Group theoretic analysis of structured elastic plates: nonsymmorphic crystals and topological waveguiding

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Abstract

The study of wave propagation through structured periodic media depends critically upon the periodic lattice from which the medium is constructed. That is unsurprising, but perhaps what is slightly more surprising, is that pieces of pure mathematics play a key role - in particular, group and representation theory. Group theory is the natural language that encodes the symmetries of shape and form. Here we use it to consider a class of $2D$ periodic crystals whose lattice is encoded by *nonsymmorphic* space groups. These are often overlooked due to their relative complexity compared to the symmorphic space groups. We demonstrate that nonsymmorphic groups have possible practical interest in terms of coalescence of dispersion curves, Dirac points and band-sticking, using both theory and simulation. Once we've laid out the group theoretical framework in the context of the nonsymmorphic crystals, we use it to illustrate how accidental degeneracies can arise in symmorphic square lattices. We combine this phenomenon with topological valley effects to design highly-efficient topological waveguides and energy-splitters.

Contents

1 Introduction

From quantum mechanics to the study of optical devices based on photonic crystals and mechanical waves through so-called platonic crystals, wave-like systems are ubiquitous in nature. Many also exhibit crystalline structure - that is, the system repeats itself in space, and translating the entire lattice by any *Bravais lattice vector*, $\boldsymbol{t}$, leaves the system indistinguishable from before.

These systems can be described and interpreted using *dispersion relations*, the relationships between the angular frequency ω and wavevector $\boldsymbol{k}$ of the propagating wave. These lead to dispersion curves that are used throughout the periodic media community, often used practically as part of the design of devices. Many numerical schemes have been devised for their accurate computation. Specific, frequency dependent features are often desired and during the design process these curves must be re-computed depending on the lattice, material constants and other parameters. Group and representation theory are powerful tools because they can predict properties of dispersion curves based purely on the symmetries, regardless of the type of system at hand. Importantly, this means that symmetry-induced effects are universal across different systems and a full understanding then circumvents, or aids, in the identification of desirable features.

One such wave-like system is the Mass-Loaded Kirchhoff-Love (MLKL) equation. Physically, it describes flexural waves on a 2D thin elastic plate with pinned point masses. This is an abstraction, and entry-level model, of many real physical mechanical wave systems - for instance of vibration modes on the thin metal skin of an aircraft [1] or waves on thin ice sheets [2].

The dimensionaless, simplified MLKL equation is given by

$$\nabla^4\Psi(\boldsymbol{x},\tau) = \Big(1+V(\boldsymbol{x})\Big)\frac{\partial^2\Psi(\boldsymbol{x},\tau)}{\partial\tau^2}, \tag{1.1}$$

where $\Psi(\boldsymbol{x})$ is the displacement of the flexural wave with position $\boldsymbol{x}$ and time τ and $V(\boldsymbol{x}) = \sum_{\boldsymbol{t}}\sum_p M^{(p)}\delta(\boldsymbol{x}-\boldsymbol{x}^{(p)}-\boldsymbol{t})$ is the contribution from point masses, each positioned relative to the lattice at $\boldsymbol{x}^{(p)}$, and repeated infinitely over lattice vectors $\boldsymbol{t}$.

Using separation of variables, the general solution can be taken in the form $\Psi(\boldsymbol{x},\tau) = \psi(\boldsymbol{x})e^{-i\omega\tau}$ where this harmonic behaviour is henceforth considered understood. Then in terms of the frequency, ω, equation (1.1) becomes

$$\nabla^4\psi(\boldsymbol{x}) = \Big(1+V(\boldsymbol{x})\Big)\omega^2\psi(\boldsymbol{x}), \tag{1.2}$$

which is an eigenvalue equation. This article will focus on MLKL systems with 2D nonsymmorphic symmetries. Nonsymmorphic symmetries in 2D crystals, as will be explained later, contain glide reflections, which have not only rotations and reflections, but also contain fractional lattice translations. All four symmetries will be studied computationally while theoretically, two space groups will be studied in depth: $p4g$ and pgg.

2 Nonsymmorphic Group Theory

In this section we outline key group theoretical concepts focused on nonsymmorphic crystals, but which can be applied to symmorphic ones as well.

When analysing wave propagation through periodic media, the dispersion relation (relationship between the frequency and wavevector) is crucial. Exotic wave phenomena can be seen directly from the dispersion curves. For example, degenerate curves are associated with the perfect transmission of waves through the medium; whilst gaps in the frequency spectrum, known as band-gaps, forbid the propagation of waves. The apriori prediction of degeneracies and band-gaps is of great physical interest; hence this motivates a first-principles group theoretical approach to analyse waves in periodic media.

Specifically, we shall seek to apriori predict the degree of degeneracies as well as the symmetries of their eigensolutions (which represent the displacement of the medium). Thereafter, we shall systematically break these degeneracies, by reducing the symmetries of the system, thereby yielding band-gaps. Near the periphery of these band-gaps we shall demonstrate novel anisotropic behaviour.

The degree of the degeneracy is equal to the dimension of the irreducible representation (which will be defined later on); this section primarily focuses on the derivation of these irreducible representations thereby allowing us to characterise the degeneracies for nonsymmorphic crystals.

2.1 Seitz notation

When describing affine transformations, where an object is actively rotated/improperly rotated then shifted, it is useful to use Seitz notation, where for a position vector $\boldsymbol{x}$,

$$\{\boldsymbol{\alpha} \mid \boldsymbol{a}\}\boldsymbol{x} := \boldsymbol{\alpha}\boldsymbol{x} + \boldsymbol{a}, \tag{2.1}$$

where Greek letters are used for unitary matrices. For a function $f(\boldsymbol{x})$, since the function itself is rotated and shifted instead of the coordinate system,

$$\{\boldsymbol{\alpha} \,\hat{|}\, \boldsymbol{a}\}f(\boldsymbol{x}) = f(\{\boldsymbol{\alpha} \mid \boldsymbol{a}\}^{-1}\boldsymbol{x}) = f(\{\boldsymbol{\alpha}^{-1} \mid -\boldsymbol{\alpha}^{-1}\boldsymbol{a}\}\boldsymbol{x}) = f(\boldsymbol{\alpha}^{-1}\boldsymbol{x} - \boldsymbol{\alpha}^{-1}\boldsymbol{a}). \tag{2.2}$$

It is easy to show that these Seitz operators obey an algebra as below:

$$\{\boldsymbol{\alpha} \mid \boldsymbol{a}\}\{\boldsymbol{\beta} \mid \boldsymbol{b}\} = \{\boldsymbol{\alpha}\boldsymbol{\beta} \mid \boldsymbol{\alpha}\boldsymbol{b} + \boldsymbol{a}\};\ \{\boldsymbol{\alpha} \mid \boldsymbol{a}\}^{-1} = \{\boldsymbol{\alpha}^{-1} \mid -\boldsymbol{\alpha}^{-1}\boldsymbol{a}\}. \tag{2.3}$$

2.2 Representation theory

Consider the eigenvalue problem

$$\hat{H}\psi(\boldsymbol{x}) = \lambda\psi(\boldsymbol{x}), \tag{2.4}$$

where $\hat{H}$ is an operator, called the Hamiltonian (a homage to quantum mechanics), and $\psi(\boldsymbol{x})$ is some solution to be determined. Now consider a set of operators $\{\hat{g}\}_g$ (where subscript denotes what is being iterated) that commutes with the Hamiltonian, $[\hat{H}, \hat{g}] = 0$, and form a *group*.

Representation theory tells us that the solutions of the partial differential equation belong to an irreducible representation (hereafter referred to as irrep) $D^{(n)}$ of $\{\hat{g}\}_g$, and that the solutions transform as

$$\hat{g}\psi_i^{(n)}(\boldsymbol{x}) = \sum_{j=1}^{n} D_{ji}^{(n)}(g)\psi_j^{(n)}(\boldsymbol{x}), \tag{2.5}$$

where $D_{ji}^{(n)}(g)$ is entry ji of the irrep $D^{(n)}$ of element g of $\{\hat{g}\}_g$, and $\{\psi_i^{(n)}(x)\}_i$ are the basis functions of $D^{(n)}$ [7].

From this we can see that n-dimensional irreducible representations will guarantee a n-fold degeneracy for a particular λ, as there will be n basis functions for the same λ. This is called *symmetry induced degeneracy*, normally just referred to as degeneracy. However, it could be that two irreps simply happen to share the same λ; this case is called *accidental degeneracy* and will be studied in section 5. Eq. (2.5) which relates the symmetry operators, $\hat{g}$, with the irrep matrix $D^{(n)}(g)$ and the basis functions $\psi_i^{(n)}(\mathbf{x})$, is imperative and will be used throughout this project.

2.3 Blochs theorem

When dealing with periodic systems, the eigenvalue problem, Eq. (2.4), is greatly simplified. Consider a two-dimensional system with wavelike solutions,

$$\hat{H}(\boldsymbol{x})\psi(\boldsymbol{x}) = \omega^m \psi(\boldsymbol{x}), \tag{2.6}$$

where $\hat{H}$ is the Hamiltonian, ω^m is the angular frequency raised to some power (power depending on the system), and ψ is the wavelike solution with $\boldsymbol{x}$ being the coordinate vector.

