SYMMETRY AND DIRAC POINTS IN GRAPHENE SPECTRUM

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ABSTRACT. Existence and stability of Dirac points in the dispersion relation of operators periodic with respect to the hexagonal lattice is investigated for different sets of additional symmetries. The following symmetries are considered: rotation by $2\pi/3$ and inversion, rotation by $2\pi/3$ and horizontal reflection, inversion or reflection with weakly broken rotation symmetry, and the case where no Dirac points arise: rotation by $2\pi/3$ and vertical reflection.

All proofs are based on symmetry considerations and are elementary in nature. In particular, existence of degeneracies in the spectrum is proved by a transplantation argument (which is deduced from the (co)representation of the relevant symmetry group). The conical shape of the dispersion relation is obtained from its invariance under rotation by $2\pi/3$. Persistence of conical points when the rotation symmetry is weakly broken is proved using a geometric phase in one case and parity of the eigenfunctions in the other.

1. INTRODUCTION

Many interesting physical properties of graphene are consequences of existence of special points in its dispersion relation [21, 7, 17, 10]. These points, sometimes referred to as Dirac points, are conical singularities, where two sheets of the dispersion relation touch at a point and are linear in any outward direction.

Most mathematical analysis of the dispersion relation of graphene is performed in physics literature in the tight-binding approximation. This is equivalent to modeling the material as a discrete graph with vertices at the carbon molecules’ locations and with edges indicating chemical bonds. A richer mathematical model for graphene was considered by Kuchment and Post in [19], who studied quantum graphs with potential on edges, arranged to form a honeycomb lattice.

The $\mathbb{R}^2$ Schrödinger operator with potential that has honeycomb symmetry was considered by Grushin [14]. A condition for a multiple eigenvalue to be a conical point was established and checked in the perturbative regime of a weak potential. The multiplicity of the eigenvalue was proved from the symmetry point of view, an approach that we fully develop here.

The case of potential of arbitrary strength was studied by Fefferman and Weinstein [9]. Their results can be schematically broken into three parts: (a) establish that the dispersion relation has a double degeneracy at the known values of quasi-momenta; (b) establish that the dispersion relation is conical in the vicinity of the degeneracy; (c) prove that the conical singularities survive under weak perturbation destroying some of the symmetries of the potential (namely, the rotational symmetry).

These results are contained in Theorem 5.1(1), 4.1 and 9.1 of ref. [9], correspondingly. The proof of the existence of degeneracy (part (a) in the above classification) is especially technical and lengthy, using, in particular, the boundedness from below of the considered operator.

The purpose of this article is to make explicit the role of symmetry in the results (a)–(c) and to give proofs that are at the same time simpler and more general. Our methods apply to many different settings: graphs (discrete or quantum), Schrödinger and Dirac operators on $\mathbb{R}^2$. We use Schrödinger operator as our primary focus, and give numerical examples using discrete graphs. We also consider the effect of different symmetries, substituting inversion symmetry, usually assumed in the literature, with horizontal reflection symmetry (the results are analogous or stronger, as explained below).

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We will now briefly review our results and the methods employed. The operator is assumed to be shift-invariant with respect to the hexagonal lattice. We also consider the following symmetries (see Fig. 1 for an illustration): rotation by $2\pi/3$ (henceforth, “rotation”), inversion (reflection with respect to the point $(0,0)$), horizontal reflection and, to a lesser extent, vertical reflection. We remark that horizontal and vertical reflections are substantially different because the hexagonal lattice is not invariant with respect to rotation by $\pi/2$. We study the question of existence of Dirac points when the operator has various subsets of the above symmetries.

We show that existence of the degeneracy is a direct consequence of symmetries of the operator. The natural tool for studying this is, of course, representation theory. It is well known that existence of a two- (or higher) dimensional representation suggests that some eigenvalues will be degenerate. However, rotation combined with inversion — the most usual choice of symmetries [14, 9] — is an abelian group, whose representations are all one-dimensional. The resolution of this question lies in the fact that the relevant symmetry is inversion combined with complex conjugation and one should look at representations combining unitary and antiunitary operators, the so-called corepresentations introduced and fully classified by Wigner [30, Chap. 26].

