Nonsymmorphic Symmetries and Their Consequences*

Bolin Liao
Department of Mechanical Engineering, Massachusetts Institute of Technology†
(Dated: May 15, 2012)

In this report, a brief review of the general space group theory is given, and a particular focus is put on the nonsymmorphic groups, of which the corresponding point group is not a subgroup, but isomorphic to a factor group with the translation group as normal divisor. A significant consequence of the nonsymmorphic symmetries is the so called "bands-sticking-together" effect at the Brillouin zone boundaries, where extra degeneracies can be observed. This effect is demonstrated using a "shifted" 2D photonic waveguide with a glide plane and spiral staircase waveguides with screw axes.

I. A LITTLE BIT OF SPACE GROUP THEORY

Space groups[1] describe the symmetry operations of a "crytal", or a geometrical configuration consisting of a "lattice", which can be generated by successive translations of primitive vectors, and a "basis" that may possess arbitrary point symmetries. It is tempting to think of space group operations as simple combinations of the translation and point operations, which, as will be shown later, is not always true. The translation symmetries is conventionally denoted by "lattice translations" that can be generally written as

$$\boldsymbol{t} = t_1\boldsymbol{a_1} + t_2\boldsymbol{a_2} + t_3\boldsymbol{a_3} \tag{1}$$

where $\boldsymbol{a_1}$,$\boldsymbol{a_2}$,$\boldsymbol{a_3}$ are primitive vectors and t_1,t_2,t_3 are integers. In terms of point symmetries, it is well known that only rotations (proper and improper) with 1, 2, 3, 4, 6-fold axis are compatible with the translation symmetry, based on which 32 crystallographic point groups can be derived[2]. A convenient way of representing members of a space group $\mathfrak{G}$ is using the *Seitz operators*[3], $\{\alpha|\boldsymbol{\tau}\}$, where α is a point symmetry operation (proper or improper rotation) and $\boldsymbol{\tau}$ is a spatial translation, which may not be a lattice translation (Here $\boldsymbol{\tau}$ is used to denote a generic spatial translation, while $\boldsymbol{t}$ is used specifically for lattice translations). The effect of a Seitz operator on a spatial point $\boldsymbol{x}$ is

$$\{\alpha|\boldsymbol{\tau}\}\boldsymbol{x} = \alpha\boldsymbol{x} + \boldsymbol{\tau} \tag{2}$$

And the basic algebra of Seitz operators can be easily shown as[4]

$$\begin{aligned} \{\alpha|\boldsymbol{\tau_1}\}\{\beta|\boldsymbol{\tau_2}\} &= \{\alpha\beta|\alpha\boldsymbol{\tau_2} + \boldsymbol{\tau_1}\} \\ \{\alpha|\boldsymbol{\tau}\}^{-1} &= \{\alpha^{-1}| - \alpha^{-1}\boldsymbol{\tau}\} \end{aligned} \tag{3}$$

Since any spatial translation $\boldsymbol{\tau}$ can be written as $\boldsymbol{\tau} = \boldsymbol{v} + \boldsymbol{t}$, where $\boldsymbol{v}$ is a vector within a primitive cell, Seitz operators can be cast into the form $\{\alpha|\boldsymbol{v}(\alpha) + \boldsymbol{t}\}$. The operations with $\boldsymbol{t} = \boldsymbol{0}$, i.e. $\{\alpha|\boldsymbol{v}(\alpha)\}$, are the non-translation operations. The "fractional" translation vectors $\boldsymbol{v}(\alpha)$ depend on the choice of the origin. Suppose the origin is shifted by a vector $\boldsymbol{b}$, the non-translational operator with respect to the new origin would change to $\{E|\boldsymbol{b}\}\{\alpha|\boldsymbol{v}(\alpha)\}\{E|\boldsymbol{b}\}^{-1} = \{\alpha|\boldsymbol{v}(\alpha) + \boldsymbol{b} - \alpha\boldsymbol{b}\}$. Thus a proper choice of the origin ($\boldsymbol{b} = (I - \alpha)^{-1}\boldsymbol{v}(\alpha)$) can make the fractional translation vector vanish. It can be shown[4] that if $\boldsymbol{v}(\alpha)$ is parallel to the axis of α (when α is a rotation) or parallel to the mirror plane (when α is a reflection), the operator $(I - \alpha)$ is singular, hence the fractional translation can not be eliminated by shifting the origin. Those operations are called nonsymmorphic (otherwise symmorphic) operations, and the former are called screw axes, and the latter glide planes. If all the non-translation elements in a space group can be chosen to be symmorphic by picking a proper origin, the space group is called a symmorphic group, otherwise a nonsymmorphic group. For a symmorphic space group, all the elements are in the form $\{\alpha|\boldsymbol{t}\}$, and the non-translation elements $\{\alpha|\boldsymbol{0}\}$ form a group, i.e. the point group, which is a subgroup of the space group. For a nonsymmorphic space group, however, the non-translation elements $\{\alpha|\boldsymbol{v}(\alpha)\}$ do not form a group, since their combination may turn out to be a pure lattice translation. Althought in this case the elements $\{\alpha|\boldsymbol{0}\}$ still form the point group, it is no longer a subgroup of the space group.

