General Theory of Momentum-Space Nonsymmorphic Symmetry

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As a fundamental concept of all crystals, space groups are partitioned into symmorphic groups and nonsymmorphic groups. Each nonsymmorphic group contains glide reflections or screw rotations with fractional lattice translations, which are absent in symmorphic groups. Although nonsymmorphic groups ubiquitously exist on real-space lattices, on the reciprocal lattices in momentum space, the ordinary theory only allows symmorphic groups. In this work, we develop a novel theory for momentum-space nonsymmorphic space groups (k-NSGs), utilizing the projective representations of space groups. The theory is quite general: Given any k-NSGs in any dimensions, it can identify the real-space symmorphic space groups (r-SSGs) and construct the corresponding projective representation of the r-SSG that leads to the k-NSG. To demonstrate the broad applicability of our theory, we show these projective representations and therefore all k-NSGs can be realized by gauge fluxes over real-space lattices. Our work fundamentally extends the framework of crystal symmetry, and therefore can accordingly extend any theory based on crystal symmetry, for instance, the classification crystalline topological phases.

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Introduction.—Space groups fundamentally characterize symmetries for all forms of natural crystals, including electronic materials, spin liquids, and crystalline superconductors, as well as various artificial crystals, including photonic or acoustic crystals, cold atoms in optical lattices, periodic mechanical systems, and electric-circuit arrays [1]. Each crystal symmetry can be either nonsymmorphic or symmorphic, depending on whether it involves a fractional lattice translation. Two elementary examples are the glide reflection and screw rotation. The pure reflection or rotation changes the crystal, and the associated fractional lattice translation should be followed to leave the crystal invariant. Hence, as a qualitative categorization, a space group is either symmorphic or nonsymmorphic groups, according to whether it contains nonsymmorphic symmetries.

In three dimensions (two dimensions), there are 157 (4) nonsymmorphic groups among 230 (17) space groups. In fact, as the dimensionality increases, the proportion of nonsymmorphic groups becomes more and more dominant among all space groups [2]. As we know, nonsymmorphic groups ubiquitously exist on *real space* lattices. It has been a hot topic to discuss nontrivial (topological) properties arising from real-space nonsymmorphic space groups (r-NSGs) [3–6].

The situation is radically changed in *momentum space* according to the ordinary theory of space groups [1]. The *momentum space* is dual to the *real space* under the Fourier transform. We have the reciprocal lattice in momentum space for each real-space lattice. And the momentum-space Hamiltonian $\mathcal{H}(\boldsymbol{k})$ is invariant under integral reciprocal-lattice translations, i.e., $\mathcal{H}(\boldsymbol{k}+\boldsymbol{K})=\mathcal{H}(\boldsymbol{k})$ for any reciprocal lattice vector $\boldsymbol{K}$. However, every symmetry operator only rotates $\boldsymbol{k}$ with NO fractional reciprocal-lattice translation [7], and therefore no nonsymmorphic group exists in momentum space [1,8].

Hence, a natural question arises: *Is it possible to have nonsymmorphic groups in momentum space?*

Here, we establish a novel theory of momentum-space nonsymmorphic space groups (k-NSGs) based on the *projective* representations of space groups. Recall that a projective representation ρ of a group G is characterized by a multiplier ν, i.e.,

$$\rho(g_1)\rho(g_2)=\nu(g_1,g_2)\rho(g_1g_2). \qquad (1)$$

Here, $\rho(g)$ is the symmetry operator of $g\in G$, and $\nu(g_1,g_2)\in U(1)$ is a phase factor for any $g_1,g_2\in G$. It is appropriate multipliers that endow symmetry operators fractional reciprocal-lattice translations.

Our theory can exhaustively represent k-NSGs in any dimensions, i.e., for each dD k-NSG we can identify a real-space symmorphic space group (r-SSG) and the multiplier ν of the r-SSG that leads to the k-NSG. Particularly, we have explicitly tabulated the representations of all 157 3D k-NSGs, and 4 2D k-NSGs.

All these multipliers of r-SSG and therefore all k-NSGs, can be realized by lattice models with gauge fluxes. This connects k-NSGs to spin liquids with emergent gauge fields [23,24], crystalline superconductors [25], and various artificial crystals with engineerable gauge fluxes [9–15,26–29].

Under a k-NSG, the Hamiltonian is constrained by

$$U_R(\boldsymbol{k})\mathcal{H}(\boldsymbol{k})[U_R(\boldsymbol{k})]^\dagger = \mathcal{H}(R\boldsymbol{k} + \boldsymbol{\kappa}_R). \tag{2}$$

Here, for each symmetry R, $\boldsymbol{\kappa}_R$ is the associated fractional reciprocal-lattice translation, and $U_R(\boldsymbol{k})$ is the unitary operator. Since crystalline topological phases rely on symmetry constraints [4,30–32], and the novel constraints of Eq. (2) can significantly extend the existing topological classifications [33–35]. Recently, it has been shown that projective symmetry can lead to fascinating topological phases [36–44]. Hence, Eq. (2) can open a broad avenue along this direction.

An example: k-NSG Pg from projective Pm.—Let us start with presenting a simple example to illustrate the main ideas before introducing our general theory.

