

# Primitive quantum gates for an $SU(2)$ discrete subgroup: Binary octahedral

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We construct a primitive gate set for the digital quantum simulation of the 48-element binary octahedral ( $\mathbb{BO}$ ) group. This non-Abelian discrete group better approximates  $SU(2)$  lattice gauge theory than previous work on the binary tetrahedral group at the cost of one additional qubit—for a total of six—per gauge link. The necessary primitives are the inversion gate, the group multiplication gate, the trace gate, and the  $\mathbb{BO}$  Fourier transform.

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## I. INTRODUCTION

The possibilities for quantum utility in lattice gauge theories (LGT) are legion [1–4]. Perhaps foremost, it provides an elegant solution to the sign problem which results in exponential scaling of classical computing resources [5] which precludes large-scale simulations of dynamics, at finite fermion density, and in the presence of topological terms. In order to study these fundamental physics topics, a number of quantum subroutines are required.

The first task is preparing strongly-coupled states of interest including ground states [6–12], thermal states [13–23], and colliding particles [24–34]. For applications to dynamics, the time-evolution operator  $U(t) = e^{-iHt}$  must be approximated and many different choices exist; Trotterization [35,36], random compilation [37,38], Taylor series [39], qubitization [40], quantum walks [41], signal processing [42], linear combination of unitaries [38,43], and variational approaches [44–47], each with their own trade-offs. Important alongside state preparation and evolution is the need to develop efficient techniques [48–51] and formulations [52–63] for measuring physical observables. Necessary for achieving this, one may further use algorithmic improvements such as error mitigation and correction

[64–79], improved Hamiltonians [80,81] and quantum smearing [82] to reduce errors from quantum noise and theoretical approximations. Beyond direct simulations, quantum computers could also accelerate classical lattice gauge theory simulations by reducing autocorrelation [83–86] and optimizing interpolating operators [87,88].

Across this cornucopia, there exist a set of fundamental group theoretic operations that LGT requires [52]. Via this identification of primitive subroutines, the problem of formulating quantum algorithms for LGT can be divided into deriving said group-dependent primitives [89–91] and group-independent algorithmic design [80,82,91,92].

With this notion in mind, one can turn to digitizing the infinite-dimensional Hilbert space of the gauge bosons. Many proposals exist that prioritizing theoretical and algorithmic facets of the problem differently [93–133]. For some digitized theories, there may be no nontrivial continuum limit [122,123,125,134–141]. Furthermore, the efficacy of a gauge digitization can be dimension dependent [89,90,117,142]. While all digitizations consider the relative quantum memory costs, the consequences of digitization on gate costs are more limited. Despite this, recent work has made abundantly clear that the number of expensive fixed-point arithmetic required can vary by orders of magnitude [36,143].

One promising digitization that uses comparatively few qubits and avoids fixed-point arithmetic is the discrete subgroup approximation [66,101,103–107,128,144,145]. This method was explored in the 1970s and 1980s to reduce memory and runtime of Euclidean LGT on classical computers. The replacement of  $U(1)$  by  $\mathbb{Z}_N$  was considered first [146,147] and eventually extended to the crystal-like subgroups of  $SU(N)$  [103,104,128,148–153]. Some studies

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were even performed with dynamical fermions [154,155]. Theoretical work has established that the discrete subgroup approximation corresponds to continuous groups broken by a Higgs mechanism [156–160].

LGT calculations are performed at fixed lattice spacing  $a = a(\beta)$  which for asymptotically free theories approach zero as  $\beta \rightarrow \infty$ . Finite  $a$  leads to discrepancies from the continuum results, but provided one simulates in the *scaling regime* below  $a_s(\beta_s)$ , these errors are well-behaved. On the lattice, the breakdown of the discrete subgroup approximation manifests as a *freeze-out*  $a_f$  (or coupling  $\beta_f$ ) where the gauge links become “frozen” to the identity. Despite this, the approximation error for Euclidean calculations can be tolerable provided  $a_s \gtrsim a_f$  ( $\beta_s \lesssim \beta_f$ ) [104,152]. Further, a connection between the couplings and lattice spacings of Minkowski and Euclidean lattice field theories has been shown [144,153,161], which suggests similarly controllable digitization error on large-scale quantum simulations and a way for determining viable approximations.

The freezing transitions are known in  $3 + 1d$  when the Wilson action is used. Given the known connection between the Wilson action and the Kogut-Susskind Hamiltonian  $H_{KS}$  [162], this provides insight into the viable groups for quantum simulations. Approximating  $U(1)$  by  $\mathbb{Z}_{n \geq 5}$  satisfies  $\beta_f > \beta_s$ , with  $\beta_f \propto 1 - \cos^{-1}(2\pi/n)$ . In the case of non-Abelian gauge groups, there are limited number of crystal-like subgroups.  $SU(2)$ , with  $\beta_s = 2.2$  has three; the 24-element binary tetrahedral  $\mathbb{BT}$  ( $\beta_f = 2.24(8)$ ), the 48-element binary octahedral  $\mathbb{BO}$  ( $\beta_f = 3.26(8)$ ), and the 120-element binary icosahedral  $\mathbb{BI}$  ( $\beta_f = 5.82(8)$ ) [104]. Thus, while  $\mathbb{BT}$  require only 5 qubits, due to its low  $\beta_f$  it is unlikely  $H_{KS}$  can be used for quantum simulation but a modified or improved Hamiltonians  $H_I$  [80,81] could prove sufficient [104,128,151,152]. The effects on the scaling regime when including fermions is a more subtle question. The structure of discrete groups makes it difficult to leverage traditional Monte Carlo schemes to investigate the transition such as shown in Fig. 1. Qualitatively one could make the following insights; for sufficiently heavy fermions one would expect the scaling behavior to be slightly increased, while the effects for lighter fermions could drastically change the scaling regime in  $\beta$  due to the lower cost of pair creation.

