

Invariants for (2+1)D bosonic crystalline topological insulators for all 17 wallpaper groups

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We study bosonic symmetry-protected topological (SPT) phases in (2+1) dimensions with symmetry $G = G_{\text{space}} \times K$, where G_{space} is a general wallpaper group and $K = \text{U}(1), \mathbb{Z}_N, \text{SO}(3)$ is an internal symmetry. In each case we propose a set of many-body invariants that can detect all the different phases predicted from real space constructions and group cohomology classifications. They are obtained by applying partial rotations and reflections to a given ground state, combined with suitable operations in K . The reflection symmetry invariants that we introduce include ‘double partial reflections’, ‘weak partial reflections’ and their ‘relative’ or ‘twisted’ versions which also depend on K . We verify our proposal through exact calculations on ground states constructed using real space constructions. We demonstrate our method in detail for the groups p4m and p4g, and in the case of p4m also derive a topological effective action involving gauge fields for orientation-reversing symmetries. Our results provide a concrete method to fully characterize (2+1)D crystalline topological invariants in bosonic SPT ground states.

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I. INTRODUCTION

The characterization and classification of topological phases with crystalline symmetries has seen remarkable progress over the last several years (for a partial list of references, see Refs. [1–39]). It is now well understood how to both classify and characterize free fermion phases with crystalline symmetries in (2+1) dimensions based on their topological band structure [10–19]. Beyond free fermions, one can consider symmetry-protected topological (SPT) states, which can be adiabatically connected to a trivial product state through a finite-depth circuit that breaks symmetry, but not through one that preserves symmetry [40–45]. We can also consider invertible topological states, which have the property that any invertible state $|\Psi\rangle$ has an inverse, denoted $|\Psi^{-1}\rangle$, such that $|\Psi\rangle \otimes |\Psi^{-1}\rangle$ can be adiabatically connected to a trivial product state [46, 47]¹. In these cases, where the system can have arbitrarily strong interactions, our understanding is less complete than for free fermions. It is now

quite well understood how to *classify* crystalline topological states in these cases using a combination of physical constructions [26–28] and mathematical techniques based on topological quantum field theory (TQFT) and higher category theory [29–31, 38, 46–50]. However, we still do not fully understand how to extract a complete set of crystalline topological invariants given a microscopic lattice model or ground state wave function.

Previous work on this question has proceeded in two broad directions. The first is to measure the invariants using the response of the system to inserting symmetry defects, specifically fluxes of internal symmetries and lattice defects such as disclinations and dislocations. This approach has been explored in detail in systems with orientation-preserving crystalline symmetries [3, 32–36, 51–53]. While defects have also been studied theoretically in the orientation-reversing case [54, 55], they are not as well understood.

A second approach is to apply *partial* symmetry operations, that is, to measure the expectation value of the ground state with respect to a symmetry operator which is restricted to act only on a subregion [37, 39, 56, 57]. Ref. [37, 39] showed that partial rotations can completely characterize invertible fermionic states with G_{space} wallpaper group and $\text{U}(1)$ charge conservation symmetries, where G_{space} is orientation-preserving. Indeed, if we additionally know the charge per unit cell (filling), the Chern number and the chiral central charge c_- of the system, this characterization was shown to be complete. While partial reflections have analogously been shown to characterize certain topological invariants associated with reflection symmetries [56], there is currently no systematic procedure to obtain a full set of invariants for each wallpaper group G_{space} using partial symmetry operations.

The goal of this paper is to obtain a complete characterization of crystalline topological invariants based on partial symmetry operations for bosonic SPT states with symmetry $G = G_{\text{space}} \times K$ where G_{space} is a *general* wallpaper group in $2d$ (d denotes the space dimension), and $K = \text{U}(1), \mathbb{Z}_N$ or $\text{SO}(3)$ is an internal unitary symmetry group. These symmetries determine a rich classification of SPT phases; detecting them requires new types of invariants, which we develop in this paper. Although we focus on bosonic SPT states in this work, we expect that our results should generalize to invertible fermionic states, with some modifications. Note that all the invariants we propose are expected to be well-defined for SPT states with arbitrarily strong interactions.

We use the classification of crystalline SPTs based on the ‘crystalline equivalence principle’ (CEP), which states that we should treat spatial symmetries as on-site symmetries, with the only caveat that space-time orientation-reversing symmetries become anti-unitary symmetries [29]. The classification for on-site symmetries is obtained using the group cohomology framework [40]. The CEP has been extensively checked for bosonic SPTs by matching its predictions to independent real-

¹ Note that SPT states are always invertible, but in (2+1) dimensions the converse is true if and only if the invertible state has vanishing chiral central charge, that is, it does not have gapless chiral edge states when defined on open boundaries.

Group cohomology classification of crystalline SPTs: $\mathcal{H}^3(G_{\text{space}} \times K, \text{U}(1)^{\text{or}})$

#	G_{space}	$\mathcal{H}^3(G_{\text{space}}, \text{U}(1)^{\text{or}})$	$K = \text{U}(1)$	$K = \mathbb{Z}_N$	$K = \text{SO}(3)$
1	p1	$\mathbb{Z}_1$	$\mathbb{Z} \times \mathbb{Z}$	$\mathbb{Z}_N \times \mathbb{Z}_N$	$\mathbb{Z}$
2	p2	$\mathbb{Z}_2^4$	$\mathbb{Z} \times \mathbb{Z}_2^3 \times \mathbb{Z}$	$\mathbb{Z}_N \times \mathbb{Z}_{(2,N)}^3 \times \mathbb{Z}_N$	$\mathbb{Z}_2^3 \times \mathbb{Z}$
3	pm	$\mathbb{Z}_2^2$	$\mathbb{Z} \times \mathbb{Z}_2$	$\mathbb{Z}_N \times \mathbb{Z}_{(2,N)}^3 \times \mathbb{Z}_{(N,2)}$	$\mathbb{Z}_2^2$
4	pg	$\mathbb{Z}_1$	$\mathbb{Z}$	$\mathbb{Z}_N \times \mathbb{Z}_{(N,2)}$	$\mathbb{Z}_2$
5	cm	$\mathbb{Z}_2$	$\mathbb{Z}$	$\mathbb{Z}_N \times \mathbb{Z}_{(2,N)} \times \mathbb{Z}_{(N,2)}$	$\mathbb{Z}_2$
6	pmm	$\mathbb{Z}_2^8$	$\mathbb{Z} \times \mathbb{Z}_2^3$	$\mathbb{Z}_N \times \mathbb{Z}_{(2,N)}^7 \times \mathbb{Z}_{(N,2)}$	$\mathbb{Z}_2^4$
7	pmg	$\mathbb{Z}_2^3$	$\mathbb{Z} \times \mathbb{Z}_2^2$	$\mathbb{Z}_N \times \mathbb{Z}_{(2,N)}^3 \times \mathbb{Z}_{(N,2)}$	$\mathbb{Z}_2^3$
8	pgg	$\mathbb{Z}_2^2$	$\mathbb{Z} \times \mathbb{Z}_2$	$\mathbb{Z}_N \times \mathbb{Z}_{(2,N)} \times \mathbb{Z}_{(N,2)}$	$\mathbb{Z}_2^2$
9	cmm	$\mathbb{Z}_2^5$	$\mathbb{Z} \times \mathbb{Z}_2^2$	$\mathbb{Z}_N \times \mathbb{Z}_{(2,N)}^4 \times \mathbb{Z}_{(N,2)}$	$\mathbb{Z}_2^3$
10	p4	$\mathbb{Z}_4^2 \times \mathbb{Z}_2$	$\mathbb{Z} \times \mathbb{Z}_4 \times \mathbb{Z}_2 \times \mathbb{Z}$	$\mathbb{Z}_N \times \mathbb{Z}_{(2,N)} \times \mathbb{Z}_{(4,N)} \times \mathbb{Z}_N$	$\mathbb{Z}_2^2 \times \mathbb{Z}$
11	p4m	$\mathbb{Z}_2^6$	$\mathbb{Z} \times \mathbb{Z}_4 \times \mathbb{Z}_2$	$\mathbb{Z}_N \times \mathbb{Z}_{(2,N)}^4 \times \mathbb{Z}_{(4,N)} \times \mathbb{Z}_{(N,2)}$	$\mathbb{Z}_2^3$
12	p4g	$\mathbb{Z}_4 \times \mathbb{Z}_2^2$	$\mathbb{Z} \times \mathbb{Z}_4$	$\mathbb{Z}_N \times \mathbb{Z}_{(2,N)} \times \mathbb{Z}_{(4,N)} \times \mathbb{Z}_{(N,2)}$	$\mathbb{Z}_2^2$
13	p3	$\mathbb{Z}_3^3$	$\mathbb{Z} \times \mathbb{Z}_3^2 \times \mathbb{Z}$	$\mathbb{Z}_N \times \mathbb{Z}_{(3,N)}^2 \times \mathbb{Z}_N$	$\mathbb{Z}$
14	p3m1	$\mathbb{Z}_2$	$\mathbb{Z} \times \mathbb{Z}_3^2$	$\mathbb{Z}_N \times \mathbb{Z}_{(3,N)}^2 \times \mathbb{Z}_{(2,N)} \times \mathbb{Z}_{(N,2)}$	$\mathbb{Z}_2$
15	p31m	$\mathbb{Z}_6$	$\mathbb{Z} \times \mathbb{Z}_3$	$\mathbb{Z}_N \times \mathbb{Z}_{(3,N)} \times \mathbb{Z}_{(2,N)} \times \mathbb{Z}_{(N,2)}$	$\mathbb{Z}_2$
16	p6	$\mathbb{Z}_6^2$	$\mathbb{Z} \times \mathbb{Z}_6 \times \mathbb{Z}$	$\mathbb{Z}_N \times \mathbb{Z}_{(6,N)} \times \mathbb{Z}_N$	$\mathbb{Z}_2 \times \mathbb{Z}$
17	p6m	$\mathbb{Z}_2^4$	$\mathbb{Z} \times \mathbb{Z}_6$	$\mathbb{Z}_N \times \mathbb{Z}_{(6,N)} \times \mathbb{Z}_{(2,N)}^2 \times \mathbb{Z}_{(N,2)}$	$\mathbb{Z}_2^2$

TABLE I. The group cohomology classification of (2+1)D bosonic SPTs with only G_{space} wallpaper group symmetry is given in the third column. To obtain the classification for $G = G_{\text{space}} \times K$, with $K = \text{U}(1), \mathbb{Z}_N, \text{SO}(3)$, we take the direct product between the third column and the desired K column. The groups in black on the third, fourth and fifth column are protected by G_{space} and corresponding K , while the red invariants are protected solely by K (we have accounted for a possible reduction by the presence of reflections). We denote the greatest common divisor between N and k by (N, k) .

space classifications [26, 28].

For each pair (G_{space}, K) , the known classification is comprised of three groups of topological invariants: 1) pure crystalline invariants; 2) pure internal invariants; and 3) mixed invariants. This is summarized in Table I. The ‘pure’ invariants are those invariants that are protected only by G_{space} (crystalline) or K (internal). The mixed invariants are protected by both K and G_{space} . Note that the allowed values of pure internal invariants may be constrained in the presence of reflection symmetry; for example, the Hall conductance is forced to be zero if there are reflections.

Assuming that the pure K invariants are known, our main result is that partial symmetries are able to detect the pure crystalline and mixed invariants, except for the $\text{U}(1)$ filling and $\mathbb{Z}_N$ filling (charge per unit cell). We confirm this by constructing exactly solvable ground states for each type of invariant and analytically demonstrating that the quantities defined in Table II take the expected nontrivial values. In particular, several of our schemes that detect invariants for reflection symmetries have not appeared in previous work.

We obtain our main result as follows. First, we define a general set of partial symmetry expectation values that are summarized in Table II; these quantities are defined with respect to a specific point or line within a real-space unit cell, and can be applied to different G_{space} . For convenience we refer to them as Type-A, Type-B, and so on; this notation will be further explained below in Sec. II B. Using them, we propose a complete set of crystalline invariants² for each G_{space} in Tables IV (pure crystalline) and V, VI (mixed between G_{space} and K). We do so by repeatedly evaluating selected invariants from Table II at different locations in the real-space unit cell. Our procedure reproduces the mathematical classification of SPT states based on group cohomology, which is summarized in Table I. Note that our methods are equally applicable

² In this draft, we use the term ‘invariant’ to refer to two different objects: (1) the quantized coefficients appearing in a topological field theory; and (2) the quantized numbers extracted from expectation values of partial symmetry operations, both of which can be related to each other.

Real-space invariants for crystalline SPTs

Invariant	Symbol	Type	Point group	K	Definition	Quantization
Partial rotation	Θ_o	A1	C_{M_o}	-	Eq. (2)	$\mathbb{Z}_{M_o} (*)$
Partial double reflection	$\Sigma_{o,l}$	A2	D_2	-	Eq. (10)	$\mathbb{Z}_2$
Partial weak reflection	Λ_l	A3	$\mathbb{Z} \times D_1$	-	Eq. (13)	$\mathbb{Z}_2$
Discrete shift	$\mathcal{S}_o^{U(1)}$	B1	C_{M_o}	U(1)	Eq. (6)	$\mathbb{Z}_{M_o}$
	$\mathcal{S}_o^{\mathbb{Z}_N}$	C1	C_{M_o}	$\mathbb{Z}_N$	Eq. (7)	$\mathbb{Z}_{(M_o, N)}$
	$\mathcal{S}_o^{SO(3)}$	D1	C_{M_o}	SO(3)	Eq. (8)	$\mathbb{Z}_{(M_o, 2)}$
Twisted relative partial reflection	$\Upsilon_l^{\mathbb{Z}_N}$	C4	D_1	$\mathbb{Z}_N$	Eq. (15)	$\mathbb{Z}_{(2, N)}$
	$\Upsilon_l^{SO(3)}$	D4	D_1	SO(3)	Eq. (16)	$\mathbb{Z}_2$
Relative partial double reflection	$\tilde{\Sigma}_{o,l}^{\mathbb{Z}_N}$	C2	D_2	$\mathbb{Z}_N$	Eq. (20)	$\mathbb{Z}_{(N, 2)}$
	$\tilde{\Sigma}_{o,l}^{SO(3)}$	D2	D_2	SO(3)	Eq. (21)	$\mathbb{Z}_2$
Relative partial weak reflection	$\tilde{\Lambda}_l^{U(1)}$	B3	D_1	U(1)	Eq. (22)	$\mathbb{Z}_2$
	$\tilde{\Lambda}_l^{\mathbb{Z}_N}$	C3	D_1	$\mathbb{Z}_N$	Eq. (22)	$\mathbb{Z}_{(N, 2)}$

TABLE II. Summary of SPT invariant types with symmetry $G_{\text{space}} \times K$, for G_{space} a point group and $K = \text{U}(1), \mathbb{Z}_N, \text{SO}(3)$. Type-A invariants are protected solely by G_{space} while the other invariants also require K . Here o denotes a rotation center of order M_o , l denotes a reflection axis. C_{M_o} is an M -fold rotation around o , D_1 is reflection about line l , D_2 is the dihedral group generated by a two-fold rotation around o and a reflection along l , and $\mathbb{Z}$ is the group of translations parallel to line l . (a, b) denotes the greatest common divisor of a and b , and $\mathbb{Z}_1 = \{e\}$ is the trivial group. These invariants together with the filling form a complete set. However, they are not all independent: there are non-trivial relations between different types of invariants, and also between the same type of invariant for different positions ‘ o ’ or lines ‘ l ’. (*) The partial rotation invariant Θ_o satisfies $2\Theta_o = 0 \pmod{M_o}$ if there exists a reflection line passing through o . To the best of our knowledge, only partial rotation and discrete shift have appeared before in the literature.

to symmorphic and non-symmorphic lattices, and can therefore handle glide symmetries as well.

The formulas cited in Table II make the assumption that all pure K SPT invariants are trivial. In general, some of them need to be modified when the K invariant is non-trivial, but to simplify our formulas we do not consider this most general case. The given formulas correctly predict the difference between the crystalline invariants of two states which share the same K invariant. We will briefly discuss the case with nontrivial K invariants in Sec. VIA. Furthermore, note that type 1 and 2 invariants require only the density matrix for a single ground state on a open disk. This adds to a growing body of work devoted to extracting topological invariants from a single ground state wave function [37, 56, 58–64]. We elaborate on this in Sec. VIB.

To further illustrate our approach, we consider in detail the wallpaper groups p4m (# 11) and p4g (# 12). p4m is the symmetry group of the square lattice that is a symmorphic group that is an extension of p4 (# 10). The p4g group is also an extension of p4 but is nonsymmorphic. We show how the invariants in Table II reproduce the group cohomology classification. In the p4m case, we also construct a topological effective action involving gauge fields for the wallpaper group symmetry, and relate the field theory coefficients to the above partial symme-

try invariants. Our method of deriving the action can be generalized to all G_{space} . Although we do not explore this here, these effective actions may be useful to motivate alternative characterizations based on symmetry defects.

A. Prior work

1. Real space constructions/invariants:

A number of previous works have developed real-space constructions of bosonic SPT ground states with the symmetries of interest in this paper. These include [26, 27] (for $G = G_{\text{space}}$), and [28] (for $G = G_{\text{space}} \times K$).

In particular, Ref. [27] studied SPT phases protected by $G = G_{\text{space}}$. They argued that 2d bosonic crystalline SPTs can be built from 0-dimensional blocks, which can be thought of as the bosonic version of ‘atomic insulators (AI)’. Additionally, [27] argued that their classification can be understood in terms of ‘point group SPT invariants’ and related ‘weak invariants’, which are defined in terms of the atomic limit. The main result of [27] relevant to us is summarized in their Table III.

Ref. [28] extended the above construction to $G =$

List of notations

Symbol	Meaning
G_{space}	2d wallpaper group
G_{pt}	Point group
K	Internal symmetry ($K = \text{U}(1), \mathbb{Z}_N, \text{SO}(3)$)
o	Origin of rotations in G_{pt}
M_{o}	Order of rotations about o
$\alpha, \beta, \gamma, \delta$	Maximal Wyckoff positions
l	Reflection axis
$\lambda, \mu, \nu, \kappa$	Unit cell reflection axes
$\mathbf{0}$	Identity group element
$\mathbf{r}_l$	Reflection about line l
$\mathbf{h}_{\text{o}}$	Elementary rotation about o
$\mathbf{x}, \mathbf{y}$	Elementary translation
$\mathbf{S}$	$\mathbb{Z}_N$ internal symmetry generator
$\mathbf{X}, \mathbf{Z}$	Generators of $\mathbb{Z}_2 \times \mathbb{Z}_2 \subset \text{SO}(3)$
$\tilde{C}_{M_{\text{o}}}$	M_{o} -fold rotation operator about o
R_l	Reflection operator along line l
$T_{\vec{a}}$	Operator for translations by $\vec{a}$
$U_{\mathbf{g}}$	Operator for internal symmetry $\mathbf{g} \in K$
$\tilde{C}_{k,\text{o}}(\mathbf{g})$	$2\pi/k$ rotation about o dressed with $U_{\mathbf{g}}$, see Eq. (3)
D	Region in which partial symmetry acts
σ	Reflection gauge field (here and below, see Footnote 7)
ω	Rotation gauge field
$\vec{R}$	Translation gauge field

TABLE III. List of notations used in this paper.

$G_{\text{space}} \times K$ SPT phases with arbitrary K ³. They argued that their method reproduces the classification using the crystalline equivalence principle (CEP) of Ref. [29] in the sense that both methods give the same abelian group of distinct SPT phases. In particular, Table I in their Supplemental Material gives the classification for various K (G_0 in their notation) in terms of d -dimensional blocks (column labeled by $E_{d,\infty}^d$).

Note that while these past works focused on computing various cohomology classifications of SPT phases, our

goal is rather to explicitly give the ground state expectation values which detect these SPT phases.

2. Fermions

Fermionic analogs of the partial rotation invariants Θ_{o} in Table II have been studied numerically in Refs. [20, 37, 56]; these works have established that partial rotations are indeed a viable method of extracting rotational SPT invariants in microscopic models. Analogous numerical studies have not yet been carried out for the other invariants relevant to reflection symmetry, particularly those that depend on both K and G_{space} .

B. Organization of paper

The rest of the paper is organized as follows. In Sec. II we give the basic definition and properties of each invariant in Table II. In Secs. III, IV we consider the groups p4m and p4g respectively, and illustrate how to use these invariants to obtain a full characterization. In Sec. V we consider the 17 wallpaper groups in general and discuss how the invariants we define fully capture their group cohomology classification. Then in Sec. VI we conclude and discuss future directions. Some background details and several technical derivations have been placed in the appendices. A summary of the notation we use is given in Table III. A brief summary of crystallographic notation is given in App. G.

II. MAIN RESULTS

A. Conceptual origin of invariants

Before getting into the specifics of each invariant, let us explain some general ideas that are useful in deriving them. These ideas also help us verify their robustness as topological invariants to some extent.

First, the classification of SPT phases using group cohomology, combined with the crystalline equivalence principle, suggests a connection between SPT phases and topological quantum field theories (TQFTs). TQFT invariants for internal symmetries can be obtained by computing partition functions on manifolds with specific background gauge field configurations, but for an arbitrary crystalline symmetry it is not clear what manifold we should consider even after applying the CEP. This was only known previously for the partial rotation invariants in (2+1)D that we will introduce below [56, 65]. In this paper we give a TQFT interpretation for most of the remaining invariants involving reflection symmetry. Altogether, we now have an understanding for almost every invariant we propose based on TQFT partition functions, except for the ‘weak’ invariants in Table II that depend

³ They actually consider a more general setting where G is not necessarily a direct product of the wallpaper group and an internal symmetry group.

Independent set of pure crystalline invariants for each wallpaper group

#	G_{space}	Type-A1: Θ_o		Type-A2: $\Sigma_{o,l}$		Type-A3: Λ_l	
		Class.	Invariants	Class.	Invariants	Class.	Invariants
1	p1	$\mathbb{Z}_1$	-	$\mathbb{Z}_1$	-	$\mathbb{Z}_1$	-
2	p2	$\mathbb{Z}_2^4$	$\Theta_\alpha, \Theta_\beta, \Theta_\gamma, \Theta_\delta$	$\mathbb{Z}_1$	-	$\mathbb{Z}_1$	-
3	pm	$\mathbb{Z}_1$	-	$\mathbb{Z}_1$	-	$\mathbb{Z}_2^2$	$\Sigma_\lambda, \Sigma_\mu$
4	pg	$\mathbb{Z}_1$	-	$\mathbb{Z}_1$	-	$\mathbb{Z}_1$	-
5	cm	$\mathbb{Z}_1$	-	$\mathbb{Z}_1$	-	$\mathbb{Z}_2$	Σ_λ
6	pmm	$\mathbb{Z}_2^4$	$\Theta_\alpha, \Theta_\beta, \Theta_\gamma, \Theta_\delta$	$\mathbb{Z}_2^4$	$\Sigma_{\alpha,\lambda}, \Sigma_{\delta,\lambda}, \Sigma_{\beta,\mu}, \Sigma_{\gamma,\mu}$	$\mathbb{Z}_1$	-
7	pmg	$\mathbb{Z}_2^2$	$\Theta_\alpha, \Theta_\beta$	$\mathbb{Z}_1$	-	$\mathbb{Z}_2$	Σ_λ
8	pgg	$\mathbb{Z}_2^2$	$\Theta_\alpha, \Theta_\beta$	$\mathbb{Z}_1$	-	$\mathbb{Z}_1$	-
9	cmm	$\mathbb{Z}_2^3$	$\Theta_\alpha, \Theta_\beta, \Theta_\gamma$	$\mathbb{Z}_2^2$	$\Sigma_{\alpha,\lambda}, \Sigma_{\alpha,\mu}$	$\mathbb{Z}_1$	-
10	p4	$\mathbb{Z}_4^2 \times \mathbb{Z}_2$	$\Theta_\alpha, \Theta_\beta, \Theta_\gamma$	$\mathbb{Z}_1$	-	$\mathbb{Z}_1$	-
11	p4m	$\mathbb{Z}_2^3$	$\frac{\Theta_\alpha}{2}, \frac{\Theta_\beta}{2}, \Theta_\gamma$	$\mathbb{Z}_2^3$	$\Sigma_{\alpha,\lambda}, \Sigma_{\gamma,\lambda}, \Sigma_{\beta,\mu}$	$\mathbb{Z}_1$	-
12	p4g	$\mathbb{Z}_4 \times \mathbb{Z}_2$	$\Theta_\alpha, \Theta_\beta$	$\mathbb{Z}_2$	Σ_β	$\mathbb{Z}_1$	-
13	p3	$\mathbb{Z}_3^3$	$\Theta_\alpha, \Theta_\beta, \Theta_\gamma$	$\mathbb{Z}_1$	-	$\mathbb{Z}_1$	-
14	p3m1	$\mathbb{Z}_1$	-	$\mathbb{Z}_1$	-	$\mathbb{Z}_2$	Σ_λ
15	p31m	$\mathbb{Z}_3$	Θ_β	$\mathbb{Z}_1$	-	$\mathbb{Z}_2$	Σ_λ
16	p6	$\mathbb{Z}_6 \times \mathbb{Z}_3 \times \mathbb{Z}_2$	$\Theta_\alpha, \Theta_\beta, \Theta_\gamma$	$\mathbb{Z}_1$	-	$\mathbb{Z}_1$	-
17	p6m	$\mathbb{Z}_2^2$	$\frac{\Theta_\alpha}{3}, \Theta_\gamma$	$\mathbb{Z}_2^2$	$\Sigma_{\alpha,\mu}, \Sigma_{\gamma,\mu}$	$\mathbb{Z}_1$	-

TABLE IV. An independent set of bosonic SPT invariants associated only to wallpaper group symmetry. The product of the terms in each row equals the pure G_{space} classification listed in Table I. We follow the unit cell conventions in App. G 2; For concreteness, when ‘o’ or ‘l’ are degenerate, the invariant is evaluated using ‘o₁’ or ‘l₁’, respectively. The invariants constitute a generating set for the respective abelian groups, listed under the ‘Class.’ column, associated with type-A1, A2, and A3. The notation $\frac{1}{(M_o/2)}\Theta_o$ in the rows 11 and 17 arises because, in these cases, $\Theta_o = (M_o/2)k \bmod M_o$, indicating that k serves as the generator of a $\mathbb{Z}_2$ subgroup in the classification.

on system size and are therefore different from the other cases.

Another perspective comes from studying the entanglement spectrum of an SPT state, certain features of which are expected to be universal within the SPT phase. The low-lying ground state entanglement spectrum in many examples coincides with that of a (1+1)D conformal field theory (CFT). We start by assuming that the density matrix ρ_D of the SPT state within a suitably chosen region D equals ρ_{CFT} , the density matrix of the CFT living on the boundary of D . Then the real space invariant can be calculated in terms of correlation functions in the CFT. This CFT calculation has been done for partial rotation invariants (Type A1, B1, C1, D1) in Ref. [37] (similar calculations were done in Ref. [56]). For bosonic SPT states, the expected answer from TQFT is contained in the leading term of the CFT correlation function, while the remaining terms become negligible for sufficiently large $|\partial D|$. However this calculation has not been done for the remaining invariants.

A third, independent motivation comes from performing explicit evaluations in simple lattice models. In this paper we construct multiple exactly solvable ground states in spin models motivated by known real-space constructions. For these states, the SPT invariants have a clear interpretation in terms of symmetry charges or one-dimensional SPT states localized at specific points or lines in the real-space unit cell. We verify that each partial symmetry invariant does take nontrivial values in at least one of the states we construct, is related to the real-space invariants in a simple way, and obeys the quantization conditions predicted by group cohomology.

The new invariants we propose in this paper were motivated by a combination of the above ideas. The fact that we can provide intuition for these invariants both from TQFT and microscopic real-space calculations gives us confidence that our partial symmetry invariants are indeed robust signatures of a topological phase.

Independent set of mixed invariants between each wallpaper group and $U(1)$ or $\mathbb{Z}_N$

#	G_{space}	$K = U(1)$		$K = \mathbb{Z}_N$			
		B1: $\mathcal{S}_o^{U(1)}$	o	C1: $\mathcal{S}_o^{\mathbb{Z}_N}$	o	C4: $\Upsilon_l^{\mathbb{Z}_N}$	l
1	p1	$\mathbb{Z}_1$	-	$\mathbb{Z}_1$	-	$\mathbb{Z}_1$	-
2	p2	$\mathbb{Z}_2^3$	α, β, γ	$\mathbb{Z}_{(2,N)}^3$	α, β, γ	$\mathbb{Z}_1$	-
4	pg	$\mathbb{Z}_1$	-	$\mathbb{Z}_1$	-	$\mathbb{Z}_1$	-
5	cm	$\mathbb{Z}_1$	-	$\mathbb{Z}_1$	-	$\mathbb{Z}_{(2,N)}$	λ
6	pmm	$\mathbb{Z}_2^3$	α, β, γ	$\mathbb{Z}_{(2,N)}^3$	α, β, γ	$\mathbb{Z}_{(2,N)}^4$	$\lambda, \mu, \nu, \kappa$
7	pmg	$\mathbb{Z}_2^2$	α, β	$\mathbb{Z}_{(2,N)}^2$	α, β	$\mathbb{Z}_{(2,N)}$	λ
8	pgg	$\mathbb{Z}_2$	α	$\mathbb{Z}_{(2,N)}$	α	$\mathbb{Z}_1$	-
9	cmm	$\mathbb{Z}_2^2$	α, γ	$\mathbb{Z}_{(2,N)}^2$	α, γ	$\mathbb{Z}_{(2,N)}^2$	λ, μ
10	p4	$\mathbb{Z}_4 \times \mathbb{Z}_2$	α, γ	$\mathbb{Z}_{(4,N)} \times \mathbb{Z}_{(2,N)}$	α, γ	$\mathbb{Z}_1$	-
11	p4m	$\mathbb{Z}_4 \times \mathbb{Z}_2$	α, γ	$\mathbb{Z}_{(4,N)} \times \mathbb{Z}_{(2,N)}$	α, γ	$\mathbb{Z}_{(2,N)}^3$	λ, μ, ν
12	p4g	$\mathbb{Z}_4$	α	$\mathbb{Z}_{(4,N)}$	α	$\mathbb{Z}_{(2,N)}$	λ
13	p3	$\mathbb{Z}_3^2$	α, β	$\mathbb{Z}_{(3,N)}^2$	α, β	$\mathbb{Z}_1$	-
14	p3m1	$\mathbb{Z}_3^2$	α, β	$\mathbb{Z}_{(3,N)}^2$	α, β	$\mathbb{Z}_{(2,N)}$	λ
15	p31m	$\mathbb{Z}_3$	α	$\mathbb{Z}_{(3,N)}$	α	$\mathbb{Z}_{(2,N)}$	λ
16	p6	$\mathbb{Z}_6$	α	$\mathbb{Z}_{(6,N)}$	α	$\mathbb{Z}_1$	-
17	p6m	$\mathbb{Z}_6$	α	$\mathbb{Z}_{(6,N)}$	α	$\mathbb{Z}_{(2,N)}^2$	λ, μ

#	G_{space}	$K = U(1)$		$K = \mathbb{Z}_N$			
		B3: $\tilde{\Lambda}_l^{U(1)}$	l	C3: $\tilde{\Lambda}_l^{\mathbb{Z}_N}$	l	C4: $\Upsilon_l^{\mathbb{Z}_N}$	l
3	pm	$\mathbb{Z}_2$	λ	$\mathbb{Z}_{(2,N)}$	λ	$\mathbb{Z}_{(2,N)}^2$	λ, μ

TABLE V. For each type of invariant, we list the rotation center ('o') or reflection line ('l') about which the invariant needs to be evaluated. The unit cell notation is from App. G 2. For $K = U(1), \mathbb{Z}_N$, there is an additional filling invariant valued in $\mathbb{Z}, \mathbb{Z}_N$ respectively; the type-B1 and C1 invariants around the rotation centers not included in the table can be used to determine the filling invariant modulo some integer (see Sec. II C). The product of terms in each row, together with the filling, equals the mixed classification listed in Table I. The group pm is an exception that is handled with type B3 and C3 invariants instead of type B1 and C1, respectively (Sec. II B 7).

