

Clifford Quantum Cellular Automata from Topological Quantum Field Theories and Invertible Subalgebras

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We present a general framework for constructing quantum cellular automata (QCAs) from topological quantum field theories (TQFTs) and invertible subalgebras (ISAs) using the cup-product formalism. This approach explicitly realizes all $\mathbb{Z}_2$ and $\mathbb{Z}_p$ Clifford QCAs (for prime p) in all admissible dimensions, in precise agreement with the classification predicted by algebraic L -theory. We determine the orders of these QCAs by explicitly showing that finite powers reduce to the identity up to finite-depth quantum circuits (FDQCs) and lattice translations. In particular, we demonstrate that the $\mathbb{Z}_2$ Clifford QCAs in $(4l + 1)$ spatial dimensions can be disentangled by non-Clifford FDQCs. Our construction applies beyond cubic lattices, allowing $\mathbb{Z}_2$ QCAs to be defined on arbitrary cellulations. Furthermore, we explicitly construct invertible subalgebras in higher dimensions, obtaining $\mathbb{Z}_2$ ISAs in $2l$ spatial dimensions and $\mathbb{Z}_p$ ISAs in $(4l - 2)$ spatial dimensions. These ISAs give rise to $\mathbb{Z}_2$ QCAs in $(2l + 1)$ dimensions and $\mathbb{Z}_p$ QCAs in $(4l - 1)$ dimensions. We further prove that the QCAs in 3 spatial dimensions constructed via TQFTs and ISAs are equivalent by identifying their boundary algebras and show that this approach extends to higher dimensions. Together, these results establish a unified and dimension-periodic framework for Clifford QCAs, connecting their explicit lattice realizations to field theories.

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I. INTRODUCTION

Quantum cellular automata (QCAs) are locality-preserving automorphisms of operator algebras defined on lattices. By definition, a QCA maps any strictly local operator to another whose support increases by at most a finite radius [1]. On a finite lattice, such automorphisms can always be realized by a unitary operator; however, in the thermodynamic limit, QCAs need not decompose into finite-depth quantum circuits (FDQCs). This distinction makes QCAs both mathematically appealing

and physically significant. Mathematically, they provide a complete characterization of locality-preserving unitaries. Physically, they capture nontrivial structures in symmetries and many-body dynamics. QCAs have become central to the modern understanding of lattice symmetries, offering a natural framework for extending symmetry-protected topological phases beyond cohomology [2–6]. They also serve as a foundational tool in the homotopical study of higher symmetries and lattice ’t Hooft anomalies [7–15]. Moreover, QCAs have found wide-ranging applications, including discretized quantum field theories [16], the classification of Floquet phases [17–23], tensor-network unitary operators [24–28], and entanglement growth in quantum dynamics [29–31].

A complete classification of QCAs is known only in one and two spatial dimensions. In these cases, QCAs are labeled by the rational Gross-Nesme-Vogts-Werner (GNVW) index, which quantifies the net flow of quantum information along a given direction [32]. Every one- or two-dimensional QCA can be expressed as a composition

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of finite-depth quantum circuits and lattice translations [33]. In higher dimensions, the structure is considerably richer. Prominent examples include the 3-fermion QCA [1], which disentangles the time-reversal-protected topological phase in three spatial dimensions, along with generalizations constructed from chiral topological orders [34,35]. Many of these higher-dimensional QCAs are *Clifford* QCAs, mapping Pauli operators to Pauli operators. The study of Clifford QCAs lies at the intersection of operator algebras, quantum information theory, and condensed matter physics, connecting algebraic L -theory [36,37], fault-tolerant protocols in measurement-based quantum computation [38–41], and the construction of topological phases [3,42].

Despite significant progress, several fundamental issues remain unresolved. First, although a classification of Clifford QCAs exists [36,37], no general procedure is known for constructing all nontrivial Clifford QCAs in arbitrary dimensions. Second, the algebraic tools for determining their order and composition laws remain incomplete. Third, existing constructions are restricted to (hyper-)cubic lattices and do not extend naturally to arbitrary triangulations or cellulations.

In this work, we address these challenges by constructing Clifford QCAs through two complementary approaches: one based on **topological quantum field theories (TQFTs)** and the other on **invertible subalgebras (ISAs)**. In the first approach, we discretize TQFT actions in the cup-product formalism on cellulations and realize the corresponding topological phases on the lattice through Pauli stabilizer models. In the second approach, we generalize the ISA construction of Ref. [43] to higher dimensions—also using the cup product—extending its applicability to arbitrary cellulations.

Using these frameworks, we construct explicit $\mathbb{Z}_2$ and $\mathbb{Z}_p$ Clifford QCAs in all spatial dimensions, where p is an odd prime. The two approaches yield consistent results, and the resulting families of QCAs align precisely with

the predictions of algebraic L -groups reported in Ref. [36], providing strong evidence that our construction captures all nontrivial Clifford classes. For each QCA, we further show that some finite power reduces to a finite-depth quantum circuit up to a lattice translation, thereby determining its exact order in the quotient group of QCAs modulo circuits and shifts. Moreover, we find that $\mathbb{Z}_2$ Clifford QCAs in $(4l + 1)$ spatial dimensions can be disentangled by non-Clifford finite-depth circuits, whereas their $(4l - 1)$ counterparts remain intrinsically nontrivial. Tables I and II summarize all $\mathbb{Z}_2$ and $\mathbb{Z}_p$ QCAs constructed in this work. The tables list the associated topological actions, indicate whether each QCA is trivialized under non-Clifford finite-depth quantum circuits with shifts, and specify the order of each QCA.

In summary, this paper develops a unified and dimension-periodic method for generating Clifford QCAs, establishes their correspondence with TQFT data, and clarifies their algebraic properties. We expect these results to provide both a conceptual advance in the classification of locality-preserving unitaries and a practical toolkit for designing Floquet protocols and fault-tolerant logical gates in quantum devices.

A. Organization of the paper

This paper is organized as follows. Section II reviews the necessary background on simplicial (co)homology, higher cup products, and the polynomial formalism, and introduces the notations and conventions used throughout this work. Section III constructs the $3 + 1$ D $\mathbb{Z}_2$ and $\mathbb{Z}_p$ QCAs from the TQFT approach and determines their orders. In Sec. IV, we generalize the construction to $\mathbb{Z}_2$ QCAs in $(2l + 1) + 1$ D and to $\mathbb{Z}_p$ QCAs in $(4l - 1) + 1$ D, establishing their periodicities in spatial dimensions. Section V develops the ISA framework, first in $2 + 1$ D and then in higher dimensions, including $\mathbb{Z}_2$ ISAs in $(2l + 1)$ D and $\mathbb{Z}_p$ ISAs in $(4l - 2) + 1$ D, which is consistent with the

TABLE I. Summary of $\mathbb{Z}_2$ Clifford quantum cellular automata in even spacetime dimensions. The $3 + 1$ D $\mathbb{Z}_2$ quantum cellular automata correspond to the 3-fermion Walker-Wang model [44], which can be understood as a gauged $\mathbb{Z}_2 \times \mathbb{Z}_2$ 1-form symmetry-protected topological phase. The corresponding topological actions admit a direct generalization to higher dimensions, from which we construct the associated $\mathbb{Z}_2$ Clifford quantum cellular automata. In spacetime dimensions $D = 4l$, these quantum cellular automata are conjectured to be nontrivial under non-Clifford finite-depth quantum circuits, based on the expectation that the corresponding anomalous boundary theories do not admit commuting-projector Hamiltonians. On the other hand, in $D = 4l + 2$ they become trivial upon allowing non-Clifford circuits, since the term $\frac{1}{2}A_{2l+1} \cup A_{2l+1}$ is a coboundary. Consequently, the classification of $\mathbb{Z}_2$ Clifford quantum cellular automata exhibits a periodicity of 2 in dimension, while allowing non-Clifford circuits reveals that the 3-fermion-type quantum cellular automata occur only every 4 dimensions.

Spacetime dimension D	Topological action in $H^D(K(\mathbb{Z}_2 \times \mathbb{Z}_2, D/2), \mathbb{R}/\mathbb{Z})$	Trivializable by FDQC + shift	Order of QCA
4 (Sec. III A)	$\frac{1}{2}(A_2 \cup A_2 + A_2 \cup B_2 + B_2 \cup B_2)$	No*	2
6 (Sec. IV A)	$\frac{1}{2}(A_3 \cup A_3 + A_3 \cup B_3 + B_3 \cup B_3)$	Yes	2
$4l$ (Sec. IV C)	$\frac{1}{2}(A_{2l} \cup A_{2l} + A_{2l} \cup B_{2l} + B_{2l} \cup B_{2l})$	No*	2
$4l + 2$ (Sec. IV C)	$\frac{1}{2}(A_{2l+1} \cup A_{2l+1} + A_{2l+1} \cup B_{2l+1} + B_{2l+1} \cup B_{2l+1})$	Yes	2

TABLE II. Summary of $\mathbb{Z}_p$ Clifford quantum cellular automata in even spacetime dimensions. These quantum cellular automata exist only in spacetime dimensions $D = 4l$ and are conjectured to remain nontrivial even upon allowing non-Clifford FDQCs. Depending on the residue of $p \bmod 4$, the order of the $\mathbb{Z}_p$ quantum cellular automata is either 2 or 4.

Spacetime dimension D	Topological action in $H^D(K(\mathbb{Z}_p, D/2), \mathbb{R}/\mathbb{Z})$	Trivializable by FDQC + shift	Order of QCA
4 (Sec. III B)	$\frac{k}{p} A_2 \cup A_2$	No*	2 if $p \equiv 1 \pmod{4}$ 4 if $p \equiv 3 \pmod{4}$
$4l$ (Sec. IV D)	$\frac{k}{p} A_{2l} \cup A_{2l}$	No*	2 if $p \equiv 1 \pmod{4}$ 4 if $p \equiv 3 \pmod{4}$

TQFT construction. In Sec. VI, we rigorously establish the equivalence between the 3 + 1D QCAs obtained from the TQFT and ISA constructions by explicitly comparing their associated skew-Hermitian forms. We also present a cup-product analysis of the boundary algebra, which admits a natural extension to higher dimensions. Sec. VII reformulates Clifford QCAs in terms of band-diagonal symplectic matrices, connects them to bounded algebraic K -theory of Pedersen and Weibel, and demonstrates that two Clifford QCAs are equivalent when they disentangle the same stabilizer group. We anticipate that this formalism may be useful in future work.

Technical details and background material are collected in the Appendixes. Appendix A reviews the Laurent polynomial formalism, and Appendix B summarizes higher cup products on hypercubes. Appendix C lists the matrix representations of the 3-fermion-type QCAs in 3 + 1D and 5 + 1D.

By providing explicit constructions that are general across dimensions, together with a comprehensive algebraic analysis, we aim for this work to serve both as a practical toolkit for quantum information applications, such as Floquet engineering in interacting many-body systems, and as a step toward a unified classification of locality-preserving unitaries.

II. NOTATION

Our constructions are formulated using topological quantum field theories (TQFTs) and invertible subalgebras (ISAs), both of which rely on higher cup products and the Laurent polynomial ring. This section reviews the notational conventions used throughout the main text.

We begin with a brief overview of simplicial cohomology, following the conventions of Refs. [42,45]. We define cochains, the coboundary operator, and various cup products, including their higher versions. For extensions to group and higher-group cohomology, we refer the reader to Refs. [46,47]. We then introduce a new compact Einstein summation notation tailored for the Laurent polynomial formalism of Pauli stabilizer codes. The latter was developed in Refs. [48–51], and our summation notation can be

considered an extension of that. A detailed review of the polynomial formalism is provided in Appendix A.

A. Simplicial cohomology

Consider a simplicial complex or cellulation of a manifold M . We may label an n -dimensional simplex/cell as σ_n . In low dimensions, we will also call $\sigma_0 \equiv v$ as vertices, $\sigma_1 = e$ as edges, $\sigma_2 = f$ as faces, and $\sigma_3 = t$ as tetrahedron or $\sigma_3 = c$ as cubes. In general, a p -simplex is denoted by vertices as $\langle 0, 1, 2, \dots, p \rangle$. A p -chain is a formal sum of p -simplices in M with coefficients in the ring R , where R is typically $\mathbb{Z}$ or $\mathbb{Z}_N$. The p -chains form the basis of the chain group $C_p(M, R)$. That is, denoting an arbitrary p -chain as c_p , we have $c_p = \sum_{\sigma_p} a_{\sigma_p} \sigma_p$ with $a_{\sigma_p} \in R$.

Consider the boundary map,

$$\partial : C_p(M, R) \rightarrow C_{p-1}(M, R), \quad (1)$$

which maps a p -simplex to the sum of its boundary simplices in one lower dimension while taking the orientation into account. Specifically, for the oriented p -simplex $\langle 0, 1, \dots, p \rangle$, its boundary is defined as

$$\partial \langle 0, 1, \dots, p \rangle = \sum_{i=0}^p (-1)^i \langle 0, \dots, \hat{i}, \dots, p \rangle, \quad (2)$$

where $\langle 0, \dots, \hat{i}, \dots, p \rangle$ denotes the i th face of $\langle 0, 1, \dots, p \rangle$, obtained by deleting the vertex i .

A p -cochain on M is an R -valued linear function acting on p -chains. The set of all p -cochains on M is $C^p(M, R)$. We use boldface symbols for cochains on M , e.g., $\mathbf{c} \in C^p(M, R)$. Each simplex can be associated with a dual basis element. For instance, a 0-cochain $\mathbf{v}$ is dual to a vertex v via

$$\mathbf{v}(v') = \begin{cases} 1 & \text{if } v' = v, \\ 0 & \text{otherwise.} \end{cases} \quad (3)$$

Similarly, $\mathbf{e}$ is a 1-cochain dual to an edge e , and $\mathbf{f}$ is a 2-cochain dual to a face f and so forth. The cochain dual to $c_p = \sum_{\sigma_p} a_{\sigma_p} \sigma_p$ is $\mathbf{c}_p = \sum_{\sigma_p} a_{\sigma_p} \sigma_p$.

Dual to the boundary operator is the coboundary operator δ , which maps a p -cochain to a $(p + 1)$ -cochain,

$$\delta : C^p(M, R) \rightarrow C^{p+1}(M, R). \quad (4)$$

For a p -cochain c and a $(p + 1)$ -simplex s , we define δ via ∂ as

$$\delta c(s) = c(\partial s). \quad (5)$$

The cup product $\cup$ combines a p -cochain and a q -cochain to produce a $(p + q)$ -cochain,

$$\cup : C^p(M, R) \times C^q(M, R) \rightarrow C^{p+q}(M, R). \quad (6)$$

For instance, for $c \in C^p(M, \mathbb{Z}_2)$ and $d \in C^q(M, \mathbb{Z}_2)$, $c \cup d$ evaluates on a $(p + q)$ -simplex $\langle 0, 1, 2, \dots, p + q \rangle$ as

$$\begin{aligned} (c \cup d)(\langle 0, 1, \dots, p + q \rangle) \\ = c(\langle 0, 1, \dots, p \rangle) d(\langle p, p + 1, \dots, p + q \rangle). \end{aligned} \quad (7)$$

The coboundary operator satisfies the derivation (Leibniz) rule,

$$\delta(c \cup d) = \delta c \cup d + (-1)^p c \cup \delta d, \quad (8)$$

for any p -cochain c and q -cochain d .

We can similarly define higher cup products. A cup- i product $\cup_i$ takes a p -cochain and a q -cochain to a $(p + q - i)$ -cochain,

$$\cup_i : C^p(M, R) \times C^q(M, R) \rightarrow C^{p+q-i}(M, R). \quad (9)$$

Closed-form expressions for higher cup products on simplicial complexes are given in Refs. [52–55]. They satisfy the following recursive relation:

$$\begin{aligned} \delta(c \cup_i d) &= \delta c \cup_i d + (-1)^p c \cup_i \delta d \\ &\quad + (-1)^{p+q-i} c \cup_{i-1} d + (-1)^{pq+p+q} d \cup_{i-1} c, \end{aligned} \quad (10)$$

where $\cup_0 \equiv \cup$. Next, we give a few examples.

For the cup-1 product we have

$$\begin{aligned} (c_p \cup_1 d_q)(\langle 0, \dots, p + q - 1 \rangle) &= \sum_{i=0}^{p-1} (-1)^{(p-i)(q+1)} c_p(\langle 0, \dots, i, q + i, \dots, p + q - 1 \rangle) d_q(\langle i, \dots, q + i \rangle) \\ &:= \sum_{i=0}^{p-1} (-1)^{(p-i)(q+1)} c_p(\langle 0 \rightarrow i, q + i \rightarrow p + q - 1 \rangle) d_q(\langle i \rightarrow q + i \rangle). \end{aligned} \quad (11)$$

For the cup-2 product (nonzero only when $2 \leq p, q$), we obtain

$$\begin{aligned} (c_p \cup_2 d_q)(\langle 0, \dots, p + q - 2 \rangle) &= \sum_{0 \leq i_1 < i_2 \leq p+q-2} (-1)^{(p-i_1)(i_2-i_1-1)} c_p(\langle 0 \rightarrow i_1, i_2 \rightarrow p + i_2 - i_1 - 1 \rangle) \\ &\quad d_q(\langle i_1 \rightarrow i_2, p + i_2 - i_1 - 1 \rightarrow p + q - 2 \rangle). \end{aligned} \quad (12)$$

For a general integer k with $0 \leq k \leq \min\{p, q\}$, the cup- k product is

$$\begin{aligned} (c_p \cup_k d_q)(\langle 0, 1, \dots, p + q - k \rangle) \\ = \sum_{0 \leq i_1 < \dots < i_k \leq p+q-k} (-1)^{\text{sgn}} c_p(\langle 0 \rightarrow i_1, i_2 \rightarrow i_3, \dots \rangle) d_q(\langle i_1 \rightarrow i_2, i_3 \rightarrow i_4, \dots \rangle), \end{aligned} \quad (13)$$

where $\text{sgn}(i_1, \dots, i_k)$ counts the permutations required to rearrange the interleaved sequence

$$0 \rightarrow i_1, \quad i_2 \rightarrow i_3, \dots; \quad i_1 + 1 \rightarrow i_2 - 1, \quad i_3 + 1 \rightarrow i_4 - 1, \dots$$

into the natural order $0 \rightarrow p + q - k$.

Finally, as a convenient shorthand, we write

$$\int_{N_p} c_p := \sum_{s_p \in N_p} c_p(s_p), \quad (14)$$

where N_p is a p -dimensional manifold. When it is clear from the context, we will suppress the subscripts and write $\int_{N_p} c_p$ as $\int c$.

B. Einstein notation for linear maps

We introduce a new notation reminiscent of the Einstein notation that will be useful in bookkeeping many linear maps in cohomology. Readers who prefer to first see the concrete setup may proceed directly to later sections and refer back to this subsection as needed.

First, in this notation, because chains and cochains are dual, we will not use the bold symbol to distinguish cochains from chains to avoid cluttering expressions. Second, the linear maps in this notation will be denoted in bold sans serif font to distinguish it from the bold operators denoting cochains.

In the basis of simplices, the coboundary operator $\delta : C^p \rightarrow C^{p+1}$ may be represented as a linear map, with matrix elements $\delta_{\sigma_{p+1}, \sigma_p}$. Our new notation will be

$$\delta_{\sigma_{p+1}, \delta \sigma_p} := \delta_{\sigma_{p+1}, \sigma_p}. \quad (15)$$

The notational convenience of introducing δ is that we will no longer treat it as the coboundary operator, but as if it is a Kronecker delta. Thus, the above notation means that it is a matrix setting σ_{p+1} equal to $\delta \sigma_p$.

The canonical pairing of chains and cochains allows us to lift the action of the boundary operator on chains, into an action on cochains $\delta^\dagger$, where $\dagger$ denotes the matrix transpose. (Later when using the polynomial formalism, e.g. in Sec. IIC, $\dagger$ will denote the transpose followed by the antipode.) Thus, as a slight abuse of notation, we will take $\partial = \delta^\dagger$ when acting on cochains. With this, we may also define

$$\delta_{\sigma_p, \partial \sigma_{p+1}} = \delta_{\delta \sigma_p, \sigma_{p+1}} := (\delta^\dagger)_{\sigma_{p+1}, \delta \sigma_p}, \quad (16)$$

which intuitively means that we may move the δ from one side to ∂ on the other side and vice versa. In this notation, the (co)chain complex condition reads

$$\delta_{\sigma_{p+1}, \delta \sigma_p} \delta_{\sigma_p, \delta \sigma_{p-1}} = 0, \quad \delta_{\partial \sigma_{p-1}, \sigma_p} \delta_{\partial \sigma_p, \sigma_{p+1}} = 0, \quad (17)$$

where in the above, we implicitly sum over the repeated “index” σ_p .

Next, for any map $Q : C^q \rightarrow C^p$ with matrix elements Q_{σ_p, σ_q} we may define the matrix with “contracted” indices

as follows:

$$Q_{\sigma_p, \delta \sigma_{q-1}} := Q_{\sigma_p, \sigma_q} \delta_{\sigma_q, \delta \sigma_{q-1}}, \quad (18)$$

$$Q_{\sigma_p, \partial \sigma_{q+1}} := Q_{\sigma_p, \sigma_q} \delta_{\sigma_q, \partial \sigma_{q+1}}, \quad (19)$$

$$Q_{\delta \sigma_{p-1}, \sigma_q} := \delta_{\delta \sigma_{p-1}, \sigma_p} Q_{\sigma_p, \sigma_q}, \quad (20)$$

$$Q_{\partial \sigma_{p+1}, \sigma_q} := \delta_{\partial \sigma_{p+1}, \sigma_p} Q_{\sigma_p, \sigma_q}. \quad (21)$$

The above notation allows us to simplify expressions by performing a sum over the repeated index. In particular, this also applies to the matrices δ themselves. For example, by summing over σ_p using the Kronecker delta, in the complex condition Eq. (17), we may write

$$\delta_{\sigma_{p+1}, \delta \sigma_p} \delta_{\sigma_p, \delta \sigma_{p-1}} = \delta_{\sigma_{p+1}, \delta^2 \sigma_{p-1}} = 0, \quad (22)$$

where we “substituted” σ_p for $\delta \sigma_{p-1}$ and used the fact that $\delta^2 = 0$.

We now turn to the linear map corresponding to cup products. Because the cup- i product is a pairing between p -cochains and $d - p + i$ -cochains, for each $p = 1, \dots, d$, we can use it to define multiple linear maps. For each p , we define $M^{(p,i)} : C^p \rightarrow C^{d-p+i}$, which acts as

$$M^{(p,i)}(c_p) = \sum_{\sigma_{d+i-p}} \left(\int \sigma_{d+i-p} \cup_i c_p \right) \sigma_{d+i-p}. \quad (23)$$

Said differently, in the basis of $\sigma_p \in C^p$ and $\sigma_{d+p-i} \in C^{d+p-i}$, the matrix element is exactly

$$M_{\sigma_{d+p-i}, \sigma_p}^{(p,i)} = \int \sigma_{d+p-i} \cup_i \sigma_p. \quad (24)$$

We note that an analogous map was defined in Ref. [5] in order to obtain higher dimensional analogs of the 3F QCA. Here, we slightly improve on the notation of the matrix as follows. We will denote in Einstein notation the matrix elements as

$$\mathbf{M}_{\sigma_{d+p-i} \cup_i \sigma_p} := M_{\sigma_{d+p-i}, \sigma_p}^{(p,i)}, \quad (25)$$

where we opt to use the cup symbol in lieu of the comma for the following esthetic reason: any relation between cup products automatically gives rise to similar looking relations between these linear maps. For example, starting with the Leibniz rule for higher cup products Eq. (10), performing the integral and matching the terms with the matrix

elements gives rise to the following identity:

$$\begin{aligned} \mathbf{M}_{\delta\sigma_q \cup_i \sigma_p} + (-1)^p \mathbf{M}_{\sigma_q \cup_i \delta\sigma_p} \\ + (-1)^{p+q-i} \mathbf{M}_{\sigma_q \cup_{i-1} \sigma_p} + (-1)^{pq+p+q} \mathbf{M}_{\sigma_p \cup_{i-1} \sigma_q}^\dagger = 0, \end{aligned} \quad (26)$$

where $q = d - p + i - 1$. In particular, for $d = 3$ we have

$$\begin{aligned} -\mathbf{M}_{\delta e \cup f} + \mathbf{M}_{e \cup f \delta} - \mathbf{M}_{e \cup f} + \mathbf{M}_{f \cup e}^\dagger = 0, \\ \mathbf{M}_{\delta f' \cup_2 f} + \mathbf{M}_{f' \cup_2 \delta f} + \mathbf{M}_{f' \cup f} + \mathbf{M}_{f' \cup f}^\dagger = 0. \end{aligned} \quad (27)$$

Last, one can show that these matrices satisfy

$$\mathbf{M}_{\partial\sigma_{d-p+2} \cup \partial\sigma_p} = 0. \quad (28)$$

C. Symplectic representation of Pauli matrices

We will now apply this formalism to the symplectic representation of Pauli matrices. See Appendix A for a review of the symplectic representation. We place d -dimensional qudits on each p -dimensional simplex σ_p . The total Hilbert space is then $\bigotimes_{|\mathcal{C}^p|} \mathbb{C}^d$. The generalized Pauli matrices can be represented in symplectic form as

$$\mathbf{Z}_{\sigma_p} = \begin{pmatrix} 0 \\ \mathbb{1} \end{pmatrix}, \quad \mathbf{X}_{\sigma_p} = \begin{pmatrix} \mathbb{1} \\ 0 \end{pmatrix}, \quad (29)$$

where $\mathbb{1}$ is the $|\mathcal{C}^p| \times |\mathcal{C}^p|$ identity matrix. Let us restrict our attention for now to $d = 3$ and consider qudits placed on faces $f = \sigma_2$. Using the index notation, we may write this as

$$\mathbf{Z}_f = \begin{pmatrix} 0 \\ \delta_{f_0 f} \end{pmatrix}, \quad \mathbf{X}_f = \begin{pmatrix} \delta_{f_0 f} \\ 0 \end{pmatrix}, \quad (30)$$

where f_0 denotes a dummy index for the rows of $\mathbf{Z}_f$ and $\mathbf{X}_f$, and $\delta_{f_0 f}$ is, as expected, the Kronecker delta representing the identity matrix. The symplectic inner product in this notation corresponds to summing over the index f_0 ,

$$\langle \mathbf{X}_f, \mathbf{Z}_{f'} \rangle = \sum_{f_0} \mathbf{X}_f^\dagger \mathbf{Z}_{f'} = \delta_{f, f_0} \delta_{f_0 f'} = \delta_{f, f'}. \quad (31)$$

As a further warmup of this notation, we may define the stabilizers of the 3d toric code as

$$\begin{aligned} \mathbf{W}_c &:= \mathbf{Z}_{\partial c} = \begin{pmatrix} 0 \\ \delta_{f_0, \partial c} \end{pmatrix}, \\ \mathbf{B}_e &:= \mathbf{X}_{\delta e} = \begin{pmatrix} \delta_{f_0, \delta e} \\ 0 \end{pmatrix}. \end{aligned} \quad (32)$$

Indeed, we can verify that they commute

$$\langle \mathbf{B}_e, \mathbf{W}_c \rangle = \delta_{\partial e, f} \langle \mathbf{X}_f, \mathbf{Z}_{f'} \rangle \delta_{f', \partial c} = \delta_{e, \partial f} \delta_{f, \partial c} = 0. \quad (33)$$

In specific constructions, we will often meet terms like $\prod_{\sigma_p} P_p^{f_{\sigma_p \cup_i \sigma_q}}$, where P_p is a Pauli operator Z or X living

on a p -simplex σ_p . The σ_p and σ_q in the integral denote the cochains corresponding to the simplexes σ_p and σ_q according to Eq. (3). In our Einstein notation, we can express it as $P_p \times \mathbf{M}_{\sigma_p \cup_i \sigma_q}$. Likewise, the term $P_q^{f_{\sigma_p \cup_i \sigma_q}}$ can be represented by $P_q \times \mathbf{M}_{\sigma_p \cup_i \sigma_q}^\dagger$. Note that the dagger is required for the index to contract correctly in the latter case.

D. Einstein notation in polynomial formalism

In the case of a hypercubic lattice with translation invariance, the notation can be further simplified using a polynomial representation. More specifically, the matrices become circulant matrices, which can be represented by their associated polynomials [50,56]. We denote x_i as the translation in the i th direction, with periodic boundary conditions $x_i^{L_i} = 1$ for integers L_i . The polynomials are elements of the ring $R[x_1, \dots, x_d]/(x_1^{L_1} - 1, \dots, x_d^{L_d} - 1)$. In lower dimensions, we use $x_1 = x$, $x_2 = y$, and $x_3 = z$. A detailed review is given in Appendix A. The polynomial formalism has been used to construct QCAs in three and higher dimensions in Ref. [5]. In this work, we develop the framework systematically and introduce new notations that allow us to express the resulting QCAs more compactly.

Figure 1 illustrates how Pauli operators on a two-dimensional square lattice can be represented by a 4×1 polynomial matrix. The first and second entries correspond to Pauli- X operators pointing in the x - and y -directions, while the third and fourth entries correspond to Pauli- Z operators in each direction. The entries of the matrix depend on the choice of base point, which in Fig. 1 is

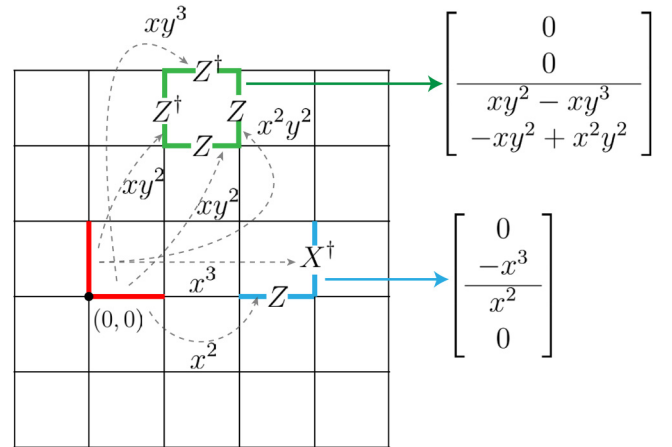


FIG. 1. Examples of polynomial expressions for Pauli operators adapted from Ref. [57]. The flux operator on a plaquette and the XZ operator on edges are shown. Red edges mark the chosen base edge, while all other edges follow from it by lattice translations. Monomials such as x^2y^2 and x^2 specify operator locations relative to the origin. A detailed review is provided in Appendix A.

taken to be the origin (0, 0). Shifting the base point corresponds to multiplying the matrix representation by an overall monomial factor.

Let us consider the three-dimensional cubic lattice in particular. The cochain complex takes the form of a tensor product of one-dimensional complexes and expands as

$$\begin{aligned} C^0 &\xrightarrow{\delta_{e,v}} C_x^1 \oplus C_y^1 \oplus C_z^1 \\ &\xrightarrow{\delta_{f,e}} C_{yz}^2 \oplus C_{xz}^2 \oplus C_{xy}^2 \\ &\xrightarrow{\delta_{c,f}} C^3, \end{aligned} \quad (34)$$

where C_x^1 denotes edges oriented in the x direction, C_{yz}^2 denotes faces oriented along the yz plane, and similarly for the other orientations.

Likewise, the corresponding chain complex expands as

$$\begin{aligned} C^0 &\xleftarrow{\partial_{v,e}} C_x^1 \oplus C_y^1 \oplus C_z^1 \\ &\xleftarrow{\partial_{e,f}} C_{yz}^2 \oplus C_{xz}^2 \oplus C_{xy}^2 \\ &\xleftarrow{\partial_{f,c}} C^3. \end{aligned} \quad (35)$$

The (co)boundary operators are defined as the maps between the respective (co)chains on the direct lattice, using the polynomial representation. However, throughout this work, we will adopt a polynomial representation defined on the dual lattice. This is because our figures are drawn on the dual lattice where faces are depicted as edges for visual clarity. In our Einstein notation, we have

$$\delta_{e,\delta v} = \delta_{\partial e,v} = \begin{pmatrix} 1-x \\ 1-y \\ 1-z \end{pmatrix}, \quad (36)$$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \times \begin{pmatrix} 0 & z-1 & 1-y \\ z-1 & 0 & 1-x \\ y-1 & 1-x & 0 \end{pmatrix} = \begin{pmatrix} 0 & z-1 & 1-y \\ z-1 & 0 & 1-x \\ y-1 & 1-x & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

FIG. 2. An illustration on the dual lattice showing the construction of the flux terms B_e via the action of the coboundary matrix $\delta_{f,\delta e}$ on the vector of operators X_f . A Pauli operator X_f is supported on each face f , and the product $X_f \delta_{f,\delta e}$ yields the flux term $X_{\delta e} = B_e$. The three colored plaquettes correspond to the yz , xy , and xz orientations, with the associated polynomial expressions shown below.

$$\delta_{f,\delta e} = \delta_{\partial f,e} = \begin{pmatrix} 0 & z-1 & 1-y \\ z-1 & 0 & 1-x \\ y-1 & 1-x & 0 \end{pmatrix}, \quad (37)$$

$$\delta_{c,\delta f} = \delta_{\partial c,f} = (1-x \quad y-1 \quad 1-z). \quad (38)$$

If we want to construct the Pauli-X or Z operators on coboundaries like δe , we just multiply the original X_f or Z_f matrix by the coboundary operator $\delta_{f,\delta e}$. Similar rules hold in higher dimensions. In Fig. 2, we give an example of constructing stabilizers using our Einstein notation on the dual cubic lattice. Specifically, in polynomial representation, the stabilizers of the 3d toric code are constructed as

$$\mathbf{W}_e = \mathbf{Z}_{\delta e} = \mathbf{Z}_f \delta_{f,\delta e} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1-\bar{x} \\ \bar{y}-1 \\ 1-\bar{z} \end{pmatrix}, \quad (39)$$

$$\mathbf{B}_e = \mathbf{X}_{\delta e} = \mathbf{X}_f \delta_{f,\delta e} = \begin{pmatrix} 0 & z-1 & 1-y \\ z-1 & 0 & 1-x \\ y-1 & 1-x & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (40)$$

III. CLIFFORD QCAs IN 3 + 1D FROM TQFTs

In this section, we use cup products to construct all $\mathbb{Z}_2$ and $\mathbb{Z}_p$ Clifford QCAs in 3 + 1D associated with the (classical) Witt group. These QCAs generate bulk states whose truncations yield commuting-projector models on the 2 + 1D boundary, supporting chiral Abelian anyon theories. The $\mathbb{Z}_2$ Clifford QCA was first obtained in Ref. [1], while the $\mathbb{Z}_p$ cases were later developed in Ref. [34]. Here, we unify these constructions within a TQFT framework,

showing that they arise from the same method under different choices of topological actions. Previous approaches were restricted to cubic lattices, whereas our formulation of the $\mathbb{Z}_2$ Clifford QCA applies to arbitrary cellulations. In addition, the construction extends naturally to higher dimensions, as we demonstrate in Sec. IV.

First, we briefly review the Walker-Wang framework, which provides a systematic construction of $3 + 1$ D lattice models with nontrivial boundary anyon theories [44]. When the input data consist of a *premodular* anyon theory (braided fusion category containing nontrivial transparent anyons) the resulting Walker-Wang model exhibits a nontrivial bulk Hamiltonian whose $(2 + 1)$ D boundary realizes precisely the input anyon theory [58]. In contrast, when the input theory is *modular*, the bulk Hamiltonian is trivial, in the sense that it supports no deconfined excitations, and the unitary mapping from a product state to the ground state defines a QCA.

An Abelian anyon theory is specified by a finite Abelian group A together with a quadratic function $q : A \rightarrow \mathbb{Q}/\mathbb{Z}$ [59], where the topological spin of an anyon $a \in A$ is given by $q(a)$. Such quadratic functions are in one-to-one correspondence with cohomology classes in $H^4(K(A, 2), \mathbb{R}/\mathbb{Z})$ [47,60–63], which classify 2-form Dijkgraaf-Witten TQFT [64]. Consequently, the Abelian Walker-Wang model can be naturally interpreted as a gauged 1-form symmetry-protected topological (SPT) phase [46].

We are interested in constructing QCAs corresponding to the generators of the Witt group of Abelian anyon theories. The Witt group gives an equivalence class of anyon theories up to stacking with anyon theories that admit a gapped boundary (Drinfeld center of some fusion category) [65]. Formally, two modular tensor categories $\mathcal{A}$ and $\mathcal{B}$ lie in the same Witt class if their product $\mathcal{A} \otimes \mathcal{B}$ admits a gapped boundary, or equivalently, if a set of bosons can be condensed to trivialize the combined theory. Intuitively, the Witt group captures the “indecomposable” topological orders that cannot be removed by boson condensation. Its group operation is stacking of anyon theories, and the inverse of a theory is given by its time-reversal. In this work, we restrict to Abelian anyon theories, and the Witt group reduces to the classical Witt group of quadratic forms over finite Abelian groups.