In this work, we consider the smallest crystal-like subgroup of a  $SU(2)$  with  $a_f > a_s$ — $\mathbb{BO}$  which requires 6 qubits per register. A number of smaller non-Abelian groups have been considered previously. Quantum simulations of the  $2N$ -element dihedral groups,  $D_N$ , while not crystal-like, have been extensively studied [52,89,101,163]. The 8-element  $\mathbb{Q}_8$  subgroup of  $SU(2)$  has also been investigated [145]. In [90], quantum circuits for  $\mathbb{BT}$  were constructed and resource estimates were obtained using the  $H_I$  of [80].

In the interest of studying near-term quantum simulations, we should consider  $2 + 1d$  theories in addition to

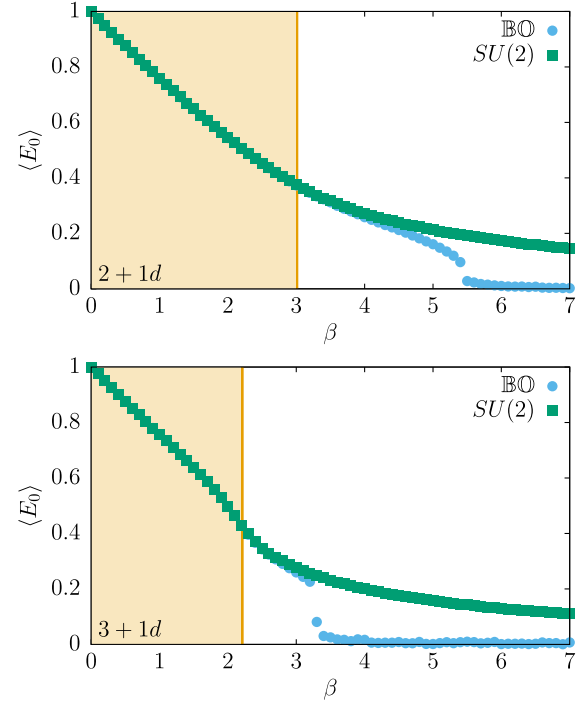


FIG. 1. Euclidean calculations of lattice energy density  $\langle E_0 \rangle$  of  $\mathbb{BO}$  as measured by the expectation value of the plaquette as a function of Wilson coupling  $\beta$  on  $8^d$  lattices for (top)  $2 + 1d$  (bottom)  $3 + 1d$ . The shaded region indicates  $\beta \leq \beta_s$ .

$3 + 1d$  ones. Using classical lattice simulations, we determined  $\beta_f > \beta_s$  in both space-times for the Wilson action (See Fig. 1). Thus quantum simulations with  $\mathbb{BO}$  can be performed with the Kogut-Susskind Hamiltonian [164], although using an improved Hamiltonian can reduce either qubits or lattice spacing errors [80].

In this paper, the four necessary primitive quantum gates (inversion, multiplication, trace, and Fourier) for quantum simulation of  $\mathbb{BO}$  theories on qubit-based computers are constructed. In Sec. II, important group theory for  $\mathbb{BO}$  is summarized and the qubit encoding is presented. A brief review of entangling gates used is found in Sec. III. Section IV provides an overview of the primitive gates. This is followed by explicit quantum circuits for each gate for  $\mathbb{BO}$ ; the inversion gate in Sec. V, the multiplication gate in Sec. VI, the trace gate in Sec. VII, and the Fourier transform gate in Sec. VIII. Using these gates, Sec. IX presents a resource estimates for simulating  $3 + 1d$   $SU(2)$ . We conclude and discuss future work in Sec. X.

## II. PROPERTIES OF $\mathbb{BO}$

The simulation of LGT requires defining a register where one can store the state of a bosonic link variable which we call a  $G$  – register. To construct the  $\mathbb{BO}$ -register in term of integers, it is necessary to map the 48 elements of  $\mathbb{BO}$  to the integers  $[0, 47]$ . A clean way to obtain this is to write every element of  $\mathbb{BO}$  as an ordered product of five generators with

exponents written in terms of the binary variables  $x_i$  with  $i = [1, 6]$ :

$$g = (-1)^{x_1} \mathbf{j}^{x_2} \mathbf{k}^{x_3} \mathbf{u}^{2x_4+x_5} \mathbf{t}^{x_6}, \quad (1)$$

with

$$\mathbf{u} = -\frac{1}{2}(\mathbb{1} + \mathbf{i} + \mathbf{j} + \mathbf{k}) \quad \text{and} \quad \mathbf{t} = \frac{1}{\sqrt{2}}(\mathbb{1} + \mathbf{i}) \quad (2)$$

and  $\mathbf{i}$ ,  $\mathbf{j}$ ,  $\mathbf{k}$  are the unit quaternions which in the 2d irreducible representation (irrep) correspond to Pauli matrices. With the construction of Eq. (1), the  $\mathbb{B}\mathbb{O}$ -register is given by a binary qubit encoding with the ordering  $|x_6 x_5 x_4 x_3 x_2 x_1\rangle$ . While there exist  $2^6$  possible state in a 6 qubit register, we only consider the 48 states where  $x_4 + x_5 \leq 1$  represent the group elements. The states where  $x_4 = x_5 = 1$  correspond to *forbidden states*. In this work we will use a short hand  $|N\rangle$  where  $N$  is the decimal representation of the binary  $x_6 x_5 x_4 x_3 x_2 x_1$ . For example,

$$\frac{1}{\sqrt{2}} \begin{pmatrix} -i & -1 \\ 1 & i \end{pmatrix} = (-1)^1 \mathbf{j}^0 \mathbf{k}^1 \mathbf{u}^{2 \times 0 + 0} \mathbf{t}^1 \rightarrow |100101\rangle = |37\rangle. \quad (3)$$