B. Definition of invariants

Consider a bosonic SPT state $|\Psi\rangle$ on a torus or an open disk. We organize the different invariants into the following classes:

1. Type-A refers to pure crystalline invariants. There are three sub-classes, which we denote by A1, A2, A3.
2. The remaining invariants are all mixed invariants between G_{space} and K . We refer to these invariants as Type-B, C or D for $K = U(1), \mathbb{Z}_N, \text{SO}(3)$ respectively.
3. Invariants of type A1, B1, C1 and D1 can all be detected by performing suitable partial rotations

on a given ground state.

4. The remaining invariants can all be detected by performing suitable partial reflections on a ground state, possibly on tori with twisted boundary conditions or different system sizes.
5. 'Weak' invariants are partly protected by a translation symmetry, and must be computed by taking ratios of expectation values for different system sizes.
6. The invariants which depend on both K and G_{space} come in two types:
 - (a) The 'relative' invariants are defined as the difference between two quantities extracted from

**Independent set of mixed invariants
between each wallpaper group and SO(3)**

#	G_{space}	D1	o	D4	l
1	p1	$\mathbb{Z}_1$	-	$\mathbb{Z}_1$	-
2	p2	$\mathbb{Z}_2^3$	α, β, γ	$\mathbb{Z}_1$	-
3	pm	$\mathbb{Z}_1$	-	$\mathbb{Z}_2^2$	λ, μ
4	pg	$\mathbb{Z}_1$	-	$\mathbb{Z}_2$	λ
5	cm	$\mathbb{Z}_1$	-	$\mathbb{Z}_2$	λ
6	pmm	$\mathbb{Z}_1$	-	$\mathbb{Z}_2^4$	$\lambda, \mu, \nu, \kappa$
7	pmg	$\mathbb{Z}_2^2$	α, β	$\mathbb{Z}_2$	λ
8	pgg	$\mathbb{Z}_2^2$	α, β	$\mathbb{Z}_1$	-
9	cmm	$\mathbb{Z}_2^2$	α, γ	$\mathbb{Z}_2$	λ
10	p4	$\mathbb{Z}_2^2$	α, β	$\mathbb{Z}_1$	-
11	p4m	$\mathbb{Z}_1$	-	$\mathbb{Z}_2^3$	λ, μ, ν
12	p4g	$\mathbb{Z}_2$	α	$\mathbb{Z}_2$	λ
13	p3	$\mathbb{Z}_1$	-	$\mathbb{Z}_1$	-
14	p3m1	$\mathbb{Z}_1$	-	$\mathbb{Z}_2$	λ
15	p31m	$\mathbb{Z}_1$	-	$\mathbb{Z}_2$	λ
16	p6	$\mathbb{Z}_2$	α	$\mathbb{Z}_1$	-
17	p6m	$\mathbb{Z}_1$	-	$\mathbb{Z}_2^2$	λ, μ

TABLE VI. An independent set of mixed bosonic SPT invariants between an internal SO(3) symmetry and G_{space} . These are of type D1 ($\mathcal{S}_o^{\text{SO}(3)}$) and type D4 ($\Upsilon_l^{\text{SO}(3)}$). The unit cell notation is from App. G 2. The product of invariants on each row is equal to $\mathcal{H}^1(G_{\text{space}}, \mathbb{Z}_2)$, or equivalently the mixed-SO(3) classification in Table I.

partial symmetry expectation values defined using the same space group symmetry but different internal symmetries; they can be computed on an open patch with arbitrary boundary conditions.

- (b) The ‘twisted’ invariants need to be defined on a torus with specific boundary conditions along one direction.

Below we give some general intuition behind deriving the different invariants, before giving their explicit definition and quantization rules. In Sec. II C, we explain with examples how suitable combinations of these invariants can be used to characterize a given SPT state. Note that there are several relations between the different invariants, some of which we will point out as we go along. In Sec. V, we give a more mathematical discussion of the precise group cohomology classes measured by each invariant. The analysis there allows us to conclude that the above invariants fully distinguish all bosonic SPT invariants predicted by group cohomology, except for filling

invariants which must be obtained separately.

1. Type A1: Partial rotation

The results in this section appeared previously in Ref. [37] in the context of invertible fermionic states. First we define $\tilde{C}_{M_o}|_D$ to be the restriction of the rotation operator $\tilde{C}_{M_o}$ to some symmetric open region D centered at o .

As in the case of invertible fermionic states, the expectation value of the partial rotation behaves as

$$\langle \Psi | \tilde{C}_{M_o}|_D | \Psi \rangle = e^{-\gamma|\partial D| + i\frac{2\pi}{M_o}\Theta_o(1 + O(e^{-\epsilon|\partial D|}))}, \quad (1)$$

γ sets the amplitude of the expectation value, while ϵ is some positive number that captures subleading contributions. As $\tilde{C}_{M_o}$ is a symmetry, $|\Psi\rangle$ and $\tilde{C}_{M_o}|_D|\Psi\rangle$ will look locally the same away from the boundary of D , except for a possible phase. The exponential decay in ∂D comes from correlations between points close to ∂D .

We summarize the expression in Eq. 1 as

$$\arg \langle \Psi | \tilde{C}_{M_o}|_D | \Psi \rangle \rightarrow \frac{2\pi}{M_o}\Theta_o \pmod{2\pi}. \quad (2)$$

$\arg z$ stands for the argument of the complex number z and the symbol ‘ $\rightarrow$ ’ means that the quantization is obtained for a large enough region D . While we expect that a similar scaling of the expectation values in Eq. 1 applies to all the invariants we present in this paper, we do not have such explicit formulas for them. Therefore we use the $\rightarrow$ symbol in later equations to indicate that suitable choices of large regions are required to get the correct results numerically.

We argue that Θ_o is a many-body topological invariant for bosonic states and is quantized modulo M_o . This can be shown by assuming that the ground state’s density matrix ρ_D within region D is equivalent to ρ_{CFT} , the density matrix of the conformal field theory (CFT) on the boundary ∂D . This relationship was first proposed in the context of fractional quantum Hall states [66] and has since been applied to various gapped topological states, as discussed for example in [67]. In this case, the expectation value on the left-hand side can be simplified using CFT techniques to an expression involving only the G -crossed modular data associated to defects of the rotational symmetry, which depends on the invariant Θ_o . This calculation was carried out for invertible fermionic states in Ref. [37], and can be adapted to bosonic SPT states. The result is that in bosonic SPT phases, Θ_o is defined mod M_o , is a many-body topological invariant (because it depends only on TQFT data), and it fully characterizes the SPT invariant for pure M_o -fold point group rotations about o . Furthermore, Θ_o is quantized to integer values when $c_- = 0$.

The quantization of the rotation invariants is different between bosonic SPTs and invertible fermionic states.

In the fermionic case, the partial rotation expectation value can depend on the size of D . Consider a four-fold rotation center. Enlarging D adds new states in orbits of 4, which are permuted under the rotation. In the fermionic case, the new state inside D differs by a factor $|\psi\rangle = c_1^\dagger c_2^\dagger c_3^\dagger c_4^\dagger |0\rangle$, where $|0\rangle$ is the vacuum. Due to the anticommutation relations of fermionic operators, $\langle\psi|\tilde{C}_{4,o}|\psi\rangle = -1$, if $\tilde{C}_{4,o}^4 = +1$. Therefore, the topological invariant associated to partial rotations with $\tilde{C}_{4,o}^4 = +1$ is defined mod 2 and not mod 4 [37]. On the other hand, the fact that bosonic operators commute implies that the analogous partial rotation expectation value in the bosonic SPT case is independent of the size of D , and remains quantized mod 4.

In the presence of a reflection R_l along a line l that goes through o ($l \ni o$), the SPT state must be an eigenstate of the reflection. Therefore $\langle\Psi|O|\Psi\rangle = \langle\Psi|R_l^\dagger O R_l|\Psi\rangle$ for any operator O . In the case $O = \tilde{C}_{M_o}|_D$, we obtain the constraint $\langle\Psi|\tilde{C}_{M_o}|_D|\Psi\rangle = \left[\langle\Psi|\tilde{C}_{M_o}|_D|\Psi\rangle\right]^\dagger$, thus $2\Theta_o/M_o = 0 \pmod{1}$. As reflections also forces a vanishing chiral central charge ($c_- = 0$), Θ_o is constrained to take certain values: 1) If M_o is even, $\Theta_o \in \{0, M_o/2\}$; 2) If M_o is odd, $\Theta_o = 0$. We remark that any reflection lines which do not intersect o will not affect the quantization of Θ_o . This is relevant to understanding certain $\mathbb{Z}_4$ rotation invariants that appear in the classification of SPT phases with $G_{\text{space}} = p4g$.

Eq. (2) along with the quantization conditions on Θ_o can be analytically verified in different exactly solvable models. First, we consider fixed-point wavefunctions for general bosonic SPT states with G_{space} symmetry, which were previously constructed in Refs. [26, 27]. It is straightforward to apply partial rotation operations to these wavefunctions and analytically verify Eq. (2). We can also consider exactly solvable models for bosonic SPTs based on stacking Affleck-Kennedy-Lieb-Tasaki model (AKLT) chains; these are not in a fixed point limit but are nonetheless analytically trackable. We compute Θ_o for these models in App. D 1 b.

2. Type B1, C1, D1: Discrete shift

Next we define a set of mixed invariants between the rotation point group at o and the internal symmetry K . When $K = \text{U}(1)$, this invariant is called the ‘discrete shift’, and has been studied in several recent works [33–36].

For each K , we define a ‘dressed’ rotation operator $\tilde{C}_{k,o}(\mathbf{g})$ which corresponds to a $2\pi/k$ rotation about o composed with an element $\mathbf{g} \in K$, such that $\mathbf{g}^k$ is the identity in K :

$$\tilde{C}_{k,o}(\mathbf{g}) := \tilde{C}_{\frac{M_o}{k}}^{\frac{M_o}{k}} \times U_{\mathbf{g}}. \quad (3)$$

These operators are of order k , and are used to define

$\Theta_{k,o}(\mathbf{g})$ as

$$\frac{k}{2\pi} \arg \langle\psi|\tilde{C}_{k,o}(\mathbf{g})|_D|\psi\rangle \rightarrow \Theta_{k,o}(\mathbf{g}) \pmod{k}. \quad (4)$$

Similar CFT arguments to those of Ref. [37] show that $\Theta_{k,o}(\mathbf{g})$ measures a many-body topological invariant defined modulo k . When $c_- = 0$, $\Theta_{k,o}(\mathbf{g})$ is integer valued and gets contributions from the pure internal invariant ($\mathbb{Z}_k$ Hall conductance $\sigma_{\mathbf{g}}$), the pure crystalline invariant (Θ_o), and the mixed invariant ($\mathcal{S}_{k,o}(\mathbf{g})$). We can thus extract $\mathcal{S}_{k,o}(\mathbf{g})$ if we know $\sigma_{\mathbf{g}}$. In this work, we will assume that $\sigma_{\mathbf{g}} = 0$ and thus (from the CFT calculation in [37]):

$$\Theta_{k,o}(\mathbf{g}) = \Theta_o + \mathcal{S}_{k,o}(\mathbf{g}) \pmod{k}. \quad (5)$$

Note that the expressions we obtain can be used to detect difference in crystalline invariants (either mixed or pure) between two SPTs with the same $\sigma_{\mathbf{g}}$. The case with non-trivial $\sigma_{\mathbf{g}}$ is discussed further in Sec. VI.

In a real space picture, $\mathcal{S}_{k,o}(\mathbf{g})$ measures the $\mathbf{g}$ charge localized at o . However, even if $\mathbf{g}$ is an element of a larger Abelian group, the charge is defined at most modulo M_o because one can always move charge away from o in an M_o -fold symmetric way. Furthermore, whenever there is an internal symmetry element, $\mathbf{k}$, such that $\mathbf{k}^{-1}\mathbf{g}\mathbf{k} = \mathbf{g}^{-1}$, we expect that $\mathcal{S}_{k,o}(\mathbf{g}) = -\mathcal{S}_{k,o}(\mathbf{g}) \pmod{k}$ from the same argument used for the Class A1 invariants.

We now identify a set of invariants that are complete for each $K \in \{\text{U}(1), \mathbb{Z}_N, \text{SO}(3)\}$. When $K = \text{U}(1)$, we take $k = M_o$ and $U_{\mathbf{g}} = e^{\frac{2\pi i}{M_o} \hat{N}}$ where $\hat{N}$ is the boson number operator, and $\Theta_o^{\text{U}(1)} := \Theta_{M_o,o}(\mathbf{g})$ for this $\mathbf{g}$. Following Eq. 5, we can extract the mixed invariant $\mathcal{S}_o^{\text{U}(1)}$ as

$$\mathcal{S}_o^{\text{U}(1)} := \Theta_o^{\text{U}(1)} - \Theta_o \pmod{M_o}. \quad (6)$$

Here Θ_o is the pure rotation SPT invariant discussed above, while $\mathcal{S}_o^{\text{U}(1)}$ is the mixed SPT invariant. Note that spatial reflections do not constrain the value of $\mathcal{S}_o^{\text{U}(1)}$.

When $K = \mathbb{Z}_N$, we take $k = (M_o, N)$ and $\mathbf{g} = \mathbf{S}^{N/(N,k)}$ where $\mathbf{S}$ is the generator of $\mathbb{Z}_N$, and $\Theta_o^{\mathbb{Z}_N} := \Theta_{k,o}(\mathbf{g})$ for this $k, \mathbf{g}$. Following Eq. 5, we can extract the mixed invariant $\mathcal{S}_o^{\mathbb{Z}_N}$ as

$$\mathcal{S}_o^{\mathbb{Z}_N} := \Theta_o^{\mathbb{Z}_N} - \Theta_o \pmod{(M_o, N)}. \quad (7)$$

When $K = \text{SO}(3)$, we can take $k = M_o$ and $\mathbf{g}$ to be a $2\pi/M_o$ spin rotation about any axis. We define $\Theta_o^{\text{SO}(3)} := \Theta_{M_o,o}(\mathbf{g})$. Applying the above CFT arguments to the $\mathbb{Z}_{M_o}$ subgroup of $\text{SO}(3)$, we can define the mixed invariant

$$\mathcal{S}_o^{\text{SO}(3)} := \frac{(M_o, 2)}{M_o} \left(\Theta_o^{\text{SO}(3)} - \Theta_o \right) \pmod{(M_o, 2)}. \quad (8)$$

Note that $\mathcal{S}_o^K$ fixes the K charge at disclinations centered at o . In particular, when the disclination angle is Ω ,

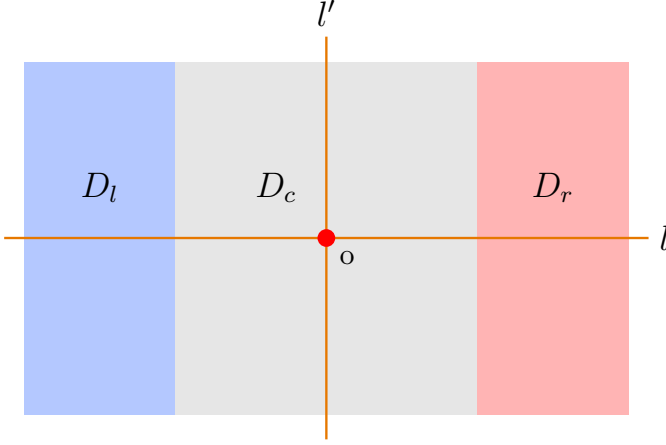


FIG. 1. Definition of the decomposition of the disk D into three regions D_l , D_c and D_r used in the definition of $\Sigma_{o,l}$.

this invariant contributes an excess K charge at a disclination given by

$$Q = \frac{\Omega}{2\pi} \times \begin{cases} \mathcal{S}_o^{\text{U}(1)} \mod 1 & , K = \text{U}(1); \\ \mathcal{S}_o^{\mathbb{Z}_N} \mod \frac{(M_o, N)}{M_o} & , K = \mathbb{Z}_N; \\ \frac{M_o}{(M_o, 2)} \mathcal{S}_o^{\text{SO}(3)} \mod 1 & , K = \text{SO}(3). \end{cases} \quad (9)$$

Furthermore, differences $\mathcal{S}_o^K - \mathcal{S}_{o'}^K$ are related to a polarization of K charge; this gives an alternative many-body definition of polarization in 2d systems with rotational symmetry. See Ref. [36] for a more complete discussion of this point.

Finally note that the filling is partially determined by partial rotation invariants. Class A1 invariants determine the $\text{U}(1)$ -filling and $\mathbb{Z}_N$ -filling modulo M and (M, N) , respectively (c.f. Sec. III C 1).

3. Type A2: Partial double reflection

Next we discuss a different class of pure crystalline invariants that explicitly depends on reflection symmetries. Suppose there is a high symmetry point o with at least a $D_2 \cong \mathbb{Z}_2 \times \mathbb{Z}_2$ site symmetry group generated by two reflections $\mathbf{r}_l, \mathbf{r}_{l'}$ about perpendicular lines l, l' passing through o . In this case, we can define an invariant $\Sigma_{o,l}$, which is protected by the pair of reflections⁴.

We choose a D_2 invariant region D that we decompose into three contiguous regions D_l, D_c and D_r as shown in Fig. 1. We choose the decomposition such that: 1) D_c is symmetric under $\mathbf{r}_l$ and $\mathbf{r}_{l'}$; 2) D_l and D_r are symmetric under $\mathbf{r}_l$; and 3) D_l and D_r are mapped to each other by

$\mathbf{r}_{l'}$. We define $\Sigma_{o,l}$ by

$$\frac{2}{2\pi} \arg \langle \Psi | R_l |_{D_c} R_{l'} |_{D_l \cup D_r} | \Psi \rangle \rightarrow \Sigma_{o,l} \mod 2. \quad (10)$$

We refer to this expectation value as ‘partial double reflection’.

In Appendix B, we show that the above expectation value simulates the partition function of the underlying TQFT on a space-time manifold $\mathcal{M}^3 \cong \mathbb{RP}_{\mathbf{r}_l}^2 \times S_{\mathbf{r}_l \mathbf{r}_{l'}}^1$:

$$(-1)^{\Sigma_{o,l}} = \mathcal{Z}(\mathbb{RP}_{\mathbf{r}_l}^2 \times S_{\mathbf{r}_l \mathbf{r}_{l'}}^1). \quad (11)$$

Here $\mathbb{RP}_{\mathbf{r}_l}^2$ (resp. $S_{\mathbf{r}_l \mathbf{r}_{l'}}^1$) is the manifold $\mathbb{RP}^2$ (resp. S^1) with $\mathbf{r}_l$ ($\mathbf{r}_l \mathbf{r}_{l'}$) holonomy along the non-trivial 1-cycle (where $\mathbf{r}_l \mathbf{r}_{l'}$ is treated as an internal symmetry).

It turns out that the partition function $\mathcal{Z}(\mathbb{RP}_{\mathbf{r}_l}^2 \times S_{\mathbf{r}_l \mathbf{r}_{l'}}^1)$, together with the partition function $\mathcal{Z}(\mathbb{RP}_{\mathbf{r}_l \mathbf{r}_{l'}}^3)$ (which is related to Θ_o) are enough to detect all the SPTs protected by $D_2 = \mathbb{Z}_2^{\mathbf{r}_l} \times \mathbb{Z}_2^{\mathbf{r}_l \mathbf{r}_{l'}}$.⁵

We verified that the partial double reflection indeed detects the topological invariant for an explicit non-trivial example. In App. D 1 a, we constructed a state by placing singlets on the bonds of the square lattice, referred to as ‘singlet covering’ in the following. This state can also be constructed by starting with AKLT states on every axis on the square lattice and removing the projector to the spin $S = 1$ sector on every lattice site. In App. D 1 c we evaluated the partial double reflection and found a non-trivial value as expected from the fact that the AKLT state belongs to a non-trivial SPT protected by reflection symmetry [68, 69].

To put the above invariant in context, recall that there is a unique non-trivial SPT in $(1+1)D$ protected by reflection symmetry. This SPT is detected by evaluating a partial reflection, which simulates the partition function on $\mathbb{RP}^2$ with $\mathbf{r}$ flux along the non-trivial 1-cycle ($\mathcal{Z}(\mathbb{RP}_{\mathbf{r}}^2)$) [69, 70]. According to the crystalline equivalence principle, SPTs protected by reflection are in one-to-one correspondence with SPTs protected by time-reversal symmetry. Therefore, there is a unique non-trivial reflection SPT in $(1+1)D$ but no non-trivial SPT in $(2+1)D$ [40] with a single reflection. An alternative perspective to understand the lack of non-trivial reflection SPTs in $(n+1)D$, is to use the folding trick [71], which roughly says that we can understand reflection SPTs protected in $(n+1)D$ by restricting to the $(n-1)d$ reflection hyperplane and treating the reflection as an on-site $\mathbb{Z}_2$ symmetry. Therefore, a non-trivial $(2+1)D$ reflection SPT corresponds to placing a $(1+1)D$ SPT protected by $\mathbb{Z}_2$ on the reflection axis. However, it is also known that there is no non-trivial $\mathbb{Z}_2$ SPT in $(1+1)D$ [40].

⁴ Note that a origin o and a line l uniquely fix the second reflection axis l' , which is why we do not include l' in the label of the invariant.

⁵ The superscript in $\mathbb{Z}_2^{\mathbf{r}_l}$ denotes that the $\mathbb{Z}_2$ generator is a reflection $\mathbf{r}_l$.

The Type A1 and A2 invariants are not all independent. For example, since $\mathbf{r}_l \mathbf{r}_{l'}$ is a C_2 rotation around o , the quantity $\Sigma_{o,l} + \Sigma_{o,l'}$ should depend on Θ_o . Indeed, when $M_o = 2$, we can show the relation

$$\Sigma_{o,l} + \Sigma_{o,l'} = \Theta_o \pmod{2} \quad (12)$$

for states that admit an atomic limit (See App. E1). In Table IV, we have presented one independent set of invariants, with the convention that we first list all possible Θ_o , followed by the remaining independent choices of $\Sigma_{o,l}$.

4. Type A3: Weak partial reflection

When the unit cell contains reflection lines but no C_2 -symmetric points lying on them (wallpaper groups pm ,

pg , cm , $p31m$, and $p3m1$), the type A2 invariant cannot be used. In this case, we introduce an alternative ‘Type A3’ invariant Λ_l , protected by the combination of D_1 reflection symmetry about the line l , generated by the operator R_l , and $\mathbb{Z}$ translation symmetry along l . Because translation symmetry is essential for its definition, we refer to this as a *weak partial reflection*. This invariant differs from A1 and A2 in that it requires evaluating the ground state on systems of different sizes.

Consider the ground state on an $L_1 \times L_2$ torus, with L_1 and L_2 much larger than the correlation length. Here L_1 is the length along the direction of l . Denote the ground state by $|\Psi(L_1, L_2)\rangle$. Let D be a region that is invariant under $\mathbf{r}_l$ and fully contains l . We define the invariant as

$$\frac{1}{\pi} \arg \frac{\langle \Psi(L_1 + 1, L_2) | R_l | \Psi(L_1 + 1, L_2) \rangle}{\langle \Psi(L_1, L_2) | R_l | \Psi(L_1, L_2) \rangle} \rightarrow \Lambda_l \pmod{2}. \quad (13)$$

This equation becomes exact in the $L_1, L_2 \rightarrow \infty$ limit. Λ_l is related to $\Sigma_{o,l}$, when they can both be defined (see App. E1 for the precise relation).

In a fixed-point limit where the degrees of freedom are all localized at specific points in the unit cell, this invariant measures the reflection eigenvalue of these degrees of freedom per unit length along the line l .

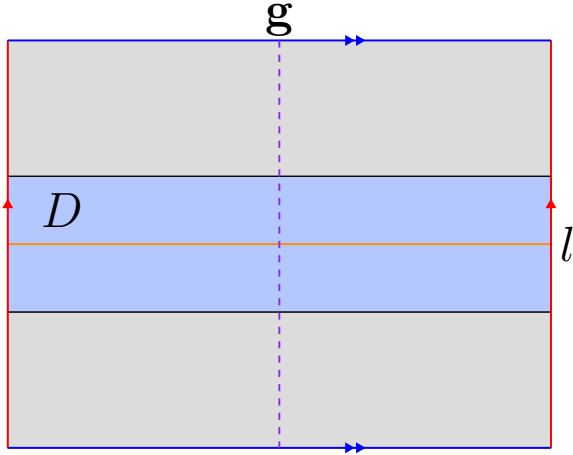


FIG. 2. Setup to evaluate $\Upsilon_l(\mathbf{g}; \mathbf{j})$. The red and blue lines denote the identification of sides of the rectangular space into a torus. D is the region in light blue. The dashed purple line denotes boundary conditions twisted by the group element $\mathbf{g}$. The reflection line l is shown in orange.

5. Type C4, D4: Twisted relative partial reflection

Given a reflection $\mathbf{r}_l$ and pair of group elements $\mathbf{j}, \mathbf{g} \in K$ such that $\mathbf{j}^2 = \mathbf{0}$ and $\mathbf{g}\mathbf{j} = \mathbf{j}\mathbf{g}$, we can define new invariants $\Upsilon_l(\mathbf{g}; \mathbf{j})$.

Let $|\Psi_{\mathbf{g}}\rangle$ be the ground state on a torus with twisted boundary conditions by $\mathbf{g}$ around a loop that intercepts the reflection line l once (see Fig. 2). Let D be a large region containing l that is $\mathbf{r}_l$ invariant. $\Upsilon_l(\mathbf{g}; \mathbf{j})$ is defined as

$$\frac{1}{\pi} \arg \frac{\langle \Psi_{\mathbf{g}} | (R_l U_{\mathbf{j}}) | \Psi_{\mathbf{g}} \rangle}{\langle \Psi_{\mathbf{g}} | (R_l) | \Psi_{\mathbf{g}} \rangle} \rightarrow \Upsilon_l(\mathbf{g}; \mathbf{j}) \pmod{2}. \quad (14)$$

We first argue that $\langle \Psi_{\mathbf{g}} | R_l | \Psi_{\mathbf{g}} \rangle$ simulates the partition function on $S^1 \times \mathbb{RP}^2$ with $\mathbf{g}$ holonomy along S^1 . The spatial manifold where $|\Psi_{\mathbf{g}}\rangle$ lives is $S_x^1 \times S_y^1$, where $S_{x/y}^1$ represents the circle along the horizontal/vertical direction. The twisted boundary conditions are understood as $\mathbf{g}$ flux along S_x^1 . For a fixed vertical cut of the spatial region, the above corresponds to the evaluation of partial reflection for a (1+1)D SPT state. This effectively "simulates" the manifold $\mathbb{RP}^2$ [56] for each point in S_x^1 , thus simulating $S^1 \times \mathbb{RP}^2$ in total. We define $\Upsilon_l(\mathbf{g}; \mathbf{j})$ using a ratio of expectation values in order to get rid of spurious bulk contributions that can depend on the size of the torus.

When $K = \mathbb{Z}_N$, we define the type C4 invariant as

$$\Upsilon_l^{\mathbb{Z}_N} := \Upsilon_l(\mathbf{S}; \mathbf{0}), \quad (15)$$

where $\mathbf{S}$ is a generator of $\mathbb{Z}_N$.

When $K = \text{SO}(3)$, we define the type D4 invariant as

$$\Upsilon_l^{\text{SO}(3)} := \Upsilon_l(\mathbf{Z}; \mathbf{X}) - \Upsilon_l(\mathbf{Z}; \mathbf{0}) \quad (16)$$

where $\mathbf{Z}$ and $\mathbf{X}$ are the elements in $\text{SO}(3)$ corresponding to π -rotations around the z and x axes, respectively.

Note that we don't define a type B4 invariant with $K = \text{U}(1)$ because the group cohomology calculation tells us that this invariant should be trivial. Furthermore, the type C4 invariant for a $\mathbb{Z}_N$ is if $\mathbb{Z}_N$ is a subgroup of a $\mathbb{Z}_{2N}$ symmetry.

In Appendix D1d we construct a state by stacking AKLT chains, and explicitly verify that the type-C4 and D4 invariants for this case take the expected non-trivial values.

6. Type C2,D2: Relative partial double reflection

The above type C4 and D4 invariants require the use of multiple ground states on a torus with twisted boundary conditions along different cycles. It may be more desirable to have an alternative scheme using a single ground state wave function on a disk, as was the case for all the partial rotation invariants. We now present such a scheme by modifying the partial double reflection operators appearing in the type A2 case. Because the type C4 and D4 invariants appearing in Tables V, VI form a complete set, the invariants presented in this section can be expressed in terms of them. We expect that, when they exist, type C2 and D2 invariants give the same information as type C4 and D4 invariants, respectively, but we have not checked this.

Pick regions D_l , D_c and D_r as in Fig. 1, as well as group elements $\mathbf{j}, \mathbf{k} \in K$ such that $\mathbf{j}^2 = \mathbf{0}$ and $\mathbf{k}\mathbf{j} = \mathbf{j}\mathbf{k}$. We define the operator

$$\mathcal{R}_{o,l}(\mathbf{k}, \mathbf{j}) = (R_l) |_{D_l \cup D_r} (R_l U_{\mathbf{j}}) |_{D_c} (U_{\mathbf{k}}) |_{D_l} \left(U_{\mathbf{k}}^\dagger \right) |_{D_r}, \quad (17)$$

and the invariant $\Sigma_{o,l}(\mathbf{k}, \mathbf{j})$ as

$$\frac{1}{\pi} \arg \langle \Psi | \mathcal{R}_{o,l}(\mathbf{k}, \mathbf{j}) | \Psi \rangle \rightarrow \Sigma_{o,l}(\mathbf{k}, \mathbf{j}) \mod 2. \quad (18)$$

The expectation value of $\mathcal{R}_{o,l}(\mathbf{k}, \mathbf{j})$ simulates the partition function on the same manifold as Type A2 but with different holonomies. In App. B3 we argue that

$$(-1)^{\Sigma_{o,l}(\mathbf{k}, \mathbf{j})} = \mathcal{Z}(\mathbb{RP}_{\mathbf{r}|\mathbf{j}}^2 \times S_{\mathbf{j}\mathbf{k}\mathbf{h}_o}^1). \quad (19)$$

As in the case of rotations, we define a quantity that measures the mixed SPT invariant by appropriately subtracting pure invariants.