In this paper, we keep the representation theory behind the scenes, in Appendix B. To prove the existence of the degeneracy in the spectrum (Theorem 2.1) we use instead the “transplantation proof”. There are three reasons for this. First, the transplantation proof is extremely simple and short, taking half a page and a figure. It requires no knowledge of representation theory and can be read immediately after the dispersion relation is defined in section 1.3. Second, the same proof works for the two cases where we establish a positive result: rotation coupled with inversion and rotation coupled with horizontal reflection. Third, to show that a two-dimensional representation leads to doubly-degenerate eigenvalue one has to show that the corresponding isotypic component of the Hilbert space is non-empty, which requires work. The transplantation proof hides that work under the hood too.

The conical nature of the dispersion relation is known to be a generic situation (see, for example, [11, Appendix 10]); to prove it in a particular case one uses perturbation theory, as done in [14] and, implicitly, in [9]. Again, we seek to make the effect of symmetry most explicit here. This is done on two levels. First, in Corollary 1.2 and Lemma 1.4 we show that the dispersion relation also has rotational symmetry and thus, by Hilbert-Weyl theory of invariant functions, is restricted to be a circular cone (which could be degenerate) plus higher order terms. Then, in Theorem 3.2 we show that the symmetries also enforce a certain relation on the first order terms of the perturbative expansion of the operator, which restricts the possible form of the terms. In spirit, this conclusion parallels the Hilbert-Weyl theory, but is somewhat more powerful: it further allows us to conclude that at quasimomentum $\vec{0}$, where we discover persistent degeneracies with only the rotational symmetry, the dispersion relation is locally flat.

Part (c) of the above classification, the survival of the Dirac points when a weak perturbation breaks the rotational symmetry can be established by perturbation theory, as done in [9]. However, such resilience of singularities indicates that there are topological obstacles to their disappearance. The method familiar to physicists is to use the Berry phase [4, 24], which works when the operator has inversion symmetry (Theorem 5.4). Interestingly, when instead of inversion symmetry we have horizontal reflection symmetry, Berry phase is not restricted to the integer multiples of $\pi$ and the topological obstacle has a different nature. The survival of the Dirac cone is shown to be a consequence of the structure of representation of the reflection symmetry (Theorem 5.4), which combines eigenfunctions of different parities at the degeneracy point. As a consequence of our proof we conclude that the perturbed cone, although shifted from the corner of the Brillouin zone, remains on a certain explicitly defined line. In particular, this restricts the location of points in the Brillouin zone where Dirac cones can be destroyed by merging with their symmetric counterparts. Naturally, this effect is also present when there is horizontal reflection symmetry in addition to the
inversion symmetry. We remark that experimentally created potentials usually possess the reflection symmetry, [26].

To summarize, in addition to providing simpler and shorter symmetry-based proofs to existing results, we discover some previously unknown consequences. In particular, we consider the case of rotational symmetry coupled with horizontal reflection symmetry; in this case when the rotational symmetry is weakly destroyed, the conical points travel on a special line. We observe degeneracies at quasimomentum $\vec{0}$ in presence of rotational symmetry only; the dispersion relation at this point is shown to be locally flat. Finally, we explain why coupling rotation and vertical reflection does not, in general, lead to the appearance of Dirac points. The tools developed in this article would be easily extensible to other lattice structures [8] and graphene superlattices [31, 23].

1.1. Symmetries. The periodicity lattice of the operators we will consider is the 2-dimensional hexagonal lattice $\Gamma$ with the basis vectors

$$a_1 = \left( \frac{\sqrt{3}/2}{1/2} \right), \quad a_2 = \left( \frac{\sqrt{3}/2}{-1/2} \right),$$

see Fig. (a). The operator considered will always be assumed to be invariant with respect to the shifts by this lattice.