Our example is the wallpaper group Pm. It is generated by translation symmetries L_x and L_y along the x and y directions, respectively, and the mirror reflection symmetry M_x that inverses the x coordinate. It is clear that in Pm

$$M_x L_y = L_y M_x, \tag{3}$$

i.e., M_x and L_y commute with each other since they act on different dimensions.

We then consider a projective representation ρ of Pm with the multiplier ν satisfying

$$\nu(M_x, L_y) = -1, \qquad \nu(L_y, M_x) = 1. \tag{4}$$

Then, according to Eq. (1), $\rho(M_x)\rho(L_y) = -\rho(M_x L_y)$ and $\rho(L_y)\rho(M_x) = \rho(L_y M_x)$. Since $\rho(M_x L_y) = \rho(L_y M_x)$, we have the projective algebraic relation,

$$\rho(M_x)\rho(L_y) = -\rho(L_y)\rho(M_x). \tag{5}$$

In momentum space, the translation operator $\rho(L_y)$ is decomposed into $\boldsymbol{k}$ components, $\rho_{\boldsymbol{k}}(L_y) = e^{ik_y b}$ with b the lattice constant along the y direction. Then, from (5), we see $\rho(M_x)\rho_{\boldsymbol{k}}(L_y)[\rho(M_x)]^\dagger = -\rho_{\boldsymbol{k}}(L_y)$, i.e., $\rho(M_x)e^{ik_y b}[\rho(M_x)]^\dagger = -e^{ik_y b} = e^{i(k_y + G_y/2)b}$, where $G_y = 2\pi/b$ is the reciprocal lattice constant along the k_y direction. Hence, under the projective representation, k_y is translated by a half of the reciprocal lattice constant, i.e.,

$$\rho(M_x): (k_x, k_y) \mapsto (-k_x, k_y + G_y/2). \tag{6}$$

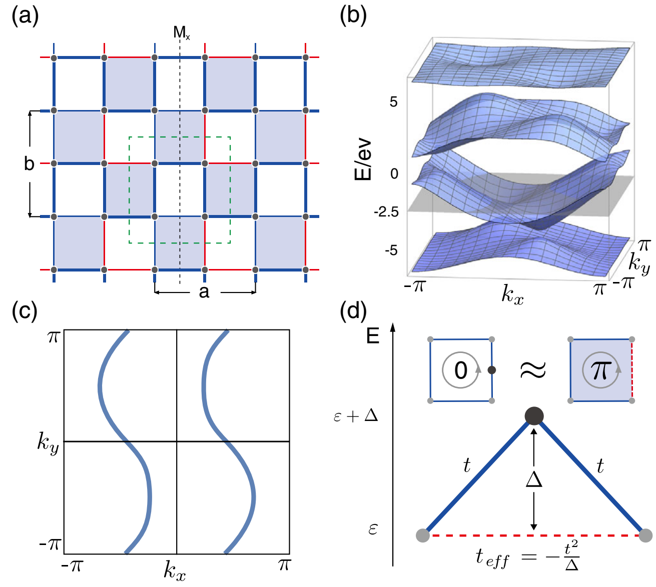

FIG. 1. (a) The lattice model with the flux pattern preserving Pm. Blue and red bonds denote positive and negative hopping amplitudes, respectively. Each plaquette with π flux is shadowed. (b) The band structure of the model. (c) The constant-energy contour of the band structure at $E = -0.25$ eV. We observe that both (b) and (c) are invariant under the glide reflection $\mathcal{G}_x$. Note that $a = b = 1$ is assumed in (b) and (c). (d) The effective negative hopping amplitude. Two (light) sites with energy ϵ hop to the (dark) site with energy $\epsilon + \Delta$ with amplitude $t > 0$. The low-energy effective hopping amplitude between the two sites with energy ϵ is $-t^2/\Delta$.

Here, the inversion of k_x comes from the ordinary relation $\rho(M_x)\rho(L_x) = \rho(L_x^{-1})\rho(M_x)$.

From the above derivations, we see $\rho(M_x)$ acts on the momentum space as a nonsymmorphic symmetry, namely, a glide reflection, which stems from the multiplier ν specified by Eq. (4).

Then, a natural question is how to realize the projective representation of Eqs. (4) or (5). It is well known that gauge fluxes can lead to projective representations. A general formulation is given in the Supplemental Material [8]. Specializing to Eq. (4), a lattice model with appropriate gauge fluxes is illustrated in Fig. 1(a).

The Hamiltonian and the unitary operator U_{M_x} for M_x can be found in the Supplemental Material [8]. Importantly, the symmetry constraint is given by

$$U_{M_x}\mathcal{H}(k_x, k_y)U_{M_x}^\dagger = \mathcal{H}(-k_x, k_y + G_y/2). \tag{7}$$

One may write $\rho(M_x)$ in momentum space as $\rho(M_x) = U_{M_x}\mathcal{G}_{k_x}$. Here, $\mathcal{G}_{k_x}$ is the glide reflection in momentum space, with $\mathcal{G}_{k_x}(k_x, k_y) = (-k_x, k_y + G_y/2)$. The energy band structure is shown in Fig. 1(b), and a constant energy cut is given in Fig. 1(c). We observe that the band structure is indeed invariant under the glide reflection. Moreover, it is easy to verify Eq. (5), since $\rho(k_y) = e^{ik_y b}$.

