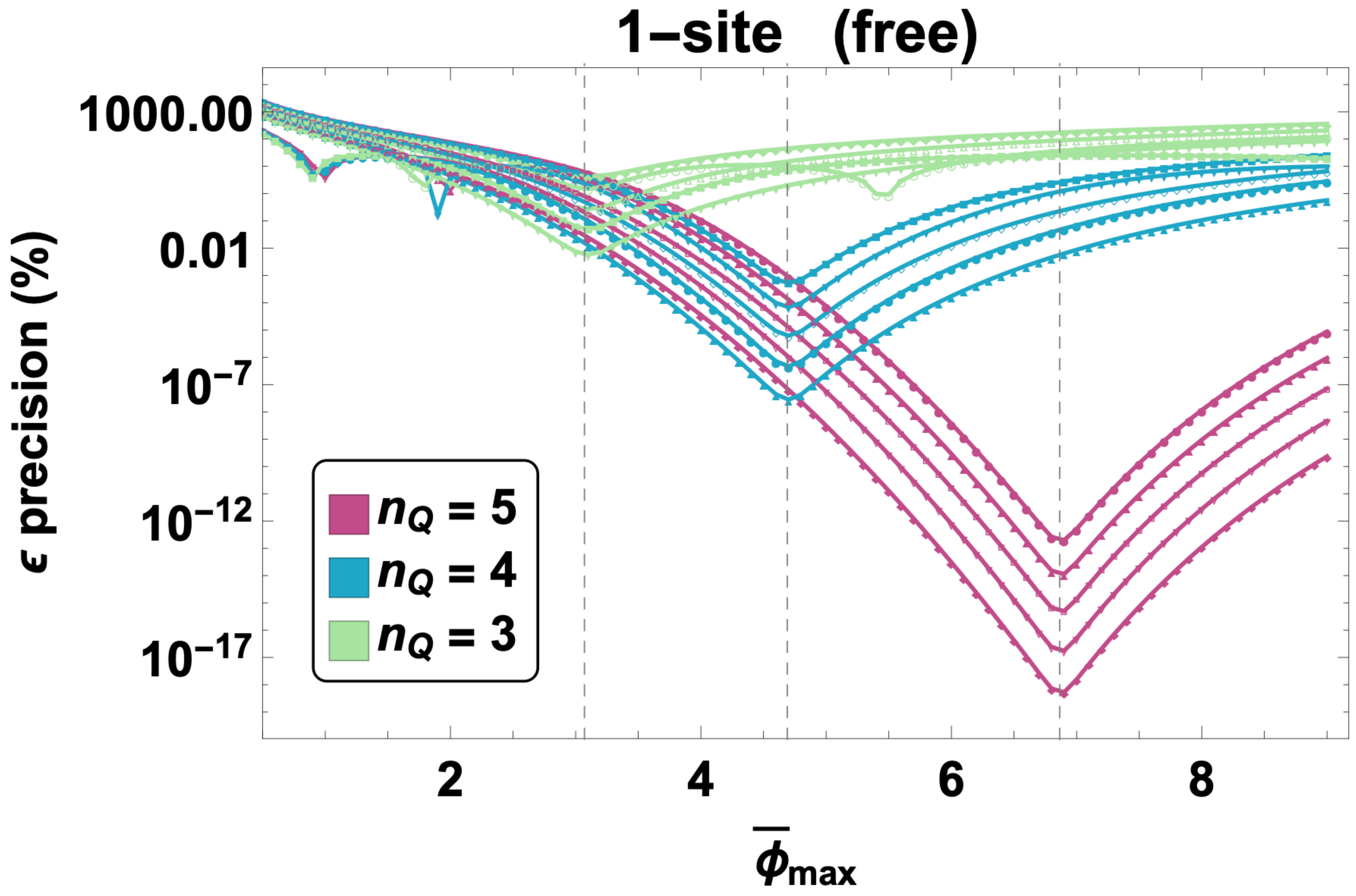
Value for optimal x_{max} can also be related to Nyquist–Shannon sampling theorem