In addition to the shifts, the lattice $\Gamma$ has several other symmetries. We now describe some of them as operators acting on functions on $\mathbb{R}^2$ (or a graph embedded in $\mathbb{R}^2$).

- Rotation $R$ of a function by $2\pi/3$ in the positive (counter-clockwise) direction. Explicitly, $R : \psi(x_1, x_2) \mapsto \psi\left( -\frac{1}{2} x_1 + \frac{\sqrt{3}}{2} x_2, -\frac{\sqrt{3}}{2} x_1 - \frac{1}{2} x_2 \right)$.

- Inversion $V$: $V : \psi(x_1, x_2) \mapsto \psi(-x_1, -x_2)$.

- Horizontal reflection $F$: $F : \psi(x_1, x_2) \mapsto \psi(-x_1, x_2)$.
Note that $R$ and $V$ together form the abelian group of rotations by multiples of $\pi/3$; $VF$ is the vertical reflection. In what follows, we will assume our operator has symmetries generated by a subset of the $R$, $V$ and $F$.

As the base operator (i.e. before we apply Floquet-Bloch analysis) we will always take an operator with real coefficients, thus it will be symmetric with respect to complex conjugation. As it turns out, an important role is played by the product of inversion and complex conjugation, $\overline{V}$:

- **Symmetry $\overline{V}$:**
  \[
  \overline{V} : \psi(x_1, x_2) \mapsto \psi(-x_1, -x_2).
  \]

Note that $\overline{V}$ is not a $\mathbb{C}$-linear operator; it is, however, a linear operator over reals.

Finally, we will also consider the vertical reflection symmetry, given by the operator $F_V$:

- **Vertical reflection $F_V$:**
  \[
  F_V : \psi(x_1, x_2) \mapsto \psi(x_1, -x_2).
  \]

Its effect is not the same as that of the horizontal reflection $F$ because the two symmetries are aligned differently with respect to the lattice $\Gamma$. In fact, in contrast to $F$, the presence of $F_V$ (in addition to symmetry $R$) does not generally lead to the appearance of conical points in the dispersion relation. This negative result is also important to understand; we explain it in section B.2.3.

In Fig. 1(b-d) we show the fundamental domain of the lattice with defects that have symmetry $R$ in addition to $V$, $F$ or $F_V$, correspondingly.

### 1.2. Operators

As our primary motivational example we use the two-dimensional Schrödinger operator $H = -\Delta + Q(x)$ with the real-valued electric potential $Q(x)$ assumed to be smooth and periodic with respect to the lattice $\Gamma$. For general properties of the dispersion relation of such operators we refer the reader to [2, 18].

To generate simple numerical examples we use discrete Schrödinger operators with potentials crafted to break or retain some of symmetries listed above. More precisely, denote by $G = (V, E)$ an infinite graph embedded in $\mathbb{R}^2$, with vertex set $V$ and edge set $E$. The embedding is realized by the mapping $\text{loc} : V \to \mathbb{R}^2$ which gives the location in $\mathbb{R}^2$ of the given vertex. A transformation $T : \mathbb{R}^2 \to \mathbb{R}^2$ preserves the graph structure if $u_1, u_2 \in V$ implies existence of $u'_1, u'_2 \in V$ such that $T(\text{loc}(u_j)) = \text{loc}(u'_j)$ and $u'_1, u'_2$ are connected by an edge if and only if $u_1, u_2$ are connected.

The graph is $\Lambda$-periodic if the graph structure is preserved by the shifts defining the lattice. A graph with space symmetry $S$ is defined analogously.

The Schrödinger operator is defined on the functions from $\ell^2(\mathbb{C}^V)$ by

\[
(2) \quad (Hf)_v = \sum_{(v,u) \in E} m_{v,u}(f_u - f_v) + q_v f_v,
\]

where the sum is over all vertices $u$ adjacent to $v$, $m_{v,u} > 0$ are weights associated to edges (often, they are taken inversely proportional to edge length) and $q : V \to \mathbb{R}$ is the discrete electric potential. In our examples, the graph structure will be compatible with all symmetries of the lattice $\Lambda$, while $m$ and $q$ will be breaking some of the point symmetries (however, they will always be periodic). The simplest $\Gamma$-periodic graph is shown in Fig. 3(a). This is the graph arising as the tight-binding approximation of graphene.