When $K = \mathbb{Z}_N$, we define the type C2 invariant as

$$\tilde{\Sigma}_{o,l}^{\mathbb{Z}_N} := \Sigma_{o,l}(\mathbf{S}, \mathbf{0}) - \Sigma_{o,l}(\mathbf{0}, \mathbf{0}) \quad (20)$$

where $\mathbf{S}$ is a generator of $\mathbb{Z}_N$.

When $K = \text{SO}(3)$, we define the type D2 invariant as

$$\tilde{\Sigma}_{o,l}^{\text{SO}(3)} := \Sigma_{o,l}(\mathbf{Z}, \mathbf{X}) - \Sigma_{o,l}(\mathbf{0}, \mathbf{X}) \quad (21)$$

where $\mathbf{Z}$ and $\mathbf{X}$ are the elements in $\text{SO}(3)$ corresponding to π -rotations around the z and x axes, respectively.

In App. D1c, we evaluate the invariants for the singlet covering state and explicitly verify that the type-C2 and D2 invariants for this case take the desired non-trivial values.

7. Type B3, C3: Relative partial weak reflection

For certain wallpaper groups, there exist $\mathbb{Z}_2$ invariants corresponding to the charge mod 2 per unit length along a reflection axis for $K = \text{U}(1), \mathbb{Z}_N$. Except for the wallpaper group pm , these invariants can be detected using the previously defined constructions.⁶

To address the above exception, we propose to use a relative version of type-A3 invariants to detect these states. In other words, let $\Lambda_l(\mathbf{j})$ be Λ_l evaluated with $R_l \rightarrow R_l U_{\mathbf{j}}$. We define the relative weak partial reflection (type B3 and C3) as

$$\tilde{\Lambda}_l^K := \Lambda_l(\pi) - \Lambda_l \mod 2; \quad (22)$$

where π is the order two element in $K = \text{U}(1), \mathbb{Z}_N$.

C. Overall classification

A central result of this work is that all the SPT invariants which depend on G_{space} can be obtained by evaluating the invariants in Table II at suitable locations in the real-space unit cell of G_{space} . The invariants which depend only on G_{space} are given in Table IV, while those that depend on both G_{space} and K are given in Table V, VI.

For a given G_{space} , each row of the table gives one independent set of invariants. This set need not be unique, as mentioned at different points in the previous section.

1. How to read the tables: an example

For a concrete example of how to read the tables, consider the group pmm (# 6). The unit cell for this group is shown in Fig. 3. There are four high symmetry points denoted $\mathbf{o} = \alpha, \beta, \gamma, \delta$; these are order two rotation centers. Each point also lies on two mutually perpendicular

⁶ One might expect that the same issue would appear for the wallpaper groups pg and cm , which also lack rotational symmetries. We find that there are no mixed invariants at all with $K = \text{U}(1)$, and the sole mixed $K = \mathbb{Z}_N$ invariant for the group cm can be detected by type C4 invariants.

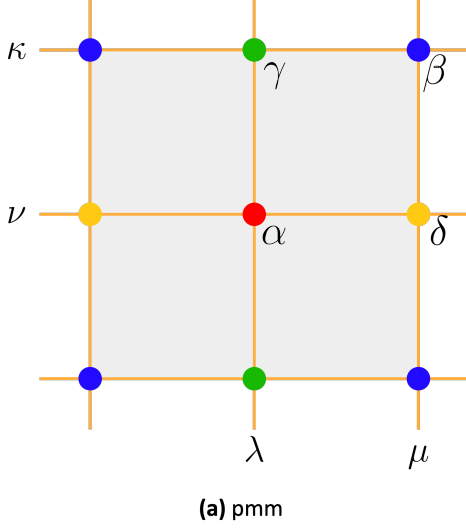


FIG. 3. Unit cell for space group pmm.

reflection axes, which we denote by $l = \lambda, \mu, \nu, \kappa$. Now the classification of pure crystalline invariants is given by $\mathcal{H}^4(\text{pmm}, \mathbb{Z}^{\text{or}}) \cong \mathbb{Z}_2^8$. As listed in Table IV, one independent set is given by Θ_o for each o (that is, four type-A1 invariants), along with four invariants of type A2. Note that an alternative but equivalent set is given by the 8 different invariants of type A2 (all possible choices of $\Sigma_{o,l}$ where o lies on l).

For pmm, the classification of mixed invariants when $K = \text{U}(1), \mathbb{Z}_N, \text{SO}(3)$ is given by $\mathbb{Z} \times \mathbb{Z}_2^3, \mathbb{Z}_N \times \mathbb{Z}_{(2,N)}^7, \mathbb{Z}_2^4$ respectively. First let $K = \text{U}(1)$. The $\mathbb{Z}$ invariant corresponds to the filling (charge per unit cell) ν . This invariant is not listed in the table, as it is common to each G_{space} and also cannot be fully determined by partial point group operations. We assume that the filling is either already specified or can be calculated separately. But the remaining $\mathbb{Z}_2^3$ classification can be obtained by evaluating $\mathcal{S}_o^{\text{U}(1)}$ at any three high symmetry points. Note that there are only three independent mixed invariants because $\sum_o \mathcal{S}_o^{\text{U}(1)} = \nu \pmod{2}$. There are no mixed invariants that depend on reflection symmetries.

When $K = \mathbb{Z}_N$, we have a $\mathbb{Z}_N$ analog of the filling as well as three independent $\mathcal{S}_o^{\mathbb{Z}_N}$ invariants, when N is even. In this case, there are four additional $\mathbb{Z}_{(2,N)}$ invariants of type C4, which can be measured by $\Upsilon_l^{\mathbb{Z}_N}$ where l runs over the four reflection lines.

Finally, when $K = \text{SO}(3)$, the mixed SPT invariants can be detected by evaluating the type-D4 invariant $\Upsilon_l^{\text{SO}(3)}$ on the four reflection lines. Note that we could alternatively measure three independent type-D1 invariants along with a single type-D4 invariant. (See App. E 2 b, which gives relations between invariants of type D1 and D2)

III. p4m

In this section we focus on the symmetries of the square lattice $\text{p4m} = \mathbb{Z}^2 \rtimes (\mathbb{Z}_4 \rtimes \mathbb{Z}_2)$. We explain the specific SPT invariants that arise in detail, and derive a topological effective action describing the response. As in previous sections we assume that: 1) the chiral central charge $c_- = 0$; and that 2) the topological invariants for internal symmetries are trivial. If these assumptions are not satisfied, the invariants may satisfy other quantization conditions [37, 65].

In this section and the next, we will repeatedly refer to a set of real-space constructions which provide representative ground states for a large class of bosonic SPT phases and which give a simple way to understand the response properties of invariants appearing in a topological field theory [26–28]. In these constructions, a crystalline SPT wave function is constructed as a tensor product of lower-dimensional states defined at the high symmetry points and lines of the real-space unit cell. These constructions generally assume a ‘Wannier limit’ in which the degrees of freedom are supported at such high symmetry regions. The various SPT invariants can then be understood in terms of the symmetry eigenvalues or quantum numbers of the localized degrees of freedom; the precise values are often obvious from the construction. When the degrees of freedom are localized on single points, we refer to the such states as atomic insulators (AI) [27]. Based on prior numerical studies on some of the invariants in this paper, for example Refs. [35–37], it is reasonable to believe that many predictions motivated by this construction should also hold away from the Wannier limit.

A. Conventions

1. Unit cell

The wallpaper group p4m has 6 Wyckoff positions with a non-trivial site-group (Fig. 4). There are three maximal Wyckoff positions, α, β, γ , that also appear in the space group p4. α and β have site-groups isomorphic to $D_4 \cong \mathbb{Z}_4 \rtimes \mathbb{Z}_2$, while γ is two-fold degenerate and has a site-group isomorphic to $D_2 \cong \mathbb{Z}_2 \times \mathbb{Z}_2$. Compared to the wallpaper group p4 = $\mathbb{Z}^2 \rtimes \mathbb{Z}_4$, there are three new Wyckoff positions. These positions lie on the reflection lines λ, μ, ν . Each of these positions have site group $D_1 \cong \mathbb{Z}_2$. There is also the generic Wyckoff position with a trivial site-group.

2. Definition of gauge fields

We fix an origin o such that $M_o = 4$, that is, o either belongs to α or β , and is contained in the horizontal line $l = \lambda_1$ or μ_1 respectively. Furthermore, we parametrize the group elements $\mathbf{g} \in \text{p4m}$ as $\mathbf{x}^{t_x, \mathbf{g}} \mathbf{y}^{t_y, \mathbf{g}} \mathbf{h}_o^{n_{\mathbf{g}}} \mathbf{r}_l^{r_{\mathbf{g}}}$ where

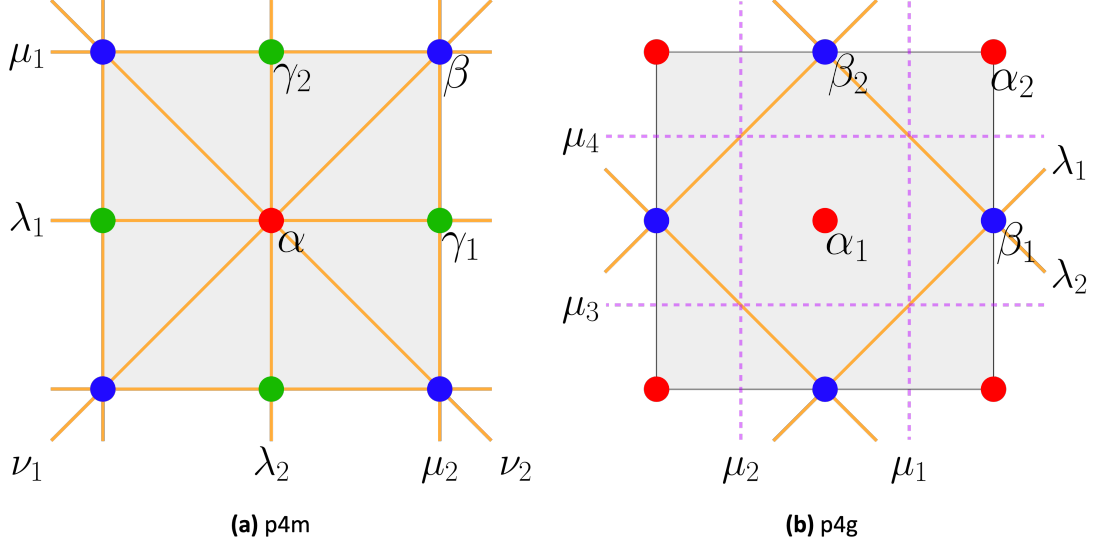


FIG. 4. Unit cell conventions for (a) p4m and (b) p4g. Maximal Wyckoff positions are labeled by early Greek letters (α, β, γ). Orange and dashed purple lines correspond to reflection and glide axes, respectively. These lines are labeled by mid-range Greek letters (λ, μ, ν). We use labels with the same subscripts to denote positions or lines that are related by a point group symmetry.

$\mathbf{x}(y)$ is translation by one unit-cell in the $x(y)$ direction, $\mathbf{r}_l$ is the reflection about l as defined above, and $\mathbf{h}_o$ is a counter-clockwise rotation by 90 degrees around o . $t_{x,\mathbf{g}}, t_{y,\mathbf{g}}, n_{\mathbf{g}}$ and $r_{\mathbf{g}}$ are integers with the redundancies $n_{\mathbf{g}} \sim n_{\mathbf{g}} + 4$ and $r_{\mathbf{g}} \sim r_{\mathbf{g}} + 2$, which follow from $\mathbf{h}_o^4 = \mathbf{r}_l^2 = 1$. Furthermore, $\mathbf{h}_o \mathbf{x} = \mathbf{y} \mathbf{h}_o$, $\mathbf{h}_o \mathbf{y} = \mathbf{x}^{-1} \mathbf{h}_o$, $\mathbf{h}_o \mathbf{r}_l = \mathbf{r}_l \mathbf{h}_o^3$, $\mathbf{r}_l \mathbf{x} = \mathbf{x} \mathbf{r}_l$, and $\mathbf{r}_l \mathbf{y} = \mathbf{y}^{-1} \mathbf{r}_l$.

Per the crystalline equivalence principle, we define the topological effective action for the group p4m in terms of a background gauge field for an internal symmetry isomorphic to p4m. Therefore we consider a closed 3-manifold $\mathcal{M}^3$ with a triangulation and define a flat gauge field on the links of the triangulation as $B = (\vec{R}, \omega, \sigma)$.⁷ The three components are gauge fields for translations, rotations and reflections respectively. The basic quantization of the three components is

$$\begin{aligned} \frac{1}{2\pi} \vec{R} &\in \mathbb{Z}^2 \\ \omega &\in \frac{2\pi}{4} \mathbb{Z}; & \omega &\sim \omega + 2\pi \\ \sigma &\in \mathbb{Z}; & \sigma &\sim \sigma + 2 \end{aligned} \quad (23)$$

Recall that the reflection gauge field should be identified with the first Stiefel-Whitney class of the space-time manifold [44].

⁷ Note that the components of the gauge field B depend on a choice of origin o and a reflection axis l . For ease of notation, we will suppress these dependencies while writing the gauge fields, and only make them explicit in the field theory coefficients.

B. Pure crystalline invariants

The pure crystalline SPT invariants are classified by $\mathcal{H}^4(\text{p4m}, \mathbb{Z}^{\text{or}}) = \mathbb{Z}_2^6$. We will explain how to understand them in terms of SPTs protected only by different site symmetry groups. Recall that the site groups of the maximal Wyckoff positions o are given by the dihedral group D_{M_o} with M_o being the order of rotations about o . M_o equals 2 or 4 for p4m.

a. Single WP: The effective Lagrangian density for D_{2n} -SPTs is (see App. C 1 for a derivation):

$$\mathcal{L}_{D_{2n}} = k_{1,o} n \omega \frac{\bar{d}\omega}{2\pi} + k_{2,o,l} \pi \sigma \frac{\bar{d}\omega}{2\pi}. \quad (24)$$

with $k_{1,o}, k_{2,o,l} \in \mathbb{Z}_2$. $\bar{d}$ is the differential twisted by orientation. $k_{1,o}$ and $k_{2,o,l}$ depend on the rotation center o and reflection line l used to define the D_{2n} gauge fields. In the case of a single WP, o is fixed uniquely, but we will need the subscript in the discussion below.

Recall that the partial symmetry operators evaluate the partition functions on certain manifolds, and these can be evaluated explicitly for the topological action in Eq. 24 [56, 72]:

$$\begin{aligned} e^{\frac{2\pi i}{2n} \Theta_o} &= \mathcal{Z}(L(2n, 1)_{\mathbf{h}_o^n}) = (-1)^{k_{1,o}} \\ (-1)^{\Sigma_{o,l}} &= \mathcal{Z}(\mathbb{RP}_{\mathbf{r}_l}^2 \times S_{\mathbf{h}_o^n}^1) = (-1)^{k_{2,o,l}}. \end{aligned} \quad (25)$$

Here $L(p, 1)_{\mathbf{g}}$ is a lens space with $\mathbf{g}$ holonomy along its non-contractible cycle. This implies

$$k_{1,o} = \frac{\Theta_o}{n} \mod 2; \quad k_{2,o,l} = \Sigma_{o,l} \mod 2. \quad (26)$$

Now that we have related the real-space invariants to coefficients of the topological action, we can easily calculate the real-space invariants for the atomic insulators previously alluded to. For each site group G_o , an AI is fully determined by how the localized degrees of freedom at o transform as a one-dimensional irreducible representation (1d-irrep) of G_o . For $G_o = D_{2n}$, there are only 4 1d-irreps that are specified by their eigenvalues under the generators $\mathbf{h}_o$ ($2n$ -fold rotation) and $\mathbf{r}_l$ (reflection). These are denoted as $\lambda_{\mathbf{h}_o}, \lambda_{\mathbf{r}_l} \in \{+1, -1\}$, where $\lambda_{\mathbf{g}}$ is the $\mathbf{g}$ -eigenvalue of the irrep. It is straightforward to evaluate the real space invariants for the AIs in terms of their eigenvalues:

$$\begin{aligned} e^{\frac{i\pi}{n}\Theta_o}|_{\text{AI}} &= \lambda_{\mathbf{h}_o}; \\ (-1)^{\Sigma_{o,l}}|_{\text{AI}} &= \lambda_{\mathbf{r}_l}. \end{aligned} \quad (27)$$

Combining the above equation and Eq. 26, we find that a state described by Eq. 24 is in the same phase as an atomic insulator of localized degrees of freedom with angular momentum $nk_{1,o} \bmod 2n$, and even(odd) parity under $\mathbf{r}_l$ when $k_{2,o,l} = 0(1)$.

b. p4m: Mathematically, the most general effective action has the Lagrangian

$$\mathcal{L} = B^* \varphi_3 \quad (28)$$

where $[\varphi_3]$ is an element of $\mathcal{H}^3(\text{p4m}, \text{U}(1)^{\text{or}})$, where we have identified $\text{U}(1)$ with the real numbers modulo 2π . B^* denotes the pullback operation using B .⁸ That is, $B^* \varphi_3$ is a cocycle defined on the 3-simplices of the trian-

gulation of $\mathcal{M}^3$, and the cocycle condition ensures that the associated partition function $e^{i \int_{\mathcal{M}^3} \mathcal{L}}$ is invariant under retriangulations. Therefore, to get a general form for $\mathcal{L}$ we first need to find a general expression for φ_3 .

The generators of $\mathcal{H}^3(\text{p4m}, \text{U}(1)^{\text{or}})$ can be obtained as cup products of generators of $\mathcal{H}^2(\text{p4m}, \mathbb{Z}^{\text{or}}) \cong \mathbb{Z}_4 \times \mathbb{Z}_2 \times \mathbb{Z}$ with the generators of $\mathcal{H}^1(\text{p4m}, \text{U}(1)) \cong \mathbb{Z}_2^3$.⁹ Roughly speaking, the elements of the former group correspond to symmetry fluxes, while those of the latter correspond to symmetry charges, and the cup product implements flux-charge attachment.

Any element $[\Xi_1] \in \mathcal{H}^1(\text{p4m}, \text{U}(1))$ can be written as

$$B^* \Xi_1 = q_{1,o} 2\omega + q_{2,o,l} \pi \sigma + q_{3,o} \vec{m} \cdot \vec{R} \in 2\pi \mathbb{R} / \mathbb{Z}, \quad (29)$$

with $q_{1,o}, q_{2,o,l}, q_3 \in \mathbb{Z}_2$ and $\vec{m} = [1/2, 1/2]$. The quantities $2q_{1,o}, q_{2,o,l}$, and q_3 correspond to the charge under $\mathbf{h}_o, \mathbf{r}_l, \mathbf{x}$, respectively.

Similarly, an element $[\Xi_2] \in \mathcal{H}^2(\text{p4m}, \mathbb{Z}^{\text{or}})$ can be written as

$$B^* \Xi_2 = j_{1,o} \frac{\bar{d}\omega}{2\pi} + j_{2,o} \frac{\bar{d}(\vec{R} \cdot \vec{m})}{2\pi} + j_3 A_{XY}, \quad (30)$$

where A_{XY} is the "area form" which reduces to $A_{XY} = \frac{1}{2\pi} R_x \wedge R_y$ in the absence of rotation or reflection fluxes [30]. The coefficients are quantized as $(j_{1,o}, j_2, j_3) \in \mathbb{Z}_4 \times \mathbb{Z}_2 \times \mathbb{Z}$.

Taking the cup product of both types of terms, and eliminating the redundant terms, we find the response action to be

$$\mathcal{L}_{\text{p4m}} = k_{1,\alpha} 2\omega \frac{\bar{d}\omega}{2\pi} + k_{2,\alpha,\lambda_1} \pi \sigma \frac{\bar{d}\omega}{2\pi} + k_{3,\alpha} (\vec{R} \cdot \vec{m}) \frac{\bar{d}\omega}{2\pi} + k_{4,\alpha,\lambda_1} \pi \sigma \frac{\bar{d}(\vec{R} \cdot \vec{m})}{2\pi} + k_5 2\omega A_{XY} + k_6 \pi \sigma A_{XY}. \quad (31)$$

A physical interpretation of each field theory coefficient will be given below. However, following the general strategy of this paper, we will first relate the coefficients to the invariants $\Theta_o, \Sigma_{o,l}$ defined previously, for different o and l . We start by restricting the space group G_{space} to site groups $G_{o'}$ for different o' . This restriction induces a map at the cohomology level $\mathcal{H}^3(G_{\text{space}}, \text{U}(1)^{\text{or}}) \rightarrow \mathcal{H}^3(G_{o'}, \text{U}(1)^{\text{or}})$ that, after pulling back by B , allows us to express $k_{1,o'}$ and $k_{2,o',l'}$ in terms of the k -invariants

appearing in Eq. 31:

$$\begin{aligned} k_{1,\alpha} &= k_{1,\alpha} \\ k_{2,\alpha,\lambda_1} &= k_{2,\alpha,\lambda_1} \\ k_{1,\beta} &= k_{1,\alpha} + k_{3,\alpha} + k_5 \\ k_{2,\beta,\mu_1} &= k_{2,\alpha,\lambda_1} + k_{3,\alpha} + k_6 \\ k_{1,\gamma_1} &= k_{3,\alpha} \\ k_{2,\gamma_1,\lambda_1} &= k_{2,\alpha,\lambda_1} + k_{4,\alpha,\lambda_1} \\ k_{1,\gamma_2} &= k_{3,\alpha} \\ k_{2,\gamma_2,\mu_1} &= k_{2,\alpha,\lambda_1} + k_{3,\alpha} + k_{4,\alpha,\lambda_1}. \end{aligned} \quad (32)$$

⁸ In reality, G gauge fields are constructed by pulling back cochains along the classifying map $f_B : \mathcal{M} \rightarrow BG$, where BG is the classifying space of principal G -bundles and $\mathcal{M}$ is the space-time manifold. Accordingly, the notation B^* is short-hand for the pullback f_B^* .

⁹ See Sec. V for a sketch of the argument, and App. C for more explicit calculations for p4m.

Then we solve for $k_{j,\alpha}$:

$$\begin{aligned}
k_{1,\alpha} &= k_{1,\alpha} \\
k_{2,\alpha,\lambda_1} &= k_{2,\alpha,\lambda_1} \\
k_{3,\alpha} &= k_{1,\gamma_1} \\
k_{4,\alpha,\lambda_1} &= k_{2,\gamma_1,\lambda_1} + k_{2,\alpha,\lambda_1} \\
k_5 &= k_{1,\alpha} + k_{1,\gamma_1} + k_{1,\beta} \\
k_6 &= k_{2,\alpha,\lambda_1} + k_{2,\gamma_1,\lambda_1} + k_{2,\gamma_2,\mu_1} + k_{2,\beta,\mu_1} \\
&= k_{2,\alpha,\lambda_1} + k_{2,\beta,\mu_1} + k_{1,\gamma_1}
\end{aligned} \quad . \quad (33)$$

Given that $k_{1,o}, k_{2,o,l}$ can be directly obtained from $\Theta_o, \Sigma_{o,l}$, we can extract all the field theory coefficients from an SPT wavefunction in terms of the real space invariants Θ_o and $\Sigma_{o,l}$. This is summarized in Table IV. See Table VII for a list of all the relations between SPT invariants for p4m, and App. E 1 for a general discussion of the relations between Type A invariants.

We now give a direct interpretation of the coefficients in Eq. 33 that is motivated by the field theory:

1. $k_{1,\alpha}$: $\ell_\alpha = 2k_{1,\alpha}$ is the C_{M_α} angular momentum of the ground state on a subregion. It has been well studied in the absence of reflection symmetry [37].
2. k_{2,α,λ_1} : As mentioned previously, in the Wannier limit real-space construction, $p_{\alpha,\lambda_1} = k_{2,\alpha,\lambda_1} \bmod 2$ is the parity under the reflection $\mathbf{r}_{\lambda_1}$ of the degrees of freedom localized at α . Although we have not numerically checked it, we expect this interpretation to hold away from the Wannier limit, analogous to how fractional U(1) charges are found to be localized at crystalline defects in topological insulators or Chern insulators away from the Wannier limit [35, 36]. A second interpretation suggested by the field theory is that it determines the angular momentum of defects of the reflection symmetry, but establishing this requires a further study of reflection symmetry defects which we do not pursue here.
3. $k_{3,\alpha}$: The quantity $\vec{\mathcal{P}}_{\alpha,s} := k_{3,\alpha}(1/2, 1/2)$ can be understood as an angular momentum polarization, consistent with the fact that it can be expressed as a difference between $k_{1,o}$ at different o . (See [36, 39] for a discussion on relating angular momentum polarization to other field theory coefficients.)
4. k_{4,α,λ_1} : Analogously, $\vec{\mathcal{P}}_{\alpha,\lambda_1,p} := k_{4,\alpha,\lambda_1}(1/2, 1/2)$ is a **polarization of the reflection eigenvalue** $k_{2,o,l}$, or equivalently a difference between $k_{2,o,l}$ for two different choices of o measured with respect to a single reflection axis l .
5. k_5 : The quantity $k_5 := \nu_s$ is interpreted as an ‘angular momentum per unit-cell’ [30, 39], and can be thought of as a generalized filling invariant. It is origin-independent, assuming we only consider the origins α, β which have the maximal site group D_4 .

Invariants being related	Relation
All coefficients of Eq. (31) in terms of $k_{1,o}, k_{2,o,l}$	Eq. (33)
$\nu, \mathcal{S}_o^{U(1)}$	Eq. (37)
$\bar{\nu}, \mathcal{S}_o^{U(1)}$ for p4g	Eq. (56)
$\overline{\mathcal{P}}_o, \mathcal{S}_{o'}^{U(1)}$	Eq. (39)
$\mathcal{S}_o^{SO(3)}, \Upsilon_l^{SO(3)}$	Eq. (51)

TABLE VII. Partial list of relations between the SPT invariants with symmetry p4m $\times K$, $K = U(1), SO(3)$. For comparison, one analogous relation for wallpaper group p4g is given in blue. Relations for $K = \mathbb{Z}_N$ can be obtained from those for $K = U(1)$ after reducing modulo N , and changing superscripts to $\mathbb{Z}_N$.

6. k_6 : Finally, the quantity $k_6 := \nu_r$ measures a weighted sum of reflection eigenvalues for different points about a horizontal axis, and is also origin-independent. It can be thought of as a measure of the **total reflection eigenvalue per unit cell**.

We emphasize that $k_{4,\alpha}, k_6$ and the partial reflection invariants which extract them have not appeared previously in the literature.

C. Mixed invariants

Next we discuss the invariants that are protected by both p4m and K . The full effective action capturing these mixed invariants is given in Eq. 53. The relations between the invariants that we have derived are summarized in Table VII.

1. $K = U(1)$:

We begin with $K = U(1)$. Note that the Hall conductance is forced to vanish because of reflection symmetry, therefore there are no pure K -SPT invariants.

a. Single WP: Let A be a U(1) gauge field. The most general mixed $U(1) \times D_{M_o}$ topological action is

$$\mathcal{L}_{D_{M_o}, U(1)}^{\text{mixed}} = \mathcal{S}_o^{U(1)} A \frac{\bar{d}\omega}{2\pi}, \quad (34)$$

with $\mathcal{S}_o^{U(1)} \in \mathbb{Z}_{M_o}$. In the absence of reflections, the above action appeared in Refs. [35, 36] and defines the discrete shift. Although those works studied systems without reflection symmetry, the quantization of the shift is unaffected by reflections. $\mathcal{S}_o^{U(1)}$ is extracted by a type-B1 invariant, which is a relative partial rotation. Previous real-space constructions in the Wannier limit interpret $\mathcal{S}_o^{U(1)}$ as the U(1) charge localized at o . Note that $\mathcal{S}_o^{U(1)}$ is only defined modulo reduction mod M_o because

one can move charge away from $\mathbf{o}$ in multiples of M_o symmetrically.

b. p4m: According to the group cohomology calculation, the most general action is

$$\mathcal{L}_{\text{p4m}, \text{U}(1)}^{\text{mixed}} = \mathcal{S}_o^{\text{U}(1)} A \frac{\bar{d}\omega_o}{2\pi} + \bar{\mathcal{P}}_o A \frac{\bar{d}\vec{R} \cdot \vec{m}}{2\pi} + \nu A A_{XY}, \quad (35)$$

where $\mathcal{S}_o^{\text{U}(1)}, \bar{\mathcal{P}}_o, \nu \in \mathbb{Z}_4 \times \mathbb{Z}_2 \times \mathbb{Z}$ and $\vec{m} = (1/2, 1/2)$. Note that $\bar{\mathcal{P}}_o := \frac{\bar{\mathcal{P}}_o}{2}(1, 1)$ is the charge polarization, and ν is the filling; these quantities were studied previously in Refs. [36, 39].

We can measure $\bar{\mathcal{P}}_o$ by reexpressing it in terms of $\mathcal{S}_{o'}^{\text{U}(1)}$ for different o' , see Eq. (39) below. The filling ν needs to be computed separately, for example by finding the $\text{U}(1)$ charge of the ground state for different system sizes. However, ν can be partially determined if we know $\mathcal{S}_{o'}^{\text{U}(1)}$ at each o' . In the Wannier limit, we can calculate ν as the sum of charge at high symmetry positions (counted with multiplicity) and the charge away from them:

$$\nu = Q_\alpha + Q_\beta + 2Q_\gamma + Q_{\text{away}}. \quad (36)$$

However, because of rotation symmetry any charge assigned to Q_{away} always appears in multiples of 4. Using $Q_o = \mathcal{S}_o^{\text{U}(1)} \bmod M_o$, we obtain

$$\nu = \mathcal{S}_\alpha^{\text{U}(1)} + \mathcal{S}_\beta^{\text{U}(1)} + 2\mathcal{S}_\gamma^{\text{U}(1)} \bmod 4. \quad (37)$$

This implies that one of the $\mathbb{Z}_4$ factors is redundant assuming ν is known.

