Efficient Hamiltonian bases for quantum simulation of non-Abelian gauge theories

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Motivation

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

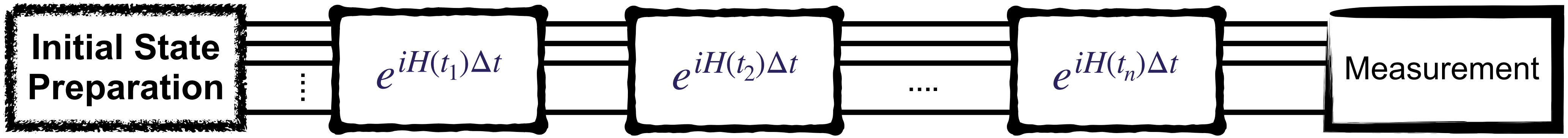
Rich phenomena of non-perturbative quantum field theories is a profitable place to look for new answers to the big questions

Digital Quantum Simulation

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

Overarching Research Goal

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

Simulating Lattice Gauge Theories

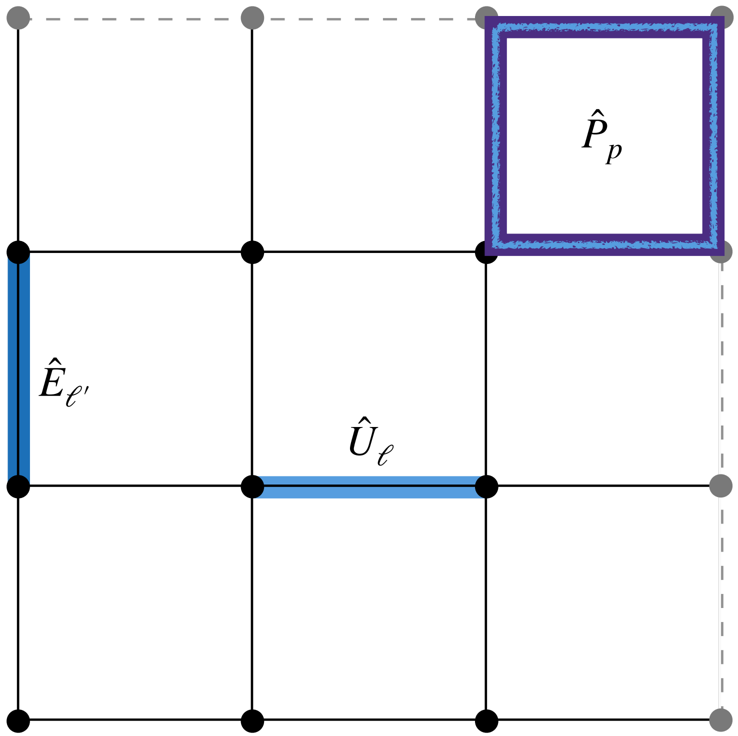
Three fundamental hurdles must be addressed to carry out quantum simulations of lattice gauge theories Hamiltonian

Phys Rev D 11, 395 (1975)

Hamiltonian Lattice Gauge Theory, Abelian

Quantum simulations utilize Hamiltonian formulations

- Continuous time, but discrete space
- Use Weyl Gauge ($A_0 = 0$)
- Can be derived from Wilson's action



These define the theory and therefore the circuit

Phys Rev D 11, 395 (1975)