The relation to the L -theoretic classification of Clifford QCAs can be summarized as follows. Any finite abelian group admits a primary decomposition,

$$\bigoplus_i \mathbb{Z}_{p_i^{r_i}},$$

where the $p_i^{r_i}$ are powers of (not necessarily distinct) primes. Quadratic forms on finite abelian groups decompose compatibly with this primary decomposition (Proposition 76 of Ref. [66]). Consequently, the associated Witt

group decomposes as a direct sum of its p_i -primary components (Proposition 5.16 of Ref. [67]).

Restricting to a fixed prime- p power cyclic group, one may realize its quadratic forms by reduction from quadratic forms on free $\mathbb{Z}_{p^r}$ -modules, for r sufficiently large. The classification of Clifford QCAs for qudit dimension p^r developed in Refs. [36,37] identifies the relevant invariant as $L_{3D}(\mathbb{Z}_{p^r})$. In spatial dimension $D = 3$, this reduces to $L_0(\mathbb{Z}_{p^r})$. This group is precisely the Witt group of free $\mathbb{Z}_{p^r}$ -modules equipped with a quadratic form and hence reproduces the corresponding p -primary direct summand of the Witt group upon allowing all possible values of r .

For Abelian anyon theories with a single generator (i.e., A cyclic), we follow the notation of Ref. [68] and denote the anyon theory described by the group $A = \mathbb{Z}_n$ and the quadratic form $q(a) = (m/n)a^2 : \mathbb{Z}_n \rightarrow \mathbb{Q}/\mathbb{Z}$ as $\mathbb{Z}_n^{(m)}$. The generators of the Witt group decompose according to prime numbers as follows [65]:

- (1) For $p = 2$ (anyon groups of order 2^k), the Witt group contains the subgroup $\mathbb{Z}_8 \times \mathbb{Z}_2$. The relevant elements include:
 - (a) $(1, 0) \in \mathbb{Z}_8 \times \mathbb{Z}_2$: the chiral semion theory $(\mathbb{Z}_2^{(1/2)})$,
 - (b) $(1, 1) \in \mathbb{Z}_8 \times \mathbb{Z}_2$: the $U(1)_4$ theory $(\mathbb{Z}_4^{(1/2)})$,
 - (c) $(4, 0) \in \mathbb{Z}_8 \times \mathbb{Z}_2$: the 3-fermion theory, with $A = \mathbb{Z}_2 \times \mathbb{Z}_2$ and $q((a, b)) = \frac{1}{2}(a^2 + ab + b^2)$.

Among these, only the 3-fermion theory gives rise to a Clifford QCA.

- (2) For each prime $p \equiv 3 \pmod{4}$, the Witt group contributes a $\mathbb{Z}_4$ subgroup generated by $\mathbb{Z}_p^{(1)}$, all of which correspond to Clifford QCAs.
- (3) For each prime $p \equiv 1 \pmod{4}$, the Witt group contributes a $\mathbb{Z}_2 \times \mathbb{Z}_2$ subgroup generated by $\mathbb{Z}_p^{(1)}$ and $\mathbb{Z}_p^{(r)}$, where r is a quadratic nonresidue modulo p . All of these also correspond to Clifford QCAs.

To construct these QCAs explicitly, we first review the definition of a QCA in terms of *separators* and *flippers*.

Definition 1 (Separators and flippers [69]). A locally flippable $\mathbb{Z}_p$ separator consists of a set of operators $\{\bar{Z}_a\}$ together with another set of operators $\{\tilde{X}_a\}$, called flippers. Each operator is supported within a disk of finite radius, and the following conditions are satisfied:

- (1) $(\bar{Z}_a)^p = 1$.
- (2) $[\bar{Z}_a, \bar{Z}_b] = 0$ for all a, b .
- (3) $\bar{Z}_a \tilde{X}_b = e^{2\pi i/p} \tilde{X}_b \bar{Z}_a$ if $a = b$; otherwise, $\bar{Z}_a$ and $\tilde{X}_b$ commute.
- (4) For an arbitrary assignment $a \mapsto \omega(a)$, where $\omega(a)$ is a p th root of unity, the space of states $|\psi\rangle$

satisfying

$$\bar{Z}_a |\psi\rangle = \omega(a) |\psi\rangle$$

for all a is one-dimensional.

In the above definition, the flippers $\tilde{X}_a$ are not required to commute with one another. However, this issue can be resolved by appropriately decorating them with the operators $\bar{Z}_a$, yielding modified flippers $\bar{X}_a$ that commute mutually. With these ingredients, a QCA α is then defined by its action on the Pauli generators,

$$\alpha(Z_a) = \bar{Z}_a, \quad \alpha(X_a) = \bar{X}_a. \quad (41)$$

Our construction of QCAs proceeds as follows. We begin with TQFT data, namely a cohomology class, and follow the standard procedure to obtain the ground-state wave function of a symmetry-protected topological (SPT) phase [46]. Upon gauging the symmetry, this yields the ground-state wave function of a Dijkgraaf-Witten TQFT [64], whose special cases include the Walker-Wang models considered in this work.

Given a ground-state wave function, however, there are infinitely many possible choices of parent Hamiltonians. Our goal is to identify a particular parent Hamiltonian that can be written as a sum of locally flippable separators,

$$H_{\text{parent}} = - \sum_i \bar{Z}_i, \quad (42)$$

such that the operators $\bar{Z}_i$ admit flippers in the sense of Definition 1. Organizing a parent Hamiltonian into this form is generally a highly nontrivial task. Fortunately, the cup-product formalism provides a systematic and efficient way to construct such Hamiltonians in our setting.

A. 3-fermion QCA from topological action

$$S = \frac{1}{2} (A_2 \cup A_2 + B_2 \cup B_2 + A_2 \cup B_2)$$

We begin with the QCA constructed from the 3-fermion Walker-Wang model on arbitrary cellulations. When restricted to the cubic lattice, our construction here reproduces the QCA obtained in Ref. [35], which is equivalent to the original construction in Ref. [1] up to a finite-depth quantum circuit.

The 3-fermion anyon theory corresponds to the anyon group $A = \mathbb{Z}_2 \times \mathbb{Z}_2$ and $q(a, b) = \frac{1}{2}(a^2 + ab + b^2)$, where a, b are the generators of the group. The terms a^2 and b^2 endow the generating anyons with fermionic self-statistics, while the term ab gives the mutual statistics, resulting in their bound state also having fermionic self-statistics. To write down the corresponding Walker-Wang model on the lattice, we place two qubits (denoted by its sublattices A and B) on each face f . We then write down the

gauge theory with the following topological action on a (3+1)-dimensional manifold [42]:

$$S = \frac{1}{2} \int A_2 \cup A_2 + B_2 \cup B_2 + A_2 \cup B_2, \quad (43)$$

where the subscript denotes the A_2 and B_2 are 2-cocycles. Here, and throughout the paper, we will implicitly assume that all gauge fields are dynamical, rather than background gauge fields. This means that we implicitly sum over all configurations which are flat $\delta A_2 = \delta B_2 = 0$.

Following Refs. [42,70], we write the Hamiltonian for the gauge theory described above on a three-dimensional lattice. On each face f , we introduce Pauli operators Z_f^A, X_f^A and Z_f^B, X_f^B . The Hamiltonian takes the form

$$H^{3f} = - \sum_t Z_{\partial t}^A - \sum_t Z_{\partial t}^B - \sum_e G_e^B \prod_f Z_f^{A f \cup e} - \sum_e G_e^A \prod_f Z_f^{B f \cup e}, \quad (44)$$

where t denotes a 3-cell, f a 2-cell, and G_e^α is the gauge constraint of the 3 + 1D bosonization [71], defined as

$$G_e^\alpha := X_{\delta e}^\alpha \prod_{f'} Z_{f'}^{\alpha f \cup \delta e \cup f'}, \quad \alpha \in \{A, B\}. \quad (45)$$

Here, $Z_{\partial t}^\alpha$ denotes the flux term, defined as the product of Z_f^α over the surface of a three-dimensional cell,

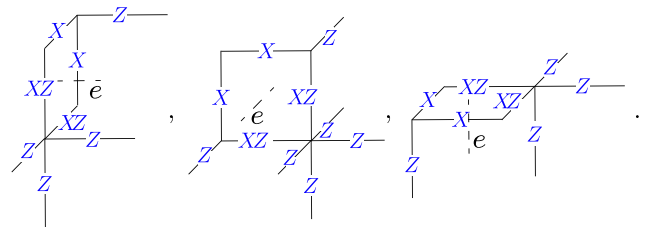
$$Z_{\partial t} := \prod_f Z_f^{f(\partial t)} = \prod_f Z_f^{f \cup \delta f \cup t}, \quad (46)$$

$$X_{\delta e} := \prod_f X_f^{e(\partial f)}.$$

In the special case of a cubic lattice, where edges e and faces f are in one-to-one correspondence through $e \cup f$ or $f \cup e$, the Hamiltonian simplifies to

$$H^{3f} = - \sum_c Z_{\partial c}^A - \sum_c Z_{\partial c}^B - \sum_f Z_f^A \prod_e G_e^{B f \cup e} - \sum_f Z_f^B \prod_e G_e^{A f \cup e}. \quad (47)$$

The 3-cell is now labeled by a cube c , and the operator G_e^α in Eq. (45) can be represented diagrammatically:



where, for clarity, all operators are illustrated on the dual lattice (solid lines), while the dashed line marks the edge e on the original lattice. Consequently, the third and fourth terms of Eq. (47) can be depicted as

$$Z_f^A \prod_e G_e^{Bf} f^{\cup e} = \text{[Diagram 1]}, \text{[Diagram 2]}, \text{[Diagram 3]}, \quad (48)$$

$$Z_f^B \prod_e G_e^{Af} e^{\cup f} = \text{[Diagram 4]}, \text{[Diagram 5]}, \text{[Diagram 6]}. \quad (49)$$

Note that if we multiply G_e^α around faces of a closed membrane on the dual lattice (equivalently, around a vertex on the direct lattice), the product becomes the identity

$$\prod_{e \supset v} G_e^\alpha = 1, \quad \forall \alpha \in \{A, B\}. \quad (50)$$

Consequently, we observe that the third and fourth terms of Eq. (47) generate the first and second terms. Thus, we may remove these two terms from the Hamiltonian without affecting its ground state.

Since the ground state is uniquely determined by the last two terms, we may define the separators of the QCA as

$$\begin{aligned} \bar{Z}_f^A &= Z_f^A \prod_e G_e^{Bf} f^{\cup e}, \\ \bar{Z}_f^B &= Z_f^B \prod_e G_e^{Af} e^{\cup f} \end{aligned} \quad (51)$$

on each face. They are the original Z operators decorated with the G operator for the other species of qubits. In the 3 + 1D bosonization [71], the fermion hopping operators are given by

$$\begin{aligned} U_f^A &:= X_f^A \prod_{f'} Z_{f'}^{Af} f'^{\cup f}, \\ U_f^B &:= X_f^B \prod_{f'} Z_{f'}^{Bf} f'^{\cup f}, \end{aligned} \quad (52)$$

where the cup-1 product encodes the interaction between Pauli operators on adjacent faces. They satisfy the commutation relations

$$U_f^\alpha U_{f'}^\alpha = (-1)^{f \cup f' + f' \cup f} U_{f'}^\alpha U_f^\alpha, \quad (53)$$

$\forall \alpha \in \{A, B\}$. The explicit realizations on the cubic lattice are

$$U_f = \text{[Diagram 7]}, \text{[Diagram 8]}, -\text{[Diagram 9]}. \quad (54)$$

Since $[U_f^\alpha, G_e^\beta] = 0$ for all $\alpha, \beta \in \{A, B\}$, we also find $[\bar{Z}_f^A, U_{f'}^B] = [\bar{Z}_f^B, U_{f'}^A] = 0$. Therefore, we have

$$\begin{aligned} \bar{Z}_f^A U_{f'}^A &= (-1)^{\delta_{f,f'}} U_{f'}^A \bar{Z}_f^A, \\ \bar{Z}_f^B U_{f'}^B &= (-1)^{\delta_{f,f'}} U_{f'}^B \bar{Z}_f^B. \end{aligned} \quad (55)$$

Hence, the hopping operators U_f^A and U_f^B act as (noncommuting) flippers for the separators $\bar{Z}_f^A$ and $\bar{Z}_f^B$. We may fix this noncommutation by attaching separators to cancel the sign coming from the commutation relation in Eq. (53).

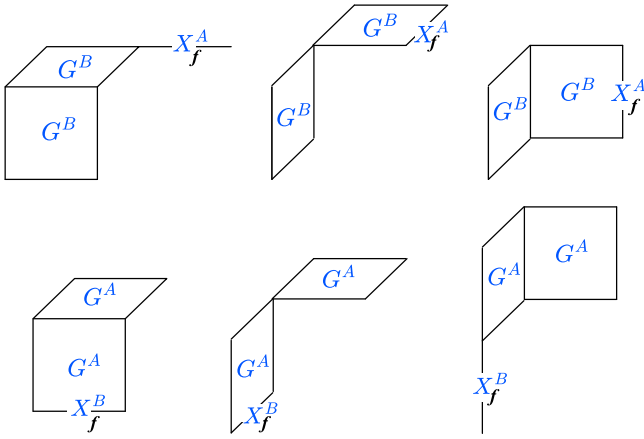


FIG. 3. The flippers $\bar{X}_f^A$ and $\bar{X}_f^B$ of the 3-fermion quantum cellular automata on the dual lattice, with G^A and G^B defined in Eq. (45).

Define

$$\begin{aligned}\bar{X}_f^A &:= U_f^A \prod_{f'} \bar{Z}_{f'}^A \int f' \cup_1 f = X_f^A \prod_{f'} \left(Z_{f'}^A \bar{Z}_{f'}^A \right)^{\int f' \cup_1 f} \\ &= X_f^A \prod_{e, f'} \left(G_e^B \int f' \cup_e \right)^{\int f' \cup_1 f}, \\ \bar{X}_f^B &:= U_f^B \prod_{f'} \bar{Z}_{f'}^B \int f' \cup_1 f = X_f^B \prod_{f'} \left(Z_{f'}^B \bar{Z}_{f'}^B \right)^{\int f' \cup_1 f} \\ &= X_f^B \prod_{e, f'} \left(G_e^A \int e \cup f' \right)^{\int f' \cup_1 f}.\end{aligned}\quad (56)$$

These flippers on the cubic lattice can be visualized in Fig. 3. We may also separately verify that $[\bar{X}_f^A, \bar{X}_{f'}^A] = [\bar{X}_f^B, \bar{X}_{f'}^B] = 0$ using the final expression by noting that G_e^α commutes for distinct edges e (this property holds only for $\mathbb{Z}_2$ qubits).

The 3-fermion quantum cellular automaton (QCA) is defined as

$$\begin{aligned}X^A &\rightarrow \bar{X}^A, & Z^A &\rightarrow \bar{Z}^A, \\ X^B &\rightarrow \bar{X}^B, & Z^B &\rightarrow \bar{Z}^B.\end{aligned}\quad (57)$$

1. Order of 3-fermion QCA

We will show that this QCA squares to the identity. To prove this, it suffices to show that G_e^α is invariant under the QCA, since the action of the QCA attaches an appropriate set of G_e to both X and Z . Thus, if this is the case, then we have

$$X \rightarrow X \prod G_e \rightarrow \left(X \prod G_e^2 \right) = X \quad (58)$$

and similarly for Pauli Z . To verify this, observe that

$$\begin{aligned}U_f^A &\rightarrow \bar{X}_f^A \prod_{f'} \bar{Z}_{f'}^A \int f' \cup_1 f \\ &= \left[U_f^A \prod_{f'} \bar{Z}_{f'}^A \int f' \cup_1 f \right] \prod_{f'} \bar{Z}_{f'}^A \int f' \cup_1 f = U_f^A,\end{aligned}\quad (59)$$

$$\begin{aligned}U_f^B &\rightarrow \bar{X}_f^B \prod_{f'} \bar{Z}_{f'}^B \int f' \cup_1 f \\ &= \left[U_f^B \prod_{f'} \bar{Z}_{f'}^B \int f' \cup_1 f \right] \prod_{f'} \bar{Z}_{f'}^B \int f' \cup_1 f = U_f^B.\end{aligned}\quad (60)$$

Thus, the hopping operator remains invariant under the QCA. By construction, the flux term $Z_{\partial c}^\alpha$ is also invariant under the QCA, due to Eq. (50). Consequently, the gauge constraint G_e^α is invariant under the QCA. Explicitly, we have

$$\begin{aligned}G_e &= \left(X_{\delta e} \prod_{f'} Z_{f'}^{\int f' \cup_1 \delta e} \right) \prod_{f'} Z_{f'}^{\int \delta e \cup_1 f' + f' \cup_1 \delta e} \\ &= U_{\delta e} \prod_{f'} Z_{f'}^{\int \delta e \cup_2 \delta f'} = U_{\delta e} \prod_c Z_{\partial c}^{\delta e \cup_2 c},\end{aligned}\quad (61)$$

where $U_{\delta e} := X_{\delta e} \prod_{f'} Z_{f'}^{\int f' \cup_1 \delta e}$ represents a product of U_f around an edge e , up to an overall $\pm$ sign. It is important to emphasize that the property of G_e being a product of U_f and $Z_{\partial c}$ is specific to $\mathbb{Z}_2$ qubits. In the QCA with $\mathbb{Z}_p$ qudits discussed in the next section, G_e is no longer expressible as a simple product of U_f and $Z_{\partial c}$. Therefore, while it is generally true in our construction that U_f and $Z_{\partial c}$ (as well as their generalization in higher dimensions) remain invariant under the QCA, the invariance of G_e under the QCA is unique to $\mathbb{Z}_2$ qubit systems.

2. Polynomial expression for 3-fermion QCA

Since we have two qubits species A and B , we define

$$\mathbf{Z}^A = \begin{pmatrix} 0 \\ 0 \\ \delta_{f_0, f} \\ 0 \end{pmatrix}, \quad \mathbf{Z}^B = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \delta_{f_0, f} \end{pmatrix}, \quad (62)$$

$$\mathbf{X}^A = \begin{pmatrix} \delta_{f_0, f} \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad \mathbf{X}^B = \begin{pmatrix} 0 \\ \delta_{f_0, f} \\ 0 \\ 0 \end{pmatrix}. \quad (63)$$

The hopping operators and the gauge constraint can be written in polynomial form as

$$\mathbf{U}_f^\alpha = \mathbf{X}_f^\alpha + k\mathbf{Z}_{f'}^\alpha \mathbf{M}_{f' \cup 1f}, \quad (64)$$

$$\tilde{\mathbf{U}}_f^\alpha = \mathbf{X}_f + k\mathbf{Z}_{f'}^\alpha \mathbf{M}_{f' \cup 1f}^\dagger, \quad (65)$$

$$\mathbf{G}_e^{(k)} = \tilde{\mathbf{U}}_{\delta e}^\alpha. \quad (66)$$

Finally, we can write the separators and flippers as

$$\bar{\mathbf{Z}}_f^A = \mathbf{Z}_f^A + \mathbf{G}_e^B \mathbf{M}_{f' \cup e}^\dagger,$$

$$\bar{\mathbf{Z}}_f^B = \mathbf{Z}_f^B + \mathbf{G}_e^A \mathbf{M}_{e \cup f},$$

$$\bar{\mathbf{X}}_f^A = \mathbf{U}_f^A + \bar{\mathbf{Z}}_{f'}^A \mathbf{M}_{f' \cup 1f} = \mathbf{X}_f^A + \mathbf{G}_e^B \mathbf{M}_{f' \cup e}^\dagger \mathbf{M}_{f' \cup 1f},$$

$$\bar{\mathbf{X}}_f^B = \mathbf{U}_f^B + \bar{\mathbf{Z}}_{f'}^B \mathbf{M}_{f' \cup 1f} = \mathbf{X}_f^B + \mathbf{G}_e^A \mathbf{M}_{e \cup f} \mathbf{M}_{f' \cup 1f}.$$

In matrix form,

$$\begin{aligned} \bar{\mathbf{Z}}^A &= \begin{pmatrix} 0 & & & \\ & \mathbf{M}_{f' \cup \partial f_0}^\dagger & & \\ & \delta_{f_0 f} & & \\ & \mathbf{M}_{f' \cup 1f_0}^\dagger & \mathbf{M}_{f' \cup \partial f'}^\dagger & \end{pmatrix}, \quad \bar{\mathbf{Z}}^B = \begin{pmatrix} \mathbf{M}_{\partial f_0 \cup f} & & & \\ & 0 & & \\ \mathbf{M}_{f' \cup 1f_0}^\dagger & \mathbf{M}_{\partial f' \cup f} & & \\ & \delta_{f_0 f} & & \end{pmatrix}, \\ \bar{\mathbf{X}}^A &= \begin{pmatrix} & \delta_{f_0 f} & & \\ & \mathbf{M}_{f' \cup \partial f_0}^\dagger & \mathbf{M}_{f' \cup 1f} & \\ & & 0 & \\ \mathbf{M}_{f'' \cup 1f_0}^\dagger & \mathbf{M}_{f' \cup \partial f''}^\dagger & \mathbf{M}_{f' \cup 1f} & \end{pmatrix}, \quad \bar{\mathbf{X}}^B = \begin{pmatrix} & \mathbf{M}_{\partial f_0 \cup f'} \mathbf{M}_{f' \cup 1f} & & \\ & \delta_{f_0 f} & & \\ \mathbf{M}_{f'' \cup 1f_0}^\dagger & \mathbf{M}_{\partial f'' \cup f'} \mathbf{M}_{f' \cup 1f} & & \\ & 0 & & \end{pmatrix}. \end{aligned} \quad (67)$$

This allows us to define the 3F QCA as

$$\alpha = \begin{pmatrix} \bar{\mathbf{X}}^A & \bar{\mathbf{X}}^B & \bar{\mathbf{Z}}^A & \bar{\mathbf{Z}}^B \end{pmatrix}. \quad (68)$$

The above QCA has been presented in polynomial form in Ref. [35], albeit in a different basis. The matrix elements of our 3F QCA can be found in Appendix C 1. We will later show in Sec. IV that higher-dimensional generalizations of the 3F QCA can be straightforwardly written by replacing the simplices to higher-dimensional ones. In fact, in $5 + 1\text{D}$, these matrices coincide with those constructed in Ref. [5].

We may show explicitly that the QCA squares exactly to the identity. Before that, we first prove some simple identities. Let us show that

$$\begin{pmatrix} \mathcal{O}_{f_0 f}^{(11)} & \cdots & \mathcal{O}_{f_0 f}^{(14)} \\ \vdots & \ddots & \vdots \\ \mathcal{O}_{f_0 f}^{(41)} & \cdots & \mathcal{O}_{f_0 f}^{(44)} \end{pmatrix} := \begin{pmatrix} \mathbf{M}_{\partial f_0 \cup f'} \\ \mathbf{M}_{f' \cup \partial f_0}^\dagger \\ \mathbf{M}_{f_0 \cup \partial f'} \\ \mathbf{M}_{\partial f' \cup f_0}^\dagger \end{pmatrix} (\mathbf{M}_{f' \cup 1f''} + \mathbf{M}_{f'' \cup 1f'}^\dagger) \times \begin{pmatrix} \mathbf{M}_{\partial f'' \cup f}^\dagger & \mathbf{M}_{f'' \cup \partial f} & \mathbf{M}_{f' \cup \partial f''}^\dagger & \mathbf{M}_{\partial f'' \cup f} \end{pmatrix} = 0. \quad (69)$$

For example,

$$\begin{aligned} \mathcal{O}_{f_0 f}^{(13)} &= \mathbf{M}_{\partial f_0 \cup f'} (\mathbf{M}_{f' \cup 1f''} + \mathbf{M}_{f'' \cup 1f'}^\dagger) \mathbf{M}_{f' \cup \partial f''}^\dagger = \mathbf{M}_{\partial f_0 \cup f'} (\mathbf{M}_{\delta f' \cup 2f''} + \mathbf{M}_{f' \cup 2\delta f''}^\dagger) \mathbf{M}_{f' \cup \partial f''}^\dagger \\ &= \mathbf{M}_{\partial f_0 \cup \partial c} \mathbf{M}_{c \cup 2f''} \mathbf{M}_{f' \cup \partial f''}^\dagger + \mathbf{M}_{\partial f_0 \cup f'} \mathbf{M}_{f' \cup 2c}^\dagger \mathbf{M}_{f' \cup \partial 2c}^\dagger = 0 \end{aligned}$$

and

$$\begin{aligned} \mathcal{O}_{f_0 f}^{(24)} &= \mathbf{M}_{f' \cup \partial f_0}^\dagger (\mathbf{M}_{f' \cup 1f''} + \mathbf{M}_{f'' \cup 1f'}^\dagger) \mathbf{M}_{\partial f'' \cup f} = \mathbf{M}_{f' \cup \partial f_0}^\dagger (\mathbf{M}_{\delta f' \cup 2f''} + \mathbf{M}_{f' \cup 2\delta f''}^\dagger) \mathbf{M}_{\partial f'' \cup f} \\ &= \mathbf{M}_{f' \cup \partial 2c}^\dagger \mathbf{M}_{c \cup 2f''} \mathbf{M}_{\partial f'' \cup f} + \mathbf{M}_{f' \cup \partial f_0}^\dagger \mathbf{M}_{f' \cup 2c}^\dagger \mathbf{M}_{\partial 2c \cup f} = 0 \end{aligned}$$

evaluate to zero using the relation of the $\cup_1$ and $\cup_2$ products in Eq. (26), similarly for all other entries. Returning to the squaring of the QCA, a direct computation shows that

$$\alpha^2 = \begin{pmatrix} \delta_{f_0 f} & 0 & \mathbf{O}_{f_0 f}^{(13)} & 0 \\ 0 & \delta_{f_0 f} + \mathbf{O}_{f_0 f'}^{(31)} \mathbf{M}_{f' \cup_1 f} & 0 & \mathbf{O}_{f_0 f}^{(31)} \\ \mathbf{M}_{f' \cup_1 f_0}^\dagger \mathbf{O}_{f' f''}^{(13)} \mathbf{M}_{f'' \cup_1 f} & 0 & \delta_{f_0 f} + \mathbf{M}_{f' \cup_1 f_0}^\dagger \mathbf{O}_{f' f}^{(13)} & 0 \\ 0 & \mathbf{M}_{f' \cup_1 f_0}^\dagger \mathbf{O}_{f' f''}^{(24)} \mathbf{M}_{f'' \cup_1 f} & 0 & \delta_{f_0 f} \end{pmatrix} = \mathbb{I}_{12 \times 12}. \quad (70)$$

3. 3-fermion QCA on arbitrary cellulations

We emphasize that our QCA construction applies to arbitrary cellulations. We place qubits of type A on the faces of the cellulation, and qubits of type B on the faces of its dual cellulation. The separators in Eq. (51) are then

$$\bar{Z}_f^A = Z_f^A G_{\text{PD}(f)}^B, \quad \bar{Z}_f^B = Z_f^B G_{\text{PD}(f')}^A, \quad (71)$$

while the flippers in Eq. (56) become

$$\begin{aligned} \bar{X}_f^A &= X_f^A \prod_{f'} \left(G_{\text{PD}(f')}^B \right)^{f' \cup_1 f}, \\ \bar{X}_f^B &= X_f^B \prod_{f'} \left(G_{\text{PD}(f')}^A \right)^{f' \cup_1 f}. \end{aligned} \quad (72)$$

Here PD denotes the Poincaré dual: PD(f) is the edge in the dual (direct) lattice intersecting the face f in the direct (dual) lattice. We use the dual cellulation because, in passing from Eq. (44) to Eq. (47), we exploited the correspondence between edges e and faces f on the cubic lattice, which is naturally interpreted as the Poincaré duality between two lattices. The definition of cup products on arbitrary cellulations can be found in Refs. [42,72].

B. $\mathbb{Z}_p^{(k)}$ QCA from topological action $S = (k/p)B_2 \cup B_2$

In this section, we construct the QCA associated with the anyon theory $\mathbb{Z}_p^{(k)}$. This theory consists of anyons

$\mathcal{A} = \{1, a, a^2, \dots, a^{p-1}\}$ with fusion rules and topological spins given by

$$a^p = 1, \quad \theta_a = \exp\left(\frac{2\pi i k}{p}\right). \quad (73)$$

Although a representative of this QCA has been constructed before in Ref. [34] via the shifting of invertible subalgebras [43], we provide here a novel construction through TQFTs and the cup-product formalism. This approach places the $\mathbb{Z}_p$ QCA in 3 + 1D on the same footing as other $\mathbb{Z}_2$ QCAs in 3 + 1D and higher dimensions. Moreover, we explicitly show that the order of these QCAs, matches that of the Witt group.

The Hamiltonian of the gauged $\mathbb{Z}_p$ 1-form SPT phase with action $S = (k/p)B_2 \cup B_2 \in H^4(B^2\mathbb{Z}_p, \mathbb{R}/\mathbb{Z})$ is

$$\begin{aligned} H_{\mathbb{Z}_p}^{(k)} &= - \sum_t Z_{\partial t} - \sum_e X_{\delta e} \prod_{f'} Z_{f'}^k f' \cup_e e \cup f' \\ &+ h.c., \end{aligned} \quad (74)$$

where $Z_{\partial t}$ is the flux operator, defined as the product of Z_f over the 2-cell faces of a 3-cell t , and $X_{\delta e}$ is the product of X_f around an edge e , with orientations specified as in Eq. (46). On the cubic lattice, the corresponding Hamiltonian terms are shown in Fig. 4.

Unlike the 3-fermion case in Eq. (47), we cannot simply remove the $Z_{\partial c}$ term on the cubic lattice (here we use

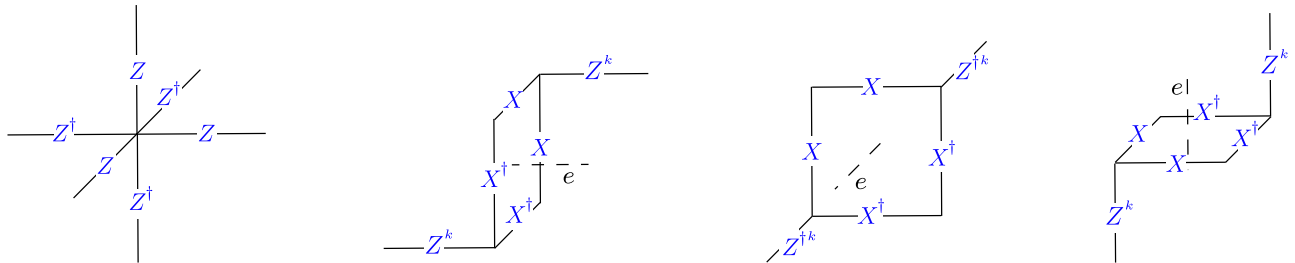


FIG. 4. A valid choice of parent Hamiltonian for the gauged 1-form symmetry-protected topological phase associated with the cocycle $S = (k/p)B_2 \cup B_2 \in H^4(B^2\mathbb{Z}_p, \mathbb{R}/\mathbb{Z})$, illustrated on the dual lattice. However, the Hamiltonian terms are not independent and therefore cannot be used directly as separators in the quantum cellular automata construction.

c instead of t to indicate that the construction is defined on the cubic lattice). The second term in Eq. (74) is an X plaquette operator multiplied by two Z operators. Consequently, taking the product around a cube leaves behind two $Z_{\partial c}$ terms instead of one. To address this, we look for a better set of stabilizer generators that eliminates $Z_{\partial t}$. These new generators will serve as separators for the QCA construction. Our approach is to multiply the second term by $Z_{\partial c}$, which preserves the stabilizer group. This allows us to rewrite it as a Z_f operator times an additional operator G defined below in Eq. (78) definition. First, using the identity

$$\begin{aligned} f' \cup e - e \cup f' \\ = \delta e \cup_1 f' - e \cup_1 \delta f' - \delta(e \cup_1 f'), \end{aligned} \quad (75)$$

we can transform the second term of Eq. (74) to

$$- \sum_e X_{\delta e} \prod_{f'} Z_{f'}^{k \int 2e \cup f' + \delta e \cup_1 f' - e \cup_1 \delta f'}. \quad (76)$$

Multiplying by $Z_{\partial c}^k$ does not change the stabilizer group generated by these operators, which leads to

$$\begin{aligned} & - \sum_e \left[\prod_c Z_{\partial c}^{k \int e \cup_1 c} X_{\delta e} \prod_{f'} Z_{f'}^{k \int 2e \cup f' + \delta e \cup_1 f' - e \cup_1 \delta f'} \right] \\ & = - \sum_e X_{\delta e} Z_{f'}^{k \int 2e \cup f' + \delta e \cup_1 f'} \\ & = - \sum_e G_e^{(k)} \prod_{f'} Z_{f'}^{2k \int e \cup f'}, \end{aligned} \quad (77)$$

where by analogy with the 3 + 1D bosonization [71], we define

$$G_e^{(k)} := X_{\delta e} \prod_{f'} Z_{f'}^{k \int \delta e \cup_1 f'}. \quad (78)$$

In the $\mathbb{Z}_p$ case, the operators $G_e^{(k)}$ on different edges do not commute. However, as shown in Eq. (77), the combinations $G_e^{(k)} \prod_{f'} Z_{f'}^{2k \int e \cup f'}$ for different edges do commute.

Next, since $e \cup f'$ defines a one-to-one correspondence between edges and faces on the cubic lattice, we can rewrite this term as

$$- \sum_f Z_f^{2k} \prod_e G_e^{(k) \int e \cup f}, \quad (79)$$

and we will show that it generates the entire stabilizer group. In fact, the product of these terms around a cube

reproduces $Z_{\partial c}^{2k}$, with all $G_e^{(k)}$ factors canceling. An alternative way to see this is by substituting $e = \delta v$ into $G_e^{(k)}$, which gives

$$\prod_{e \supset v} G_e^{(k)} = X_{\delta(\delta v)} Z_{f'}^{k \int \delta(\delta v) \cup_1 f'} = 1. \quad (80)$$

For odd p , the operator $Z_{\partial c}^{2k}$ already generates $Z_{\partial c}$, ensuring that the entire stabilizer group is captured. Consequently, we obtain an equivalent Hamiltonian with the same ground state,

$$\begin{aligned} H_{\text{separator}}^{Z_p^{(k)}} &= - \sum_f Z_f^{2k} \prod_e G_e^{(k) \int e \cup f} + h.c. \\ &= - \sum_f \left(\bar{Z}_f^{(k)} \right)^{2k} + h.c., \end{aligned} \quad (81)$$

where we define

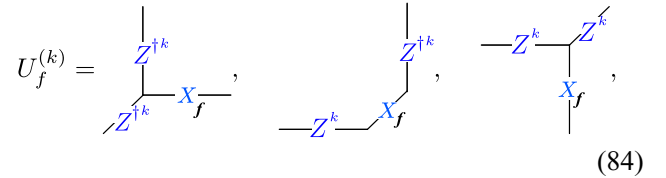
$$\bar{Z}_f^{(k)} := Z_f \prod_e G_e^{(k) \frac{1}{2k} \int e \cup f}, \quad (82)$$

with $1/2k$ denoting the multiplicative inverse of $2k$ in $\mathbb{Z}_p$. The construction is illustrated in Fig. 5.