In experiments, we need to realize the particular pattern of π fluxes or negative hopping amplitudes of the model. A simple mechanism is illustrated in Fig. 1(d). The low-energy effective hopping amplitude of two low-energy sites through a high-energy site is negative if the energy gap Δ is large enough. Thus, in principle, one can engineer negative hopping amplitudes by appropriately inserting high-energy sites [see Fig. 1(d)]. More details and other mechanisms for realizing gauge fluxes can be found in the Supplemental Material [8].

Two questions.—We shall generalize the main ideas of the simple example into a general theory for all k-NSGs in any dimensions. Specifically, for each k-NSG, we shall answer two questions: (i) What is the corresponding r-SSG? (ii) With the r-SSG obtained, what is the multiplier that leads to the k-NSG?

To answer the two questions, we first look into how certain multipliers of projective representations can lead to fractional translations of momenta in the following two sections.

The canonical multiplier.—To spell out the multipliers that we are interested in, we first introduce a basic formulation of r-SSGs. Each r-SSG contains two natural subgroups, namely, the translation group $\mathcal{L}$ and the point group P. $\mathcal{L}$ consists of lattice translations with lengths $\boldsymbol{t} = \sum_i n^i \boldsymbol{e}_i$, where n^i are integers, and $\boldsymbol{e}_i$ the primitive lattice vectors. Hence, the group elements can be written as

$$\mathcal{L} = \{\boldsymbol{t} = \sum_i n^i \boldsymbol{e}_i, n^i \in \mathbb{Z}\}. \tag{8}$$

$\mathcal{L}$ can equally be interpreted as the collection of lattice sites related to the origin by lattice translations. Hereafter, we refer to $\mathcal{L}$ as the real-space translation group and lattice, interchangeably. The point group P is a finite subgroup of the orthogonal group $O(d)$. P compatibly operates on the lattice $\mathcal{L}$, i.e., $R\boldsymbol{t} \in \mathcal{L}$ for any $R \in P$ and $\boldsymbol{t} \in \mathcal{L}$. Such a compatible pair $(P, \mathcal{L})$ is referred to as a crystal class D. Accordingly, each r-SSG can be denoted by $\mathcal{L} \rtimes_D P$, consisting of group elements $(\boldsymbol{t}, R)$ with $\boldsymbol{t} \in \mathcal{L}$ and $R \in P$. The group multiplication is given by

$$(\boldsymbol{t}_1, R_1)(\boldsymbol{t}_2, R_2) = (\boldsymbol{t}_1 + R_1\boldsymbol{t}_2, R_1R_2). \tag{9}$$

Notably, a point group may compatibly operate on more than one kind of lattices, and therefore corresponds to a number of crystal classes. Consequently, in three dimensions, there are 32 point groups, but 73 crystal classes and therefore 73 symmorphic space groups.

We are now ready to state one of the key results, namely, the multiplier, which is given by

$$\nu((\boldsymbol{t}_1, R_1), (\boldsymbol{t}_2, R_2)) = e^{-i\boldsymbol{\kappa}_{R_1}\cdot R_1\boldsymbol{t}_2}. \tag{10}$$

We shall show that $\boldsymbol{\kappa}_R$ is the fractional reciprocal-lattice translation associated to R, i.e., R transforms $\boldsymbol{k}$ as

$$R\colon \boldsymbol{k} \mapsto R\boldsymbol{k} + \boldsymbol{\kappa}_R. \tag{11}$$

Moreover, to make Eq. (10) a multiplier, $\boldsymbol{\kappa}_R$ must satisfy the relation

$$\boldsymbol{\kappa}_{R_1} + R_1\boldsymbol{\kappa}_{R_2} - \boldsymbol{\kappa}_{R_1R_2} \in \hat{\mathcal{L}} \tag{12}$$

for any $R_1, R_2 \in P$. Here, $\hat{\mathcal{L}}$ is the reciprocal lattice dual to $\mathcal{L}$. From $\boldsymbol{e}_i$, we can derive the primitive reciprocal-lattice vectors $\boldsymbol{G}_i$ [45], and write $\hat{\mathcal{L}}$ as

$$\hat{\mathcal{L}} = \left\{\boldsymbol{K} = \sum_i m^i \boldsymbol{G}_i, m^i \in \mathbb{Z}\right\}. \tag{13}$$

Note that $e^{i\boldsymbol{t}\cdot\boldsymbol{K}} = 1$ for any $\boldsymbol{t} \in \mathcal{L}$ and $\boldsymbol{K} \in \hat{\mathcal{L}}$. Just like $\mathcal{L}$, $\hat{\mathcal{L}}$ is referred to as the momentum-space translation group and reciprocal lattice interchangeably.

The rigorous derivations of Eqs. (10) and (12) can be found in Appendix A, which are based on Mackey's canonical form of multipliers for semi-direct product groups [16,46].

Fractional translations of momenta.—We then elucidate the meaning of $\boldsymbol{\kappa}_R$ in a projective representation ρ with the multiplier of Eq. (10). It is significant to note that with the multiplier of Eq. (10), we can derive from Eq. (1) the projective algebraic relation,

$$\rho(\boldsymbol{t}', R)\rho(\boldsymbol{t}, 1) = e^{-i\boldsymbol{\kappa}_R\cdot R\boldsymbol{t}}\rho(R\boldsymbol{t}, 1)\rho(\boldsymbol{t}', R). \tag{14}$$

Here, $(\boldsymbol{t}, 1)$ is an arbitrary element of the translation subgroup of the r-SSG $\mathcal{L} \rtimes_D P$ [8].