The  $\mathbf{i}$ ,  $\mathbf{j}$ , and  $\mathbf{k}$  generators anticommute with each other. Additional useful relations are

$$\begin{aligned} \mathbf{i}^2 = \mathbf{j}^2 = \mathbf{k}^2 &= -\mathbb{1}, & \mathbf{u}^3 &= \mathbb{1}, & \mathbf{t}^2 &= \mathbf{i}, \\ \mathbf{i}\mathbf{j} &= \mathbf{k}, & \mathbf{j}\mathbf{k} &= \mathbf{i}, & \mathbf{k}\mathbf{i} &= \mathbf{j}, \\ \mathbf{i}\mathbf{u} &= \mathbf{u}\mathbf{k}, & \mathbf{j}\mathbf{u} &= \mathbf{u}\mathbf{i}, & \mathbf{k}\mathbf{u} &= \mathbf{u}\mathbf{j}, \\ \mathbf{i}\mathbf{t} &= \mathbf{t}\mathbf{i}, & -\mathbf{j}\mathbf{t} &= \mathbf{t}\mathbf{k}, & \mathbf{k}\mathbf{t} &= \mathbf{t}\mathbf{j}, \end{aligned} \quad (4)$$

The character table (Table I) lists important group properties; the different irreps, denoted as  $\rho_i$ , can be identified by the value of their character, which correspond to the columns in Table I, acting on each element. The final row indicates the binary state corresponding to group elements in a given character. An irrep's dimension is the value of the character of 1. There are three 1d irreps, three 2d irreps (one real and two complex), and one 3d irrep. To derive the Fourier transform, it is necessary to know a matrix presentation of each irrep. Based on our qubit mapping, given a presentation of  $-1$ ,  $\mathbf{i}$ ,  $\mathbf{j}$ , and  $\mathbf{k}$  we can construct any element of the group from Eq. (1). With the  $n$ th root of unity  $\omega_n = e^{2\pi i/n}$ , the matrix presentations of our generators in each irrep are found in Table II.

### III. QUBIT GATES

To construct our primitive gates, we chose a universal, albeit redundant, basic qubit quantum gate set. We use the

TABLE I. Character table of  $\mathbb{B}\mathbb{O}$  from [165] and an enumeration of the elements in the given class.

Size	1	1	12	6	8	8	6	6
Order	1	2	4	4	6	3	8	8
$\rho_1$	1	1	1	1	1	1	1	1
$\rho_2$	1	1	-1	1	1	1	-1	-1
$\rho_3$	2	2	0	2	-1	-1	0	0
$\rho_4$	2	-2	0	0	1	-1	$\sqrt{2}$	$-\sqrt{2}$
$\rho_5$	2	-2	0	0	1	-1	$-\sqrt{2}$	$\sqrt{2}$
$\rho_6$	3	3	-1	-1	0	0	1	1
$\rho_7$	3	3	1	-1	0	0	-1	-1
$\rho_8$	4	-4	0	0	-1	1	0	0
$ g\rangle$	$ 0\rangle 1\rangle 34\rangle -  37\rangle 2\rangle -  7\rangle 9\rangle,  11\rangle 8\rangle,  10\rangle$		$ 44\rangle -  49\rangle$		$ 13\rangle,  15\rangle,  17\rangle,  18\rangle,  20\rangle,  22\rangle$	$ 12\rangle,  14\rangle,  16\rangle,  19\rangle,  21\rangle,  23\rangle$	$ 32\rangle,  39\rangle,  41\rangle,  43\rangle,  50\rangle,  54\rangle$	$ 33\rangle,  38\rangle,  40\rangle,  42\rangle,  51\rangle,  55\rangle$

Pauli gates  $p = X, Y, Z$  and their arbitrary rotation generalizations  $R_p(\theta) = e^{i\theta p/2}$ . When decomposing onto fault-tolerant devices, how these are decomposed in terms of the  $T = \text{diag}(1, e^{i\pi/4})$  gate becomes relevant to resource estimations.

We also use the SWAP gate

$$\text{SWAP}|a\rangle \otimes |b\rangle = |b\rangle \otimes |a\rangle,$$

and CNOT gate

$$\text{CNOT}|a\rangle \otimes |b\rangle = |a\rangle \otimes |b \oplus a\rangle.$$

We further use the multiqubit  $C^n\text{NOT}$ —of which  $C^2\text{NOT}$  is called the Toffoli gate—and CSWAP (Fredkin) gates. The  $C^n\text{NOT}$  gate consists of one target qubit and  $n$  control qubits. For example, the Toffoli in terms of modular arithmetic is

$$C^2\text{NOT}|a\rangle \otimes |b\rangle \otimes |c\rangle = |a\rangle \otimes |b\rangle \otimes |c \oplus ab\rangle.$$

The CSWAP gate swaps two qubit states if the control is in the  $|1\rangle$  state:

$$\begin{aligned} \text{CSWAP}|a\rangle \otimes |b\rangle \otimes |c\rangle &= |a\rangle \otimes |b(1 \oplus a) \oplus ac\rangle \\ &\quad \otimes |c(1 \oplus a) \oplus ab\rangle. \end{aligned}$$

### IV. OVERVIEW OF PRIMITIVE GATES

One can define any quantum circuit for gauge theories via a set of primitive gates, of which one choice is inversion  $\mathcal{U}_{-1}$ , multiplication  $\mathcal{U}_\times$ , trace  $\mathcal{U}_T$ , and Fourier transform  $\mathcal{U}_F$  [52]. The inversion gate,  $\mathcal{U}_{-1}$ , takes a  $G$ -register to its inverse:

TABLE II. Matrix representations of the generators used for digitization of  $\mathbb{BO}$ .