We also define the ‘‘hopping term’’ as

$$U_f^{(k)} := X_f \prod_{f'} Z_{f'}^{k \int f' \cup_1 f}. \quad (83)$$

On a cubic lattice, $U_f^{(k)}$ can be depicted as

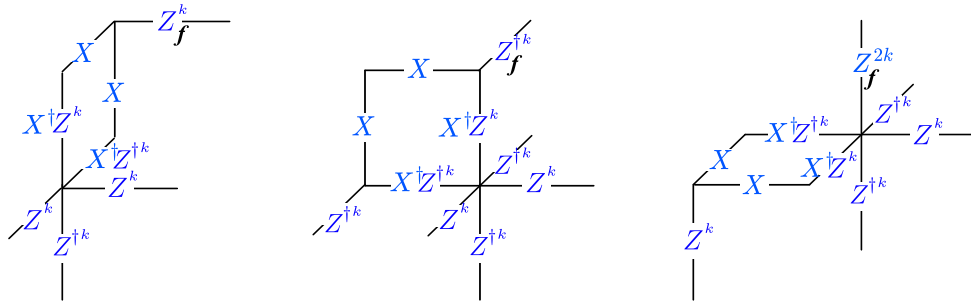


$$U_f^{(k)} = \begin{array}{c} \text{Diagram 1: } Z_{\text{edges}}^k \text{ around face } f \\ \text{Diagram 2: } X_{\text{edges}}^k \text{ around face } f \\ \text{Diagram 3: } Z_{\text{edges}}^k \text{ around face } f \text{ and } X_f^k \end{array}, \quad (84)$$

where faces on the original lattice are represented as edges on the dual lattice. One checks that $U_f^{(k)}$ commutes with $G_e^{(k)}$,

$$\begin{aligned} U_f^{(k)} G_e^{(k)} &= \left(X_f \prod_{f'} Z_{f'}^{k \int f' \cup_1 f} \right) \left(X_{\delta e} \prod_{f''} Z_{f''}^{k \int \delta e \cup_1 f''} \right) \\ &= \exp \left(\frac{2\pi i k}{p} \left[\int \delta e \cup_1 f - \delta e \cup_1 f \right] \right) \\ &\quad \left(X_{\delta e} \prod_{f''} Z_{f''}^{k \int \delta e \cup_1 f''} \right) \left(X_f \prod_{f'} Z_{f'}^{k \int f' \cup_1 f} \right) \\ &= G_e^{(k)} U_f^{(k)}. \end{aligned} \quad (85)$$

As a result, each $U_f^{(k)}$ fails to commute with exactly one Z_f^2 term in Eq. (79). Hence, $\{U_f^{(k)}\}$ are the noncommuting

FIG. 5. Separators $\bar{Z}_f^{2k}$ shown on the dual lattice.

“flippers” used to build the QCA, just as in Eq. (52) for the 3-fermion example.

To define the commuting flippers, we decorate $U_f^{(k)}$ with a product of $\bar{Z}_f$,

$$\begin{aligned} \bar{X}_f^{(k)} &:= U_f^{(k)} \prod_{f'} \bar{Z}_{f'}^{k f f' \cup 1 f} \\ &= X_f \prod_{f'} \left(Z_{f'} \bar{Z}_{f'} \right)^{k f f' \cup 1 f} \\ &= X_f \prod_{f'} \left[\prod_e G_e^{(k) - \frac{1}{2k} f e \cup f} \right]^{k f f' \cup 1 f} \\ &= X_f \prod_{f'} \left[\prod_e G_e^{(k) - \frac{1}{2} f e \cup f} \right]^{f f' \cup 1 f}, \end{aligned} \quad (86)$$

in analogy to Eq. (56). Hence, the complete $\mathbb{Z}_p^{(k)}$ QCA, denoted $\alpha_p^{(k)}$, is defined by

$$\begin{aligned} \alpha_p^{(k)} : Z_f &\rightarrow \alpha_p^{(k)}(Z_f) = \bar{Z}_f^{(k)} \\ &= Z_f \prod_e G_e^{(k) \frac{1}{2k} f e \cup f}, \\ \alpha_p^{(k)} : X_f &\rightarrow \alpha_p^{(k)}(X_f) = \bar{X}_f^{(k)} \\ &= X_f \prod_{f'} \left[\prod_e G_e^{(k) - \frac{1}{2} f e \cup f} \right]^{f f' \cup 1 f}. \end{aligned} \quad (87)$$

As in Eqs. (59) and (60), we find that $U_f^{(k)}$ remains invariant under this QCA,

$$\begin{aligned} U_f^{(k)} &\rightarrow \bar{X}_f \prod_{f'} \bar{Z}_{f'}^{k f f' \cup 1 f} \\ &= U_f^{(k)} \prod_{f'} \bar{Z}_{f'}^{k f f' \cup 1 f} \prod_{f'} \bar{Z}_{f'}^{k f f' \cup 1 f} = U_f^{(k)}. \end{aligned} \quad (88)$$

It also follows from Eq. (86) that $Z_{\partial c} \bar{Z}_f^{(k)}$ is invariant under this QCA,

$$\bar{Z}_{\partial c}^{(k)} = \prod_f \left(\bar{Z}_f^{(k)} \right)^{[f](\partial c)} = \prod_f Z_f^{[f](\partial c)} = Z_{\partial c}. \quad (89)$$

We stress, however, that $G_e^{(k)}$ is *not* invariant under the QCA, because in the $\mathbb{Z}_p$ case, $G_e^{(k)}$ cannot be expressed as a product of $U_f^{(k)}$ and $Z_{\partial c}$. Concretely, there is a leftover term of Z^2 , which vanishes only when $p = 2$,

$$\begin{aligned} G_e^{(k)} &= X_{\delta e} \prod_{f'} Z_{f'}^{k f \delta e \cup 1 f'} \\ &= \left(X_{\delta e} \prod_{f'} Z_{f'}^{k f f' \cup 1 e} \right) \prod_{f'} Z_{f'}^{k f \delta e \cup 1 f' - f' \cup 1 \delta e} \\ &= U_{\delta e}^{(k)} \prod_{f'} Z_{f'}^{k f \delta e \cup 2 \delta f' + 2 \delta e \cup 1 f'} \\ &= U_{\delta e}^{(k)} \prod_{f'} Z_{f'}^{k f \delta e \cup 2 \delta f' + 2(f' \cup e - e \cup f' + e \cup 1 \delta f')} \\ &= U_{\delta e}^{(k)} \prod_c Z_{\partial c}^{k f \delta e \cup 2 c + 2 e \cup 1 c} \prod_{f'} Z_{f'}^{2k f f' \cup e - e \cup f'}, \end{aligned} \quad (90)$$

where we have employed Eq. (75) and the recursive formula for higher cup products

$$\begin{aligned} \delta(A_2 \cup_2 B_2) &= \delta A_2 \cup_2 B_2 + A_2 \cup_2 \delta B_2 \\ &\quad + A_2 \cup_1 B_2 + B_2 \cup_1 A_2. \end{aligned} \quad (91)$$

Notably, on the cubic lattice, there is a one-to-one correspondence between edges and faces, characterized by $f e \cup f \neq 0$ (and similarly a dual correspondence given by $f f \cup e \neq 0$). More precisely, the following identity holds

on the cubic lattice, but not on a generic triangulation:

$$\prod_e \left(\prod_{f'} Z_{f'}^{f \cup f'} \right)^{f \cup f} = Z_f. \quad (92)$$

We can now decompose $\alpha_p^{(k)}(Z_f)$ as

$$\begin{aligned} \alpha_p^{(k)}(Z_f) &= Z_f \prod_e G_e^{\frac{1}{2k} \int f \cup f} \\ &= \prod_e \left(U_{\delta e}^{(k)} \prod_c Z_{\partial c}^{k \int \delta e \cup 2c + 2e \cup 1c} \right)^{\frac{1}{2k} \int f \cup f} \\ &\quad \times \prod_e \left(\prod_{f'} Z_{f'}^{f \cup f'} \right)^{f \cup f} \\ &= Z_{T(f)} \prod_e \left(U_{\delta e}^{(k)} \prod_c Z_{\partial c}^{k \int \delta e \cup 2c + 2e \cup 1c} \right)^{\frac{1}{2k} \int f \cup f}, \end{aligned} \quad (93)$$

in which we have used

$$\prod_e \left(\prod_{f'} Z_{f'}^{f \cup f'} \right)^{f \cup f} = Z_{T(f)}, \quad (94)$$

where $T(f)$ denotes the face f shifted by $(-1, -1, -1)$ on the cubic lattice. Thus, $\bar{Z}_f$ is simply $Z_{T(f)}$ multiplied

by $U_{f'}^{(k)}$ and $Z_{\partial c}$. When we apply $\alpha_p^{(k)}$ once again, the $U_{f'}^{(k)}$ and $Z_{\partial c}$ factors remain unchanged, and only $Z_{T(f)}$ is translated to $Z_{T(T(f))}$ (up to some additional $U_{f'}^{(k)}$ and $Z_{\partial c}$ factors), as illustrated in Fig. 6. We emphasize that the QCA constructed in Eq. (87) is not the unique way to disentangle the ground state of the $\mathbb{Z}_p^{(k)}$ Walker-Wang Hamiltonian in Eq. (74). For example, Eq. (76) can be instead written as

$$- \sum_e X_{\delta e} \prod_{f'} Z_{f'}^{k \int 2f' \cup e - \delta e \cup 1f' + e \cup 1\delta f'}. \quad (95)$$

Following the same procedure, we obtain separators and flippers

$$\begin{aligned} \beta_p^{(k)} : Z_f &\rightarrow \beta_p^{(k)}(Z_f) \\ &= Z_f \prod_e G_e^{(-k) \frac{1}{2k} \int f \cup e}, \\ \beta_p^{(k)} : X_f &\rightarrow \beta_p^{(k)}(X_f) \\ &= U_f^{(-k)} \prod_{f'} [\beta_p^{(k)}(Z_{f'})^\dagger]^{-k \int f' \cup 1f} \\ &= X_f \prod_{f'} [Z_{f'} \beta_p^{(k)}(Z_{f'})^\dagger]^{-k \int f' \cup 1f} \\ &= X_f \prod_{f'} \left[\prod_e G_e^{(k) \frac{1}{2} \int f \cup e} \right]^{f' \cup 1f}. \end{aligned} \quad (96)$$

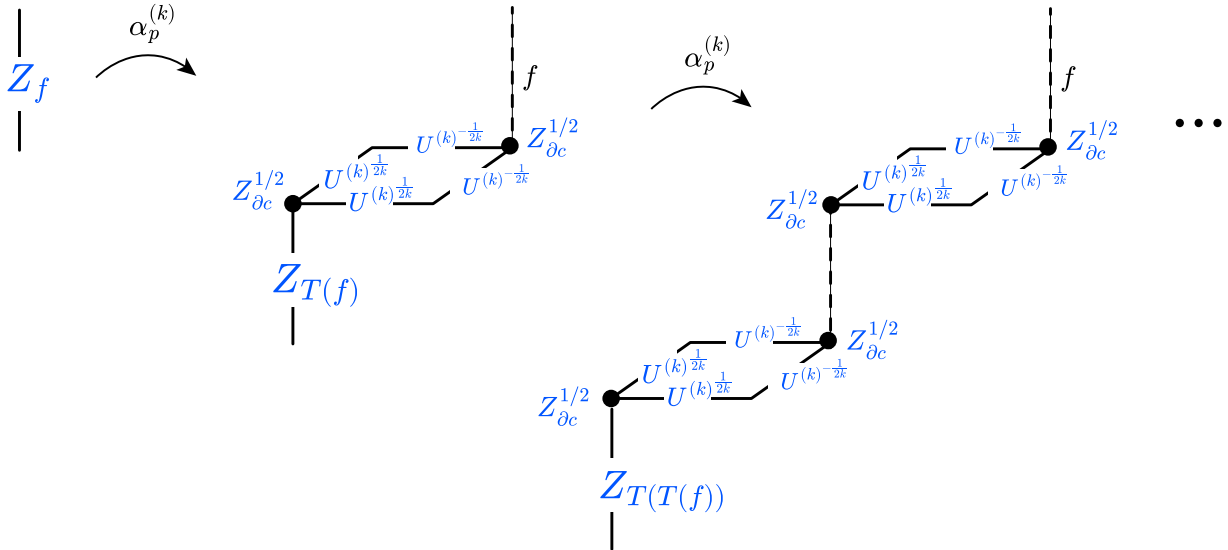


FIG. 6. An illustration of the action of $\alpha_p^{(k)}$ quantum cellular automata on a single Pauli-Z operator on an xy face (shown here as a z edge on the dual lattice). Repeated applications form a stair-like structure, where face f is represented by an edge and cube c is represented by a dot. The Pauli-Z operators in other directions follow a similar inductive law.

The QCA $\beta_p^{(k)}$ preserves both $U_f^{(-k)}$ and $Z_{\partial c}$. Combined with Eqs. (93) and (96), it is straightforward to verify that

$$\beta_p^{(-k)}(\alpha_p^{(k)}(Z_f)) = Z_f, \quad (97)$$

on the cubic lattice. Therefore, $\beta_p^{(-k)}$ is the inverse of $\alpha_p^{(k)}$ on the cubic lattice.

Both $\alpha_p^{(-k)}$ and $\beta_p^{(-k)}$ disentangle the same Walker-Wang ground state, suggesting that these two QCAs belong to the same class. In Sec. VII, we will establish the operator algebra formalism to show that if two QCAs disentangle the same stabilizer group, they are equivalent up to finite-depth quantum circuits (FDQC) and translations. Consequently, we conclude that $\alpha_p^{(-k)} \circ \alpha_p^{(k)} \sim \mathbf{1}$, where $\mathbf{1}$ is the identity operator and $\sim$ denotes equivalence up to FDQC and translations.

At the end of this section, we will prove that the order of $\mathbb{Z}_p^{(k)}$ QCA is 2 or 4, depending on $p \bmod 4$ be 1 or 3. The proof will be divided into two parts.

1. Order of $\mathbb{Z}_p$ QCA for $p \equiv 1 \pmod{4}$

We will prove that when $p \equiv 1 \pmod{4}$, the $\mathbb{Z}_p^{(k)}$ QCA can be transformed into the $\mathbb{Z}_p^{(-k)}$ QCA $\alpha_p^{(-k)}$ —with action $S = -(k/p)B_2 \cup B_2$ —by an on-site unitary transformation. Furthermore, in Appendix C 2, we use a polynomial representation to show that $\mathbb{Z}_p^{(-k)}$ QCA $\alpha_p^{(-k)}$ is the inverse of $\mathbb{Z}_p^{(k)}$ QCA $\alpha_p^{(k)}$ up to a finite-depth circuit.

When $p \equiv 1 \pmod{4}$, -1 is a quadratic residue mod p , i.e., there exists a such that $a^2 \equiv -1 \pmod{p}$.

We now define the following transformation c_p on each face:

$$c_p(Z_f) := Z_f^a, \quad c_p(X_f) := X_f^{-a}. \quad (98)$$

This transformation is unitary because $-a$ is the multiplicative inverse of $a \bmod p$. Moreover, it can be viewed as a squareroot of charge conjugation. In the cochain language, this corresponds to the map $B \rightarrow aB$. Substituting $B \rightarrow aB$ into the original $\mathbb{Z}_p^{(k)}$ action $S = (k/p)B_2 \cup B_2$ yields the action $S' = -(k/p)B_2 \cup B_2$, with the corresponding $\mathbb{Z}_p^{(-k)}$ QCA defined as $c_p \circ \alpha_p^{(k)} \circ c_p^{-1}$. Indeed, we can verify that this matches the expression for $\alpha_p^{(-k)}(Z_f)$ defined in Eq. (87),

$$\begin{aligned} & c_p(\alpha_p^{(k)}(c_p^{-1}(Z_f))) \\ &= c_p^{-1} \left(Z_f \prod_e \left[X_{\delta e} \prod_{f'} Z_{f'}^{k \int \delta e \cup 1 f'} \right]^{\frac{1}{2k} \int e \cup f} \right)^{-a} \end{aligned}$$

$$\begin{aligned} &= Z_f \prod_e \left[X_{\delta e}^\dagger \prod_{f'} Z_{f'}^{k \int \delta e \cup 1 f'} \right]^{\frac{1}{2k} \int e \cup f} \\ &= Z_f \prod_e G_e^{(-k) - \frac{1}{2k} \int e \cup f} = \alpha_p^{(-k)}(Z_f). \end{aligned} \quad (99)$$

There is another way to express the above quantity as

$$\begin{aligned} & Z_f \prod_e \left[X_{\delta e}^\dagger \prod_{f'} Z_{f'}^{k \int \delta e \cup 1 f'} \right]^{\frac{1}{2k} \int e \cup f} \\ & \times \prod_{ef'} \left[Z_{f'}^{\int \delta e \cup 1 f'} \right]^{\int e \cup f} \\ &= Z_f \prod_e G_e^{(k) - \frac{1}{2k} \int e \cup f} \prod_{ef'} \left[Z_{f'}^{\int \delta e \cup 1 f'} \right]^{\int e \cup f}. \end{aligned} \quad (100)$$

Now, we focus on the cubic lattice to proceed. Note that $\int e \cup f \neq 0$ induces a one-to-one correspondence between edges e and faces f on the cubic lattice. Hence, we can rewrite the above expression as

$$\begin{aligned} & G_e^{(k) - \frac{1}{2k} \int e \cup f} \prod_f Z_f^{\int e \cup f} \prod_{f'} Z_{f'}^{\int \delta e \cup 1 f'} \\ &= G_e^{(k) - \frac{1}{2k} \int e \cup f} \prod_f Z_f^{\int f \cup e + \int \delta f \cup 1 e}, \end{aligned} \quad (101)$$

where we have used Eq. (75). By applying the other duality between e and f for $\int f \cup e \neq 1$, we can rearrange it into

$$\begin{aligned} & \alpha_p^{(-k)}(Z_{T^{-1}(f)}) \\ &= Z_f \prod_e G_e^{(k) - \frac{1}{2k} \int f \cup e} \prod_{ef'} \left[Z_{f'}^{\int e \cup 1 \delta f'} \right]^{\int f \cup e} \\ &= Z_f \prod_e G_e^{(k) - \frac{1}{2k} \int f \cup e} \prod_{e,c} \left[Z_{\partial c}^{\int e \cup 1 c} \right]^{\int f \cup e}, \end{aligned} \quad (102)$$

where the overall shift along $(-1, -1, -1)$ comes from Eq. (94).

Comparing $\beta_p^{(-k)}(Z_f)$ from Eq. (96) with $\alpha_p^{(-k)}(Z_{T^{-1}(f)})$ in Eq. (102), we find that they differ only by a $Z_{\partial c}$ term. Since such $Z_{\partial c}$ factors lie in the stabilizer group, we conclude that both $\alpha_p^{(-k)}$ and $\beta_p^{(-k)}$ disentangle the same $\mathbb{Z}_p^{(-k)}$ Walker-Wang ground state, which corresponds to the action $S' = -(k/p)B_2 \cup B_2$.

Before proceeding, we emphasize a key result stating that any Clifford QCAs that disentangle the same stabilizer group are equivalent. Corollary 1, proved in Sec. VII B, is essential for our argument. Even though two QCAs disentangle the same Walker-Wang ground state, it is not immediately obvious that these two QCAs should be equivalent

since they map the stabilizers differently. The corollary guarantees that it suffices to consider a single representative QCA that disentangles the given ground state, without concerning that different choices of Hamiltonian lead to inequivalent QCAs.

Therefore, by Corollary 1, $\alpha_p^{(-k)}$ and $\beta_p^{(-k)}$ are related by a finite-depth quantum circuit (FDQC) and translations. In Sec. III B 4, we write $\alpha_p^{(-k)}$ explicitly as matrices over polynomial rings and exhibit the FDQC and translations that relate these two matrices.

2. Order of $\mathbb{Z}_p$ QCA for $p \equiv 3 \pmod{4}$

In the case that $p \equiv 3 \pmod{4}$, we will show that two copies of $\mathbb{Z}_p^{(1)}$ QCA are transformed into two copies of $\mathbb{Z}_p^{(-1)}$ QCA by a local unitary communicating the two copies. In the case where $p \equiv 3 \pmod{4}$, the term $e^{\frac{p-1}{4}}$ is no longer valid, so we should seek help from another copy of QCA. To begin with, we present a number theory proposition, that there exist two integers a and b , satisfying $a^2 + b^2 \equiv -1 \pmod{p}$. To prove this, we first modify the equation to be $(1 + x^2)a^2 \equiv -1 \pmod{p}$. There must exist an x for $1 + x^2$ to be quadratic nonresidue. Otherwise quadratic residue can be extended to the whole residue class, which is obviously contradictory. Since quadratic nonresidues correspond to the odd power of any primitive roots, the quotient of two quadratic nonresidues (in number theory that means the multiplication of one and the other's inverse) is exactly a quadratic residue. Namely, there must exist an a for $(1 + x^2)a^2 \equiv -1 \pmod{p}$ when $1 + x^2$ is a quadratic nonresidue. Denoting $x \times a$ as b , we obtain the solution for $a^2 + b^2 \equiv -1 \pmod{p}$.

We label the qudits of the two QCA copies as Z_f^1 and Z_f^2 . The transformation is then given by

$$Z_f^1 \rightarrow (Z_f^1)^a (Z_f^2)^b, \quad (103)$$

$$Z_f^2 \rightarrow (Z_f^1)^b (Z_f^2)^{-a}, \quad (104)$$

$$X_f^1 \rightarrow (X_f^1)^{-a} (X_f^2)^{-b}, \quad (105)$$

$$X_f^2 \rightarrow (X_f^1)^{-b} (X_f^2)^a. \quad (106)$$

While in the cochain representation, that can be shown as $B^1 \rightarrow aB^1 + bB^2, B^2 \rightarrow bB^1 - aB^2$. Substituting the transformation into the two-copy $\mathbb{Z}_p^{(1)}$ action, we obtain $S' = -(1/p)(B^1 \cup B^1 + B^2 \cup B^2)$, the action for two-copy $\mathbb{Z}_p^{(-1)}$ QCA.

As we have proved that $\mathbb{Z}_p^{(1)}$ QCA and $\mathbb{Z}_p^{(-1)}$ QCA are inverse in the Appendix, we finally reached the conclusion that $\mathbb{Z}_p^{(1)}$ QCA has order 2 when $p \equiv 1 \pmod{4}$, and that it has order 4 when $p \equiv 3 \pmod{4}$.

3. Polynomial expression of odd prime QCA

First, we have

$$\mathbf{U}_f^{(k)} = \mathbf{X}_f^{(k)} + k\mathbf{Z}_{f'} \mathbf{M}_{f' \cup 1f}, \quad (107)$$

$$\tilde{\mathbf{U}}_f^{(k)} = \mathbf{X}_f^{(k)} + k\mathbf{Z}_{f'} \mathbf{M}_{f' \cup 1f}^\dagger, \quad (108)$$

$$\mathbf{G}_e^{(k)} = \tilde{\mathbf{U}}_{\delta e}^{(k)}. \quad (109)$$

In term of the polynomial, they are

$$\mathbf{U}^{(k)} = \begin{pmatrix} \delta_{f_0 f} \\ k\mathbf{M}_{f_0 \cup 1f} \end{pmatrix}, \quad (110)$$

$$\tilde{\mathbf{U}}^{(k)} = \begin{pmatrix} \delta_{f_0 f} \\ k\mathbf{M}_{f_0 \cup 1f}^\dagger \end{pmatrix}, \quad (111)$$

$$\mathbf{G}^{(k)} = \begin{pmatrix} \delta_{f_0, \delta e} \\ k\mathbf{M}_{\delta e \cup 1f_0}^\dagger \end{pmatrix}. \quad (112)$$

Then separators and flippers for the odd prime QCA are

$$\bar{\mathbf{Z}}_f^{(k)} = \mathbf{Z}_f + \frac{1}{2k} \mathbf{G}_e^{(k)} \mathbf{M}_{e \cup f}, \quad (113)$$

$$\begin{aligned} \bar{\mathbf{X}}_f^{(k)} &= \mathbf{U}_f^{(k)} - k\mathbf{Z}_{f'} \mathbf{M}_{f' \cup 1f} \\ &= \mathbf{X}_f - \frac{1}{2} \mathbf{G}_e^{(k)} \mathbf{M}_{e \cup f} \mathbf{M}_{f' \cup 1f}. \end{aligned} \quad (114)$$

In polynomial form, we have

$$\bar{\mathbf{Z}}^{(k)} = \begin{pmatrix} \frac{1}{2k} \mathbf{M}_{\partial f_0 \cup f} \\ \delta_{f_0 f} + \frac{1}{2} \mathbf{M}_{f' \cup 1f_0}^\dagger \mathbf{M}_{\partial f' \cup f} \end{pmatrix}, \quad (115)$$

whose matrix elements are

$$\begin{pmatrix} 0 & \frac{1}{2kx} - \frac{1}{2kx} & \frac{1}{2kxy} - \frac{1}{2kx} \\ \frac{1}{2ky} - \frac{1}{2kyz} & 0 & \frac{1}{2kxy} - \frac{1}{2ky} \\ \frac{1}{2kz} - \frac{1}{2kyz} & \frac{1}{2kz} - \frac{1}{2kxz} & 0 \\ \frac{1}{2yz} + \frac{1}{2} & \frac{1}{2xz} - \frac{1}{2z} & \frac{1}{2} - \frac{1}{2x} \\ \frac{1}{2y^2z} - \frac{1}{2yz} & \frac{1}{2xyz} - \frac{1}{2yz} + \frac{1}{2z} + \frac{1}{2} & \frac{1}{2y} - \frac{1}{2} \\ \frac{1}{2yz} - \frac{1}{2yz^2} & \frac{1}{2z^2} - \frac{1}{2z} & \frac{1}{2xyz} - \frac{1}{2z} + 1 \end{pmatrix}$$

and

$$\bar{\mathbf{X}}^{(k)} = \begin{pmatrix} \delta_{f_0 f} - \frac{1}{2} \mathbf{M}_{\partial f_0 \cup f} \mathbf{M}_{f' \cup 1f} \\ -\frac{k}{2} \mathbf{M}_{\delta e \cup 1f_0}^\dagger \mathbf{M}_{e \cup f} \mathbf{M}_{f' \cup 1f} \end{pmatrix}, \quad (116)$$

whose matrix elements are

$$\begin{pmatrix} \frac{1}{2xyz} - \frac{1}{2x} + 1 & \frac{1}{2x} - \frac{y}{2x} & \frac{z}{2x} - \frac{1}{2x} \\ \frac{1}{2xy} - \frac{1}{2y} & \frac{1}{2xyz} - \frac{1}{2xy} + \frac{1}{2x} + \frac{1}{2} & \frac{1}{2xy} - \frac{z}{2xy} \\ \frac{1}{2yz} - \frac{1}{2xyz} & \frac{1}{2xyz} - \frac{1}{2xz} & \frac{1}{2xy} + \frac{1}{2} \\ \frac{k}{2xyz} - \frac{k}{2x} - \frac{k}{2yz} + \frac{k}{2} & -\frac{k}{2xyz} - \frac{ky}{2x} + \frac{k}{2x} + \frac{ky}{2} & -\frac{k}{2xy} + \frac{kz}{2x} - \frac{k}{2x} + \frac{k}{2} \\ \frac{k}{2xy^2z} - \frac{k}{2y^2z} + \frac{k}{2yz} - \frac{k}{2} & -\frac{k}{2xy^2z} + \frac{k}{2xyz} - \frac{ky}{2} + \frac{k}{2} & -\frac{k}{2xy^2} + \frac{k}{2y} + \frac{kz}{2} - \frac{k}{2} \\ \frac{k}{2xyz} + \frac{k}{2yz^2} - \frac{k}{2yz} - \frac{k}{2z} & \frac{k}{2xyz^2} - \frac{k}{2xyz} + \frac{k}{2xz} - \frac{ky}{2z} & \frac{k}{2xyz} - \frac{k}{2xy} - \frac{k}{2z} + \frac{k}{2} \end{pmatrix}. \quad (117)$$

We can confirm that $\bar{\mathbf{Z}}_f^{(k)}$ generates $\mathbf{Z}_{\partial c}$ since

$$\bar{\mathbf{Z}}_{\partial c} = \mathbf{Z}_{\partial c} + \frac{1}{2k} \tilde{\mathbf{G}}_e^{(k)} \mathbf{M}_{e \cup \partial c} = \mathbf{Z}_{\partial c} + \frac{1}{2k} \mathbf{G}_e^{(k)} \mathbf{M}_{e \cup \partial c} = \mathbf{Z}_{\partial c} + \frac{1}{2k} \tilde{\mathbf{U}}_{\delta_e}^{(k)} \mathbf{M}_{\delta_e \cup \partial c} \rightarrow 0$$

With this, we can now define the QCA as

$$\alpha^{(k)} = \begin{pmatrix} \bar{\mathbf{X}}^{(k)} & \bar{\mathbf{Z}}^{(k)} \end{pmatrix} = \begin{pmatrix} \delta_{f_0 f} - \frac{1}{2} \mathbf{M}_{\partial f_0 \cup f'} \mathbf{M}_{f' \cup 1f} & \frac{1}{2k} \mathbf{M}_{\partial f_0 \cup f} \\ -\frac{k}{2} \mathbf{M}_{f' \cup 1f_0}^\dagger \mathbf{M}_{\partial f' \cup f'} \mathbf{M}_{f' \cup 1f} & \delta_{f_0 f} + \frac{1}{2} \mathbf{M}_{f' \cup 1f_0}^\dagger \mathbf{M}_{\partial f' \cup f} \end{pmatrix}. \quad (118)$$

From the expression above, it is clear that $\alpha^{(k)} \mathbf{U}^{(k)} = \mathbf{U}^{(k)}$.

4. $p \equiv 1 \pmod{4}$

In this case, there exists a such that $a^2 \equiv -1 \pmod{p}$. The onsite basis transformation is given by $\mathbf{c} = \begin{pmatrix} -a & 1 \\ 0 & a \end{pmatrix}$, which is a symplectic matrix. Conjugating a matrix results in

$$\begin{pmatrix} -a & 1 \\ 0 & a \end{pmatrix} \begin{pmatrix} \alpha_{11} & \alpha_{12} \\ \alpha_{21} & \alpha_{22} \end{pmatrix} \begin{pmatrix} a & 0 \\ 0 & -a \end{pmatrix} = \begin{pmatrix} \alpha_{11} & -\alpha_{12} \\ -\alpha_{21} & \alpha_{22} \end{pmatrix}. \quad (119)$$

Since the dependence of k in α is exactly off-diagonal, we can immediately see that $\mathbf{c} \alpha^{(k)} \mathbf{c}^{-1} = \alpha^{(-k)}$. Let us now compute the square of the QCA (up to circuits),

$$\alpha^{(-k)} \alpha^{(k)} = \begin{pmatrix} \delta_{f_0 f} + (\frac{1}{4} \mathbf{O}_{f_0 f'}^{(14)} - \mathbf{M}_{\partial f_0 \cup f'}) \mathbf{M}_{f' \cup 1f} & 0 \\ 0 & \delta_{f_0 f} + \mathbf{M}_{f' \cup 1f_0}^\dagger (\frac{1}{4} \mathbf{O}_{f' f}^{(14)} + \mathbf{M}_{\partial f' \cup f}) \end{pmatrix} \quad (120)$$

$$= \begin{pmatrix} \delta_{f_0 f} - \mathbf{M}_{\partial f_0 \cup f'} \mathbf{M}_{f' \cup 1f} & 0 \\ 0 & \delta_{f_0 f} + \mathbf{M}_{\delta_e \cup 1f_0}^\dagger \mathbf{M}_{e \cup f} \end{pmatrix} \quad (121)$$

$$= \begin{pmatrix} \delta_{f_0 f} - \mathbf{M}_{\partial f_0 \cup f'} \mathbf{M}_{f' \cup 1f} & 0 \\ 0 & \delta_{f_0 f} + (\mathbf{M}_{f_0 \cup e} - \mathbf{M}_{e \cup f_0}^\dagger + \mathbf{M}_{e \cup 1f_0}^\dagger) \mathbf{M}_{e \cup f} \end{pmatrix}. \quad (122)$$

Thus, this QCA does not mix Z and X stabilizers. The result of Sec. VII therefore implies that this QCA can be decomposed into circuits and shifts.

We may further explicitly find such a decomposition on the cubic lattice. Specifically, due to the unique pairing of edges and faces via the cup product, we have a special property that $\mathbf{M}_{e \cup f_0}^\dagger \mathbf{M}_{e \cup f} = \delta_{f_0 f}$. Thus,

$$\alpha^{(-k)} \alpha^{(k)} = \begin{pmatrix} \delta_{f_0 f} - \mathbf{M}_{\partial f_0 \cup f'} \mathbf{M}_{f' \cup 1f} & 0 \\ 0 & (\mathbf{M}_{f_0 \cup e} + \mathbf{M}_{e \cup 1f_0}^\dagger) \mathbf{M}_{e \cup f} \end{pmatrix}. \quad (123)$$

Next, we show that $\alpha^{(-k)}\alpha^{(k)}$ is composed of circuits together with shifts. Consider the following transformation:

$$\mathbf{U} = \begin{pmatrix} \mathbf{M}_{f_0 \cup e}^\dagger + \mathbf{M}_{e \cup_1 \delta f_0} & 0 \\ 0 & (\mathbf{M}_{f_0 \cup e} + \mathbf{M}_{e \cup_1 \delta f_0}^\dagger)^{-1} \end{pmatrix} \quad (124)$$

$$= \begin{pmatrix} 1 & y-1 & 1-z & 0 & 0 & 0 \\ \frac{1}{x}-1 & \frac{y}{x}-\frac{1}{x}-y & \frac{1}{x}-\frac{z}{x} & 0 & 0 & 0 \\ \frac{1}{xy}-\frac{1}{y} & \frac{1}{x}-\frac{1}{xy} & -\frac{z}{xy}+\frac{1}{xy}+z & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{x}{yz}+x+\frac{1}{yz} & \frac{x}{z}-\frac{1}{z} & 1-x \\ 0 & 0 & 0 & \frac{1}{yz}-\frac{1}{z} & \frac{y}{z}-y-\frac{1}{z} & 1-y \\ 0 & 0 & 0 & \frac{1}{yz}-\frac{1}{y} & 1-\frac{1}{z} & 1 \end{pmatrix}. \quad (125)$$

This can be decomposed in terms of CNOT gates, and so it is a circuit. In particular,

$$\mathbf{U} = \text{diag}(1, -1, 1, 1, -1, 1) \mathbf{U}_1 \mathbf{U}_2 \mathbf{U}_3 \mathbf{U}_4, \quad (126)$$

where

$$\mathbf{U}_1 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ \bar{x}-1 & 1-\bar{y} & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1-x \\ 0 & 0 & 0 & 0 & 1 & y-1 \end{pmatrix}, \quad \mathbf{U}_2 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1-\bar{x} & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & x-1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad (127)$$

$$\mathbf{U}_3 = \begin{pmatrix} 1 & 0 & 1-z & 0 & 0 & 0 \\ 0 & 1 & z-1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \bar{z}-1 & 1-\bar{z} & 1 \end{pmatrix}, \quad \mathbf{U}_4 = \begin{pmatrix} 1 & y-1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1-\bar{y} & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \quad (128)$$

Acting $\mathbf{U}$ on $\alpha^{(-k)}\alpha^{(k)}$, we have

$$\mathbf{U}\alpha^{(-k)}\alpha^{(k)} = \begin{pmatrix} \mathbf{M}_{e \cup f} & 0 \\ 0 & \mathbf{M}_{e \cup f} \end{pmatrix} = \text{diag}(\bar{y}\bar{z}, -\bar{x}\bar{z}, \bar{x}\bar{y}, \bar{y}\bar{z}, -\bar{x}\bar{z}, \bar{x}\bar{y}). \quad (129)$$

Thus, we have shown that the QCA is order two up to circuits and shifts.

5. $p \equiv 3 \pmod{4}$

In this case, we consider two copies of QCA, which is just the direct sum $\alpha^{(k)} \oplus \alpha^{(k)}$. In the matrix notation, it can be expressed as a block-diagonal matrix $\begin{pmatrix} \alpha^{(k)} & 0 \\ 0 & \alpha^{(k)} \end{pmatrix}$. When $p \equiv 3 \pmod{4}$, there exists a and b satisfying $a^2 + b^2 = -1 \pmod{p}$. We can consider the following transformation matrix:

$$\mathbf{c} = \begin{pmatrix} a\mathbb{1} & 0 & b\mathbb{1} & 0 \\ 0 & -a\mathbb{1} & 0 & -b\mathbb{1} \\ b\mathbb{1} & 0 & -a\mathbb{1} & 0 \\ 0 & -b\mathbb{1} & 0 & a\mathbb{1} \end{pmatrix}. \quad (130)$$

This corresponds to a transformation connecting the same sites in each QCA copy. Applying this transformation to the original QCA, we obtain

$$\begin{aligned} c \begin{pmatrix} \alpha^{(k)} & 0 \\ 0 & \alpha^{(k)} \end{pmatrix} c^{-1} &= \begin{pmatrix} a\mathbb{1} & 0 & b\mathbb{1} & 0 \\ 0 & -a\mathbb{1} & 0 & -b\mathbb{1} \\ b\mathbb{1} & 0 & -a\mathbb{1} & 0 \\ 0 & -b\mathbb{1} & 0 & a\mathbb{1} \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & 0 & 0 \\ a_{21} & a_{22} & 0 & 0 \\ 0 & 0 & a_{11} & a_{12} \\ 0 & 0 & a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} -a\mathbb{1} & 0 & -b\mathbb{1} & 0 \\ 0 & a\mathbb{1} & 0 & b\mathbb{1} \\ -b\mathbb{1} & 0 & a\mathbb{1} & 0 \\ 0 & b\mathbb{1} & 0 & -a\mathbb{1} \end{pmatrix} \\ &= \begin{pmatrix} a_{11} & -a_{12} & 0 & 0 \\ -a_{21} & a_{22} & 0 & 0 \\ 0 & 0 & a_{11} & -a_{12} \\ 0 & 0 & -a_{21} & a_{22} \end{pmatrix} = \begin{pmatrix} \alpha^{(-k)} & 0 \\ 0 & \alpha^{(-k)} \end{pmatrix}. \end{aligned} \quad (131)$$

This implies that after transformation, the original QCA is again decomposed into two copies of $\alpha^{(-k)}$ QCA.