Let us recall that each $\boldsymbol{k}$ corresponds to the irreducible representation $\rho_{\boldsymbol{k}}$ of the translation subgroup $\mathcal{L}$, with $\rho_{\boldsymbol{k}}(\boldsymbol{t}, 1) = e^{i\boldsymbol{k}\cdot\boldsymbol{t}}$. Then, the transformation of $\rho(\boldsymbol{t}', R)$ on $\boldsymbol{k}$ is given by $\rho_{\boldsymbol{k}}(\boldsymbol{t}, 1) \mapsto \rho(\boldsymbol{t}', R)\rho_{\boldsymbol{k}}(\boldsymbol{t}, 1)[\rho(\boldsymbol{t}', R)]^\dagger$. From Eq. (14), we find that

$$e^{i\boldsymbol{k}\cdot\boldsymbol{t}} \mapsto e^{-i\boldsymbol{\kappa}_R\cdot R\boldsymbol{t}} e^{i\boldsymbol{k}\cdot R\boldsymbol{t}} = e^{i(-R^T\boldsymbol{\kappa}_R + R^T\boldsymbol{k})\cdot\boldsymbol{t}}. \tag{15}$$

Here, R^T is the transpose of R with $R^{-1} = R^T$. Note that $\boldsymbol{\kappa}_{R^T} + R^T\boldsymbol{\kappa}_R \in \hat{\mathcal{L}}$, which comes from Eq. (12) with $R_1 = R^T$ and $R_2 = R$. The transformation can be simplified to be

$$e^{i\boldsymbol{k}\cdot\boldsymbol{t}} \mapsto e^{i(R^T\boldsymbol{k} + \boldsymbol{\kappa}_{R^T})\cdot\boldsymbol{t}}. \tag{16}$$

Thus, we conclude that each $R \in P$ operates on momentum space as Eq. (11). Thus, we have proved that $\rho(\boldsymbol{t}', R)$ acts as a nonsymmorphic symmetry in momentum space.

It is insightful to compare k-NSGs with r-NSGs. Recall that for a r-NSG with the point group P. Each $R \in P$ is associated with a fractional lattice translation $\boldsymbol{\tau}_R$, and we have the relation,

$$\boldsymbol{\tau}_{R_1} + R_1\boldsymbol{\tau}_{R_2} - \boldsymbol{\tau}_{R_1R_2} \in \mathcal{L} \tag{17}$$

for any $R_1, R_2 \in P$ [1,2,8]. Here, $\mathcal{L}$ is the translation subgroup of the r-NSG. We observe that Eqs. (12) and (17) have exactly the same form, except that one is in momentum space and the other in real space. This further confirms that the projective representations of Eq. (10) give rise to k-NSGs through Eq. (11).

Remarkably, the duality between k-NSGs and projective representations of r-SSGs with Eq. (10) can be rigorously established at the cohomological level, which is treated in Appendix B.

Answers and algorithm for all k-NSGs.—We are almost ready to answer the two questions that we initially proposed. One last piece needed is the concept called the Fourier duality between crystal classes, which is introduced below.

By the Fourier transform of the real-space lattice $\mathcal{L}$, we obtain the reciprocal lattice $\hat{\mathcal{L}}$. Both $\mathcal{L}$ and $\hat{\mathcal{L}}$ are invariant under the same point group P. But, in terms of the P actions, the crystal class $\hat{D}$ of $\hat{\mathcal{L}}$ may be different from D of $\mathcal{L}$. $\hat{D}$ is referred to as the Fourier dual of D. Since the Fourier transform is invertible, we have $\hat{\hat{D}} = D$, i.e., D and $\hat{D}$ are dual to each other, resembling the duality between $\mathcal{L}$ and $\hat{\mathcal{L}}$. Hence, each crystal class is either self-dual or paired with its Fourier dual. For instance, in three dimensions, among the four crystal classes of point group D_{2h}, $mmmP$ and $mmmC$ are both self dual, while $mmmI$ and $mmmF$ are dual to each other. As illustrated in Figs. 2(a) and 2(b), the dual crystal classes $mmmF$ and $mmmI$ correspond to the face-centered cubic and body-centered cubic lattices, respectively.

For any given k-NSG with reciprocal lattice $\hat{\mathcal{L}}$, point group P, and crystal class $\hat{D}$, it is now straightforward to answer the two questions. (i) The r-SSG is $\mathcal{L}\rtimes_D P$, with D dual to $\hat{D}$ under the Fourier transform. (ii) To realize the k-NSG, the multiplier of the r-SSG, $\mathcal{L}\rtimes_D P$, is given by Eq. (10).

The answers lead to the following algorithm for constructing an arbitrary k-NSG.

First, we write down the fractional translations $\boldsymbol{\kappa}_R$ satisfying Eq. (12). From standard textbooks, e.g., Ref. [1], we can find the fractional translations $\boldsymbol{\tau}_R$ for the nonsymmorphic group. To get $\boldsymbol{\kappa}_R$, we just need to formally replace the real-space basis $\boldsymbol{e}_i$ by the reciprocal lattice basis $\boldsymbol{G}_i$.