We now establish the relation between $\bar{\mathcal{P}}_o$ and $\mathcal{S}_{o'}^{\text{U}(1)}$. From the results in Table IX, and noting that upon restriction to p1 the generator A_{XY} remains while all others vanish, we find

$$\begin{aligned} \mathcal{S}_\alpha^{\text{U}(1)} &= \mathcal{S}_\alpha^{\text{U}(1)} \bmod 4 \\ \mathcal{S}_\beta^{\text{U}(1)} &= \mathcal{S}_\alpha^{\text{U}(1)} + 2\bar{\mathcal{P}}_\alpha + \nu \bmod 4 \\ \mathcal{S}_\gamma^{\text{U}(1)} &= \mathcal{S}_\alpha^{\text{U}(1)} + \bar{\mathcal{P}}_\alpha \bmod 2. \end{aligned} \quad (38)$$

This implies that

$$\begin{aligned} \mathcal{S}_\alpha^{\text{U}(1)} &= \mathcal{S}_\alpha^{\text{U}(1)} \\ \bar{\mathcal{P}}_\alpha &= \mathcal{S}_\gamma^{\text{U}(1)} - \mathcal{S}_\alpha^{\text{U}(1)} \bmod 2. \end{aligned} \quad (39)$$

2. $K = \mathbb{Z}_N$:

Next, we consider $K = \mathbb{Z}_N$. In what follows, we assume that the pure $\mathbb{Z}_N$ -SPT invariant is trivial in the ground state; we discuss the consequences of relaxing this assumption in Sec. VI.

a. Single WP: mixed $D_1 \times \mathbb{Z}_N$ SPTs are classified by $\mathbb{Z}_{(2,N)}$.¹⁰ The corresponding action is

$$\mathcal{L}_{D_1, \mathbb{Z}_N}^{\text{mixed}} = t_{1,l} \frac{N}{(N, 2)} A \sigma, \quad (40)$$

where σ is the reflection gauge field, A is the $\mathbb{Z}_N$ gauge field (taking values in $\frac{2\pi}{N}\mathbb{Z}$), and $t_{1,l} \in \mathbb{Z}_2$.

Since $\mathbf{r}_l$ acts as a $\mathbb{Z}_2$ on-site symmetry on l , the mixed SPT can be understood as decorations of l with $(1+1)\text{D}$ $\mathbb{Z}_2 \times \mathbb{Z}_N$ SPTs. An example of a non-trivial decoration is the AKLT chain. In this case, we can evaluate the type C4 invariant (Eq. 15) $\Upsilon_l^{\mathbb{Z}_N} = 1 \bmod 2$ explicitly. Therefore, $\Upsilon_l^{\mathbb{Z}_N} = t_{1,l}$.

In the presence of D_{2n} symmetry around $\mathbf{o}$, the mixed terms are

$$\begin{aligned} \mathcal{L}_{D_{2n}, \mathbb{Z}_N}^{\text{mixed}} &= \frac{N}{(N, 2)} A \sigma \left[t_{1,o,l} \sigma + t_{2,o} \frac{n\omega_o}{2\pi} \right] \\ &\quad + \mathcal{S}_o^{\mathbb{Z}_N} A \frac{\bar{d}\omega}{2\pi}, \end{aligned} \quad (41)$$

where we have added a subscript $\mathbf{o}$ to the coefficients for later convenience. $t_{2,o}$ measures the difference of $t_{1,o,l} - t_{1,o,l'}$ for $\mathbf{r}_{l'} = \mathbf{h}_o \mathbf{r}_l$, which can be shown by restricting the action to the two $D_1 \times \mathbb{Z}_N$ subgroups. $\mathcal{S}_o^{\mathbb{Z}_N}$ is the $\mathbb{Z}_N$ version of shift and can be detected by $\Theta_o^{\mathbb{Z}_{2n}}$.

Note that when N is odd, the only allowed term is $\mathcal{S}_o^{\mathbb{Z}_N} A \frac{\bar{d}\omega}{2\pi}$ with $\mathcal{S}_o^{\mathbb{Z}_N}$ is defined modulo (N, n) .

b. p4m: The mixed SPT states are classified by

$$\begin{aligned} \mathcal{H}^2(\text{p4m}, \mathbb{Z}_N^{\text{or}}) &\cong (\mathcal{H}^2(\text{p4m}, \mathbb{Z}^{\text{or}}) \otimes \mathbb{Z}_N) \\ &\quad \oplus \text{Tor}[\mathcal{H}^3(\text{p4m}, \mathbb{Z}^{\text{or}}), \mathbb{Z}_N]. \end{aligned} \quad (42)$$

The first term corresponds to the $\mathbb{Z}_N$ version of the $\text{p4m} \times \text{U}(1)$ invariants. The tensor product means that we need to reduce the various invariants modulo N , which is expected as charge is now defined modulo N :

$$\mathcal{H}^2(\text{p4m}, \mathbb{Z}^{\text{or}}) \otimes \mathbb{Z}_N = \mathbb{Z}_{(N,4)} \times \mathbb{Z}_{(N,2)} \times \mathbb{Z}_N. \quad (43)$$

An effective action capturing these invariants is the same as Eq. 35 (now with $\mathbb{Z}_N$ superscripts):

$$\begin{aligned} \mathcal{L}_{\text{p4m}, \mathbb{Z}_N}^{\text{mixed}} &= \mathcal{S}_o^{\mathbb{Z}_N} A \frac{\bar{d}\omega_o}{2\pi} + \bar{\mathcal{P}}_o^{\mathbb{Z}_N} A \frac{\bar{d}\vec{R} \cdot \vec{m}}{2\pi} \\ &\quad + \nu^{\mathbb{Z}_N} A A_{XY}, \end{aligned} \quad (44)$$

The coefficients have the quantization $(\mathcal{S}_o^{\mathbb{Z}_N}, \bar{\mathcal{P}}_o^{\mathbb{Z}_N}, \nu^{\mathbb{Z}_N}) \in \mathbb{Z}_{(N,4)} \times \mathbb{Z}_{(N,2)} \times \mathbb{Z}_N$.

Now consider the second piece. The group cohomology calculation shows that $\mathcal{H}^3(\text{p4m}, \mathbb{Z}^{\text{or}}) = \mathbb{Z}_2^3$ and is trivial

¹⁰ See also Ref. [73] where an effective boundary field theory approach was used.

upon restriction to p4. Evaluating the torsion, we get

$$\text{Tor}[\mathcal{H}^3(\text{p4m}, \mathbb{Z}^{\text{or}}), \mathbb{Z}_N] = \mathbb{Z}_{(2,N)} \times \mathbb{Z}_{(2,N)} \times \mathbb{Z}_{(2,N)}. \quad (45)$$

The topological action describing these ‘torsion’ mixed SPTs is

$$\mathcal{L}_{\text{p4m}, \mathbb{Z}_N}^{\text{Tor}} = \frac{2N}{(N, 2)} A \sigma (t_{1,o,l} \frac{\sigma}{2} + t_{2,o} \frac{2\omega}{2\pi} + t_3 \frac{\vec{R} \cdot \vec{m}}{2\pi}), \quad (46)$$

where $t_{1,o,l}, t_{2,o}, t_3 \in \mathbb{Z}_2^3$.

In p4m, any reflection is in the conjugacy class of one of the following reflections: $\mathbf{r}_{\lambda_1}$, $\mathbf{r}_{\mu_1}$ or $\mathbf{r}_{\nu_1}$ (see Fig. 4). For N even, there are 3 root phases according to the real space construction. Corresponding ideal states are constructed by placing $\mathbb{Z}_2 \times \mathbb{Z}_N$ (1+1)D SPTs on each conjugacy class of reflection lines. By restricting the action in Eq. 46 from p4m to the three different D_1 subgroups generated by each of the three reflections, we find the following relation between the topological action and the invariants:

$$\begin{aligned} \Upsilon_{\lambda_1}^{\mathbb{Z}_N} &= t_{1,\alpha,\lambda_1} \mod 2; \\ \Upsilon_{\nu_1}^{\mathbb{Z}_N} &= t_{1,\alpha,\lambda_1} + t_{2,\alpha} \mod 2; \\ \Upsilon_{\mu_1}^{\mathbb{Z}_N} &= t_{1,\alpha,\lambda_1} + t_3 \mod 2. \end{aligned} \quad (47)$$

See App. D1c for an explicit computation of the $\Upsilon_l^{\mathbb{Z}_2}$ invariant in an ideal SPT ground state with p4m symmetry.

3. $K = \text{SO}(3)$:

We now consider spin rotation symmetry, $K = \text{SO}(3)$. The spin Hall conductivity is forced to be trivial due to spatial reflections.

a. single WP: $D_1 \times \text{SO}(3)$ mixed SPTs are classified by $\mathbb{Z}_2$. The corresponding action is

$$\mathcal{L}_{D_1, \text{SO}(3)}^{\text{mixed}} = u_l \pi w_2 \sigma, \quad (48)$$

where w_2 (the Stiefel-Whitney class of the $\text{SO}(3)$ bundle) is the pullback of the generator of $\mathcal{H}^2(\text{SO}(3), \mathbb{Z}_2)$ and $u_l \in \mathbb{Z}_2$. The $u_l = 1$ case can be understood as placing an AKLT chain (the non-trivial $\text{SO}(3)$ (1+1)D SPT phase) on l . We can detect this using the Type-C4 invariant $\Upsilon_l^{\text{SO}(3)}$ (see Eq. (16)).

The AKLT chain is characterized by fractionalized $\text{SO}(3)$ spins in the presence of open boundary conditions. Consequently, a non-trivial u_l (or $\Upsilon_l^{\text{SO}(3)}$) signals the presence of fractionalized spins at the points where l intersects the system boundary.

For D_{2n} symmetry, the classification is $\mathbb{Z}_2 \times \mathbb{Z}_2$, with corresponding topological action

$$\mathcal{L}_{D_{2n}, \text{SO}(3)}^{\text{mixed}} = 2\pi w_2 (u_{1,o,l} \frac{\sigma}{2} + u_{2,o} \frac{n\omega}{2\pi}), \quad (49)$$

where $u_{1,o,l}, u_{2,o} \in \mathbb{Z}_2$. Analogously to the $\mathbb{Z}_N$ case: $u_{1,o,l}$ corresponds to the invariant $u_{1,l}$ for the D_1 subgroup generated by $\mathbf{r}_l$.

We can understand $2\pi w_2 \frac{n\omega}{2\pi}$ by restricting $\text{SO}(3)$ to a $\text{SO}(2)$ ($\cong \text{U}(1)$) subgroup. Under this restriction, $w_2 \rightarrow \frac{dA}{2\pi} \mod 2$, where A is the $\text{SO}(2)$ gauge field. Integrating by parts then gives $2\pi w_2 \frac{n\omega}{2\pi} \rightarrow nA \frac{d\omega}{2\pi}$. Therefore, there is charge $nu_{2,o}$ localized at o , which implies that a disclination of angle $\pm\pi/n$ carries charge $u_{2,o}/2$ under $\text{SO}(2)$. In other words, the $\text{SO}(3)$ spin at a disclination core S_o satisfies $S_o = \frac{u_{2,o}}{2} \mod 1$. From the action restricted to $\text{SO}(2)$, together with the known relation between dressed partial rotations and the coefficients of the topological action, we obtain $u_{2,o} = \delta_o^{\text{SO}(3)}$.

b. p4m: The new mixed SPT invariants are classified by $\mathcal{H}^1(\text{p4m}, \mathcal{H}^2(\text{SO}(3), \text{U}(1))) = \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2$. The topological action for these mixed invariants is

$$\mathcal{L}_{\text{p4m}, \text{SO}(3)}^{\text{mixed}} = 2\pi w_2 (u_{1,o,l} \frac{\sigma}{2} + u_{2,o} \frac{2\omega}{2\pi} + u_3 \frac{\vec{R} \cdot \vec{m}}{2\pi}), \quad (50)$$

where $u_{1,o,l}, u_{2,o}, u_3 \in \mathbb{Z}_2$. The real space construction and the folding trick suggest, that the root states are obtained by placing AKLT states on the conjugacy classes of the reflection lines λ_1 , μ_1 , and ν_1 .

From the analysis of a single WP, we have $u_{1,\alpha,\lambda_1} = \Upsilon_{\lambda_1}^{\text{SO}(3)}$ and $u_{2,\alpha} = \delta_\alpha^{\text{SO}(3)}$. We now derive the relation

$$\delta_\alpha^{\text{SO}(3)} = \Upsilon_{\lambda_1}^{\text{SO}(3)} + \Upsilon_{\nu_1}^{\text{SO}(3)}. \quad (51)$$

One approach is to start from the action in Eq. 50 and restrict to the two D_1 subgroups generated by $\mathbf{r}_{\lambda_1}$ and $\mathbf{r}_{\nu_1}$, which allow us to relate the corresponding coefficients in the action (See App. E2a for details).

Another approach is to observe that, according to the real-space construction, the three root states for mixed p4m- $\text{SO}(3)$ SPTs can be obtained by placing Haldane chains (the nontrivial (1+1)D $\text{SO}(3)$ SPT) along each of the conjugacy classes of reflection lines. In these idealized states, the only sources of fractional spins are the dangling ends of the Haldane chains. In particular, when constructing a $\pi/2$ disclination, one effectively removes half of the λ_1 and ν_1 reflection lines. Since $\Upsilon_l^{\text{SO}(3)} = 1$ only if a Haldane chain is placed on l , the spin at a disclination core is $\frac{\delta_\alpha^{\text{SO}(3)}}{2} = \frac{\Upsilon_{\lambda_1}^{\text{SO}(3)} + \Upsilon_{\nu_1}^{\text{SO}(3)}}{2} \mod 1$.

Upon restricting p4m to p1, the mixed SPT invariants are classified by $u_{3,o} \in \mathbb{Z}_2$.¹¹ The invariant associated with this $\mathbb{Z}_2$ is the translation- $\text{SO}(3)$ Lieb-Shultz-Mattis anomaly of the edge theory – the parity of fractional spins per unit cell on the edge theory. By restricting the action in Eq. 50 to the site groups at α and β (see App. E2a),

¹¹ The mixed SPTs are classified by $\mathbb{Z}_2^3$ but the C_4 rotation imposes that the two indices to be equal, thus reducing the classification to $\mathbb{Z}_2$

we obtain

$$u_3 = u_{1,\alpha,\lambda_1} + u_{1,\beta,\mu_1} = \Upsilon_{\lambda_1}^{\text{SO}(3)} + \Upsilon_{\mu_1}^{\text{SO}(3)}. \quad (52)$$

We can interpret this as follows: if translations and reflection symmetries are present on the edge, the fractional SO(3) charge on the unit cell can be determined by considering only the center ($\Upsilon_{\lambda_1}^{\text{SO}(3)}$) and middle ($\Upsilon_{\mu_1}^{\text{SO}(3)}$) of the

edge unit cell because any contribution away from these two points comes in pairs and thus cancels out.

4. Summary

The full crystalline action for SPT with wallpaper group p4m and internal symmetry $K = \text{U}(1), \mathbb{Z}_N, \text{SO}(3)$ is

$$\begin{aligned} \mathcal{L}_{\text{p4m},K} &= \mathcal{L}_{\text{p4m}} + \mathcal{L}_{\text{p4m},K}^{\text{mix}} \\ \mathcal{L}_{\text{p4m}} &= k_{1,\alpha} 2\omega \frac{\bar{d}\omega}{2\pi} + k_{2,\alpha,\lambda_1} \pi \sigma \frac{\bar{d}\omega}{2\pi} + k_{3,\alpha} (\vec{R} \cdot \vec{m}) \frac{\bar{d}\omega}{2\pi} + k_{4,\alpha,\lambda_1} \pi \sigma \frac{\bar{d}\vec{R} \cdot \vec{m}}{2\pi} + k_5 2\omega A_{XY} + k_6 \pi \sigma A_{XY}. \\ \mathcal{L}_{\text{p4m},K}^{\text{mix}} &= \begin{cases} \mathcal{S}_o^{\text{U}(1)} A \frac{\bar{d}\omega_o}{2\pi} + \overline{\mathcal{P}}_o A \frac{\bar{d}\vec{R} \cdot \vec{m}}{2\pi} + \nu A A_{XY} & ; K = \text{U}(1); \\ \mathcal{S}_o^{\mathbb{Z}_N} A \frac{\bar{d}\omega_o}{2\pi} + \overline{\mathcal{P}}_o^{\mathbb{Z}_N} A \frac{\bar{d}\vec{R} \cdot \vec{m}}{2\pi} + \nu^{\mathbb{Z}_N} A A_{XY} + \frac{2N}{(N,2)} A \sigma (t_{1,o,l} \frac{\sigma}{2} + t_{2,o} \frac{2\omega}{2\pi} + t_3 \frac{\vec{R} \cdot \vec{m}}{2\pi}) & ; K = \mathbb{Z}_N \\ 2\pi w_2 (u_{1,o,l} \frac{\sigma}{2} + u_{2,o} \frac{2\omega}{2\pi} + u_3 \frac{\vec{R} \cdot \vec{m}}{2\pi}) & ; K = \text{SO}(3) \end{cases} \end{aligned} \quad (53)$$

For $K = \mathbb{Z}_N$ and N even, we are allowed to have a term $\sigma_{\mathbb{Z}_N} A \frac{\bar{d}A}{2\pi}$, with $\sigma_{\mathbb{Z}_N}$ a multiple of $N/2$. This term likely modifies the relations between the real space invariants and the effective action coefficients presented above.

IV. p4g

Next, we study a non-symmorphic example, $G_{\text{space}} = \text{p4g}$, which is a non-trivial extension of D_1 by p4. In this extension, the generator of D_1 squares to a translation—i.e., the generator of D_1 becomes a glide symmetry in p4g. We take the unit cell to be as in Fig. 4. Because of the glide symmetry, every WP is degenerate. Therefore the MWP contains only two orbits invariant under a rotation, α and β . We have $G_{\alpha_j} \cong C_4$ and $G_{\beta_j} \cong D_2$, where $j = 1, 2$. The extra glide transformation relates the two MWPs with $M_o = 4$ of p4. Moreover, every point in the unit cell is mapped to a distinct point under the glide, which has direct consequences for the filling invariants, as discussed below.

First we study the pure crystalline invariants. The group cohomology result is

$$\mathcal{H}^3(\text{p4g}, \text{U}(1)^{\text{or}}) = \mathbb{Z}_4 \times \mathbb{Z}_2^2. \quad (54)$$

This can be understood as $\mathcal{H}^3(\text{p4g}, \text{U}(1)^{\text{or}}) \cong \mathcal{H}^3(G_{\alpha_1}, \text{U}(1)^{\text{or}}) \times \mathcal{H}^3(G_{\beta_1}, \text{U}(1)^{\text{or}})$. In other words, there is a $\mathbb{Z}_4$ type-A1 invariant for α and a $\mathbb{Z}_2^2$ invariant (one $\mathbb{Z}_2$ from type A1 and A2 respectively) for β . Since there is no reflection line passing through α , the $\mathbb{Z}_4$ invariant is not reduced by reflections, as it would have been in a symmorphic lattice.

Next we study the mixed invariants. We note the following group cohomology results (obtained with GAP):

$$\begin{aligned} \mathcal{H}^1(\text{p4g}, \mathbb{Z}^{\text{or}}) &= \mathbb{Z}_2 \\ \mathcal{H}^2(\text{p4g}, \mathbb{Z}^{\text{or}}) &= \mathbb{Z} \times \mathbb{Z}_4 \\ \mathcal{H}^3(\text{p4g}, \mathbb{Z}^{\text{or}}) &= \mathbb{Z}_2. \end{aligned} \quad (55)$$

When $K = \text{U}(1)$, the mixed phases are classified by $\mathcal{H}^2(\text{p4g}, \mathcal{H}^1(\text{U}(1), \text{U}(1)^{\text{or}})) \cong \mathcal{H}^2(\text{p4g}, \mathbb{Z}^{\text{or}})$. The $\mathbb{Z}_4$ factor corresponds to having an integer invariant $\mathcal{S}_o^{\text{U}(1)} \bmod 4$ at α_1 , and the $\mathbb{Z}$ factor is equal to the total charge in each fundamental domain. The fundamental domain is a subset of the unit cell that generates the full unit cell upon action of translations or glides. For symmorphic groups, the unit cell is the same as the fundamental domain, but this is not true in non-symmorphic groups. An important result is that the true integer invariant in the non-symmorphic case is the filling per fundamental domain $\bar{\nu}$, while in contrast the filling per unit cell $\nu = 2\bar{\nu}$ is an even integer.

Consider the AI limit. Let Q_o be the charge localized at o . Note that $Q_o = \mathcal{S}_o^{\text{U}(1)} \bmod M_o$, $Q_{\alpha_1} = Q_{\alpha_2}$ and $Q_{\beta_1} = Q_{\beta_2}$. Due to the C_4 symmetry around α_1 , the charge away from high symmetry points $\alpha_1, \alpha_2, \beta_1, \beta_2$ appear in multiples of 4, i.e. $Q_{\text{away}} = 0 \bmod 4$. We can calculate the total filling as $\nu = 2\bar{\nu} = 2Q_{\alpha_1} + 2Q_{\beta_1} + Q_{\text{away}}$. Taking a mod 4 reduction and dividing by 2, we find $\bar{\nu} = Q_{\alpha_1} + Q_{\beta_1} \bmod 2$. Therefore, Q_{β_1} is determined from Q_{α_1} and $\bar{\nu}$, and thus

$$\bar{\nu} = \mathcal{S}_{\alpha_1}^{\text{U}(1)} + \mathcal{S}_{\beta_1}^{\text{U}(1)} \bmod 2. \quad (56)$$

We have thus shown that $\mathcal{S}_{\beta_1}^{\text{U}(1)}$ is not an independent invariant. (The analogous relation for p4m is Eq. (37).)

When $K = \mathbb{Z}_N$, the mixed phases are classified by two pieces: the first is $\mathcal{H}^2(\text{p4g}, \mathbb{Z}^{\text{or}}) \otimes \mathbb{Z}_N$ (charges modulo N), and the second is a new piece $\text{Tor}[\mathcal{H}^3(\text{p4g}, \mathbb{Z}^{\text{or}}), \mathbb{Z}_N] \cong \mathbb{Z}_{(N,2)}$. From our previous discussion of the group p4m, this piece can be detected by type-C1 invariants. In p4g, all reflections are conjugate to $\mathbf{r}_{\lambda_1}$. Therefore, this new

mixed SPT state can be constructed by placing mixed $\mathbb{Z}_2 \times \mathbb{Z}_N$ SPT states along the reflection axis λ_1 .

For $K = \text{SO}(3)$, the mixed SPT states are classified by $\mathbb{Z}_2$. As above, they correspond to placing a (1+1)D $\text{SO}(3)$ -SPT state on λ_1 .

In principle, one could construct the effective actions for p4g directly from the corresponding group cohomology cocycles, but we will leave this for future work. An interesting feature of these cocycles is that the area form¹² of p4g restricts to *twice* the area form of p4. This can be understood geometrically: the area form of p4g actually represents the fundamental domain which is half as large as the unit cell of p4 due to the glide symmetry.

V. GROUP COHOMOLOGY INTERPRETATION OF INVARIANTS

The previous two sections studied two specific wallpaper groups at length. In this section, we consider the 17 wallpaper groups in general and discuss how the various invariants in this paper fit into the group cohomology classification of bosonic SPTs. We also argue why the invariants listed in the tables give a complete classification as per group cohomology (possibly up to specifying some filling invariants). All the cohomology groups we actually need to compute have integer coefficients and can be evaluated using the GAP program [74]. These groups have been tabulated in Tables XIII, XIV. A physicist's introduction to the group cohomology definitions and formulas that we use in this paper can be found in Refs. [40, 46].

Table IV lists the classification of Type A1, A2 and A3 invariants, which are pure crystalline invariants. Consider a high-symmetry point o . If $G_o = C_{M_o}$, the classification of G_o SPTs is $\mathcal{H}^4(G_o, \mathbb{Z}) \cong \mathbb{Z}_{M_o}$, and this is detected by the type A1 invariant. If $G_o = D_{2M_o}$, the classification of G_o SPTs is $\mathcal{H}^4(G_o, \mathbb{Z}^{\text{or}}) \cong \mathbb{Z}_2 \times \mathbb{Z}_{(2, M_o)}$, and the two factors are detected by the type A1 and A2 invariants at o , respectively. Finally, suppose G_{space} has a $\mathbb{Z} \rtimes \mathbb{Z}_2^r$ subgroup generated by a translation and a reflection about an axis orthogonal to the translation direction. In this case $\mathcal{H}^4(\mathbb{Z} \rtimes \mathbb{Z}_2^r, \mathbb{Z}^{\text{or}}) \cong \mathbb{Z}_2$, and this is the class detected by the type A3 invariant.

For every wallpaper group G_{space} we have shown that type A1, A2 and A3 invariants evaluated for different o and l measure enough information to fully determine the SPT class. An independent and complete set of invariants for each wallpaper group is shown in Table IV. To obtain this result we used the following steps: first we constructed candidate generators for $\mathcal{H}^3(G, \text{U}(1)^{\text{or}})$ by taking the cup product between generators of $\mathcal{H}^1(G, \text{U}(1))$ and $\mathcal{H}^2(G, \mathbb{Z}^{\text{or}})$. To check that these classes are indeed generators, we evaluated the cohomology invariants associated to the type A invariants

in Table IV, and found that the set of candidate generators are indeed independent and complete.

Next, consider $G = G_{\text{space}} \times \text{U}(1)$. Using the Kunneth formula, we have

$$\mathcal{H}^4(G, \mathbb{Z}^{\text{or}}) \cong \mathcal{H}^4(G_{\text{space}}, \mathbb{Z}^{\text{or}}) \times \mathcal{H}^2(G_{\text{space}}, \mathbb{Z}^{\text{or}}). \quad (57)$$

The second term classifies the different assignments of $\text{U}(1)$ charge at points in the unit cell. This term always includes a $\mathbb{Z}$ factor, which gives the filling per fundamental domain (the usual filling ν for symmorphic wallpaper groups and $\nu/2$ for non-symmorphic wallpaper groups). The remaining factors can be determined using Type-B1 invariants. (Note that we can also recover partial information about ν from Type-B1 invariants.)

For $G = G_{\text{space}} \times \mathbb{Z}_N$, the mixed invariants are classified by the following term in the Kunneth decomposition:

$$\begin{aligned} \mathcal{H}^2(G_{\text{space}}, \mathcal{H}^1(\mathbb{Z}_N, \text{U}(1)^{\text{or}})) &= \mathcal{H}^2(G_{\text{space}}, \mathbb{Z}_N^{\text{or}}) \\ &= \mathcal{H}^2(G_{\text{space}}, \mathbb{Z}^{\text{or}}) \otimes \mathbb{Z}_N \\ &\quad \times \text{Tor}[\mathcal{H}^3(G_{\text{space}}, \mathbb{Z}^{\text{or}}), \mathbb{Z}_N]. \end{aligned} \quad (58)$$

The second equality uses the Universal Coefficient Theorem. The first term is a $\mathbb{Z}_N$ analog of the mixed invariant that appeared above with $K = \text{U}(1)$. This term always contains a $\mathbb{Z}_N$ factor which corresponds to the $\mathbb{Z}_N$ filling per unit cell. There are additional pieces, which are detected by the Type-C1 invariants. In all cases except for the group pm, these pieces can be interpreted as classifying the different assignments of $\mathbb{Z}_N$ charge at points in the unit cell. The special case of pm was addressed in Sec. IIB 7.

The Tor term on the last line is nontrivial only in the presence of reflection symmetries. It classifies (1+1)D SPTs of $\mathbb{Z}_N \times \mathbb{Z}_2^r$ symmetry that can be placed on the reflection axes in the unit cell. These correspond to the Type-C4 invariants in Table V.

Finally, for $G = G_{\text{space}} \times \text{SO}(3)$, the mixed invariants are classified by

$$\begin{aligned} \mathcal{H}^1(G_{\text{space}}, H^2(\text{SO}(3), \text{U}(1)^{\text{or}})) &= \mathcal{H}^1(G_{\text{space}}, \mathbb{Z}_2) \\ &= \text{Tor}[\mathcal{H}^2(G_{\text{space}}, \mathbb{Z}^{\text{or}}), \mathbb{Z}_2] \\ &\quad \times \mathcal{H}^1(G_{\text{space}}, \mathbb{Z}^{\text{or}}) \otimes \mathbb{Z}_2. \end{aligned} \quad (59)$$

The Tor term on the last line captures two distinct types of invariants. One type consists of mixed invariants between $\text{SO}(3)$ and C_{M_o} subgroups of G_{space} ; specifically, these invariants measure SPTs in which AKLT chains are placed on the boundaries of fundamental domains of the rotation symmetry. This subgroup can be detected by invariants of type D1. The second type classifies mixed invariants between $\text{SO}(3)$ and reflection subgroups of G_{space} . Specifically, these invariants measure SPTs in which AKLT chains are placed on the reflection axes. The corresponding invariants are of type D2. In general, there is some freedom in attributing a given factor of this Tor classification to type D1 or D2, if both rotations and

¹² By ‘area form’, we mean the generator of the $\mathbb{Z}$ factor in $\mathcal{H}^2(G_{\text{space}}, \mathbb{Z}^{\text{or}})$.

reflections are present.

The final term containing the tensor product $\otimes$ is non-trivial only in the presence of reflections. In this case, the classification is always a single factor of $\mathbb{Z}_2$, and the state carrying this invariant is constructed by stacking AKLT chains along the reflection axis. This topological phase can also be detected by an invariant of type D2.

Based on this discussion, we conclude that the new invariants we propose in this paper do capture the full mathematical classification of bosonic SPTs predicted by group cohomology.

VI. DISCUSSION

We have considered bosonic SPT states in (2+1)D with symmetry $G = G_{\text{space}} \times K$ where G_{space} is any of the 17 2d wallpaper groups and the internal symmetry $K = \text{U}(1), \mathbb{Z}_N$ or $\text{SO}(3)$. We have provided formulas to extract all the SPT invariants that depend on G_{space} , including pure crystalline invariants as well as mixed invariants between G_{space} and K . It was known that all the new invariants involving reflection symmetry can be physically understood in terms of lower-dimensional states decorated on a reflection axis. That they can all be detected with expectation values of partial reflections, suitably combined with other operations in G , is the main new result of this paper.

Below we address some related issues. First we consider the case where the given state does have pure K invariants. Next, we address to what extent the invariants presented here can be obtained from a single ground state wave function, and whether we might instead need a family of wave functions in some cases. Finally, we comment on future directions suggested by this work.

A. The case where pure K SPT invariants are nontrivial

So far in this paper, we have made the assumption that all topological invariants associated to K symmetry alone are trivial. In this section we consider the case where the given state might have nontrivial K SPT invariants, and to what extent our partial symmetry approaches can capture them.

When $K = \text{U}(1)$ the only pure K invariant is the bosonic Hall conductance $\sigma_H = 2C_{\text{U}(1)}e_b^2/h$ where e_b is the charge of an elementary boson. The Chern number $C_{\text{U}(1)}$ is a $\mathbb{Z}$ invariant. When $K = \mathbb{Z}_N$ we have a $\mathbb{Z}_N$ analog of this, whose coefficient $C_{\mathbb{Z}_N}$ is defined mod N . Finally, for $K = \text{SO}(3)$ there is a spin Hall conductance which is $\mathbb{Z}$ classified. Note that C_K and $-C_K$ must necessarily be equal for any G_{space} with orientation-reversing elements whenever $G = G_{\text{space}} \times K$ and G_{space} is unitary. Interestingly, our approach turns out to give partial information about these invariants, as we now discuss.