According to the previous subsection, the composition of these two QCAs can be decomposed into two separate sets of finite-depth circuits $\mathbf{U} \oplus \mathbf{U}$,

$$\begin{pmatrix} \mathbf{U} & 0 \\ 0 & \mathbf{U} \end{pmatrix} \begin{pmatrix} \alpha^{(-k)} & 0 \\ 0 & \alpha^{(-k)} \end{pmatrix} \begin{pmatrix} \alpha^{(k)} & 0 \\ 0 & \alpha^{(k)} \end{pmatrix} = \text{diag}(\bar{y}\bar{z}, -\bar{x}\bar{z}, \bar{x}\bar{y}, \bar{y}\bar{z}, -\bar{x}\bar{z}, \bar{x}\bar{y}, \bar{y}\bar{z}, -\bar{x}\bar{z}, \bar{x}\bar{y}, \bar{y}\bar{z}, -\bar{x}\bar{z}, \bar{x}\bar{y}). \quad (132)$$

Since two copies of a QCA are equivalent to a single QCA applied twice, the order of this QCA is 4.

IV. $\mathbb{Z}_2$ AND $\mathbb{Z}_p$ CLIFFORD QCAs IN HIGHER DIMENSIONS FROM TQFTs

In this section, we generalize the 3-fermion QCA from the previous section to arbitrary $2k + 1$ spatial dimensions. The construction is derived directly from the corresponding topological action, allowing the QCA to be defined on arbitrary cellulations and thereby providing greater flexibility in lattice realizations. When restricted to the hypercubic lattices, our formulation reproduces the construction of Ref. [5].

A. $\mathbb{Z}_2$ QCA in 5 + 1D from topological action

$$S = \frac{1}{2} \int A_3 \cup A_3 + A_3 \cup B_3 + B_3 \cup B_3$$

The action for this QCA is given by

$$S = \frac{1}{2} \int A_3 \cup A_3 + A_3 \cup B_3 + B_3 \cup B_3. \quad (133)$$

This expression closely resembles the 3-fermion Walker-Wang QCA in 3 + 1D, with the primary difference being the change in the dimensionality of the cocycles. Consequently, the lattice construction for this QCA follows the same general framework as in the 3-fermion Walker-Wang case. The corresponding separators and (noncommuting) flippers on hypercubic lattices are

$$\begin{aligned} \bar{Z}_c^A &= Z_c^A \prod_f G_f^{B \int c \cup f}, \quad \bar{Z}_c^B = Z_c^B \prod_f G_f^{A \int f \cup c}, \\ U_c^A &= X_c^A \prod_{c'} Z_{c'}^{A \int c' \cup 1^t}, \quad U_c^B = X_c^B \prod_{c'} Z_{c'}^{B \int c' \cup 1^t}, \end{aligned} \quad (134)$$

where qubits are placed on cubes c , and G_f^α is defined in analogy with Eq. (45),

$$G_f^\alpha := X_{\delta f}^\alpha \prod_{c'} Z_{c'}^{\alpha \int \delta f \cup 1^{c'}}, \quad \alpha \in \{A, B\}. \quad (135)$$

See Appendix C 2 for the polynomial formalism of this QCA on the hypercubic lattice. On a general cellulation, we place qubit A on each 3-cell of the direct lattice and qubit B on each 3-cell of the dual lattice. The separators and (noncommuting) flippers then take the form

$$\begin{aligned} \bar{Z}_t^A &= Z_t^A G_{\text{PD}(t)}^B, \quad \bar{Z}_t^B = Z_t^B G_{\text{PD}(t)}^A, \\ U_t^A &= X_t^A \prod_{t'} Z_{t'}^{A \int t' \cup 1^t}, \quad U_t^B = X_t^B \prod_{t'} Z_{t'}^{B \int t' \cup 1^t}, \end{aligned} \quad (136)$$

where PD denotes the Poincaré dual: PD(t) is the face in the dual lattice intersecting the tetrahedron t in the direct lattice. For simplicity, we focus on hypercubic lattices in the following construction, while noting that the argument extends straightforwardly to arbitrary cellulations.

As noted in Ref. [5], this QCA should be disentangled by a non-Clifford finite-depth quantum circuit, and we argue that our construction indeed possesses this property. First, observe that

$$\frac{1}{2} A_3 \cup A_3 \quad (137)$$

is a trivial cocycle in $H^6(B^3\mathbb{Z}_2, \mathbb{R}/\mathbb{Z})$ when A is a closed 3-form. Indeed, consider the coboundary

$$\begin{aligned} & \frac{1}{4} \delta (A_3 \cup_1 A_3 + A_3 \cup_2 \delta A_3) \\ &= -\frac{1}{2} A_3 \cup A_3 - \frac{1}{2} A_3 \cup_1 \delta A_3 + \frac{1}{4} \delta A_3 \cup_2 \delta A_3, \end{aligned} \quad (138)$$

where we have used the standard coboundary identity for higher cup products. To be consistent with the denominator 4, we lift the cochain A from $\mathbb{Z}_2$ to $\mathbb{Z}$. Since A is closed, we have $\delta A \equiv 0 \pmod{2}$. Consequently,

$$\frac{1}{2} A_3 \cup_1 \delta A_3 - \frac{1}{4} \delta A_3 \cup_2 \delta A_3 \equiv 0 \pmod{1}. \quad (139)$$

Thus, $\frac{1}{2} A_3 \cup A_3$ is a coboundary. Adding this coboundary to the topological action modifies the ground state only by a finite-depth quantum circuit (FDQC) parameterized by $\frac{1}{4} (A_3 \cup_1 A_3 + A_3 \cup_2 \delta A_3)$. Because the denominator is 4, the resulting circuit is non-Clifford, acting on the $\mathbb{Z}_2$ qubits located on tetrahedra (in particular, it includes the controlled- S gate).

We note that although two topological actions that differ by a coboundary give rise to the same ground state, the corresponding Hamiltonian-to-QCA constructions may *a priori* yield different QCAs. Corollary 1 guarantees that it suffices to consider a representative QCA that disentangles the given ground state, without concerning that different choices of Hamiltonian may lead to inequivalent QCAs.

The coboundary term $\frac{1}{2} A_3 \cup A_3$ transforms the gauged SPT ground state via the circuit

$$\begin{aligned} & V_{\text{FDQC}}^a |a_t\rangle \\ &:= \exp \left(-\frac{2\pi i}{4} \int_{M_5} a_t \cup_1 a_t + a_t \cup_2 \delta a_t \right) |a_t\rangle, \end{aligned} \quad (140)$$

where a_t is the 3-cochain labeling the A -type qubit configuration on tetrahedra, and M_5 is the spatial manifold. Consequently, the two Clifford QCAs defined with or without the $\frac{1}{2} A_3 \cup A_3$ term differ only by V_{FDQC}^a and are therefore equivalent. The same reasoning applies to the term $\frac{1}{2} B_3 \cup B_3$, for which we define the associated V_{FDQC}^b . Hence, the QCA generated by

$$\frac{1}{2} (A_3 \cup A_3 + A_3 \cup B_3 + B_3 \cup B_3), \quad (141)$$

conjugated by the non-Clifford circuit $V_{\text{FDQC}}^a V_{\text{FDQC}}^b$, is identical to the QCA generated by

$$\frac{1}{2} A_3 \cup B_3. \quad (142)$$

Finally, we show that the QCA from $\frac{1}{2} A_3 \cup B_3$ is in fact a Clifford circuit. The Hamiltonian associated with this

action is

$$H = - \sum_f X_{\delta f}^A \prod_c Z_c^{B f \cup c} - \sum_f X_{\delta f}^B \prod_c Z_c^{A f \cup c}. \quad (143)$$

On a hypercubic lattice, separators can be written as

$$\begin{aligned} \bar{Z}_c^A &= Z_c^A \prod_f X_{\delta f}^{B f \cup c}, \\ \bar{Z}_c^B &= Z_c^B \prod_f X_{\delta f}^{A f \cup c}, \end{aligned} \quad (144)$$

while the flippers remain X_c^A and X_c^B . We define the Clifford circuit

$$U = \prod_{c, c'} CZ(X_c^A, X_{c'}^B)^{f \cup \partial c'}. \quad (145)$$

Here $\partial c'$ means a 2-cochain taking value 1 on ∂c and 0 on other faces. It can be checked geometrically that $\prod_f Z_{\delta f}^{f \cup c} = \prod_{c'} Z_{c'}^{f \cup \partial c} = \prod_{c'} Z_{c'}^{c' \cup \partial c}$. Then it is direct that

$$\bar{Z}_c^A = U Z_c^A U^\dagger, \quad \bar{Z}_c^B = U Z_c^B U^\dagger. \quad (146)$$

Thus, the QCA derived from $S = \frac{1}{2} A_3 \cup B_3$ is realized by a Clifford circuit.

B. $\mathbb{Z}_2$ QCA in 7 + 1D from topological action

$$S = \frac{1}{2} \int A_4 \cup A_4 + A_4 \cup B_4 + B_4 \cup B_4$$

The topological action in 7 + 1D is

$$S = \frac{1}{2} \int A_4 \cup A_4 + A_4 \cup B_4 + B_4 \cup B_4. \quad (147)$$

The resulting QCA is structurally similar to the 3 + 1D case, and the separators and flippers can be written directly as

$$\begin{aligned} \bar{Z}_{s_4}^A &= Z_{s_4}^A \prod_{s_4} G_t^{B f s_4 \cup t}, \\ \bar{Z}_{s_4}^B &= Z_{s_4}^B \prod_{s_4} G_t^{A f t \cup s_4}, \\ U_{s_4}^A &= X_{s_4}^A \prod_{s_4'} Z_{s_4'}^{A f s_4' \cup_1 s_4}, \\ U_{s_4}^B &= X_{s_4}^B \prod_{s_4'} Z_{s_4'}^{B f s_4' \cup_1 s_4}, \end{aligned} \quad (148)$$

where s_4 denotes a 4-simplex.

Unlike the 5 + 1D case, however, the term $\frac{1}{2} A_4 \cup A_4$ is no longer a trivial cocycle. In 7 + 1D there is no analog

of Eq. (138), and therefore this cocycle cannot be removed by adding a coboundary. As a result, we expect that the corresponding QCA cannot be simplified to a non-Clifford circuit. This conclusion is consistent with the fact that w_8 is a nontrivial Stiefel-Whitney class in $7 + 1D$, which indeed classifies a nontrivial QCA. A polynomial representation of this QCA can be obtained by translating the cup products of cochains into matrices, as in the previous cases. The resulting matrix coincides with that obtained in Ref. [5].

C. $\mathbb{Z}_2$ QCA in $(2l - 1) + 1D$ from topological action

$$S = \frac{1}{2} \int A_l \cup A_l + A_l \cup B_l + B_l \cup B_l$$

In a general even dimension, the action can be written as

$$S = \frac{1}{2} \int A_l \cup A_l + A_l \cup B_l + B_l \cup B_l. \quad (149)$$

We denote a $(l - 1)$ -simplex by s_{l-1} and a l -simplex by s_l . The corresponding QCA is then

$$\begin{aligned} \bar{Z}_{s_l}^A &= Z_{s_l}^A \prod_{s_{l-1}} G_{s_{l-1}}^{B \int s_l \cup s_{l-1}}, \\ \bar{Z}_{s_l}^B &= Z_{s_l}^B \prod_{s_{l-1}} G_{s_{l-1}}^{A \int s_{l-1} \cup s_l}, \\ U_{s_l}^A &= X_{s_l}^A \prod_{s'_l} Z_{s'_l}^{A \int s'_l \cup s_l}, \\ U_{s_l}^B &= X_{s_l}^B \prod_{s'_l} Z_{s'_l}^{B \int s'_l \cup s_l}. \end{aligned} \quad (150)$$

In an arbitrary dimension, Eq. (138) generalizes to

$$\begin{aligned} &\frac{1}{4} \delta (A_l \cup_1 A_l + A_l \cup_2 \delta A_l) \\ &= \frac{1}{4} \delta A_l \cup_2 \delta A_l + \frac{(-1)^l - 1}{4} (A_l \cup A_l + A_l \cup_1 \delta A_l). \end{aligned} \quad (151)$$

When l is odd, using the fact that $\delta A_l \equiv 0 \pmod{2}$, we obtain

$$\frac{1}{2} A_l \cup A_l = -\frac{1}{4} \delta (A_l \cup_1 A_l + A_l \cup_2 \delta A_l), \quad (152)$$

so that $\frac{1}{2} A_l \cup A_l$ is a coboundary in $H^{2l}(B^l \mathbb{Z}_2, \mathbb{R}/\mathbb{Z})$. In this case, as in $5 + 1D$, the corresponding QCA is trivial up to a non-Clifford circuit.

When l is even, the $A_l \cup A_l$ term in Eq. (151) cancels, leaving a nontrivial cocycle. Consequently, the associated QCA is also nontrivial. We therefore establish a 4-periodicity in the spatial dimensions for the generalized “3-fermion” Walker-Wang QCAs. Moreover, if non-Clifford circuits are not allowed, the QCAs exhibit only a 2-periodicity in the spatial dimensions.

D. $\mathbb{Z}_p$ Clifford QCAs in $(4l - 1) + 1D$ from TQFTs

The generalization of the $\mathbb{Z}_2$ 3-fermion QCA to higher dimensions can be extended to $\mathbb{Z}_p^{(k)}$ QCAs as well. However, in this case, the construction exhibits a 4-periodicity in the spatial dimension, so that nontrivial QCAs appear only in $(4l - 1)$ spatial dimensions.

Consider the action

$$S = \frac{k}{p} \int A_{2l} \cup A_{2l} \in H^{4l}(B^{2l} \mathbb{Z}_p, \mathbb{R}/\mathbb{Z}). \quad (153)$$

Following the framework of the $3 + 1D$ case, the corresponding separators and flippers are

$$\begin{aligned} \bar{Z}_{s_l} &= Z_{s_l} \prod_{s_{l-1}} \left(G_{s_{l-1}}^{(k)} \right)^{\frac{1}{2k} \int s_{l-1} \cup s_l}, \\ \bar{X}_{s_l} &= X_{s_l} \prod_{s'_l} \left[\prod_{s_{l-1}} \left(G_{s_{l-1}}^{(k)} \right)^{-\frac{1}{2} \int s_{l-1} \cup s_l} \right]^{\int s'_l \cup s_l}, \end{aligned} \quad (154)$$

where s_{l-1} and s_l denote $(l - 1)$ - and l -simplices, and

$$G_{s_{l-1}}^{(k)} := X_{\delta s_{l-1}} \prod_{s'_l} Z_{s'_l}^{k \int \delta s_{l-1} \cup s'_l}. \quad (155)$$

This construction is valid because the coboundary identities for higher cup products repeat with a 4-periodicity. Specifically, the formulas

$$\begin{aligned} \delta(c_p \cup_i d_q) &= \delta c_p \cup_i d_q \\ &\quad + (-1)^p c_p \cup_i \delta d_q \\ &\quad + (-1)^{p+q-i} c_p \cup_{i-1} d_q \\ &\quad + (-1)^{pq+p+q} d_q \cup_{i-1} c_p, \\ \delta(c_{p+2} \cup_i d_{q+2}) &= \delta c_{p+2} \cup_i d_{q+2} \\ &\quad + (-1)^p c_{p+2} \cup_i \delta d_{q+2} \\ &\quad + (-1)^{p+q-i} c_{p+2} \cup_{i-1} d_{q+2} \\ &\quad + (-1)^{pq+p+q} d_{q+2} \cup_{i-1} c_{p+2} \end{aligned} \quad (156)$$

have identical sign structures. Promoting each cochain by two degrees therefore preserves the relations, implying a 4-periodicity. Thus, our $\mathbb{Z}_p$ QCA constructions are valid in every fourth spatial dimension, consistent with the classification of Ref. [36].

We now argue that QCAs in $(4l + 1)$ spatial dimensions are always trivial, even when restricted to Clifford circuits.

Consider the identity

$$\begin{aligned}
 & \frac{k(p-1)}{2p} \delta(A_{2l+1} \cup_1 A_{2l+1}) \\
 &= \frac{k(p-1)}{2p} (\delta A_{2l+1} \cup_1 A_{2l+1} - A_{2l+1} \cup_1 \delta A_{2l+1} \\
 & \quad - A_{2l+1} \cup A_{2l+1} - A_{2l+1} \cup A_{2l+1}) \\
 &= \frac{k}{p} A_{2l+1} \cup A_{2l+1}. \tag{157}
 \end{aligned}$$

Hence, $(k/p)A_{2l+1} \cup A_{2l+1}$ is a coboundary. More importantly,

$$\begin{aligned}
 & \frac{k(p-1)}{2p} \delta(A_{2l+1} \cup_1 A_{2l+1}) \\
 &= \delta \left(\frac{k(p-1)/2}{p} A_{2l+1} \cup_1 A_{2l+1} \right) \tag{158}
 \end{aligned}$$

is implemented by a Clifford circuit, since the denominator involves only p . (By contrast, in the $\mathbb{Z}_2$ case the denominator is 4, which goes beyond Clifford.) Therefore, the QCA derived from

$$S = \frac{k}{p} A_{2l+1} \cup A_{2l+1} \tag{159}$$

is a Clifford circuit, and thus no nontrivial QCA arises in $(4l+1)$ spatial dimensions.

We conclude that $\mathbb{Z}_p$ QCAs exhibit a 4-periodicity in spatial dimensions, nontrivial only in $(4l-1)$ spatial dimensions.

V. INVERTIBLE SUBALGEBRAS IN 2 + 1D AND HIGHER DIMENSIONS

A closely related notion to QCAs is that of *invertible subalgebras* (ISAs), introduced by Haah in Ref. [43]. An ISA $\mathcal{A}$ is defined as a subalgebra of operators on a Hilbert space such that every operator can be locally expressed using elements of $\mathcal{A}$ and its commutant $\bar{\mathcal{A}}$. This induces a decomposition of the Hilbert space as

$$\mathcal{H} = \mathcal{H}_{\mathcal{A}} \otimes \mathcal{H}_{\bar{\mathcal{A}}}, \tag{160}$$

where $\mathcal{H}_{\mathcal{A}}$ is the Hilbert space generated by operators in $\mathcal{A}$. A nontrivial ISA arises when a tensor product Hilbert space $\mathcal{H}$ splits into factors $\mathcal{H}_{\mathcal{A}}$ and $\mathcal{H}_{\bar{\mathcal{A}}}$ that do not themselves form a tensor product structure.

Haah showed that an ISA in d spatial dimensions can be used to construct a QCA in $(d+1)$ dimensions. Concretely, consider a stack of d -dimensional ISAs layered along the extra dimension. The total Hilbert space takes

the form

$$\bigotimes_i \mathcal{H}_{\mathcal{A}}^{(i)} \otimes \mathcal{H}_{\bar{\mathcal{A}}}^{(i)}, \tag{161}$$

where i labels the layers. The QCA acts by shifting operators in $\mathcal{H}_{\mathcal{A}}^{(i)}$ forward to $\mathcal{H}_{\mathcal{A}}^{(i+1)}$ while leaving $\mathcal{H}_{\bar{\mathcal{A}}}^{(i)}$ invariant. This establishes a one-to-one correspondence between ISAs in d dimensions and QCAs in $d+1$ dimensions.

To date, the only known example of a nontrivial ISA appears in two spatial dimensions on the square lattice. Reference [43] constructed $\mathbb{Z}_p^{(k)}$ ISAs in this setting, showing that each such ISA uniquely generates a QCA in one higher dimension.

In this section, we introduce a new construction of $\mathbb{Z}_2$ ISAs on arbitrary two-dimensional cellulations, where the subalgebra $\mathcal{A}$ realizes the 3-fermion chiral topological order, and extend this construction to all even spatial dimensions. In addition, we reformulate the $\mathbb{Z}_p^{(k)}$ ISAs in two spatial dimensions and generalize them to all $(4l-2)$ dimensions. These constructions are consistent with the classification of algebraic L -groups over Laurent polynomial rings given in Ref. [36].

A. 2 + 1D $\mathbb{Z}_2$ invertible subalgebras

We present the invertible subalgebra on the 2 + 1D square lattice with two $\mathbb{Z}_2$ qubits per edge, which corresponds to the 3 + 1D 3-fermion QCA. First, we can rearrange two copies of $\mathbb{Z}_2$ toric codes $\{1, e_A, m_A, f_A\} \times \{1, e_B, m_B, f_B\}$ into the 3-fermion topological order $\mathcal{A}$ and its antichiral copy $\bar{\mathcal{A}}$ as follows:

$$\begin{aligned}
 \mathcal{A} \times \bar{\mathcal{A}} &:= \{1, e_A f_B, m_A f_B, f_A\} \\
 &\quad \times \{1, e_B f_A, m_B f_A, f_B\}. \tag{162}
 \end{aligned}$$

We define two shorthands that will be useful later on

$$\begin{aligned}
 U_e^\alpha &:= X_e^\alpha \prod_{e'} Z_{e'}^{\alpha f_{e' \cup e}}, \\
 \tilde{U}_e^\alpha &:= X_e^\alpha \prod_{e'} Z_{e'}^{\alpha f_{e \cup e'}}, \tag{163}
 \end{aligned}$$

$\alpha \in \{A, B\}$. Diagrammatically, they are

$$\begin{aligned}
 U_e^\alpha &= \begin{array}{c} \text{---} X_e^\alpha \text{---} \\ | \\ Z_e^\alpha \\ | \end{array}, \quad \begin{array}{c} | \\ X_e^\alpha \\ \text{---} Z_e^\alpha \text{---} \end{array}, \\
 \tilde{U}_e^\alpha &= \begin{array}{c} | \\ Z_e^\alpha \\ \text{---} X_e^\alpha \text{---} \end{array}, \quad \begin{array}{c} \text{---} Z_e^\alpha \text{---} \\ | \\ X_e^\alpha \\ | \end{array}. \tag{164}
 \end{aligned}$$

For simplicity, we define the flux operator W_f^α as

$$W_f^\alpha = Z_{\partial f}^\alpha = \begin{array}{c} \boxed{\begin{array}{ccc} & Z^\alpha & \\ Z^\alpha & f & Z^\alpha \\ & Z^\alpha & \end{array}} \end{array}. \quad (165)$$

The following are the generators of the ISA for the 3-fermion theory:

$$\begin{aligned} A_e^A &= \tilde{U}_e^A \prod_f W_f^{A f \cup_1 e}, \\ A_e^B &= \tilde{U}_e^B \prod_f W_f^{B f \cup_1 e} \prod_{e'} Z_{e'}^{A f \cup e'}, \\ \bar{A}_e^A &= \tilde{U}_e^A \prod_f W_f^{A f \cup_1 e} \prod_{e'} Z_{e'}^{B f \cup e'}, \\ \bar{A}_e^B &= \tilde{U}_e^B \prod_f W_f^{B f \cup_1 e}. \end{aligned} \quad (166)$$

These generators are constructed by attaching the flux terms $W_f^{A/B}$ and single-qubit Pauli operators $Z_f^{A/B}$ to the hopping terms $\tilde{U}_e^{A/B}$, in accordance with the pattern specified by the cup and cup-1 products. This structure ensures that the resulting operators satisfy the definition of an ISA.

On the square lattice, these terms are

$$\begin{aligned} A_e^A &= \begin{array}{c} \boxed{\begin{array}{ccc} & Z^A & \\ Z^A & X^A Z^A & \\ & Z^A & \end{array}} \quad , \quad \begin{array}{c} \boxed{\begin{array}{c} Z^A \\ X^A Z^A \end{array}} \end{array}, & A_e^B &= \begin{array}{c} \boxed{\begin{array}{ccc} & Z^A & \\ X^B Z^B & & Z^B \\ & Z^B & \end{array}} \quad , \quad \begin{array}{c} \boxed{\begin{array}{ccc} & Z^A Z^B & \\ X^B Z_e^B & & Z^B \\ & Z^B & \end{array}} \end{array}, \\ \bar{A}_e^A &= \begin{array}{c} \boxed{\begin{array}{ccc} & X^A Z^A & \\ Z^B & e & Z^A \\ & Z^B & \end{array}} \quad , \quad \begin{array}{c} \boxed{\begin{array}{ccc} & X^A Z_e^A & \\ Z^A Z^B & & Z^A \\ & Z^A & \end{array}} \end{array}, & \bar{A}_e^B &= \begin{array}{c} \boxed{\begin{array}{ccc} & Z^B & \\ Z^B & X^B Z^B & \\ & Z^B & \end{array}} \quad , \quad \begin{array}{c} \boxed{\begin{array}{ccc} & Z^B & \\ Z^B & X^B Z_e^B & \end{array}} \end{array}. \end{aligned} \quad (167)$$

Next, we prove that it is invertible, which means that the single X and Z terms can be generated from A and $\bar{A}$. We first construct the flux operator of B qubits from A_e^A and $\bar{A}_e^A$ as $W_f^B = \prod_v (A_{\delta v}^A \bar{A}_{\delta v}^A)^{f \cup v}$,

The diagram shows a 2x2 grid of Z^B operators on the left, which is equal to a product of eight 2x2 grids. Each grid contains a combination of X^A and Z^A operators. The first row has four grids, and the second row has four grids. The operators are arranged in a way that their product reproduces the original Z^B operators.

With this W_f^B , we construct single Z_e^A from A_e^B and $\bar{A}_e^B$

$$Z_e^A = \prod_{e'} (A_{e'}^B \bar{A}_{e'}^B \prod_f W_f^B)^{f \cup 1_{e'} + e' \cup 1_f} f e' \cup e, \quad (168)$$

which can be shown diagrammatically as

The diagram shows a single Z^A operator (represented by a vertical rectangle) is equal to a product of two rows of four 2x2 grids each. Each grid contains a combination of X^B and Z^B operators. The first row of grids has X^B operators on the left and Z^B operators on the right. The second row of grids has Z^B operators on the left and X^B operators on the right. The product of these grids reproduces the Z^A operator.

With this single Z^A obtained, the construction of other single Pauli operators are obvious. In cup-product formalism, they can be shown as

$$\begin{aligned} X_e^A &= A_e^A \prod_{e'} Z_{e'}^{A f e \cup e'} \prod_f W_f^{A f f \cup 1_e}, \\ Z_e^B &= \prod_{e'} \left(X_{e'}^A \bar{A}_{e'}^A \prod_{e''} Z_{e''}^{A f e' \cup e''} \prod_f W_f^{A f e' \cup f} \right)^{f e \cup e'}, \\ X_e^B &= \bar{A}_e^B \prod_{e'} Z_{e'}^{B f e \cup e'} \prod_f W_f^{B f f \cup 1_e}. \end{aligned} \quad (169)$$

Operators A_e^α and $\bar{A}_e^\alpha$ are related by the unitary

$$U = \prod_{e, f'} CZ(Z_e^A, W_{f'}^A)^{f f \cup 1_e + e \cup 1_f} CZ(Z_e^B, W_{f'}^B)^{f f \cup 1_e + e \cup 1_f} \times \prod_{e, e'} CZ(Z_e^A, Z_{e'}^B)^{f e' \cup e}, \quad (170)$$

where $CZ(P_1, P_2) = (-1)^{\frac{1-P_1}{2} \frac{1-P_2}{2}}$ is the generalized controlled gate of two commuting Pauli operators P_1 and P_2 . Note that $W_f^{f f \cup 1_e + e \cup 1_f}$ on the square lattice does not contain Z_e so the CZ operator is well defined.

1. Polynomial form

The hopping operators in polynomial form are

$$\mathbf{U}_e^\alpha = \mathbf{X}_e^\alpha + \mathbf{Z}_e^\alpha \mathbf{M}_{e' \cup e}^\alpha, \quad (171)$$

$$\tilde{\mathbf{U}}_e^\alpha = \mathbf{X}_e^\alpha + \mathbf{Z}_e^\alpha \mathbf{M}_{e \cup e'}^\dagger, \quad (172)$$

$$\mathbf{W}_f^\alpha = \mathbf{Z}_{\delta e}^\alpha, \quad (173)$$

where $\alpha \in \{A, B\}$. The generators of the ISA are

$$\mathbf{A}_e^A = \tilde{\mathbf{U}}_e^A + \mathbf{W}_f^A \mathbf{M}_{f \cup_1 e}, \quad (174)$$

$$\bar{\mathbf{A}}_e^A = \tilde{\mathbf{U}}_e^A + \mathbf{W}_f^A \mathbf{M}_{e \cup_1 f}^\dagger + \mathbf{Z}_{e'}^B \mathbf{M}_{e' \cup e}, \quad (175)$$

$$\mathbf{A}_e^B = \tilde{\mathbf{U}}_e^B + \mathbf{W}_f^B \mathbf{M}_{e \cup_1 f}^\dagger + \mathbf{Z}_{e'}^A \mathbf{M}_{e \cup e'}^\dagger, \quad (176)$$

$$\bar{\mathbf{A}}_e^B = \tilde{\mathbf{U}}_e^B + \mathbf{W}_f^B \mathbf{M}_{f \cup_1 e}. \quad (177)$$

In other words, we have

$$\mathbf{A} = (\mathbf{A}^A \quad \mathbf{A}^B) = \begin{pmatrix} \mathbb{1} \\ \mathcal{M} \end{pmatrix}, \quad (178)$$

$$\bar{\mathbf{A}} = (\bar{\mathbf{A}}^A \quad \bar{\mathbf{A}}^B) = \begin{pmatrix} \mathbb{1} \\ \bar{\mathcal{M}} \end{pmatrix}, \quad (179)$$

where

$$\mathcal{M} = \begin{pmatrix} \mathbf{M}_{e \cup e_0}^\dagger + \mathbf{M}_{\delta e_0 \cup_1 e} & \mathbf{M}_{e \cup e_0}^\dagger \\ 0 & \mathbf{M}_{e \cup e_0}^\dagger + \mathbf{M}_{e \cup_1 \delta e_0}^\dagger \end{pmatrix}, \quad (180)$$

$$\bar{\mathcal{M}} = \begin{pmatrix} \mathbf{M}_{e \cup e_0}^\dagger + \mathbf{M}_{e \cup_1 \delta e_0}^\dagger & 0 \\ \mathbf{M}_{e_0 \cup e} & \mathbf{M}_{e \cup e_0}^\dagger + \mathbf{M}_{\delta e_0 \cup_1 e} \end{pmatrix}. \quad (181)$$

In fact, $\mathcal{M}^\dagger = \bar{\mathcal{M}}$, where the equality for the diagonal terms follows from the Leibniz rule for the $\cup_1$ product.

A QCA can be constructed from the ISA by pushing $\mathbf{A}$ in an arbitrary direction of $m = x^i y^j z^k$ as

$$\mathbf{H} \begin{pmatrix} m & 0 \\ 0 & 1 \end{pmatrix} \mathbf{H}^{-1}, \quad \text{where } \mathbf{H} = (\mathbf{A} \quad \bar{\mathbf{A}}), \quad (182)$$

of which the simplest is to take $m = z$. We may write

$$\alpha_{\text{ISA}}^{3F} = \mathbf{H} \begin{pmatrix} z & 0 \\ 0 & 1 \end{pmatrix} \mathbf{H}^{-1}. \quad (183)$$

2. $\mathbb{Z}_2$ invertible subalgebra on dual triangular-honeycomb lattices

In this subsection, we generalize our cubic lattice construction for $\mathbb{Z}_2$ invertible subalgebra to other lattices. Specifically, we introduce the dual triangular-honeycomb lattices illustrated in Fig. 7(a).

We place A qubits on the edges of the triangular lattice and B qubits on the edges of the honeycomb lattice.

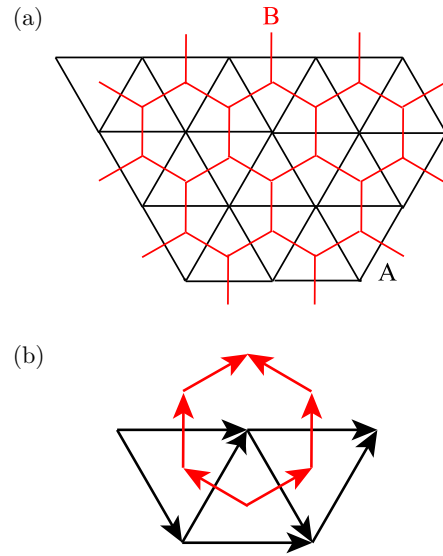


FIG. 7. (a) The lattice is constructed by stacking a triangular lattice together with its dual, the honeycomb lattice. (b) Branching structure of the mixed lattice.

To incorporate this model into our cup-product framework, we introduce the rules for cup products on the mixed lattice.

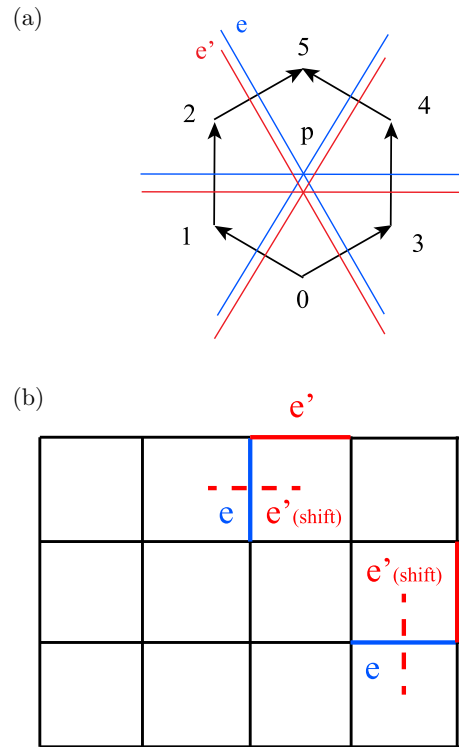


FIG. 8. (a) The intersections of shifted dual lines indicate the cup-product definition. (b) An illustration of the cup product on a square lattice, realized as the intersection of one edge with the other after a left-downward shift.

We begin by establishing the branching structure of the lattice, illustrated in Fig. 7(b). The cup product and coboundary operators on the triangular lattice follow directly from simplicial cohomology, as reviewed in Sec. II A. Our main focus, therefore, is on defining the cup products on the honeycomb lattice and the mixed cup products such as $e^A \cup e^B$ across the two lattices.

Following the geometric definition of the cup product on the cubic lattice, we define the cup and cup-1 products on the honeycomb lattice as illustrated in Fig. 8(a):

$$\begin{aligned} e \cup_1 f(p) &= e(01) + e(12) + e(25)]f(p), \\ f \cup_1 e(p) &= [e(03) + e(34) + e(45)]f(p), \\ e \cup e'(p) &= e(03)e'(34) + e(03)e'(45) + e(34)e'(45) \\ &\quad + e(01)e'(12) + e(01)e'(25) + e(12)e'(25). \end{aligned} \quad (184)$$

Next, we derive the formula for $e^A \cup e^B$. On the square lattice, the cup product of two edges corresponds

geometrically to the intersection of one edge with the dual edge shifted toward the down-left direction, as illustrated in Fig. 8(b). Motivated by this, we define $\int e^A \cup e^B \neq 0$ whenever e^A and e^B are Poincaré dual to each other. As an example, the operator A_e^A can be written as

$$\begin{aligned} A_e^A &= \tilde{U}_e^A \prod_f W_f^A \int e \cup_1 f \prod_{e'} Z_{e'}^B \int e \cup e' \\ &= \tilde{U}_e^A \left(\prod_f W_f^A \int e \cup_1 f \right) Z_{\text{PD}(e)}^B, \end{aligned} \quad (185)$$

where $\text{PD}(e)$ denotes the edge Poincaré dual to e .