If a system is *periodic*, it means that the system is invariant under any discrete lattice translations by

$$\boldsymbol{t} = n_1 \boldsymbol{a}_1 + n_2 \boldsymbol{a}_2, \tag{2.7}$$

for $n_i \in \mathbb{Z}$ and where $\boldsymbol{a}_i$ are primitive lattice vectors, as illustrated in Fig. 1. Mathematically, this is represented as the Hamiltonian commuting with translation operators, $[\hat{H}, \widehat{\{\mathbb{1} \mid \boldsymbol{t}\}}] = 0$.

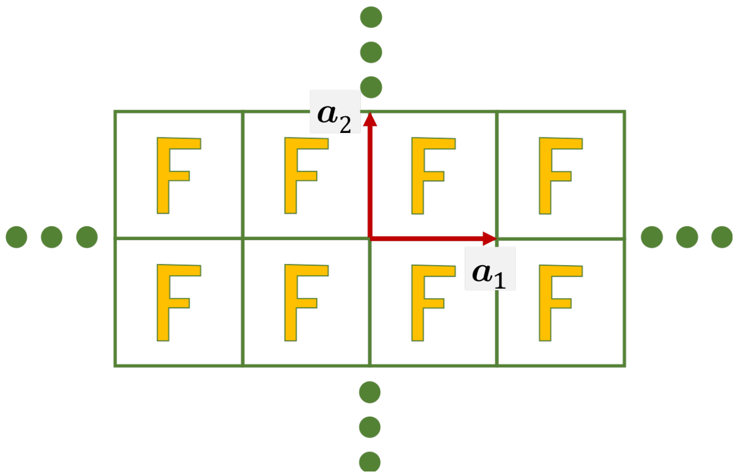

Figure 1: An illustration of a periodic medium with translational symmetry. a_1, a_2 represent lattice translations along the x and y axes, respectively.

It can be shown, through Bloch's theorem (which uses representation theory), that such systems have Bloch wave solutions:

$$\psi_{n,\boldsymbol{k}}(\boldsymbol{x}) = e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} u_{n,\boldsymbol{k}}(\boldsymbol{x}), \tag{2.8}$$

where we label the solutions with band index n and wavevector $\boldsymbol{k}$, and $u_{n,\boldsymbol{k}}(\boldsymbol{x}) = u_{n,\boldsymbol{k}}(\boldsymbol{x} \pm \boldsymbol{t})$ contains the symmetry of the crystal [7].

Eq. (2.8) will be crucial in the subsequent subsection, and will be used to define the subgroup of a crystal's space group, as well as to reduce the domain of wavevectors in reciprocal space.

2.4 Translation Subgroup T

The translational operators $\left\{\{\mathbb{1} \mid \boldsymbol{t}\}\right\}_{\boldsymbol{t}}$ form a group, called the translational group, T. For a given $\boldsymbol{k}$, $\psi_{n,\boldsymbol{k}}(\boldsymbol{x})$ is the basis function for the $D_T^{(k)} = \{e^{-i\boldsymbol{k}\cdot\boldsymbol{t}}\}_{\boldsymbol{t}}$ one-dimensional irrep of T, since

$$\{\mathbb{1} \mid \boldsymbol{t}\}\psi_{n,\boldsymbol{k}}(\boldsymbol{x}) = e^{-i\boldsymbol{k}\cdot\boldsymbol{t}}\psi_{n,\boldsymbol{k}}(\boldsymbol{x}), \tag{2.9}$$

which fulfills the requirement of a basis function, since $\psi_{n,\boldsymbol{k}}(\boldsymbol{x})$ is an eigenfunction of the translation operator.

Another consequence of the translational symmetry is that the wavevector, $\boldsymbol{k}$, can be reduced into a restricted area within reciprocal space, namely, the First Brillouin Zone (FBZ); this greatly simplifies the eigenvalue problem. Physically, this implies that two wavevectors, seperated by a reciprocal lattice vector, are equivalent.

$$\boldsymbol{k} \Leftrightarrow \boldsymbol{k} + \boldsymbol{K}, \tag{2.10}$$

where $\boldsymbol{K} = m_1\boldsymbol{b}_1 + m_2\boldsymbol{b}_2$ is the reciprocal lattice vector, such that $\boldsymbol{a}_i \cdot \boldsymbol{b}_j = 2\pi\delta_{ij}$.

In this subsection, we've demonstrated that Bloch's theorem gives rise to a translation subgroup, T, aswell as how it is used to simplify the eigenvalue problem by reducing the domain of the problem(equation (2.10)).

2.5 Nonsymmorphic space groups

2.5.1 Identifying nonsymmorphic groups

In addition to the translational symmetries, the system may be invariant under other affine operators, $\left\{\{\boldsymbol{\alpha} \mid \boldsymbol{a}\}\right\}_{\{\boldsymbol{\alpha}|\boldsymbol{a}\}}$. Together, these affine transformations and the translations, form a group called the space group, G. An example of a space group, pmg, is shown in Fig. 2.

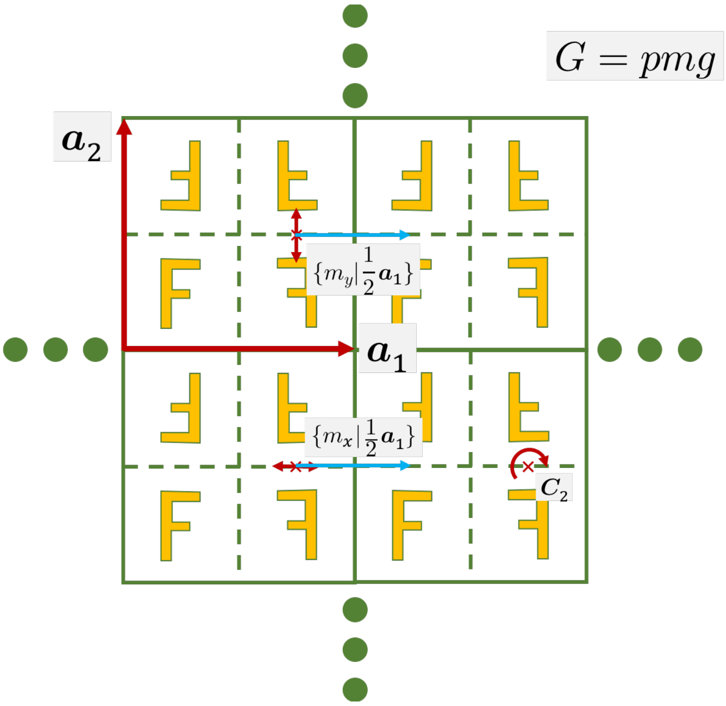

Figure 2: An illustration of a periodic medium with pmg symmetry. Filled green squares indicate the unit cell, while the dotted squares indicate the smallest pattern the unit cell can be made out of. m_x, m_y denote reflections in the x and y axis respectively, and C_2 denote a 180°rotation.

Any element $\{\boldsymbol{\alpha} \mid \boldsymbol{a}\}$ of the space group can always be decomposed into primitive lattice vectors and non-primitive ones:

$$\{\boldsymbol{\alpha} \mid \boldsymbol{a}\} = \{\mathbf{1} \mid \boldsymbol{t}\}\{\boldsymbol{\alpha} \mid \boldsymbol{v}\}, \tag{2.11}$$

where $\boldsymbol{v}$ represents a fractional translational vector.

Note that we can shift the origin of the transformation by a similarity relation,

$$\{\boldsymbol{\alpha} \mid \boldsymbol{v}\} \to \{\boldsymbol{\alpha}' \mid \boldsymbol{v}'\} = \{\mathbb{1} \mid \boldsymbol{b}\}\{\alpha \mid \boldsymbol{v}\}\{\mathbb{1} \mid \boldsymbol{b}\}^{-1} = \{\boldsymbol{\alpha} \mid \boldsymbol{v} + \boldsymbol{b} - \boldsymbol{\alpha}\boldsymbol{b}\}, \tag{2.12}$$

where $\boldsymbol{b}$ the shift transformation. To try to set $\boldsymbol{v}' = 0$, we let

$$\boldsymbol{b} = (\mathbb{1} - \boldsymbol{\alpha})^{-1}\boldsymbol{v}. \tag{2.13}$$

However, if $(\mathbb{1} - \boldsymbol{\alpha})$ is singular, fractional translations cannot be removed by changing the origin. We define space group G to be symmorphic if $(\mathbb{1} - \boldsymbol{\alpha})$ is not singular for all $\boldsymbol{\alpha}$. If this is the case then every element can be decomposed into $\{\mathbb{1} \mid \boldsymbol{t}\}\{\boldsymbol{\alpha} \mid 0\}$; hence, G is a semi-direct product of T and a point group, P, $G = T \rtimes P$.

Conversely, G is non-symmorphic if there exist some $\boldsymbol{\alpha}$ such that $(\mathbb{1} - \boldsymbol{\alpha})$ is singular, and in general elements are $\{\mathbb{1} \mid t\}\{\boldsymbol{\alpha} \mid \boldsymbol{v}\}$, where $\boldsymbol{v}$ is a fractional translation.