$g$	$-1$	$j$	$k$	$u$	$t$
$\rho_1$	1	1	1	1	1
$\rho_2$	1	1	1	1	-1
$\rho_3$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \omega_3^2 & 0 \\ 0 & \omega_3 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
$\rho_4$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$	$\frac{1}{2} \begin{pmatrix} -1-i & -1+i \\ 1+i & -1+i \end{pmatrix}$	$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix}$
$\rho_5$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$	$\frac{1}{2} \begin{pmatrix} -1-i & -1+i \\ 1+i & -1+i \end{pmatrix}$	$\frac{1}{\sqrt{2}} \begin{pmatrix} -1 & i \\ i & -1 \end{pmatrix}$
$\rho_6$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
$\rho_7$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
$\rho_8$	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & -i & 0 & 0 \\ -i & 0 & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \end{pmatrix}$	$\begin{pmatrix} i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & -i & 0 \end{pmatrix}$	$\frac{\omega_3}{2} \begin{pmatrix} (-1-i)\omega_3 & (1+i)\omega_3 & 0 & 0 \\ (-1+i)\omega_3 & (-1+i)\omega_3 & 0 & 0 \\ 0 & 0 & -1+i & 1+i \\ 0 & 0 & -1+i & -1-i \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$

$$\mathcal{U}_{-1}|g\rangle = |g^{-1}\rangle. \quad (5)$$

$\mathcal{U}_\times$  takes a target  $G$ -register and changes it to the left product controlled by a second  $G$ -register:

$$\mathcal{U}_\times|g\rangle|h\rangle = |g\rangle|gh\rangle. \quad (6)$$

Left multiplication is sufficient for a minimal set as right multiplication can be obtained from two applications of  $\mathcal{U}_{-1}$  and  $\mathcal{U}_\times$ , albeit resource costs can be further reduced by an explicit construction [80].

Traces of group elements generally define the lattice Hamiltonian. We can implement the evolution with respect to these terms via:

$$\mathcal{U}_F = \begin{pmatrix} \tilde{\rho}_{1,0} & \tilde{\rho}_{1,1} & \tilde{\rho}_{1,2} & \cdots & \tilde{\rho}_{1,|G|-2} & \tilde{\rho}_{1,|G|-1} \\ \tilde{\rho}_{2,0} & \tilde{\rho}_{2,1} & \tilde{\rho}_{2,2} & \cdots & \tilde{\rho}_{2,|G|-2} & \tilde{\rho}_{2,|G|-1} \\ \tilde{\rho}_{3,0} & \tilde{\rho}_{3,1} & \tilde{\rho}_{3,2} & \cdots & \tilde{\rho}_{3,|G|-2} & \tilde{\rho}_{3,|G|-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \tilde{\rho}_{4,0} & \tilde{\rho}_{4,1} & \tilde{\rho}_{4,2} & \cdots & \tilde{\rho}_{4,|G|-2} & \tilde{\rho}_{4,|G|-1} \end{pmatrix}$$

FIG. 2. Example  $\mathcal{U}_F$  from Eq. (8) using  $\tilde{\rho}_{i,j} = \sqrt{d_\rho/|G|}\rho_{i,j}$  where  $\rho_{i,j} = \rho_i(g_j)$ . This example has four irreps with  $d_1 = d_2 < d_3 < d_4$ .  $\mathcal{U}_F$  is square since  $\sum_\rho d_\rho^2 = |G|$ .

$$\mathcal{U}_{\text{Tr}}(\theta)|g\rangle = e^{i\theta \text{Re Tr } g}|g\rangle. \quad (7)$$

The final gate of this set is  $\mathcal{U}_F$ . The Fourier transform,  $\hat{f}$ , of a function  $f$  over a finite  $G$  is

$$\hat{f}(\rho) = \sum_{g \in G} \sqrt{\frac{d_\rho}{|G|}} f(g) \rho(g), \quad (8)$$

where  $|G|$  is the size of the group,  $d_\rho$  is the dimensionality of the irrep  $\rho$ . The inverse transform is given by

$$f(g) = \sum_{\rho \in \hat{G}} \sqrt{\frac{d_\rho}{|G|}} \text{Tr}(\hat{f}(\rho) \rho(g^{-1})), \quad (9)$$

where the dual  $\hat{G}$  is the set of irrep of  $G$ . A paradigm of this unitary matrix is shown in Fig. 2 which can then be transformed into a gate.  $\mathcal{U}_F$  then acts on a single  $G$ -register with some amplitudes  $f(g)$  which rotate it into the irrep basis:

$$\mathcal{U}_F \sum_{g \in G} f(g) |g\rangle = \sum_{\rho \in \hat{G}} \hat{f}(\rho)_{ij} |\rho, i, j\rangle. \quad (10)$$

## V. INVERSION GATE

Consider a  $\mathbb{BO}$ -register storing the group element given by  $g = (-1)^{x_1} \mathbf{j}^{x_2} \mathbf{k}^{x_3} \mathbf{u}^{2x_4+x_5} \mathbf{t}^{x_6}$ . The effect of the inversion gate on this register is to transform it to

$$|g\rangle = |x_1 x_2 x_3 x_4 x_5 x_6\rangle \rightarrow |g^{-1}\rangle = |y_1 y_2 y_3 y_4 y_5 y_6\rangle. \quad (11)$$

Where  $y_i$  must be determined. With Eq. (1),  $g^{-1}$  is

$$g^{-1} = \mathbf{t}^{8-x_6} \mathbf{u}^{3-(2x_4+x_5)} \mathbf{k}^{x_3} \mathbf{j}^{x_2} (-1)^{x_1+x_2+x_3}. \quad (12)$$

A systematic way to build the  $\mathcal{U}_{-1}$  of  $\mathbb{B}\mathbb{O}$  is to embed the inverse gates of subgroups of  $\mathbb{B}\mathbb{O}$ . We start with the expression of Eq. (12), and begin by reordering the  $\mathbb{Q}_8$  subgroup so that the element is of the form:

$$\mathbf{k}^{x_3} \mathbf{j}^{x_2} (-1)^{x_1+x_2+x_3} = (-1)^{a_1} \mathbf{j}^{a_2} \mathbf{k}^{a_3}, \quad (13)$$

where  $a_1 = x_1 + x_2 + x_3 + x_2x_3$  and  $a_2 = x_2$ ,  $a_3 = x_3$ . The next step is commuting through  $\mathbf{u}$  to obtain

$$\mathbf{u}^{3-(2x_4+x_5)} (-1)^{a_1} \mathbf{j}^{a_2} \mathbf{k}^{a_3} = (-1)^{b_1} \mathbf{j}^{b_2} \mathbf{k}^{b_3} \mathbf{u}^{2b_4+b_5}, \quad (14)$$

which corresponds to the  $\mathbb{B}\mathbb{T}$  inverse gate where

$$\begin{aligned} b_2 &= a_2(1+x_4) + a_3(x_4+x_5), \\ b_3 &= a_3(1+x_5) + a_2(x_4+x_5), \\ b_4 &= x_5, \\ b_5 &= x_4, \end{aligned} \quad (15)$$

while  $b_1 = a_1$  is unchanged. Finally, commuting through  $\mathbf{t}$ ,

$$\mathbf{t}^{8-x_6} (-1)^{b_1} \mathbf{j}^{b_2} \mathbf{k}^{b_3} \mathbf{u}^{2b_4+b_5} = (-1)^{y_1} \mathbf{j}^{y_2} \mathbf{k}^{y_3} \mathbf{u}^{2y_4+y_5} \mathbf{t}^{y_6}. \quad (16)$$