An important fact about a space group $\mathfrak{G}$ (whether symmorphic or not) is that the translation group $\mathfrak{T}$ is an invariant subgroup of $\mathfrak{G}$, since

$$\{\alpha|\boldsymbol{\tau'}\}^{-1}\{E|\boldsymbol{\tau}\}\{\alpha|\boldsymbol{\tau'}\} = \{E|\alpha^{-1}\boldsymbol{\tau}\} \tag{4}$$

where $\{E|\alpha^{-1}\boldsymbol{\tau}\}$ is apparently also a lattice translation. An invariant subgroup has equivalent right and left cosets, and the cosets form a group under the definition of coset multiplication (given cosets $\mathfrak{C}_1$, $\mathfrak{C}_2$ and $\mathfrak{C}_3$, $\mathfrak{C}_1\mathfrak{C}_2 = \mathfrak{C}_3$ means that for any elements $g_1 \in \mathfrak{C}_1$ and $g_2 \in \mathfrak{C}_2$, their product $g_1g_2 \in \mathfrak{C}_3$), which is called the factor group of the original group, and the invariant subgroup is called a normal divisor[5]. In the case of the space group, the factor group $\mathfrak{G}/\mathfrak{T}$ can be shown to be isomorphic to the point group $\mathfrak{P}$[6], which is crucial in discussing the irreducible representations of space groups. Suppose we know an irreducible representation of the factor group, usually an irreducible representation

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* This is the course project report for Spring 2012 18.369: Mathematical Methods in Nanophotonics, by Prof. Steven Johnson
† bolin@mit.edu; http://web.mit.edu/bolin/www

of the full group can be deduced based on it. A trivial one is that where all elements in the invariant subgroup are represented by a unity matrix, thus all elements in a certain coset are represented by one matrix, which is the representation matrix of the coset in the factor group. In dealing with space groups, however, a more convenient way is to work with Bloch waves, which are parner functions of irreducible representations of the translation group.

First of all, one can always *choose* the translation operations to be diagonal in an irreducible representation[2], or in other words, one can always restrict the basis functions to Bloch waves in generating irreducible representations of $\mathfrak{G}$, because of the translational symmetry. For a specific irreducible representation of the translation group labeled by $\boldsymbol{k}$, or in other words, a specific $\boldsymbol{k}$ point in the Brillouin zone, the effects of any space group elements on the Bloch wave with wavevector $\boldsymbol{k}$ is to transform it into another irreducible representation with a "rotated" $\boldsymbol{k}$[7]. As can be shown as

$$\begin{aligned}\{E|\boldsymbol{t}\}\{\alpha|\boldsymbol{\tau}\}\psi_{\boldsymbol{k}} &= \{\alpha|\boldsymbol{\tau}\}\{E|\alpha^{-1}\boldsymbol{t}\}\psi_{\boldsymbol{k}} \\ &= \exp(i\boldsymbol{k}\cdot\alpha^{-1}\boldsymbol{t})\{\alpha|\boldsymbol{\tau}\}\psi_{\boldsymbol{k}} \\ &= \exp(i\alpha\boldsymbol{k}\cdot\boldsymbol{t})\{\alpha|\boldsymbol{\tau}\}\psi_{\boldsymbol{k}} \end{aligned} \tag{5}$$

Thus $\{\alpha|\boldsymbol{\tau}\}\psi_{\boldsymbol{k}}$ is a partner function of the representation labeled by $\alpha\boldsymbol{k}$. All the elements in the space group $\mathfrak{G}$ that leave the $\boldsymbol{k}$ vector of a Bloch wave invariant, in the sense that $\boldsymbol{k}$ and $\alpha\boldsymbol{k}$ are related by a reciprocal lattice vector, form the "group of $\boldsymbol{k}$", denoted as $\mathfrak{G}_{\boldsymbol{k}}$, of which the translation group $\mathfrak{T}$ is apparently an invariant subgroup since a pure translation doen not affect the $\boldsymbol{k}$ vector. The corresponding point group of each $\mathfrak{G}_{\boldsymbol{k}}$ is denoted as $\mathfrak{P}_{\boldsymbol{k}}$. Irreducible representations of $\mathfrak{G}_{\boldsymbol{k}}$ are of special interest because they contain the information of degeneracy at each $\boldsymbol{k}$ point and also the irreducible representations of $\mathfrak{G}$ with Bloch waves as basis functions can be derived from them. Since we restrict the basis functions to be Bloch waves, the representation $\boldsymbol{D}^{\boldsymbol{k}}$ for all the translations are naturally[2]

$$\boldsymbol{D}^{\boldsymbol{k}}(\{E|\boldsymbol{t}\}) = \exp(i\boldsymbol{k}\cdot\boldsymbol{t})\boldsymbol{I}^{d} \tag{6}$$

where $\boldsymbol{I}^{d}$ is the unity matrix with the dimention of the representation.

There are three different cases when determining the irreducible representaions of $\mathfrak{G}_{\boldsymbol{k}}$[5]:

1. $\boldsymbol{k}$ is inside the Brillouin zone;
2. $\boldsymbol{k}$ is at the zone boundary and $\mathfrak{G}_{\boldsymbol{k}}$ is symmorphic;
3. $\boldsymbol{k}$ is at the zone boundary and $\mathfrak{G}_{\boldsymbol{k}}$ is nonsymmorphic.

For the first two cases, the irreducible representation of $\mathfrak{G}_{\boldsymbol{k}}$ can be simply generated by combining the irreducible representation of the point group $\mathfrak{P}_{\boldsymbol{k}}$ and the translation group as shown in equation 6. Suppose the representation matrix of an element α in $\mathfrak{P}_{\boldsymbol{k}}$ is $\boldsymbol{\Gamma}(\alpha)$, then the representation matrix of a general element $\{\alpha|\boldsymbol{\tau}\}$ in $\mathfrak{G}_{\boldsymbol{k}}$ can be written as

$$\boldsymbol{D}^{\boldsymbol{k}}(\{\alpha|\boldsymbol{\tau}\}) = \exp(i\boldsymbol{k}\cdot\boldsymbol{\tau})\boldsymbol{\Gamma}(\alpha) \tag{7}$$