The only way in which the pure K invariants affect our previous results is to modify the formulas for the partial rotation invariants Θ_o^K . (Formulas to isolate the pure K invariants have been given in [65].) Using CFT arguments, it was shown [37] that the most general formula in this case is

$$\Theta_o^K - \Theta_o - C_K = \begin{cases} \mathcal{S}_o^{\text{U}(1)} \mod M_o & K = \text{U}(1) \\ \mathcal{S}_o^{\mathbb{Z}_N} \mod (M_o, N) & K = \mathbb{Z}_N \\ \frac{M_o}{(M_o, 2)} \mathcal{S}_o^{\text{SO}(3)} \mod M_o & K = \text{SO}(3) \end{cases} \quad (60)$$

Thus for a given M_o -fold rotation about o , $\Theta_o^{\text{U}(1)}$ contains information about $C_{\text{U}(1)} \mod M_o$, while $\Theta_o^{\mathbb{Z}_N}$ contains information about $C_{\mathbb{Z}_N} \mod (M_o, N)$. In defining $\Theta_o^{\text{SO}(3)}$, we consider an M_o -fold rotation instead of the 2-fold rotation used previously. Note that the pure $\text{SO}(3)$ SPT invariant $C_{\text{SO}(3)}$ manifests as a Hall conductance which must be an even multiple of the elementary BIQH conductance $C_{\text{U}(1)} = 1$; therefore it only contributes when M_o is even and $M_o \geq 4$. We can thus conclude that if M is the largest possible value of M_o for the given lattice, partial rotations can at best determine $C_{\text{U}(1)} \mod M$ and $C_{\mathbb{Z}_N} \mod (M, N)$. However, in order to extract even this information, we need to determine Θ_o and $\mathcal{S}_o^K$ separately for sufficiently many origins o . The precise extent to which this is possible depends on G_{space} .

B. Requirement of a single ground state wave function

In general, a partial symmetry invariant of the form $\langle \psi | \hat{O} | \psi \rangle$ only requires a single ground state wave function $|\psi\rangle$, while an invariant involving an expression such as $\langle \psi_{\mathbf{g}_1} | \hat{O} | \psi_{\mathbf{g}_2} \rangle$ requires a family of ground states with boundary conditions twisted by $\mathbf{g}_1, \mathbf{g}_2 \in K$. From our definitions we can see that all the invariants except for the ‘weak’ invariants, and Types C4 and D4 can be obtained from a single wave function. For the weak invariants, we need to consider the ground state on different system sizes, while in the other two cases we need to consider twisted boundary conditions. Note that we can alternatively measure type C4 and D4 invariants using type C2 and D2 respectively, and these use a single wave function. Therefore the only case in which we still need multiple wave functions is the weak case.

There are 5 wallpaper groups in which it is necessary to measure weak invariants: pm, cm, pmg, p3m1, and p31m. The common feature of these lattices is that they have a reflection axis which does not pass through any C_2 rotation center. Indeed, whenever such a point with D_2 symmetry exists, we can measure the same invariant differently: for example, we can replace the type A3 invariant with a type A2 invariant, which does not require multiple ground states. It is not clear to us whether there is an alternative way to measure the weak invariants us-

ing a single ground state wave function.

C. Future directions

A natural extension of this work is to consider invertible fermionic states with general wallpaper group symmetries. Real-space classifications of such states are already available, for various K [75]. In this case, the full symmetry is given by a group extension of the ‘bosonic’ symmetry group G_b by fermion parity $\mathbb{Z}_2^f$. We expect that the main additional step is to properly define partial symmetry invariants for operations in G_b that extend fermion parity in different ways. It would also be interesting to fully understand the relations between the different invariants studied here, since we have not derived all possible relations in this paper.

Another important direction is to numerically test the various predictions made here in ground states that are away from any ideal limit, and also to potentially simplify the formulas to make them more natural to implement in an experiment or a quantum simulation.

Finally, the invariants described in this paper are also relevant to symmetry-enriched topological (SET) phases, which harbor topologically degenerate ground states and anyonic excitations. Recent work has already shown the applicability of partial rotations in obtaining the symmetry fractionalization data and response invariants for fractional Chern insulators (FCI) [76]. We expect that the partial reflection invariants defined here will prove similarly useful in studying SET phases with reflection symmetry, such as quantum spin liquids.

VII. ACKNOWLEDGEMENTS

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Appendix A: Review of real space construction

According to Ref. [27], crystalline SPTs when K is trivial can be constructed by placing G_p charges at p for all maximal Wyckoff positions p for the wallpaper group G_{space} .

For a non-trivial K , Ref. [28] tells us that the real space construction is done by decorating n -simplices of an equivariant decomposition of the unit cell. Each n -simplex is decorated by an SPT in $(n+1)$ D protected by K and any lattice symmetry that leaves the simplex invariant. There are additional relations and restrictions between the possible decorations. We can read off how many decorations for each n are needed to construct states in each of the different phases from Table III of Ref. [28]. Using this result, we see that

1. For $K = \text{U}(1)$, we only need to decorate 0-simplices, which corresponds to placing $\text{U}(1)$ charges at the Wyckoff positions.
2. For $K = \text{SO}(3)$, we need to decorate 1-simplices. Only reflections can leave 1-simplices invariant and there are no $\mathbb{Z}_2 \times \text{SO}(3)$ mixed SPT phases in $(1+1)$ D. Then, the decorations correspond to placing $\text{SO}(3)$ SPT states on the 1-simplices. Simple examples of this include singlets made of two $S = 1/2$ spins.
3. For $K = \mathbb{Z}_N$, we need to decorate both 0- and 1-simplices. The decorations on 0 simplices correspond to placing $\mathbb{Z}_N$ charges at different Wyckoff positions. The 1-simplex decorations come from $\mathbb{Z}_N \times \mathbb{Z}_2$ mixed $(1+1)$ D SPTs, which are only present when there are reflections.

Appendix B: Relation between $\Sigma_{o,l}$ and TQFT partition function

The aim of this appendix is to relate the expectation value which defines $\Sigma_{o,l}$ to a TQFT partition function that evaluates to the invariant $k_{2,o,l}$ in the topological action of D_{2n} (Eq. 24). This is summarized by the result

$$\Sigma_{o,l} = k_{2,o,l}. \quad (\text{B1})$$

In App. B 1, we relate the partial double reflection to a particular TQFT partition function, which we evaluate in App. B 2. App. B 3 extends these calculations to the dressed partial double reflection $\Sigma_{o,l}(\mathbf{k}, \mathbf{j})$.

1. Relation with TQFT

We start with the ground state Ψ on a disk and choose a region $D = D_l \cup D_c \cup D_r$ as in Fig. 1. Then, the reduced density matrix $\rho = \text{Tr}_{\bar{D}}[|\Psi\rangle\langle\Psi|]$, representing the state in the region D , is represented as a solid sphere.

The northern and southern hemispheres correspond to the ket and bra parts of the state, respectively. We then triangulate the bra and ket parts of the surface as shown in panels (a) and (b) of Fig. 5, respectively.

Next, we determine the surface gluing prescription by analyzing the partial symmetry operator: $R_l|_{D_c} \cdot (R_{l'})|_{D_l \cup D_r}$. Recall that l and l' denote horizontal and vertical reflection lines, respectively (see Fig. 1).

The partial vertical reflection $R_{l'}|_{D_l \cup D_r}$ acts on the side regions, interchanging the red and blue regions, which dictates the gluing of $D_l \leftrightarrow D_r^*$ and $D_r \leftrightarrow D_l^*$.

Similarly, the partial horizontal reflection $R_l|_{D_c}$ dictates the following gluing of regions $D_{c,1} \leftrightarrow D_{c,4}^*$, $D_{c,2} \leftrightarrow D_{c,3}^*$, $D_{c,3} \leftrightarrow D_{c,2}^*$, and $D_{c,4} \leftrightarrow D_{c,1}^*$.

Having established an intuitive understanding of the gluing process based on the symmetries, we now provide a formal description using a specific triangulation of the sphere, which we deform to a cylinder for simplicity.

2. Evaluation of partition function

The analysis below follows the detailed discussion of state-sum constructions in Ref. [54].

We triangulate the cylinder representing the state on region D as shown in Fig. 6. We used the same vertex labeling as in Fig. 5. We denote the n -simplices by $\Delta_{i_1 \dots i_n}^n$, where $i_1 < i_2 < \dots < i_n$ are the vertices. The plane containing the 2-simplex Δ_{045}^2 separates the ‘bra’ and ‘ket’ regions of the state. For reference, the faces in Fig. 5 correspond to 2-simplices Δ_{ijk}^2 , where i, j, k are the vertices on the boundary of said face. We now use the previously defined surface gluing prescription to identify 2-simplices. For example, we need to identify $\Delta_{012}^2 \sim \Delta_{457}^2$ and $\Delta_{026}^2 \sim \Delta_{137}^2$.

Since all 0-simplices and 1-simplices on the boundary of the 2-simplices also need to be identified, the resulting cellulation has: 2 0-simplices (Δ_0^0, Δ_2^0), 6 1-simplices ($\Delta_{01}^1, \Delta_{02}^1, \Delta_{03}^1, \Delta_{04}^1, \Delta_{05}^1, \Delta_{26}^1$), 8 2-simplices, and 6 3-simplices. To simplify the expressions, we define the group element $\mathbf{c} \equiv \mathbf{h}_o^{M_o/2}$ and $\mathbf{r} \equiv \mathbf{r}_l$. Since the invariant is solely determined by the $D_2 = \{\mathbf{0}, \mathbf{c}, \mathbf{r}, \mathbf{cr}\}$ subgroup of D_{2n} , we evaluate the state sum using $G = D_2$.

Even though we identify the 0-simplices associated to vertices 0, 1, 4, 5 and 2, 3, 6, 7, the corresponding group elements are related by multiplication with the appropriate group element. Explicitly, we have

$$\begin{aligned} \mathbf{g}_1 &= \mathbf{r}\mathbf{g}_0, & \mathbf{g}_4 &= \mathbf{r}\mathbf{c}\mathbf{g}_0, & \mathbf{g}_5 &= \mathbf{c}\mathbf{g}_0, \\ \mathbf{g}_3 &= \mathbf{r}\mathbf{g}_2, & \mathbf{g}_6 &= \mathbf{c}\mathbf{g}_2, & \mathbf{g}_7 &= \mathbf{r}\mathbf{c}\mathbf{g}_2. \end{aligned} \quad (\text{B2})$$

To each 3-simplex and configuration of group elements $\{\mathbf{g}_j\}$, we assign a complex phase

$$\mathcal{Z}(\Delta_{j_1 j_2 j_3 j_4}^3; \{\mathbf{g}_j\}) = \tilde{\nu}_3(\mathbf{g}_{j_1}, \mathbf{g}_{j_2}, \mathbf{g}_{j_3}, \mathbf{g}_{j_4})^{s(\Delta_{j_1 j_2 j_3 j_4}^3)}, \quad (\text{B3})$$

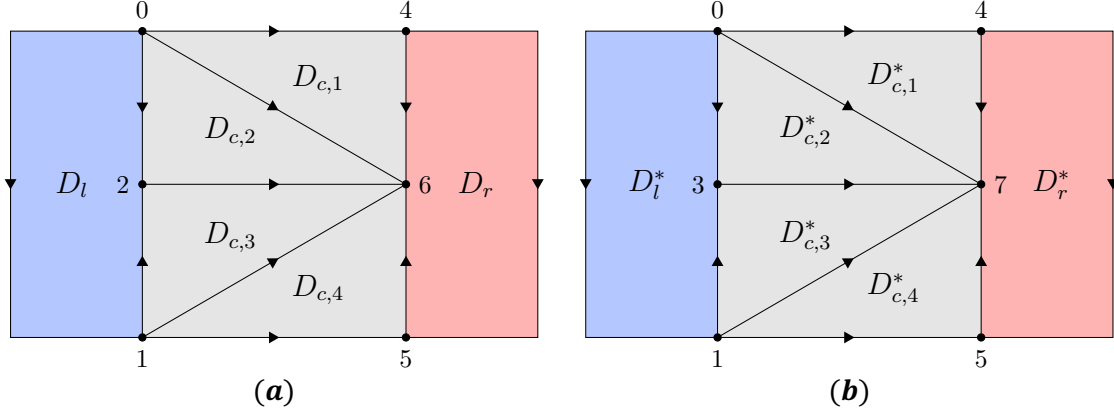


FIG. 5. The state on the region $D = D_l \cup D_c \cup D_r$ is represented by a solid sphere, whose boundary is a sphere. The northern hemisphere is the ‘ket’ part of the state, which we triangulate as shown in panel (a). We have broken region D_c into four smaller regions to accommodate the triangulation. Panel (b) shows the triangulation of the ‘bra’ part. Note that the boundaries of the regions in panels (a) and (b) are the same because it corresponds to the equator of the sphere representing the state.

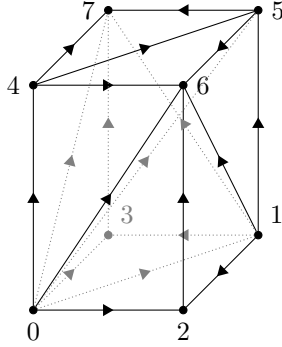


FIG. 6. Triangulation of the square prism used to evaluate the partial double reflection as a state sum construction. The 2-simplices Δ_{012}^2 and Δ_{456}^2 are identified with the region D_r and D_l , respectively, of the ‘bra’ when evaluating the double partial reflection.

where $\tilde{\nu}_3$ is a homogeneous cocycle, satisfying

$$\tilde{\nu}_3(\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3, \mathbf{g}_4) = \tilde{\nu}_3(\mathbf{g}_0 \mathbf{g}_1, \mathbf{g}_0 \mathbf{g}_2, \mathbf{g}_0 \mathbf{g}_3, \mathbf{g}_0 \mathbf{g}_4)^{p(\mathbf{g}_0)} \quad (\text{B4})$$

for $\mathbf{g}_0, \dots, \mathbf{g}_4 \in G$. $p(\mathbf{g}_0) = 1$ if $\mathbf{g}_0$ is orientation pre-

serving, and $p(\mathbf{g}_0) = *$ is complex conjugation if $\mathbf{g}_0$ is orientation reversing. There is a one to one map between homogeneous and inhomogeneous cocycles:

$$\nu_3(\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3) = \tilde{\nu}_3(\mathbf{0}, \mathbf{g}_1, \mathbf{g}_1 \mathbf{g}_2, \mathbf{g}_1 \mathbf{g}_2 \mathbf{g}_3), \quad (\text{B5})$$

where ν_3 is the inhomogeneous cocycle we have used in most of the paper.

The partition function is

$$\mathcal{Z}(\mathcal{M}^3) = \frac{1}{|G|^{N_v}} \sum_{\{\mathbf{g}_j\}} \prod_{\Delta^3 \in \mathcal{I}_3} \mathcal{Z}(\Delta^3; \{\mathbf{g}_j\})^{s(\Delta^3)}, \quad (\text{B6})$$

where $\mathcal{I}_n$ is the set of n -simplices of the cellulation of the manifold $\mathcal{M}^3$, and N_v is the number of 0-simplices. $s(\Delta^3)$ is the orientation of the 3-simplex relative to a reference 3-simplex. Then $s(\Delta^3) = 1(*)$ if Δ^3 has the same (opposite) orientation as the reference 3-simplex. As our cellulation is constructed from a triangulation, the orientation is such that any two 3-simplices sharing a 2-simplex must have opposite orientation. In our case, $\Delta_{0126}^3, \Delta_{9456}^3$ and Δ_{0157}^3 have the same orientation, while $\Delta_{0156}^3, \Delta_{0137}^3$ and Δ_{0457}^3 have orientation opposite to Δ_{0126}^3 . Therefore, for a given configuration $\{\mathbf{g}_j\}$ (which is specified by $\mathbf{g}_0$ and $\mathbf{g}_2$ in our case), the summand in Eq. B6 is then

$$\begin{aligned} e^{iS[\{\mathbf{g}_j\}]} &= \frac{\tilde{\nu}_3(\mathbf{g}_0, \mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_6) \tilde{\nu}_3(\mathbf{g}_0, \mathbf{g}_4, \mathbf{g}_5, \mathbf{g}_6) \nu_3(\mathbf{g}_0, \mathbf{g}_1, \mathbf{g}_5, \mathbf{g}_7)}{\tilde{\nu}_3(\mathbf{g}_0, \mathbf{g}_1, \mathbf{g}_5, \mathbf{g}_6) \nu_3(\mathbf{g}_0, \mathbf{g}_4, \mathbf{g}_5, \mathbf{g}_7) \nu_3(\mathbf{g}_0, \mathbf{g}_1, \mathbf{g}_3, \mathbf{g}_7)} \\ &= \left[\frac{\nu_3(\mathbf{r}, \mathbf{r}\mathbf{g}, \mathbf{c}) \nu_3(\mathbf{r}\mathbf{c}, \mathbf{r}, \mathbf{g}) \nu_3(\mathbf{g}, \mathbf{r}\mathbf{c}, \mathbf{r}\mathbf{g})}{\nu_3(\mathbf{r}, \mathbf{c}\mathbf{r}, \mathbf{g}) \nu_3(\mathbf{r}\mathbf{c}, \mathbf{r}, \mathbf{r}\mathbf{g}) \nu_3(\mathbf{r}, \mathbf{g}, \mathbf{c})} \right]^{p(\mathbf{g}_0)} \end{aligned} \quad (\text{B7})$$

where we have defined $\mathbf{g} := \mathbf{g}_0^{-1} \mathbf{g}_2$. We need to simplify the above action.

By combining the following expressions

$$\begin{aligned}
1 &= \bar{d}\nu_3(\mathbf{r}, \mathbf{c}, \mathbf{r}, \mathbf{rg}) = \frac{\nu_3(\mathbf{r}, \mathbf{cr}, \mathbf{rg})\nu_3(\mathbf{r}, \mathbf{c}, \mathbf{r})}{\nu_3(\mathbf{c}, \mathbf{r}, \mathbf{rg})\nu_3(\mathbf{cr}, \mathbf{r}, \mathbf{rg})\nu_3(\mathbf{r}, \mathbf{c}, \mathbf{g})}; \\
1 &= \bar{d}\nu_3(\mathbf{r}, \mathbf{r}, \mathbf{c}, \mathbf{g}) = \frac{\nu_3(\mathbf{r}, \mathbf{rc}, \mathbf{g})\nu_3(\mathbf{r}, \mathbf{r}, \mathbf{c})}{\nu_3(\mathbf{r}, \mathbf{c}, \mathbf{g})\nu_3(\mathbf{0}, \mathbf{c}, \mathbf{g})\nu_3(\mathbf{r}, \mathbf{r}, \mathbf{cg})}; \\
1 &= \bar{d}\nu_3(\mathbf{c}, \mathbf{r}, \mathbf{r}, \mathbf{g}) = \frac{\nu_3(\mathbf{r}, \mathbf{r}, \mathbf{g})\nu_3(\mathbf{c}, \mathbf{0}, \mathbf{g})\nu_3(\mathbf{c}, \mathbf{r}, \mathbf{r})}{\nu_3(\mathbf{cr}, \mathbf{r}, \mathbf{g})\nu_3(\mathbf{c}, \mathbf{r}, \mathbf{rg})}; \\
1 &= \bar{d}\nu_3(\mathbf{r}, \mathbf{r}, \mathbf{g}, \mathbf{c}) = \frac{\nu_3(\mathbf{r}, \mathbf{rg}, \mathbf{c})\nu_3(\mathbf{r}, \mathbf{r}, \mathbf{g})}{\nu_3(\mathbf{r}, \mathbf{g}, \mathbf{c})\nu_3(\mathbf{0}, \mathbf{g}, \mathbf{c})\nu_3(\mathbf{r}, \mathbf{r}, \mathbf{gc})}; \\
\iota_{\mathbf{c}}\nu_3(\mathbf{r}, \mathbf{r}) &= \frac{\nu_3(\mathbf{c}, \mathbf{r}, \mathbf{r})\nu_3(\mathbf{r}, \mathbf{r}, \mathbf{c})}{\nu_3(\mathbf{r}, \mathbf{c}, \mathbf{r})}; \\
\iota_{\mathbf{c}}\nu_3(\mathbf{0}, \mathbf{g}) &= \frac{\nu_3(\mathbf{c}, \mathbf{0}, \mathbf{g})\nu_3(\mathbf{0}, \mathbf{g}, \mathbf{c})}{\nu_3(\mathbf{0}, \mathbf{c}, \mathbf{g})},
\end{aligned} \tag{B8}$$

we obtain

$$e^{iS[\{\mathbf{g}_j\}]} = [\iota_{\mathbf{c}}\nu_3(\mathbf{r}, \mathbf{r})\iota_{\mathbf{c}}\nu_3(\mathbf{0}, \mathbf{c})]^{p(\mathbf{g}_0)}. \tag{B9}$$

Given that ν_3 can be taken to be normalized (i.e., $\nu_3 = 1$ whenever any of its arguments equals $\mathbf{0}$), we identify

$$\iota_{\mathbf{c}}\nu_3(\mathbf{r}, \mathbf{r}) = \mathcal{Z}(\mathbb{RP}_{\mathbf{r}}^2 \times S_{\mathbf{c}}^1) \tag{B10}$$

(see App. C 1 a). Since this partition function can only take real values ± 1 , we may omit the factor $p(\mathbf{g}_0)$. Consequently,

$$\begin{aligned}
\mathcal{Z}(\mathcal{M}^3) &= \frac{1}{4^2} \sum_{\mathbf{g}_0, \mathbf{g}_2 \in D_2} \mathcal{Z}(\mathbb{RP}_{\mathbf{r}}^2 \times S_{\mathbf{c}}^1) \\
&= \mathcal{Z}(\mathbb{RP}_{\mathbf{r}}^2 \times S_{\mathbf{c}}^1).
\end{aligned} \tag{B11}$$

3. Dressed Partial double reflection

The dressed partial double reflection is obtained from the operator defined in Eq. 17. The difference compared to the bare partial double reflection is the additional action of $\mathbf{j}$, $\mathbf{k}$, and $\mathbf{k}^{-1}$ on the regions D_c , D_l , and D_r , respectively. The identification of 2-simplices is the same as for the bare partial double reflection. However, the identification of group elements becomes

$$\begin{aligned}
\mathbf{g}_1 &= \mathbf{rjg}_0, & \mathbf{g}_4 &= \mathbf{rckg}_0, & \mathbf{g}_5 &= \mathbf{cjk g}_0, \\
\mathbf{g}_3 &= \mathbf{rjg}_2, & \mathbf{g}_6 &= \mathbf{cjk g}_2, & \mathbf{g}_7 &= \mathbf{rckg}_2.
\end{aligned} \tag{B12}$$

The group elements now belong to $G = \mathbb{Z}_2^{\mathbf{r}} \times \mathbb{Z}_2^{\mathbf{c}} \times \mathbb{Z}_2^{\mathbf{j}} \times \mathbb{Z}_{2n}^{\mathbf{k}}$. The summand in the partition function now becomes

$$e^{iS[\{\mathbf{g}_j\}]} = \left[\frac{\nu_3(\tilde{\mathbf{r}}, \tilde{\mathbf{r}}\mathbf{g}, \mathbf{s})\nu_3(\tilde{\mathbf{r}}\mathbf{s}, \tilde{\mathbf{r}}, \mathbf{g})\nu_3(\mathbf{g}, \tilde{\mathbf{r}}\mathbf{s}, \tilde{\mathbf{r}}\mathbf{g})}{\nu_3(\tilde{\mathbf{r}}, \tilde{\mathbf{s}}\mathbf{r}, \mathbf{g})\nu_3(\tilde{\mathbf{r}}\mathbf{s}, \tilde{\mathbf{r}}, \tilde{\mathbf{r}}\mathbf{g})\nu_3(\tilde{\mathbf{r}}, \mathbf{g}, \mathbf{s})} \right]^{p(\mathbf{g}_0)}, \tag{B13}$$

where $\tilde{\mathbf{r}} = \mathbf{rj}$ and $\mathbf{s} = \mathbf{cjk}$. Using the same steps to get from Eq. B7 to Eq. B9, we obtain¹³

$$e^{iS[\{\mathbf{g}_j\}]} = [\iota_{\mathbf{s}}\nu_3(\tilde{\mathbf{r}}, \tilde{\mathbf{r}})]^{p(\mathbf{g}_0)}, \tag{B14}$$

where we have assumed that ν_3 is a normalized cocycle. From the Künneth formula, $\mathcal{H}^3(\mathbb{Z}_{2n} \times \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2^{\mathbf{r}}, \mathbf{U}(1)^{\text{or}}) = \mathbb{Z}_2^J$ for some integer J . This implies that the invariant $\iota_{\mathbf{s}}\nu_3(\tilde{\mathbf{r}}, \tilde{\mathbf{r}})$ can only take the values ± 1 . Then, we can remove $p(\mathbf{g}_0)$ in Eq. B9 and obtain

$$\mathcal{Z}(\mathcal{M}^3) = [\iota_{\mathbf{s}}\nu_3(\tilde{\mathbf{r}}, \tilde{\mathbf{r}})], \tag{B15}$$

after summing over $\mathbf{g}_0$ and $\mathbf{g}_2$. Using the same arguments to interpret the bare partial double reflection, we obtain

$$\mathcal{Z}(\mathcal{M}^3) = \mathcal{Z}(\mathbb{RP}_{\mathbf{jr}}^2 \times S_{\mathbf{cjk}}^1). \tag{B16}$$

Appendix C: Details on group cohomology for p4m

This appendix contains the explicit cocycles and cohomology invariants we used in Sec. III. App. C 1 focuses on dihedral groups D_{2n} , providing the ground work for the full analysis of the wallpaper group p4m in App. C 2.

1. Group cohomology of D_{2n}

Recall that D_{2n} is the dihedral group with $4n$ elements, generated by a reflection $\mathbf{r}$ and $2n$ -fold rotation $\mathbf{h}$. These elements satisfy the relations

$$\mathbf{r}^2 = \mathbf{h}^{2n} = (\mathbf{rh})^2 = \mathbf{0}, \tag{C1}$$

¹³ To obtain the relations in Eq. B8 used that $\mathbf{r}^2 = \mathbf{0}$ but never that $\mathbf{g}^2 = \mathbf{c}^2 = \mathbf{0}$. Therefore, they remain valid after replacing $(\mathbf{r}, \mathbf{c}) \rightarrow (\tilde{\mathbf{r}}, \mathbf{s})$.

where $\mathbf{0}$ is the identity. Then, a general element in D_{2n} can be written as $\mathbf{h}^a \mathbf{r}^b$ with $a \in \{0, 1, \dots, 2n-1\}$ and $b \in \{0, 1\}$. See Ref. [77] for a calculation of the group cohomology groups we cite below.

Consider the following cochains $f_0, f_1, f_2 \in C^1(D_{2n}, \mathbb{Z})$:

$$\begin{aligned} f_0(\mathbf{h}^a \mathbf{r}^b) &= [a]_{2n}; & f_1(\mathbf{h}^a \mathbf{r}^b) &= [a]_2; \\ f_2(\mathbf{h}^a \mathbf{r}^b) &= [b]_2. \end{aligned} \quad (\text{C2})$$

Recall that $[s]_m$ is the residue of s modulo m , with

$$\tilde{z}_1(\mathbf{h}^{a_1} \mathbf{r}^{b_1}, \mathbf{h}^{a_2} \mathbf{r}^{b_2}) = \frac{[a_1]_{2n} + (-1)^{b_1} [a_2]_{2n} - [a_1 + (-1)^{b_1} a_2]_{2n}}{2n}. \quad (\text{C4})$$

According to Ref. [77], $\mathcal{H}^4(D_{2n}, \mathbb{Z}^{\text{or}})$ is isomorphic to $\mathbb{Z}_2 \times \mathbb{Z}_2$ as an Abelian group, and its generators are precisely the cup product of the generators of $\mathcal{H}^2(D_{2n}, \mathbb{Z})$ with the generator of $\mathcal{H}^2(D_{2n}, \mathbb{Z}^{\text{or}})$. In other words, the generators are $\tilde{Z}_j = z_j \cup \tilde{z}_1$ for $j = 1, 2$, or more explicitly:

$$\tilde{Z}_j(\mathbf{h}^{a_1} \mathbf{r}^{b_1}, \mathbf{h}^{a_2} \mathbf{r}^{b_2}, \mathbf{h}^{a_3} \mathbf{r}^{b_3}, \mathbf{h}^{a_4} \mathbf{r}^{b_4}) = z_j(\mathbf{h}^{a_1} \mathbf{r}^{b_1}, \mathbf{h}^{a_2} \mathbf{r}^{b_2}) (-1)^{b_1+b_2} \tilde{z}_1(\mathbf{h}^{a_3} \mathbf{r}^{b_3}, \mathbf{h}^{a_4} \mathbf{r}^{b_4}). \quad (\text{C5})$$

The factor $(-1)^{b_1}$ appears because we are dealing with cocycles with twisted coefficients¹⁴, e.g. see Appendix A.1 of Ref. [78].

Finally, by the Bockstein homomorphism one has $\mathcal{H}^3(D_{2n}, \text{U}(1)^{\text{or}}) \cong \mathcal{H}^4(D_{2n}, \mathbb{Z}^{\text{or}})$, and representative cocycles can be obtained by finding cochains $\Phi \in C^3(D_{2n}, \mathbb{R})$ satisfying $\bar{d}\Phi = 2\pi\tilde{Z}$ for $\tilde{Z} \in Z^4(D_{2n}, \mathbb{Z}^{\text{or}})$. The respective cocycle $\zeta \in Z^3(D_{2n}, \text{U}(1)^{\text{or}})$ is $\zeta = e^{i\Phi}$. We can solve for Φ easily using: (1) $\bar{d}^2 = 0$, and (2) the Leibnitz rule. These conditions give $\bar{d}\Phi_j = \tilde{Z}_j$ is $\Phi_j = \pi f_j \cup \tilde{z}_1$ for $j = 1, 2$.