Second, from the reciprocal lattice $\hat{\mathcal{L}}$ and the crystal class $\hat{D}$ of the k-NSG, we determine the dual lattice $\mathcal{L}$ and dual class D. $\mathcal{L}$ and D uniquely give the r-SSG $\mathcal{L}\rtimes_D P$ with P the point group of the k-NSG.

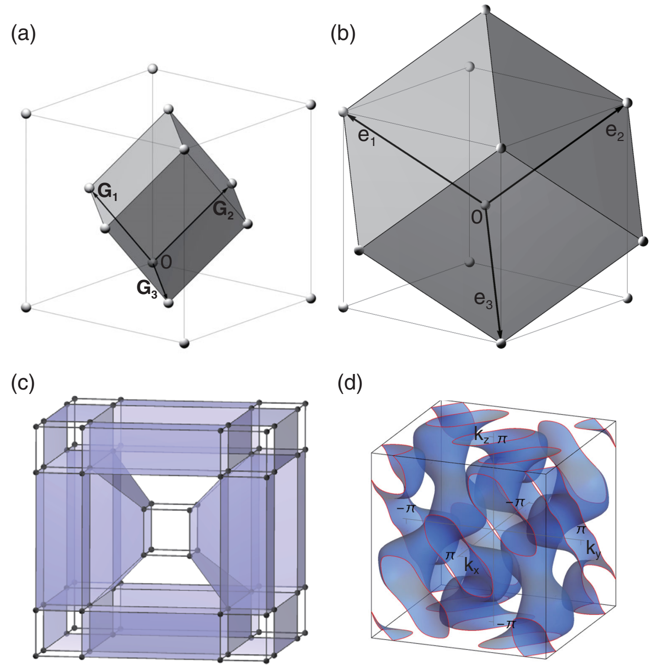

FIG. 2. (a) and (b) are the dual face-centered and body-centered cubic lattices, respectively. The primitive translations are denoted by $\boldsymbol{G}_i$ and $\boldsymbol{e}_i$, and accordingly the fundamental domains are shadowed. The length of cube edge in (a) [(b)] is 2π (2). (c) The model for k-NSG $Fddd$. Each lattice site in (b) is substituted by a small cube, and π fluxes are inserted through shadowed plaquettes connecting these small cubes. (d) A constant-energy contour of (c) preserving the k-NSG $Fddd$. See the Supplemental Material for more details [8].

Third, using Eq. (10), we write down the multiplier ν of $\mathcal{L}\rtimes_D P$ from $\boldsymbol{\kappa}_R$. The projective representation of $\mathcal{L}\rtimes_D P$ with multiplier ν gives the k-NSG.

2D and 3D k-NSGs.—Clearly, following the above algorithm, we can realize any k-NSG in any dimensions by constructing the r-SSG with the multiplier of Eq. (10). The projective representations for all k-NSGs in two and three dimensions can be found in the Supplemental Material [8].

All the four 2D nonsymmorphic space groups act on rectangular or square lattices, and therefore their crystal classes are all self dual. The case of two different crystal classes dual to each other occurs in three dimensions. Hence, we demonstrate our algorithm by such an example, namely, k-NSG $Fddd$.

The lattice $\hat{\mathcal{L}}$ of the MNSG $Fddd$ corresponds to the face-centered cube as illustrated in Fig. 2(b). The basis of $\hat{\mathcal{L}}$ is given by

$$\boldsymbol{G}_1 = \pi(0,1,1), \qquad \boldsymbol{G}_2 = \pi(1,0,1), \qquad \boldsymbol{G}_3 = \pi(1,1,0).$$

The point group of $Fddd$ is D_{2h}, which is generated by three reflections M_{k_i} with $i = 1, 2, 3$. Here, $M_{k_{1,2,3}}$ inverse

$k_{x,y,z}$, respectively. The three reflections are associated with fractional translations: $\boldsymbol{\kappa}_{M_{k_i}} = \boldsymbol{G}_i/2$. The fractional translations for other elements of D_{2h} can be derived from (12). The crystal class of $Fddd$ is $mmmF$, which is dual to $mmmI$. Hence, the corresponding real-space symmorphic group is $Immm$ on the body-centered-cubic lattice $\mathcal{L}$ [see Figs. 2(a) and 2(b)]. The basis of $\mathcal{L}$ is given by

$$\boldsymbol{e}_1 = (-1, 1, 1), \quad \boldsymbol{e}_2 = (1, -1, 1), \quad \boldsymbol{e}_3 = (1, 1, -1). \tag{18}$$

The independent multiplier components are derived from Eq. (10) as

$$\nu[(\boldsymbol{t}_1, M_{k_i}), (\boldsymbol{t}_2, R)] = (-1)^{n_2^i}, \tag{19}$$

which corresponds to the projective representation ρ satisfying

$$\rho(M_{k_i})\rho(\boldsymbol{e}_i)\rho(M_{k_i}) = -\rho(\boldsymbol{e}_1 + \boldsymbol{e}_2 + \boldsymbol{e}_3) \tag{20}$$

with $i = 1, 2, 3$. Other multiplier components and projective algebraic relations can be derived from them.

Gauge-flux models for k-NSGs.—Although not all projective representations of space groups can be realized by lattice models with gauge fluxes, the projective representations for k-NSGs can be realized in this way. This can be inferred from the particular form of Eq. (10). It only modifies the algebraic relations between translations and point-group symmetries, namely, modifying the operation of the point group on the real-space lattice with additional phase factors [see Eq. (14)]. These phase factors can be realized by gauge fluxes, resembling the Aharonov-Bohm effect. See the Supplemental Material for a general formulation [8].