With all these cup products defined, we can now derive the invertible subalgebra on this triangular-honeycomb lattice from the original formalism. Starting with the $\tilde{U}$ operator defined in Eq. (163),

$$\begin{aligned} \tilde{U}_e^A &= X_e^A \prod_{e'} Z_{e'}^A \int e \cup e' = \begin{array}{c} \text{Diagram 1: } X_e^A \text{ on edge } e, Z_{e'}^A \text{ on edges } e' \text{ forming a triangle with } e. \\ \text{Diagram 2: } X_e^A \text{ on edge } e, Z_{e'}^A \text{ on edges } e' \text{ forming a triangle with } e. \\ \text{Diagram 3: } X_e^A \text{ on edge } e, Z_{e'}^A \text{ on edges } e' \text{ forming a triangle with } e. \end{array}, \\ \tilde{U}_e^B &= X_e^B \prod_{e'} Z_{e'}^B \int e \cup e' = \begin{array}{c} \text{Diagram 4: } X_e^B \text{ on edge } e, Z_{e'}^B \text{ on edges } e' \text{ forming a triangle with } e. \\ \text{Diagram 5: } X_e^B \text{ on edge } e, Z_{e'}^B \text{ on edges } e' \text{ forming a triangle with } e. \\ \text{Diagram 6: } X_e^B \text{ on edge } e, Z_{e'}^B \text{ on edges } e' \text{ forming a triangle with } e. \end{array}. \end{aligned} \quad (186)$$

We can then derive the entire invertible subalgebra as follows:

$$\begin{aligned} A_e^A &= \tilde{U}_e^A \prod_f W_f^A \int e \cup_1 f \prod_{e'} Z_{e'}^B \int e \cup e' = \begin{array}{c} \text{Diagram 7: } X_e^A \text{ on edge } e, Z_{e'}^B \text{ on edges } e' \text{ forming a triangle with } e. \\ \text{Diagram 8: } X_e^A \text{ on edge } e, Z_{e'}^B \text{ on edges } e' \text{ forming a triangle with } e. \\ \text{Diagram 9: } X_e^A \text{ on edge } e, Z_{e'}^B \text{ on edges } e' \text{ forming a triangle with } e. \end{array}, \\ A_e^B &= \tilde{U}_e^B \prod_f W_f^B \int f \cup_1 e = \begin{array}{c} \text{Diagram 10: } X_e^B \text{ on edge } e, Z_{e'}^B \text{ on edges } e' \text{ forming a triangle with } e. \\ \text{Diagram 11: } X_e^B \text{ on edge } e, Z_{e'}^B \text{ on edges } e' \text{ forming a triangle with } e. \\ \text{Diagram 12: } X_e^B \text{ on edge } e, Z_{e'}^B \text{ on edges } e' \text{ forming a triangle with } e. \end{array}, \end{aligned} \quad (187)$$

and

$$\begin{aligned} \bar{A}_e^A &= \tilde{U}_e^A \prod_f W_f^A f^{\cup_1 e} = \text{diagram 1}, \text{diagram 2}, \text{diagram 3}, \\ \bar{A}_e^B &= \tilde{U}_e^B \prod_f W_f^B f^{e \cup_1 f} \prod_{e'} Z_{e'}^A f^{e' \cup e} = \text{diagram 4}, \text{diagram 5}, \text{diagram 6}. \end{aligned} \quad (188)$$

Following the similar calculation of Eq. (169), we conclude that these operators also generate the entire qubit algebra, meaning that they form an invertible subalgebra.

Thus, we generalize the cubic $\mathbb{Z}_2$ invertible subalgebra to a specific noncubic lattice. Before moving on, we claim that this kind of generalization only works for $\mathbb{Z}_2$ cases because in other cases the additional $\pm$ sign would break the commutativity of A and $\bar{A}$. From a mathematical point of view, the $\mathbb{Z}_2$ invertible subalgebra (and its corresponding QCA) is guided by a $\mathbb{Z}_2$ topological invariant w_2^2 , while $\mathbb{Z}_k$ cases are not. So the cup-product formula for $\mathbb{Z}_2$ ISA is robust to lattice changes, but $\mathbb{Z}_k$ ISA only lives on a certain lattice (the cubic one).

B. 2 + 1D $\mathbb{Z}_p^{(k)}$ invertible subalgebras

On the 2d square lattice, we put one $\mathbb{Z}_p$ qudit on each edge, spanning the whole Pauli algebra. We can define a subalgebra of the Pauli group generated by the operator

$$A_e^{(k)} := X_e \prod_{e'} Z_{e'}^{k f^{e' \cup e}} \prod_f Z_{\partial f}^{\frac{k}{2} f(e \cup_1 f - f \cup_1 e)}, \quad (189)$$

where we again emphasize that $\frac{1}{2}$ in the exponent stands for the integer $(p+1)/2$, which is the multiplicative inverse of 2 mod p . The orthogonal subalgebra is generated by

$$\bar{A}_e^{(k)} := X_e \prod_{e'} Z_{e'}^{-k f^{e' \cup e}} \prod_f Z_{\partial f}^{-\frac{k}{2} f(e \cup_1 f - f \cup_1 e)}, \quad (190)$$

which is the charge conjugation, $Z \rightarrow Z^{-1}$, of the subalgebra generated by $A_e^{(k)}$.

These two terms can be shown in the following diagrams:

$$A_e^{(k)} = \text{diagram 1}, \text{diagram 2}, \quad (191)$$

$$\bar{A}_e^{(k)} = \text{diagram 3}, \text{diagram 4}. \quad (192)$$

First, we verify elements in $\{A_e^{(k)}\}$ and $\{\bar{A}_e^{(k)}\}$ mutually commute, i.e.,

$$A_{e_1}^{(k)} \bar{A}_{e_2}^{(k)} = \exp\left(\frac{2\pi i}{p} \chi\right) \bar{A}_{e_2}^{(k)} A_{e_1}^{(k)}, \quad (193)$$

with

$$\begin{aligned} \chi &= \frac{k}{2} \int -2e_1 \cup e_2 - e_2 \cup_1 \delta e_1 + \delta e_1 \cup_1 e_2 \\ &\quad - 2e_2 \cup e_1 - e_1 \cup_1 \delta e_2 + \delta e_2 \cup_1 e_1 \\ &= 0, \end{aligned} \quad (194)$$

where we have used

$$\begin{aligned}\delta(A_1 \cup B_1) &= \delta A_1 \cup B_1 - A_1 \cup \delta B_1 \\ &\quad - A_1 \cup B_1 - B_1 \cup A_1.\end{aligned}\quad (195)$$

Next, we need to show that the single Pauli X_e or Z_e can be generated from $\{A_e^{(k)}\}$ and $\{\bar{A}_e^{(k)}\}$. We note that this scenario is specific to the square lattice. For a generic triangulation, $\{A_e^{(k)}\}$ and $\{\bar{A}_e^{(k)}\}$ might not generate all operators in the Hilbert space, and $\{A_e^{(k)}\}$ will not realize an invertible subalgebra.

First, it is useful to notice the following identity:

$$\begin{aligned}A_{\delta v}^{(k)} &= X_{\delta v} \prod_{e'} Z_{e'}^{k \int e' \cup \delta v + \frac{k}{2} \int (\delta v \cup_1 \delta e' - \delta e' \cup_1 \delta v)} \\ &= X_{\delta v} \prod_f Z_{\partial f}^{k \int v \cup f},\end{aligned}\quad (196)$$

where we have used

$$\begin{aligned}\delta(e' \cup v) &= \delta e' \cup v - e' \cup \delta v, \\ \delta(\delta v \cup_2 \delta e') &= -\delta v \cup_1 \delta e' - \delta e' \cup_1 \delta v, \\ \delta(v \cup_1 \delta e') &= \delta v \cup_1 \delta e' - v \cup \delta e' + \delta e' \cup v.\end{aligned}\quad (197)$$

We then multiply $A_e^{(k)}$ and $\bar{A}_e^{(k)}$ to obtain X_e^2 and therefore single Pauli X_e ,

$$X_e = \left(A_e^{(k)} \bar{A}_e^{(k)} \right)^{\frac{1}{2}}. \quad (198)$$

Diagrammatically, they are

$$\begin{aligned}-X_e^2 &= \begin{array}{|c|} \hline Z^{\frac{k}{2}} \\ \hline Z^{\frac{k}{2}} \\ \hline \end{array} \begin{array}{|c|} \hline Z^{-\frac{k}{2}} \\ \hline Z^{-\frac{k}{2}} \\ \hline \end{array} \times \begin{array}{|c|} \hline Z^{-\frac{k}{2}} \\ \hline Z^{-\frac{k}{2}} \\ \hline \end{array} \begin{array}{|c|} \hline Z^{\frac{k}{2}} \\ \hline Z^{\frac{k}{2}} \\ \hline \end{array}, \\ |X_e^2|_e &= \begin{array}{|c|} \hline Z^{\frac{k}{2}} \\ \hline Z^{\frac{k}{2}} \\ \hline \end{array} \begin{array}{|c|} \hline X \\ \hline X \\ \hline \end{array} \begin{array}{|c|} \hline Z^{-\frac{k}{2}} \\ \hline Z^{-\frac{k}{2}} \\ \hline \end{array} \times \begin{array}{|c|} \hline Z^{-\frac{k}{2}} \\ \hline Z^{-\frac{k}{2}} \\ \hline \end{array} \begin{array}{|c|} \hline X \\ \hline X \\ \hline \end{array} \begin{array}{|c|} \hline Z^{\frac{k}{2}} \\ \hline Z^{\frac{k}{2}} \\ \hline \end{array}.\end{aligned}\quad (199)$$

Subsequently, on the square lattice, we use Pauli X_e and Eq. (196) to obtain a single $Z_{\partial f}$ term,

$$Z_{\partial f} = \prod_v (A_{\delta v} X_{\delta v}^{-1})^{\frac{1}{k} \int v \cup f} = \prod_v (A_{\delta v} \bar{A}_{\delta v}^{-1})^{\frac{1}{2k} \int v \cup f}. \quad (200)$$

This product can be illustrated by the following diagram:

$$\begin{array}{|c|} \hline Z^{-k} \\ \hline Z^k \\ \hline \end{array} = \begin{array}{|c|} \hline Z^{-\frac{k}{2}} \\ \hline X^\dagger \\ \hline Z^{\frac{k}{2}} \\ \hline \end{array} \times \begin{array}{|c|} \hline Z^{-\frac{k}{2}} \\ \hline X^\dagger \\ \hline Z^{\frac{k}{2}} \\ \hline \end{array} \times \begin{array}{|c|} \hline Z^{\frac{k}{2}} \\ \hline X \\ \hline Z^{-\frac{k}{2}} \\ \hline \end{array} \times \begin{array}{|c|} \hline Z^{\frac{k}{2}} \\ \hline X \\ \hline Z^{-\frac{k}{2}} \\ \hline \end{array} \times \begin{array}{|c|} \hline X \\ \hline X^\dagger \\ \hline X \\ \hline \end{array}.\quad (201)$$

Finally, we multiply the Pauli X_e and plaquette term $Z_{\partial f}$ to $A_e^{(k)}$, to derive single Pauli Z_e as

$$Z_{e'} = \prod_e \left(A_e^{(k)} X_e^{-1} \prod_f Z_{\partial f}^{-\frac{k}{2} \int (e \cup_1 f - f \cup_1 e)} \right)^{\frac{1}{k} \int e' \cup e}. \quad (202)$$

Graphically, this is

$$\begin{aligned}\begin{array}{|c|} \hline Z^k \\ \hline \end{array} &= \begin{array}{|c|} \hline Z^{\frac{k}{2}} \\ \hline X \\ \hline Z^{-\frac{k}{2}} \\ \hline \end{array} \times \begin{array}{|c|} \hline X^\dagger \\ \hline \end{array} \times \begin{array}{|c|} \hline Z^{-\frac{k}{2}} \\ \hline Z^{\frac{k}{2}} \\ \hline \end{array} \times \begin{array}{|c|} \hline Z^{-\frac{k}{2}} \\ \hline Z^{\frac{k}{2}} \\ \hline \end{array}, \\ \begin{array}{|c|} \hline Z^{-k} \\ \hline \end{array} &= \begin{array}{|c|} \hline Z^{\frac{k}{2}} \\ \hline X \\ \hline Z^{-\frac{k}{2}} \\ \hline \end{array} \times \begin{array}{|c|} \hline X^\dagger \\ \hline \end{array} \times \begin{array}{|c|} \hline Z^{\frac{k}{2}} \\ \hline Z^{-\frac{k}{2}} \\ \hline \end{array} \times \begin{array}{|c|} \hline Z^{-\frac{k}{2}} \\ \hline Z^{\frac{k}{2}} \\ \hline \end{array}.\end{aligned}\quad (203)$$

Thus, this can be expressed entirely in terms of $A_e^{(k)}$ and $\bar{A}_e^{(k)}$ as

$$Z_{e'} = \prod_e \left[\left(A_e^{(k)} (\bar{A}_e^{(k)})^{-1} \right) \times \prod_{v,f} \left(A_{\delta v}^{(k)} (\bar{A}_{\delta v}^{(k)})^{-1} \right)^{-\frac{1}{2} \int v \cup f \int (e \cup_1 f - f \cup_1 e)} \right]^{\frac{1}{2k} \int e' \cup e}. \quad (204)$$

When $p \equiv 1 \pmod{4}$, the element -1 is a quadratic residue in $\mathbb{Z}_p$. Let $a \in \mathbb{Z}_p$ satisfy $a^2 \equiv -1 \pmod{p}$. Then the diagonal symplectic transformation

$$\begin{pmatrix} a & 0 & 0 & 0 \\ 0 & a & 0 & 0 \\ 0 & 0 & -a & 0 \\ 0 & 0 & 0 & -a \end{pmatrix} \quad (205)$$

maps $A_e^{(k)}$ to its conjugate $\bar{A}_e^{(k)}$. Consequently, two copies of the invertible subalgebra $A_e^{(k)}$ are equivalent to one copy of $A_e^{(k)}$ and one copy of $\bar{A}_e^{(k)}$. This tensor product Hilbert space is reducible to a trivial factorization, implying that the combined system of two copies of $A_e^{(k)}$ is trivial ISA. This conclusion is fully consistent with the Witt group classification, where for primes $p \equiv 1 \pmod{4}$ the corresponding quadratic forms yield only order-two elements, so stacking two copies indeed produces a trivial class.

1. Polynomial form

In the odd prime cases, the ISA are constructed as

$$\mathbf{A}_e^{(k)} = \mathbf{U}_e^{(k)} + \frac{k}{2} \mathbf{Z}_{e'} (\mathbf{M}_{e \cup_1 \delta e'}^\dagger - \mathbf{M}_{\delta e' \cup_1 e}), \quad (206)$$

$$\mathbf{A}^{(k)} = \begin{pmatrix} \mathbb{1} \\ \mathcal{M} \end{pmatrix}, \quad (207)$$

where

$$\mathcal{M}_{e_0, e} = k \mathbf{M}_{e_0 \cup e} + \frac{k}{2} (\mathbf{M}_{e \cup_1 \delta e_0}^\dagger - \mathbf{M}_{\delta e_0 \cup_1 e}). \quad (208)$$

Define $\bar{\mathbf{A}}^{(k)} \equiv \mathbf{A}^{(-k)}$. One can check that

$$\langle \mathbf{A}^{(k)}, \bar{\mathbf{A}}^{(k)} \rangle = 0. \quad (209)$$

$\mathbf{A}^{(k)}$ defines an invertible subalgebra if $\mathbf{A}^{(k)}$ and $\bar{\mathbf{A}}^{(k)}$ generates all Pauli operators. That is, the matrix

$$\mathbf{H} = \begin{pmatrix} \mathbf{A}^{(k)} & \bar{\mathbf{A}}^{(k)} \end{pmatrix} \quad (210)$$

is invertible. An explicit form of the inverse is

$$\mathbf{H}^{-1} = \frac{1}{2} \begin{pmatrix} \mathbb{1} & \mathcal{M}^{-1} \\ \mathbb{1} & -\mathcal{M}^{-1} \end{pmatrix}. \quad (211)$$

Thus, $\mathcal{M}$ needs to be invertible. A sufficient condition for being invertible is if $\mathbf{M}_{v \cup f}$ and $\mathbf{M}_{e' \cup e}$ are invertible matrices, which is the case for the square lattice. Since the columns of $\mathbf{H}^{-1}$ describe the coefficients of $\mathbf{A}^{(k)}$ and $\bar{\mathbf{A}}^{(k)}$ that give $\mathbf{X}$ and $\mathbf{Z}$, we can directly obtain the expression for $\mathcal{M}^{-1}$ in terms of the cup products from Eq. (204) as

$$\begin{aligned} \mathcal{M}_{e_0, e}^{-1} &= \frac{1}{k} \left[\delta_{e_0, e} - \frac{1}{2} (\mathbf{M}_{\delta e_0, f}^\dagger)^{-1} \right. \\ &\quad \left. \times (\mathbf{M}_{e' \cup_1 f}^\dagger - \mathbf{M}_{f \cup_1 e'}) \right] (\mathbf{M}_{e \cup e'})^{-1}. \end{aligned} \quad (212)$$

A QCA can then be constructed from the ISA by again pushing, for example $\mathbf{A}^{(k)}$, in an arbitrary direction of $m = x^i y^j z^k$ as

$$\mathbf{H} \begin{pmatrix} m & 0 \\ 0 & 1 \end{pmatrix} \mathbf{H}^{-1}. \quad (213)$$

Take $m = x^{-1} y^{-1} z^{-1}$ as an example, we have

$$\alpha_{\text{ISA}}^{(k)} = A + z^{-1} B, \quad (214)$$

where

$$A = \begin{pmatrix} \frac{1}{2} & 0 & \frac{x}{4k} - \frac{1}{4kx} & \frac{y}{4kx} + \frac{1}{4kx} + \frac{y}{4k} - \frac{1}{4k} \\ 0 & \frac{1}{2} & -\frac{x}{4ky} - \frac{x}{4k} - \frac{1}{4ky} + \frac{1}{4k} & \frac{1}{4ky} - \frac{y}{4k} \\ \frac{k}{4y} - \frac{ky}{4} & -\frac{ky}{4x} - \frac{k}{4x} - \frac{ky}{4} + \frac{k}{4} & \frac{1}{2} & 0 \\ \frac{kx}{4y} + \frac{kx}{4} + \frac{k}{4y} - \frac{k}{4} & \frac{kx}{4} - \frac{k}{4x} & 0 & \frac{1}{2} \end{pmatrix}$$

and

$$B = \begin{pmatrix} \frac{1}{2xy} & 0 & \frac{1}{4kx^2y} - \frac{1}{4ky} & -\frac{1}{4kx^2y} - \frac{1}{4kx^2} + \frac{1}{4kxy} - \frac{1}{4kx} \\ 0 & \frac{1}{2xy} & \frac{1}{4kxy^2} - \frac{1}{4kxy} + \frac{1}{4ky^2} + \frac{1}{4ky} & \frac{1}{4kx} - \frac{1}{4kxy^2} \\ \frac{k}{4x} - \frac{k}{4xy^2} & \frac{k}{4x^2y} + \frac{k}{4x^2} - \frac{k}{4xy} + \frac{k}{4x} & \frac{1}{2xy} & 0 \\ -\frac{k}{4xy^2} + \frac{k}{4xy} - \frac{k}{4y^2} - \frac{k}{4y} & \frac{k}{4x^2y} - \frac{k}{4y} & 0 & \frac{1}{2xy} \end{pmatrix}.$$

Further, we may explicitly construct a QCA that squares to translation in an arbitrary direction. In particular, let the desired translation be given by a monomial $m = x^i y^j z^k$ for $p = 1 \bmod 4$. Define

$$\alpha_{\text{ISA}} = \mathbf{H} \begin{pmatrix} m & 0 \\ 0 & 1 \end{pmatrix} \mathbf{H}^{-1} \begin{pmatrix} -a\mathbb{1} & 0 \\ 0 & a\mathbb{1} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} -a(m+1)\mathbb{1} & a(m-1)\mathcal{M}^{-1} \\ -a(m-1)\mathcal{M} & a(m+1)\mathbb{1} \end{pmatrix}, \quad (215)$$

where we choose $a^2 = -1 \pmod{p}$ such that α_{ISA} is a symplectic transformation. Then, we see that

$$\alpha_{\text{ISA}}^2 = \begin{pmatrix} -m\mathbb{1} & 0 \\ 0 & -m\mathbb{1} \end{pmatrix}, \quad (216)$$

which is a translation in the direction m followed by charge conjugation.

When $p = -1 \pmod{4}$, there exists no $a^2 = -1 \pmod{p}$, but there always exist a and b that $a^2 + b^2 \equiv -1 \pmod{p}$. In this case, we must consider the stack of two invertible subalgebras $\mathbf{H} \oplus \mathbf{H}$ represented by a block-diagonal matrix $\text{diag}(\mathbf{H}, \mathbf{H})$. We can then consider a QCA induced by this double subalgebra,

$$\alpha_{\text{ISA}} = \begin{pmatrix} \mathbf{H} & 0 \\ 0 & \mathbf{H} \end{pmatrix} \begin{pmatrix} m\mathbb{1} & 0 & 0 & 0 \\ 0 & \mathbb{1} & 0 & 0 \\ 0 & 0 & m\mathbb{1} & 0 \\ 0 & 0 & 0 & \mathbb{1} \end{pmatrix} \begin{pmatrix} \mathbf{H}^{-1} & 0 \\ 0 & \mathbf{H}^{-1} \end{pmatrix} \begin{pmatrix} a\mathbb{1} & 0 & b\mathbb{1} & 0 \\ 0 & -a\mathbb{1} & 0 & -b\mathbb{1} \\ b\mathbb{1} & 0 & -a\mathbb{1} & 0 \\ 0 & -b\mathbb{1} & 0 & a\mathbb{1} \end{pmatrix}. \quad (217)$$

It is straightforward to check that this α_{ISA} also satisfies

$$\alpha_{\text{ISA}}^2 = \begin{pmatrix} -m\mathbb{1} & 0 & 0 & 0 \\ 0 & -m\mathbb{1} & 0 & 0 \\ 0 & 0 & -m\mathbb{1} & 0 \\ 0 & 0 & 0 & -m\mathbb{1} \end{pmatrix}, \quad (218)$$

which represents a shift along the direction m along with a charge conjugation on both pieces of the invertible subalgebra.

C. 4 + 1D and 2I + 1D $\mathbb{Z}_2$ invertible subalgebras

For $\mathbb{Z}_2$ ISAs, the overall signs in front of higher cup products can be ignored. Hence, each cochain can simply be promoted by one degree, and the same analysis applies. For instance, Eq. (166) generalizes to 4 + 1D as

$$\begin{aligned} A_f^A &= \tilde{U}_f^A \prod_t W_t^{A \int t \cup_1 f}, \\ A_f^B &= \tilde{U}_f^B \left(\prod_t W_t^{B \int f \cup_1 t} \right) Z_{\text{PD}(f)}^A, \\ \bar{A}_f^A &= \tilde{U}_f^A \left(\prod_t W_t^{A \int f \cup_1 t} \right) Z_{\text{PD}(f)}^B, \\ \bar{A}_f^B &= \tilde{U}_f^B \prod_t W_t^{B \int t \cup_1 f}, \end{aligned} \quad (219)$$

where qubits of type A are placed on the faces of the direct lattice and qubits of type B on the faces of the dual lattice. Here $\text{PD}(f)$ denotes the face in the dual (direct) lattice that intersects the face f in the direct (dual) lattice. The hopping and flux terms are defined as

$$\tilde{U}_f^\alpha := X_{f'}^\alpha \prod_{f'} (Z_{f'}^\alpha)^{f \cup f'}, \quad W_t^\alpha := Z_{\partial t}^\alpha, \quad (220)$$

$\alpha \in \{A, B\}$. It is straightforward to verify that these operators satisfy the definition of an ISA. ISAs in $6 + 1\text{D}$ and higher dimensions can be constructed analogously by continuing to increase the cochain degree.

D. $6 + 1\text{D}$ and $(4l - 2) + 1\text{D}$ $\mathbb{Z}_p^{(k)}$ invertible subalgebras

The recursive relation for cup products, introduced in the derivation of the $2 + 1\text{D}$ invertible subalgebras in Eqs. (194) and (197), generalizes naturally to higher dimensions, reappearing every fourth dimension.

As shown in Sec. IV D, promoting each cochain by two degrees yields the same structure. On a hypercubic lattice, each nonvanishing product $c_i \cup c_{d-i}$ establishes a one-to-one correspondence between c_i and c_{d-i} , ensuring that the subalgebra remains invertible.

As a concrete example, the $6 + 1\text{D}$ $\mathbb{Z}_p^{(k)}$ invertible subalgebras are defined by

$$A_{c_3}^{(k)} = X_{c_3} \prod_{c_3'} Z_{c_3'}^{k \int c_3' \cup c_3} \prod_{c_4} Z_{\partial c_3}^{\frac{k}{2} \int (c_3 \cup_1 c_4 - c_4 \cup_1 c_3)}, \quad (221)$$

$$\bar{A}_{c_3}^{(k)} = A_{c_3}^{(-k)},$$

where c_3 and c_4 denote three- and four-dimensional (hyper)cubes, respectively. For higher dimensions, the construction proceeds analogously by increasing the cochain degree by two.

VI. EQUIVALENCE OF QCAs CONSTRUCTED FROM TQFTs AND ISAs

In this section, we first explicitly demonstrate that the $3 + 1\text{D}$ Clifford QCAs constructed from TQFTs and from ISAs are equivalent by comparing their skew-Hermitian forms within the polynomial formalism. While this approach is, in principle, applicable to higher dimensions, the required explicit computations rapidly become prohibitively time-consuming. To overcome this difficulty, we develop an algebraic approach based on the cup-product formalism to analyze the boundary excitations. We show that the excitations obtained from the TQFT construction and those from the ISA construction coincide, implying that the two approaches yield equivalent QCAs. This argument applies to arbitrary dimensions.

We begin by reviewing the definition of boundary algebra introduced in Ref. [73] and further developed in Ref. [66]. Related constructions and perspectives have appeared in Refs. [74–77], as well as in studies of phase transitions Refs. [78,79].

Given a translation-invariant topological stabilizer code, we truncate the system by removing all qudits below the plane $z = 0$ and discarding all stabilizers that involve any of the truncated qudits. The remaining stabilizers are referred to as **bulk stabilizers**.

The **boundary algebra** is defined as the algebra generated by local Pauli operators that commute with all bulk stabilizers, modulo the bulk stabilizers themselves. This algebra captures the independent boundary degrees of freedom that are invisible to the bulk Hamiltonian. The structure of the boundary algebra can be encoded by a finitely generated module over a polynomial ring in one fewer variable, together with a skew-Hermitian form describing the commutation relations. In general, this module need not be free, nor is the form necessarily non-degenerate. This reflects the presence of nontrivial bulk excitation and braiding [73,74]. Such modules are referred to as **quasi-symplectic** in Ref. [66].

Let α be a translationally invariant Clifford QCA acting on $\mathbb{Z}_p$ qudits, with p a prime. The separators of α generate the stabilizer group of an associated stabilizer code. In this special case, there are no bulk excitation, and the boundary algebra constructed as above is a free module equipped with a nondegenerate skew-Hermitian form. Section 4.3 of Ref. [66] shows that this boundary algebra is Witt equivalent to the boundary algebra defined for a Clifford QCA in Ref. [34], thereby realizing the boundary algebra of a Clifford QCA as a special case of the boundary algebra of a topological stabilizer code.

Theorem 1 (Classification of Clifford QCAs by skew-Hermitian forms [34]). Two Clifford QCAs are equivalent if and only if their boundary algebras are equivalent. More precisely, suppose their boundary algebras are free modules equipped with skew-Hermitian forms Ξ and Ξ' , respectively. Then the QCAs are equivalent if and only if there exist integers q, q' and an invertible matrix E such that

$$E^\dagger (\Xi \oplus \lambda_q) E = \Xi' \oplus \lambda_{q'}, \quad (222)$$

where λ_q and $\lambda_{q'}$ denote the standard symplectic matrices of dimensions $2q$ and $2q'$, respectively.

A. Polynomial formalism

In this section, we represent the QCA α by a polynomial matrix Q . First, we briefly describe how to obtain a skew-Hermitian form Ξ that appears in Theorem 1. As a representation of α , each column of Q encodes the image of the onsite Pauli X, Z operators. Assume we fixed some

ordering such that the first q columns are the flippers and the last q columns are the respective separators/stabilizers. It is always possible to coarse-grain the sites so that the separators and flippers have a width of at most two in the x_D -direction. In other words, $Q = A + x_D B$ where A, B do not involve the variable x_D . The columns of matrix B are the flippers and separators truncated above the hyperplane $x_D = 0$. *A priori*, Q is symplectic following from the fact that flippers and separators have a commutation relation governed by the standard symplectic matrix λ_q . After the truncation, the commutation relation is governed by a different skew-Hermitian form. Focusing on the truncated separators, i.e., the last q columns B_0 of B , we denote their commutation relation by the form $\Xi = B_0^\dagger \lambda_q B_0$. These truncated separators corresponding to the columns of B_0 are boundary gauge operators in Ref. [73]. The boundary algebra of a stabilizer code determines a Witt class that is independent of the choice of truncation procedure and of basis transformations of B [34,66].

The skew-Hermitian form Ξ associated with the boundary algebra of a QCA can be computed using the following lemma.

Lemma 1 (Lemma III.8 of Ref. [34]). Let $Q = A + x_D B$ be a $2q \times 2q$ symplectic matrix where A, B do not involve the variable x_D (e.g. in $3 + 1D$, x_D can be chosen to be $x^\pm, y^\pm, z^\pm$). Let B_0 be the last q columns of B , and put $\Xi = B_0^\dagger \lambda_q B_0$. If the matrix Ξ is invertible, then Ξ is a skew-Hermitian form of Theorem 1.

In addition, we will need the following Clifford gates expressed in terms of polynomial matrices:

(1) *Hadamard*:

$$H_i := E_{i,i+q}(-1) E_{i+q,i}(1) E_{i,i+q}(-1), \quad 1 \leq i \leq q.$$

(2) *Controlled-phase*:

$$\text{CPhase}_f^i := E_{i+q,i}(f), \quad f = \bar{f}, \quad 1 \leq i \leq q.$$

(3) *Controlled-NOT*:

$$CX_a^{ij} := E_{ij}(a) E_{j+q,i+q}(-\bar{a}), \quad 1 \leq i \neq j \leq q.$$

Here, for $i \neq j$, $E_{ij}(a)$ denotes the row-addition elementary $2q \times 2q$ matrix with entries

$$[E_{ij}(a)]_{\mu\nu} = \delta_{\mu\nu} + \delta_{\mu i} \delta_{\nu j} a, \quad (223)$$

where a is a polynomial. We refer the reader to Sec. 2 of Ref. [80] for a detailed discussion of these gates and illustrative examples.

1. $\mathbb{Z}_2$ case

We are ready to show that the 3F QCA $\alpha_{\text{TQFT}}^{3F}$ obtained from the TQFT approach Eq. (68) is equivalent to α_{ISA}^{3F} obtained from the invertible subalgebra Eq. (183). Observe that α_{ISA}^{3F} is already of the form $A + z B$. Using Lemma 1, we find the skew-Hermitian form of

$$\Xi_{\text{ISA}}^{3F} = \begin{pmatrix} x + \frac{1}{x} & \frac{y}{x} + \frac{1}{x} + y + 1 & 0 & y \\ \frac{x}{y} + x + \frac{1}{y} + 1 & y + \frac{1}{y} & x & 0 \\ 0 & \frac{1}{x} & x + \frac{1}{x} & \frac{y}{x} + \frac{1}{x} + y + 1 \\ \frac{1}{y} & 0 & \frac{x}{y} + x + \frac{1}{y} + 1 & y + \frac{1}{y} \end{pmatrix}. \quad (224)$$

Now consider $\alpha_{\text{TQFT}}^{3F}$ whose matrix elements are given in Appendix C 1. Recall that QCAs are defined up to FDQC and shifts. Applying a shift circuit of

$$S = \begin{pmatrix} x \mathbb{I}_{3 \times 3} & 0 & 0 & 0 \\ 0 & \mathbb{I}_{3 \times 3} & 0 & 0 \\ 0 & 0 & x \mathbb{I}_{3 \times 3} & 0 \\ 0 & 0 & 0 & \mathbb{I}_{3 \times 3} \end{pmatrix}, \quad (225)$$

we find $S \alpha_{\text{TQFT}}^{3F}$ is of the form $A + x B$, where A and B are matrices that do not involve the variable x . However, we cannot yet use Lemma 1, as a skew-Hermitian form needs to be invertible. We act further by the basis transformation

$$U(\cdot) = U_{\text{FDQC}}(\cdot) E, \quad (226)$$

where

$$U_{\text{FQDC}} = H_6 H_4 H_3 H_2 C X_{1+\frac{1}{z}}^{6,4} C X_{\frac{1}{yz^2}+\frac{1}{yz}}^{3,4} C X_{\frac{1}{y^2z}+\frac{1}{yz}}^{2,4} H_6 H_3 H_2 C X_{1+\frac{1}{yz}}^{5,4} C X_{\frac{1}{z}+\frac{1}{yz}}^{3,4} C X_{\frac{1}{y}+\frac{1}{yz}}^{2,4} H_4 H_1 C X_{1+yz}^{6,1} C X_{1+\frac{1}{yz}}^{5,1} \\ \times H_6 H_5 C X_{1+\frac{1}{z}}^{6,1} C X_{1+z}^{5,1} H_1 H_2 H_3 C X_1^{3,1} C X_{\frac{1}{y}}^{2,1} H_2 H_3 C X_1^{6,4} H_6 C X_y^{6,5} \quad (227)$$

is a finite-depth quantum circuit and

$$E = T_1^{4,12} T_{\frac{1}{y}}^{4,11} T_{1+yz}^{1,4} T_{yz+y^2z}^{2,4} T_{yz+yz^2}^{3,4} T_{y+yz}^{8,4} T_{z+yz}^{9,4} T_1^{1,9} T_{\frac{1}{y}}^{1,8} T_y^{2,7} T_1^{3,7} T_{\frac{1}{yz^2}+\frac{1}{z}+\frac{1}{yz}+z+yz+yz^2}^{7,1} \\ \times T_{1+\frac{1}{y}}^{10,11} T_{1+\frac{1}{z}}^{10,12} T_{yz+y^2z}^{2,4} T_{yz+yz^2}^{3,4} T_{1+y}^{5,4} T_{1+z}^{6,4} T_{y+yz}^{8,4} T_{z+yz}^{9,4} T_y^{5,10} T_1^{6,10} T_{1+\frac{y}{z}}^{5,12} T_{1+\frac{1}{z}}^{6,12} T_{1+\frac{1}{y}}^{5,11}, \quad (228)$$

with $T_f^{i,j}$ is the matrix of elementary column operation that adds to the i th column by the j th column multiplied by f . The column operation is just multiplying our stabilizers generators, and it does not change the stabilizer group. Note that we have designed E such that the transformed QCA is symplectic. Acting these transformations on our QCA, we find

$$U(\mathcal{S}\alpha_{\text{TQFT}}^{3F}) = \begin{pmatrix} x & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & * & 0 & 0 & * & * & 0 & 0 & 0 & 0 & 0 & * \\ 0 & 0 & * & 0 & * & * & 0 & 0 & 0 & 0 & * & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & * & * & 0 & * & * & 0 & * & * & 0 & * & * \\ 0 & * & * & 0 & * & * & 0 & * & * & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & x & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & * & * & 0 & * & 0 & 0 & * & * \\ 0 & 0 & 0 & 0 & * & * & 0 & 0 & * & 0 & * & * \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & * & * & 0 & * & 0 & 0 & 0 & * & 0 & 0 & 0 \\ 0 & * & * & 0 & * & 0 & 0 & * & * & 0 & 0 & * \end{pmatrix}, \quad (229)$$

where the $*$ terms are nonzero polynomials which are given below. Observe that the first and fourth qubits are disentangled from the rest of the system. They can be removed. We now have the transformed QCA

$$\alpha_{\text{TQFT, transformed}}^{3F} = A + xB, \quad (230)$$

where

$$A = \begin{pmatrix} 0 & 0 & \frac{1}{yz} & \frac{z+1}{y} & 0 & 0 & 0 & \frac{1}{y} \\ 0 & 0 & \frac{y+1}{z} & \frac{y+z+1}{yz} & 0 & 0 & \frac{1}{z} & 0 \\ \frac{1}{yz} & \frac{1}{y} & y+1 & \frac{1}{y}+1 & 1 & \frac{1}{y} & 1 & \frac{1}{y} \\ y(y+1)z+1 & z(yz+y+1) & y & 1 & y & yz & 0 & 0 \\ 0 & 0 & \frac{(y+1)(yz+1)}{y^2z} & \frac{z}{y} & 0 & 0 & \frac{1}{y} & \frac{y+1}{y^2} \\ 0 & 0 & \frac{yz(yz+y+z)+z+1}{yz^2} & z+\frac{1}{z} & 0 & 0 & \frac{1}{z}+1 & \frac{yz+z+1}{yz} \\ yz+z+1 & z(z+1) & 1 & 0 & 0 & z & 0 & 0 \\ (y+1)yz+y+\frac{1}{z}+1 & (z+1)(yz+1) & y+1 & 0 & y(z+1) & yz+z+1 & 0 & 1 \end{pmatrix}$$

and

$$B = \begin{pmatrix} 1 & 0 & \frac{1}{y} + \frac{1}{z} + 1 & \frac{z+1}{yz} & 0 & 0 & 0 & \frac{1}{y} \\ 0 & 1 & \frac{y+1}{yz} & 1 & 0 & 0 & \frac{1}{z} & 0 \\ y(y+1)z + \frac{1}{z} & yz(z+1) + \frac{1}{yz} & 0 & 0 & yz + y + \frac{1}{z} & yz + z + 1 & 0 & 0 \\ y & 1 & 0 & 0 & y & yz & 0 & 0 \\ 0 & 0 & \frac{y^3+1}{y^2z} + y + 1 & \frac{\frac{1}{y}+z^2+1}{z} & 1 & 0 & \frac{\frac{1}{y}+1}{z} + 1 & \frac{1}{y} + 1 \\ 0 & 0 & \frac{y^2(z+1)+y+z+1}{yz^2} & \frac{1}{z^2} + 1 & 0 & 1 & \frac{z+1}{z^2} & \frac{1}{z} \\ y & z+1 & 0 & 0 & 0 & z & 0 & 0 \\ y(y + \frac{1}{z} + 1) & yz + y + \frac{1}{z} + 1 & 0 & 0 & y(\frac{1}{z} + 1) & y & 0 & 0 \end{pmatrix}.$$

Applying Lemma 1, we have

$$\Xi_{\text{TQFT}}^{3\text{F}} = \begin{pmatrix} z + \frac{1}{z} & \frac{z}{y} + \frac{1}{y} + z + 1 & 0 & \frac{1}{y} \\ \frac{y}{z} + y + \frac{1}{z} + 1 & y + \frac{1}{y} & \frac{1}{z} & 0 \\ 0 & z & z + \frac{1}{z} & \frac{z}{y} + \frac{1}{y} + z + 1 \\ y & 0 & \frac{y}{z} + y + \frac{1}{z} + 1 & y + \frac{1}{y} \end{pmatrix}, \quad (231)$$

which is exactly equal to $\Xi_{\text{ISA}}^{3\text{F}}$ of Eq. (224) by re-defining our coordinate system by sending $z \rightarrow x^{-1}, y \rightarrow y^{-1}$. Thus, Theorem 1 tells us $\alpha_{\text{TQFT}}^{3\text{F}}$ and $\alpha_{\text{ISA}}^{3\text{F}}$ are equivalent.