Thus a general element $\mathcal{H}^3(D_{2n}, \text{U}(1)^{\text{or}})$ is represented by a cocycle of the form

$$\varphi_3 = k_1 \Phi_1 + k_2 \Phi_2; \quad k_1, k_2 \in \mathbb{Z}_2, \quad (\text{C6})$$

or, equivalently,

$$\nu_3 = \zeta_1^{k_1} \zeta_2^{k_2}. \quad (\text{C7})$$

a. Cohomology invariants

To extract the invariants k_1 and k_2 from a generic cocycle $\nu_3 \in Z^3(D_{2n}, \text{U}(1)^{\text{or}})$, consider the following quan-

$[s]_m$ taking values in $\{0, 1, \dots, m-1\}$. Representative cochains for the generators of $\mathcal{H}^2(D_{2n}, \mathbb{Z}) \cong \mathbb{Z}_2 \times \mathbb{Z}_2$ are $z_1 := \frac{df_1}{2}$ and $z_2 := \frac{df_2}{2}$. More explicitly

$$\begin{aligned} z_1(\mathbf{h}^{a_1} \mathbf{r}^{b_1}, \mathbf{h}^{a_2} \mathbf{r}^{b_2}) &= [a_1]_2 [a_2]_2; \\ z_2(\mathbf{h}^{a_1} \mathbf{r}^{b_1}, \mathbf{h}^{a_2} \mathbf{r}^{b_2}) &= [b_1]_2 [b_2]_2. \end{aligned} \quad (\text{C3})$$

Similarly, $\mathcal{H}^2(D_{2n}, \mathbb{Z}^{\text{or}}) \cong \mathbb{Z}_{2n}$ is generated by $\tilde{z}_1 := \frac{\bar{d}f_0}{2n}$, or more explicitly:

tities :

$$\begin{aligned} \mathcal{I}_1[\nu_3] &:= \prod_{j=0}^{2n-1} \nu_3(\mathbf{h}, \mathbf{h}^j, \mathbf{h}) \\ \mathcal{I}_2[\nu_3] &:= \prod_{j=0}^1 \frac{\nu_3(\mathbf{h}^n, \mathbf{r}^j, \mathbf{r}) \nu_3(\mathbf{r}^j, \mathbf{r}, \mathbf{h}^n)}{\nu_3(\mathbf{r}^j, \mathbf{h}^n, \mathbf{r})}. \end{aligned} \quad (\text{C8})$$

It is a standard result that $\mathcal{I}_1$ is coboundary-invariant, e.g. see [72]. $\mathcal{I}_2$ is an invariant if $\mathcal{I}_2[\bar{d}\alpha] = 1$ for any $\alpha \in C^2(D_{2n}, \text{U}(1))$. Note that

$$\bar{d}\alpha(\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3) = \frac{\mathbf{g}_1 \alpha(\mathbf{g}_2, \mathbf{g}_3) \alpha(\mathbf{g}_1, \mathbf{g}_2 \mathbf{g}_3)}{\alpha(\mathbf{g}_1 \mathbf{g}_2, \mathbf{g}_3) \alpha(\mathbf{g}_1, \mathbf{g}_2)}. \quad (\text{C9})$$

Recall that $\mathbf{g}_1 \alpha(\mathbf{g}_2, \mathbf{g}_3) = [\alpha(\mathbf{g}_2, \mathbf{g}_3)]^{(-1)^b}$ for $\mathbf{g} = \mathbf{h}^a \mathbf{r}^b$. It is straightforward to show that $\mathcal{I}_2[\bar{d}\alpha] = 1$ by combining Eqs. C9 and C8.

We then evaluate the invariants for ν_3 in Eq. C6:

$$\mathcal{I}_1[\nu_3] = (-1)^{k_1}; \quad \mathcal{I}_2[\nu_3] = (-1)^{k_2}. \quad (\text{C10})$$

We have thus shown that $\{\mathcal{I}_1, \mathcal{I}_2\}$ is an independent and complete set of invariants.

A well-known interpretation of the invariant $\mathcal{I}_1$ is that it evaluates the partition function of the TQFT on a lens space with appropriate fluxes along its non-trivial cycle

¹⁴ Recall that $\tilde{z}_1$ is a cocycle with values in $\mathbb{Z}^{\text{or}}$.

[72]. To interpret $\mathcal{I}_2$, we note that

$$\begin{aligned}\mathcal{I}_2[\nu_3] &= \mathcal{J}[\iota_{\mathbf{h}^n} \nu_3]; \\ (\iota_{\mathbf{g}_0} \nu_3)(\mathbf{g}_1, \mathbf{g}_2) &:= \frac{\nu_3(\mathbf{g}_0, \mathbf{g}_1, \mathbf{g}_2) \nu_3(\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_0)}{\nu_3(\mathbf{g}_1, \mathbf{g}_0, \mathbf{g}_2)}; \\ \mathcal{J}[\mu] &:= \mu(\mathbf{r}, \mathbf{r}) \mu(\mathbf{0}, \mathbf{r}),\end{aligned}\quad (\text{C11})$$

where $\iota_{\mathbf{g}}$ denotes the Slant product and $\mathcal{J}$ is an invariant defined for 2-cochains. On the non-orientable manifold $\mathbb{RP}^2$, the partition function evaluates precisely the invariant $\mathcal{J}$ [54]. The action of the Slant product with a group element $\mathbf{g}$ can be interpreted as compactifying one direction into a circle with a $\mathbf{g}$ -flux threaded through it [72]. Therefore, $\mathcal{I}_2$ is the value of the partition function on the manifold $S^1 \times \mathbb{RP}^2$, with $\mathbf{h}^n$ flux through S^1 .

Note that D_{2n} has $2n$ distinct reflections, given by $\mathbf{r}_a = \mathbf{h}^a \mathbf{r}$ with $a = 0, 1, \dots, 2n-1$. For each reflection, we can define an invariant $\mathcal{I}_{2,a}[\nu_3] = \prod_{j=0,1} (\iota_{\mathbf{h}^j} \nu_3)(\mathbf{r}_a^j, \mathbf{r}_l)$. We can evaluate $\mathcal{I}_{2,a}[\nu_3] = (-1)^{ak_1+k_2}$. In this sense, the k_2 invariant depends on a choice of reflection axis.

b. Relation to topological action

The gauge fields are obtained by pullbacks using the map $B: \omega = \frac{2\pi}{2n} B^* f_0$ and $\sigma = B^* f_2$. Then $\frac{\bar{d}\omega}{2\pi} = B^* \tilde{z}_1 \in \mathbb{Z}$ and $n\omega = \pi B^* f_1 \mod 2\pi$. Thus,

$$\begin{aligned}B^* \Phi_1 &= n\omega \frac{\bar{d}\omega}{2\pi} \mod 2\pi; \\ B^* \Phi_2 &= \pi\sigma \frac{\bar{d}\omega}{2\pi} \mod 2\pi.\end{aligned}\quad (\text{C12})$$

We can recover Eq. 24 by setting $\mathcal{L} = B^* \varphi_3$ and replacing $(k_1, k_2) \rightarrow (k_{1,o}, k_{2,o,l})$ in Eq. C6. We added the l subscript to remark that this coefficient depends on the choice of reflection axis when writing the action. The subscript o is redundant at the moment but will be important once we study p4m.

Another way to see the reflection axis dependence of k_2 is to use a different reference reflection to write gauge fields: we factorizing the group elements as $\mathbf{h}^{a'}(\mathbf{h}\mathbf{r})^{b'}$. This means that the new gauge fields (primed) are related to the old gauge fields (unprimed) by $\omega' \sim \omega + \pi\sigma/n$ and $\sigma' \sim \sigma$. Thus

$$\begin{aligned}n\omega' \frac{\bar{d}\omega'}{2\pi} &= n\omega \frac{\bar{d}\omega}{2\pi} + \omega \frac{\bar{d}\omega}{2\pi} \\ \sigma' \frac{\bar{d}\omega'}{2\pi} &= \sigma \frac{\bar{d}\omega}{2\pi}\end{aligned}\quad (\text{C13})$$

where we have used that $\bar{d}\sigma = 0$. Therefore, by changing the reference reflection axis used to define the gauge fields, the coefficients in the action change. If l' is defined by $\mathbf{r}_{l'} = \mathbf{h}\mathbf{r}_l$, the above transformations for the gauge fields confirm that

$$k_{1,o} = k_{1,o}; \quad k_{2,o,l'} = k_{2,o,l} + k_{1,o}. \quad (\text{C14})$$

c. More cohomology invariants

For future convenience, we introduce invariants to identify elements in $\mathcal{H}^1(D_{2n}, \text{U}(1))$ and $\mathcal{H}^2(D_{2n}, \mathbb{Z}^{\text{or}})$.

Any element in $\mathcal{H}^1(D_{2n}, \text{U}(1))$ can be represented by $\Xi_1 \in Z^1(D_{2n}, \mathbb{R}/\mathbb{Z})^{15}$ where

$$\Xi_1 = a_1 w_1 + a_2 w_2, \quad a_1, a_2 \in \mathbb{Z}_2; \quad (\text{C15})$$

here $w_1 = f_1/2$ and $w_2 = f_2/2$ are representative cocycles for generators of $\mathcal{H}^1(D_{2n}, \mathbb{R}/\mathbb{Z})$. $[\Xi_1]$ is fully specified by the invariants $\{\mathcal{E}_{\mathbf{h}}, \mathcal{E}_{\mathbf{r}}\}$, where

$$\mathcal{E}_{\mathbf{g}}(\Xi) := \Xi(\mathbf{g}) \quad (\text{C16})$$

for any normalized cocycle $\Xi \in Z^1(G, \mathbb{R}/\mathbb{Z})$ and $\mathbf{g} \in G$.

Similarly, any class in $\mathcal{H}^2(D_{2n}, \mathbb{Z}^{\text{or}})$ can be represented by a cocycle in $\Xi_2 \in Z^2(D_{2n}, \mathbb{Z}^{\text{or}})$ of the form

$$\Xi_2 = \frac{b_1}{2n} \tilde{z}_1; \quad b_1 \in \mathbb{Z}_{2n}. \quad (\text{C17})$$

The value of b_1 is detected by the invariant $\mathcal{F}_{\mathbf{h}}$, where we have defined

$$\mathcal{F}_{\mathbf{g}}[\Xi_2] := \sum_{j=0}^{d_{\mathbf{g}}-1} \Xi_2(\mathbf{g}^j, \mathbf{g}) \mod d_{\mathbf{g}}, \quad (\text{C18})$$

here $\Xi_2 \in Z^2(G, \mathbb{Z})$ and $\mathbf{g} \in G$ is an orientation preserving element of order $d_{\mathbf{g}}$, i.e. $\mathbf{g}^{d_{\mathbf{g}}-1} \neq \mathbf{0}$ but $\mathbf{g}^{d_{\mathbf{g}}} = \mathbf{0}$. Note that even though Ξ_2 is a 2-cocycle on twisted coefficients, its restriction to C_{2n} is a regular 2-cocycle because no element in C_{2n} reverses orientation.

2. Group cohomology of p4m

Recall that p4m is the symmetry group of the square lattice which is a semidirect product between D_4 and translations $\mathbb{Z}^2$, with generators $\mathbf{x}$ and $\mathbf{y}$. For the rest of this appendix, we take the origin of rotations as α , and the preferred reflection axis as λ_1 (see Fig. 4 for unit cell conventions). The group elements satisfy: $\mathbf{h}_{\alpha}\mathbf{x} = \mathbf{y}\mathbf{h}_{\alpha}$, $\mathbf{h}_{\alpha}\mathbf{y} = \mathbf{x}^{-1}\mathbf{h}_{\alpha}$, $\mathbf{h}_{\alpha}\mathbf{r}_{\lambda_1} = \mathbf{r}_{\lambda_1}\mathbf{h}_{\alpha}^3$, $\mathbf{r}_{\lambda_1}\mathbf{x} = \mathbf{x}\mathbf{r}_{\lambda_1}$, and $\mathbf{r}_{\lambda_1}\mathbf{y} = \mathbf{y}^{-1}\mathbf{r}_{\lambda_1}$. A general element $\mathbf{g} \in \text{p4m}$ can be written as

$$\mathbf{g} = \mathbf{x}^{c_x} \mathbf{y}^{c_y} \mathbf{h}_{\alpha}^a \mathbf{r}_{\lambda_1}^b \quad (\text{C19})$$

with $c_x, c_y \in \mathbb{Z}$, $a \in \{0, 1, 2, 3\}$ and $b \in \{0, 1\}$.

To facilitate calculations involving the various site groups (G_p), we fix a preferred reflection line (l_p) for each site $p \in \{\alpha, \beta, \gamma_1, \gamma_2\}$. We choose $l_{\alpha} = l_{\gamma_1} = \lambda_1$ and $l_{\beta} = l_{\gamma_2} = \mu_1$. All G_p gauge fields are defined with respect to their corresponding reflection axis, l_p . The

¹⁵ $\mathbb{R}/\mathbb{Z}$ is the additive group of real numbers modulo one which is isomorphic to $\text{U}(1)$ by identifying $x \in \mathbb{R}/\mathbb{Z}$ with $e^{2\pi i x} \in \text{U}(1)$.

Generators of site groups G_p				
$\backslash p$	α	β	γ_1	γ_2
$\mathbf{r}_{l_p}$	$\mathbf{r}_{\lambda_1}$	$\mathbf{y}\mathbf{r}_{\lambda_1}$	$\mathbf{r}_{\lambda_1}$	$\mathbf{y}\mathbf{r}_{\lambda_1}$
$\mathbf{h}_p$	$\mathbf{h}_\alpha$	$\mathbf{x}\mathbf{h}_\alpha$	$\mathbf{x}\mathbf{h}_\alpha^2$	$\mathbf{y}\mathbf{h}_\alpha^2$

TABLE VIII. Explicit formulas for the rotation and reflection generators for the site groups in terms of the generators of p4m with origin $\mathbf{o} = \alpha$.

expressions for generators of each G_p are provided in Table VIII. Recall that we are computing restrictions to these subgroups to determine relations between different invariants, and to identify their origin or reflection axis

We construct the area-form cocycle $\Omega \in Z^2(\text{p4m}, \mathbb{Z}^{\text{or}})$ in App. C 2 e. The result is

$$\Omega(\mathbf{x}^{c_{x1}} \mathbf{y}^{c_{y1}} \mathbf{h}_\alpha^{a_1} \mathbf{r}_{\lambda_1}^{b_1}, \mathbf{x}^{c_{x2}} \mathbf{y}^{c_{y2}} \mathbf{h}_\alpha^{a_2} \mathbf{r}_{\lambda_1}^{b_2}) := c_{x1}(\sin(\frac{\pi}{2}a_1)c_{x2} + \cos(\frac{\pi}{2}a_1)(-1)^{b_1}c_{y2}) + [b_1]_2 c_{x2}c_{y2}. \quad (\text{C21})$$

$$b. \quad \mathcal{H}^1(\text{p4m}, \mathbb{R}/\mathbb{Z}), \mathcal{H}^2(\text{p4m}, \mathbb{Z}), \mathcal{H}^2(\text{p4m}, \mathbb{Z}^{\text{or}})$$

A set of representative cocycles of the generators of $\mathcal{H}^1(\text{p4m}, \mathbb{R}/\mathbb{Z}) \cong \mathbb{Z}_2^3$ is (w_1, w_2, w_3) , where

$$w_1 := \frac{f_1}{2}; w_2 := \frac{f_2}{2}; w_3 := \frac{f_x + f_y}{2} \in \mathbb{R}.^{16} \quad (\text{C22})$$

The coefficients of $\Xi = \sum_{j=1}^3 k_j \tilde{z}_j$ can be obtained as: $k_1 = \mathcal{E}_{\mathbf{h}_\alpha}[\Xi]$, $k_2 = \mathcal{E}_{\mathbf{r}_{\lambda_1}}[\Xi]$, and $k_3 = \mathcal{E}_{\mathbf{x}}[\Xi]$. To find the restriction of $[w_j]$ to G_p , it is enough to evaluate $\mathcal{E}_{\mathbf{h}_p}$ and $\mathcal{E}_{\mathbf{r}_{l_p}}$ because these invariants fully determine classes in $\mathcal{H}^1(G_p, \mathbb{R}/\mathbb{Z}) \cong \mathbb{Z}_2^2$. Let Res_p be shorthand for restriction from p4m to G_p . Let $\vec{w} := (w_1, w_2, w_3)$, then

$$\begin{aligned} \text{Res}_\alpha \vec{w} &= (w_1, w_2, 0) \\ \text{Res}_\beta \vec{w} &= (w_1, w_2, w_1 + w_2) \\ \text{Res}_{\gamma_1} \vec{w} &= (0, w_2, w_1) \\ \text{Res}_{\gamma_2} \vec{w} &= (0, w_2, w_1 + w_2) \end{aligned} \quad (\text{C23})$$

where the above equalities hold as cohomology classes. Expressions for w_j on the RHS are given in App. C 1 c. The generators $\mathcal{H}^2(\text{p4m}, \mathbb{Z}) \cong \mathcal{H}^1(\text{p4m}, \mathbb{R}/\mathbb{Z})$ can be taken as $z_j = dw_j$, for $j = 1, 2, 3$. Their restrictions can be obtained directly from Eq. C23 because Res_p and d commute.

A set of generators of $\mathcal{H}^2(\text{p4m}, \mathbb{Z}^{\text{or}}) \cong \mathbb{Z}_4 \times \mathbb{Z}_2 \times \mathbb{Z}$ is

dependence.

a. Useful cochains

Consider the following cochains $f_j, f_x, f_y \in C^1(\text{p4m}, \mathbb{Z})$ with $j = 0, 1, 2$:

$$\begin{aligned} f_0(\mathbf{x}^{c_x} \mathbf{y}^{c_y} \mathbf{h}_\alpha^a \mathbf{r}_{\lambda_1}^b) &= [a]_4; \\ f_1(\mathbf{x}^{c_x} \mathbf{y}^{c_y} \mathbf{h}_\alpha^a \mathbf{r}_{\lambda_1}^b) &= [a]_2; \\ f_2(\mathbf{x}^{c_x} \mathbf{y}^{c_y} \mathbf{h}_\alpha^a \mathbf{r}_{\lambda_1}^b) &= [b]_2; \\ f_x(\mathbf{x}^{c_x} \mathbf{y}^{c_y} \mathbf{h}_\alpha^a \mathbf{r}_{\lambda_1}^b) &= c_x; \\ f_y(\mathbf{x}^{c_x} \mathbf{y}^{c_y} \mathbf{h}_\alpha^a \mathbf{r}_{\lambda_1}^b) &= c_y. \end{aligned} \quad (\text{C20})$$

$(\tilde{z}_1, \tilde{z}_2, \tilde{z}_3)^{17}$ where

$$\tilde{z}_1 := \frac{\bar{d}f_0}{4}; \quad \tilde{z}_2 := \frac{\bar{d}(f_x + f_y)}{2}; \quad \tilde{z}_3 := \Omega. \quad (\text{C24})$$

The coefficients of $\Xi = \sum_{j=1}^3 k_j \tilde{z}_j$ can be obtained as: $k_1 = \mathcal{F}_{\mathbf{h}_\alpha}[\Xi]$, $k_2 = \mathcal{F}_{\mathbf{x}\mathbf{h}_\alpha^2}[\Xi]$, and $k_3 = \Xi(\mathbf{x}, \mathbf{y}) - \Xi(\mathbf{y}, \mathbf{x})$.

The image of $\vec{z} = (\tilde{z}_1, \tilde{z}_2, \tilde{z}_3)$ under Res_p is fully determined by $\mathcal{F}_{\mathbf{h}_p}$, which we evaluated. From here, we obtain

$$\begin{aligned} \text{Res}_\alpha \vec{z} &= (\tilde{z}_1, 0, 0); \\ \text{Res}_\beta \vec{z} &= (\tilde{z}_1, 2\tilde{z}_1, \tilde{z}_1); \\ \text{Res}_{\gamma_1} \vec{z} &= (\tilde{z}_1, \tilde{z}_1, 0); \\ \text{Res}_{\gamma_2} \vec{z} &= (\tilde{z}_1, \tilde{z}_1, 0). \end{aligned} \quad (\text{C25})$$

$$c. \quad \mathcal{H}^3(\text{p4m}, \text{U}(1)^{\text{or}})$$

According to the GAP computation, we find that $\mathcal{H}^4(\text{p4m}, \mathbb{Z}^{\text{or}}) \cong \mathbb{Z}_2^6$. Consequently, $\mathcal{H}^4(\text{p4m}, \text{U}(1)^{\text{or}}) \cong \mathbb{Z}_2^6$ as well. We propose a basis $\{\zeta_1, \dots, \zeta_6\}$ for the latter group by defining cochains $\Phi_j \in C^3(\text{p4m}, \mathbb{R})$ for $j = 1, \dots, 6$, such that $\zeta_j = e^{i\Phi_j}$. The corresponding

¹⁶ We take w_j to be chains valued in $\mathbb{R}$ and use them as representatives of $\mathbb{R}/\mathbb{Z}$ classes by reducing modulo 1, which we leave implicit.

¹⁷ We always give the list of generators in the same order we present the cohomology group, e.g., in this case $\tilde{z}_1$ generates $\mathbb{Z}_4$, $\tilde{z}_2$ generates $\mathbb{Z}_2$, and $\tilde{z}_3$ generates $\mathbb{Z}$.

phases Φ_j are given by

$$\begin{aligned}\Phi_1 &= 2\pi w_1 \cup \tilde{z}_1; & \Phi_2 &= 2\pi w_2 \cup \tilde{z}_1; \\ \Phi_3 &= 2\pi w_3 \cup \tilde{z}_1; & \Phi_4 &= 2\pi w_2 \cup \tilde{z}_2; \\ \Phi_5 &= 2\pi w_1 \cup \tilde{z}_3; & \Phi_6 &= 2\pi w_2 \cup \tilde{z}_3.\end{aligned}\quad (\text{C26})$$

The ζ_j are clearly co-cycles by construction. To show that they form a basis, consider the invariants in Eq. C8 evaluated for different $\mathbf{o}$ and l :

$$\begin{aligned}\mathcal{I}_{1,\mathbf{o}}[\nu_3] &:= \prod_{j=0}^{M_{\mathbf{o}}-1} \nu_3(\mathbf{h}_{\mathbf{o}}, \mathbf{h}_{\mathbf{o}}^j, \mathbf{h}_{\mathbf{o}}); \\ \mathcal{I}_{2,\mathbf{o},l}[\nu_3] &:= \prod_{j=0}^1 \iota_{\mathbf{h}_{\mathbf{o}}^{M_{\mathbf{o}}/2}} \nu_3(\mathbf{r}_l^j, \mathbf{r}_l),\end{aligned}\quad (\text{C27})$$

where $\mathbf{o}$ lies on l . Let

$$\nu_3 = \prod_{j=1}^j \zeta_j^{k_j}; \quad k_j \in \{0, 1\}, \quad (\text{C28})$$

be a generic element in $\mathcal{H}^3(\text{p4m}, \text{U}(1)^{\text{or}})$. Then,

$$\begin{aligned}\mathcal{I}_{1,\alpha}[\nu_3] &= (-1)^{k_1} \\ \mathcal{I}_{2,\alpha,\lambda_1}[\nu_3] &= (-1)^{k_2} \\ \mathcal{I}_{1,\beta}[\nu_3] &= (-1)^{k_1+k_3+k_5} \\ \mathcal{I}_{2,\beta,\mu_1}[\nu_3] &= (-1)^{k_2+k_3+k_6} \\ \mathcal{I}_{1,\gamma_1}[\nu_3] &= (-1)^{k_3} \\ \mathcal{I}_{2,\gamma_1,\lambda_1}[\nu_3] &= (-1)^{k_2+k_4}\end{aligned}\quad (\text{C29})$$

It is clear that the above invariants are independent. Thus the proposed set indeed gives a basis.

d. Topological action

The gauge fields used in the main text are

$$\begin{aligned}\omega &= \frac{2\pi}{4} B^* f_0, \\ \sigma &= B^* f_2,\end{aligned}\quad (\text{C30})$$

$$\vec{R} = 2\pi[B^* f_x, B^* f_y]^\top.$$

Therefore, the actions in Eq. C26 after pulling back by B become

$$\begin{aligned}B^* \Phi_1 &= 2\omega \cup \frac{\bar{d}\omega}{2\pi}; \\ B^* \Phi_2 &= \pi\sigma \cup \frac{\bar{d}\omega}{2\pi}; \\ B^* \Phi_3 &= (\vec{R} \cdot \vec{m}) \cup \frac{\bar{d}\omega}{2\pi}; \\ B^* \Phi_4 &= \pi\sigma \cup \frac{\bar{d}(\vec{R} \cdot \vec{m})}{2\pi}; \\ B^* \Phi_5 &= 2\omega \cup A_{XY}; \\ B^* \Phi_6 &= \pi\sigma \cup A_{XY}.\end{aligned}\quad (\text{C31})$$

We can then recover Eq. 31 in the main text by pulling back the most general element of $\mathcal{H}^3(G_{\text{space}}, \mathbb{R}/2\pi\mathbb{Z})$:

$$\mathcal{L} = B^*(k_{1,\alpha}\Phi_1 + k_{2,\alpha,\lambda_1}\Phi_2 + k_{3,\alpha}\Phi_3 + k_{4,\alpha,\lambda_1}\Phi_4 + k_5\Phi_5 + k_6\Phi_6). \quad (\text{C32})$$

Where we have added a subscript α and λ_1 to the coefficients used in Eq. C28 to indicate dependence on origin and reference reflection line.

To study topological actions of terms protected by p4m and internal symmetries it is useful to use the restrictions in Eqs. C23 and C25. We summarize these restrictions after pulling back by the gauge field in Table IX.

e. Area form cocycle

We construct the cocycle corresponding to the area form for p4m. More precisely, we want $\Omega \in Z^2(\text{p4m}, \mathbb{Z}^{\text{or}})$ such that $\iota_{\mathbf{y}} \iota_{\mathbf{x}} \Omega = \Omega(\mathbf{x}, \mathbf{y}) - \Omega(\mathbf{y}, \mathbf{x}) = 1$. We considered the area form separately because its construction was not obvious to us, even though the final expression (Eq. C21) is simple.

The twisted cup product gives an obvious starting

point. Consider $\vec{t}(\mathbf{g}) = [f_x(\mathbf{g}), f_y(\mathbf{g})]^\top \in \mathbb{Z}^2$ is the ‘translation cocycle’ that satisfies

$$\mathbf{g}_1 \vec{t}(\mathbf{g}_2) - \vec{t}(\mathbf{g}_1 \mathbf{g}_2) + \vec{t}(\mathbf{g}_1) = 0 \quad (\text{C33})$$

for the action

$$\mathbf{g} \vec{t} = \begin{pmatrix} \cos(\pi a/2) & -\sin(\pi a/2)(-1)^b \\ \sin(\pi a/2) & \cos(\pi a/2)(-1)^b \end{pmatrix} \cdot \vec{t}. \quad (\text{C34})$$

where $a = f_0(\mathbf{g})$ and $b = f_2(\mathbf{g})$ are the powers of $\mathbf{h}_{\mathbf{o}}$ and $\mathbf{r}_l$ in $\mathbf{g}$, respectively. Equivalently, $\mathbf{g} \vec{t}(\mathbf{g}_1) = \vec{t}(\mathbf{g} \mathbf{g}_1 \mathbf{g}^{-1})$.

Recall that the wedge product $(\vec{V} \wedge \vec{U} := V_1 U_2 - V_2 U_1)$ of two $\text{O}(2)$ vectors (V, U) transforms under the sign rep-

$B^* \text{Res}_o \Xi_1; [\Xi_1] \in \mathcal{H}^1(\text{p4m}, \text{U}(1))$				
$B^* \Xi_1 \backslash o$	α	β	γ_1	γ_2
2ω	2ω	2ω	0	0
$\pi\sigma$	$\pi\sigma$	$\pi\sigma$	$\pi\sigma$	$\pi\sigma$
$\vec{m} \cdot \vec{R}$	0	$2\omega + \pi\sigma$	ω	$\omega + \pi\sigma$

$B^* \text{Res}_o \Xi_2; [\Xi_2] \in \mathcal{H}^2(\text{p4m}, \mathbb{Z}^{\text{or}})$				
$B^* \Xi_2 \backslash o$	α	β	γ_1	γ_2
$\frac{\vec{d}\omega_\alpha}{2\pi}$	$\frac{\vec{d}\omega}{2\pi}$	$\frac{\vec{d}\omega}{2\pi}$	$\frac{\vec{d}\omega}{2\pi}$	$\frac{\vec{d}\omega}{2\pi}$
$\frac{\vec{d}\vec{m} \cdot \vec{R}}{2\pi}$	0	$2\frac{\vec{d}\omega}{2\pi}$	$\frac{\vec{d}\omega}{2\pi}$	$\frac{\vec{d}\omega}{2\pi}$
A_{XY}	0	$\frac{\vec{d}\omega}{2\pi}$	0	0

TABLE IX. Entries of the tables are the image under the restriction map (Res_o) for generators the generators of $\mathcal{H}^1(\text{p4m}, \text{U}(1))$ (left) and $\mathcal{H}^2(\text{p4m}, \mathbb{Z}^{\text{or}})$ (right).

resentation of $\text{O}(2)$. This still holds upon restriction to any finite subgroup $D_n \subset \text{O}(2)$, in particular the subgroup D_4 . This implies that the twisted cup product

$$\tilde{\Omega}(\mathbf{g}_1, \mathbf{g}_2) = \vec{t}(\mathbf{g}_1) \wedge^{\mathbf{g}_1} \vec{t}(\mathbf{g}_2), \quad (\text{C35})$$

is closed under the twisted cup product, i.e. $\vec{d}\tilde{\Omega} = 0$. However, $\iota_{\mathbf{y}} \iota_{\mathbf{x}} \tilde{\Omega} = 2$.

Consider now the cochain $\varpi \in C^1(\text{p4m}, \mathbb{Z})$:

$$\varpi(\mathbf{x}^{c_x} \mathbf{y}^{c_y} \mathbf{h}_o^a \mathbf{r}_l^b) = c_x c_y, \quad (\text{C36})$$

which satisfies

$$\vec{d}\varpi(\mathbf{g}_1, \mathbf{g}_2) = \tilde{\Omega}(\mathbf{g}_1, \mathbf{g}_2) \pmod{2}. \quad (\text{C37})$$

To see this, let $b_1 = f_2(\mathbf{g}_1)$, $[x_1, y_1] := \vec{t}(\mathbf{g}_1)^\top$, $[x_2, y_2] := \vec{t}(\mathbf{g}_2)^\top$ and $[x_3, y_3] :=^{\mathbf{g}_1} \vec{t}(\mathbf{g}_1)^\top$. Then

$$\begin{aligned} \vec{d}\varpi(\mathbf{g}_1, \mathbf{g}_2) &= (-1)^{b_1} x_2 y_2 + x_1 y_1 - (x_1 + x_3)(y_1 + y_3) \\ &= -2[b_1]_2 x_2 y_2 - (x_1 y_3 + x_3 y_1) \\ &= x_1 y_3 - x_3 y_1 \pmod{2} \\ &= \tilde{\Omega}(\mathbf{g}_1, \mathbf{g}_2) \pmod{2}. \end{aligned} \quad (\text{C38})$$

Therefore, we can take $\Omega := \frac{\tilde{\Omega} - \vec{d}\varpi}{2} \in Z^2(\text{p4m}, \mathbb{Z}^{\text{or}})$. We write the explicit expression for Ω in Eq. C21, which can be used to check that $\iota_{\mathbf{y}} \iota_{\mathbf{x}} \Omega = +1$.

Appendix D: Analytical verification of partial symmetry invariants

In this appendix, we explicitly evaluate the partial symmetry invariants mentioned in the main text for two classes of examples. In App. D1 we study a state with zero correlation length, and in App. D2 we study a state constructed using AKLT chains.