Propagating  $\mathbf{t}^{x_6}$  through the  $\mathbb{Q}_8$  portion yields  $g^{-1} = (-1)^{c_1} \mathbf{j}^{c_2} \mathbf{k}^{c_3} \mathbf{t}^{x_6} \mathbf{u}^{2b_4+b_5}$ , where

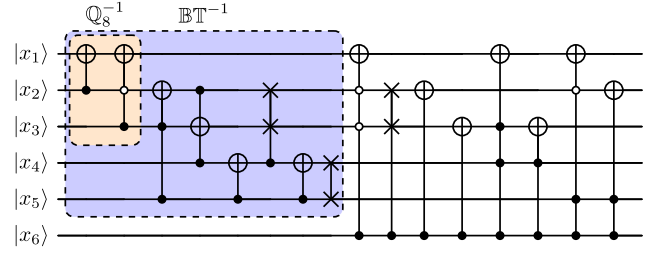


FIG. 3. Quantum circuit for  $\mathcal{U}_{-1}$  for  $\mathbb{B}\mathbb{O}$ . The subgates correspond to  $\mathcal{U}_{-1}$  for  $\mathbb{Q}_8$  ( $\mathbb{B}\mathbb{T}$ ) in orange (blue).

$$c_1 = b_1 + x_6(1-b_3)(1-b_2),$$

$$c_2 = (1-b_3)x_6 + (1-x_6)b_2,$$

$$c_3 = (1-b_2)x_6 + (1-x_6)b_3.$$

Finally, propagating through  $\mathbf{t}^{x_6}$  through  $\mathbf{u}^{2b_4+b_5}$  yields,

$$y_1 = c_1 + x_6(b_4(1-c_2) + c_3b_5),$$

$$y_2 = c_2 + b_4x_6,$$

$$y_3 = c_3 + (b_4 + b_5)x_6,$$

$$y_4 = x_6b_5 + (1-x_6)b_4,$$

$$y_5 = x_6b_4 + (1-x_6)b_5, \quad (17)$$

with  $y_6 = x_6$ . Together, this yields for  $|g\rangle$  to  $|g^{-1}\rangle$ :

$$\begin{aligned} y_1 &= x_1 + x_2x_3x_6 + x_2x_3 + x_2x_5x_6 + x_2x_6 + x_2 + x_3x_4x_6 + x_3x_6 + x_3 + x_4x_6 + x_6, \\ y_2 &= x_2x_4 + x_2x_5x_6 + x_2x_6 + x_2 + x_3x_4x_6 + x_3x_4 + x_3x_5 + x_3x_6 + x_5x_6 + x_6, \\ y_3 &= (x_2 + x_3)(x_5 + x_6) + x_6(x_4(x_3 + 1) + x_5(x_2 + 1)) + x_2x_4 + x_3 + x_6, \\ y_4 &= (x_4 + x_5)x_6 + x_5, \\ y_5 &= (x_4 + x_5)x_6 + x_4, \end{aligned} \quad (18)$$

where  $y_6 = x_6$  is unaffected. We provide the quantum circuit for this gate in Fig. 3.

## VI. MULTIPLICATION GATE

Given two  $\mathbb{B}\mathbb{O}$ -registers  $|g\rangle = |\prod x_i\rangle$  and  $|h\rangle = |\prod y_i\rangle$ , we want  $|gh\rangle = |\prod z_i\rangle$ . Here, we again decompose

$$\mathcal{U}_\times = \mathcal{U}_{\times,-1} \mathcal{U}_{\times,j} \mathcal{U}_{\times,k} \mathcal{U}_{\times,u_2} \mathcal{U}_{\times,u_1} \mathcal{U}_{\times,t} \quad (19)$$

into gates controlled by a single qubits. For each step, we use temporary variables indexed by other letters, e.g.  $a_i$ . The first gate,  $\mathcal{U}_{\times,t}$ , controlled by  $x_6$ , sets:

$$\begin{aligned} a_1 &= y_2y_4y_6 + y_3y_4y_6 + y_2y_5y_6 + y_2y_3 + y_2y_4 \\ &\quad + y_3y_5 + y_3y_6 + y_4y_6 + y_1 + y_3 + y_5, \end{aligned}$$

$$a_2 = y_4y_6 + y_3 + y_5 + y_6,$$

$$a_3 = y_5y_6 + y_2 + y_4 + y_5 + y_6,$$

$$a_4 = y_5,$$

$$a_5 = y_4,$$

$$z_6 = y_6 + 1. \quad (20)$$

Then one acts with  $\mathcal{U}_{\times,u_1}$  which is controlled by  $x_5$ :