2.5.2 Translation subgroups of the nonsymmorphic groups

The translational subgroup T is an invariant subgroup of G, so G can be decomposed into cosets of T:

$$G = T \cdot r_1 + ... + T \cdot r_s;\ r_1 := \{\mathbb{1} \mid 0\}, \tag{2.14}$$

where $\{r_i\}_i$ are the coset representatives. Physically, they are the non-translational elements of the space group. All elements of G can be compactly written in this form. All four two-dimensional nonsymmorphic space groups are down in the table below:

Group G	Coset Representatives of G/T	P
pg	$\{\mathbb{1} \mid 0\}, \{\sigma_y \mid \frac{1}{2}a_1\}$	σ_y
pmg	$\{\mathbb{1} \mid 0\}, \{\sigma_y \mid \frac{1}{2}a_1\}, \{\sigma_x \mid \frac{1}{2}a_1\}, \{C_2 \mid 0\}$	C_{2v}
pgg	$\{\mathbb{1} \mid 0\}, \{\sigma_x \mid \frac{1}{2}a_1 + \frac{1}{2}a_2\}, \{\sigma_y \mid \frac{1}{2}a_1 + \frac{1}{2}a_2\}, \{C_2 \mid 0\}$	C_{2v}
$p4g$	$\{\mathbb{1} \mid 0\}, \{\sigma_x \mid \frac{1}{2}a_1 + \frac{1}{2}a_2\}, \{\sigma_y \mid \frac{1}{2}a_1 + \frac{1}{2}a_2\}, \{\sigma_{da} \mid \frac{1}{2}a_1 + \frac{1}{2}a_2\},$ $\{\sigma_{db} \mid \frac{1}{2}a_1 + \frac{1}{2}a_2\}, \{C_4 \mid 0\}, \{C_4^{-1} \mid 0\}, \{C_2 \mid 0\}$	C_{4v}

The rotations/improper rotations of the operators of G, form a point group. We define this to be the point group of the space group, and label it P. For symmorphic groups, the rotational and reflectional elements, form P, whereas for nonsymmorphic groups, only the coset representatives form P. This is an important distinction, as when we deal with the group of the wavevector $\boldsymbol{k}$, that group will be isomorphic, albeit not identical, to a subgroup of the nonsymmorphic group.

2.5.3 Irreducible Brillouin Zone (IBZ)

The point group symmetry is reflected in the reciprocal space. Therefore, the First Brillouin Zone (FBZ) exhibits symmetry of the point group of the space group, P. We define the Irreducible Brillouin Zone (IBZ) as smallest part of the Brillouin zone that can be tessellated to form the entire Brillouin zone. Apart from the point group symmetry of the crystal, many systems also exhibit Time Reversal Symmetry (TRS), where in terms of reciprocal space, $\boldsymbol{k}$ is equivalent to $-\boldsymbol{k}$. This can 'fold' the IBZ into a smaller one. The High-Symmetry Points (HSP) on the IBZ are conventionally labeled, as shown below in Fig. 3 for the square lattice:

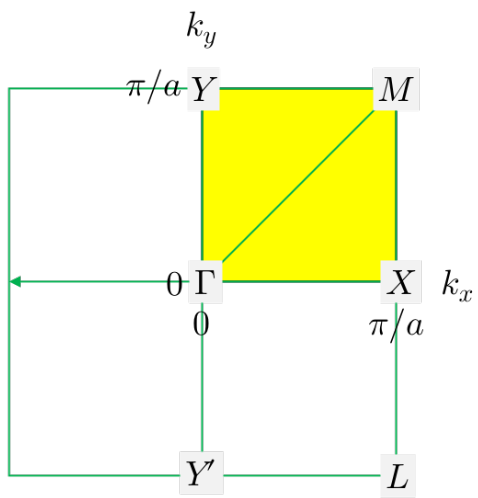

Figure 3: The First Brillouin Zone (FBZ) can be retreived via tesslation of the Irreducible Brillouin Zone (IBZ), whose High Symmetry Points (HSP) are labelled as the figure for the case of a square lattice.

For pmg, pgg, because the point group of the space group is C_{2v}, the IBZ is the square ΓXMY, while for $p4g$, the IBZ is the triangle ΓXM. For pg, even though P is $\{E, \sigma_y\}$ and therefore IBZ is $YY'LM$, the IBZ folds again for systems with TRS and becomes the square ΓXMY.

The IBZ is used when we examine the wave properties of the medium. Dispersion relations, which relate the frequency to the wavevector, are plotted along the edge of the IBZ where interesting wave phenomena are more likely to occur; this is due to the higher-degree of symmetry at these points, compared with those lieing within the IBZ.

2.6 Group of the wavevector *k*

Recall that from Bloch's theorem, the argument of the exponential function is $(i\boldsymbol{k} \cdot \boldsymbol{x})$. We have already discussed how the translational component (associated to $\boldsymbol{x}$) is reflected in the representations of the nonsymmorphic group; in this subsection we now examine more closely the group of $\boldsymbol{k} \in$ edge of IBZ. This group, $G_{\boldsymbol{k}}$, is also known as the 'little group'.

Consider an element of the space group, $\{\boldsymbol{\alpha} \mid \boldsymbol{a}\} \in G$. It acts on a Bloch wave as

$$\begin{aligned} \{\boldsymbol{\alpha} \hat{\mid} \boldsymbol{a}\}\psi_{\boldsymbol{k}}(\boldsymbol{x}) &= \psi_{\boldsymbol{k}}(\{\boldsymbol{\alpha} \mid \boldsymbol{a}\}^{-1}\boldsymbol{x}) = \psi_{\boldsymbol{k}}(\{\boldsymbol{\alpha}^{-1} \mid -\boldsymbol{\alpha}^{-1}\boldsymbol{a}\}\boldsymbol{x}) \\ &= \psi_{\boldsymbol{k}}(\boldsymbol{\alpha}^{-1}\boldsymbol{x} - \boldsymbol{\alpha}^{-1}\boldsymbol{a}) = e^{i\boldsymbol{k}\cdot(\boldsymbol{\alpha}^{-1}\boldsymbol{x} - \boldsymbol{\alpha}^{-1}\boldsymbol{a})} u_{\boldsymbol{k}}(\boldsymbol{\alpha}^{-1}\boldsymbol{x} - \boldsymbol{\alpha}^{-1}\boldsymbol{a}). \end{aligned} \tag{2.15}$$

Since the dot product is invariant under unitary transformations, $i\boldsymbol{k} \cdot (\boldsymbol{\alpha}^{-1}\boldsymbol{x} - \boldsymbol{\alpha}^{-1}\boldsymbol{a}) = i(\boldsymbol{\alpha}\boldsymbol{k}) \cdot (\boldsymbol{x} - \boldsymbol{a})$, and since $u_{\boldsymbol{k}}(\boldsymbol{x})$ follows the symmetry of the crystal,

$$\{\boldsymbol{\alpha} \hat{\mid} \boldsymbol{a}\}\psi_{\boldsymbol{k}}(\boldsymbol{x}) = e^{i\boldsymbol{\alpha}\boldsymbol{k}\cdot(\boldsymbol{x} - \boldsymbol{a})} u_{\boldsymbol{k}}(\boldsymbol{x}). \tag{2.16}$$

Now if $\boldsymbol{k}$ is at Brillouin zone boundaries (also known as high symmetry points), certain $\{\boldsymbol{\alpha} \mid \boldsymbol{a}\}$ will result in $\boldsymbol{\alpha}\boldsymbol{k} = \boldsymbol{k} + \boldsymbol{K}$. This means that $\{\boldsymbol{\alpha} \mid \boldsymbol{a}\}\psi_{\boldsymbol{k}}(\boldsymbol{x})$ is the basis function of the same irrep of T as $\psi_{\boldsymbol{k}}(\boldsymbol{x})$.

Define the group of $\boldsymbol{k}$, also known as 'little group of $\boldsymbol{k}$', $G_{\boldsymbol{k}}$, as

$$G_{\boldsymbol{k}} := \Big\{\{\boldsymbol{\alpha} \mid \boldsymbol{a}\} \in G \mid \boldsymbol{\alpha}\boldsymbol{k} = \boldsymbol{k} + \boldsymbol{K}\Big\}. \tag{2.17}$$

For a specific ω and $\boldsymbol{k}$, by group theory, the dimension of the irrep of $G_{\boldsymbol{k}}$ is equal to the degeneracy of the solutions. Note that by this definition, it is always the case that $\{\mathbb{1} \mid \boldsymbol{t}\} \in G_{\boldsymbol{k}}$.

In a similar way to G, we can compactly write down elements of $G_{\boldsymbol{k}}$ through coset decomposition $G_{\boldsymbol{k}}/T$.

Rotations/improper rotations of elements of $G_{\boldsymbol{k}}$ form a point group. We define this to be the point group of $\boldsymbol{k}$, $P_{\boldsymbol{k}}$. We can see that it is isomorphic to the coset decomposition of $G_{\boldsymbol{k}}$: $G_{\boldsymbol{k}}/T \cong P_{\boldsymbol{k}}$.

Most importantly, note that for symmorphic groups, the coset representatives of $G_{\boldsymbol{k}}/T$ are the same operators as the operators of $P_{\boldsymbol{k}}$ itself. However, for nonsymmorphic groups, because there are fractional translations that cannot be removed, the coset representatives of $G_{\boldsymbol{k}}/T$ are not the same as the operators of $P_{\boldsymbol{k}}$.

2.7 Irreducible representation of $G_{\boldsymbol{k}}$

By utilising all the knowledge accrued in the previous subsections we are now in a position to construct the irreps of a nonsymmorphic group.

For symmorphic groups, since $G = T \rtimes P$, it is also true that $G_{\boldsymbol{k}} = T \rtimes P_{\boldsymbol{k}}$.