Note that the discrete Schrödinger operator of graphs with more than two atoms per unit cell is not a mere mathematical curiosity since it arises in studying the twisted graphene and graphene in a periodic potential (superlattice), see [20, 31, 27] and references therein.

### 1.3. Floquet-Bloch reduction

Floquet theory can be thought of as a version of Fourier expansion, mapping the spectral problem on a non-compact manifold into a continuous sum of spectral problems on a compact manifold. The compact spectral problems are parametrized by the representations of the abelian group of periods (shifts).
Figure 2. Floquet-Bloch reduction on the plane with hexagonal lattice generated by $\vec{a}_1$ and $\vec{a}_2$.

Denote by $\mathcal{H}(\vec{k})$, $\vec{k} = (k_1, k_2) \in [0, 2\pi)^2$ the space of Bloch functions, i.e. locally $L^2$ functions satisfying
\begin{equation}
\psi(\vec{x} + n_1 \vec{a}_1 + n_2 \vec{a}_2) = e^{i(n_1 k_1 + n_2 k_2)} \psi(x), \quad n_1, n_2 \in \mathbb{Z}.
\end{equation}
For $\psi \in \mathcal{H}(\vec{k})$ which also belong to the domain of $H$ it can be immediately seen that
\begin{equation}
(H\psi)(x + n_1 \vec{a}_1 + n_2 \vec{a}_2) = e^{i(n_1 k_1 + n_2 k_2)} H\psi(x),
\end{equation}
i.e. the space $\mathcal{H}(\vec{k})$ is invariant under $H$. By $H(\vec{k})$ we will denote the restriction of the operator $H$ to the space $\mathcal{H}(\vec{k})$. Its domain is $\mathcal{H}^2(\vec{k})$, the dense subspace of $\mathcal{H}(\vec{k})$ consisting of functions that locally belong to $L^2$ together with their derivatives up to the second order.

Choosing a fundamental domain\footnote{A domain having the property that each trajectory $\{\vec{x} + n_1 \vec{a}_1 + n_2 \vec{a}_2 : n_1, n_2 \in \mathbb{Z}\}$ has exactly one representative in it} of the action of the group of periods, we can reduce the problem to the fundamental domain with quasi-periodic boundary conditions.

The result of the Floquet-Bloch reduction is shown in Fig. 2. In Fig. 2(a), the lattice generating vectors $\vec{a}_1$ and $\vec{a}_2$ are shown together with a convenient choice of the fundamental region (shaded) and its three translations, by $\vec{a}_1$, $\vec{a}_2$ and $\vec{a}_1 - \vec{a}_2$. The values of a Bloch function in four regions, according to equation (3), are indicated in Fig. 2(b), using the notation
\begin{equation}
\omega_j = e^{ik_j}.
\end{equation}
The continuity of the function and its derivative across the boundaries of copies of the fundamental region impose boundary conditions shown schematically in Fig. 2(c). They should be understood as follows: taking the bottom and top boundaries as an example, and parametrizing them left to right, the conditions read
\begin{align*}
\psi\big|_{\text{top}} &= e^{i\omega_1} \psi\big|_{\text{bottom}}, \\
-\partial_{\vec{n}} \psi\big|_{\text{top}} &= e^{i\omega_1} \partial_{\vec{n}} \psi\big|_{\text{bottom}},
\end{align*}
where the normal derivative is taken in the outward direction (this causes the minus sign to appear). We stress again that in Fig. 2(c) we use letters $f$, $g$ and $h$ as placeholder labels, connecting the values of the function and its derivative on similarly labelled sides.
Figure 3. The dual basis (a) to the vectors \( \vec{a}_1 \) and \( \vec{a}_2 \) and two choices of the Brillouin zone in terms of (b) coordinates \( k_1, k_2 \) (drawn as if they are Cartesian) and (c) coordinates \( \kappa_1, \kappa_2 \) (which are Cartesian); part (c) also shows the correct position for the axes \( k_1 \) and \( k_2 \). The axis of symmetry of the operator \( \hat{F} \) is shown in dashed line (equation \( k_1 = -k_2 \)). Fixed points of the operator \( \hat{R} \) are shown by circles (different fill styles correspond to different points of symmetry).