Hamiltonian Lattice Gauge Theory, Abelian

Kogut-Susskind Hamiltonian

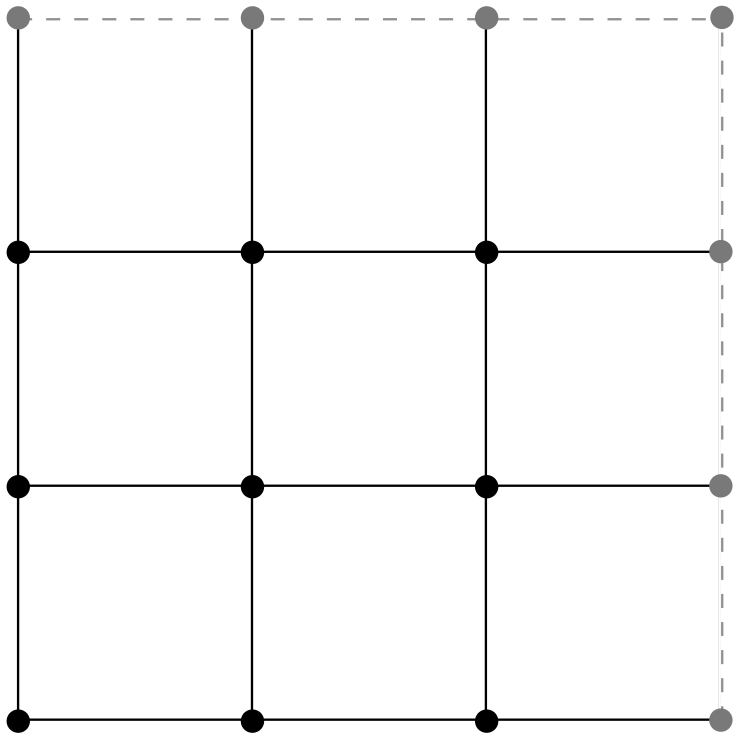
$$H = \frac{1}{2a}\left[g^2 \sum_{\ell \in links} E_\ell E_\ell + \frac{1}{g^2} \sum_{p \in plaquettes} \mathrm{Tr}\left(2I - P_p - P_p^\dagger\right)\right]$$

- Commutation relations inform how operators map onto qubits

$$\left[\hat{E}_\ell, \hat{U}_{\ell'}\right] = \hat{U}_\ell \delta_{\ell\ell'}$$

Indicates that $\hat{U}$ is raising operator

- Precise mapping will depend on choice of ***BASIS***



Action of plaquette on a given state

Phys Rev D 11, 395 (1975)

Hamiltonian Lattice Gauge Theory, SU(N) Version

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

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

.

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

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

Coupling Strength and Basis Choices

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

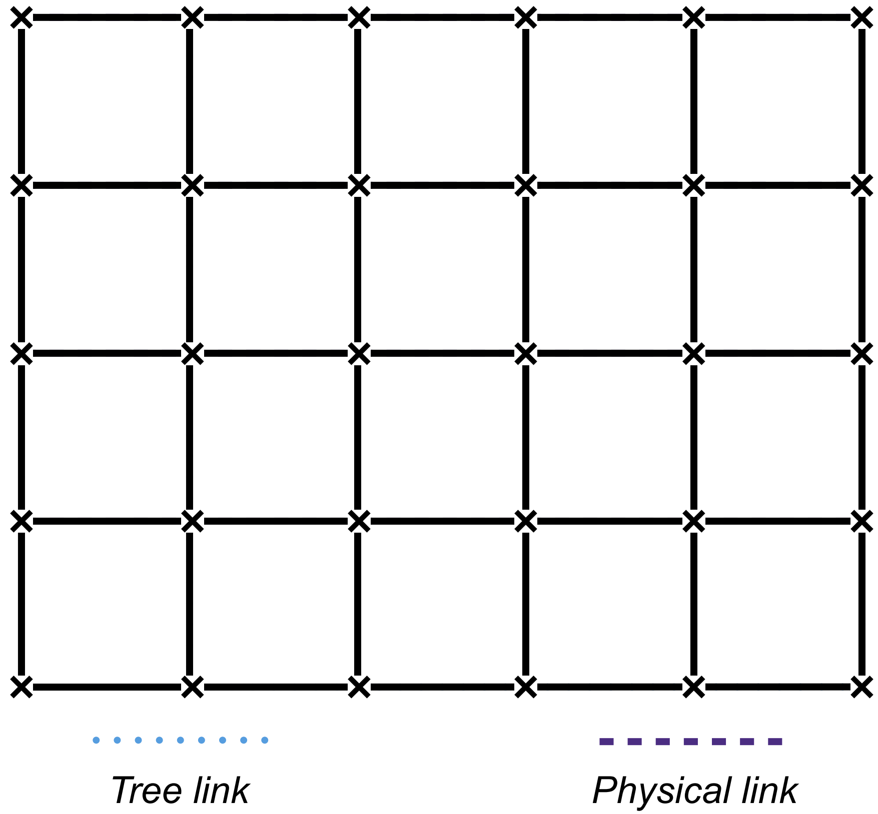
$$H = \frac{1}{2a}\left[g^2 \sum_{\ell \in links} E^a_\ell E^a_\ell + \frac{1}{g^2} \sum_{p \in plaquettes} \mathrm{Tr}\left(2I - P_p - P_p^\dagger\right)\right]$$