Let $D_T^{(\boldsymbol{k})}$ be the irrep $\boldsymbol{k}$ of T, and $D_{P_{\boldsymbol{k}}}^{(\gamma)}$ be the irrep γ of $P_{\boldsymbol{k}}$. Hence, for symmorphic groups, irreps of $G_{\boldsymbol{k}}$ can be deconstructed as follows,

$$D_{G_{\boldsymbol{k}}}^{(\gamma)}(\{\boldsymbol{\alpha} \mid \boldsymbol{t}\}) = D_T^{(\boldsymbol{k})}(\{\mathbb{1} \mid \boldsymbol{t}\}) D_{P_{\boldsymbol{k}}}^{(\gamma)}(\{\boldsymbol{\alpha} \mid 0\}) = \exp(i\boldsymbol{k}\cdot\boldsymbol{t}) D_{P_{\boldsymbol{k}}}^{(\gamma)}(\{\boldsymbol{\alpha} \mid 0\}). \tag{2.18}$$

For nonsymmorphic groups, the irreducible representations cannot be deconstructed in a similar manner; hence other methods must be used to simplify the total irrep. One method is to use Herring's method.

We define the translational subgroup of k, $T_{\boldsymbol{k}}$, as

$$T_{\boldsymbol{k}} := \Big\{ \{\mathbb{1} \mid \boldsymbol{t}_k\} \in T \mid \exp(i\boldsymbol{k}\cdot\boldsymbol{t}_k) = 1 \Big\}. \tag{2.19}$$

We note that the irrep of $T_{\boldsymbol{k}}$ is unity, i.e. 1, for all elements. Therefore, if the irrep of $G_{\boldsymbol{k}}/T_{\boldsymbol{k}}$ is known, then the irrep of $G_{\boldsymbol{k}}$ is the same as the irrep of $G_{\boldsymbol{k}}/T_{\boldsymbol{k}}$. Now $G_{\boldsymbol{k}}/T_{\boldsymbol{k}}$ can be isomorphic to a point group bigger than $G_{\boldsymbol{k}}/T$, because the coset representatives of $G_{\boldsymbol{k}}/T_{\boldsymbol{k}}$ will contain translations not in $T_{\boldsymbol{k}}$, $\{\mathbb{1} \mid \boldsymbol{t}_m\} \notin T_{\boldsymbol{k}}$ (i.e. non-lattice translations).

However, this method can create spurious irreps, as any $\boldsymbol{t}_k$ such that $\exp(i\boldsymbol{k}\cdot\boldsymbol{t}_k) = 1$ will also mean that $\exp(in\boldsymbol{k}\cdot\boldsymbol{t}_k) = 1$ for any $n \in \mathbb{Z}$. To remove the spurious irreps of $G_{\boldsymbol{k}}$, we check whether

$$\chi_{G_{\boldsymbol{k}}}^{(\alpha)}(\{\mathbb{1} \mid t_m\}) = \dim\left(D_{G_{\boldsymbol{k}}/T_{\boldsymbol{k}}}^{(\alpha)}\right) \exp(i\boldsymbol{k}\cdot\boldsymbol{t}_m). \tag{2.20}$$

Any irreps that do not hold the requirement above are spurious irreps [5].

For points away from the high symmetry points, T_k cannot be constructed; in these cases, ray representations are used, which will not be covered here but are shown in Inui [7].

3 $\boldsymbol{k}\cdot\boldsymbol{p}$ Theory for the MLKL System

In this section we elucidate the $\boldsymbol{k}\cdot\boldsymbol{p}$ perturbation method, a method that can be used to analyse the dispersive behaviour in the vicinity of critical points in the Bloch spectrum, focusing on the case of the MLKL system for concreteness. $\boldsymbol{k}\cdot\boldsymbol{p}$ theory will be used in conjunction with group theoretical concepts, from Sec. 2, to simplify the local eigenvalue problem to reveal whether there are degeneracies, their order if one exists, and how they can be broken to yield band-gaps.

For a mass-loaded Kirchhoff-Love system, the simplified PDE is

$$\Big(\nabla^4 - \omega_{n,\boldsymbol{k}}^2[1 + V(\boldsymbol{x})]\Big)\psi_{n,\boldsymbol{k}} = 0, \tag{3.1}$$

where $V(\boldsymbol{x}) = V(\boldsymbol{x} - \boldsymbol{t}) = \sum_{\boldsymbol{t},p} M^{(p)}\delta(\boldsymbol{x} - \boldsymbol{x}^{(p)} - \boldsymbol{t})$.

For a given $\boldsymbol{k}_0$, the periodic waves $\{u_{n,\boldsymbol{k}_0}\}_n$ form a complete basis set [8]. Therefore any solution $\psi_{n,\boldsymbol{k}}$ can be written as

$$\begin{aligned}\psi_{n,\boldsymbol{k}} &= e^{i\boldsymbol{k}\cdot\boldsymbol{x}} u_{n,\boldsymbol{k}} = e^{i\boldsymbol{k}\cdot\boldsymbol{x}} \sum_m a_{m,n}(\boldsymbol{k}) u_{m,\boldsymbol{k}_0} \\ &= e^{-i(\boldsymbol{k}-\boldsymbol{k}_0)\cdot\boldsymbol{x}} \sum_m a_{m,n}(\boldsymbol{k})\psi_{m,\boldsymbol{k}_0} =: e^{-i\Delta\boldsymbol{k}\cdot\boldsymbol{x}} \sum_m a_{m,n}(\boldsymbol{k})\psi_{m,\boldsymbol{k}_0}.\end{aligned} \tag{3.2}$$

Now it can be shown that

$$\nabla^4(e^{-i\Delta\boldsymbol{k}\cdot\boldsymbol{x}}\psi_{m,\boldsymbol{k}_0}) = e^{-i\Delta\boldsymbol{k}\cdot\boldsymbol{x}}[\nabla^4 + 6i\Delta\boldsymbol{k}\cdot\nabla^3 - 6\Delta\boldsymbol{k}^2\nabla^2 + O(\Delta\boldsymbol{k}^3)]\psi_{m,\boldsymbol{k}_0}, \tag{3.3}$$

and since at $\boldsymbol{k}_0$

$$\nabla^4\psi_{m,\boldsymbol{k}_0} = \omega_{\boldsymbol{k}_0}^2[1 + V(\boldsymbol{x})]\psi_{m,\boldsymbol{k}_0}, \tag{3.4}$$

we find that we require

$$a_{n,m}(\boldsymbol{k})\{[\omega_{\boldsymbol{k}_0}^2 - \omega_{\boldsymbol{k}}^2][1 + V(\boldsymbol{x})] + 6i\Delta\boldsymbol{k}\cdot\nabla^3 - 6\Delta k^2\nabla^2\}\psi_{m,\boldsymbol{k}_0} = 0 \tag{3.5}$$

for any n, m.

In the neighbourhood of $\boldsymbol{k}_0$, $\omega_{k_0}^2 - \omega_k^2 \approx -2\omega_{k_0}\Delta\omega$, where $\Delta\omega := \omega_k - \omega_{k_0}$. Taking the overlap with some arbitrary ψ_{l,k_0}, we get the following:

$$(H_{lm}^{(1)} + H_{lm}^{(2)})a_{n,m}(k) = \Lambda_{lm}a_{n,m}(k) \tag{3.6}$$

where
$H_{lm}^{(1)} := 6i\Delta k\cdot\langle l \mid \nabla^3 \mid m\rangle$,
$H_{lm}^{(2)} := -6\Delta k^2\langle l \mid \nabla^2 \mid m\rangle$, and
$\Lambda_{lm} := 2\omega_{k_0}\Delta\omega[\delta_{l,m} + \langle l \mid V(x) \mid m\rangle]$.

If $H_{lm}^{(1)} = 0$ and $H_{lm}^{(2)} \neq 0$, we get quadratic degeneracy. Whether these matrix elements are going to be equal to zero can be predicted by selection rules of space group using group theory.

4 Results For Nonsymmorphic Platonic Crystal

Lin J. et al. computationally showed that when a photonic crystal adiabatically transitions from a $p4g$ symmetry to a pgg symmetry, a quadratic degeneracy at Γ becomes a linear one along ΓX or ΓY [4]. In this section we demonstrate how these results are transposed to a structure elastic plate.

We first show group theoretically that these effects should occur for the MLKL system, along with other effects. Then, we compute the dispersion curves for all four nonsymmorphic space groups to verify Lin J. et al's assertions. Then, we demonstrate highly anisotropic oscillations which arise following a symmetry breaking perturbation.

4.1 Theoretical results

4.1.1 Proof of two-fold degeneracy for any $p4g$ system

Firstly, we prove, using group theoretical concepts from section 2, that there will be a two-fold degeneracy at $\boldsymbol{k} = \Gamma$ for any system with $p4g$ symmetry.

For $G = p4g$, there are 8 coset representatives of G/T. So,

$$\begin{aligned} G = {} & T\{\mathbb{1} \mid 0\} + T\{C_4 \mid 0\} \\ & + T\{C_4^{-1} \mid 0\} + T\{C_2 \mid 0\} \\ & + T\{\sigma_x \mid \frac{1}{2}a_1 + \frac{1}{2}a_2\} + T\{\sigma_y \mid \frac{1}{2}a_1 + \frac{1}{2}a_2\} \\ & + T\{\sigma_{da} \mid \frac{1}{2}a_1 + \frac{1}{2}a_2\} + T\{\sigma_{db} \mid \frac{1}{2}a_1 + \frac{1}{2}a_2\}. \end{aligned} \tag{4.1}$$

Now, at $\boldsymbol{k} = \Gamma$, G_Γ has the same coset representatives as G, that is $G_\Gamma/T = G/T$. Also, $T_\Gamma = T$, since $\exp(i0 \cdot \boldsymbol{t}) = 1 \; \forall \; \{\mathbb{1} \mid \boldsymbol{t}\} \in T$.