A lattice model for k-NSGs $Fddd$ has been illustrated in Fig. 2(c). Each lattice site in Fig. 2(b) is substituted by a small cube without flux, and π fluxes are inserted for shadowed plaquettes connecting these cubes. The lattice model realizes the projective representation of $Immm$ with the multiplier (19). A constant-energy contour of the model is shown in Fig. 2(d), which visualizes the k-NSG $Fddd$. The technical details for the lattice realization and all lattice realizations for the four 2D k-NSGs can be found in the Supplemental Material [8].

In fact, realizing negative hopping amplitudes is sufficient for all 2D k-NSGs and 119 3D k-NSGs among the 157 ones in total. This is because these k-NSGs involve only half reciprocal-lattice translations, and therefore the multipliers are equal to ± 1 according to Eq. (10). Thus, all 2D and most 3D k-NSGs can be readily realized by artificial crystals [see Fig. 1(d)].

Summary and discussions.—In summary, we have revealed the intrinsic connection between projective representations and k-NSGs, based on Mackey's canonical form of multipliers for semidirect product groups. From the connection, we can systematically construct any k-NSG by the projective representation of the corresponding r-SSG with the multiplier given by Eq. (10), which can be physically realized on the dual lattice with appropriate gauge fluxes.

Our work substantially extends the scope of crystal symmetry, and deepens our understanding of the interplay between gauge structures and symmetry. We expect new avenues to be opened in topological physics and artificial crystals under the grand framework of k-NSGs.

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Appendix A: On canonical form of multipliers.—Mackey formulated a canonical form for multipliers of semidirect product groups in the classic work [16]. The canonical form is introduced in the Supplemental Material with slightly changed conventions for our application [8]. Since each r-SSG is a semidirect product of the translation group $\mathcal{L}$ and the point group P, we can apply Mackey's canonical form to analyze the multipliers of r-SSGs.

Remarkably, according to Mackey's canonical form, any multiplier ν of an r-SSG can be decomposed as $\nu = \sigma\gamma\alpha$, with σ, α and γ three elementary multipliers of the r-SSG. σ and α are the restrictions of ν on the two subgroups $\mathcal{L}$ and P, respectively. Importantly, the multiplier of Eq. (10) is in fact the γ component, and any γ component can be cast into the form of Eq. (10). γ is a multiplier that connects $\mathcal{L}$ and P. Hence, it is γ that changes the algebraic relations between translation and point-group operators, and therefore leads to fractional reciprocal-lattice translations.

For our purpose, it is sufficient to presume that the restrictions of the r-SSG multiplier ν on the two subgroups $\mathcal{L}$ and P are trivial, namely, $\sigma = \alpha = 1$. Then, in accord with Mackey's canonical form, the multiplier can be written as

$$\nu[(\boldsymbol{t}_1, R_1), (\boldsymbol{t}_2, R_2)] = \gamma(R_1\boldsymbol{t}_2, R_1). \tag{A1}$$

Here, $\gamma(\boldsymbol{t}, R)$ is valued in $U(1)$, and satisfies the following conditions:

$$\gamma(\boldsymbol{t}_1 + \boldsymbol{t}_2, R) = \gamma(\boldsymbol{t}_1, R)\gamma(\boldsymbol{t}_2, R), \tag{A2}$$

and

$$\gamma(\boldsymbol{t}, R_1R_2) = \gamma(\boldsymbol{t}, R_1)\gamma(R_1^T\boldsymbol{t}, R_2). \tag{A3}$$

It is straightforward to check that the two conditions Eqs. (A1) and (A3) are sufficient for making ν a multiplier, i.e., $\nu(g_1, g_2)\nu(g_1 g_2, g_3) = \nu(g_1, g_2 g_3)\nu(g_2, g_3)$ for all $g_1, g_2, g_3 \in \mathcal{L} \rtimes_D P$.

The first equation implies $\gamma(*, R)$ with R fixed is a homomorphism from $\mathcal{L}$ to $U(1)$, and therefore γ takes the form:

$$\gamma(\boldsymbol{t}, R) = e^{-i\boldsymbol{\kappa}_R \cdot \boldsymbol{t}}, \tag{A4}$$

where $\boldsymbol{\kappa}_R$ specifies the homomorphism for each $R \in P$. Substituting Eq. (A4) into Eq. (A1), we obtain Eq. (10). Substituting Eq. (A4) into Eq. (A3) gives the significant relation in Eq. (12).

Appendix B: On cohomological equivalence.—In fact, the duality between k-NSGs and projective representations of r-SSGs with Eq. (10) can be solidly established at the cohomological level.