This can be shown in a following way. Consider the product of two general group elements $\{\alpha_1|\boldsymbol{\tau_1}\}$ and $\{\alpha_2|\boldsymbol{\tau_2}\}$ in $\mathfrak{G}_{\boldsymbol{k}}$. The product of the matrices is

$$\begin{aligned}\boldsymbol{D}^{\boldsymbol{k}}(\{\alpha_1|\boldsymbol{\tau_1}\})\boldsymbol{D}^{\boldsymbol{k}}(\{\alpha_2|\boldsymbol{\tau_2}\}) &= \exp(i\boldsymbol{k}\cdot(\boldsymbol{\tau_1}+\boldsymbol{\tau_2}))\boldsymbol{\Gamma}(\alpha_1)\boldsymbol{\Gamma}(\alpha_2) \\ &= \exp(i\boldsymbol{k}\cdot(\boldsymbol{\tau_1}+\boldsymbol{\tau_2}))\boldsymbol{\Gamma}(\alpha_1\alpha_2) \end{aligned} \tag{8}$$

And the representation matrix of the product element is

$$\boldsymbol{D}^{\boldsymbol{k}}(\{\alpha_1\alpha_2|\alpha_1\boldsymbol{\tau_2}+\boldsymbol{\tau_1}\}) = \exp(i\boldsymbol{k}\cdot(\alpha_1\boldsymbol{\tau_2}+\boldsymbol{\tau_1}))\boldsymbol{\Gamma}(\alpha_1\alpha_2) \tag{9}$$

Thus Eq.7 is an irreducible representation of $\mathfrak{G}_{\boldsymbol{k}}$ if and only if

$$\exp(i(\alpha_1^{-1}\boldsymbol{k}-\boldsymbol{k})\cdot\boldsymbol{\tau_2}) = 1 \tag{10}$$

For case 1, $\alpha_1^{-1}\boldsymbol{k}=\boldsymbol{k}$ because they can never differ by a reciprocal lattice vector other than $\boldsymbol{0}$ for α_1^{-1} is unitary, thus Eq.10 always holds. For case 2, $\alpha_1^{-1}\boldsymbol{k}-\boldsymbol{k}$ can be a reciprocal lattice vector, but since $\boldsymbol{\tau_2}$ is a real space lattice vector, so Eq.10 also holds. For case 3, however, since $\boldsymbol{\tau_2}$ can be a fractional translation vector in a nonsymmorphic group, Eq.10 does not generally hold. To find the irreducible representations of a nonsymmophic $\mathfrak{G}_{\boldsymbol{k}}$ when $\boldsymbol{k}$ is at zone boundary, special methods have to be used, of which the most intuitive one was proposed by Herring in 1942[8].

The basic idea is to deduce the irreducible representation of $\mathfrak{G}_{\boldsymbol{k}}$ from that of a factor group. As discussed before, the simplest way is to assign unity matrices to all elements in the invariant subgroup and elements in one coset are given the same representation matrix as the one of the coset in the factor group. Here since we want to pick Bloch waves as the basis functions, the elements in the invariant subgroup must bahave like unity operators when applied to Bloch waves with wavevector $\boldsymbol{k}$. Based on this observation, a natural choice of the invariant subgroup is the one with translation operations $\boldsymbol{t}_{\boldsymbol{k}}$ such that

$$\exp(i\boldsymbol{k}\cdot\boldsymbol{t}_{\boldsymbol{k}}) = 1 \tag{11}$$

The resulting subgroup is denoted $\mathfrak{T}_{\boldsymbol{k}}$, and can be easily shown to be an invariant subgroup. Thus if one can find an irreducible representation of the factor group $\mathfrak{G}_{\boldsymbol{k}}/\mathfrak{T}_{\boldsymbol{k}}$, the irreducible representation of $\mathfrak{G}_{\boldsymbol{k}}$ then follows.

There is a subtle problem with this method, however, that may generate spurious representations for $\mathfrak{G}_{\boldsymbol{k}}$. This comes from the fact that Eq.11 also implies

$$\exp(i(n\boldsymbol{k})\cdot\boldsymbol{t}_{\boldsymbol{k}}) = 1 \tag{12}$$

where n is any integer. Now suppose we have three cosets in $\mathfrak{G}_{\boldsymbol{k}}/\mathfrak{T}_{\boldsymbol{k}}$, $\{E|\boldsymbol{t}_m\}\mathfrak{T}_{\boldsymbol{k}}$, $m=1,2,3$, (of course $\boldsymbol{t}_m$ are translations that are not in $\mathfrak{T}_{\boldsymbol{k}}$ by definition) that satisfy $\{E|\boldsymbol{t}_1\}\mathfrak{T}_{\boldsymbol{k}}\{E|\boldsymbol{t}_2\}\mathfrak{T}_{\boldsymbol{k}} = \{E|\boldsymbol{t}_3\}\mathfrak{T}_{\boldsymbol{k}}$ in the sense of coset multiplication, which indicates $\{E|\boldsymbol{t}_1\}\{E|\boldsymbol{t}_2\} = \{E|\boldsymbol{t}_3+\boldsymbol{t}_{\boldsymbol{k}}\}$, where $\boldsymbol{t_k}$ is certain element in $\mathfrak{T}_{\boldsymbol{k}}$. To preserve this product relation, we can of course assign $\exp(i\boldsymbol{k}\cdot\boldsymbol{t}_m\}$ times the unity matrix to the three cosets because of Eq.11, which is the "true" representation as required by Eq.6, but we may as well assign $\exp(i(n\boldsymbol{k})\cdot\boldsymbol{t}_m)$ times the unity matrix to the cosets, because Eq.12 also guarantees the product relation be preserved. Thus after obtaining the irreducible representations of the factor group $\mathfrak{G}_{\boldsymbol{k}}/\mathfrak{T}_{\boldsymbol{k}}$, one has to remove the spurious representations (such as $\exp(i(n\boldsymbol{k})\cdot\boldsymbol{t}_m)$) stemmed from the ambiguity discussed above.