Step One: Gauge-Fixing Procedure

Motivation: Gauge fixing allows for “importance sampling” when working in magnetic basis without worrying about breaking gauge-invariance

General Idea: Residual (spatial) gauge transformations allow for certain number of links to be set to identity

- Maximal-tree procedure provides a systematic method for determining which links can be eliminated



Step One: Gauge-Fixing Procedure

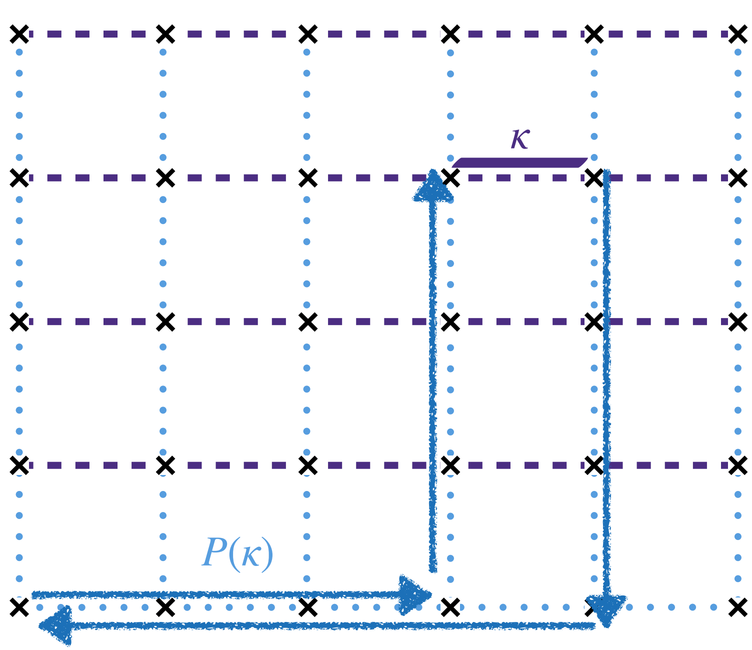
Motivation: Gauge fixing allows for "importance sampling" when working in magnetic basis without worrying about breaking gauge-invariance

Non-Local Hamiltonian: Hamiltonian written in terms of new gauge-fixed variables is more complicated

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

Max. Tree Gauge Fixing

$$H = \frac{g^2}{2a}\sum_\ell \left(\sum_{\kappa \in t_+(\ell)} \hat{\mathscr{E}}^a_{L\kappa} - \sum_{\kappa \in t_-(\ell)} \hat{\mathscr{E}}^a_{R\kappa}\right)^2 + \left(\frac{1}{2g^2 a}\sum_p Tr\left(I - \prod_{\kappa \in p} \hat{X}(\kappa)^{\sigma(\kappa)}\right) + \mathrm{h.c.}\right)$$