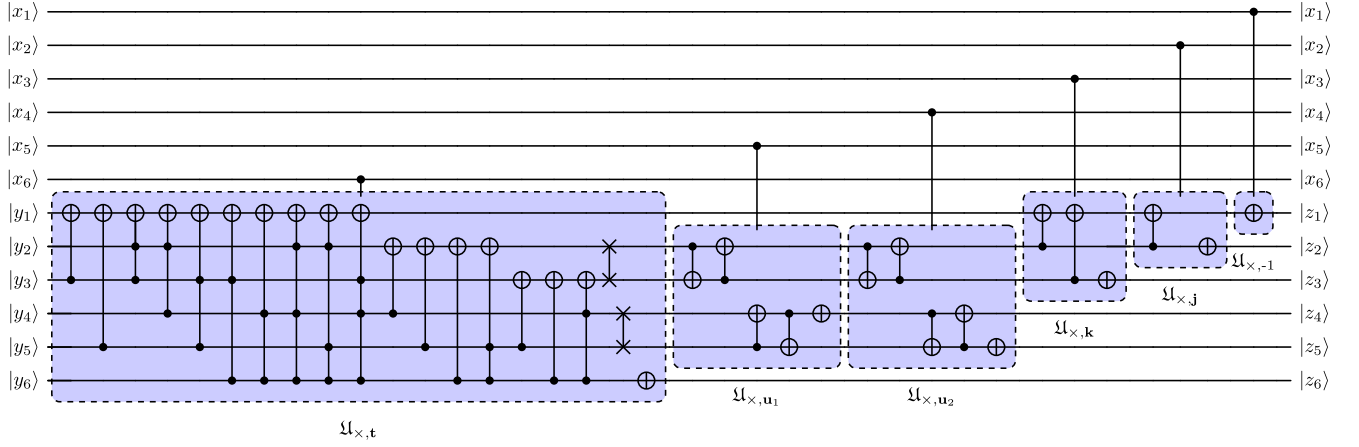


FIG. 4. The decomposition of the multiplication gate,  $\mathfrak{U}_x$ , into a product of multiplication by each generator.

$$\begin{aligned}
 b_2 &= a_2 + a_3, \\
 b_3 &= a_2, \\
 b_4 &= a_5, \\
 b_5 &= a_4 + a_5 + 1,
 \end{aligned} \tag{21}$$

where  $a_1$  and  $z_6$  do not change. Next, applying  $\mathfrak{U}_{x,u_2}$  controlled by  $x_4$ ,

$$\begin{aligned}
 c_2 &= b_3, \\
 c_3 &= b_2 + b_3, \\
 z_4 &= b_4 + b_5 + 1, \\
 z_5 &= b_4,
 \end{aligned} \tag{22}$$

with  $a_1$  and  $z_6$  unchanged.  $\mathfrak{U}_{x,k}$ , controlled by  $x_3$ , sets

$$\begin{aligned}
 d_1 &= a_1 + c_2 + c_3, \\
 z_3 &= c_3 + 1,
 \end{aligned} \tag{23}$$

where  $c_2$ ,  $z_4$ ,  $z_5$ , and  $z_6$  are unchanged. Then,  $\mathfrak{U}_{x,j}$  controlled by  $x_2$  is

$$\begin{aligned}
 e_1 &= d_1 + c_2, \\
 z_2 &= c_2 + 1,
 \end{aligned} \tag{24}$$

with  $z_3$  through  $z_6$  unchanged. Finally,  $\mathfrak{U}_{x,-1}$  needs  $z_1 = e_1 + 1$  controlled by  $x_1$  i.e. a CNOT. The full  $\mathfrak{U}_x$  is in Fig. 4.

## VII. TRACE GATE

For simulating LGT, the Hamiltonian requires gauge-invariant operators. Without matter, all terms can be constructed from traces of  $g$ —and thus  $\mathfrak{U}_{\text{Tr}}$ —in the fundamental irrep,  $\rho_4$ . Table I provides us with  $\text{ReTr}(g_i)$ . In previous works [52,89,90],  $\mathfrak{U}_{\text{Tr}}$  was derived from a Hamiltonian,  $H_{\text{Tr}}$

with  $\text{ReTr}(g_i)$  as eigenvalues. For our  $\mathbb{BQ}$ -register,  $H_{\text{Tr}}$  would require 20 Pauli strings which results in  $\mathfrak{U}_{\text{Tr}} = e^{i\theta H_{\text{Tr}}}$  decomposing into at least 20  $R_Z(\theta)$  gates. In a fault-tolerant calculation,  $R_Z$  gates require synthesis from T gates, and thus can be unduly expensive.

Here, we explore a different implementation of  $\mathfrak{U}_{\text{Tr}}$  that is advantageous for discrete groups where  $\text{ReTr}(g)$  are limited by the number of conjugacy classes. In this case,  $\mathfrak{U}_{\text{Tr}}$  could be decomposed into two gates; a gate  $U_{\text{conj}}$  to map the 48  $|g\rangle$  to the 8 conjugacy classes  $|c\rangle$ , and a gate  $U_{\text{Tr}}$  which computes the traces for each conjugacy class. Together, we obtain a circuit for  $\mathfrak{U}_{\text{Tr}} = U_{\text{conj}} U_{\text{Tr}}(\theta) U_{\text{conj}}^\dagger$  which should have fewer  $R_Z(\theta)$  at the cost of additional CNOT gates which have  $\epsilon$ -independent T gate costs. Taking the assignment of Table III for the traces we derive

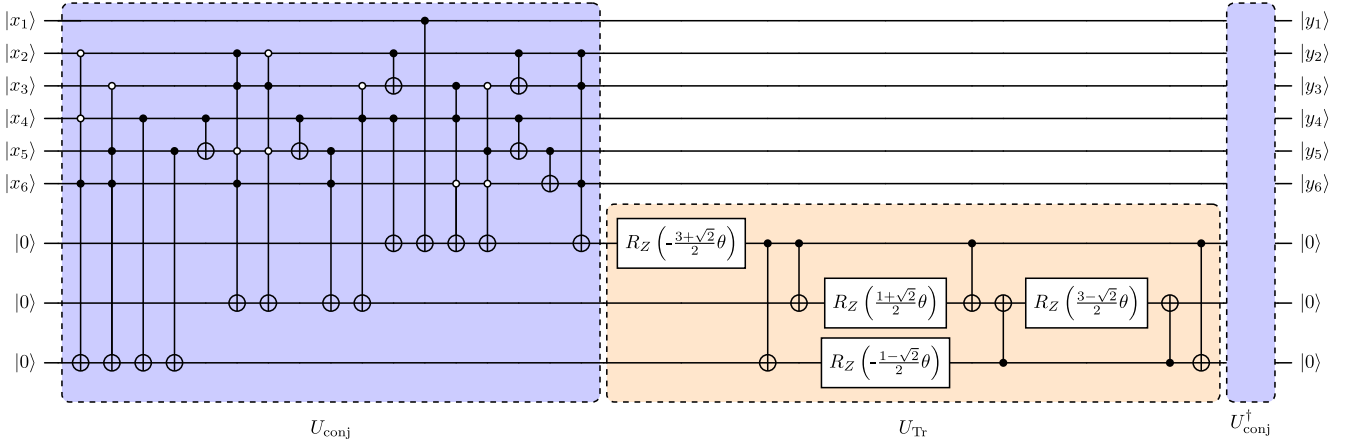
$$(-1)^{x_1} \mathbf{j}^{x_2} \mathbf{k}^{x_3} \mathbf{u}^{2x_4+x_5} \mathbf{t}^{x_6} \mapsto (v_1, v_2, v_3),$$