1. Calculations for the singlet covering state

Below we present calculations for the singlet coveringstate with symmetry $G = \text{SO}(3) \times \text{p4m}$. By identifying suitable subgroups of $\text{SO}(3)$ with $\text{U}(1)$ or $\mathbb{Z}_N$, this

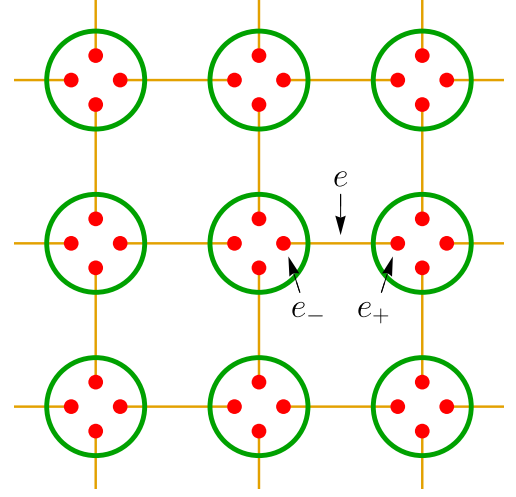


FIG. 7. Pictorial representation of singlet coveringstate. Red dots denote a spin $S = 1/2$, and green circles represent sites/vertices of the square lattice. Orange lines connect spins that form singlets. Each orange line lies on an edge e . The spins lying on the ends of e are denoted by e_+ and e_- .

example allows us to compute and verify all the independent invariant types studied in this paper except type A3. We compute a complete set of invariants to characterize the SPT phase of this state and summarize the results in several tables.

In App. D1 a we explicitly define the state. App. D1 b evaluates the partial rotation $(\Theta_{k,o}(\mathbf{g}))$, App. D1 c evaluates the partial double reflection $(\Sigma_{o,l}(\mathbf{g}, \mathbf{j}))$, and App. D1 d evaluates the phase of the partial reflection with twisted boundary conditions $(\Upsilon_l(\mathbf{g}; \mathbf{j}))$.

a. Definition of state

In this section, we explicitly define the singlet coveringstate $(|\psi_0\rangle)$. The overall Hilbert space is constructed by placing two $S = 1/2$ spins on the ends of every bond of the square lattice (see Fig. 7). At any vertex, the local Hilbert space is the tensor product of four spins from the four incident edges $\mathcal{H}_{\text{local}} = \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2 = (\mathbb{C}^2)^{\otimes 4}$. Since this local space involves an even number of $S = 1/2$

spins, $\mathcal{H}_{\text{local}}$ transforms under a linear representation of $\text{SO}(3)$ (the group of spatial rotations), rather than the double cover $\text{SU}(2)$. Consider the exactly solvable Hamiltonian

$$H = \sum_e \vec{S}_{e_+} \cdot \vec{S}_{e_-} \quad (\text{D1})$$

where $\vec{S}_s$ is the spin operator for spin s . e_+ and e_- denote the two spins living at the ends of the edge e (see Fig. 7). The singlet covering state $|\psi_0\rangle$ is the ground state of the above Hamiltonian, which is the tensor product of singlets

$$|\psi_0\rangle = \bigotimes_e \frac{1}{\sqrt{2}} \left(|\uparrow\rangle_{e_+} |\downarrow\rangle_{e_-} - |\downarrow\rangle_{e_+} |\uparrow\rangle_{e_-} \right), \quad (\text{D2})$$

where $|\uparrow\rangle_s$ and $|\downarrow\rangle_s$ denote the spin up and spin down states of spin s .

This state and Hamiltonian are invariant under: 1) the geometric action of $G_{\text{space}} = \text{p4m}$ on the edges of the square lattice¹⁸; and 2) $\text{SO}(3)$ generated by $\vec{S}_{\text{tot}} = \sum_e (\vec{S}_{e_+} + \vec{S}_{e_-})$. In particular, every $\mathbf{g} \in \text{SO}(3)$ acts on a spin $S = 1/2$ as a 2×2 matrix $V_{\mathbf{g}} \in \text{SU}(2)$ that satisfies

$$V_{\mathbf{g}_1} V_{\mathbf{g}_2} = \mu(\mathbf{g}_1, \mathbf{g}_2) V_{\mathbf{g}_1 \mathbf{g}_2}, \quad (\text{D3})$$

$\mu(\mathbf{g}_1, \mathbf{g}_2) \in \{+1, -1\}$ is a sign that appears because the spins transform as projective representations of $\text{SO}(3)$. In particular, μ is a group cocycle representative of the non-trivial class in $\mathcal{H}^2(\text{SO}(3), \text{U}(1))$.

To evaluate the type B invariants we use the subgroup of rotations around the x-axis as the $K = \text{U}(1)$ group. For type C invariants, we identify $K = \mathbb{Z}_2$ with the group generated by π rotations around the x-axis.

In what follows, we consider the state $|\psi_0\rangle$ where the vertices of the square lattice lie on the Wyckoff position α . The region D will be taken to be a rectangle whose boundary crosses $2N_x$ vertical bonds and $2N_y$ horizontal bonds. We denote the ‘interior’ of D by $\bar{D}$ and its ‘boundary’ by ∂D .

The evaluation of the invariants can be simplified by noting that

$$\mathcal{O}_D := \langle \psi_0 | \mathcal{O} | \psi_0 \rangle = \text{Tr}[\mathcal{O} \rho_D], \quad (\text{D4})$$

where the reduced density matrix decomposes as

$$\rho_D = \text{Tr}_{\bar{D}}[|\psi_0\rangle \langle \psi_0|] = \rho_{\bar{D}} \otimes \rho_{\partial D}. \quad (\text{D5})$$

Here, $\rho_{\bar{D}}$ is the pure state of singlets entirely contained within $\bar{D}$, while $\rho_{\partial D}$ is a maximally mixed state for spins forming singlets with those outside D (see Fig. 8). Consequently, the calculation factorizes into contributions from

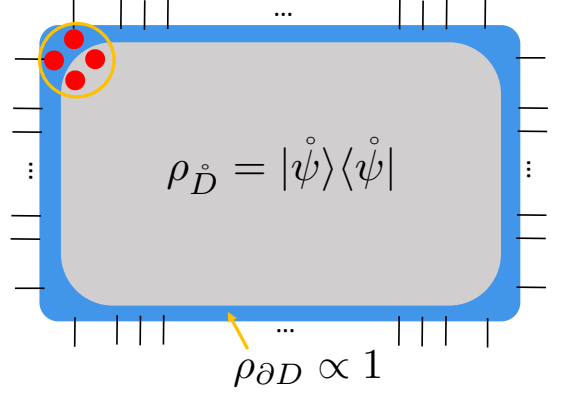


FIG. 8. Decomposition of reduced density matrix for the singlet covering state. The four red dots surrounded by a circle aim to illustrate the four spins belonging to site closest to the top left corner of region D .

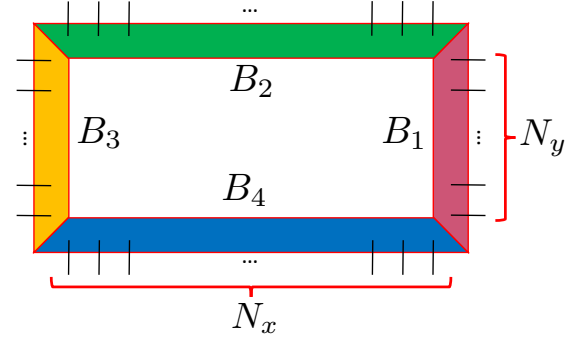


FIG. 9. Decomposition used in the calculation of partial symmetry operations.

the boundary ($\mathcal{O}_{\partial D}$) and the interior ($\mathcal{O}_{\bar{D}}$),

$$\mathcal{O}_D = \mathcal{O}_{\partial D} \cdot \mathcal{O}_{\bar{D}}. \quad (\text{D6})$$

b. Partial rotations (type A1/B1/C1/D1)

In this section, we evaluate Eq. D4 with

$$\mathcal{O} = \tilde{C}_{M_o}^m U_{\mathbf{g}}. \quad (\text{D7})$$

for $\mathbf{g} \in \text{SO}(3)$. We consider the cases where the order of $\mathcal{O}$ is 4 and 2 separately. We show in Tab. X the real space invariants for $|\psi_0\rangle$.

a. $\mathcal{O}$ is order 4: This corresponds to $\mathbf{o} \in \alpha, \beta$ with $n = 1$. We take the region D to be a square ($N_x = N_y$) centered at $\mathbf{o} = \alpha$ or β . Due to the geometry of the square lattice, N_x is odd for $\mathbf{o} = \alpha$ and even for $\mathbf{o} = \beta$.

The boundary ∂D is the disjoint union of 4 sides B_1 , B_2 , B_3 and B_4 that are permuted cyclically under C_4 (see Fig. 9). On each B_j , there are N_x boundary spin-

¹⁸ Geometric action means that it just acts by permuting sites.

1/2 variables.

The boundary contribution to Eq. D4 is

$$\mathcal{O}_{\partial D} = \frac{\text{Tr}[\text{SWAP}_{1,2,3,4} \otimes_{j \in \partial D} (V_{\mathbf{g}})_j]}{2^{2N_x + 2N_y}} \quad (\text{D8})$$

where $\text{SWAP}_{1,2,3,4} = \text{SWAP}_{3,4} \text{SWAP}_{2,3} \text{SWAP}_{1,2}$, and $\text{SWAP}_{i,j}$ acts by exchanging the states on subsystems B_i and B_j . Recall that $V_{\mathbf{g}}$ is the local action of $\text{SO}(3)$ on each spin-1/2 (Eq. D3). $\mathcal{O}_{\partial D}$ can be simplified to

$$\mathcal{O}_{\partial D} = \left(\frac{\text{Tr}[V_{\mathbf{g}}^4]}{2^4} \right)^{N_x} = e^{iN_x \phi_{\mathbf{g}} - 3 \log(2) N_x} \quad (\text{D9})$$

with

$$e^{i\phi_{\mathbf{g}}} = \prod_{j=0}^3 \mu(\mathbf{g}, \mathbf{g}^j) \in \{+1, -1\}. \quad (\text{D10})$$

The sign of the interior contribution, $\mathcal{O}_{\hat{D}}$, can be computed by assigning an orientation to each edge in $\hat{D}$ and counting the bonds that are flipped under the rotation. Each flipped bond contributes a factor of -1 , since the spatial wavefunction of a singlet is antisymmetric. The contribution from $U_{\mathbf{g}}$ vanishes because the state in $\hat{D}$ is a product of singlets. By grouping bonds into sets of four that are closed under rotations, one sees that exactly two bonds are flipped in each group, making the overall interior contribution trivial.

The partial rotation evaluates to

$$\langle \psi_0 | (\tilde{C}_{M_o} U_{\mathbf{g}})_D | \psi_0 \rangle = \frac{1}{2^{3N_x}} \begin{cases} e^{i\phi_{\mathbf{g}}} & , o = \alpha \\ 1 & , o = \beta \end{cases}, \quad (\text{D11})$$

here $\phi_{\mathbf{g}}$ is defined in Eq. D10.

b. $\mathcal{O}$ is order 2 In this case, $o \in \{\alpha, \beta, \gamma\}$ and $n = (M_o, 4)/2$. Now the internal symmetry element $\mathbf{g}$ satisfies $\mathbf{g}^2 = \mathbf{0}$. From the geometry of the square lattice,

$$(N_x + N_y) = \begin{cases} 0 \pmod{2} & , o \in \{\alpha, \beta\} \\ 1 \pmod{2} & , o \in \{\gamma\} \end{cases}. \quad (\text{D12})$$

The boundary contribution is

$$\mathcal{O}_{\partial D} = \frac{\text{Tr}[\text{SWAP}_{1,3} \text{SWAP}_{2,4} \otimes_{j \in \partial D} (V_{\mathbf{g}})_j]}{2^{2N_x + 2N_y}}. \quad (\text{D13})$$

where now $\text{SWAP}_{j,k}$ swaps regions B_j and B_k in Fig. 9. $\mathcal{O}_{\partial D}$ simplifies to

$$\mathcal{O}_{\partial D} = \left(\frac{\mu(\mathbf{g}, \mathbf{g})}{2} \right)^{N_x + N_y}. \quad (\text{D14})$$

The bulk contribution for $o \in \{\alpha, \beta\}$ is still trivial. However, for $o = \gamma$, $\mathcal{O}_{\hat{D}} = -1$ because of the bond passing

Invariant	value	$\mathbf{g}$	n
Θ_{α}	0	$\mathbf{0}$	1
Θ_{β}	0	$\mathbf{0}$	1
Θ_{γ}	1	$\mathbf{0}$	1
$\Theta_{\alpha}^{\text{SO}(3)}$	2	$[\pi/2, \hat{x}]$	1
$\Theta_{\beta}^{\text{SO}(3)}$	0	$[\pi/2, \hat{x}]$	1
$\Theta_{\gamma}^{\text{SO}(3)}$	0	$[\pi, \hat{x}]$	1
$\Theta_{\alpha}^{\mathbb{Z}_2}$	0	$[\pi, \hat{x}]$	2
$\Theta_{\beta}^{\mathbb{Z}_2}$	0	$[\pi, \hat{x}]$	2
$\Theta_{\gamma}^{\mathbb{Z}_2}$	0	$[\pi, \hat{x}]$	1

TABLE X. Dressed partial rotation invariants for the singlet covering state $|\psi_0\rangle$ using Eq. D4 with $O = \tilde{C}_{M_o}^n U_{\mathbf{g}}$, $\mathbf{g} \in \text{SO}(3)$.

$o \backslash$	Θ_o	$\mathcal{S}_o^{\text{U}(1)}$	$\mathcal{S}_o^{\mathbb{Z}_2}$	$\mathcal{S}_o^{\text{SO}(3)}$
α	0	2	0	2
β	0	0	0	0
γ	1	1	1	1

TABLE XI. Type A1, B1, C1 and D1 invariants for the state $|\psi_0\rangle$.

through the rotation center. Putting things together

$$\langle \psi_0 | (\tilde{C}_{M_o}^{\frac{(M_o, 4)}{2}} U_{\mathbf{g}})_D | \psi_0 \rangle = \begin{cases} \frac{1}{2^{N_x + N_y}} & , o = \alpha, \beta \\ \frac{-\mu(\mathbf{g}, \mathbf{g})}{2^{N_x + N_y}} & , o = \gamma \end{cases}. \quad (\text{D15})$$

c. Evaluation of real space invariants: We evaluated the real space invariants using Eq. D11 and Eq. D15. In Table X, we summarize the real space invariant and the group element $\mathbf{g}$ used to evaluate them. Note that $\Theta_o^{\text{U}(1)} = \Theta_o^{\text{SO}(3)}$ by our choice of $\text{U}(1) \cong \text{SO}(2)$.

We summarize the type A1, B1, C1 and D1 invariants in Table XI, which are calculated by taking differences of the appropriate invariants in Table X.

c. Partial double reflections (Type A2/C2/D2)

The main result of this section is Eq. (D21), which evaluates $\Sigma_{o,l}(\mathbf{g}, \mathbf{j})$, and the numerical result for the singlet covering state, which is summarized in Table XII. We decompose the region D into three subregions D_l, D_c, D_r as in Fig. 1 in the main text.

a. l is horizontal: we orient l parallel to the x axis. We take the boundary of the region D to cross $2N_y$ horizontal bonds and $2N_x$ vertical bonds. Let $2N_1$ and $2N_2$ be the number of vertical bonds the boundary of regions D_l and D_c cross, respectively. The group elements $\mathbf{g}, \mathbf{j} \in \text{SO}(3)$ satisfy $\mathbf{g}\mathbf{j} = \mathbf{j}\mathbf{g}$ and $\mathbf{j}^2 = \mathbf{0}$.

The expectation value $\mathcal{O}$ now decomposes as

$$\mathcal{O} = \mathcal{O}_{B_{lr}} \mathcal{O}_{B_v} \mathcal{O}_{B_h} \mathcal{O}_{\dot{D}_{lr}} \mathcal{O}_{\dot{D}_c}. \quad (\text{D16})$$

The subscripts correspond to the regions in Fig. 10 and $B_{lr} = B_l \cup B_r$ and $\dot{D}_{lr} = \dot{D}_l \cup \dot{D}_r$.

The contribution from $\dot{D}_{lr}$ (B_{lr}) is 2^{-N} , where N is the number of singlets on $\dot{D}_l$ (B_l), because we can choose the orientation of singlets in $\dot{D}_l$ (B_l) to be the mirror image of those in $\dot{D}_r$ (B_r). For the same reason, only singlets lying on or crossing l can contribute a non-trivial phase to $\mathcal{O}_{D_c}$. A direct calculation shows that only the singlets crossing l can contribute a phase.

Let's consider the contribution to $\mathcal{O}_{B_v}$ from the two singlets lying on l . Their wavefunction is¹⁹

$$|\phi\rangle = \frac{1}{2} \sum_{s_1, s_2, s_3, s_4=0,1} \varepsilon_{s_1 s_2} \varepsilon_{s_3 s_4} |s_1 s_2 s_3 s_4\rangle, \quad (\text{D17})$$

where we have numbered the spins from left to right (e.g., spin 2 is in region D_c , near its left boundary), and $\varepsilon_{ss'}$ is the Levi-Civita tensor.

Their contribution to $\mathcal{O}_{B_v}$ is

$$A_{\mathbf{g}, \mathbf{j}} := \langle \phi | \text{SWAP}_{1,4} (V_{\mathbf{g}} \otimes V_{\mathbf{j}} \otimes V_{\mathbf{j}} \otimes V_{\mathbf{g}}^\dagger) | \phi \rangle, \quad (\text{D18})$$

because, to calculate $\Sigma_{o,l}(\mathbf{g}, \mathbf{j})$, we act with $\mathbf{g}$ on D_l (where spin 1 lies), with $\mathbf{g}^{-1}$ on D_r (where spin 4 lies), and with $\mathbf{j}$ on D_c (where spins 2 and 3 are located).

Using the fact that for any $\mathbf{g} \in \text{SO}(3)$, $V_{\mathbf{g}} \otimes V_{\mathbf{g}} |\varphi_0\rangle = |\varphi_0\rangle$, where $|\varphi_0\rangle$ is the spin-singlet state, we can rewrite

$$A_{\mathbf{g}, \mathbf{j}} = \langle \phi | \text{SWAP}_{1,4} (\mathbb{I} \otimes V_{\mathbf{j}} V_{\mathbf{g}}^\dagger \otimes V_{\mathbf{j}} V_{\mathbf{g}} \otimes \mathbb{I}) | \phi \rangle. \quad (\text{D19})$$

Using the relation $\sum_s \varepsilon_{s_1 s} \varepsilon_{s_2 s} = \delta_{s_1 s_2}$, A simplifies to

$$A_{\mathbf{g}, \mathbf{j}} = \frac{1}{4} \text{Tr} [V_{\mathbf{g}} V_{\mathbf{j}} V_{\mathbf{g}}^\dagger V_{\mathbf{j}}] = \frac{\mu(\mathbf{j}, \mathbf{j}) \mu(\mathbf{g}, \mathbf{j})}{2 \mu(\mathbf{j}, \mathbf{g})}. \quad (\text{D20})$$

The ratio $\mu(\mathbf{g}, \mathbf{j})/\mu(\mathbf{j}, \mathbf{g})$ arises when commuting $V_{\mathbf{g}}$ past $V_{\mathbf{j}}$, while the factor $\mu(\mathbf{j}, \mathbf{j})$ comes from the product $V_{\mathbf{j}}^2$.

The remaining singlets on B_v appear in groups of four, each forming an orbit under the action of D_2 , generated by $\mathbf{r}_l$ and $\mathbf{r}_{l'}$. Their contribution can be rewritten as $A_{\mathbf{g}, \mathbf{j}}^2$. The singlets in B_h come in pairs, related by l . Each pair contributes $A_{\mathbf{0}, \mathbf{j}}$.

Putting everything together, we obtain

$$\mathcal{O} = \frac{1}{2^{N_x+2N_y}} \begin{cases} \frac{\mu(\mathbf{g}, \mathbf{j})}{\mu(\mathbf{j}, \mathbf{g})} & , o = \alpha \\ \mu(\mathbf{j}, \mathbf{j}) \times \frac{\mu(\mathbf{g}, \mathbf{j})}{\mu(\mathbf{j}, \mathbf{g})} & , o = \gamma_1 \\ -\mu(\mathbf{j}, \mathbf{j}) & , o = \gamma_2 \\ 1 & , o = \beta \end{cases}. \quad (\text{D21})$$

We see that non-trivial phases are only contributed by

Invariant	value
$\Sigma_{\alpha, \lambda_1}$	0
$\Sigma_{\gamma_1, \lambda_1}$	0
Σ_{β, μ_1}	0
$\tilde{\Sigma}_{\alpha, \lambda_1}^{\text{SO}(3)}$	1
$\tilde{\Sigma}_{\beta, \mu_1}^{\text{SO}(3)}$	0
$\tilde{\Sigma}_{\alpha, \nu_1}^{\text{SO}(3)}$	0
$\tilde{\Sigma}_{\alpha, \lambda_1}^{\mathbb{Z}_N}$	1
$\tilde{\Sigma}_{\beta, \mu_1}^{\mathbb{Z}_N}$	0
$\tilde{\Sigma}_{\alpha, \nu_1}^{\mathbb{Z}_N}$	0

TABLE XII. Type-A2 ($\Sigma_{o,l}$), type-D2 ($\tilde{\Sigma}_{o,l}^{\text{SO}(3)}$) and type-C2 ($\tilde{\Sigma}_{o,l}^{\mathbb{Z}_{2m}}$) invariants for the singlet covering state. Type A2 and D2 are calculated with geometric reflections, while type C2 are calculated by combining the geometric reflection with $\mathbf{X} \in \text{SO}(3)$.

degrees of freedom on l and l' .

b. l is diagonal: now l is parallel to the line $y = x$, and $o = \alpha$ or β . The calculation can be done as in the previous case, but we always find that the phase of $\mathcal{O}$ is trivial.

c. Evaluation of real space invariants: The A2 and D2 invariants calculated using geometric reflection are tabulated in Table XII. In the same table, we tabulated C2 invariants with reflections given by combining geometric reflections with $\mathbf{X}$, and $\mathbf{S} = [2\pi/N, \hat{z}]$.

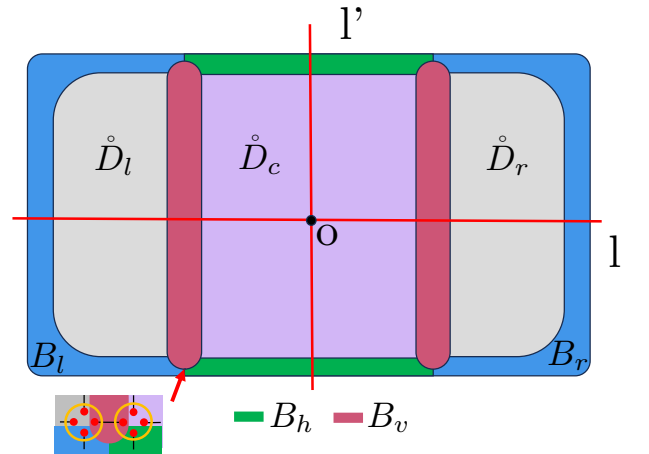


FIG. 10. Decomposition of the regions used in the evaluation of $\Sigma_{o,l}$. The inset illustrates how spins located at the corners of the regions D_l and D_r are assigned to the regions used to evaluate the partial symmetry.

¹⁹ we identify $|\uparrow\rangle = |0\rangle$ and $|\downarrow\rangle = |1\rangle$.

d. Partial reflection with twisted boundary conditions

For the Hamiltonian in Eq. D1, $\mathbf{g}$ -twisted boundary conditions amount to replacing $\vec{S}_{e-} \rightarrow U_{\mathbf{g}} \vec{S}_{e-} U_{\mathbf{g}}^\dagger$ for all bonds e that cross one vertical line l_* that lies between two vertical axes of the square lattice. We are taking e_- to be the spin lying to the right of l_* . The new ground state is given by

$$|\psi_{0,\mathbf{g}}\rangle = \prod_{e \in \mathcal{L}} U_{\mathbf{g}} |e_-\rangle |\psi_0\rangle. \quad (\text{D22})$$

Since we are after the evaluation of type C4 and D4 invariants, we need the *relative phase* of the expectation value $\langle (\mathbf{r}_l U_{\mathbf{j}}) |_D \rangle$ between $|\psi_0\rangle$ and $|\psi_{0,\mathbf{g}}\rangle$. It is clear that this relative phase will come from the spins where $\mathbf{g}$ acts in Eq. D22.

By doing manipulations similar to the ones done for $\Sigma_{o,l}(\mathbf{g}, \mathbf{j})$, we arrive at

$$(-1)^{\Upsilon_l(\mathbf{g}; \mathbf{j})} = \left(\frac{\mu(\mathbf{g}, \mathbf{j})}{\mu(\mathbf{j}, \mathbf{g})} \right)^{N_y}, \quad (\text{D23})$$

where N_y is the number horizontal bonds inside D that intersect l_* . Therefore, N_y is odd (even) when $l = [\alpha, \gamma_1][\beta, \gamma_2]$.

2. Calculations for stacked AKLT chains

Here we briefly outline the calculation for a state with finite correlation length that lies in the same phase as the singlet covering. This state is constructed by placing Affleck–Kennedy–Lieb–Tasaki (AKLT) chains along each line of the square lattice. At every vertex of the square lattice, we place two $S = 1$ spins. The Hamiltonian for each line is

$$H_{\text{AKLT}} = \sum_i \vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{3} \left(\vec{S}_i \cdot \vec{S}_{i+1} \right)^2, \quad (\text{D24})$$

where the sum is over sites on the line.

It is well known that the ground state of H_{AKLT} can be understood by decomposing each $S = 1$ spin into two virtual $S = 1/2$ spins, which form singlets with neighboring sites. This state admits an explicit representation as a matrix product state (MPS) with finite correlation length.

Using the explicit MPS representation, the evaluation of partial symmetries can be simplified considerably when the system and the size of D are both large. This is because the correlation functions for the MPS are dominated by a single eigenvector of the transfer matrix. To leading order in system and D size, the results agree with the singlet covering state. For partial rotations, we analytically checked that expectation value $\langle \psi | (\tilde{C}_{M_o}) |_D | \psi \rangle$ behaves as 1 for a rectangular region D .

Appendix E: Relation between invariants

1. Relations between type-A invariants

As in Ref. [27], we assume that any short-range state can be deformed to an ‘atomic limit’ while preserving G_{space} . We derive the relations assuming that $|\Psi\rangle$ is already in its atomic limit.

First notice that Θ_o and $\Sigma_{o,l}$, when they exist, satisfy

$$\begin{aligned} \tilde{C}_{M_o} |_{\{o\}} |\Psi\rangle &= e^{2\pi i \Theta_o / M_o} |\Psi\rangle \\ R_l |_{\{o\}} |\Psi\rangle &= (-1)^{\Sigma_{o,l}} |\Psi\rangle \end{aligned} \quad (\text{E1})$$

where $\mathbf{h}_o$ is anticlockwise rotation by $2\pi/M_o$ radians around o and $\mathbf{r}_l$ is reflection along l . To see that Eq. E1 is true, note that we choose the regions D in the definitions of Θ_o and $\Sigma_{o,l}$ such that the contributions away from o come in groups of M_o and 2 for Θ_o and $\Sigma_{o,l}$, respectively. Therefore, all contributions away from the origin cancel out.

Consider the case when $D_2 \subset G_o$, then if we define l' by $\mathbf{r}_{l'} = \mathbf{h}_o \mathbf{r}_l$, we can write

$$R_{l'} |_{\{o\}} |\Psi\rangle = \tilde{C}_{M_o} |_{\{o\}} R_l |_{\{o\}} |\Psi\rangle \quad (\text{E2})$$

and use Eq. E1 to show that

$$\Sigma_{o,l'} = \frac{2}{M_o} \Theta_o + \Sigma_{o,l} \pmod{2}. \quad (\text{E3})$$

Similarly, consider the case when there are two maximal Wyckoff positions o and o' lying on a line l , whose site group includes a D_2 subgroup (i.e. M_o and $M_{o'}$ are even). Λ_l also needs a translation parallel to l , which we denote as $\mathbb{Z}^{(l)}$. Let $n_o(n_{o'})$ be the number of sites in the MWP $o(o')$ appearing in the unit cell of $\mathbb{Z}^{(l)}$. Then from the definition

$$\frac{\langle \Psi(L_x + 1) | R_l | \Psi(L_x + 1) \rangle}{\langle \Psi(L_x) | R_l | \Psi(L_x) \rangle} \propto (-1)^{\Lambda_l}, \quad (\text{E4})$$

where $|\Psi(L_x)\rangle$ is the state on a cylinder (or torus) with L_x unit cells along the direction parallel to l .

From Eq. E1,

$$\begin{aligned} R_l | \Psi(L_x) \rangle &= (-1)^{[n_o \Sigma_{o',l} + n_{o'} \Sigma_{o,l}] L_x} | \Psi(L_x) \rangle \\ \Rightarrow \Lambda_l &= n_o \Sigma_{o,l} + n_{o'} \Sigma_{o',l} \pmod{2}. \end{aligned} \quad (\text{E5})$$

2. Relations between type-D invariants

$$a. \quad p4m$$

In this section we derive Eq. 51 using group cohomology methods. Recall that for $\mathbf{g}, \mathbf{j} \in K$ such that $\mathbf{g}\mathbf{j} = \mathbf{j}\mathbf{g}$, we get

$$(-1)^{\Upsilon_{\mathbf{g}; \mathbf{j}}} = \mathcal{Z}(S_{\mathbf{g}}^1 \times \mathbb{RP}_{\mathbf{j}\mathbf{r}_l}^2) = \iota_{\mathbf{g}} \nu_3(\mathbf{j}\mathbf{r}_l, \mathbf{j}\mathbf{r}_l), \quad (\text{E6})$$

where ν_3 is a 3-cochain, such that $B^*\nu_3 = e^{i\mathcal{L}}$, where $\mathcal{L}$ is the Lagrangian of the topological action.

When we evaluate the type D invariants, we evaluate suitable differences that get rid of any contribution from pure invariants. Therefore, we can express $\Upsilon_l^{\text{SO}(3)}$ solely in terms of the coefficients in Eq. 50. A choice of $\varphi_3 \in Z^3(\text{p4m} \times \text{SO}(3), \text{U}(1)^\sigma)$, such that $B^*\varphi_3$ returns Eq. 50, is

$$\varphi_3 = 2\pi w_2(u_{1,\alpha,\lambda_1} \frac{f_2}{2} + u_{2,\alpha} \frac{f_1}{2} + u_3 \frac{f_x + f_y}{2}). \quad (\text{E7})$$

Here we used the cocycles from App. C, and w_2 is a cocycle representing the Stiefel-Whitney class of the $\text{SO}(3)$ bundle. Then by applying Eq. (E6), we find

$$\begin{aligned} \Upsilon_{\lambda_1}^{\text{SO}(3)} &= u_{1,\alpha,\lambda_1} \\ \Upsilon_{\nu_1}^{\text{SO}(3)} &= u_{1,\alpha,\lambda_1} + u_{2,\alpha} \\ \Upsilon_{\mu_1}^{\text{SO}(3)} &= u_{1,\alpha,\lambda_1} + u_3 \\ \Rightarrow \Upsilon_{\lambda_1}^{\text{SO}(3)} + \Upsilon_{\nu_1}^{\text{SO}(3)} &= u_{2,\alpha} \pmod{2}, \\ \Rightarrow \Upsilon_{\lambda_1}^{\text{SO}(3)} + \Upsilon_{\mu_1}^{\text{SO}(3)} &= u_3 \pmod{2}. \end{aligned} \quad (\text{E8})$$

To derive Eq. 51 we finally note that $u_{2,\alpha} = \mathcal{S}_\alpha^{\text{SO}(3)}$.

b. pmm

The analogous equation to Eq. E7 for pmm is

$$\varphi_3 = \pi w_2(u_{1,\alpha,\lambda} f_2 + u_{2,\alpha} f_1 + u_{3,x} f_x + u_{3,y} f_y), \quad (\text{E9})$$

where the cocycles $f_{\dots}$ are the same as those in Eq. C20, with the only modification that the variable a is now

defined modulo 2.