Commutation relations of new variables are canonical

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

Bauer, D'Andrea, Freytsis and **DMG**,
Phys.Rev.D 109 (2024) 7, 074501

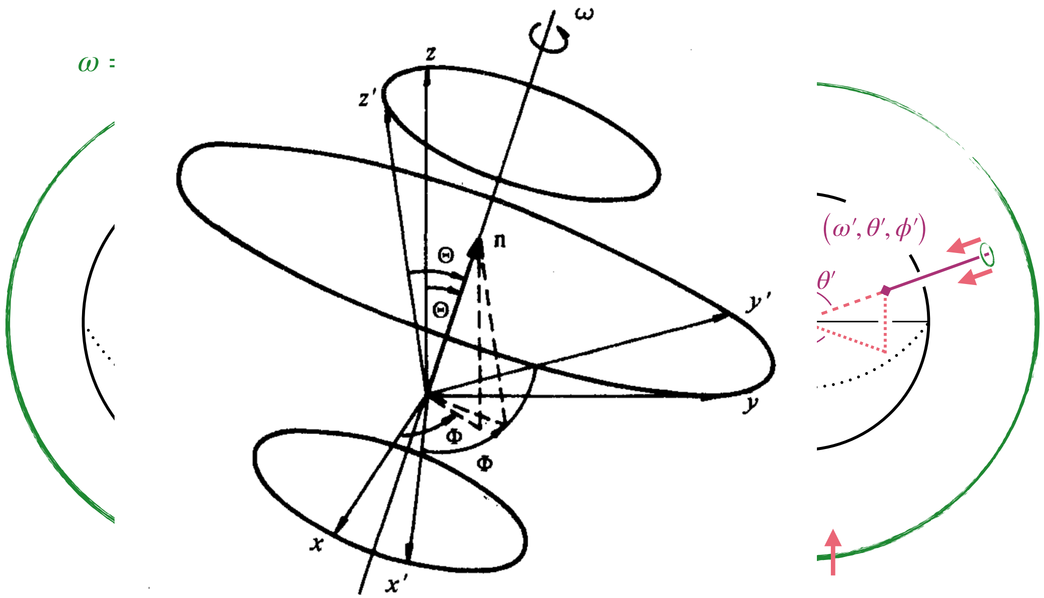
Step Two: Parameterizing Operators

Motivation: Three quantum numbers of SU(2) Hamiltonian can be thought of as total angular momentum and projected angular momentums in lab frame and body frame: $\hat{L}^2$, $\hat{L}^z$, $\hat{L}'^z$

Eye towards Digitization: Axis-angle coordinates are particularly convenient parameterization of SU(2)

- Each loop variable is simply an SU(2) matrix

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



"Quantum Theory of Angular Momentum"
Varshalovich, Moskalev, Khersonskii

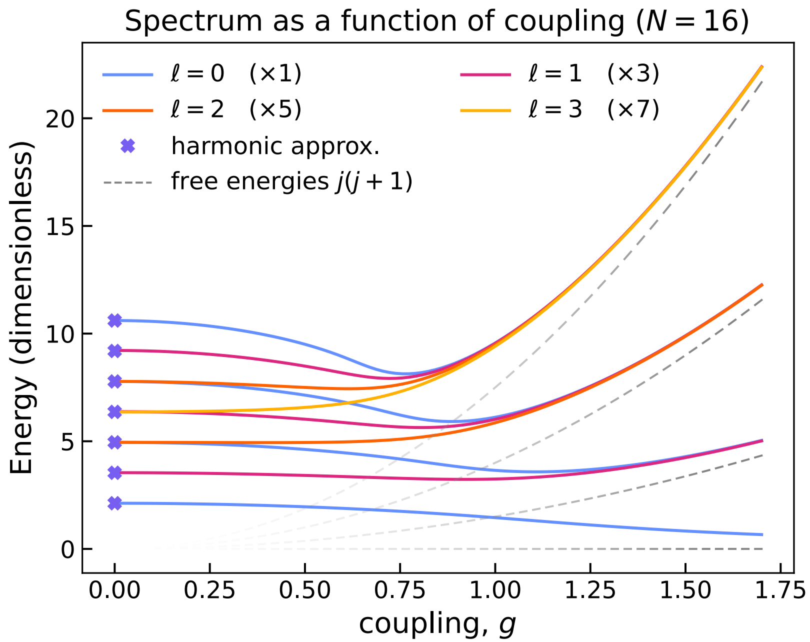
Step Three: Digitize Operators

Are we done?

Bauer, D'Andrea, Freytsis and ***DMG****,*
Phys.Rev.D 109 (2024) 7, 074501

Motivation: As currently written, $(\omega_i, \theta_i, \phi_i)$ are all continuous variables and so cannot yet be implemented onto digital quantum computers

Small Change of Basis: Angular coordinates (θ_i, ϕ_i) can be recast as spherical harmonic quantum numbers (ℓ_i, m_i)



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

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

Global Conservation Laws

Recall: All gauge transformations are carried out relative to the origin and so an overall global gauge transformation remains

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

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

Similarly, fully gauge-fixed Hamiltonians are thought to be highly non-local and thus expensive to implement on any machine - are we being foolhardy?