2. $\mathbb{Z}_p$ case

Let us now show that the QCAs, $\alpha_{\text{TQFT}}^{(k)}$ obtained from the TQFT Eq. (118) and $\alpha_{\text{ISA}}^{(k)}$ obtained from the invertible subalgebra Eq. (214), are equivalent. First, we bring Eq. (118) into the form of $A + z^{-1}B$ through an FDQC, which we pick to be

$$\begin{aligned} \mathbf{U} = & \text{CPhase}^3_{\frac{1}{4}kxyz + \frac{k}{4xy} - \frac{k}{4} - \frac{kz}{4xy} - \frac{k}{4} - \frac{k}{4z} + \frac{k}{2}} \text{CX}^{1,3}_{-\frac{1}{2x} - \frac{yz}{2}} \text{CX}^{2,3}_{\frac{1}{2xy} + \frac{z}{2}} \text{H}_1 \text{H}_2 \text{CX}^{2,3}_{-\frac{k}{2} - \frac{k}{2xy^2} + \frac{k}{2y} + \frac{kz}{2}} \text{CX}^{1,3}_{\frac{k}{2} - \frac{k}{2x} - \frac{k}{2xy} + \frac{kz}{2x}} \\ & \times \text{H}_3 \text{H}_1 \text{H}_2 \text{CX}^{2,3}_{\frac{1}{2ky} - \frac{1}{2kxy}} \text{CX}^{1,3}_{\frac{1}{2kx} - \frac{1}{2kxy}} \text{H}_2 \text{H}_1 \text{CX}^{2,3}_{\frac{1}{2} - \frac{1}{2y}} \text{CX}^{1,3}_{-\frac{1}{2} + \frac{1}{2x}} \text{CX}^{3,2}_{-\frac{1}{z}} \text{CX}^{3,1}_{\frac{1}{yz}} \text{H}_3 \text{H}_2 \text{H}_1. \end{aligned} \quad (232)$$

And, we have

$$\mathbf{U} \alpha_{\text{TQFT}}^{(k)} = \begin{pmatrix} * & 0 & 0 & * & * & 0 \\ 0 & * & 0 & * & * & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ * & * & 0 & * & 0 & 0 \\ * & * & 0 & 0 & * & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix}, \quad (233)$$

where the $*$ terms are given below. Observe that the third qudit is now disentangled from the rest of the system and can be dropped. We then obtain the transformed QCA

$\alpha_{\text{TQFT,transformed}}^{(k)}$

$$= \begin{pmatrix} \frac{1}{2xyz} + \frac{1}{2} & 0 & -\frac{1}{2kxy^2z} + \frac{1}{2kxyz} - \frac{y}{2k} + \frac{1}{2k} & \frac{1}{2kxy} + \frac{y}{2kx} - \frac{1}{2kx} - \frac{y}{2k} \\ 0 & \frac{1}{2xyz} + \frac{1}{2} & -\frac{1}{2kxy^2z} + \frac{1}{2kxyz} - \frac{1}{2kyz} + \frac{1}{2k} & \frac{1}{2kxy} - \frac{1}{2kx} - \frac{1}{2kyz} + \frac{1}{2k} \\ \frac{k}{2xyz} - \frac{k}{2x} - \frac{k}{2yz} + \frac{k}{2} & -\frac{k}{2xyz} - \frac{ky}{2x} + \frac{k}{2x} + \frac{ky}{2} & \frac{1}{2xyz} + \frac{1}{2} & 0 \\ \frac{k}{2xy^2z} - \frac{k}{2y^2z} + \frac{k}{2yz} - \frac{k}{2} & -\frac{k}{2xy^2z} + \frac{k}{2xyz} - \frac{ky}{2} + \frac{k}{2} & 0 & \frac{1}{2xyz} + \frac{1}{2} \end{pmatrix}.$$

Applying Lemma 1, we find the skew-Hermitian form to be

$$\Xi_{\text{TQFT}} = \begin{pmatrix} \frac{1}{4ky} - \frac{y}{4k} & \frac{y}{4kx} - \frac{1}{4kx} - \frac{y}{4k} - \frac{1}{4k} \\ \frac{x}{4k} + \frac{1}{4ky} + \frac{1}{4k} - \frac{x}{4ky} & \frac{x}{4k} - \frac{1}{4kx} \end{pmatrix}. \quad (234)$$

It is then straightforward to show that $\Xi_{\text{TQFT}} = E^\dagger \Xi_{\text{ISA}} E$ for the Ξ_{ISA} computed from Eq. (214), where

$$E = \begin{pmatrix} 0 & y^{-1}x \\ 1 & 0 \end{pmatrix}. \quad (235)$$

By Theorem 1, the QCAs obtained from the TQFT approach and the invertible subalgebra approach are equivalent.

We have computed the matrix representation of the skew-Hermitian form for the TQFT-based 3 + 1D QCA and compared it with that obtained from the ISA construction, thereby explicitly verifying this equivalence. However, this comparison involves numerous intermediate basis transformations. Furthermore, in higher-dimensional QCAs, the matrix size grows rapidly, rendering it impractical to explicitly determine the required basis transformations or the corresponding unitary circuits that relate the QCAs constructed from TQFTs and ISAs.

B. Cup-product formalism

Motivated by the limitations of the polynomial approach, we develop an alternative method to extract the boundary algebra that does not rely on an explicit matrix representation. In this subsection, we reformulate the boundary algebra using the cup-product formalism, which is directly applicable in arbitrary spatial dimensions.

1. $\mathbb{Z}_2$ case

We begin by studying the three-fermion Walker-Wang model on a spatial manifold M_3 with an open boundary $N_2 = \partial M_3$. We review the auxiliary-vertex approach (also known as the boundary cone construction) introduced in Refs. [4,45], which is consistent with the boundary Hamiltonian presented in Ref. [42].

To extend our bulk construction to manifolds with boundary, we embed the system into a closed manifold by adjoining a set of auxiliary simplices. Concretely, we introduce an auxiliary vertex v_0 and connect it to every vertex on the boundary manifold N_2 . This generates auxiliary edges $\langle 0i \rangle$ for each $i \in N_2$, auxiliary faces $\langle 0ij \rangle$ for each boundary edge $\langle ij \rangle \subset N_2$, and higher-dimensional auxiliary simplices defined analogously. The union of these auxiliary simplices with N_2 defines the cone over N_2 , which we denote by CN_2 . By gluing CN_2 to the original manifold M_3 along N_2 , we obtain a closed spatial three-manifold,

$$\tilde{M}_3 \equiv M_3 \sqcup CN_2, \quad \partial \tilde{M}_3 = 0. \quad (236)$$

With this closed manifold in hand, we may directly apply the bulk formalism. Given cochains $a, b \in C^1(M_4, \mathbb{Z}_2)$, we extend them to cochains in $C^1(\tilde{M}_4, \mathbb{Z}_2)$ by setting $a(e) = b(e) = 0$ on all auxiliary edges e . Upon gauging the 1-form $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry, the state $|a|_{\tilde{M}_4}, b|_{\tilde{M}_4}\rangle$ is mapped to

$$|\delta a|_{\tilde{M}_3}, \delta b|_{\tilde{M}_3}\rangle = |\delta a|_{M_3}, \delta b|_{M_3}, a|_{N_2}, b|_{N_2}\rangle, \quad (237)$$

where $(\cdot)|_S$ denotes restriction of a cochain to the subspace S .

To interpret the boundary degrees of freedom, we identify the value of δa on an auxiliary face $\langle 0ij \rangle$ with the edge variable $a(\langle ij \rangle)$ on N_2 , using the condition $a(\langle 0i \rangle) = 0$. The same identification applies to δb and $b|_{N_2}$. We denote the Pauli operators acting on the four components appearing in Eq. (237) by $Z_f^A, Z_f^B, \mathcal{Z}_e^A$, and $\mathcal{Z}_e^B$, respectively.

We now analyze the Hamiltonian terms in Eq. (44) defined on $\tilde{M}_3$. We decorate the terms involving G_e with appropriate flux factors $Z_{\partial t}$, which preserves the stabilizer group,

$$\begin{aligned} G_e^A \prod_f \tilde{Z}_f^{B \int_{\tilde{M}_3} e \cup f} \\ = \tilde{X}_{\delta e}^A \prod_f \tilde{Z}_f^{A \int_{\tilde{M}_3} \delta e \cup 1f} \prod_f \tilde{Z}_f^{B \int_{\tilde{M}_3} e \cup f} \\ \sim \tilde{X}_{\delta e}^A \prod_f \tilde{Z}_f^{A \int_{\tilde{M}_3} e \cup f + f \cup e} \prod_f \tilde{Z}_f^{B \int_{\tilde{M}_3} e \cup f} \end{aligned} \quad (238)$$

and

$$\begin{aligned}
G_e^B \prod_f \tilde{Z}_f^{A \int_{\tilde{M}_3} f \cup e} \\
= \tilde{X}_{\delta e}^B \prod_f \tilde{Z}_f^{B \int_{\tilde{M}_3} \delta e \cup f} \prod_f \tilde{Z}_f^{A \int_{\tilde{M}_3} f \cup e} \\
\sim \tilde{X}_{\delta e}^B \prod_f \tilde{Z}_f^{B \int_{\tilde{M}_3} e \cup f + f \cup e} \prod_f \tilde{Z}_f^{A \int_{\tilde{M}_3} f \cup e}. \quad (239)
\end{aligned}$$

We now focus on the behavior of these stabilizers in the vicinity of the boundary N_2 .

- (1) $t = \langle 0ijk \rangle$ denotes an auxiliary tetrahedron, and let $f = \langle ijk \rangle$ be the corresponding boundary face. The associated flux term can be written as

$$Z_{\partial t}^\alpha = Z_f^\alpha \prod_{e \in N_2 | e \subset f} Z_e^\alpha := Z_f^\alpha Z_{\partial f}^\alpha, \quad (240)$$

for $\alpha = A, B$. Here, Z_f^α acts on the bulk degrees of freedom in M_3 , while $Z_{\partial f}^\alpha$ acts on the boundary degrees of freedom associated with CN_2 . In other words, the Pauli Z_f on the boundary face f of M_3 is equal to the product of Z_e around edge e such that $e \in \partial f$.

- (2) $e = \langle 0i \rangle$ denotes an auxiliary edge, and let $v = \langle i \rangle$ be the corresponding boundary vertex. In this case, we obtain the stabilizer as

$$\begin{aligned}
\tilde{X}_{\delta e}^A \prod_f \tilde{Z}_f^{A \int_{\tilde{M}_3} e \cup f + f \cup e} \prod_f \tilde{Z}_f^{B \int_{\tilde{M}_3} e \cup f} \\
= \mathcal{X}_{\delta v}^A \prod_{f \in N_2} (Z_f^A Z_f^B)^{\int_{N_2} v \cup f} \\
= \mathcal{X}_{\delta v}^A \prod_{f \in N_2} (Z_{\partial f}^A Z_{\partial f}^B)^{\int_{N_2} v \cup f}, \quad (241)
\end{aligned}$$

where $\sim$ indicates equality up to multiplication by flux terms. Similarly,

$$\begin{aligned}
\tilde{X}_{\delta e}^B \prod_f \tilde{Z}_f^{B \int_{\tilde{M}_3} e \cup f + f \cup e} \prod_f \tilde{Z}_f^{A \int_{\tilde{M}_3} f \cup e} \\
= \mathcal{X}_{\delta v}^B \prod_{f \in N_2} Z_{\partial f}^B \int_{N_2} v \cup f. \quad (242)
\end{aligned}$$

- (3) $e = \langle ij \rangle$ denotes a boundary edge. In this case, we obtain

$$\begin{aligned}
\tilde{X}_{\delta e}^A \prod_f \tilde{Z}_f^{A \int_{\tilde{M}_3} e \cup f + f \cup e} \prod_f \tilde{Z}_f^{B \int_{\tilde{M}_3} e \cup f} \\
= X_{\delta e}^A \mathcal{X}_e^A \prod_{f \in M_3} Z_f^{A \int_{M_3} e \cup f + f \cup e} \prod_{e' \in N_2} Z_{e'}^{A \int_{N_2} e' \cup e} \\
\times \prod_f Z_f^{B \int_{M_3} e \cup f} \\
= \mathcal{X}_e^A \prod_{e' \in N_2} Z_{e'}^{A \int_{N_2} e' \cup e} \times \text{bulk terms}
\end{aligned}$$

and

$$\begin{aligned}
\tilde{X}_{\delta e}^B \prod_f \tilde{Z}_f^{B \int_{\tilde{M}_3} e \cup f + f \cup e} \prod_f \tilde{Z}_f^{A \int_{\tilde{M}_3} f \cup e} \\
= X_{\delta e}^B \mathcal{X}_e^B \prod_{f \in M_3} Z_f^{B \int_{M_3} e \cup f + f \cup e} \prod_{e' \in N_2} Z_{e'}^{B \int_{N_2} e' \cup e} \\
\times \prod_{f \in M_3} Z_f^{A \int_{M_3} f \cup e} \prod_{e' \in N_2} Z_{e'}^{A \int_{N_2} e' \cup e} \\
= \mathcal{X}_e^B \prod_{e' \in N_2} (Z_{e'}^A Z_{e'}^B)^{\int_{N_2} e' \cup e} \times \text{bulk terms}.
\end{aligned}$$

To summarize, the boundary Hamiltonian takes the form

$$\begin{aligned}
H_{\text{boundary}} \\
= - \sum_{v \in N_2} \mathcal{X}_{\delta v}^A \prod_{f \in N_2} (Z_{\partial f}^A Z_{\partial f}^B)^{\int_{N_2} v \cup f} \\
- \sum_{v \in N_2} \mathcal{X}_{\delta v}^B \prod_{f \in N_2} Z_{\partial f}^B \int_{N_2} v \cup f \\
- \sum_{f \in N_2} \left(Z_f^A Z_{\partial f}^A + Z_f^B Z_{\partial f}^B \right) \\
- \sum_{e \in N_2} \mathcal{X}_e^A \prod_{e' \in N_2} Z_{e'}^{A \int_{N_2} e' \cup e} \times \text{bulk terms} \\
- \sum_{e \in N_2} \mathcal{X}_e^B \prod_{e' \in N_2} (Z_{e'}^A Z_{e'}^B)^{\int_{N_2} e' \cup e} \times \text{bulk terms}. \quad (243)
\end{aligned}$$

We now swap the roles of the bulk and the boundary, treating the cone CN_2 as the “bulk,” with Hilbert space generated by $\mathcal{X}_e^{A,B}$ and $Z_e^{A,B}$. From this perspective, the first two lines can be interpreted as bulk stabilizers on CN_2 , while the $\mathcal{X}$ and Z operators appearing in the remaining terms generate the boundary algebra.

In particular, we focus on the last two lines, which correspond to the anyons $m_A e_A$ and $m_B e_A e_B$ in the $\mathbb{Z}_2^A \times \mathbb{Z}_2^B$ toric code. These are precisely the same anyon generators that appear in the ISA construction.

Explicitly, the bulk stabilizer on CN_2 is given by

$$S_{\text{bulk}} = \left\langle \begin{array}{c} \text{---} \mathcal{X}^A \text{---} \\ \text{---} \mathcal{X}^A \mathcal{Z}^A \mathcal{Z}^B \text{---} \\ \text{---} \mathcal{X}^A \text{---} \end{array} \right\rangle, \left\langle \begin{array}{c} \text{---} \mathcal{X}^B \text{---} \\ \text{---} \mathcal{X}^B \mathcal{Z}^B \text{---} \\ \text{---} \mathcal{X}^B \text{---} \end{array} \right\rangle. \quad (244)$$

The boundary algebra is defined as

$$\mathcal{A}_{\text{boundary}} = \frac{S_{\text{bulk}}^\perp}{S_{\text{bulk}}}, \quad (245)$$

where $S_{\text{bulk}}^\perp$ consists of all finite Pauli operators generated by $\mathcal{X}_e^{A,B}$ and $\mathcal{Z}_e^{A,B}$ that commute with S_{bulk} . From the last three lines of Eq. (243), the corresponding boundary algebra is generated by the following operators:

$$\forall \alpha \in \{A, B\}, \quad \mathcal{Z}_{\partial f}^\alpha = \begin{array}{c} \mathcal{Z}^\alpha \\ \mathcal{Z}^\alpha f \mathcal{Z}^\alpha \\ \mathcal{Z}^\alpha \end{array},$$

$$\mathcal{X}_e^A \prod_{e' \in N_2} \mathcal{Z}_{e'}^{A \int_{N_2} e' \cup e} = \begin{array}{c} \text{---} \mathcal{X}^A \text{---} \\ \text{---} \mathcal{Z}^A \text{---} \end{array}, \begin{array}{c} \text{---} \mathcal{X}^A \text{---} \\ \text{---} \mathcal{Z}^A \text{---} \end{array},$$

$$\mathcal{X}_e^B \prod_{e' \in N_2} (\mathcal{Z}_{e'}^A \mathcal{Z}_{e'}^B)^{\int_{N_2} e' \cup e} = \begin{array}{c} \text{---} \mathcal{X}^B \text{---} \\ \text{---} \mathcal{Z}^A \mathcal{Z}^B \text{---} \end{array}, \begin{array}{c} \text{---} \mathcal{X}^B \text{---} \\ \text{---} \mathcal{Z}^A \mathcal{Z}^B \text{---} \end{array}. \quad (246)$$

However, these generators are not independent. A straightforward analysis shows that the following two operators are sufficient to generate the entire boundary algebra (up

to multiplication by bulk stabilizers),

$$\mathcal{X}_e^A \prod_{e' \in N_2} \mathcal{Z}_{e'}^{A \int_{N_2} e' \cup e + e \cup_1 \delta e'}$$

$$= \begin{array}{c} \text{---} \mathcal{X}^A \text{---} \\ \text{---} \mathcal{Z}^A \text{---} \end{array}, \begin{array}{c} \text{---} \mathcal{X}^A \mathcal{Z}^A \text{---} \\ \text{---} \mathcal{Z}^A \text{---} \end{array},$$

$$\mathcal{X}_e^B \prod_{e' \in N_2} \mathcal{Z}_{e'}^{A \int_{N_2} e' \cup e} \mathcal{Z}_{e'}^{B \int_{N_2} e' \cup e + \delta e' \cup_1 e}$$

$$= \begin{array}{c} \text{---} \mathcal{Z}^B \text{---} \\ \text{---} \mathcal{Z}^B \text{---} \end{array}, \begin{array}{c} \text{---} \mathcal{Z}^B \text{---} \\ \text{---} \mathcal{X}^B \mathcal{Z}^B \text{---} \end{array}. \quad (247)$$

We note that this boundary algebra is exactly the ISA for the 3-fermion theory, up to a reordering of the cup products.

The same analysis extends to higher dimensions with a periodicity of 2: one simply shifts the degree of each cochain by 1, and the recursive relations for the cup products continue to hold modulo 2.

2. $\mathbb{Z}_p$ case

In this section, we study the $\mathbb{Z}_p^{(k)}$ Walker-Wang Hamiltonian defined in Eq. (74), which consists of the following two types of terms:

$$Z_{\partial t}, \quad X_{\delta e} \prod_f \mathcal{Z}_f^{k \int f \cup e + e \cup f}. \quad (248)$$

As in the previous section, we construct the Hamiltonian on the closed manifold $\tilde{M}_3 \equiv M_3 \sqcup CN_2$. We place $\mathbb{Z}_p$ qudits on each face $f \in M_3$ and each edge $e \in N_2$, equipped with Pauli operators X_f, Z_f and $\mathcal{X}_e, \mathcal{Z}_e$, respectively.

We now analyze the Hamiltonian terms supported near N_2 ,

- (1) Let $t = \langle 0ijk \rangle$ denote an auxiliary tetrahedron, and let $f = \langle ijk \rangle$ be the corresponding boundary face. The associated flux term can be written as

$$Z_{\partial t} = Z_{(ijk)} \mathcal{Z}_{(jk)}^{-1} \mathcal{Z}_{(ik)} \mathcal{Z}_{(ij)}^{-1} := Z_f \mathcal{Z}_{\partial f}^{-1}. \quad (249)$$

- (2) Let $e = \langle 0i \rangle$ denote an auxiliary edge, and let $v = \langle i \rangle$ be the corresponding boundary vertex. In this

case, the stabilizer takes the form

$$\begin{aligned} \tilde{X}_{\delta e} \prod_f \tilde{Z}_f^{k \int_{M_3} (f \cup e + e \cup f)} \\ = \mathcal{X}_{\delta v}^{-1} \prod_{f \in N_2} Z_f^{k \int_{N_2} v \cup f} \\ = \mathcal{X}_{\delta v}^{-1} \prod_{f \in N_2} \mathcal{Z}_{\partial f}^{k \int_{N_2} v \cup f}, \end{aligned} \quad (250)$$

where the minus sign in the exponent of $\mathcal{X}_{\delta v}$ arises because when $e = \langle 0i \rangle$ appears with positive orientation in $\partial \langle 0ij \rangle$, the corresponding boundary vertex $v = \langle i \rangle$ appears with negative orientation in $\partial \langle ij \rangle$.

- (3) Let $e = \langle ij \rangle$ denote a boundary edge. In this case, we obtain

$$\begin{aligned} \tilde{X}_{\delta e} \prod_f \tilde{Z}_f^{k \int_{M_3} f \cup e + e \cup f} \\ = X_{\delta e} \mathcal{X}_e \prod_{f \in M_3} Z_f^{k \int_{M_3} f \cup e + e \cup f} \prod_{e' \in N_2} \mathcal{Z}_{e'}^{k \int_{N_2} e' \cup e} \\ = \mathcal{X}_e \prod_{e' \in N_2} \mathcal{Z}_{e'}^{k \int_{N_2} e' \cup e} \times \text{bulk terms}. \end{aligned} \quad (251)$$

Collecting the above results, the boundary Hamiltonian takes the form

$$\begin{aligned} H_{\text{boundary}} \\ = - \sum_{v \in N_2} \mathcal{X}_{\delta v} \prod_{f \in N_2} \mathcal{Z}_{\partial f}^{-k \int_{N_2} v \cup f} - \sum_{f \in N_2} Z_f \mathcal{Z}_{\partial f}^{-1} \\ - \sum_{e \in N_2} \mathcal{X}_e \prod_{e' \in N_2} \mathcal{Z}_{e'}^{k \int_{N_2} e' \cup e} \times \text{bulk terms} + h.c. \end{aligned} \quad (252)$$

As in the previous case, we treat the operators $\mathcal{X}_e$ and $\mathcal{Z}_e$ supported on CN_2 as bulk degrees of freedom. With this convention, the first term in Eq. (252) defines a bulk stabilizer,

$$\mathcal{X}_{\delta v} \prod_{f \in N_2} \mathcal{Z}_{\partial f}^{-k \int_{N_2} v \cup f} = \text{diagram} \quad (253)$$

The remaining two terms in Eq. (252) generate the boundary algebra. In particular, the boundary operators can

be taken as

$$\mathcal{Z}_{\partial f} = \text{diagram} \quad (254)$$

and

$$\mathcal{X}_e \prod_{e'} \mathcal{Z}_{e'}^{k \int_{N_2} e' \cup e} = \text{diagram} \quad (255)$$

These operators are not independent: they generate redundant elements of the boundary algebra. By appropriately combining them, we obtain a single free generator,

$$= \text{diagram} \quad (256)$$

which coincides exactly with the generator of the $\mathbb{Z}_p$ ISA construction in Sec. VB. Therefore, the QCAs constructed via the TQFT and ISA approaches are equivalent.

The same analysis applies in higher dimensions, repeating every 4 dimensions: one simply increases the degree of each cochain by 2, and the recursive relations for the cup products continue to hold.

VII. ALGEBRAIC FORMALISM FOR CLIFFORD QCA

In this section, we develop an algebraic framework for analyzing Clifford QCAs. We model them as automorphisms of the generalized Pauli group, modulo phase, subject to a locality-preserving condition. This reformulation reduces the study of Clifford QCAs to symplectic automorphisms of an abelian group with a band-diagonality constraint. It also enables a natural connection to the questions in algebraic K -theory. We begin with the definition of generalized Pauli operators and show how Clifford QCAs correspond to the locality-preserving automorphisms of their group.

A. Preliminaries

Recall from Sec. IIC, we place n -dimensional qudits on each p -dimensional simplex σ_p . Throughout Sec. VII, we denote the collection of qudits by Λ , which is equipped with a distance function $d : \Lambda \times \Lambda \rightarrow \mathbb{R}_{\geq 0}$.

Definition 2. Denote by X_i, Z_i the generalized Pauli matrices supported on $i \in \Lambda$. Let *generalized Pauli operators* $\mathbf{P}$ be the group generated by $\{X_i, Z_i\}_{i \in \Lambda}$.

Proposition 1. A Clifford QCA α is completely determined by the images $\alpha(X_i), \alpha(Z_i) \in \mathbf{P}$ for every $i \in \Lambda$. In other words, a Clifford QCA is reduced to an automorphism $\alpha \in \text{Aut}(\mathbf{P})$ that meets the locality-preserving condition.

Proof. Generalized Pauli X_i, Z_i generate the entire algebra of local operators. Therefore, the image under α of another operator is determined by automorphism properties. ■

It is possible to express $\mathbf{P}$ modulo its center $\mathbb{Z}_d$ using an abelian group [81]. The clock and shift operators X_i and Z_i defined are represented respectively by $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$. Each generalized Pauli operator has a corresponding sum of $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$, which is uniquely defined up to a phase. For example, both $X_i^2 Z_i$ and $X_i Z_i X_i$ are represented by $\begin{pmatrix} 2 \\ 1 \end{pmatrix}$. As $X_i^d = Z_i^d = I$, we have $\begin{pmatrix} d \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ d \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$. All calculations shall therefore be done modulo d , where d is the dimension of the qudit. We denote the set of all length-2 column vectors modulo d by $\mathbb{Z}_d^2$.

Moreover, the commutation relation between two operators is recovered by the matrix $\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$: two Pauli operators represented by $\begin{pmatrix} a \\ b \end{pmatrix}$ and $\begin{pmatrix} c \\ d \end{pmatrix}$ commute up to some $\exp(2\pi i(m/d)) \in \mu_d$ with

$$m = \omega_i \left(\begin{pmatrix} a \\ b \end{pmatrix}, \begin{pmatrix} c \\ d \end{pmatrix} \right) = (a \ b) \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} c \\ d \end{pmatrix}.$$

This is also called the standard symplectic form on $\mathbb{Z}_d^2$,

$$\omega_i : \mathbb{Z}_d^2 \times \mathbb{Z}_d^2 \rightarrow \mathbb{Z}_d. \quad (257)$$

Definition 3. Motivated by this, we define $P := \bigoplus_{\Lambda} \mathbb{Z}_d^2$ and $\omega := \sum_{i \in \Lambda} \omega_i$. Let $\text{Aut}^\omega(P) = \{\theta \in \text{Aut}(P) : \omega(\theta(p_1), \theta(p_2)) = \omega(p_1, p_2) \text{ for } p_1, p_2 \in P\}$ be the collection of symplectic automorphisms.

Lemma 2. There is a surjective homomorphism

$$\kappa : \text{Aut}(\mathbf{P}) \rightarrow \text{Aut}^\omega(P).$$

Furthermore, $\ker \kappa$ consists of only Clifford circuits.

Proof. An automorphism $\alpha \in \text{Aut}(\mathbf{P})$ has to map the center to itself. Therefore, it induces an automorphism $\kappa(\alpha)$ of P . Since α respects the commutation relation in $\mathbf{P}$, $\kappa(\alpha) \in \text{Aut}^\omega(P)$. If $\alpha \in \ker \kappa$, then $\alpha(X_i) = \exp(2\pi i(m_i/d))X_i$ and $\alpha(Z_i) = \exp(2\pi i(n_i/d))Z_i$. Therefore, α is the single-layer quantum circuit $\prod_{i \in \Lambda} X_i^{m_i} Z_i^{-n_i}$. ■

As Clifford circuits are deemed trivial, it suffices to study $\text{Aut}^\omega(P)$. As for the locality-preserving condition, the following representation is convenient. An automorphism $\theta \in \text{Aut}^\omega(P)$ has an explicit representation

$$\theta = \begin{pmatrix} \Theta^{XX} & \Theta^{XZ} \\ \Theta^{ZX} & \Theta^{ZZ} \end{pmatrix},$$

where $\Theta^{\bullet\bullet} : \Lambda \times \Lambda \rightarrow \mathbb{Z}_d$ are 2-tensors indexed by Λ . Here $\Theta^{\bullet\bullet} \in \{\Theta^{XX}, \Theta^{XZ}, \Theta^{ZX}, \Theta^{ZZ}\}$. Viewed as Λ -indexed square matrices, multiplication between 2-tensors is defined as matrix multiplication. We will refer to these 2-tensors simply as matrices. The automorphism being θ symplectic is equivalent to the identities

$$\theta^T J_\Lambda \theta = J_\Lambda \quad \text{and} \quad \theta J_\Lambda \theta^T = J_\Lambda,$$

where

$$J_\Lambda = \begin{pmatrix} 0 & I_\Lambda \\ -I_\Lambda & 0 \end{pmatrix}.$$

Observe that θ is invertible with inverse $-J_\Lambda \theta^T J_\Lambda$. The locality-preserving condition translates into a “band-diagonality” condition: there exists $r > 0$ such that $\Theta^{\bullet\bullet}(i, j) = 0$ for all $i, j \in \Lambda$ satisfying $d(i, j) > r$. Let $\text{Sp}_\Lambda^{bd}(\mathbb{Z}_d)$ denote the subgroup of band-diagonal elements in $\text{Aut}^\omega(P)$. Similar objects have been considered in topology under the name controlled linear algebra [82].

A single-layer Clifford circuit corresponds to θ where $\Theta^{\bullet\bullet}$ are identically block-diagonal. In other words, there exists a partition of Λ into disjoint blocks $\Lambda = \bigsqcup_\beta \Lambda_\beta$ of finite block sizes $\text{diam}(\Lambda_\beta) < \infty$. And $\Theta^{\bullet\bullet} = \sum_\beta \Theta_\beta^{\bullet\bullet}$ with $\Theta_\beta^{\bullet\bullet}(i, j) = 0$ unless $i, j \in \Lambda_\beta$. Furthermore, the band-diagonal condition forces the block sizes to be uniformly bounded. Let $\text{ESp}_\Lambda^{bd}(\mathbb{Z}_d)$ denote the group generated by them. It corresponds to finite-depth Clifford circuits.

A QCA which only permutes qudits corresponds to θ with $\Theta^{XZ} = \Theta^{ZX} = 0$ and $\Theta^{XX} = \Theta^{ZZ}$ a band-diagonal permutation matrix [83]. Let $\text{PSp}_\Lambda^{bd}(\mathbb{Z}_d)$ denote the group generated by them.

In conclusion, the classification of Clifford QCA is reduced to

$$\frac{\text{Sp}_\Lambda^{bd}(\mathbb{Z}_d)}{\langle \text{ESp}_\Lambda^{bd}(\mathbb{Z}_d), \text{PSp}_\Lambda^{bd}(\mathbb{Z}_d) \rangle},$$

up to a procedure called stabilization (see below). Elements in $\langle \text{ESp}_\Lambda^{bd}(\mathbb{Z}_d), \text{PSp}_\Lambda^{bd}(\mathbb{Z}_d) \rangle$ are referred to as trivial Clifford QCAs.

Above, we implicitly assume that there is a single qudit at each site $i \in \Lambda$. However, it is customary to allow multiple qudits on each site. Stabilization allows one to compare QCAs defined on the same Λ with different on-site qudits. A QCA may be extended to additional on-site qudits by the identity action on operators supported on them. These extended QCA are regarded equivalent to the original. The

procedure is called stabilization. In view of this, we should allow

$$P = \bigoplus_{i \in \Lambda} \mathbb{Z}_d^{2q_i},$$

with different numbers q_i of qudits on site i and its symplectic form ω accordingly. This generalizes

$$\Theta^{\bullet\bullet}(j, k) \in \text{Mat}_{q_k \times q_j}(\mathbb{Z}_d),$$

for $j, k \in \Lambda$.

B. QCAs with the same stabilizer group

This section addresses a fundamental question: *Are two Clifford QCAs with the same stabilizer group (or flipper group) always equivalent?* We begin by introducing a special class of QCAs for which this question reduces to a particularly simple form.

Definition 4. A Clifford QCA α is called **separated** if

$$\alpha(\langle X_i \rangle_{i \in \Lambda}) = \langle X_i \rangle_{i \in \Lambda}, \quad \alpha(\langle Z_i \rangle_{i \in \Lambda}) = \langle Z_i \rangle_{i \in \Lambda}.$$

Here, $\langle X_i \rangle_{i \in \Lambda}$ (resp. $\langle Z_i \rangle_{i \in \Lambda}$) denotes the group of Pauli operators generated purely by X (resp. purely by Z) operators and phase. For a separated QCA α , the associated symplectic transformation $\kappa(\alpha)$ necessarily takes the block-diagonal form

$$\kappa(\alpha) = \begin{pmatrix} \Theta & 0 \\ 0 & (\Theta^T)^{-1} \end{pmatrix} \in \text{Sp}_\Lambda^{\text{bd}}(\mathbb{Z}_d).$$

We refer to such elements of $\text{Sp}_\Lambda^{\text{bd}}(\mathbb{Z}_d)$ as **separated** symplectic transformations.

Note that a separated Clifford QCA maps CSS codes to CSS codes, and hence preserves the CSS structure.

Theorem 2. Two Clifford QCAs with the same stabilizer group (or the same flipper group) are equivalent up to finite-depth quantum circuits if and only if every separated Clifford QCA is trivial.

Lemma 3. Any θ with $\Theta^{XZ} = 0$ is equivalent to a separated $\theta' = \begin{pmatrix} \Theta & 0 \\ 0 & (\Theta^T)^{-1} \end{pmatrix} \in \text{Sp}_\Lambda^{\text{bd}}(\mathbb{Z}_d)$.