In the following section, several example photonic crystal waveguides with nonsymmorphic operations will be discussed, and the "bands-sticking-together" effect[7] at the zone boundaries originating from the complexity discussed above will be demonstrated and analyzed using Herring's method.

II. STUDY OF MODEL STRUCTURES

A. A "Shifted" 1D Photonic Crystal Waveguide

In this section, the result of an earlier work in literature[9] is reproduced. Instead of considering a line defect in a 2D photonic crystal as the original work, here two kinds of 1D-periodic index waveguides as shown in Fig.1 are investigated to show the effect induced by a glide plane. Illustrated in Fig.1(a) is a simple "normal" waveguide consisting of two rows of dielectric cylinders, whose point group is $C_{2v} = \{E, C_2, \sigma_x, \sigma_y\}$. At the boundary $k = \frac{\pi}{a}$, the group of k $\mathfrak{G}_{\boldsymbol{k}}$ is also C_{2v}, which only has one-dimentional irreducible representations, thus no "essential" degeneracies (not accidental) are supposed to be observed at the zone boundary. Fig.2(a) shows the band diagram of the guided modes in a normal waveguide calculated using MPB[10], a frequency-domain electromagnetic eigensolver, and as expected bands are separated at the zone boundary. In Fig.1(b) a modified version of the waveguide is shown, where one row of the cylinders is shifted by half a lattice constant, giving rise to a glide plane operation: mirror reflection with respect to the x-axis, and then shifting the structure along x-direction by half a lattice constant. As shown in Fig.2(b), two-fold degeracies appear at the zone boudaries. Now we use Herring's method to analyze this bands-pairing effect.

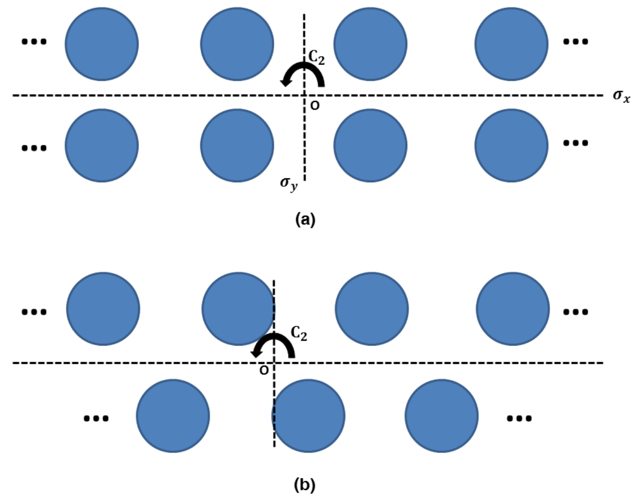

FIG. 1. (a) a normal 1D periodic waveguide; (b) a shifted 1D periodic waveguide.

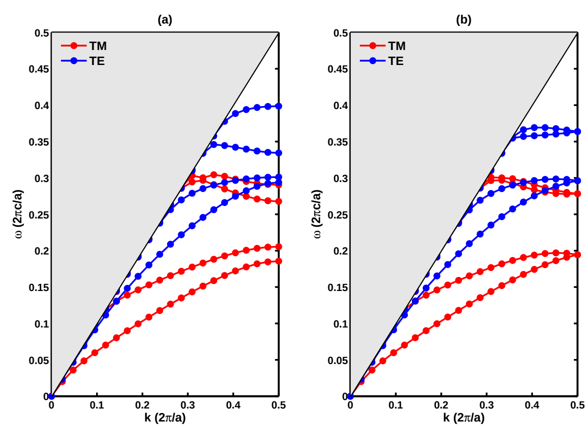

FIG. 2. (a) band diagram for the normal waveguide; (b) band diagram for the "shifted" waveguide.

Choose the origin as shown in Fig.1(b) for convenience (the C_2 rotation is easy to be defined), thus there are 4 nontranslation symmetries:

$$\begin{aligned} e &= \{E|\mathbf{0}\}, \\ c &= \{C_2|\mathbf{0}\}, \\ m &= \{\sigma_x|a/2\}, \\ g &= \{\sigma_y|a/2\}. \end{aligned} \tag{13}$$

And immediately it can be seen that all the 4 operations keep the $\boldsymbol{k}$ vector at the zone boundary ($\boldsymbol{k} = \pi/a$) invariant for their corresponding point operations E, σ_x leave k unchanged, and C_2, σ_y switch $\boldsymbol{k}$ to $-\boldsymbol{k}$, which is equivalent to $\boldsymbol{k}$ since they are connected by a reciprocal lattice vector. Thus the group of $\boldsymbol{k} = \pi/a$ consists of the 4 nontranslation operations, the full translation group $\mathfrak{T}$ and their combinations. Following Herring's method, the next step is to identify the invariant subgroup $\mathfrak{T}_{\boldsymbol{k}}$, defined by Eq.11. At $\boldsymbol{k} = \pi/a$, the translations that satisfy Eq.11 are $\boldsymbol{t_k} = 2na$, where n is any integer. Thus the invariant subgroup $\mathfrak{T}_{\boldsymbol{k}} = \{E|2na\}$. To find the factor group $\mathfrak{G}_{\boldsymbol{k}}/\mathfrak{T}_{\boldsymbol{k}}$, we first list the representative elements of the cosets. Since $\mathfrak{T}_{\boldsymbol{k}}$ has roughly half the size of $\mathfrak{T}$, we expect 8 cosets to be identified (there are 4 in the factor group $\mathfrak{G}_{\boldsymbol{k}}/\mathfrak{T}$, with the 4 nontranslation elements as representative elements). The 8 cosets can be enumerated by choosing the representative elements to be combinations of the 4 nontranslation elements with the