To represent the exponent of the Bloch phase \( n_1 k_1 + n_2 k_2 \) as a scalar product, we introduce the vectors

\[
\vec{b}_1 = \left( \frac{1}{\sqrt{3}}, 1 \right)^T, \quad \vec{b}_2 = \left( \frac{1}{\sqrt{3}}, -1 \right)^T,
\]

see Fig. 3(a). Then

\[
\vec{b}_1^T \cdot \vec{a}_j = \delta_{i,j}.
\]

The vectors \( \vec{b}_1, \vec{b}_2 \) define a lattice which is known as the dual lattice. For a hexagonal lattice, the dual lattice is also hexagonal.

Due to (6), one can write \( n_1 k_1 + n_2 k_2 \) as the dot product of the vector of the shift \( n_1 \vec{a}_1 + n_2 \vec{a}_2 \) the vector which has \( k_j, j = 1, 2 \), as components:

\[
n_1 k_1 + n_2 k_2 = (k_1 \vec{b}_1 + k_2 \vec{b}_2) \cdot (n_1 \vec{a}_1 + n_2 \vec{a}_2).
\]

Let us comment on using coordinates \( k_1, k_2 \) which are the coordinates with respect to the basis \( \vec{b}_1, \vec{b}_2 \) versus the corresponding Cartesian coordinates \( \kappa_1, \kappa_2 \) given by

\[
\vec{\kappa} = \begin{pmatrix} 1/\sqrt{3} & 1/\sqrt{3} \\ 1 & -1 \end{pmatrix} \vec{k} =: B \vec{k}.
\]

In Fig. 3(b) we show two choices of the Brillouin zone drawn in terms of coordinates \( k_1, k_2 \) and coordinates \( \kappa_1, \kappa_2 \). The first picture one gets if one uses \( k_1 \) and \( k_2 \) as parameters for the dispersion relation (which is natural) ranging from \(-\pi\) to \( \pi \) (black square) and then plots the result using \( k_1 \) and \( k_2 \) as Cartesian coordinates. The resulting plot of the dispersion relation will be skewed similarly to the blue hexagon in Fig. 3(b) (cf. Figures 5 and 6 of [19]). A more correct way of plotting is over a domain in Fig. 3(c), as it will highlight the symmetries of the result (see Figs. 4 and 5 and the explanations in the following section).

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2 By “Brillouin zone” we understand any choice of the fundamental domain of the dual lattice. What is known as the “first Brillouin zone” is the hexagonal domain in blue in Fig. 3(c).
1.4. Symmetries of the reduced operator. As mentioned before, the operator $H(\vec{k})$ is the restriction of the operator $H$ to the space $\mathcal{H}(\vec{k})$. Equivalently, it can be considered as the operator on the compact domain of Fig. 2(c) with the specified boundary conditions. The operator $H(\vec{k})$ has discrete spectrum; its spectrum as a function of $\vec{k}$ is called the dispersion relation.

An example of the dispersion relation is shown in Fig. 4. Here, the first three eigenvalues of a particular choice of the operator $H$ are shown as functions of $\vec{k}$ (or, rather, of coordinates $\tilde{\vec{x}}$, see Eq. (7)). The most prominent feature is the presence of the conical degeneracies, whose existence and persistence under perturbation we study in this article.