Finish Step One: Gauge Fix Fully

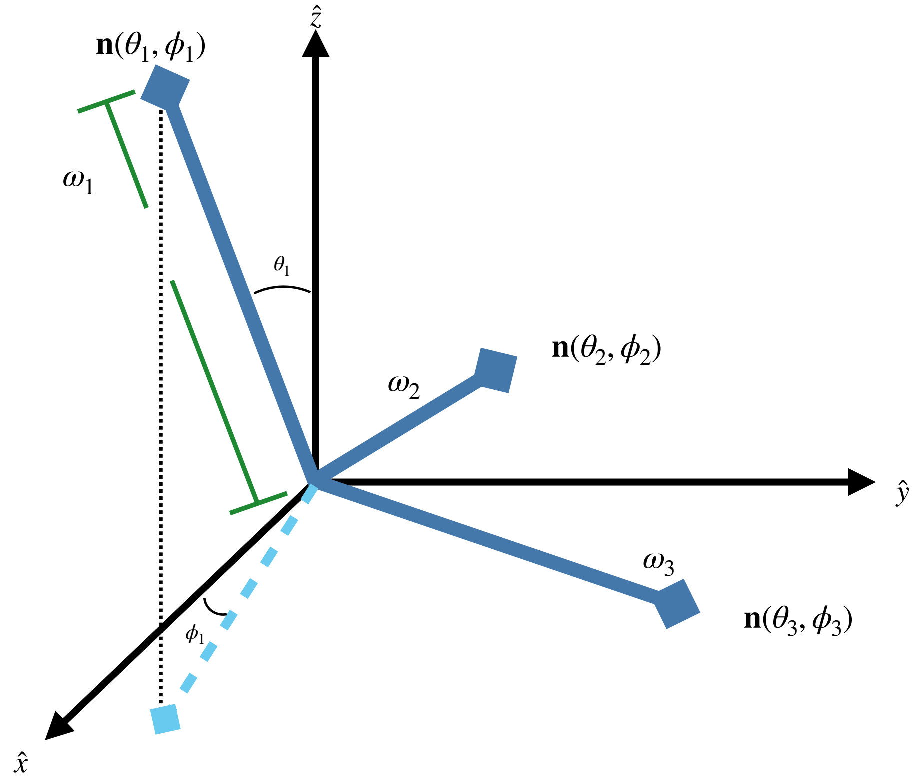
Observation: SU(2) Hamiltonian can be thought of as a system of rigid rods fixed together at the origin (axis-angle are hyperspherical coordinates)

Motivation: The quantum numbers $\left(\ell_i, m_i\right)$ are related to the total color charge of the system

$$\hat{G}^a(n_0) = \sum_{\kappa} \left[\hat{E}^a_L(\kappa) - \hat{E}^a_R(\kappa)\right] = -\sum_i L^a_i$$

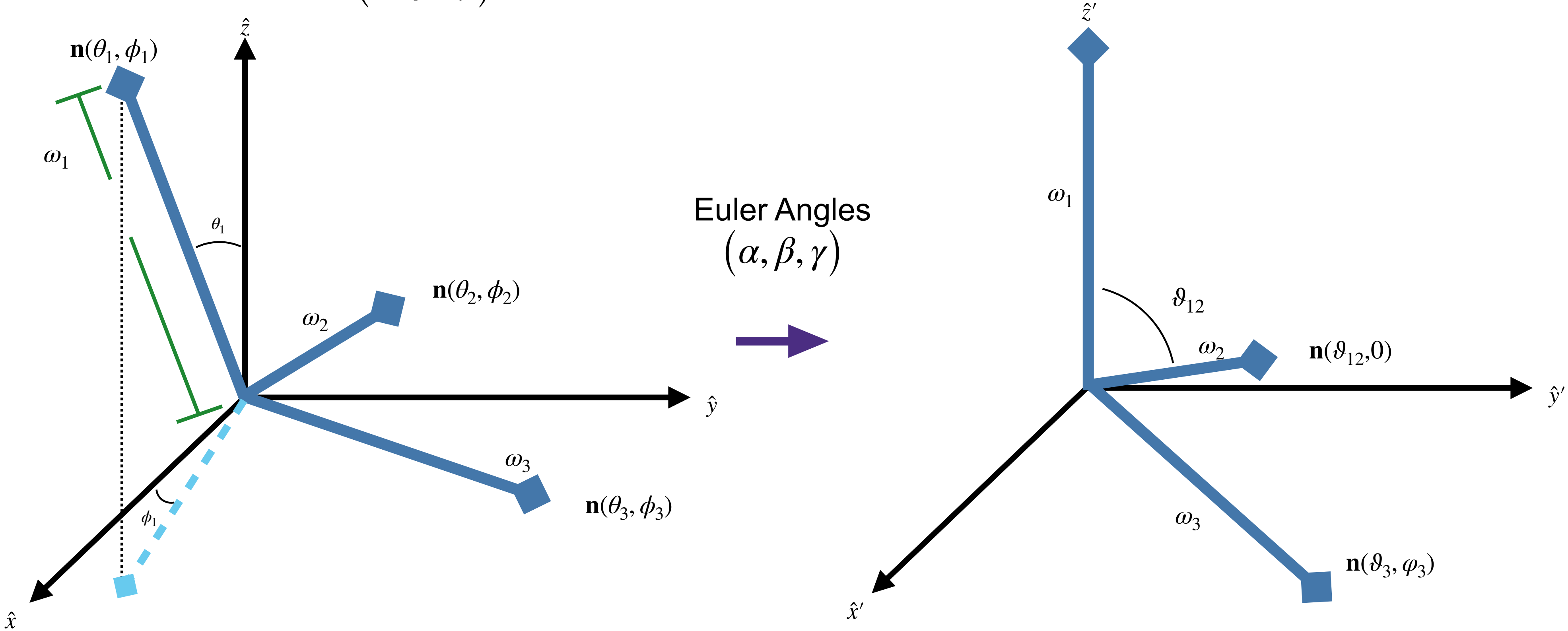
("difference between lab and body frame")