TABLE I. Mulplication table of the factor group $\mathfrak{G}_{\boldsymbol{k}}/\mathfrak{T}_{\boldsymbol{k}}$ at $\boldsymbol{k} = \pi/a$. It can be recognized to be isomorphic to the familiar group C_{4v}.

	e'	$\overline{e}'$	c'	$\overline{c}'$	m'	$\overline{m}'$	g'	$\overline{g}'$
e'	e'	$\overline{e}'$	c'	$\overline{c}'$	m'	$\overline{m}'$	g'	$\overline{g}'$
$\overline{e}'$	$\overline{e}'$	e'	$\overline{c}'$	c'	$\overline{m}'$	m'	$\overline{g}'$	g'
c'	c'	$\overline{c}'$	e'	$\overline{e}'$	$\overline{g}'$	g'	$\overline{m}'$	m'
$\overline{c}'$	$\overline{c}'$	c'	$\overline{e}'$	e'	g'	$\overline{g}'$	m'	$\overline{m}'$
m'	m'	$\overline{m}'$	g'	$\overline{g}'$	$\overline{e}'$	e'	$\overline{c}'$	c'
$\overline{m}'$	$\overline{m}'$	m'	$\overline{g}'$	g'	e'	$\overline{e}'$	c'	$\overline{c}'$
g'	g'	$\overline{g}'$	m'	$\overline{m}'$	c'	$\overline{c}'$	e'	$\overline{e}'$
$\overline{g}'$	$\overline{g}'$	g'	$\overline{m}'$	m'	$\overline{c}'$	c'	$\overline{e}'$	e'

TABLE II. Character table of the factor group $\mathfrak{G}_{\boldsymbol{k}}/\mathfrak{T}_{\boldsymbol{k}}$ at $\boldsymbol{k} = \pi/a$, deduced from that of C_{4v}.

	e'	$\overline{e}'$	c',$\overline{c}'$	m',$\overline{m}'$	g',$\overline{g}'$
$\boldsymbol{\Gamma}_1$	1	1	1	1	1
$\boldsymbol{\Gamma}_2$	1	1	1	-1	-1
$\boldsymbol{\Gamma}_3$	1	1	-1	1	-1
$\boldsymbol{\Gamma}_4$	1	1	-1	-1	1
$\boldsymbol{\Gamma}_5$	2	-2	0	0	0

translation elements that are not in $\mathfrak{T}_{\boldsymbol{k}}$:

$$
\begin{aligned}
e' &= \{E|2na\},\\
\overline{e}' &= \{E|a+2na\},\\
c' &= \{C_2|2na\},\\
\overline{c}' &= \{C_2|a+2na\},\\
m' &= \{\sigma_x|a/2+2na\},\\
\overline{m}' &= \{\sigma_x|3a/2+2na\},\\
g' &= \{\sigma_y|a/2+2na\},\\
\overline{g}' &= \{\sigma_y|3a/2+2na\}.
\end{aligned} \tag{14}
$$

The multiplication table of this group is shown in Table I. From the multiplication table, the factor group can be recognized to be isomorphic to the familiar point group C_{4v}, thus the character table can be written down immediately as shown in Table II. We can not conclude, however, that there would be 1-fold and 2-fold degeneracies at $\boldsymbol{k} = \pi/a$ from the character table as we usually do, because of the caveat provided at the end of Section I. Some of the representations listed in Table II might be spurious, and we have to sift them out using Eq.6. Consider the coset $\overline{e}'$, which according to Eq.6 should be represented by $\exp(i\frac{\pi}{a}\cdot a)\boldsymbol{I}^d = -\boldsymbol{I}^d$, whose character is $-d$ (d is the dimensionality of the representation). Thus only $\boldsymbol{\Gamma}_5$ is the "true" irreducible representation of $\mathfrak{G}_{\boldsymbol{k}}/\mathfrak{T}_{\boldsymbol{k}}$, based on which the representation of $\mathfrak{G}_{\boldsymbol{k}}$ can be derived by assigning unity matrices to the elements in $\mathfrak{T}_{\boldsymbol{k}}$. Since this representation is 2-dimentional and is the only irreducible representaion , it explains the fact that at the zone boundary all bands are paired and "sticking together". The existence of a unique irreducible representation of $\mathfrak{G}_{\boldsymbol{k}}$ implies all elements of it are in a single conjugate class, which originates from the degrees of freedom supplied by the full translation group $\mathfrak{T}$ as a subgroup. With these observations, we can furthur discuss the spatial distribution of the two degenerate eigen fields. First we notice that any Bloch waves with the wavevector $\boldsymbol{k} = \pi/a$ are partner functions of $\boldsymbol{\Gamma}_5$ by applying the projection operator

$$
\begin{aligned}
\boldsymbol{P}^{(5)}\psi_{\frac{\pi}{a}} &= \frac{1}{2}(e' - \overline{e}')u_{\frac{\pi}{a}}(x,y)\exp{(i\frac{\pi}{a}x)}\\
&= \frac{1}{2}u_{\frac{\pi}{a}}(x,y)(\exp{(i\frac{\pi}{a})} - (-\exp{(i\frac{\pi}{a})}))\\
&= \psi_{\frac{\pi}{a}}
\end{aligned} \tag{15}
$$

which is guaranteed by our initial restrictions on the basis functions. To understand the two-fold degeneracy, consider a Bloch wave ψ with $\boldsymbol{k} = \frac{\pi}{a}$. First assume functions generated by applying operations e', c', m', g' ($\overline{e}'$, $\overline{c}'$, $\overline{m}'$ and $\overline{g}'$ are not considered here because they just add an extra minus sign when applied on ψ) on ψ:

$$
\begin{aligned}
\psi_1 &= e'\psi,\\
\psi_2 &= c'\psi,\\
\psi_3 &= m'\psi,\\
\psi_4 &= g'\psi.
\end{aligned} \tag{16}
$$