where

$$\begin{aligned}
 v_1 &= (x_6 + 1)(x_1 + (x_4 + x_5)(1 + x_2)(1 + x_3)) \\
 &\quad + x_6(x_5x_1 + x_4(1 + x_1) + (1 + x_4 + x_5)(x_2x_3 + x_1)), \\
 v_2 &= (x_6 + 1)((1 + x_2)(1 + x_3)(1 + x_4 + x_5)) \\
 &\quad + x_6(x_5x_2 + x_4(1 + x_3) + (1 + x_4 + x_5)(1 + x_2 + x_3)), \\
 v_3 &= (x_6 + 1)(x_4 + x_5) + x_6(x_5x_2 + x_4(1 + x_3) \\
 &\quad + (1 + x_4 + x_5)(1 + x_2 + x_3)).
 \end{aligned} \tag{25}$$

TABLE III. Trace elements and associated bit strings for the conjugacy classes stored in the ancilla. Note,  $v_1$  is a sign bit.

$\text{ReTr}(g)$	0	0	2	-2	1	-1	$\sqrt{2}$	$-\sqrt{2}$
$v_1$	0	1	0	1	0	1	0	1
$v_2$	0	0	1	1	0	0	1	1
$v_3$	0	0	0	0	1	1	1	1

FIG. 5. A qubit implementation of  $\mathcal{U}_{\text{Tr}}$ .

A qubit-based circuit for  $\mathcal{U}_{\text{Tr}}$  is shown in Fig. 5. With this, we will estimate the reduction in fault-tolerant resource gate costs in Sec. IX compared to the  $H_{\text{Tr}}$  method.

### VIII. FOURIER TRANSFORM

The standard  $n$ -qubit quantum Fourier transform (QFT) [166] corresponds to the quantum version of the fast Fourier transform of  $\mathbb{Z}_{2^n}$ . Quantum Fourier transforms over some non-Abelian groups exist [89,167–170]. Alas, for the crystal-like subgroups, efficient QFT circuits are currently unknown [171]. In general, no clear algorithmic way to construct the QFT exists. Thus, we instead construct a suboptimal  $\mathcal{U}_F$  from Eq. (8) from the irreps.

Since  $\mathbb{B}\mathbb{O}$  has 48 elements, on a qubit device  $\mathcal{U}_F$  must be embedded into a larger  $2^d \times 2^d$  unitary. The columns index qubit bitstrings from  $|0\rangle$  to  $|63\rangle$  where the physical states are given by the subset of  $|g\rangle$  in Table I. We then index the irreducible representation  $\rho_i$  sequentially from  $i = 1$  to  $i = 8$ , and construct the matrix, including appropriate padding for the forbidden states. This matrix was then passed to the Qiskit v0.43.1 transpiler, and an optimized version of  $\mathcal{U}_F$  needed 1839 CNOTs, 166  $R_X$ , 1996  $R_Y$ , and 3401  $R_Z$  gates<sup>1</sup>; the Fourier gate is the most expensive qubit primitive and dominates simulation costs.

### IX. RESOURCE ESTIMATES

Clearly quantum practicality with  $\mathbb{B}\mathbb{O}$  will require error corrections. Since the Eastin-Knill theorem restricts QEC codes from having a universal transversal sets of gates [172], compromises must be made. Typically, the Clifford gates are transversal [173–177] while the T gate is not. Thus T gate counts are often used in fault-tolerant resource analysis [173,178]. Recently, novel universal sets have been

proposed with transversal  $\mathbb{B}\mathbb{T}$ ,  $\mathbb{B}\mathbb{O}$ ,  $\mathbb{B}\mathbb{I}$  gates [179–182] which deserve investigation for use with LGT.

The Toffoli gate requires 7 T gates [173] and one method for constructing the  $C^n$ NOT gates is with  $2\lceil \log_2 n \rceil - 1$  Toffoli gates and  $n - 2$  dirty ancilla qubits<sup>2</sup> which can be reused later [173,183,184]. We arrive at the cost for the  $R_Z$  gates via [185] where these gates can be approximated to precision  $\epsilon$  with on average  $1.15\log_2(1/\epsilon)$  T gates (and at worst  $-9 + 4\log_2(1/\epsilon)$  [186]). Further,  $R_Y$  and  $R_X$  can be replaced by at most 3  $R_Z$ . With these, we can construct gate estimates for  $\mathbb{B}\mathbb{O}$  (See Table IV). We note that for  $\epsilon \lesssim 10^{-6}$ , the 20  $R_Z(\theta)$  required for  $e^{i\theta H_{\text{Tr}}}$  is more expensive than the  $\mathcal{U}_{\text{Tr}}$  constructed using  $U_{\text{conj}}$ .