Now, the factor group is isomorphic to $G_\Gamma/T_\Gamma \cong C_{4v}$, with the cosets of G_Γ/T_Γ equivalent to the elements of C_{4v} of the same names. That is,

$$\{\alpha \mid v\} \Leftrightarrow \alpha \;\; \forall \; \{\alpha \mid v\} \in G_\Gamma/T_\Gamma, \;\; \forall \; \alpha \in C_{4v}. \tag{4.2}$$

The C_{4v} character table is as below:

C_{4v} (G_Γ) classes $\Rightarrow$ irreps $\Downarrow$	E	$2\,C_4$	C_2	$2\sigma_v$	$2\sigma_d$	Linear	Quadratic	Cubic
A_1	+1	+1	+1	+1	+1	z	x^2+y^2, z^2	$z^3, z(x^2+y^2)$
A_2	+1	+1	+1	-1	-1	R_z	-	-
B_1	+1	-1	+1	+1	-1	-	x^2-y^2	$z(x^2-y^2)$
B_2	+1	-1	+1	-1	+1	-	xy	xyz
E	+2	0	-2	0	0	(x,y), (R_x,R_y)	(xz,yz)	(xz^2,yz^2), $(xy^2,x^2y),(x^3,y^3)$

We see that the E irrep of C_{4v} is two-dimensional. This guarantees a two-fold degeneracy at $\boldsymbol{k} = \Gamma$ for any system with $p4g$ symmetry.

4.1.2 Proof of quadratic degeneracy for an MLKL $p4g$ system

Secondly, using the perturbation theory of Sec. 3, we can demonstrate that this degeneracy is quadratic.

Consider the matrix element $H^{(1)}_{lm} := 6i\Delta\boldsymbol{k} \cdot \langle l \mid \nabla^3 \mid m\rangle$, between the basis function of the irrep E of G_Γ. To see whether it vanishes for any l, m, we inspect the operator ∇^3:

$$\nabla^3 = \left(\frac{\partial^3}{\partial x^3} + \frac{\partial}{\partial x}\frac{\partial^2}{\partial y^2}\right)\hat{i} + \left(\frac{\partial^3}{\partial y^3} + \frac{\partial}{\partial y}\frac{\partial^2}{\partial x^2}\right)\hat{j} \tag{4.3}$$

Inside the inner product, which integrates over a unit cell, the translation operators do not change the result of the integral. Noting this, the form of Eq. (4.3), and the character table of C_{4v}, we can see that ∇^3 transforms as the two-dimensional irrep E of G_Γ, named E after the irrep of C_{4v}, and is an irreducible tensor operator.

Now, in order for an inner product

$$\langle l^{(\gamma)} \mid \hat{T}^{(\alpha)} \mid m^{(\beta)}\rangle, \tag{4.4}$$

where $\hat{T}^{(\alpha)}$ is a irreducible tensor operator, $\mid m^{(\beta)}\rangle, \mid m^{(\gamma)}\rangle$ are basis functions for irreps $D^{(\gamma)}, D^{(\beta)}$ respectively, to not vanish, we require that $D^{(\alpha\times\beta)}$ contain $D^{(\gamma)}$ [7]. Inspecting the first order term in the effective Hamiltonian,

$$H^{(1)}_{lm} = 6i\Delta\boldsymbol{k} \cdot \langle l \mid \nabla^3 \mid m\rangle, \tag{4.5}$$

Now, all three $\mid m\rangle, \mid l\rangle, \nabla^3$ transform as the irrep E. However, $D^{(E\times E)} = A_1 + A_2 + B_1 + B_2$, which doesn't contain E. Therefore, the matrix element vanishes, and we have no linear term in the dispersion relation.

Now consider the quadratic term, $H^{(2)}_{lm} := -6\Delta k^2 \langle l \mid \nabla^2 \mid m\rangle$. The ∇^2 operator is

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}. \tag{4.6}$$

Looking at the C_{4v} character table, we note that this operator is also an irreducible tensor operator and transform as the irrep A_1. Now $D^{(A_1 \times E)} = E$, which contains the irrep E; therefore the quadratic term does not vanish. The two results leads to a quadratic degeneracy between the two E basis functions at $\boldsymbol{k} = \Gamma$.

4.1.3 Proof of band-sticking along $M - X$ of $p4g$

In this section we demonstrate a nonsymmorphic specific phenomena, known as band-sticking; this is when bands are degenerate along entire edges of the IBZ.

We prove that this occurs along $M - X$ for any system with $G = p4g$ symmetry and TRS. To prove this, we prove that only two-dimensional irreps exist at M, X, and the line MX. We show the construction of irrep of G_X below.

G_X/T has four coset representatives

$$E = \{\mathbb{1} \mid 0\}, \tag{4.7}$$

$$C_2 = \{C_2 \mid 0\}, \tag{4.8}$$

$$\sigma_x = \{\sigma_x \mid \frac{1}{2}t_1 + \frac{1}{2}t_2\}, \tag{4.9}$$

$$\sigma_y = \{\sigma_t \mid \frac{1}{2}t_1 + \frac{1}{2}t_2\}. \tag{4.10}$$

The $\boldsymbol{t}$'s that make $\exp(i\boldsymbol{k}\cdot\boldsymbol{t}) = 1$ form $T_X = \{\{\mathbb{1} \mid 2\boldsymbol{t}_1 + \boldsymbol{t}_2\}\}$, so the translation representative not in T_X is $\{\mathbf{1} \mid a_1\}$. Now G_X/T_X has double the elements as G_X/T:

$$E' = \{\mathbb{1} \mid 0\}, \tag{4.11}$$

$$C_2' = \{C_2 \mid 0\}, \tag{4.12}$$

$$\sigma_x' = \{\sigma_x \mid \frac{1}{2}t_1 + \frac{1}{2}t_2\}, \tag{4.13}$$

$$\sigma_y' = \{\sigma_t \mid \frac{1}{2}t_1 + \frac{1}{2}t_2\}, \tag{4.14}$$

$$\bar{E}' = \{\mathbb{1} \mid t_1\}, \tag{4.15}$$

$$\bar{C_2}' = \{C_2 \mid t_1\}, \tag{4.16}$$

$$\bar{\sigma_x}' = \{\sigma_x \mid \frac{3}{2}t_1 + \frac{1}{2}t_2\}, \tag{4.17}$$

$$\bar{\sigma_y}' = \{\sigma_t \mid \frac{3}{2}t_1 + \frac{1}{2}t_2\}, \tag{4.18}$$

a total of 8 elements. From the multiplication table, we can see that this factor group is isomorphic to C_{4v}, with $\bar{E}' \Leftrightarrow C_2$. Applying the fact that we require $\chi^{(\alpha)}_{G_k}(\{\mathbf{1} \mid t_m\}) = dim(D^{(\alpha)}_{G_k/T_k})\exp(ik\cdot t_m) = -dim(D^{(\alpha)}_{G_k/T_k})$, we find that only the E representation of C_{4v} can be a representation of G_X. This means that G_X can only have two-dimensional irreps. Similarly, it can be shown that $\boldsymbol{k} = M$ point will have a G_k/T_k isomorphic to D_{4h}, with only E_g, E_u, 2-dimensional irreps allowed.

Lastly, the coset representatives for G_{MX} are

$$E = \{\mathbb{1} \mid 0\}, \quad \sigma_x = \{\sigma_x \mid \frac{1}{2}a_1 + \frac{1}{2}a_2\}. \tag{4.19}$$

Consulting Terzibaschian T. [6], we see that irreps are

G_{MX} classes $\Rightarrow$ irreps $\Downarrow$	$\{\mathbb{1} \mid 0\}$	$\{\sigma_x \mid \frac{1}{2}a_1 + \frac{1}{2}a_2\}$
$D^{(1)}_{MX}$	1	i
$D^{(2)}_{MX}$	1	$-i$

Now $D^{(2)}_{MX} = D^{(1)*}_{MX}$; in the presence of time-reversal symmetry, this means that the two irreps are degenerate. This proves that there will be a two-fold degeneracy along $X - M$, in the presence of TRS. Using the same method, it can be shown that pgg will also have band-sticking along $M - X$.

4.2 Numerical results

Below we present the computations that verify the theoretical results in the previous section.

4.2.1 Dispersion curves of the four 2D Nonsymmorphic MLKL systems

The mass pin setup analogous to [4] for the four 2D nonsymmorphic space groups were constructed, and the dispersion curves calculated using Matlab. They are shown below in Figs. 4 - 7.