Let us recall that to identify a r-NSG, it is not sufficient to only specify the fractional translation $\boldsymbol{\tau}_R$ for each point-group element R. This is because for an arbitrary vector $\bar{\boldsymbol{r}}$, we can construct the fractional translations,

$$\delta\bar{\boldsymbol{r}}_R = R\bar{\boldsymbol{r}} - \bar{\boldsymbol{r}}, \tag{B1}$$

which obviously satisfy Eq. (17). But such fractional translations are trivial, since they correspond to essentially symmorphic space groups [2]. That is, $\delta\bar{\boldsymbol{r}}_R$ comes from the displacement $\bar{\boldsymbol{r}}$ of the point-group reference point and the coordinate origin. Moreover, $\boldsymbol{\tau}_R$ and $\tilde{\boldsymbol{\tau}}_R$ are equivalent if their difference $\tilde{\boldsymbol{\tau}}_R - \boldsymbol{\tau}_R = \delta\bar{\boldsymbol{r}}_R$ for some $\bar{\boldsymbol{r}}$, since they can be equated by shifting the coordinate origin by $\bar{\boldsymbol{r}}$.

Hence, to fully establish the concept of k-NSGs, we need to check whether such momentum-space fractional translations,

$$\delta\bar{\boldsymbol{k}}_R = R\bar{\boldsymbol{k}} - \bar{\boldsymbol{k}}, \tag{B2}$$

correspond to trivial multipliers. Here, $\bar{\boldsymbol{k}}$ is an arbitrary vector in momentum space. To see this, it is noticed that the corresponding multiplier is given by

$$\nu_{\bar{\boldsymbol{k}}}[(\boldsymbol{t}_1, R_1), (\boldsymbol{t}_2, R_2)] = e^{i\bar{\boldsymbol{k}}\cdot R_1 \boldsymbol{t}_2} e^{-i\bar{\boldsymbol{k}}\cdot \boldsymbol{t}_2}. \tag{B3}$$

The multiplier is trivial, because it can be induced from an ordinary representation by multiplying each operator $\rho(\boldsymbol{t}, R)$ with the phase factor $\chi(\boldsymbol{t}, R) = e^{i\bar{\boldsymbol{k}}\cdot\boldsymbol{t}}$. That is, it is equal to $\{\chi[(\boldsymbol{t}_1, R_1)(\boldsymbol{t}_2, R_2)]/\chi(\boldsymbol{t}_1, R_1)\chi(\boldsymbol{t}_2, R_2)\}$. Hence, we have confirmed that if $\tilde{\boldsymbol{\kappa}}_R - \boldsymbol{\kappa}_R = \delta\bar{\boldsymbol{k}}_R$ for some $\bar{\boldsymbol{k}}$, $\tilde{\boldsymbol{\kappa}}_R$ and $\boldsymbol{\kappa}_R$ are equivalent, since they correspond to equivalent projective representations.

Thus, given a point group P, all possibilities of k-NSGs are characterized by equivalence classes of solutions of Eq. (12). This is just the "twisted" first cohomology group $H^{1,\hat{D}}(P, \mathbb{R}^d/\hat{\mathcal{L}})$. Here, $\mathbb{R}^d/\hat{\mathcal{L}}$ denotes the fundamental domain in momentum space, namely, the Brillouin zone, in which $\boldsymbol{\kappa}_R$ is valued. In parallel, all possible real-space nonsymmorphic groups are given by $H^{1,D}(P, \mathbb{R}^d/\mathcal{L})$. Starting with (P, D), we can first work out $H^{1,\hat{D}}(P, \mathbb{R}^d/\hat{\mathcal{L}})$ and $H^{1,D}(P, \mathbb{R}^d/\mathcal{L})$, and then exhaust all the k-NSGs and r-NSGs, respectively.

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[1] C. Bradley and A. Cracknell, *The Mathematical Theory of Symmetry in Solids: Representation Theory for Point Groups and Space Groups* (Oxford University Press, New York, 2010).

[2] A. Szczepanski, *Geometry of Crystallographic Groups* (World Scientific, Singapore, 2012), Vol. 4.

[3] L. Michel and J. Zak, Phys. Rev. B **59**, 5998 (1999).

[4] Y. X. Zhao and A. P. Schnyder, Phys. Rev. B **94**, 195109 (2016).

[5] K. Shiozaki, M. Sato, and K. Gomi, Phys. Rev. B **93**, 195413 (2016).

[6] S. M. Young and C. L. Kane, Phys. Rev. Lett. **115**, 126803 (2015).

[7] An element R of $O(d)$ is called a proper or improper rotation according to $\mathrm{Det}(R) = \pm 1$.

[8] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.130.256601 for an introduction to Mackey's canonical form, the table of all 3D k-NSGs, model realizations of 2D and 3D k-NSGs, experimental realizations of gauge fluxes, and other derivation details, which includes Refs. [9–22].

[9] T. Ozawa, H. M. Price, A. Amo, N. Goldman, M. Hafezi, L. Lu, M. C. Rechtsman, D. Schuster, J. Simon, O. Zilberberg *et al.*, Rev. Mod. Phys. **91**, 015006 (2019).

[10] G. Ma, M. Xiao, and C. T. Chan, Nat. Rev. Phys. **1**, 281 (2019).

[11] S. Imhof, C. Berger, F. Bayer, J. Brehm, L. W. Molenkamp, T. Kiessling, F. Schindler, C. H. Lee, M. Greiter, T. Neupert *et al.*, Nat. Phys. **14**, 925 (2018).

[12] R. Yu, Y. Zhao, and A. P. Schnyder, Natl. Sci. Rev. **7**, 1288 (2020).

[13] E. Prodan and C. Prodan, Phys. Rev. Lett. **103**, 248101 (2009).