Primitive gate costs for implementing  $H_{\text{KS}}$  [164] and  $H_I$  [80], per link per Trotter step  $\delta t$  are shown in Table V. Using these, we can determine the total T gate count  $N_T^H = C_T^H \times dL^d N_t$  for a  $d$  spatial lattice simulated for a time  $t = N_t \delta t$ . We find that for  $H_{\text{KS}}$

$$C_T^{\text{KS}} = 2863(d - 1) + (22737.8 + 2.3d)\log_2 \frac{1}{\epsilon}. \quad (26)$$

With this, the total synthesis error  $\epsilon_T$  can be estimated as the sum of  $\epsilon$  from each  $R_Z$ . In the case of  $H_{\text{KS}}$  this is

$$\epsilon_T = 2(9886 + d)dL^d N_t \times \epsilon. \quad (27)$$

If one looks to reduce lattice spacing errors for a fixed number of qubits, one can use  $H_I$  which would require

$$C_T^I = 11949d - 10157 + (45473.3 + 6.9d)\log_2 \frac{1}{\epsilon}, \quad (28)$$

where the total synthesis error is

<sup>1</sup>In [90], the Qiskit v0.37.2 was used, yielding for the  $\mathbb{B}\mathbb{T}$   $\mathcal{U}_F$  of 1025 CNOTs, 1109  $R_Y$ , and 2139  $R_Z$  gates. With the v0.43.1 transpiler, we obtain 442 CNOTs, 40  $R_X$ , 494  $R_Y$ , and 835  $R_Z$ .

<sup>2</sup>A *clean* ancilla is in state  $|0\rangle$ . *Dirty* ancillae have unknown states.

TABLE IV. Number of physical T gates and clean ancilla required to implement logical gates for (top) basic gates taken from [173] (bottom) primitive gates for  $\mathbb{B}\mathbb{O}$ .

Gate	T gates	Clean ancilla
$C^2\text{NOT}$	7	0
$C^3\text{NOT}$	21	1
$C^4\text{NOT}$	35	2
CSWAP	7	0
$R_Z$	$1.15 \log_2(1/\epsilon)$	0
$\mathcal{U}_{-1}$	112	1
$\mathcal{U}_\times$	392	4
$\mathcal{U}_{\text{Tr}}$	$340^a + 4.6 \log_2(1/\epsilon)$	2
$\mathcal{U}_{FT}$	$11370.1 \log_2(1/\epsilon)$	0

<sup>a</sup>With 6 additional ancilla, this can be reduced to 188.

TABLE V. Number of primitive gates per link per  $\delta t$  neglecting boundary effects as a function of  $d$  for  $H_{\text{KS}}$  and  $H_I$ .

Gate	$N[H_{\text{KS}}]$	$N[H_I]$
$\mathcal{U}_F$	2	4
$\mathcal{U}_{\text{Tr}}$	$\frac{1}{2}(d-1)$	$\frac{3}{2}(d-1)$
$\mathcal{U}_{-1}$	$3(d-1)$	$2 + 11(d-1)$
$\mathcal{U}_\times$	$6(d-1)$	$4 + 26(d-1)$

$$\epsilon_T = 2(19771 + 3d)dL^d N_t \times \epsilon. \quad (29)$$

Following [57,90,143], we will make resource estimates based on our primitive gates for the calculation of the shear viscosity  $\eta$  on a  $L^3 = 10^3$  lattice evolved for  $N_t = 50$ , and total synthesis error of  $\epsilon_T = 10^{-8}$ . Considering only the time evolution and neglecting state preparation (which can be substantial [12,14,17–21,28,30–33,51,82,84,87,187]), Kan and Nam estimated  $3 \times 10^{19}$  T gates would be required for an pure-gauge  $SU(2)$  simulation of  $H_{\text{KS}}$ . This estimate used a truncated electric-field digitization which requires substantial fixed-point arithmetic—greatly inflating the T gate cost. Using  $\mathbb{B}\mathbb{T}$ , we presently estimate that  $1.1 \times 10^{11}$  T gates would be sufficient<sup>3</sup> but only  $H_I$  could be used. Here, the  $\mathbb{B}\mathbb{O}$  group would require  $4.1 \times 10^{11}$  T gates if  $H_I$  were used—albeit with smaller lattice

<sup>3</sup>This supersedes [90] due to the improved transpiler, proper consideration of  $\epsilon_T$ , and better cost estimates of  $R_X, R_Y$ .

spacing errors than Kan and Nam since they used  $H_{\text{KS}}$ . Thus  $\mathbb{B}\mathbb{O}$  reduces the gate costs of [143] by  $10^8$  for fixed  $L$  by avoiding quantum fixed-point arithmetic while allowing for smaller lattice spacings that  $\mathbb{B}\mathbb{T}$ . If  $H_{\text{KS}}$  were used the T gate cost is reduced to  $2.0 \times 10^{11}$ . Alternatively, if we take the heuristic of [80] that for  $a = \mathcal{O}(0.1 \text{ fm})$  using  $H_I$  could reduce  $L$  by half for fixed lattice spacing errors with only  $4.9 \times 10^{10}$  T gates. Similar to  $\mathbb{B}\mathbb{T}$ ,  $\mathcal{U}_F$  dominates the simulations—99% and 98% of the total cost of simulation  $H_{\text{KS}}$  and  $H_I$ , respectively.

## X. CONCLUSIONS

In this paper, we constructed the necessary primitive gates for the simulation of  $\mathbb{B}\mathbb{O}$ —a crystal-like subgroup of  $SU(2)$ —gauge theories and quantum resource estimates were made for the simulation of pure  $SU(2)$  shear viscosity. Compared to previous fault-tolerant qubit estimates of electric basis truncations, we require  $10^8$  fewer T gates by avoiding quantum fixed point arithmetic via the discrete group approximation. Further, reducing digitization error compared to  $\mathbb{B}\mathbb{T}$  increase the total cost by a factor of  $\sim 4$  perhaps suggesting a  $|G|^2$  scaling.

Looking forward, primitive gates should be constructed for  $\mathbb{B}\mathbb{I}$  and to the subgroups of  $SU(3)$ . At the cost of more qubits,  $\mathbb{B}\mathbb{I}$  would allow smaller digitization error and lattice spacings. To further reduce the qubit-based simulation gate costs for all discrete subgroup approximations, the formalism for deriving the quantum Fourier transform for crystal-like groups remains of paramount interest.

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