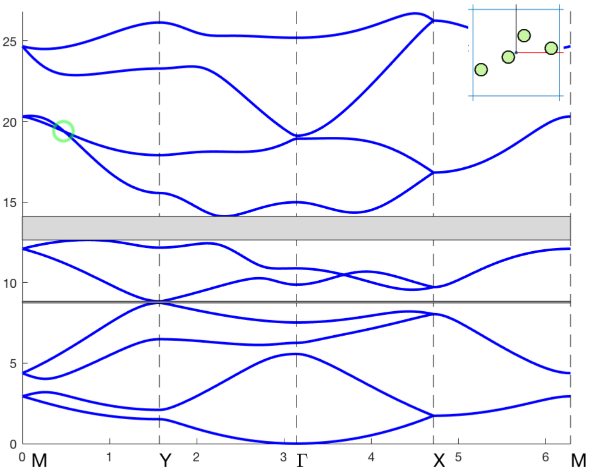

Figure 4: Dispersion curve for a pg lattice of [4]

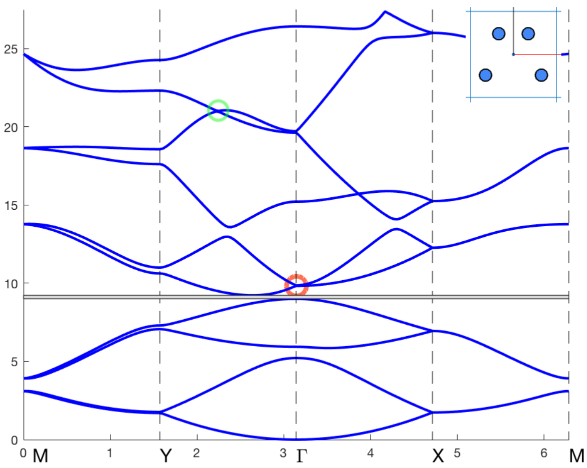

Figure 5: Dispersion curve for a pmg lattice of [4]

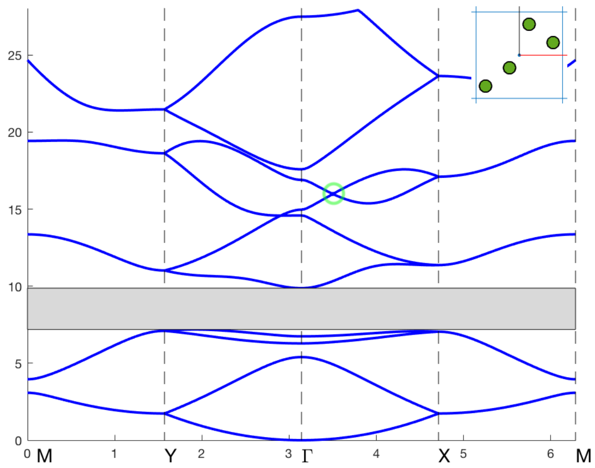

Figure 6: Dispersion curve for a pgg lattice of [4]

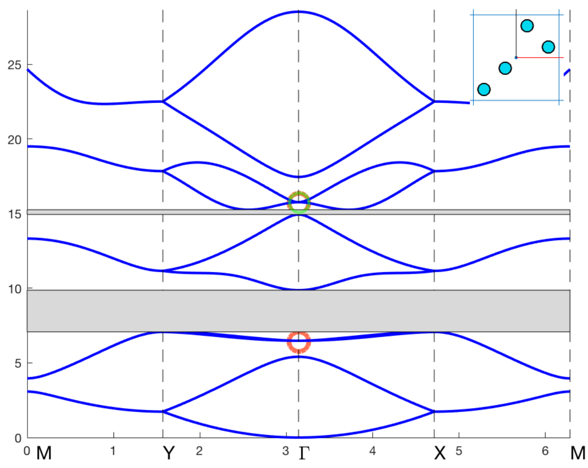

Figure 7: Dispersion curve for a p4g lattice of [4]

The $p4g$'s symmetry is broken into pgg by rotating the pairs of masses off of the $\pi/4$. One property that is common with all four dispersion curves is that there is band sticking along $X - M$. This can be attributed to the fact that there are only two-dimensional irreps along this line, as it was proven for $p4g$. This is due to the spurious irreps from fractional translations, and is unique to nonsymmorphic groups.

In the earlier section, we proved that there would be a doubly quadratic degeneracy at Γ for $p4g$ which may turn into a band crossing when transformed into pgg. Indeed, this is seen in the dispersion curves shown in Figs. 4-7.

4.3 Dispersion contours and lattice simulation for p4g and pgg

In this subsection we adiabatically transform a pgg structure to a $p4g$ structure. The dispersionless linear degeneracy of the pgg structure occurs at the same frequency as the dispersive quadratic degeneracy of the $p4g$ structure. Hence it makes sense to contrast the scattering behaviour between the two structures for a frequency in the vicinity of the degeneracies.

To demonstrate that the properties are symmetry induced, an alternate mass setup with the same symmetries were constructed for pgg and $p4g$. They are shown in Fig. 8, 9.

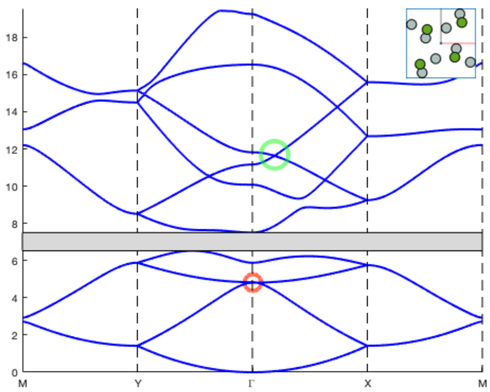

Figure 8: Dispersion Curve for an alternate lattice of pgg symmetry.

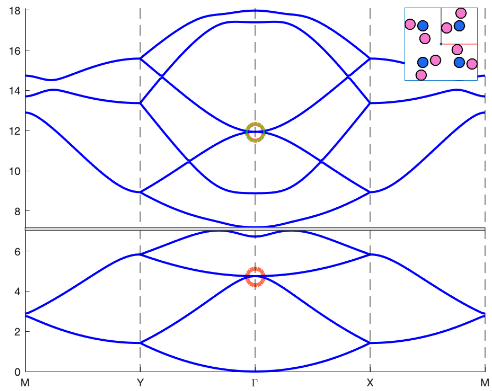

Figure 9: Dispersion Curve for an alternate lattice of p4g symmetry.

For this setup, the symmetry is broken by a shearing transformation of the four masses of C_{4v} symmetry. We see that again, there is a quadratic degeneracy that turns into a linear one between the 7 $^{\text{th}}$ and 8$^{\text{th}}$ band as $p4g \rightarrow pgg$.

To further study the dispersion relation, we plot the dispersion contours in the neighbourhood of the degeneracies, as shown in Figs. 10 - 13. We see that for pgg, we get an elliptical contour in the neighbourhood of the Dirac point, which indicates the linear behaviour, while for $p4g$ we get an anistropic dispersion of C_{4v} symmetry.

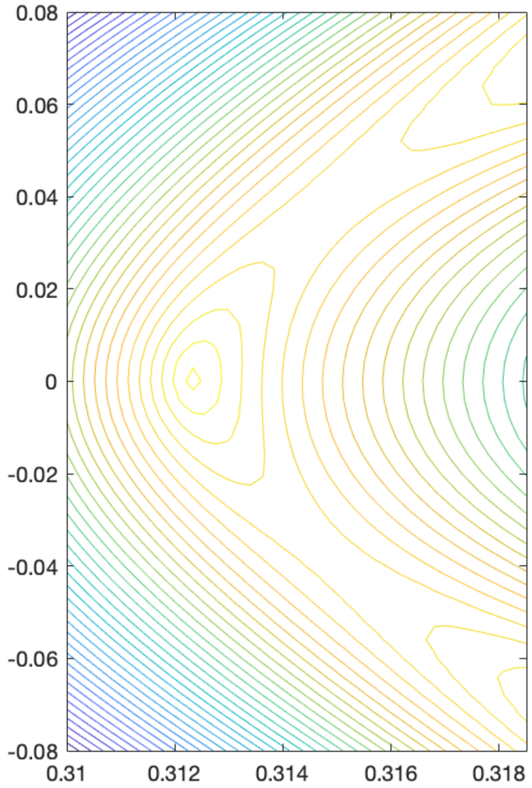

Figure 10: Dispersion contour at the neighbourhood of the Dirac point for the 7th band of pgg.

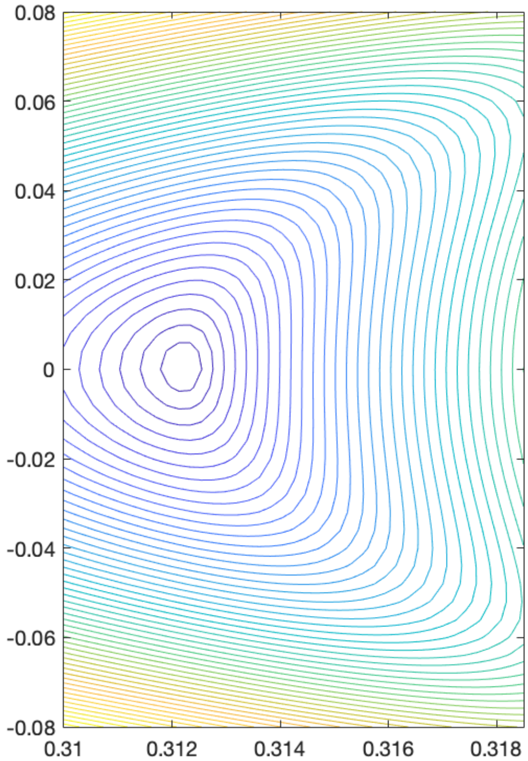

Figure 11: Dispersion contour at the neighbourhood of the Dirac point for the 8th band of pgg.