are linearly dependent of each other, i.e. $\psi_2 = p\psi_1$, $\psi_3 = q\psi_1$, $\psi_4 = r\psi_1$, where p, q, r are constants and $p^2 = 1$, $q^2 = -1$ and $r^2 = 1$ (because $c'^2 = e'$, $m'^2 = \overline{e}'$, $g'^2 = e'$ from the multiplication table). From the multiplication table, $m'^2 = g'c'g'c'$, thus we have $m'^2\psi = g'c'g'c'\psi = r^2p^2\psi$ and $m'^2\psi = q^2\psi$, hence $p^2r^2 = q^2$, which is a contradiction. Therefore the four functions can not be linearly dependent of each other, and there must be degeneracy at $\boldsymbol{k} = \frac{\pi}{a}$. Fig.3 shows the spatial distributions of the z-components of the electric field of the lowest 2 TM modes in the normal and the "shifted" waveguides. From the patterns of the two degerate modes of the "shifted" waveguide, an irreducible representation of $\boldsymbol{\Gamma}_5$ can be derived as shown in Table III.

This example demonstrates the basic idea of Herring's method of deriving the irreducible representations of the group of $\boldsymbol{k}$ at zone boundaries for nonsymmorphic groups, and the "bands-sticking-together" effect due to the fractional translations. Now we proceed to investigate a similar variation with a screw axis instead of a glide plane: a spiral staircase waveguide.

TABLE III. An irreducible representation of $\boldsymbol{\Gamma}_5$.

	e'	$\overline{e}'$	c',$\overline{c}'$	m',$\overline{m}'$	g',$\overline{g}'$
$\boldsymbol{\Gamma}_5$	$\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$	$\begin{pmatrix}-1 & 0\\ 0 & -1\end{pmatrix}$	$\begin{pmatrix}i & 0\\ 0 & -i\end{pmatrix}$	$\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & i\\ i & 0\end{pmatrix}$

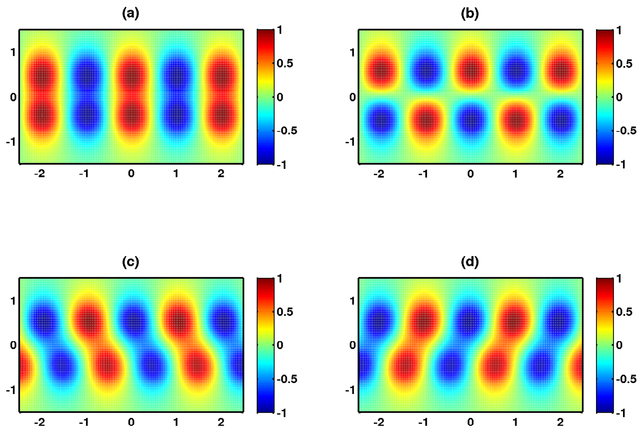

FIG. 3. z-component of the electric field of the lowest 2 TM modes of (a)(b) the normal waveguide and (c)(d) the "shifted" waveguide.

B. A Spiral Staircase Waveguide

Here we consider the other class of nonsymmorphic operations: screw axes, which are combinations of a rotation and a fractional translation. The International Notation for a screw axis is n_m, meaning it is constructed upon an n-fold rotation axis and each rotation gives a translation of $\frac{m}{n}$ of a lattice vector. To be compatible with the full translation group, it can be shown that only $n = 1, 2, 3, 4, 6$ is possible for a screw axis[4], just like the normal rotation, and m has to be an integer smaller than n. For simplicity, we consider a 1D waveguide with a 3_1 screw axis as shown in Fig.4. First step is to find all the nontranslation elements. Obvious ones are the identity and the 2 screw rotations, while there are also 3 C_2 rotations around axes with different orientations as shown in Fig.5. They are listed in Eq.17.

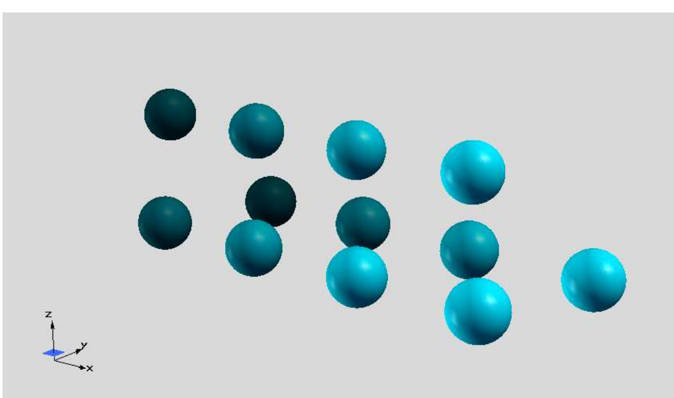

FIG. 4. Schematic of a 3-step staircase waveguide

$$\begin{aligned} e &= \{E|\mathbf{0}\} \\ s_1 &= \{C_3|\frac{1}{3}a\} \\ s_2 &= \{C_3^2|\frac{2}{3}a\} \\ c_1 &= \{C_2|\mathbf{0}\} \\ c_2 &= \{C_2|\frac{1}{3}a\} \\ c_3 &= \{C_2|\frac{2}{3}a\} \end{aligned} \tag{17}$$