The various reflections (see Fig. 3) are

$$\mathbf{r}_\mu = \mathbf{x}\mathbf{r}_\lambda; \quad \mathbf{r}_\nu = \mathbf{h}_\alpha\mathbf{r}_\lambda; \quad \mathbf{r}_\kappa = \mathbf{y}\mathbf{h}_\alpha\mathbf{r}_\lambda. \quad (\text{E10})$$

Then using Eq. E6, we obtain

$$\begin{aligned} \Upsilon_\lambda^{\text{SO}(3)} &= u_{1,\alpha,\lambda}; \\ \Upsilon_\mu^{\text{SO}(3)} &= u_{1,\alpha,\lambda} + u_{3,x}; \\ \Upsilon_\nu^{\text{SO}(3)} &= u_{1,\alpha,\lambda} + u_{2,\alpha}; \\ \Upsilon_\kappa^{\text{SO}(3)} &= u_{1,\alpha,\lambda} + u_{2,\alpha} + u_{3,y}. \end{aligned} \quad (\text{E11})$$

The various rotations are

$$\mathbf{h}_\beta = \mathbf{x}\mathbf{y}\mathbf{h}_\alpha; \quad \mathbf{h}_\gamma = \mathbf{y}\mathbf{h}_\alpha; \quad \mathbf{h}_\delta = \mathbf{x}\mathbf{h}_\alpha. \quad (\text{E12})$$

Recall also that for $\mathbf{g}$ of order two,

$$(-1)^{\Theta_o(\mathbf{g})} = \nu_3(\mathbf{g}\mathbf{h}_o, \mathbf{g}\mathbf{h}_o, \mathbf{g}\mathbf{h}_o). \quad (\text{E13})$$

Therefore, the type D1 invariants are

$$\begin{aligned} \mathcal{S}_\alpha^{\text{SO}(3)} &= u_{2,\alpha,\lambda}; \\ \mathcal{S}_\beta^{\text{SO}(3)} &= u_{2,\alpha,\lambda} + u_{3,x} + u_{3,y} \\ \mathcal{S}_\gamma^{\text{SO}(3)} &= u_{2,\alpha,\gamma} + u_{3,y} \\ \mathcal{S}_\delta^{\text{SO}(3)} &= u_{2,\alpha,\lambda} + u_{3,x}. \end{aligned} \quad (\text{E14})$$

We thus see that only 3 of the 4 D1 invariants are independent. To fully determine the invariants appearing in Eq. E9, we need to include at least one type D2 invariant.

Appendix F: Group cohomology tables

In Table XIII we present the group cohomology with $\mathbb{Z}$ coefficients for every wallpaper group up to degree 5.

Group cohomology $\mathcal{H}^n(G_{\text{space}}, \mathbb{Z})$						
#	$G_{\text{space}} \backslash n$	1	2	3	4	5
1	p1	$\mathbb{Z}^2$	$\mathbb{Z}$	$\mathbb{Z}_1$	$\mathbb{Z}_1$	$\mathbb{Z}_1$
2	p2	$\mathbb{Z}_1$	$\mathbb{Z} \times \mathbb{Z}_2^3$	$\mathbb{Z}_1$	$\mathbb{Z}_2^4$	$\mathbb{Z}_1$
3	pm	$\mathbb{Z}$	$\mathbb{Z}_2^2$	$\mathbb{Z}_2^2$	$\mathbb{Z}_2^2$	$\mathbb{Z}_2^2$
4	pg	$\mathbb{Z}$	$\mathbb{Z}_2$	$\mathbb{Z}_1$	$\mathbb{Z}_1$	$\mathbb{Z}_1$
5	cm	$\mathbb{Z}$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2$
6	pmm	$\mathbb{Z}_1$	$\mathbb{Z}_2^4$	$\mathbb{Z}_2^4$	$\mathbb{Z}_2^8$	$\mathbb{Z}_2^8$
7	pmg	$\mathbb{Z}_1$	$\mathbb{Z}_2^3$	$\mathbb{Z}_2$	$\mathbb{Z}_2^3$	$\mathbb{Z}_2$
8	pgg	$\mathbb{Z}_1$	$\mathbb{Z}_4 \times \mathbb{Z}_2$	$\mathbb{Z}_1$	$\mathbb{Z}_2^2$	$\mathbb{Z}_1$
9	cmm	$\mathbb{Z}_1$	$\mathbb{Z}_2^3$	$\mathbb{Z}_2^2$	$\mathbb{Z}_2^5$	$\mathbb{Z}_2^4$
10	p4	$\mathbb{Z}_1$	$\mathbb{Z} \times \mathbb{Z}_4 \times \mathbb{Z}_2$	$\mathbb{Z}_1$	$\mathbb{Z}_4^2 \times \mathbb{Z}_2$	$\mathbb{Z}_1$
11	p4m	$\mathbb{Z}_1$	$\mathbb{Z}_2^3$	$\mathbb{Z}_2^3$	$\mathbb{Z}_4^2 \times \mathbb{Z}_2^4$	$\mathbb{Z}_2^6$
12	p4g	$\mathbb{Z}_1$	$\mathbb{Z}_4 \times \mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_4 \times \mathbb{Z}_2^2$	$\mathbb{Z}_2^2$
13	p3	$\mathbb{Z}_1$	$\mathbb{Z} \times \mathbb{Z}_3^2$	$\mathbb{Z}_1$	$\mathbb{Z}_3^3$	$\mathbb{Z}_1$
14	p3m1	$\mathbb{Z}_1$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_3^2 \times \mathbb{Z}_6$	$\mathbb{Z}_2$
15	p31m	$\mathbb{Z}_1$	$\mathbb{Z}_6$	$\mathbb{Z}_2$	$\mathbb{Z}_3 \times \mathbb{Z}_6$	$\mathbb{Z}_2$
16	p6	$\mathbb{Z}_1$	$\mathbb{Z} \times \mathbb{Z}_6$	$\mathbb{Z}_1$	$\mathbb{Z}_6^2$	$\mathbb{Z}_1$
17	p6m	$\mathbb{Z}_1$	$\mathbb{Z}_2^2$	$\mathbb{Z}_2^2$	$\mathbb{Z}_2^2 \times \mathbb{Z}_6^2$	$\mathbb{Z}_2^4$

TABLE XIII. Group cohomology $\mathcal{H}^n(G_{\text{space}}, \mathbb{Z})$ for $n = 1, 2, 3, 4, 5$, where G_{space} acts trivially on the $\mathbb{Z}$ coefficients. Note that $\mathcal{H}^0(G_{\text{space}}, \mathbb{Z}) \cong \mathbb{Z}$. $\mathbb{Z}_1$ denotes the trivial group.

Group cohomology twisted by orientation: $\mathcal{H}^n(G_{\text{space}}, \mathbb{Z}^{\text{or}})$

#	$G_{\text{space}} \backslash n$	1	2	3	4	5
1	p1	$\mathbb{Z}^2$	$\mathbb{Z}$	$\mathbb{Z}_1$	$\mathbb{Z}_1$	$\mathbb{Z}_1$
2	p2	$\mathbb{Z}_1$	$\mathbb{Z} \times \mathbb{Z}_2^3$	$\mathbb{Z}_1$	$\mathbb{Z}_2^4$	$\mathbb{Z}_1$
3	pm	$\mathbb{Z} \times \mathbb{Z}_2$	$\mathbb{Z} \times \mathbb{Z}_2$	$\mathbb{Z}_2^2$	$\mathbb{Z}_2^2$	$\mathbb{Z}_2^2$
4	pg	$\mathbb{Z} \times \mathbb{Z}_2$	$\mathbb{Z}$	$\mathbb{Z}_1$	$\mathbb{Z}_1$	$\mathbb{Z}_1$
5	cm	$\mathbb{Z} \times \mathbb{Z}_2$	$\mathbb{Z}$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2$
6	pmm	$\mathbb{Z}_2$	$\mathbb{Z} \times \mathbb{Z}_2^3$	$\mathbb{Z}_2^4$	$\mathbb{Z}_2^8$	$\mathbb{Z}_2^8$
7	pmg	$\mathbb{Z}_2$	$\mathbb{Z} \times \mathbb{Z}_2^2$	$\mathbb{Z}_2$	$\mathbb{Z}_2^3$	$\mathbb{Z}_2$
8	pgg	$\mathbb{Z}_2$	$\mathbb{Z} \times \mathbb{Z}_2$	$\mathbb{Z}_1$	$\mathbb{Z}_2^2$	$\mathbb{Z}_1$
9	cmm	$\mathbb{Z}_2$	$\mathbb{Z} \times \mathbb{Z}_2^2$	$\mathbb{Z}_2^2$	$\mathbb{Z}_2^5$	$\mathbb{Z}_2^4$
10	p4	$\mathbb{Z}_1$	$\mathbb{Z} \times \mathbb{Z}_4 \times \mathbb{Z}_2$	$\mathbb{Z}_1$	$\mathbb{Z}_4^2 \times \mathbb{Z}_2$	$\mathbb{Z}_1$
11	p4m	$\mathbb{Z}_2$	$\mathbb{Z} \times \mathbb{Z}_4 \times \mathbb{Z}_2$	$\mathbb{Z}_2^3$	$\mathbb{Z}_2^6$	$\mathbb{Z}_2^6$
12	p4g	$\mathbb{Z}_2$	$\mathbb{Z} \times \mathbb{Z}_4$	$\mathbb{Z}_2$	$\mathbb{Z}_4 \times \mathbb{Z}_2^2$	$\mathbb{Z}_2^2$
13	p3	$\mathbb{Z}_1$	$\mathbb{Z} \times \mathbb{Z}_3^2$	$\mathbb{Z}_1$	$\mathbb{Z}_3^3$	$\mathbb{Z}_1$
14	p3m1	$\mathbb{Z}_2$	$\mathbb{Z} \times \mathbb{Z}_3^2$	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}_2$
15	p31m	$\mathbb{Z}_2$	$\mathbb{Z} \times \mathbb{Z}_3$	$\mathbb{Z}_2$	$\mathbb{Z}_6$	$\mathbb{Z}_2$
16	p6	$\mathbb{Z}_1$	$\mathbb{Z} \times \mathbb{Z}_6$	$\mathbb{Z}_1$	$\mathbb{Z}_6^2$	$\mathbb{Z}_1$
17	p6m	$\mathbb{Z}_2$	$\mathbb{Z} \times \mathbb{Z}_6$	$\mathbb{Z}_2^2$	$\mathbb{Z}_2^4$	$\mathbb{Z}_2^4$

TABLE XIV. Group cohomology $\mathcal{H}^n(G_{\text{space}}, \mathbb{Z}^{\text{or}})$ for $n = 1, 2, 3, 4, 5$, in which reflections act by changing the sign of the coefficient. Note that $\mathcal{H}^0(G_{\text{space}}, \mathbb{Z}^{\text{or}}) \cong \mathbb{Z}$ if G_{space} is orientation preserving, and is the trivial group. Furthermore, for the groups without reflections (p1, p2, p3, p4 and p6), $\mathcal{H}^n(G_{\text{space}}, \mathbb{Z}) \cong \mathcal{H}^n(G_{\text{space}}, \mathbb{Z}^{\text{or}})$. $\mathbb{Z}_1$ denotes the trivial group

#	G_{space}	G_0	$\rho(\mathbf{h})$
2	p2	$\mathbb{Z}_2$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$
10	p4	$\mathbb{Z}_4$	$\begin{pmatrix} 0 & -1 \\ +1 & 0 \end{pmatrix}$
13	p3	$\mathbb{Z}_3$	$\begin{pmatrix} -1 & -1 \\ +1 & 0 \end{pmatrix}$
16	p6	$\mathbb{Z}_6$	$\begin{pmatrix} 0 & -1 \\ +1 & 1 \end{pmatrix}$

TABLE XV. **Orientation preserving wallpaper groups:** As abstract groups $G_{\text{space}} = \mathbb{Z}^2 \rtimes_{\rho} G_0$. The point groups corresponding to $G_0 = \mathbb{Z}_M$ are denoted by C_M .

#	G_{space}	G_0	$\rho(\mathbf{h})$	$\rho(\mathbf{r})$
3	pm	$\mathbb{Z}_2$	-	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$
5	cm	$\mathbb{Z}_2$	-	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
6	pmm	$\mathbb{Z}_2^2$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$
9	cmm	$\mathbb{Z}_2^2$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
11	p4m	$\mathbb{Z}_4 \rtimes \mathbb{Z}_2$	$\begin{pmatrix} 0 & -1 \\ +1 & 0 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$
14	p3m1	$\mathbb{Z}_3 \rtimes \mathbb{Z}_2$	$\begin{pmatrix} -1 & -1 \\ +1 & 0 \end{pmatrix}$	$\begin{pmatrix} -1 & -1 \\ 0 & 1 \end{pmatrix}$
15	p31m	$\mathbb{Z}_3 \rtimes \mathbb{Z}_2$	$\begin{pmatrix} -1 & -1 \\ +1 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & +1 \\ 0 & -1 \end{pmatrix}$
17	p6m	$\mathbb{Z}_6 \rtimes \mathbb{Z}_2$	$\begin{pmatrix} 0 & -1 \\ +1 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$

TABLE XVI. **Orientation reversing symmorphic groups wallpaper groups:** As abstract groups $G_{\text{space}} = \mathbb{Z}^2 \rtimes_{\rho} G_0$, the reflection in G_0 is $\mathbf{r}$, while the generator of the rotation subgroup is $\mathbf{h}$. The point groups corresponding to $G_0 = \mathbb{Z}_M \rtimes \mathbb{Z}_2$ are denoted by D_M .

Appendix G: Crystallography concepts

This appendix gives a summary of our conventions for wallpaper groups. In App. G 1, we give a concrete definition of the 17 wallpaper groups in terms of generators. App. G 2 contains our conventions for the high symmetry points and lines used to label the invariants in the main text.

1. Definition of wallpaper groups

Recall that wallpaper groups are extensions of a finite group (G_0) by translations $\mathbb{Z}^2$. The extension is specified by ρ , an automorphism of $\mathbb{Z}^2$ enacted by G_0 , and a 2-cocycle $m \in \mathcal{Z}_{\rho}^2(G_0, \mathbb{Z}^2)$. ρ specifies the point group, while m specifies if any point group symmetry squares to a translation. m is trivial for symmorphic groups.

Two-dimensional point groups have the general form $G_0 = \mathbb{Z}_M$ or $\mathbb{Z}_M \rtimes \mathbb{Z}_2$ with $M = 1, 2, 3, 4, 6$. For the abelian groups $\mathbb{Z}_M$, $\mathbf{h}$ denotes a generator. For the dihedral groups $\mathbb{Z}_M \rtimes \mathbb{Z}_2$ we denote by $\mathbf{h}$ the generator of the $\mathbb{Z}_M$ subgroup, and by $\mathbf{r}$ the generator of $\mathbb{Z}_2$. Since ρ is a group homomorphism, it is enough to specify $\rho(\mathbf{r})$ and $\rho(\mathbf{h})$ as elements of $\text{GL}_2(\mathbb{Z})$.

The non-symmorphic groups are defined as follows. The group pg is simply $\mathbb{Z} \rtimes \mathbb{Z}$; in this case, $G_0 = \mathbb{Z}_1 \rtimes \mathbb{Z}_2$ with $\rho(\mathbf{r}) = \text{diag}(+1, -1)$ and $m(\mathbf{r}, \mathbf{r}) = [1, 0]^\top$: this indicates that there is a glide symmetry along the x axis. The groups pmg and pgg both have $G_0 = \mathbb{Z}_2 \rtimes \mathbb{Z}_2 \cong \mathbb{Z}_2 \times \mathbb{Z}_2$ and are of the form $\text{pg} \rtimes \mathbb{Z}_2^{\mathbf{h}} = (\mathbb{Z} \rtimes \mathbb{Z}) \rtimes \mathbb{Z}_2$. Let $\mathbf{g}$ be the horizontal glide and $\mathbf{y}$ the vertical translation. For pmg , we have $\mathbf{hg} = \mathbf{g}^{-1}\mathbf{h}$ and $\mathbf{hy} = \mathbf{y}^{-1}\mathbf{h}$. While for pgg , $\mathbf{hg} = \mathbf{y}^{-1}\mathbf{g}^{-1}\mathbf{h}$ and $\mathbf{hy} = \mathbf{y}^{-1}\mathbf{h}$. Finally, $\text{p4g} \cong \text{p4} \rtimes \mathbb{Z}_2^{\mathbf{r}}$ but now $\mathbf{rx} = \mathbf{y}^{-1}\mathbf{r}$, $\mathbf{ry} = \mathbf{x}^{-1}\mathbf{r}$ and $\mathbf{rh} = \mathbf{yh}^{-1}\mathbf{r}$.

Explicitly, we can think of the wallpaper groups as subgroups of $\text{GL}_3(\mathbb{Q})$ (3-by-3 matrices with rational entries). Translations are represented as

$$\mathbf{x} \mapsto \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}; \quad \mathbf{y} \mapsto \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix}. \quad (\text{G1})$$

For symmorphic groups, rotations and reflections are mapped to

$$\mathbf{h} \mapsto \begin{pmatrix} \rho(\mathbf{h}) & 0 \\ 0 & 1 \end{pmatrix}; \quad \mathbf{r} \mapsto \begin{pmatrix} \rho(\mathbf{r}) & 0 \\ 0 & 1 \end{pmatrix}. \quad (\text{G2})$$

The non-symmorphic group pg has point group D_1 . The glide $\mathbf{g}$ is represented by

$$\mathbf{g} \mapsto \begin{pmatrix} 1 & 0 & 1/2 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

For pmg and pgg , the point groups is D_2 . However, they differ in how the C_2 rotation is represented:

$$\mathbf{h}_{\text{pmg}} \mapsto \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}; \quad \mathbf{h}_{\text{pgg}} \mapsto \begin{pmatrix} -1 & 0 & 1/2 \\ 0 & -1 & 1/2 \\ 0 & 0 & 1 \end{pmatrix}.$$

Finally, the point group of p4g is D_4 . The reflection and rotation are represented as

$$\mathbf{r}_{\text{p4g}} \mapsto \begin{pmatrix} 0 & -1 & 1/2 \\ -1 & 0 & 1/2 \\ 0 & 0 & 1 \end{pmatrix}; \quad \mathbf{h}_{\text{p4g}} \mapsto \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

2. Unit cells for Wallpaper groups

The conventions used for all the wallpaper groups are shown in Figs. 11, 12 and 13. We omit wallpaper group p1 because there is nothing to label.

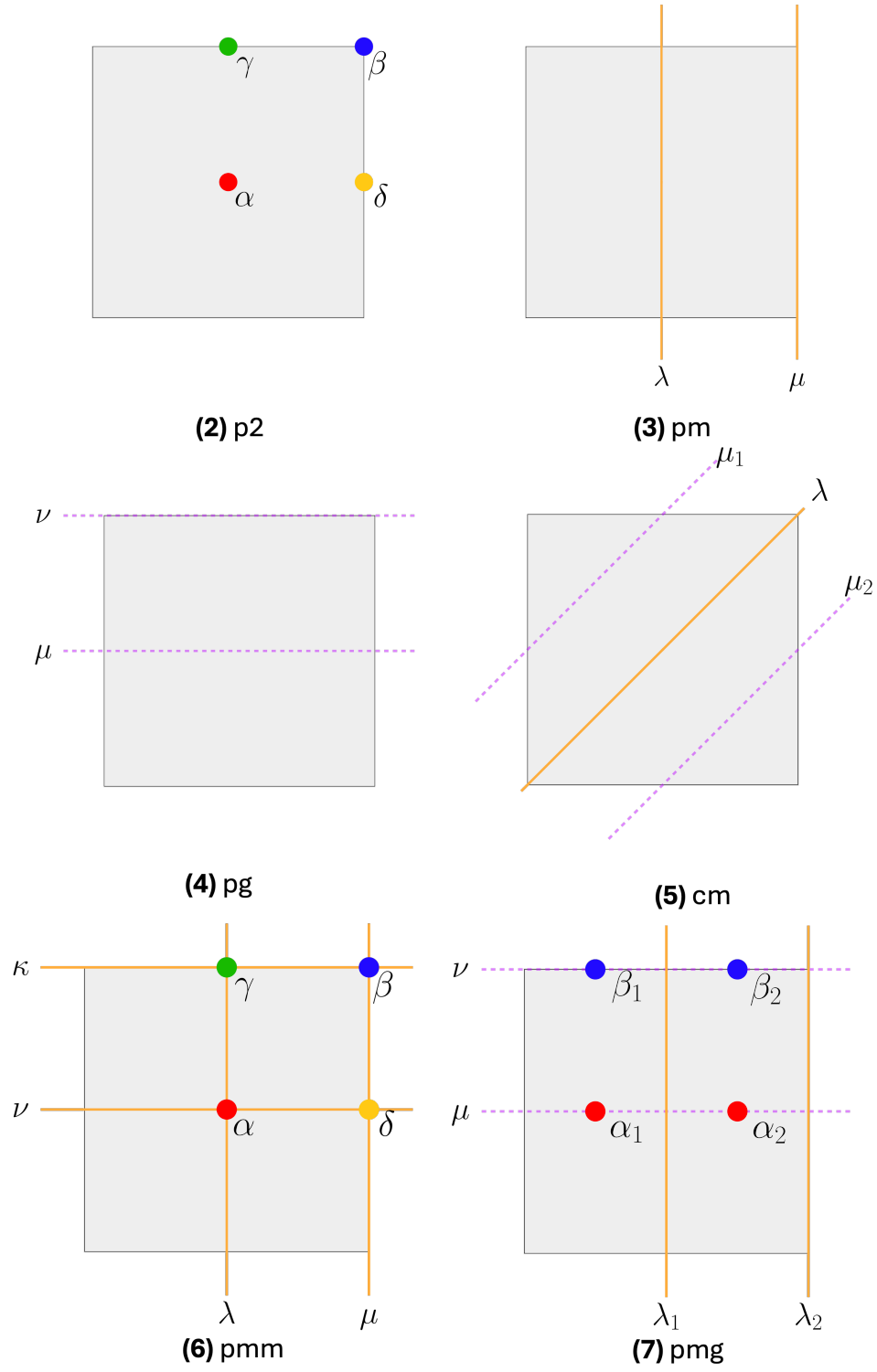


FIG. 11. Conventions for the unit cell, Wyckoff positions and symmetry lines for wallpaper groups p2, pm, pg, cm, pmm, and pmg.

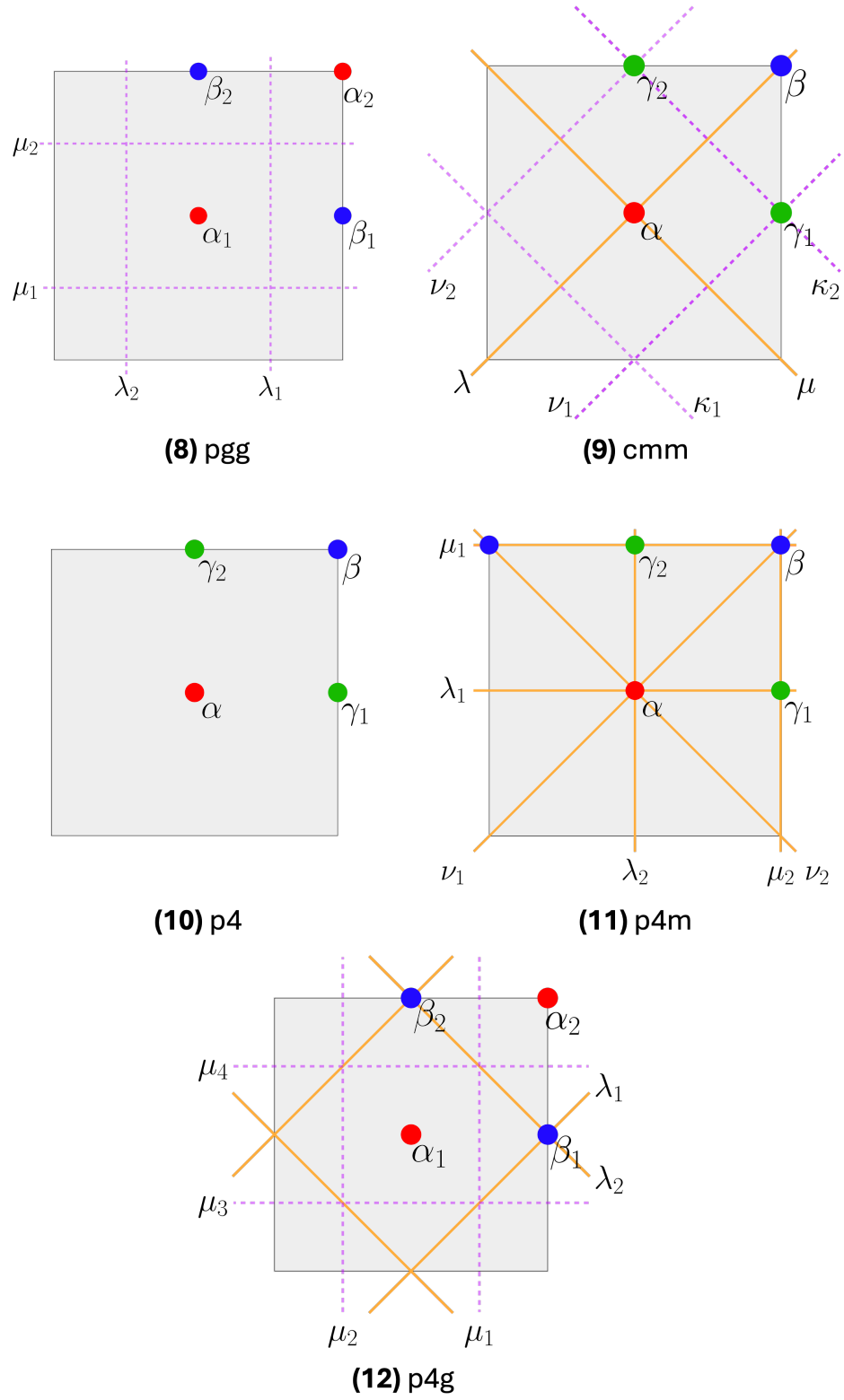


FIG. 12. Conventions for the unit cell, Wyckoff positions and symmetry lines for wallpaper groups pgg, cmm, p4, p4m, and p4g.

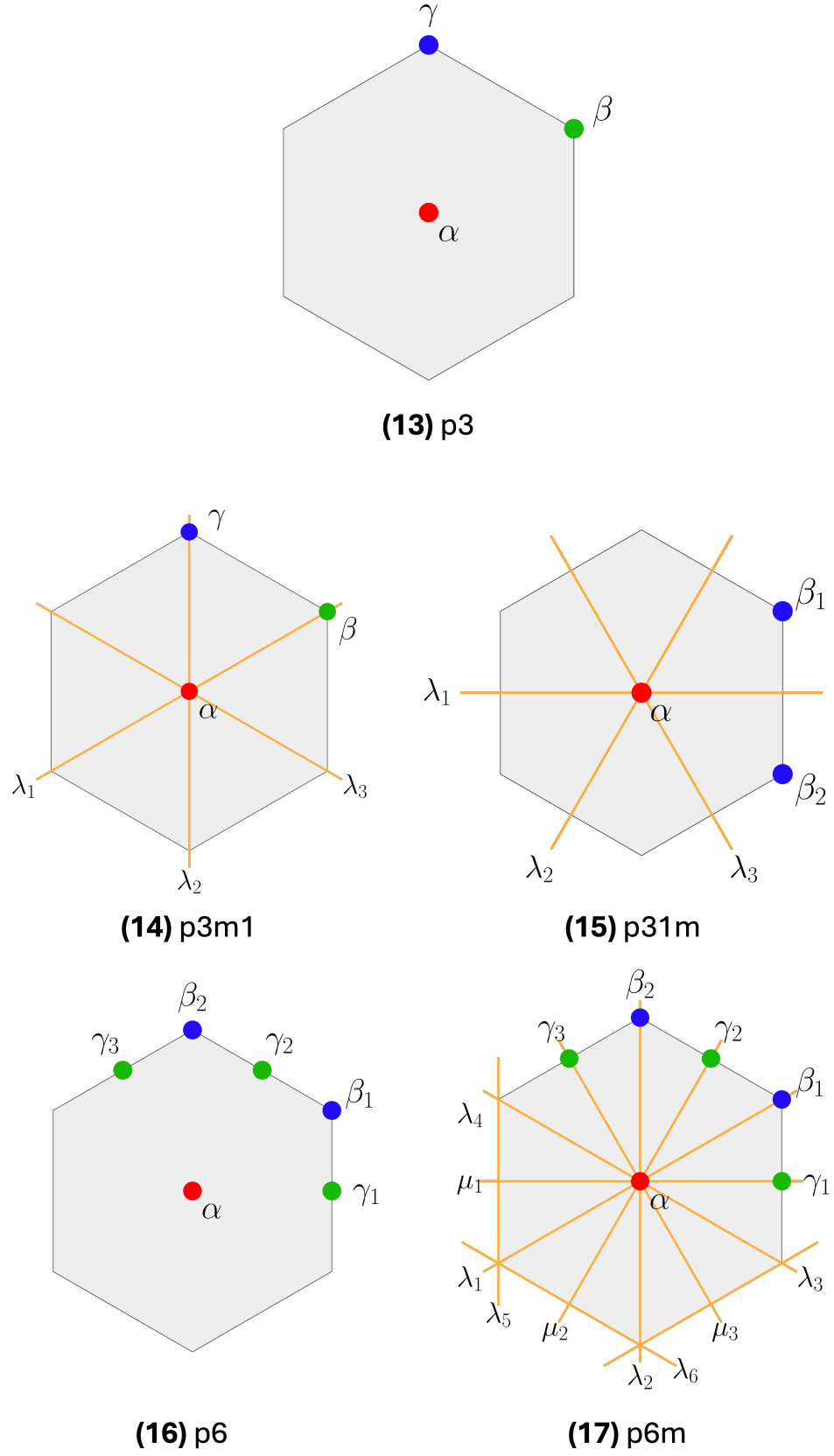


FIG. 13. Conventions for the unit cell, Wyckoff positions and symmetry lines for wallpaper groups p3, p3m1, p31m, p6, and p6m.