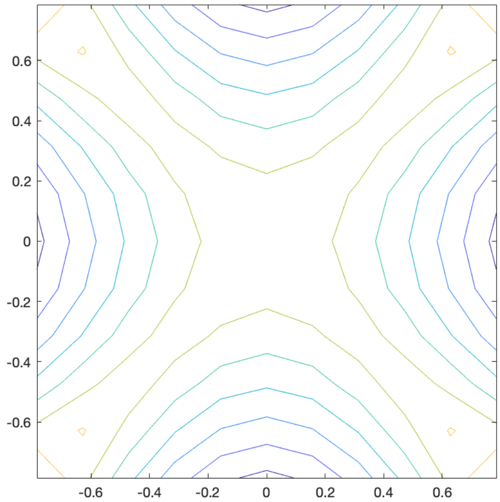

Figure 12: Dispersion contour at the neighbourhood of the quadratic degeneracy for the 7th band of p4g.

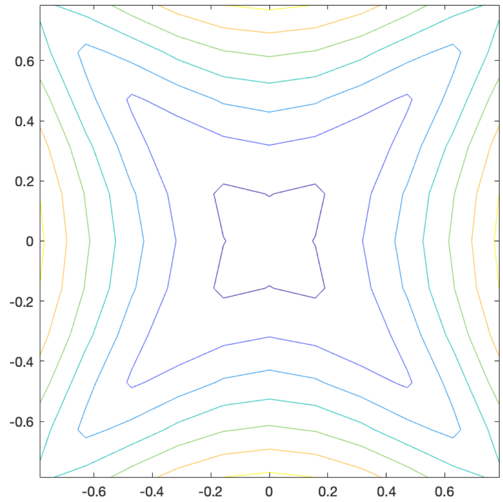

Figure 13: Dispersion contour at the neighbourhood of the quadratic degeneracy for the 8th band of p4g.

Group velocity, which is the speed in which the envelope of the wave travels at, is given by

$$\boldsymbol{v}_g = \frac{\partial \omega}{\partial \boldsymbol{k}} = \nabla_{\boldsymbol{k}} \omega(\boldsymbol{k}). \tag{4.20}$$

Note that because in the neighbourhood of a linear degeneracy, the gradient is constant with ω, we expect a dispersionless propagation, while in the neighbourhood of a quadratic degeneracy, we expect waves to disperse.

The Matlab code `Foldy` was used to find the scattering solution for structured plates due to a point source placed in the central position of a $p4g$ and pgg structure. The results are shown in Fig. 14, 15. The highly directed oscillation in the vicinity of the $p4g$ band-gap is shown in the right-hand figure.

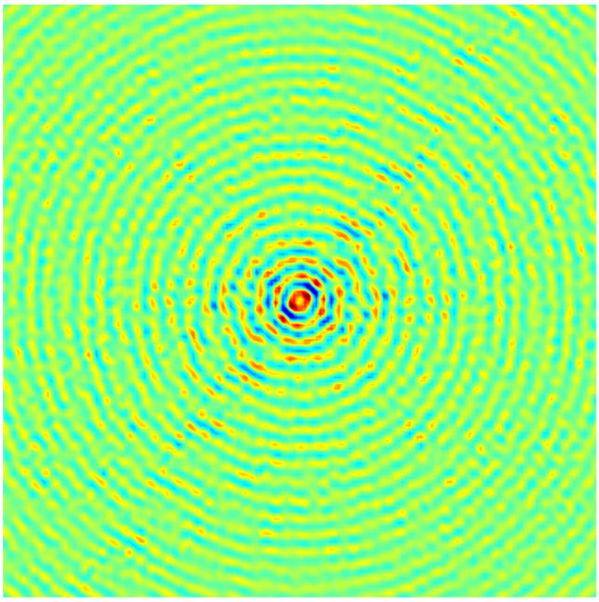

Figure 14: Dispersion-light propagation of waves from a point source at frequency near the band gap for a platonic crystal of pgg symmetry.

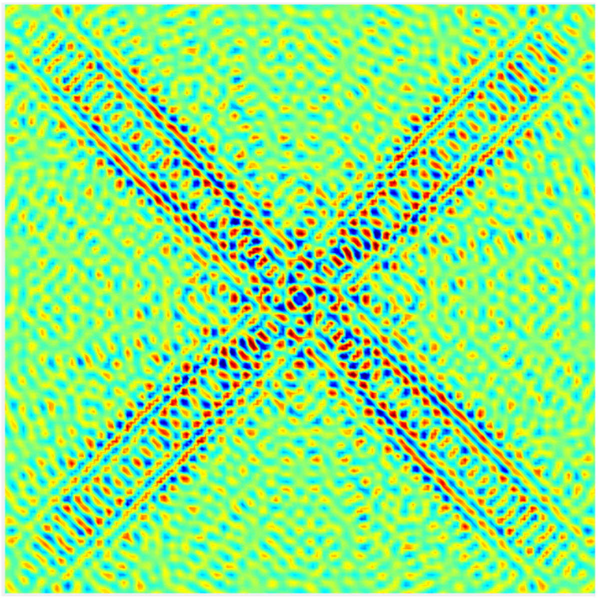

Figure 15: Highly directed propagation of waves from a point source at frequency near the band gap for a platonic crystal of p4g symmetry.

Using the knowledge of Eq. (4.20), because $p4g$ has a point group symmetry of C_{4v}, we expect propagation to be a dispersive with a C_{4v} symmetry in the neighbourhood of ω of the degeneracy. For pgg symmetry, we expect a dispersionless propagation in the neighbourhood of ω of the degeneracy. We can see that as predicted, waves propagating in a $p4g$ medium displays an X shape that has C_{4v} symmetry, which indicates dispersive propagation with C_{4v} symmetry. On the other hand, waves in pgg medium displays a circular dispersion, due to the fact that the neighbourhood of the Dirac point is dispersionless. The slight residual anistropy is due to the other modes of the same ω being excited.

These directed oscillations are reminiscent of caustics, which can occur when light rays reflect or refract off a curved surface.

5 Designing Topological Waveguides and Energy-Splitters

5.1 Accidental Degeneracies

Up until now we have solely dealt with symmetry induced degeneracies. However other degeneracies, not entirely symmetry induced, can occur; these are more commonly known as accidental degeneracies.

Varying the material parameters of a system can often bring two bands together. However, upon getting closer, sometimes the bands 'repel' from each other while other times they cross each other. This can be explained using representation theory.

Consider a two-band system at a given k and material parameter m_0, with eigenfunctions $|A\rangle, |B\rangle$ that adhere to the symmetry constraints, such that

$$\hat{H}_0|i\rangle = \omega_i|i\rangle, \tag{5.1}$$

for $i = A, B$. Then, let us assume that changing the material parameters by δm alter the Hamiltonian by $\delta\hat{H}$. Then, we can calculate the shift in energies by diagonalizing the following Hamiltonian matrix

$$\boldsymbol{H} = \begin{bmatrix} \omega_A + \delta H_{AA} & \delta H_{AB} \\ \delta H^*_{AB} & \omega_B + \delta H_{BB} \end{bmatrix}, \tag{5.2}$$

where

$$\delta H_{ij} = \langle i^{(\alpha)} \mid \delta\hat{H} \mid j^{(\beta)} \rangle. \tag{5.3}$$

Then, the solution to the eigenvalue problem is

$$\omega_\pm = \frac{1}{2}(\omega_A + \omega_B + \delta H_{AA} + \delta H_{BB}) \pm \sqrt{([\omega_A - \omega_B] + [\delta H_{AA} - \delta H_{BB}])^2 + 4|\delta H_{AB}|^2}. \tag{5.4}$$

We can see that we can bring the bands together by $[\delta H_{AA} - \delta H_{BB}] \to -[\omega_A - \omega_B]$. However, we can also see that the eigenvalues cannot become degenerate unless $H_{AB} = 0$.

Now even though the actual basis functions are complicated and change with the specific $\boldsymbol{k}$ values, their symmetries are determined by the irrep and G_k. Since $\hat{H}$ will transform as the fully symmetric group, this means that in order for H_{AB} to vanish, $|i\rangle$ and $|j\rangle$ must be of different irreps α, β such that $D^{(\alpha\times\beta)}$ does not contain the fully symmetric group.

So, if two bands are of different irreps, they can be accidentally degenerate, and therefore a Dirac point can occur. The symmetry that allows the two bands to be of different irrep is said to 'protect' the Dirac point. This theory can also explain 'gapping' of Dirac points. If the symmetry is reduced such that the two bands previously of different irreps are of the same irrep, then as shown, the two bands will repel each other, leading to a band gap (provided there are no other bands near by).

5.2 Compatibility relations

Consider a point $\boldsymbol{k}_1$ in the dispersion curve and a neighbouring $\boldsymbol{k}_2$ point. Compatibility relations can tell us which bands of $\boldsymbol{k}_1$ are connected to bands of $\boldsymbol{k}_2$. Also consider a small deformation in the crystal which brings the space group from G to a subgroup H. Compatibility relations can also tell us which irreps transform into another irrep.

In general, an irrep of a group G is 'compatible' with a direct sum of irreps of a smaller subgroup H if the elements of the irrep of G can be written as a direct sum of irreps of H [8]. This can be useful in determining the behavior of the basis functions and the dispersion curves, as shown in the example below.