[14] N. R. Cooper, J. Dalibard, and I. B. Spielman, Rev. Mod. Phys. **91**, 015005 (2019).

[15] J. Dalibard, F. Gerbier, G. Juzeliūnas, and P. Öhberg, Rev. Mod. Phys. **83**, 1523 (2011).

[16] G. W. Mackey, Acta Math. **99**, 265 (1958).

[17] S. Mittal, V. V. Orre, G. Zhu, M. A. Gorlach, A. Poddubny, and M. Hafezi, Nat. Photonics **13**, 692 (2019).

[18] H. Xue, Y. Ge, H.-X. Sun, Q. Wang, D. Jia, Y.-J. Guan, S.-Q. Yuan, Y. Chong, and B. Zhang, Nat. Commun. **11**, 2442 (2020).

[19] D.-W. Zhang, Y.-Q. Zhu, Y. Zhao, H. Yan, and S.-L. Zhu, Adv. Phys. **67**, 253 (2018).

[20] Z. Wang, X.-T. Zeng, Y. Biao, Z. Yan, and R. Yu, Phys. Rev. Lett. **130**, 057201 (2023).

[21] X.-G. Wen, Phys. Rev. B **65**, 165113 (2002).

[22] A. Kitaev, Ann. Phys. (Amsterdam) **321**, 2 (2006).

[23] G. Baskaran, Z. Zou, and P. W. Anderson, Solid State Commun. **88**, 853 (1993).

[24] X.-G. Wen, Phys. Rev. B **60**, 8827 (1999).
[25] Q. Wang, C.-C. Liu, Y.-M. Lu, and F. Zhang, Phys. Rev. Lett. **121**, 186801 (2018).
[26] L. Lu, J. D. Joannopoulos, and M. Soljačić, Nat. Photonics **8**, 821 (2014).
[27] Z. Yang, F. Gao, X. Shi, X. Lin, Z. Gao, Y. Chong, and B. Zhang, Phys. Rev. Lett. **114**, 114301 (2015).
[28] H. Xue, D. Jia, Y. Ge, Y.-J. Guan, Q. Wang, S.-Q. Yuan, H.-X. Sun, Y. D. Chong, and B. Zhang, Phys. Rev. Lett. **127**, 214301 (2021).
[29] S. D. Huber, Nat. Phys. **12**, 621 (2016).
[30] L. Fu, Phys. Rev. Lett. **106**, 106802 (2011).
[31] K. Shiozaki and M. Sato, Phys. Rev. B **90**, 165114 (2014).
[32] K. Shiozaki, M. Sato, and K. Gomi, Phys. Rev. B **93**, 195413 (2016).
[33] C.-K. Chiu, J. C. Y. Teo, A. P. Schnyder, and S. Ryu, Rev. Mod. Phys. **88**, 035005 (2016).
[34] Y. X. Zhao and Z. D. Wang, Phys. Rev. Lett. **110**, 240404 (2013).
[35] Y. X. Zhao, A. P. Schnyder, and Z. D. Wang, Phys. Rev. Lett. **116**, 156402 (2016).
[36] Z. Y. Chen, S. A. Yang, and Y. X. Zhao, Nat. Commun. **13**, 2215 (2022).
[37] Y. X. Zhao, C. Chen, X.-L. Sheng, and S. A. Yang, Phys. Rev. Lett. **126**, 196402 (2021).
[38] L. B. Shao, Q. Liu, R. Xiao, S. A. Yang, and Y. X. Zhao, Phys. Rev. Lett. **127**, 076401 (2021).
[39] H. Xue, Z. Wang, Y.-X. Huang, Z. Cheng, L. Yu, Y. X. Foo, Y. X. Zhao, S. A. Yang, and B. Zhang, Phys. Rev. Lett. **128**, 116802 (2022).
[40] T. Li, J. Du, Q. Zhang, Y. Li, X. Fan, F. Zhang, and C. Qiu, Phys. Rev. Lett. **128**, 116803 (2022).
[41] Y. Yang, H. C. Po, V. Liu, J. D. Joannopoulos, L. Fu, and M. Soljačić, Phys. Rev. B **106**, L161108 (2022).
[42] J. Herzog-Arbeitman, Z.-D. Song, L. Elcoro, and B. A. Bernevig, Phys. Rev. Lett. **130**, 236601 (2023).
[43] Y. Meng, S. Lin, B.-J. Shi, B. Wei, L. Yang, B. Yan, Z. Zhu, X. Xi, Y. Wang, Y. Ge, S.-Q. Yuan, J. Chen, G.-G. Liu, H.-X. Sun, H. Chen, Y. Yang, and Z. Gao, Phys. Rev. Lett. **130**, 026101 (2023).
[44] Z. Y. Chen, Z. Zhang, S. A. Yang, and Y. X. Zhao, Nat. Commun. **14**, 743 (2023).
[45] In three dimensions, the primitive reciprocal lattice vectors are given by $\boldsymbol{G}_i = 2\pi\epsilon_{ijk}\boldsymbol{e}_j \times \boldsymbol{e}_k / |\boldsymbol{e}_1 \cdot (\boldsymbol{e}_2 \times \boldsymbol{e}_3)|$.
[46] G. Mackey, *Unitary Group Representations in Physics, Probability, and Number Theory, Advanced Book Classics* (Addison-Wesley Publishing Company Advanced Book Program, Redwood City, CA, 1989).