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

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

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- 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

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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

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

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

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

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

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

Formulation works well for all values of the gauge coupling

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

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

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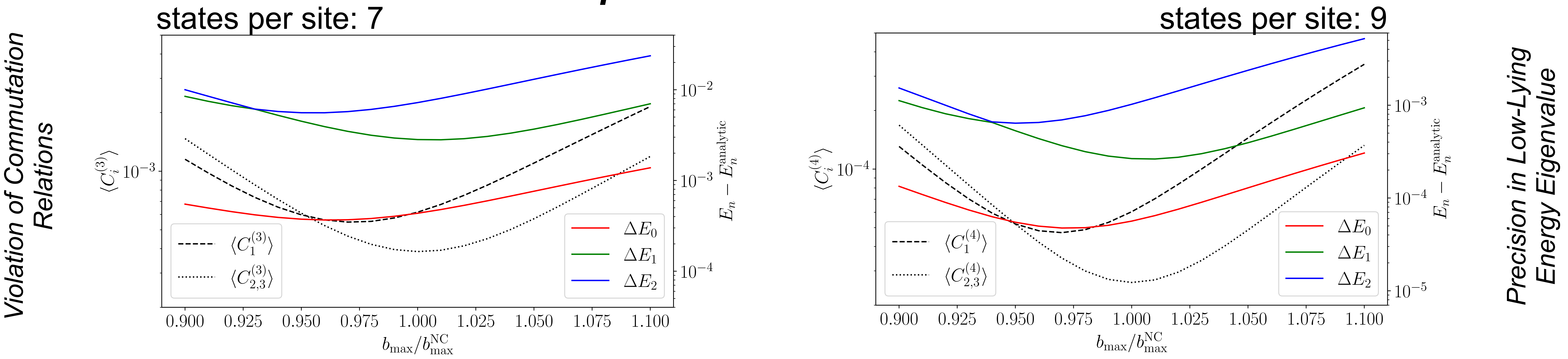
Comparison to exact solution



Scanning through truncation scale, compared to optimal truncation scale

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

Algorithmic Development: Polynomial Scaling

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

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

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

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

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

Grabowska et al, to appear shortly

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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 | 10^5 classical FLOPs to create circuit

Grabowska et al, to appear shortly

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

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

Must be real and positive

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

<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

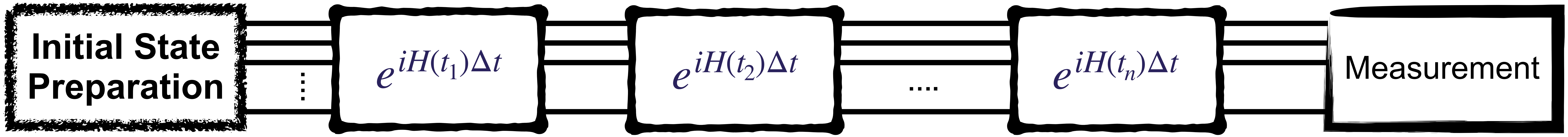
Can quantum computing help?

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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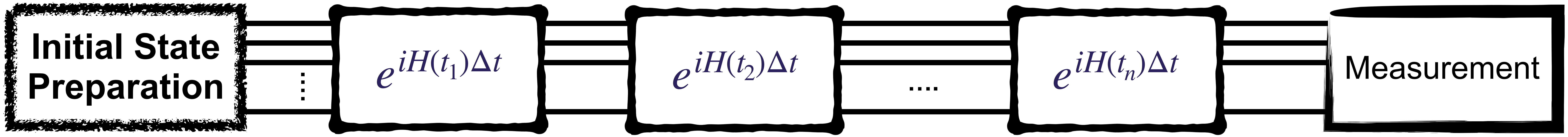

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<u>**Overarching Research Goal**</u>

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

Theoretical Development: Time Evolution Operator

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
$\|n\rangle$		$\|x\rangle$

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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