5.3 Example: accidental degeneracies for a nonsymmorphic crystal: along $\Gamma - X$ or $\Gamma - Y$ from $p4g \to pgg$

Although we cannot prove group theoretically that a Dirac point *will* occur along $\Gamma - X$ or $\Gamma - Y$ near where the quadratic degeneracy at Γ of $p4g$, we can show that

- The two-fold degeneracy will be lifted as $p4g \to pgg$
- The bands will be allowed to cross along $\Gamma - X$ or $\Gamma - Y$,

using compatibility relations and level-crossing theory.

The compatibility relations of the E irrep of $p4g_\Gamma/T_\Gamma$ to the neighbouring $\boldsymbol{k}$'s, ΓX and ΓY and to pgg's groups are illustrated in the table below.

$G \Rightarrow$	$p4g$		pgg	
$\boldsymbol{k} \Downarrow$	$G_{\boldsymbol{k}} \cong$	$D_{G_{\boldsymbol{k}}}$	$G_{\boldsymbol{k}} \cong$	$D_{G_{\boldsymbol{k}}}$
Γ	C_{4v}	E	C_{2v}	$B_1 + B_2$
ΓX	C_2	$A + B$	C_2	$A + B$
ΓY	C_2	$A + B$	C_2	$A + B$

From the compatibility relations, we can see that the E irrep of $p4g_\Gamma$ is compatible with a direct sum of irreps of different parity of pgg for all relevant $\boldsymbol{k}$'s, which means that firstly, the two-fold degeneracy is lifted, and secondly, by level-crossing theory of Sec. **??**, the two new bands are allowed to cross. This was already shown in Figs. 6, 7; the quadratic degeneracy adiabatically changes into a linear one.

5.4 Example: off-HSP Dirac points

Using the theory of accidental degeneracies, we show how to create a Dirac point at an off-HSP, induced by accidental degeneracies. An argument similar to this one was used C.T. Chan, et al. to explain the presence of a Dirac point for a photonic crystal system [3].

Consider a photonic crystal which has rods of electric permittivity ϵ. It turns out for a photonic system, that increasing the permittivity of rods has the effect of bringing bands together.

Now consider a square lattice of p4m symmetry. This is a symmorphic group, so $G = p4m = C_{4v} \rtimes T$. Now the point group of $\boldsymbol{k}$ (which the group of $\boldsymbol{k}$ trivially follows since G is a symmorphic group) near $\boldsymbol{k} = X$ is as follows:

$$P_X = C_{2v};\ P_{\Gamma X} = \{\mathbb{1}, \sigma_y\};\ P_{XM} = \{\mathbb{1}, \sigma_x\},$$

where the character tables are shown below:

$P_X = C_{2v}$ classes $\Rightarrow$ irreps $\Downarrow$	E	C_2	σ_y	σ_x
A_1	$+1$	$+1$	$+1$	$+1$
A_2	$+1$	$+1$	-1	-1
B_1	$+1$	-1	$+1$	-1
B_2	$+1$	-1	-1	$+1$

$P_{\Gamma X}$ or P_{XM} classes $\Rightarrow$ irreps $\Downarrow$	E	σ_y or σ_x
A	1	1
B	1	-1

Turns out, at $\boldsymbol{k} = X$, the bands $(A_1, B_1)^{(X)}$ are on top of each other and can be brought together by tweaking ϵ. Compatibility relations show us that $(A_1, B_1)^{(X)} \leftrightarrow (A, A)^{(\Gamma X)}$ and

$(A_1, B_1)^{(X)} \leftrightarrow (A, B)^{(XM)}$. From this result and level crossing theory, we know that the (A_1, B_1) bands will cross along XM, as they are of different irreps along XM, while they will repel along ΓX, since they are of the same irrep (A) along ΓX. This 'guarantees' a Dirac point along XM as the two bands are brought together. Now, if the mirror symmetry is broken, then the two bands will now be of the same irrep (the identity irrep); this will open up the Dirac point.

5.5 Topological waveguides and energy-splitters

It was demonstrated by C.T. Chan et al. that the Dirac points that arise from accidental degeneracies have non-trivial topological indices. Therefore, when gapped by reducing the symmetries, by the bulk-edge correspondnce, yield topologically protected edge states, which are propagating states between edges of two lattices [3]. These edge states are more robust, less prone to backscattering, than topologically trivial states. In the aformentioned paper the gapping was induced by a breaking of TRS; in this section, we demonstrate via simulations, that a reduction in the reflectional symmetries m_x and m_y, by a slight rotation of the components of the unit cell, can also yield these edge states. This passive mechanism is beneficial as no external TRS breaking field is required. Examples of a straight interfacial waveguide, a bend and a topological energy-splitter are shown below. A source was placed at the leftmost edge for all three examples.

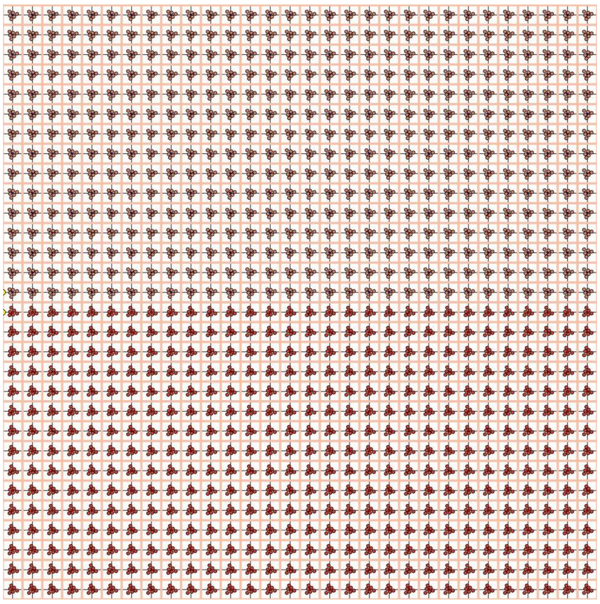

Figure 16: Mass setup for topological waveguide. Two lattices reflections of one another are sandwiched.

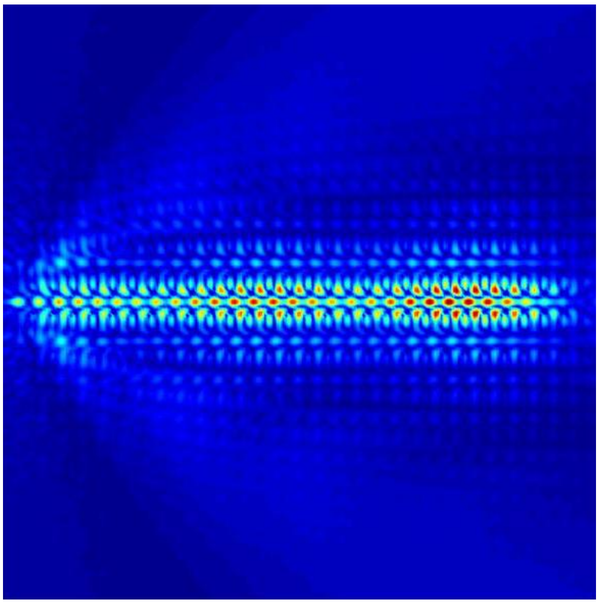

Figure 17: The aforementioned lattice allows for a propagating edge state which is directional and does not bleed into surroundings.

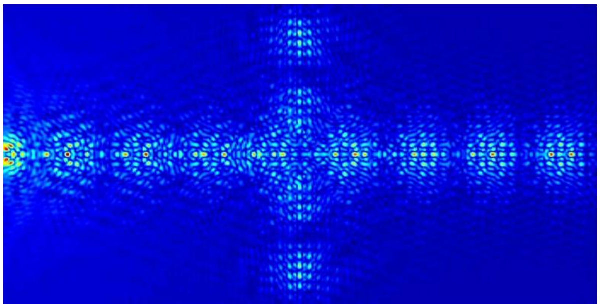

Figure 18: By altering the layout of the different lattice types, propagation of edgemodes can be split.

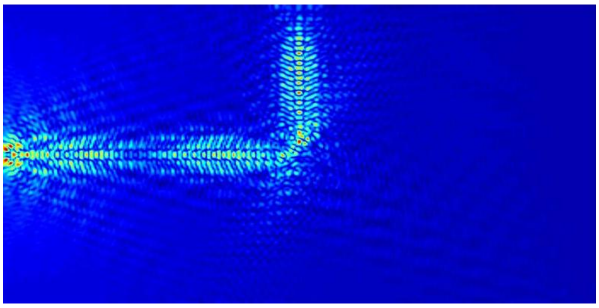

Figure 19: Propagation of edgemodes can also be bent around corners.

6 Conclusion

Using group and $\boldsymbol{k}\cdot\boldsymbol{p}$ theory, we have shown a first-principles approach to analysing wave phenomena in nonsymmorphic structured elastic plates. Degeneracies and their associated exotic phenomena, such as dynamic anisotropy, are predicted via purely analytic means. Both symmetric induced degeneracies, for nonsymmorphic crystals and accidental degeneracies were theoretically examined; for the latter we showed how they result in passive topologically protected edge states. The energy was shown to propagate cleanly around a sharp bend aswell as split at junction which lay between topologically distinct media. To the authors knowledge this is the first demonstration of topological energy-splitting in more than two directions. The uses of this splitter are far-reaching; the underlying mechanism is ideal for applications such as beam-splitters and switches.

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