All the nontranslation operations leave $\boldsymbol{k} = \frac{\pi}{a}$ invariant, thus they are all in the group $\mathfrak{G}_{\boldsymbol{k}}$. The invariant subgroup $\mathfrak{T}_{\boldsymbol{k}}$ is still $\{E|2na\}$. Similar combinations of the nontranslation elements with the invariant subgroup again generate the factor group, with cosets listed in Eq.18,

$$\begin{aligned} e' &= \{E|2na\}, \\ \overline{e}' &= \{E|a + 2na\}, \\ s_1' &= \{C_3|\frac{1}{3}a + 2na\}, \\ \overline{s}_1' &= \{C_3|\frac{4}{3}a + 2na\}, \\ s_2' &= \{C_3^2|\frac{2}{3}a + 2na\}, \\ \overline{s}_2' &= \{C_3^2|\frac{5}{3}a + 2na\}, \\ c_1' &= \{C_2|2na\}, \\ \overline{c}_1' &= \{C_2|a + 2na\}, \\ c_2' &= \{C_2|\frac{1}{3}a + 2na\}, \\ \overline{c}_2' &= \{C_2|\frac{4}{3}a + 2na\}, \\ c_3' &= \{C_2|\frac{2}{3}a + 2na\}, \\ \overline{c}_3' &= \{C_2|\frac{5}{3}a + 2na\}. \end{aligned} \tag{18}$$

The next step is to identify the conjugate classes. Notice that in dealing with factor groups, all the operations are in the sense of "modulo" $\mathfrak{T}_{\boldsymbol{k}}$. For instance, s_1' is found to be conjugate to $\overline{s}_2'$ because,

$$\begin{aligned} \{C_2|2ma\}\{C_3|\frac{1}{3}a\}\{C_2|2na\}^{-1} &= \{C_3^2|C_2(C_3(-C_2^{-1}2na) \\ &\quad + \frac{1}{3}a) + 2ma\} \\ &= \{C_3^2|\frac{5}{3}a + 2pa\} \end{aligned} \tag{19}$$

where n and m are any integers, and $p = m - n - 1$ is also an integer. Similarly, we can determine the conjugate classes as $\{e'\}$, $\{\overline{e}'\}$, $\{s_1', \overline{s}_2'\}$, $\{\overline{s}_1', s_2'\}$, $\{c_1', \overline{c}_2', c_3'\}$, $\{\overline{c}_1', c_2', \overline{c}_3'\}$. With 12 group elements and 6 conjugate classes, we expect to see two 2-dimentional irreducible

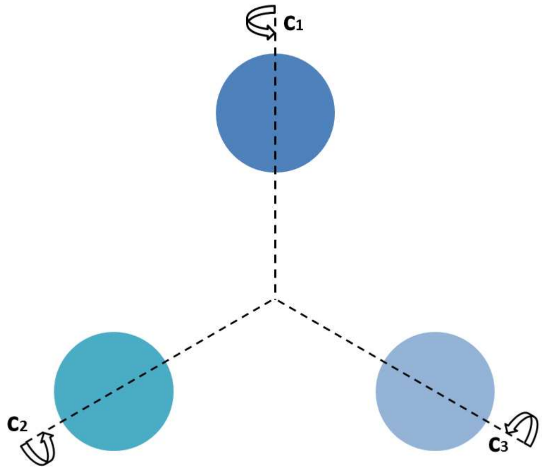

FIG. 5. Front view of the 3-step waveguide and the 3 C_2 rotations.

TABLE IV. Character table of the factor group $\mathfrak{G}_{\boldsymbol{k}}/\mathfrak{T}_{\boldsymbol{k}}$ at $\boldsymbol{k} = \pi/a$ of a spiral waveguide with a 3_1 screw axis.

	e'	$\bar{e}'$	$s'_1, \bar{s}'_2$	$\bar{s}'_1, s'_2$	$c'_1, \bar{c}'_2, c'_3$	$\bar{c}'_1, c'_2, \bar{c}'_3$
$\boldsymbol{\Gamma}_1$	1	1	1	1	1	1
$\boldsymbol{\Gamma}_2$	1	1	1	1	-1	-1
$\boldsymbol{\Gamma}_3$	1	-1	-1	1	1	-1
$\boldsymbol{\Gamma}_4$	1	-1	-1	1	-1	1
$\boldsymbol{\Gamma}_5$	2	2	-1	-1	0	0
$\boldsymbol{\Gamma}_6$	2	-2	1	-1	0	0

representations according to the character table rules. The character table is shown in Table IV, and it is recognized to be isomorphic to the point group D_{3h}. Based on a similar argument as that for the 1D "shifted" waveguide, only $\boldsymbol{\Gamma}_3$, $\boldsymbol{\Gamma}_4$, and $\boldsymbol{\Gamma}_6$ are legitimate irreducible representations. Hence both 1-fold and 2-fold degeneracy are expected at the zone boundary, which is verified by MPB simulation as shown in Fig.6.

A natural question to ask is whether there would be anything different between the band structures of the 3_1 and 3_2 screw axes. It turnes out that structures with the two kinds of screw axes are mirror images of each other, and they are called "chiral" structures, which means they have distinct "handedness". Since they are mirror images of each other, their band structures will be exactly the same. Chiral structures generally have lower symmetry because of the lack of mirror reflections (mirror reflection would change the chirality). Another interesting question to ask is whether it is possible to have higher-fold degeneracy at the zone boundary . A naive speculation is that structures with "achiral" screw axes such as 4_2 and 6_3 axes and so on, may exhibit higher symmetry and hence higher-fold degeneracy because the mirror reflections are allowed. A familiar example is the high degeneracy of electronics bands at the zone boundary of "armchair" carbon nanotubes[11]. But the simulation results

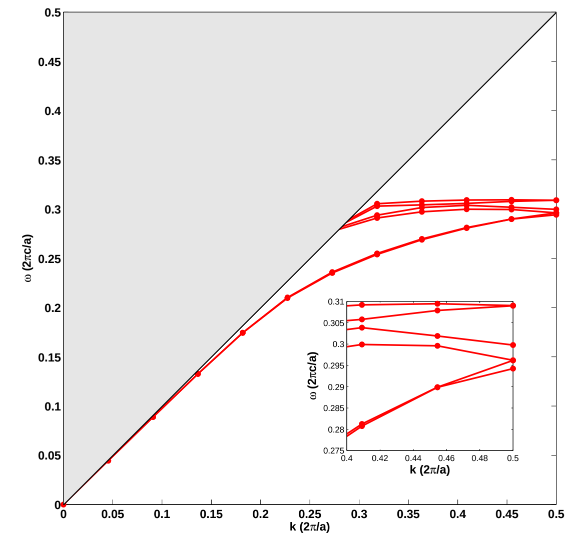

FIG. 6. Band structure of a 3-step spiral waveguide. The inset shows the bands near the zone boundary, where both 1-fold and 2-fold degeneracies are observed.