Proof. Write $\theta = \begin{pmatrix} \Theta^{XX} & 0 \\ \Theta^{ZX} & \Theta^{ZZ} \end{pmatrix}$. Then $\theta^T J_\Lambda \theta = J_\Lambda$ and $\theta J_\Lambda \theta^T = J_\Lambda$ is equivalent to

$$\Theta^{ZZ} = ((\Theta^{XX})^T)^{-1}$$

and $(\Theta^{XX})^T \Theta^{ZX}, \Theta^{ZZ} (\Theta^{ZX})^T$ are symmetric. By the first equality, $\theta' = \begin{pmatrix} \Theta^{XX} & 0 \\ 0 & \Theta^{ZZ} \end{pmatrix} \in \text{Sp}_\Lambda^{\text{bd}}(\mathbb{Z}_d)$. Moreover,

$\theta'^{-1} \theta = \begin{pmatrix} I_\Lambda & 0 \\ (\Theta^{XX})^T \Theta^{ZX} & I_\Lambda \end{pmatrix} \in \text{ESp}_\Lambda^{\text{bd}}(\mathbb{Z}_d)$. In other words, $\theta'^{-1} \theta$ lifts to a QCA with $X_j \mapsto X_j$ and $Z_j \mapsto \mathcal{X}_j Z_j$ where

$$\mathcal{X}_j = \exp\{\pi i ((\Theta^{XX})^T \Theta^{ZX})(j, j)/d\} \\ \times \prod_{k \in \Lambda} X_k^{((\Theta^{XX})^T \Theta^{ZX})(j, k)}$$

consists only of Pauli X matrices and a phase. Such a QCA is always a circuit. This proves the lemma. ■

Proof of Theorem. Let α and β be two QCAs that both bijectively map $\langle X_i \rangle_{i \in \Lambda}$ to the same image. Their difference $\beta^{-1} \circ \alpha$ is a Clifford QCA. Since $\beta^{-1} \circ \alpha$ maps $\langle X_i \rangle_{i \in \Lambda}$ bijectively to itself, $\kappa(\beta^{-1} \circ \alpha) \in A := \{\theta \in \text{Sp}_\Lambda^{\text{bd}}(\mathbb{Z}_d) : \Theta^{XZ} = 0\}$. By the lemma above, $\kappa(\beta^{-1} \circ \alpha)$ is equivalent to some $\theta' = \begin{pmatrix} \Theta & 0 \\ 0 & (\Theta^T)^{-1} \end{pmatrix}$. Hence α and β are equivalent if θ' is trivial.

Conversely, a nontrivial θ' of this form has the same stabilizer group as the identity QCA. Therefore, it provides a counterexample. ■

Define $\text{GL}_\Lambda^{\text{bd}}(\mathbb{Z}_d)$ to be the collection of invertible band-diagonal matrices indexed by Λ . There is an injective homomorphism

$$D : \Theta \mapsto \begin{pmatrix} \Theta & 0 \\ 0 & (\Theta^T)^{-1} \end{pmatrix}$$

embedding $\text{GL}_\Lambda^{\text{bd}}(\mathbb{Z}_d)$ in $\text{Sp}_\Lambda^{\text{bd}}(\mathbb{Z}_d)$. The image of D is precisely the subgroup of separated elements $\Sigma = \{\theta \in \text{Sp}_\Lambda^{\text{bd}}(\mathbb{Z}_d) : \Theta^{12} = \Theta^{21} = 0\}$. Define $E_\Lambda^{\text{bd}}(\mathbb{Z}_d) \subset \text{GL}_\Lambda^{\text{bd}}(\mathbb{Z}_d)$ to be the subgroup generated by block-diagonal matrices and $P_\Lambda^{\text{bd}}(\mathbb{Z}_d) \subset \text{GL}_\Lambda^{\text{bd}}(\mathbb{Z}_d)$ the permutation matrices. The classification group of separated QCAs is isomorphic to $\text{GL}_\Lambda^{\text{bd}}(\mathbb{Z}_d) / \langle E_\Lambda^{\text{bd}}(\mathbb{Z}_d), P_\Lambda^{\text{bd}}(\mathbb{Z}_d) \rangle$ up to stabilization.

C. Separated QCAs and K-theory

The following construction is taken from Refs. [84,85]. It provides a natural categorical setting for Clifford QCA [37].

Definition 5. Let X be a metric space and $\mathcal{A}$ a filtered additive category. We then define the filtered category $\mathcal{C}_X(\mathcal{A})$ as follows:

- (1) An object A of $\mathcal{C}_X(\mathcal{A})$ is a collection of objects $A(x)$ of $\mathcal{A}$, one for each $x \in X$, satisfying the condition that for each ball $B \subset X$, $A(x) \neq 0$ for only finitely many $x \in B$.
- (2) A morphism $\phi : A \rightarrow B$ is a collection of morphisms $\phi_x^y : A(x) \rightarrow B(y)$ in $\mathcal{A}$ such that there exists r depending only on ϕ so that

- (a) $\phi_y^x = 0$ for $d(x, y) > r$.
- (b) all ϕ_y^x are in $F, \text{Hom}(A(x), B(y))$.

(We then say that ϕ has filtration degree $\leq r$.)

Composition of $\phi : A \rightarrow B$ with $\psi : B \rightarrow C$ is given by $(\psi\phi)_z^x = \sum_{y \in X} \psi_z^y \phi_y^x$. Notice that the sum makes sense because the category is additive and because the sum will always be finite.

The categories $\mathcal{C}_X(\mathcal{A})$ and $\mathcal{C}_Y(\mathcal{A})$ are equivalent for coarsely equivalent metric spaces X, Y . See Ref. [84] for a proof.

Definition 6. Let $\mathcal{A}$ be an additive category. The *algebraic K_1 group* of $\mathcal{A}$, denoted $K_1(\mathcal{A})$, is defined as follows:

We first consider the category $\text{Aut}(\mathcal{A})$, whose objects are pairs (A, ϕ) where A is an object of $\mathcal{A}$ and $\phi : A \rightarrow A$ is an automorphism in $\mathcal{A}$. A morphism $f : (A, \alpha) \rightarrow (B, \beta)$ in $\text{Aut}(\mathcal{A})$ is a morphism $f : A \rightarrow B$ in $\mathcal{A}$ such that

$$f \circ \alpha = \beta \circ f.$$

Then $K_1(\mathcal{A})$ is defined as the abelian group obtained from the group completion of the monoid of isomorphism classes in $\text{Aut}(\mathcal{A})$, modulo the relations:

- (1) $[A, \alpha] + [A, \alpha'] = [A, \alpha \circ \alpha']$.
- (2) $[A, \alpha] + [C, \gamma] = [B, \beta]$ whenever there is a diagram with exact rows

$$\begin{array}{ccccccccc} 0 & \longrightarrow & A & \longrightarrow & B & \longrightarrow & C & \longrightarrow & 0 \\ & & \downarrow \alpha & & \downarrow \beta & & \downarrow \gamma & & \\ 0 & \longrightarrow & A & \longrightarrow & B & \longrightarrow & C & \longrightarrow & 0 \end{array}$$

In particular, $K_1(\mathcal{C}_X(\mathcal{A}))$ gives a description of the homology theory associated with any algebraic K-theory. The following theorem [86] will be useful.

Theorem 3. Let $\mathcal{A}$ be the category of finitely generated free R -modules for a ring R ,

$$K_1(\mathcal{C}_{\mathbb{Z}^{D+1}}(\mathcal{A})) \cong K_{-D}(R),$$

the negative algebraic K -theory of R .

Let $\mathcal{A}$ be the category of finitely generated free $\mathbb{Z}_d$ -modules and $X = \Lambda$. The definition of $\text{GL}_{\Lambda}^{bd}(\mathbb{Z}_d)$ coincides with $\text{Aut}(\mathcal{A})$. Moreover, $\text{GL}_{\Lambda}^{bd}(\mathbb{Z}_d)/E_{\Lambda}^{bd}(\mathbb{Z}_d)$ with stabilization is isomorphic to $K_1(\mathcal{C}_{\Lambda}(\mathcal{A}))$. Therefore, the classification of separated QCA is a quotient of $K_1(\mathcal{C}_{\Lambda}(\mathcal{A}))$.

For QCAs on Euclidean spaces, the theorem above implies

$$K_1(\mathcal{C}_{\mathbb{Z}^D}(\mathcal{A})) \cong K_{-D+1}(\mathbb{Z}_d) = \begin{cases} \mathbb{Z}^r, & \text{for } D = 1, \\ 0, & \text{for } D > 1, \end{cases}$$

where r is the number of distinct prime factors of d . In dimension 1, nontrivial K_1 -classes correspond to translations. Since separated QCAs are classified by the corresponding negative K -groups, the above result immediately implies the following corollary.

Corollary 1. On any lattice coarsely equivalent to a Euclidean space, all separated QCAs are trivial. Consequently, Clifford QCAs with the same stabilizer group are always equivalent on such lattices according to Theorem 2.

In the translation-invariant case, the same conclusion follows from Suslin's stability theorem (see Lemma IV.10 in Ref. [1]). On these lattices, Clifford QCAs with the same stabilizer group are always equivalent. On the other hand, there exist metric spaces X on which the K_1 group of $\mathcal{C}_X(\mathbb{Z}_d)$ is nontrivial. Separated QCAs on such X could be nontrivial. Examples include open cones

$$X := O(Y) = \{tx \in \mathbb{R}^{n+1} : t \geq 0 \text{ and } x \in Y \subset S^n\}$$

over certain subspaces Y of the unit n -sphere $S^n \subset \mathbb{R}^{n+1}$ with nontrivial K -theory homology groups [84]. This should motivate further study of QCAs on lattices of the form

$$\{nx \in \mathbb{R}^{n+1} : n \in \mathbb{N} \text{ and } x \in \Gamma \subset S^n\},$$

where Γ is some discrete lattice in the unit n -sphere.

D. Local flippability

Last, we record a useful result in the translation invariant setup. Consider a Pauli translation-invariant stabilizer code over $\mathbb{Z}_{p^r}$ defined by a module homomorphism (see Refs. [50,87]) $R^t \xrightarrow{\sigma} P = R^{2q}$, where $L := \text{image of } \sigma$ satisfies the topological order (aka Lagrangian) condition:

$$R^t \xrightarrow{\sigma} P \xrightarrow{\epsilon} R^t$$

is exact. For the purpose of Clifford QCA construction, we impose the additional conditions that $t = q$ and σ injective. In particular, L is free of rank q .

Theorem 4. The following are equivalent:

- (1) Separators defined by σ are locally flippable.
- (2) The short exact sequence $0 \rightarrow L \rightarrow P \rightarrow P/L \rightarrow 0$ splits.
- (3) P/L is projective.
- (4) P/L is free.

- (5) The module of topological point excitation [88] $\text{Ext}^1(P/L, R)$ vanishes.

Proof. $1 \implies 2$: the local separators provide a basis for P/L .

$2 \implies 3$: as the short exact sequence splits, P/L is a direct summand of free module P .

$3 \implies 4$: by Quillen-Suslin theorem, every projective module over $R/pR = \mathbb{Z}_p[x_1^\pm, \dots, x_D^\pm]$ is free. Assume M is a projective module over $R = \mathbb{Z}_{p^r}[x_1^\pm, \dots, x_D^\pm]$, then M/pM is a free module over R/pR . Lift a basis of M/pM to $\{m_1, \dots, m_k\} \subset M$ and denote the submodule it generates by $M' \subset M$. Notice $M/M' \subset p(M/M')$, by Nakayama's lemma $M/M' = 0$. In other words, we have a short exact sequence $0 \rightarrow K \rightarrow R^k \xrightarrow{\sigma} M \rightarrow 0$, where σ is generated by $\{m_1, \dots, m_k\}$ and $K = \ker \sigma$. By the projectivity of M , $R^k \cong K \oplus M$. Moreover, $K \cong R^k/M \subset pK$. Therefore, by Nakayama's lemma again, $K = 0$.

$4 \implies 5$: follows from the definition of Ext .

$5 \implies 1$: As L is free, $\text{Ext}^1(P/L, R) = 0$ implies $\text{Ext}^1(P/L, L) = 0$ as well. In other words, all extensions of P/L by L are trivial and $P \cong L \oplus P/L$. Since L is Lagrangian, there exists a standard symplectic basis for this direct sum decomposition of P . ■

VIII. DISCUSSIONS

Our work establishes a unified framework for constructing $\mathbb{Z}_2$ and $\mathbb{Z}_p$ Clifford QCAs from both TQFTs and ISAs, clarifying their orders, periodicities in dimensions, and realizations on arbitrary cellulations (for $\mathbb{Z}_2$ QCAs). Several natural directions for future research emerge from this framework.

A particularly important direction is to move beyond the Clifford regime. Notable examples, such as the chiral semion Walker-Wang model, already indicate the existence of intrinsically non-Clifford QCAs for qubits [35]. Developing systematic methods to construct and classify such models would extend our framework to a much broader class of topological phases.

As a concrete example, the semion QCA is associated with the topological action

$$\frac{1}{4} (B_2 \cup B_2 + B_2 \cup_1 \delta B_2) \in H^4(K(\mathbb{Z}_2, 2), \mathbb{R}/\mathbb{Z}), \quad (258)$$

whose surface anyon theory is $\{1, s\}$, where s is a semion obeying $\mathbb{Z}_2$ fusion rules and carrying topological spin $\theta(s) = i$. This theory has chiral central charge $c_- = 1$. The fourth power of the semion QCA is equivalent to the 3-fermion QCA (with $c_- = 4$), since their surface anyon theories lie in the same Witt class. Explicitly, starting from

$$\mathcal{A} = \{1, s_1\} \times \{1, s_2\} \times \{1, s_3\} \times \{1, s_4\}, \quad (259)$$

condensing the boson $b = s_1 s_2 s_3 s_4$ yields

$$\mathcal{A}' = \{1, s_1 s_2, s_1 s_3, s_1 s_4\}, \quad (260)$$

which is precisely the 3-fermion anyon theory.

Generalizing this construction to higher dimensions may lead to new families of non-Clifford QCAs. For instance, we expect that the topological action

$$\frac{1}{4} (B_{2l} \cup B_{2l} + B_{2l} \cup_1 \delta B_{2l}) \in H^{4l}(K(\mathbb{Z}_2, 2l), \mathbb{R}/\mathbb{Z}) \quad (261)$$

gives rise to semion-type QCAs in $(4l - 1)$ spatial dimensions. It would also be interesting to construct a non-Clifford ISA corresponding to the chiral semion theory and to generalize such constructions to higher dimensions.

Another promising perspective is to derive QCAs from cobordism classifications. The 3-fermion Walker-Wang model corresponds to the $3 + 1D$ w_2^2 TQFT, and its $4 + 1D$ generalization, associated with the $w_2 w_3$ TQFT, was constructed in Ref. [4] via the topological action

$$\frac{1}{2} \int A_3 \cup_1 A_3 + A_3 \cup B_2 + B_2 \cup (B_2 \cup_1 B_2), \quad (262)$$

which closely parallels the 3-fermion Walker-Wang action in Eq. (43). It is natural to conjecture that all nontrivial cobordism classes give rise to nontrivial QCAs [4, 5].

Finally, we note that whenever a topological action involves coefficients beyond $1/2$ or contains terms higher than quadratic, the resulting QCA is necessarily non-Clifford in prime-dimensional qudits, since the corresponding Hamiltonian can no longer be written as a Pauli stabilizer and must involve at least S or CZ gates. Therefore, exploring cocycles for higher-form symmetries provides a systematic route to constructing new non-Clifford QCAs. However, extracting explicit separators and flippers from such Hamiltonians is highly nontrivial and remains an important open problem.

Next, a more explicit connection between the TQFT and ISA constructions remains to be established. Although we have argued that both descriptions capture the same phases, a direct finite-depth circuit relating them has not yet been constructed in general. Constructing such a circuit would provide an operator-algebraic proof of their equivalence and elucidate the role of locality-preserving unitaries in pumping chirality [89].

Another natural direction is to explore QCAs that act on Hilbert spaces beyond simple tensor products of local qudits. Examples include the Kramers-Wannier duality, symmetry-protected QCAs, and more general categorical dualities in spin systems [14, 90]. Extending our framework to these cases would connect QCA classification to recent work on lattice anomalies and higher-form symmetries, thereby enriching the interplay between algebraic topology, category theory, and condensed matter physics.

Finally, several structural generalizations remain open. While we demonstrated that $\mathbb{Z}_2$ QCAs can be realized on arbitrary cellulations, extending $\mathbb{Z}_p$ QCAs systematically to triangulations and general cell complexes would further clarify their robustness and their relation to generalized cohomology. One key property of hypercubic lattices is that $c_i \cup c_{d-i}$ induces a one-to-one correspondence between cells. It would be interesting to identify other lattices with similar properties, or to exploit Poincaré duality, as in our $\mathbb{Z}_2$ construction. For example, vertex-face pairing seems to be important in the construction of Chern-Simons theory on the lattice [91–94].

More broadly, our results suggest a deep correspondence between TQFT classifications and QCA classifications. Making this link precise, both in the Clifford and non-Clifford regimes, would provide a unified understanding of the algebraic invariants underlying QCAs and their role in higher-dimensional phases of matter. A systematic study along these lines would not only extend the mathematical classification of QCAs in higher dimensions but also clarify their relevance to fault-tolerant quantum computation, Floquet dynamics, generalized symmetries, and lattice anomalies.

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DATA AVAILABILITY

No data were created or analyzed in this study.

APPENDIX A: REVIEW OF THE LAURENT POLYNOMIAL FORMALISM

This appendix reviews the Laurent polynomial representation and its application to translation-invariant stabilizer codes. The formalism was first introduced in Refs. [48–51]. In this work, we adopt the conventions and notations of Refs. [57,73,95,96]. We begin with a general $\mathbb{Z}_d$ qudit system, where the $d \times d$ generalized Pauli matrices are

defined as

$$X = \begin{bmatrix} 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \end{bmatrix},$$

$$Z = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & \omega & 0 & \cdots & 0 \\ 0 & 0 & \omega^2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \omega^{d-1} \end{bmatrix}, \quad (\text{A1})$$

with $\omega := \exp(2\pi i/d)$. These matrices satisfy the commutation relation

$$ZX = \omega XZ. \quad (\text{A2})$$

We develop the formalism in the setting of a two-dimensional square lattice, from which the extension to the three-dimensional cubic lattice and higher dimensions follows naturally.

We consider the case of two $\mathbb{Z}_d$ qudits per unit cell (e.g., one qudit on each edge of a square lattice), generalizable to k qudits per cell. Any Pauli operator—a finite tensor product of Pauli matrices—can be represented, up to an overall phase, as a column vector over the polynomial ring

$$R = \mathbb{Z}_d[x, y, x^{-1}, y^{-1}], \quad (\text{A3})$$

which includes all polynomials in $x^{\pm 1}, y^{\pm 1}$ with coefficients in $\mathbb{Z}_d$. We assign column vectors over $\mathbb{Z}_d$ to the (generalized) Pauli matrices X_{12}, Z_{12}, X_{14} , and Z_{14} , depicted in Fig. 9,

$$\mathcal{X}_{12} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \mathcal{Z}_{12} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \quad \mathcal{X}_{14} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix},$$

$$\mathcal{Z}_{14} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}, \quad (\text{A4})$$

where column vector representations of operators are indicated using curly letters. The coefficients in these vectors correspond to their powers,

$$\mathcal{P} = \begin{bmatrix} i \\ j \\ k \\ l \end{bmatrix} \Rightarrow \mathcal{P}^m = \begin{bmatrix} mi \\ mj \\ mk \\ ml \end{bmatrix} \quad \forall m \in \mathbb{Z}_d. \quad (\text{A5})$$

The translation of operators is achieved using polynomials of x and y to denote translations in the x and y directions,

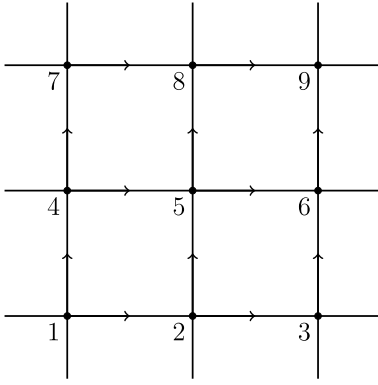


FIG. 9. A qudit is placed on each edge, with generalized Pauli operators X_e and Z_e acting on it.

respectively. To illustrate, translating the operator on edge e_{12} to edge e_{78} or to edge e_{58} involves multiplying the column vector of the operator by y^2 or xy , respectively,

$$\mathcal{Z}_{78} = y^2 \mathcal{Z}_{12} = \begin{bmatrix} 0 \\ 0 \\ y^2 \\ 0 \end{bmatrix}, \quad \mathcal{X}_{58} = xy \mathcal{X}_{14} = \begin{bmatrix} 0 \\ xy \\ 0 \\ 0 \end{bmatrix}. \quad (\text{A6})$$

A general Pauli operator can be expressed as

$$P = \eta X_{e_1}^{a_1} X_{e_2}^{a_2} \cdots X_{e_n}^{a_n} Z_{e'_1}^{b_1} Z_{e'_2}^{b_2} \cdots Z_{e'_m}^{b_m}, \quad (\text{A7})$$

where η represents a root of unity of order $2d$. After dropping the overall phase η , the corresponding column vector for this operator is a linear combination of individual Pauli matrices, expressed as

$$\mathcal{P} = a_1 \mathcal{X}_{e_1} + a_2 \mathcal{X}_{e_2} + \cdots + a_n \mathcal{X}_{e_n} + b_1 \mathcal{Z}_{e'_1} + b_2 \mathcal{Z}_{e'_2} + \cdots + b_m \mathcal{Z}_{e'_m}. \quad (\text{A8})$$

More examples are included in Fig. 1.

Next, we introduce the **antipode map** that is a $\mathbb{Z}_d$ -linear map from R to R defined by

$$x^a y^b \rightarrow \overline{x^a y^b} := x^{-a} y^{-b}. \quad (\text{A9})$$

To determine whether two Pauli operators represented by vectors v_1 and v_2 commute or anticommute, we define the dot product as

$$v_1 \cdot v_2 = \bar{v}_1^T \Lambda v_2, \quad (\text{A10})$$

where T is the transpose operation on a matrix and

$$\Lambda = \left[\begin{array}{cc|cc} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ \hline -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{array} \right] \quad (\text{A11})$$

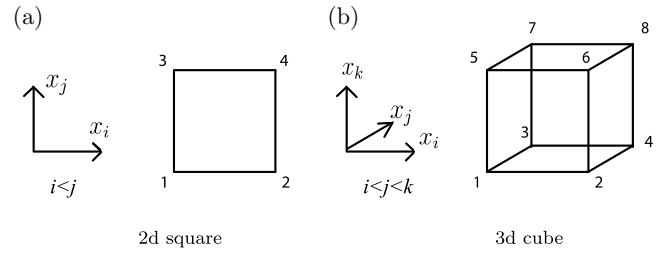


FIG. 10. (a) The conventional orientation of a 2d square. (b) The conventional orientation of a 3d cube.

is the matrix representation of the standard **symplectic bilinear form**. For simplicity, we denote $(\cdots)^T$ as $(\cdots)^\dagger$.

A translation-invariant stabilizer code corresponds to an R -submodule σ such that

$$v_1 \cdot v_2 = v_1^\dagger \Lambda v_2 = 0, \quad \forall v_1, v_2 \in \sigma, \quad (\text{A12})$$

called the **stabilizer module**. The Hamiltonian could have two (or more) terms per square to have a unique ground state on a simply-connected manifold, denoted as $H = -\sum_{\text{cells}} (S_1 + S_2)$. For example, the trivial phase $H_0 = -\sum_e \mathcal{X}_e$ is

$$S_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad S_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad (\text{A13})$$

and the standard $\mathbb{Z}_d$ toric code Hamiltonian

$$H_{\text{TC}} = -\sum_v \begin{array}{c} | \\ \textcolor{blue}{X} \\ \textcolor{blue}{X}^\dagger \textcolor{blue}{v} \textcolor{blue}{X} \\ | \end{array} - \sum_p \begin{array}{c} \textcolor{blue}{Z}^\dagger \\ \textcolor{blue}{Z}^\dagger \textcolor{blue}{p} \textcolor{blue}{Z} \\ \textcolor{blue}{Z} \end{array}, \quad (\text{A14})$$

corresponds to

$$S_1 = \begin{bmatrix} 1 - \bar{x} \\ 1 - \bar{y} \\ 0 \\ 0 \end{bmatrix}, \quad S_2 = \begin{bmatrix} 0 \\ 0 \\ 1 - y \\ -1 + x \end{bmatrix}. \quad (\text{A15})$$

APPENDIX B: REVIEW OF HIGHER CUP PRODUCTS ON HYPERCUBES

The notations and definitions in this Appendix are mostly adapted from Ref. [42], but note that the signs of boundary and coboundary operators with integer

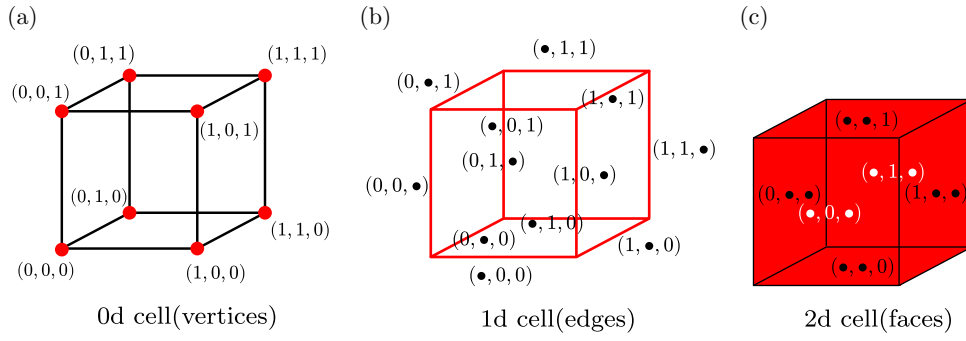


FIG. 11. (a), (b), and (c) correspond to different dimensional cells F_0 , F_1 , and F_2 .

coefficients presented previously have typos. Here, we provide a corrected sign convention and explicitly list all definitions of the higher cup products used for hypercubes in this paper.

First, let us establish the notation for cochains on a hypercube. We denote the d -dimensional hypercube by $\square_d$. As a subset of $\mathbb{R}^d$, we assign coordinates to $\square_d$ via

$$\square_d = \{(x_1, \dots, x_d) \in \mathbb{R}^d \mid x_i \in [0, 1]\}, \quad (\text{B1})$$

which will be used throughout our discussion of cochain operations. The ordering of the coordinates is shown in Fig. 10.

1. The cells

We denote the set of p -cells of $\square_d$ by $F_p(\square_d)$. For instance, the vertices of the hypercube are the 0-cells,

$$F_0(\square_d) = \{(\sigma_1, \dots, \sigma_d) \mid \sigma_i = 0, 1\}. \quad (\text{B2})$$

Equivalently, each label $(\sigma_1 \dots \sigma_d)$ can be interpreted as the vertex's coordinate in $\mathbb{R}^d$.

Next, consider the p -cells in $F_p(\square_d)$. A p -cell is spanned by p directions $\{i_1 \dots i_p\}$. However, identifying just the directions is not sufficient to specify a particular

cell because there are 2^{d-p} possible choices for the remaining coordinates, each of which can be 0 or 1. Concretely, if we let $\{\hat{i}_1 \dots \hat{i}_{d-p}\}$ denote the complementary set of directions $\{1, 2, \dots, d\} \setminus \{i_1, i_2, \dots, i_p\}$, then specifying a p -cell also requires assigning a value of 0 or 1 to each of those $\hat{i}$ -coordinates.

To organize these labels, we represent each cell in terms of a d -tuple $(z_1 \dots z_d)$. We assign $z_j = \bullet$ if $j \in \{i_1 \dots i_p\}$, indicating that the coordinate in direction j can vary in $[0, 1]$. Otherwise, z_j is fixed to be either 0 or 1, indicating that the coordinate in that direction does not vary. A cell described by $(z_1 \dots z_d)$ is a p -cell precisely when exactly p of the entries are $\bullet$. We denote such a cell by $P_{(z_1 \dots z_d)}$. As a subset of $\mathbb{R}^d$, we may write

$$P_{(z_1 \dots z_d)} := \{(x_1, \dots, x_d) \in \mathbb{R}^d \mid x_i \in [0, 1] \text{ if } z_i = \bullet, \text{ or } x_i = z_i \text{ if } z_i \in \{0, 1\}\}. \quad (\text{B3})$$

For example, the cells of $\square_2$ can be listed as

$$\begin{aligned} F_0(\square_2) &= \{(0, 0), (0, 1), (1, 0), (1, 1)\}, \\ F_1(\square_2) &= \{(\bullet, 0), (\bullet, 1), (0, \bullet), (1, \bullet)\}, \\ F_2(\square_2) &= \{(\bullet, \bullet)\}. \end{aligned} \quad (\text{B4})$$

Similarly, for a three-dimensional cube $\square_3$, the cells are

$$\begin{aligned} F_0(\square_3) &= \{(0, 0, 0), (0, 0, 1), (0, 1, 0), (0, 1, 1), (1, 0, 0), (1, 0, 1), (1, 1, 0), (1, 1, 1)\}, \\ F_1(\square_3) &= \{(\bullet, 0, 0), (\bullet, 0, 1), (\bullet, 1, 0), (\bullet, 1, 1), (0, \bullet, 0), (0, \bullet, 1), (1, \bullet, 0), (1, \bullet, 1), \\ &\quad (0, 0, \bullet), (0, 1, \bullet), (1, 0, \bullet), (1, 1, \bullet)\}, \\ F_2(\square_3) &= \{(\bullet, \bullet, 0), (\bullet, \bullet, 1), (\bullet, 0, \bullet), (\bullet, 1, \bullet), (0, \bullet, \bullet), (1, \bullet, \bullet)\}, \\ F_3(\square_3) &= \{(\bullet, \bullet, \bullet)\}, \end{aligned} \quad (\text{B5})$$

which are shown in Fig. 11.

2. Boundary of a cell

We now describe the boundary of a p -cell $P_{(z_1 \dots z_d)}$. Suppose $z_j = \bullet$ exactly for $j \in \{i_1 \dots i_p\}$. The boundary $\partial P_{(z_1 \dots z_d)}$ is formed by replacing precisely one of the $\bullet$'s

with either 0 or 1. Concretely,

$$\begin{aligned} \partial P_{(z_1 \dots z_d)} &= \left\{ P_{(z_1 \dots z_{j-1}, \tilde{z}_j, z_{j+1} \dots z_d)} \mid j \in \{i_1 \dots i_p\}, \tilde{z}_j \in \{0, 1\} \right\}. \end{aligned} \quad (\text{B6})$$

For example, using the notation $(z_1 \cdots z_d) \leftrightarrow P_{(z_1 \cdots z_d)}$,

$$\partial(\bullet, \bullet, 0) = \{(\bullet, 0, 0), (\bullet, 1, 0), (0, \bullet, 0), (1, \bullet, 0)\}. \quad (\text{B7})$$

When working with integer coefficients $\mathbb{Z}$ instead of $\mathbb{Z}_2$, the boundary acquires signs. Specifically [97],

$$\partial(\bullet_1, \dots, \bullet_d) = \sum_{\substack{\ell=1, \\ a_\ell \in \{0,1\}}}^d (-1)^{\ell+a_\ell} (\bullet_1, \dots, \underbrace{a_\ell}_{\ell^{\text{th}} \text{ coord}}, \dots, \bullet_d). \quad (\text{B8})$$

For instance, the boundary of the one-dimensional edge $\square_1 = (\bullet)$ is

$$\partial(\bullet) = -(0) + (1), \quad (\text{B9})$$

the boundary of the two-dimensional face $\square_2 = (\bullet, \bullet)$ is

$$\partial(\bullet, \bullet) = -(0, \bullet) + (1, \bullet) + (\bullet, 0) - (\bullet, 1), \quad (\text{B10})$$

and the boundary of the three-dimensional cube $\square_3 = (\bullet, \bullet, \bullet)$ is

$$\begin{aligned} \partial(\bullet, \bullet, \bullet) = & -(0, \bullet, \bullet) + (1, \bullet, \bullet) + (\bullet, 0, \bullet) - (\bullet, 1, \bullet) \\ & - (\bullet, \bullet, 0) + (\bullet, \bullet, 1). \end{aligned} \quad (\text{B11})$$

In the following parts, we will build upon these definitions to review the higher cup-product structures on the cubic lattice.

3. Higher cup products

Convention for higher cup products on a square is

$$A_1 \cup B_1(\bullet, \bullet) = A_1(\bullet, 0)B_1(1, \bullet) - A_1(0, \bullet)B_1(\bullet, 1), \quad (\text{B12})$$

$$A_1 \cup_1 B_2(\bullet, \bullet) = -A_1(0, \bullet)B_2(\bullet, \bullet) - A_1(\bullet, 1)B_2(\bullet, \bullet), \quad (\text{B13})$$

$$A_2 \cup_1 B_1(\bullet, \bullet) = A_2(\bullet, \bullet)B_1(\bullet, 0) + A_2(\bullet, \bullet)B_1(1, \bullet), \quad (\text{B14})$$

$$A_2 \cup_2 B_2(\bullet, \bullet) = A_2(\bullet, \bullet)B_2(\bullet, \bullet), \quad (\text{B15})$$

where $(\bullet, \bullet)$ represents the square spanned on the x_i and x_j coordinates, with all other indices that remain constants omitted implicitly. For example, $(\bullet, \bullet)$ could be $(\bullet, \bullet, 0)$, $(1, \bullet, \bullet)$, $(\bullet, 1, \bullet)$, or any square. In the computation, we are free to ignore all other coordinates except x_i and x_j .

$$A_1 \cup B_1(\square_{1234}) = A_1(12)B_1(24) - A_1(13)B_1(34), \quad (\text{B16})$$

$$A_1 \cup B_2(\square_{1234}) = -A_1(13)B_2(\square_{1234}) - A_1(34)B_2(\square_{1234}), \quad (\text{B17})$$

$$A_2 \cup B_1(\square_{1234}) = A_2(\square_{1234})B_1(12) + A_2(\square_{1234})B_1(24). \quad (\text{B18})$$

$$A_2 \cup B_1(\bullet, \bullet, \bullet) = A_2(0, \bullet, \bullet)B_1(\bullet, 1, 1) - A_2(\bullet, 0, \bullet)B_1(1, \bullet, 1) + A_2(\bullet, \bullet, 0)B_1(1, 1, \bullet), \quad (\text{B19})$$

$$A_1 \cup B_2(\bullet, \bullet, \bullet) = A_1(0, 0, \bullet)B_2(\bullet, \bullet, 1) - A_1(0, \bullet, 0)B_2(\bullet, 1, \bullet) + A_1(\bullet, 0, 0)B_2(1, \bullet, \bullet), \quad (\text{B20})$$

$$\begin{aligned} A_2 \cup_1 B_2(\bullet, \bullet, \bullet) = & A_2(\bullet, 1, \bullet)B_2(\bullet, \bullet, 0) - A_2(\bullet, \bullet, 1)B_2(\bullet, 0, \bullet) + A_2(0, \bullet, \bullet)B_2(\bullet, \bullet, 0) \\ & + A_2(0, \bullet, \bullet)B_2(\bullet, 1, \bullet) - A_2(\bullet, \bullet, 1)B_2(1, \bullet, \bullet) - A_2(\bullet, 0, \bullet)B_2(1, \bullet, \bullet), \end{aligned} \quad (\text{B21})$$

$$A_1 \cup_1 B_3(\bullet, \bullet, \bullet) = A_1(\bullet, 1, 1)B_3(\bullet, \bullet, \bullet) + A_1(0, \bullet, 1)B_3(\bullet, \bullet, \bullet) + A_1(0, 0, \bullet)B_3(\bullet, \bullet, \bullet), \quad (\text{B22})$$

$$A_3 \cup_1 B_1(\bullet, \bullet, \bullet) = A_3(\bullet, \bullet, \bullet)B_1(\bullet, 0, 0) + A_3(\bullet, \bullet, \bullet)B_1(1, \bullet, 0) + A_3(\bullet, \bullet, \bullet)B_1(1, 1, \bullet), \quad (\text{B23})$$

$$A_2 \cup_2 B_3(\bullet, \bullet, \bullet) = A_2(\bullet, \bullet, 0)B_3(\bullet, \bullet, \bullet) + A_2(\bullet, \bullet, 1)B_3(\bullet, \bullet, \bullet) + A_2(0, \bullet, \bullet)B_3(\bullet, \bullet, \bullet), \quad (\text{B24})$$

$$A_3 \cup_2 B_2(\bullet, \bullet, \bullet) = A_3(\bullet, \bullet, \bullet)B_2(1, \bullet, \bullet) + A_3(\bullet, \bullet, \bullet)B_2(\bullet, 0, \bullet) + A_3(\bullet, \bullet, \bullet)B_2(\bullet, \bullet, 1), \quad (\text{B25})$$

$$A_3 \cup_3 B_3(\bullet, \bullet, \bullet) = A_3(\bullet, \bullet, \bullet)B_3(\bullet, \bullet, \bullet). \quad (\text{B26})$$

In the graphic representation, that is (for simplicity, we will denote the entire cube as C , instead of [12345678])

$$A_2 \cup B_1(C) = A_2(\square_{1357})B_1(78) - A_2(\square_{1256})B_1(68) + A_2(\square_{1234})B_1(48), \quad (\text{B27})$$

$$A_1 \cup B_2(C) = A_1(15)B_2(\square_{5678}) - A_1(13)B_2(\square_{3478}) + A_1(12)B_2(\square_{2468}), \quad (\text{B28})$$

$$\begin{aligned} A_2 \cup_1 B_2(C) = & A_2(\square_{3478})B_2(\square_{1234}) - A_2(\square_{5678})B_2(\square_{1256}) + A_2(\square_{1357})B_2(\square_{1234}) \\ & + A_2(\square_{1357})B_2(\square_{3478}) - A_2(\square_{5678})B_2(\square_{2468}) - A_2(\square_{1256})B_2(\square_{2468}), \end{aligned} \quad (\text{B29})$$

$$A_1 \cup_1 B_3(C) = [A_1(79) + A_1(57) + A_1(15)] B_3(C), \quad (\text{B30})$$

$$A_3 \cup_1 B_1(C) = A_3(C) [B_1(12) + B_1(24) + B_1(48)], \quad (\text{B31})$$

$$A_2 \cup_2 B_3(C) = [A_2(\square_{1234}) + A_2(\square_{3478}) + A_2(\square_{1357})] B_3(C), \quad (\text{B32})$$

$$A_3 \cup_2 B_2(C) = A_3(C) [B_2(\square_{2468}) + B_2(\square_{1256}) + B_2(\square_{5678})]. \quad (\text{B33})$$

We can also write down some useful cup products in higher dimensions.