Recall: Three quantum numbers of link can be thought of as eigenstates of $\hat{L}^2$, $\hat{L}^z$, $\hat{L}'^z$ and therefore the total charge of the system should be $\hat{L}^2_{\text{tot}}$, $\hat{L}^z_{\text{tot}}$, $\hat{L}'^z_{\text{tot}}$



Finish Step One: Gauge Fix Fully

Motivation: Euler Angles (α, β, γ) will take total system from lab frame to body frame



If we can relate these two bases AND do a change of variable on all operators in the Hamiltonian, then we will have a fully gauge-fixed theory!

DMG, *Kane and Bauer, to appear shortly*

Finish Step One: Gauge Fix Fully

Motivation: Simple* change of variable will lead us to a fully gauge-fixed theory

Step 1: Relate the two basis by writing the position of the rods in the two frames

Original Basis

$$n_i = \{\sin\theta_i \cos\phi_i, \sin\theta_i \sin\phi_i, \cos\theta_i\}$$

Sequestered Basis

$$n_1^{(0)} = R(\alpha,\beta,\gamma)(0,0,0)$$

$$n_2^{(0)} = R(\alpha,\beta,\gamma)\left(\sin\vartheta_{12}, 0, \cos\vartheta_{12}\right)$$

$$n_\mu^{(0)} = R(\alpha,\beta,\gamma)\{\sin\vartheta_\mu \cos\varphi_\mu, \sin\vartheta_\mu \sin\varphi_\mu, \cos\vartheta_\mu\}$$

* Simple in theory, but difficult to execute; luckily, we only have to do it once and it's done now

DMG, *Kane and Bauer, to appear shortly*

Finish Step One: Gauge Fix Fully

Motivation: Simple* change of variable will lead us to a fully gauge-fixed theory

Step 3: Classify and derive all possible electric bilinear and magnetic loops

Bilinear	Changing quantum numbers	σ change	Total (four rods)	Total (N rods)
$E^1_\eta E^1_{\eta'}$	no change		1	1
	$\Delta N = \pm 1$	$\Delta\sigma = \pm 1$	2	2
	$\Delta m^{[i]}_\mu = \pm 1$	$\Delta\sigma = \pm 1$	4	$2n_\kappa - 4$
	$\Delta N = \pm 1$; $\Delta m^{[i]}_\mu = \pm 1$	$\Delta\sigma = 0$	4	$2n_\kappa - 4$
	$\Delta m^{[i]}_\mu = \pm 1$, $\Delta m^{[i]}_\nu = \pm 1$,	$\Delta\sigma = 0$	2	$(n_\kappa - 2)(n_\kappa - 3)$
	total:		13	$n_\kappa(n_\kappa - 1) + 1$
$E^2_\eta E^2_{\eta'}$	no change		1	1
	total:		1	1
$E^{\mu^{[d]}}_\eta E^{\mu^{[d]}}_{\eta'}$	no change		1	1
	total:		1	1

ıe electric (Magnetic) Hamiltonian can change more than ıour (five) quantum numbers at a time!

Conclusions

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: Basis choice can dramatically affect both the resource efficiency

Main Take-Away Point 2: It is important to explore a variety of approaches to simulating lattice gauge Hamiltonian and critically analyze commonly-heard lore.

Paper presenting fully gauge-fixed SU(2) Hamiltonian that can be simulated with polynomial resources will be on arXiv next week!