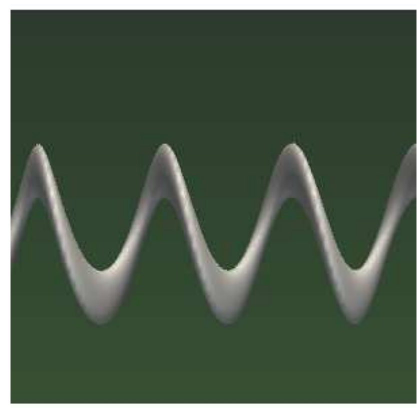

FIG. 7. Schematic of a continuous spiral waveguide.

of staircase waveguides with 4_2 and 6_3 screw axes do not exhibit higher-than-two-fold denegenary, indicating more sophiscated symmetry is required to "stick" more bands together at the zone boundary, which is still an on-going pursuit of the author.

Just out of curiosity, a spiral waveguide with a continuous screw axis as shown in Fig.7(a) is simulated. Formal analysis of continuous symmetries demands the theory of Lie groups, which is out of the scope of this report, but the simulation results still shed some light in understanding the origin of the extra degeneracy due to the screw axis. Fig.8(a) shows the band structure of the continuous spiral waveguide, where 2-fold degeneracy is again observed at the zone boundary. Fig.8(b)(c) show the contour plots of the electric field energy density distribution of the lowest two degenerate modes. They

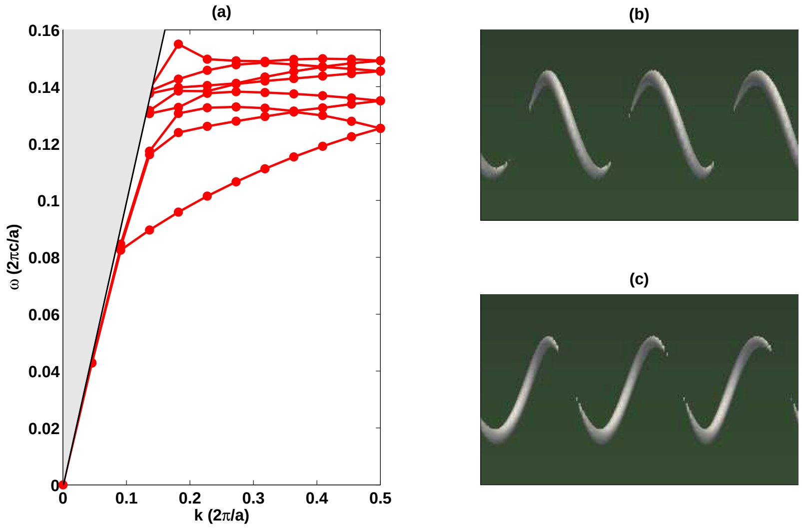

FIG. 8. (a) Band structure of a continuous spiral waveguide. (b) and (c) Contour plots of the electric field energy density of the lowest two degenerate modes.

have the same "shape", and the only difference is that the nodes of one mode is shifted by one fourth a period from those of the other mode, which resembles the relation between sine and cosine functions. In general, sine and cosine functions are not degenerate in structures with normal mirror planes, for instance, in a 1D "atomic chain" structure, where they are separated by the band gap at the zone edge. But the existence of nonsymmorphic operations make it possible for eigen fields with a similar relation to be degenerate, resulting in the double-fold degeneracy at the zone boundary.

III. SUMMARY

In summary, in this report the basic method (Herring's method) of analyzing the irreducible representations of nonsymmorphic space groups is reviewed, and the main consequency, i.e. "bands-sticking-together" effect is demonstrated via model studies of photonic crystal waveguides with glide planes and screw axes. The origin of the extra degeneracy is simply discussed and illustrated with a continuous spiral waveguide.

ACKNOWLEDGMENTS

The author wants to thank Professor Johnson for his wonderful lectures, even more wonderful talks during office hours and his introduction of the "Hairy Ball Theorem", which stimulates the author's interest in learning some topology after group theory.

[1] G. Burns and A. Glazer, *Space Groups For Solid State Scientists* (Academic Press, INC, 1990).
[2] L. M. Falicov, *Group Theory and its Physical Applications* (The University of Chicago Press, 1966).
[3] F. Seitz, Annal. Math. **37**, 17 (1935).
[4] M. Lax, *Symmetry Principles in Solid State and Molecular Physics* (John Wiley & Sons, 1974).
[5] T. Inui, Y. Tanabe, and Y. Onodera, *Group Theory and Its Applications in Physics* (Springer-Verlag, 1990).
[6] R. Mirman, *Point Groups, Space Groups, Crystals, Molecules* (World Scientific, Singapore, 1999).
[7] V. Heine, *Group Theory in Quantum Mechanics* (Pergamon Press, 1960).
[8] C. Herring, J. Franklin Inst. **233**, 525 (1942).
[9] A. Mock, L. Lu, and J. O'Brien, Phy. Rev. B **81**, 155115 (2010).
[10] S. G. Johnson and J. D. Joannopoulos, Opt. Express **8**, 173 (2001).
[11] C. T. White and T. N. Todorov, Nature **393**, 240 (1998).