For example, in five dimensions, we have

$$\begin{aligned} A_2 \cup B_3(\bullet, \bullet, \bullet, \bullet, \bullet) &= +A_2(\bullet, \bullet, 0, 0, 0)B_3(1, 1, \bullet, \bullet, \bullet) - A_2(\bullet, 0, \bullet, 0, 0)B_3(1, \bullet, 1, \bullet, \bullet) + A_2(\bullet, 0, 0, \bullet, 0)B_3(1, \bullet, \bullet, 1, \bullet) \\ &\quad - A_2(\bullet, 0, 0, 0, \bullet)B_3(1, \bullet, \bullet, \bullet, 1) + A_2(0, \bullet, \bullet, 0, 0)B_3(\bullet, 1, 1, \bullet, \bullet) - A_2(0, \bullet, 0, \bullet, 0)B_3(\bullet, 1, \bullet, 1, \bullet) \\ &\quad + A_2(0, \bullet, 0, 0, \bullet)B_3(\bullet, 1, \bullet, \bullet, 1) + A_2(0, 0, \bullet, \bullet, 0)B_3(\bullet, \bullet, 1, 1, \bullet) - A_2(0, 0, \bullet, 0, \bullet)B_3(\bullet, \bullet, 1, \bullet, 1) \\ &\quad + A_2(0, 0, 0, \bullet, \bullet)B_3(\bullet, \bullet, \bullet, 1, 1), \end{aligned} \quad (\text{B34})$$

$$\begin{aligned} A_3 \cup B_2(\bullet, \bullet, \bullet, \bullet, \bullet) &= +A_3(\bullet, \bullet, \bullet, 0, 0)B_2(1, 1, 1, \bullet, \bullet) - A_3(\bullet, \bullet, 0, \bullet, 0)B_2(1, 1, \bullet, 1, \bullet) + A_3(\bullet, 0, \bullet, \bullet, 0)B_2(1, \bullet, 1, 1, \bullet) \\ &\quad - A_3(0, \bullet, \bullet, \bullet, 0)B_2(\bullet, 1, 1, 1, \bullet) + A_3(\bullet, \bullet, 0, 0, \bullet)B_2(1, 1, \bullet, \bullet, 1) - A_3(\bullet, 0, \bullet, 0, \bullet)B_2(1, \bullet, 1, \bullet, 1) \\ &\quad + A_3(0, \bullet, \bullet, 0, \bullet)B_2(\bullet, 1, 1, \bullet, 1) + A_3(\bullet, 0, 0, \bullet, \bullet)B_2(1, \bullet, \bullet, 1, 1) - A_3(0, \bullet, 0, \bullet, \bullet)B_2(\bullet, 1, \bullet, 1, 1) \\ &\quad + A_3(0, 0, \bullet, \bullet, \bullet)B_2(\bullet, \bullet, 1, 1, 1), \end{aligned} \quad (\text{B35})$$

and

$$\begin{aligned} A_3 \cup_1 B_3(\bullet, \bullet, \bullet, \bullet, \bullet) &= +A_3(\bullet, \bullet, \bullet, 1, 1)B_3(\bullet, 0, 0, \bullet, \bullet) + A_3(\bullet, \bullet, \bullet, 1, 1)B_3(1, \bullet, 0, \bullet, \bullet) + A_3(\bullet, \bullet, \bullet, 1, 1)B_3(1, 1, \bullet, \bullet, \bullet) \\ &\quad - A_3(\bullet, \bullet, 1, \bullet, 1)B_3(\bullet, 0, \bullet, 0, \bullet) - A_3(\bullet, \bullet, 1, \bullet, 1)B_3(1, \bullet, \bullet, 0, \bullet) + A_3(\bullet, \bullet, 0, \bullet, 1)B_3(1, 1, \bullet, \bullet, \bullet) \\ &\quad + A_3(\bullet, \bullet, 1, 1, \bullet)B_3(\bullet, 0, \bullet, \bullet, 0) + A_3(\bullet, \bullet, 1, 1, \bullet)B_3(1, \bullet, \bullet, \bullet, 0) + A_3(\bullet, \bullet, 0, 0, \bullet)B_3(1, 1, \bullet, \bullet, \bullet) \\ &\quad + A_3(\bullet, 1, \bullet, \bullet, 1)B_3(\bullet, \bullet, 0, 0, \bullet) - A_3(\bullet, 0, \bullet, \bullet, 1)B_3(1, \bullet, \bullet, 0, \bullet) - A_3(\bullet, 0, \bullet, \bullet, 1)B_3(1, \bullet, 1, \bullet, \bullet) \\ &\quad - A_3(\bullet, 1, \bullet, 1, \bullet)B_3(\bullet, \bullet, 0, \bullet, 0) + A_3(\bullet, 0, \bullet, 1, \bullet)B_3(1, \bullet, \bullet, \bullet, 0) - A_3(\bullet, 0, \bullet, 0, \bullet)B_3(1, \bullet, 1, \bullet, \bullet) \\ &\quad + A_3(\bullet, 1, 1, \bullet, \bullet)B_3(\bullet, \bullet, \bullet, 0, 0) + A_3(\bullet, 0, 0, \bullet, \bullet)B_3(1, \bullet, \bullet, \bullet, 0) + A_3(\bullet, 0, 0, \bullet, \bullet)B_3(1, \bullet, \bullet, 1, \bullet) \\ &\quad + A_3(0, \bullet, \bullet, \bullet, 1)B_3(\bullet, \bullet, 0, 0, \bullet) + A_3(0, \bullet, \bullet, \bullet, 1)B_3(\bullet, 1, \bullet, 0, \bullet) + A_3(0, \bullet, \bullet, \bullet, 1)B_3(\bullet, 1, 1, \bullet, \bullet) \\ &\quad - A_3(0, \bullet, \bullet, 1, \bullet)B_3(\bullet, \bullet, 0, \bullet, 0) - A_3(0, \bullet, \bullet, 1, \bullet)B_3(\bullet, 1, \bullet, \bullet, 0) + A_3(0, \bullet, \bullet, 0, \bullet)B_3(\bullet, 1, 1, \bullet, \bullet) \\ &\quad + A_3(0, \bullet, 1, \bullet, \bullet)B_3(\bullet, \bullet, \bullet, 0, 0) - A_3(0, \bullet, 0, \bullet, \bullet)B_3(\bullet, 1, \bullet, \bullet, 0) - A_3(0, \bullet, 0, \bullet, \bullet)B_3(\bullet, 1, \bullet, 1, \bullet) \\ &\quad + A_3(0, 0, \bullet, \bullet, \bullet)B_3(\bullet, \bullet, \bullet, 0, 0) + A_3(0, 0, \bullet, \bullet, \bullet)B_3(\bullet, \bullet, 1, \bullet, 0) + A_3(0, 0, \bullet, \bullet, \bullet)B_3(\bullet, \bullet, 1, 1, \bullet). \end{aligned} \quad (\text{B36})$$

The general formula for higher cup products on a hypercubic lattice can be found in Ref. [42].

4. Polynomial expression for higher cup products

We may explicitly write down the expressions for the matrices $M_{\mathcal{T}}$ using the definitions of the cup products on the cubic lattice. We tabulate some of them used in the text here

$$\begin{aligned} \mathbf{M}_{e \cup f} &= \begin{pmatrix} \bar{y}\bar{z} & 0 & 0 \\ 0 & -\bar{x}\bar{z} & 0 \\ 0 & 0 & \bar{x}\bar{y} \end{pmatrix}, \quad \mathbf{M}_{f \cup e} = \begin{pmatrix} \bar{x} & 0 & 0 \\ 0 & -\bar{y} & 0 \\ 0 & 0 & \bar{z} \end{pmatrix}, \quad \mathbf{M}_{f' \cup_{1f}} = \begin{pmatrix} 0 & \bar{x} & \bar{x}z \\ -\bar{y} & 0 & z \\ -1 & -y & 0 \end{pmatrix}, \\ \mathbf{M}_{e \cup_{1c}} &= \begin{pmatrix} 1 \\ \bar{x} \\ \bar{x}\bar{y} \end{pmatrix}, \quad \mathbf{M}_{f \cup_{2c}} = \begin{pmatrix} \bar{x} \\ 1 \\ \bar{z} \end{pmatrix}, \quad \mathbf{M}_{c \cup_{2f}} = (1 \quad y \quad 1). \end{aligned} \quad (\text{B37})$$

APPENDIX C: EXPLICIT MATRICES FOR THE 3-FERMION-TYPE QCA

1. The 3 + 1D 3-fermion QCA

The matrix elements of the QCA obtained from the TQFT approach, Eq. (68), are

$$\bar{\mathbf{X}}^A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ yz + 1 & y^2z + yz & yz^2 + yz \\ xz + z & xyz + yz + z + 1 & z^2 + z \\ x + 1 & y + 1 & xyz + z \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ xyz + x + yz + 1 & xy^2z + y^2z + yz + 1 & xyz + yz^2 + yz + z \\ xyz + \frac{x}{y} + x + \frac{1}{y} & xy^2z + xyz + \frac{1}{y} + 1 & xyz^2 + xyz + xz + \frac{z}{y} \\ xy + \frac{x}{z} + x + 1 & xy^2 + y + \frac{1}{z} + 1 & xyz + xy + z + 1 \end{pmatrix}, \quad (\text{C1})$$

$$\bar{\mathbf{X}}^B = \begin{pmatrix} \frac{1}{xyz} + \frac{1}{x} & \frac{y}{x} + \frac{1}{x} & \frac{z}{x} + \frac{1}{x} \\ \frac{1}{xy} + \frac{1}{y} & \frac{1}{xyz} + \frac{1}{xy} + \frac{1}{x} + 1 & \frac{z}{xy} + \frac{1}{xy} \\ \frac{1}{xyz} + \frac{1}{yz} & \frac{1}{xyz} + \frac{1}{xz} & \frac{1}{xy} + 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ \frac{1}{xyz} + \frac{1}{x} + \frac{1}{yz} + 1 & \frac{1}{xyz} + \frac{y}{x} + \frac{1}{x} + y & \frac{1}{xy} + \frac{z}{x} + \frac{1}{x} + 1 \\ \frac{1}{xy^2z} + \frac{1}{y^2z} + \frac{1}{yz} + 1 & \frac{1}{xy^2z} + \frac{1}{xyz} + y + 1 & \frac{1}{xy^2} + \frac{1}{y} + z + 1 \\ \frac{1}{xyz} + \frac{1}{yz^2} + \frac{1}{yz} + \frac{1}{z} & \frac{1}{xyz^2} + \frac{1}{xyz} + \frac{1}{xz} + \frac{y}{z} & \frac{1}{xyz} + \frac{1}{xy} + \frac{1}{z} + 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (\text{C2})$$

$$\bar{\mathbf{Z}}^A = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & yz + y & yz + z \\ xz + x & 0 & xz + z \\ xy + x & xy + y & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ xyz + x & xy + y & xyz + yz \\ \frac{x}{y} + x & xyz + xy + x + 1 & xyz + xz \\ \frac{x}{z} + x & \frac{xy}{z} + xy & xy + 1 \end{pmatrix}, \quad (\text{C3})$$

$$\bar{\mathbf{Z}}^B = \begin{pmatrix} 0 & \frac{1}{xz} + \frac{1}{x} & \frac{1}{xy} + \frac{1}{x} \\ \frac{1}{yz} + \frac{1}{y} & 0 & \frac{1}{xy} + \frac{1}{y} \\ \frac{1}{yz} + \frac{1}{z} & \frac{1}{xz} + \frac{1}{z} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ \frac{1}{yz} + 1 & \frac{1}{xz} + \frac{1}{z} & \frac{1}{x} + 1 \\ \frac{1}{y^2z} + \frac{1}{yz} & \frac{1}{xyz} + \frac{1}{yz} + \frac{1}{z} + 1 & \frac{1}{y} + 1 \\ \frac{1}{yz^2} + \frac{1}{yz} & \frac{1}{z^2} + \frac{1}{z} & \frac{1}{xyz} + \frac{1}{z} \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (\text{C4})$$

And, the $\mathbf{H}$ matrix that is used to construct the QCA from 3F invertible subalgebra is

$$\mathbf{H} = \begin{pmatrix} 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ y+1 & \frac{y}{x} + \frac{1}{x} + y & 0 & y & \frac{1}{y} + 1 & 1 & 0 & 0 \\ 1 & \frac{1}{x} + 1 & x & 0 & \frac{x}{y} + x + \frac{1}{y} & x+1 & 0 & 0 \\ 0 & 0 & \frac{1}{y} + 1 & 1 & 0 & \frac{1}{x} & y+1 & \frac{y}{x} + \frac{1}{x} + y \\ 0 & 0 & \frac{x}{y} + x + \frac{1}{y} & x+1 & \frac{1}{y} & 0 & 1 & \frac{1}{x} + 1 \end{pmatrix}. \quad (\text{C5})$$

2. The 5 + 1D “3-fermion” QCA

In five spatial dimensions, we begin by writing down the matrices for the coboundary operator and the relevant (higher) cup products. For convenience, we label the coordinates by $\{a, b, c, d, e\}$,

$$\delta_{c,\delta f} = \begin{pmatrix} c-1 & 1-b & 0 & 0 & a-1 & 0 & 0 & 0 & 0 & 0 \\ d-1 & 0 & 1-b & 0 & 0 & a-1 & 0 & 0 & 0 & 0 \\ e-1 & 0 & 0 & 1-b & 0 & 0 & a-1 & 0 & 0 & 0 \\ 0 & d-1 & 1-c & 0 & 0 & 0 & 0 & a-1 & 0 & 0 \\ 0 & e-1 & 0 & 1-c & 0 & 0 & 0 & 0 & a-1 & 0 \\ 0 & 0 & e-1 & 1-d & 0 & 0 & 0 & 0 & 0 & a-1 \\ 0 & 0 & 0 & 0 & d-1 & 1-c & 0 & b-1 & 0 & 0 \\ 0 & 0 & 0 & 0 & e-1 & 0 & 1-c & 0 & b-1 & 0 \\ 0 & 0 & 0 & 0 & 0 & e-1 & 1-d & 0 & 0 & b-1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & e-1 & 1-d & c-1 \end{pmatrix}, \quad (\text{C6})$$

$$\mathbf{M}_{f \cup c} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & abc \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -abd & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & abe & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & acd & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -ace & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & ade & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -bcd & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & bce & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -bde & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ cde & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad (\text{C7})$$

$$\mathbf{M}_{c \cup f} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & ab \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -ac & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & ad & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -ae & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & bc & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -bd & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & be & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & cd & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -ce & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ de & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad (\text{C8})$$

$$\mathbf{M}_{c \cup 1c} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \frac{1}{de} & 0 & 0 & \frac{a}{de} & \frac{ab}{de} \\ 0 & 0 & 0 & 0 & -\frac{1}{ce} & 0 & 0 & -\frac{a}{ce} & 0 & \frac{ab}{e} \\ 0 & 0 & 0 & \frac{1}{cd} & 0 & 0 & \frac{a}{cd} & 0 & 0 & ab \\ 0 & 0 & \frac{1}{be} & 0 & 0 & 0 & 0 & -\frac{a}{e} & -\frac{ac}{e} & 0 \\ 0 & -\frac{1}{bd} & 0 & 0 & 0 & 0 & \frac{a}{d} & 0 & -ac & 0 \\ \frac{1}{bc} & 0 & 0 & 0 & 0 & 0 & a & ad & 0 & 0 \\ 0 & 0 & \frac{1}{e} & 0 & \frac{b}{e} & \frac{bc}{e} & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{d} & 0 & -\frac{b}{d} & 0 & bc & 0 & 0 & 0 & 0 \\ \frac{1}{c} & 0 & 0 & -b & -bd & 0 & 0 & 0 & 0 & 0 \\ 1 & c & cd & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \quad (\text{C9})$$

The original qubits A and B are

$$\mathbf{z}_c^A = \begin{pmatrix} 0 \\ 0 \\ \mathbb{1}_{10 \times 10} \\ 0 \end{pmatrix}, \quad \mathbf{z}_c^B = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \mathbb{1}_{10 \times 10} \end{pmatrix}, \quad \mathbf{x}_c^A = \begin{pmatrix} \mathbb{1}_{10 \times 10} \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad \mathbf{x}_c^B = \begin{pmatrix} 0 \\ \mathbb{1}_{10 \times 10} \\ 0 \\ 0 \end{pmatrix}. \quad (\text{C10})$$

The 5 + 1D 3F QCA can then be set up as (we do not perform the tensor contractions for clarity)

$$\begin{aligned} \bar{\mathbf{z}}_c^A &= \mathbf{z}_c^A + (\mathbf{x}_{c'}^B \delta_{c', \delta f} + \mathbf{z}_{c'}^B \mathbf{M}_{c'' \cup 1c}^\dagger \delta_{c'', \delta f}) \mathbf{M}_{c \cup f}^\dagger, \\ \bar{\mathbf{z}}_c^B &= \mathbf{z}_c^B + (\mathbf{x}_{c'}^A \delta_{c', \delta f} + \mathbf{z}_{c'}^A \mathbf{M}_{c'' \cup 1c}^\dagger \delta_{c'', \delta f}) \mathbf{M}_{f \cup c}, \\ \bar{\mathbf{x}}_c^A &= \mathbf{x}_c^A + (\mathbf{x}_{c''}^B \delta_{c'', \delta f} + \mathbf{z}_{c''}^B \mathbf{M}_{c' \cup 1c}^\dagger \delta_{c', \delta f}) \mathbf{M}_{c' \cup f}^\dagger \mathbf{M}_{c' \cup 1c}, \\ \bar{\mathbf{x}}_c^B &= \mathbf{x}_c^B + (\mathbf{x}_{c''}^A \delta_{c'', \delta f} + \mathbf{z}_{c''}^A \mathbf{M}_{c' \cup 1c}^\dagger \delta_{c', \delta f}) \mathbf{M}_{f \cup c'} \mathbf{M}_{c' \cup 1c}. \end{aligned} \quad (\text{C11})$$

The proof that the QCA squares to the identity can be performed similarly to the 3 + 1D version.

[1] J. Haah, L. Fidkowski, and M. B. Hastings, Nontrivial quantum cellular automata in higher dimensions, *Commun. Math. Phys.* **398**, 469 (2023).

-
- [2] A. Kapustin, Symmetry protected topological phases, anomalies, and cobordisms: Beyond group cohomology, [arXiv:1403.1467](#).
- [3] L. Fidkowski, J. Haah, and M. B. Hastings, Exactly solvable model for a 4 + 1D beyond-cohomology symmetry-protected topological phase, *Phys. Rev. B* **101**, 155124 (2020).
- [4] Y.-A. Chen and P.-S. Hsin, Exactly solvable lattice Hamiltonians and gravitational anomalies, *SciPost Phys.* **14**, 089 (2023).
- [5] L. Fidkowski, J. Haah, and M. B. Hastings, A quantum cellular automaton for every symmetry protected topological phase, *Phys. Rev. B* **112**, 035123 (2025).
- [6] C. Jones, P. Naaijken, and D. Penneys, Holography for bulk-boundary local topological order, [arXiv:2506.19969](#).
- [7] R. Kobayashi, Y. Li, H. Xue, P.-S. Hsin, and Y.-A. Chen, Generalized statistics on lattices, *Phys. Rev. X* **16**, 011010 (2026).
- [8] W. Shirley, C. Zhang, W. Ji, and M. Levin, Anomaly-free symmetries with obstructions to gauging and onsite ability, [arXiv:2507.21267](#).
- [9] Y.-T. Tu, D. M. Long, and D. V. Else, Anomalies of global symmetries on the lattice, [arXiv:2507.21209](#).

- [10] S. Seifnashri and W. Shirley, Disentangling anomaly-free symmetries of quantum spin chains, [arXiv:2503.09717](#).
- [11] A. Kapustin, Higher symmetries and anomalies in quantum lattice systems, [arXiv:2505.04719](#).
- [12] A. Kapustin and L. Spodyneiko, Higher symmetries, anomalies, and crossed squares in lattice gauge theory, [arXiv:2507.16966](#).
- [13] A. Kapustin and N. Sopenko, Anomalous symmetries of quantum spin chains and a generalization of the Lieb-Schultz-Mattis theorem, *Commun. Math. Phys.* **406**, 238 (2025).
- [14] R. Ma, Y. Li, and M. Cheng, Quantum cellular automata on symmetric subalgebras, [arXiv:2411.19280](#).
- [15] K. Kawagoe and W. Shirley, Anomaly diagnosis via symmetry restriction in two-dimensional lattice systems, [arXiv:2507.07430](#).
- [16] T. A. Brun and L. Mlodinow, Quantum cellular automata and quantum field theory in two spatial dimensions, *Phys. Rev. A* **102**, 062222 (2020).
- [17] C. Zhang and M. Levin, Bulk-boundary correspondence for interacting Floquet systems in two dimensions, *Phys. Rev. X* **13**, 031038 (2023).
- [18] H. C. Po, L. Fidkowski, T. Morimoto, A. C. Potter, and A. Vishwanath, Chiral Floquet phases of many-body localized bosons, *Phys. Rev. X* **6**, 041070 (2016).
- [19] H. C. Po, L. Fidkowski, A. Vishwanath, and A. C. Potter, Radical chiral Floquet phases in a periodically driven Kitaev model and beyond, *Phys. Rev. B* **96**, 245116 (2017).
- [20] A. C. Potter and T. Morimoto, Dynamically enriched topological orders in driven two-dimensional systems, *Phys. Rev. B* **95**, 155126 (2017).
- [21] A. C. Potter, A. Vishwanath, and L. Fidkowski, Infinite family of three-dimensional Floquet topological paramagnets, *Phys. Rev. B* **97**, 245106 (2018).
- [22] C. Zhang and M. Levin, Classification of interacting Floquet phases with $U(1)$ symmetry in two dimensions, *Phys. Rev. B* **103**, 064302 (2021).
- [23] P. Glorioso, A. Gromov, and S. Ryu, Effective response theory for Floquet topological systems, *Phys. Rev. Res.* **3**, 013117 (2021).
- [24] J. I. Cirac, D. Perez-Garcia, N. Schuch, and F. Verstraete, Matrix product unitaries: Structure, symmetries, and topological invariants, *J. Stat. Mech.: Theory Exp.* **2017**, 083105 (2017).
- [25] M. B. Şahinoğlu, S. K. Shukla, F. Bi, and X. Chen, Matrix product representation of locality preserving unitaries, *Phys. Rev. B* **98**, 245122 (2018).
- [26] Z. Gong, C. Sünderhauf, N. Schuch, and J. I. Cirac, Classification of matrix-product unitaries with symmetries, *Phys. Rev. Lett.* **124**, 100402 (2020).
- [27] L. Piroli, A. Turzillo, S. K. Shukla, and J. I. Cirac, Fermionic quantum cellular automata and generalized matrix-product unitaries, *J. Stat. Mech.: Theory Exp.* **2021**, 013107 (2021).
- [28] L. Piroli and J. I. Cirac, Quantum cellular automata, tensor networks, and area laws, *Phys. Rev. Lett.* **125**, 190402 (2020).
- [29] Z. Gong, L. Piroli, and J. I. Cirac, Topological lower bound on quantum chaos by entanglement growth, *Phys. Rev. Lett.* **126**, 160601 (2021).
- [30] D. Ranard, M. Walter, and F. Witteveen, A converse to Lieb-Robinson bounds in one dimension using index theory, *Ann. Henri Poincaré* **23**, 3905 (2022).
- [31] Z. Gong, A. Nahum, and L. Piroli, Coarse-grained entanglement and operator growth in anomalous dynamics, *Phys. Rev. Lett.* **128**, 080602 (2022).
- [32] D. Gross, V. Nesme, H. Vogts, and R. F. Werner, Index theory of one dimensional quantum walks and cellular automata, *Commun. Math. Phys.* **310**, 419 (2012).
- [33] M. Freedman and M. B. Hastings, Classification of quantum cellular automata, *Commun. Math. Phys.* **376**, 1171 (2020).
- [34] J. Haah, Clifford quantum cellular automata: Trivial group in 2D and Witt group in 3D, *J. Math. Phys.* **62**, 092202 (2021).
- [35] W. Shirley, Y.-A. Chen, A. Dua, T. D. Ellison, N. Tantivasadakarn, and D. J. Williamson, Three-dimensional quantum cellular automata from chiral semion surface topological order and beyond, *PRX Quantum* **3**, 030326 (2022).
- [36] J. Haah, Topological phases of unitary dynamics: Classification in Clifford category, *Commun. Math. Phys.* **406**, 76 (2025).
- [37] B. Yang, Categorifying Clifford QCA, [arXiv:2504.14811](#).
- [38] S. Roberts and D. J. Williamson, 3-fermion topological quantum computation, *PRX Quantum* **5**, 010315 (2024).
- [39] H. Bombin, D. Litinski, N. Nickerson, F. Pastawski, and S. Roberts, Unifying flavors of fault tolerance with the ZX calculus, *Quantum* **8**, 1379 (2024).
- [40] H. Bombin, C. Dawson, T. Farrelly, Y. Liu, N. Nickerson, M. Pant, F. Pastawski, and S. Roberts, Fault-tolerant complexes, [arXiv:2308.07844](#).
- [41] D. T. Stephen, H. P. Nautrup, J. Bermejo-Vega, J. Eisert, and R. Raussendorf, Subsystem symmetries, quantum cellular automata, and computational phases of quantum matter, *Quantum* **3**, 142 (2019).
- [42] Y.-A. Chen and S. Tata, Higher cup products on hypercubic lattices: Application to lattice models of topological phases, *J. Math. Phys.* **64**, 091902 (2023).
- [43] J. Haah, Invertible subalgebras, *Commun. Math. Phys.* **403**, 661 (2023).
- [44] K. Walker and Z. Wang, $(3+1)$ -TQFTs and topological insulators, *Front. Phys.* **7**, 150 (2012).
- [45] Y.-A. Chen, T. D. Ellison, and N. Tantivasadakarn, Disentangling supercohomology symmetry-protected topological phases in three spatial dimensions, *Phys. Rev. Res.* **3**, 013056 (2021).
- [46] X. Chen, Z.-C. Gu, Z.-X. Liu, and X.-G. Wen, Symmetry-protected topological orders in interacting bosonic systems, *Science* **338**, 1604 (2012).
- [47] A. Kapustin and R. Thorngren, in *Algebra, Geometry, and Physics in the 21st Century*, edited by D. Auroux, L. Katzarkov, T. Pantev, Y. Soibelman, and Y. Tschinkel, Vol. 324 (Birkhäuser, Cham, 2017), pp. 177–202.
- [48] D.-M. Schlingemann, H. Vogts, and R. F. Werner, On the structure of Clifford quantum cellular automata, *J. Math. Phys.* **49**, 112104 (2008).
- [49] J. Gütschow, Entanglement generation of Clifford quantum cellular automata, *Appl. Phys. B* **98**, 623 (2010).
- [50] J. Haah, Commuting Pauli Hamiltonians as maps between free modules, *Commun. Math. Phys.* **324**, 351 (2013).

- [51] J. Haah, Algebraic methods for quantum codes on lattices, *Rev. Colomb. Mat.* **50**, 299 (2017).
- [52] N. E. Steenrod, Products of cocycles and extensions of mappings, *Ann. Math.* **48**, 290 (1947).
- [53] D. Gaiotto and A. Kapustin, Spin TQFTs and fermionic phases of matter, *Int. J. Mod. Phys. A* **31**, 1645044 (2016).
- [54] Y.-A. Chen, Exact bosonization in arbitrary dimensions, *Phys. Rev. Res.* **2**, 033527 (2020).
- [55] L. Tsui and X.-G. Wen, Lattice models that realize $\mathbb{Z}_n - 1$ symmetry-protected topological states for even n , *Phys. Rev. B* **101**, 035101 (2020).
- [56] P. Panteleev and G. Kalachev, Quantum LDPC codes with almost linear minimum distance, *IEEE Trans. Inf. Theory* **68**, 213 (2022).
- [57] Z. Liang, Y. Xu, J. T. Iosue, and Y.-A. Chen, Extracting topological orders of generalized Pauli stabilizer codes in two dimensions, *PRX Quantum* **5**, 030328 (2024).
- [58] C. W. von Keyserlingk, F. J. Burnell, and S. H. Simon, Three-dimensional topological lattice models with surface anyons, *Phys. Rev. B* **87**, 045107 (2013).
- [59] L. Wang and Z. Wang, In and around abelian anyon models, *J. Phys. A: Math. Theor.* **53**, 505203 (2020).
- [60] S. Eilenberg and S. MacLane, On the groups $H(\Pi, n)$, I, *Ann. Math.* **58**, 55 (1953).
- [61] S. Eilenberg and S. MacLane, On the groups $H(\Pi, n)$, II: Methods of computation, *Ann. Math.* **60**, 49 (1954).
- [62] A. Kapustin and R. Thorngren, Topological field theory on a lattice, discrete theta-angles and confinement, *Adv. Theor. Math. Phys.* **18**, 1233 (2014).
- [63] C. Delcamp and A. Tiwari, On 2-form gauge models of topological phases, *J. High Energy Phys.* **2019**, 64 (2019).
- [64] R. Dijkgraaf and E. Witten, Topological gauge theories and group cohomology, *Commun. Math. Phys.* **129**, 393 (1990).
- [65] A. Davydov, M. Müger, D. Nikshych, and V. Ostrik, The Witt group of non-degenerate braided fusion categories, *J. Reine Angew. Math.* **677**, 135 (2013).
- [66] B. Ruba and B. Yang, Witt groups and bulk-boundary correspondence for stabilizer states, [arXiv:2509.10418](https://arxiv.org/abs/2509.10418).
- [67] A. Davydov, D. Nikshych, and V. Ostrik, On the structure of the Witt group of braided fusion categories, *Sel. Math.* **19**, 237 (2013).
- [68] P. H. Bonderson, Non-abelian anyons and interferometry, Ph.D. thesis, California Institute of Technology, 2007.
- [69] J. Haah, L. Fidkowski, and M. B. Hastings, Nontrivial quantum cellular automata in higher dimensions, *Commun. Math. Phys.* **398**, 469 (2023).
- [70] X. Chen, Z.-C. Gu, Z.-X. Liu, and X.-G. Wen, Symmetry protected topological orders and the group cohomology of their symmetry group, *Phys. Rev. B* **87**, 155114 (2013).
- [71] Y.-A. Chen and A. Kapustin, Bosonization in three spatial dimensions and a 2-form gauge theory, *Phys. Rev. B* **100**, 245127 (2019).
- [72] A. Bauer, Low-overhead non-Clifford fault-tolerant circuits for all non-chiral abelian topological phases, *Quantum* **9**, 1673 (2025).
- [73] Z. Liang, B. Yang, J. T. Iosue, and Y.-A. Chen, Operator algebra and algorithmic construction of boundaries and defects in $(2 + 1)$ D topological Pauli stabilizer codes, [arXiv:2410.11942](https://arxiv.org/abs/2410.11942).
- [74] T. Schuster, N. Tantivasadakarn, A. Vishwanath, and N. Y. Yao, A holographic view of topological stabilizer codes, [arXiv:2312.04617](https://arxiv.org/abs/2312.04617).
- [75] L. Kong, X.-G. Wen, and H. Zheng, Boundary-bulk relation in topological orders, *Nucl. Phys. B* **922**, 62 (2017).
- [76] A. Kitaev and L. Kong, Models for gapped boundaries and domain walls, *Commun. Math. Phys.* **313**, 351 (2012).
- [77] T. Lan and X.-G. Wen, Topological quasiparticles and the holographic bulk-edge relation in $(2 + 1)$ -dimensional string-net models, *Phys. Rev. B* **90**, 115119 (2014).
- [78] Z. Wang, X. Ma, D. T. Stephen, M. Hermele, and X. Chen, Renormalization of Ising cage-net model and generalized foliation, *Phys. Rev. B* **108**, 035148 (2023).
- [79] X. Chen, A. Dua, M. Hermele, D. T. Stephen, N. Tantivasadakarn, R. Vanhove, and J.-Y. Zhao, Sequential quantum circuits as maps between gapped phases, *Phys. Rev. B* **109**, 075116 (2024).
- [80] J. Haah, Commuting Pauli Hamiltonians as maps between free modules, *Commun. Math. Phys.* **324**, 351 (2013).
- [81] A. R. Calderbank, E. M. Rains, P. W. Shor, and N. J. A. Sloane, Quantum error correction and orthogonal geometry, *Phys. Rev. Lett.* **78**, 405 (1997).
- [82] M. H. Freedman and Z. Wang, in *Prospects in Topology: Proceedings of a Conference in Honor of William Browder* (Princeton University, Princeton, New Jersey, 1995), p. 138.
- [83] A permutation matrix is a square binary matrix that has exactly one entry of 1 in each row and each column with all other entries 0.
- [84] E. K. Pedersen and C. A. Weibel, in *Algebraic Topology: Proceedings of an International Conference held in Arcata, California, July 27–August 2, 1986* (Springer, Berlin, Heidelberg, 1989), pp. 346–361.
- [85] E. K. Pedersen and C. A. Weibel, in *Algebraic and Geometric Topology: Proceedings of a Conference held at Rutgers University, New Brunswick, USA, July 6–13, 1983* (Springer, Berlin, Heidelberg, 2006), pp. 166–181.
- [86] E. K. Pedersen, *J. Algebra* **90**, 461 (1984).
- [87] B. Ruba and B. Yang, Homological invariants of Pauli stabilizer codes, *Commun. Math. Phys.* **405**, 126 (2024).
- [88] This algebraic invariant was first defined this way in Ref. [87] but appeared already in Ref. [50].
- [89] L. Fidkowski and M. B. Hastings, Pumping chirality in three dimensions, *Phys. Rev. B* **109**, 235142 (2024).
- [90] C. Jones, K. Schatz, and D. J. Williamson, Quantum cellular automata and categorical dualities of spin chains, [arXiv:2410.08884](https://arxiv.org/abs/2410.08884).
- [91] D. Eliezer and G. Semenoff, Anyonization of lattice Chern-Simons theory, *Ann. Phys.* **217**, 66 (1992).
- [92] D. Eliezer and G. W. Semenoff, Intersection forms and the geometry of lattice Chern-Simons theory, *Phys. Lett. B* **286**, 118 (1992).
- [93] K. Sun, K. Kumar, and E. Fradkin, Discretized abelian Chern-Simons gauge theory on arbitrary graphs, *Phys. Rev. B* **92**, 115148 (2015).
- [94] J. C. M. de la Fuente, T. D. Ellison, M. Cheng, and D. J. Williamson, Topological stabilizer models on continuous variables, [arXiv:2411.04993](https://arxiv.org/abs/2411.04993).
- [95] Z. Liang, K. Liu, H. Song, and Y.-A. Chen, Generalized toric codes on twisted tori for quantum error correction, *PRX Quantum* **6**, 020357 (2025).
- [96] Z. Liang, J. N. Eberhardt, and Y.-A. Chen, Planar quantum low-density parity-check codes with open boundaries, [arXiv:2504.08887](https://arxiv.org/abs/2504.08887).
- [97] Note that our sign convention differs from Ref. [42], which has a typo in the overall factor.