It is immediate from the definition of $H(\vec{k})$ that the dispersion relation is invariant with respect to shifts by $2\pi$,

$$\vec{k} \mapsto \vec{k} + (2\pi, 0) \quad \text{and} \quad \vec{k} \mapsto \vec{k} + (0, 2\pi).$$

In other words, the dispersion relation is periodic with respect to the dual lattice. We will now study other symmetries of the dispersion relation.

For given values of $k_1, k_2$ (or, equivalently, $\omega_1, \omega_2$), the operator $H(\vec{k})$ may no longer have all the symmetries of the original operator $H$: while the differential expression defining the operator is still invariant, the domain of definition has been restricted and may not be invariant anymore.

We start with the rotation operator $R$. We first need to understand the effect of $R$ on the space $\mathcal{H}(\vec{k})$. This can be understood by rotating the picture in Fig. 2(b) by $2\pi/3$ and finding the “new $\omega_1, \omega_2$”:

$$\omega'_1 = \overline{\omega_1}, \quad \omega'_2 = \overline{\omega_2}, \quad \overline{\omega'_2} \omega'_1 = \omega_2.$$

The last equation clearly follows from the first two. For the exponents $k'_1, k'_2$, defined as in (4), we have

$$\begin{pmatrix} k'_1 \\ k'_2 \end{pmatrix} = \begin{pmatrix} -1 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} k_1 \\ k_2 \end{pmatrix} =: \hat{R} \begin{pmatrix} k_1 \\ k_2 \end{pmatrix}.$$

With respect to the dual basis $\vec{b}_1, \vec{b}_2$, the matrix $\hat{R}$ is unitary; it is the rotation of coordinates by $2\pi/3$, see Fig. 3(a) (and Appendix A for further discussion).

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3If the operator $H$ is specified on discrete graphs, the “boundary conditions” require special interpretation, see Section 2.1 for some examples.
Since the operator $H(\vec{k})$ is the restriction of the operator $H$, which is invariant under the rotation $R$, to the space $\mathcal{H}(\vec{k})$, we get

**Lemma 1.1.** $R$ acts as a unitary operator from $\mathcal{H}(\vec{k})$ to $\mathcal{H}(\hat{R}\vec{k})$. Therefore,

\begin{equation}
H(\vec{k}) = R^* H(\hat{R}\vec{k}) R.
\end{equation}

As a consequence, each sheet $\lambda_n(\vec{k})$ of the dispersion relation is invariant under the mapping

\begin{equation}
\vec{k} \mapsto \hat{R}\vec{k} \mod 2\pi,
\end{equation}

which maps a Brillouin zone to itself. The fixed points of this mapping are the points

\begin{equation}
\vec{0} := (0,0), \quad \vec{\kappa} := (2\pi/3, -2\pi/3), \quad -\vec{\kappa} := (-2\pi/3, 2\pi/3),
\end{equation}

and their shifts by $2\pi$. In coordinates $\kappa$, the mapping acts as a rotation by $2\pi/3$ around each of the fixed points

\begin{equation}
\vec{\xi} := (0,0), \quad \vec{\xi}^* := (0, 4\pi/3), \quad -\vec{\xi}^* := (0, -4\pi/3),
\end{equation}

**Proof.** Equation (10) follows immediately from $R$ being a symmetry of $H$ (i.e. $H = R^* H R$) and $H$ leaving spaces $\mathcal{H}(\vec{k})$ to $\mathcal{H}(\hat{R}\vec{k})$ invariant.

From (10), we immediately conclude that the spectra of $H(\vec{k})$ and $H(\hat{R}\vec{k})$ are the same, i.e. the dispersion relation is invariant under the rotation $\hat{R}$. The invariance under the shift by $2\pi$ in either coordinate was already explained above. The rest is a simple calculation. \hfill \Box

Analogous considerations for the horizontal reflection $F$ result in

\begin{equation}
\omega'_1 = \overline{\omega}_2, \quad \omega'_2 = \overline{\omega}_1,
\end{equation}

and, eventually, in

\begin{equation}
FH(\vec{k})F^* = H(\hat{F}\vec{k}), \quad \text{where} \quad \hat{F} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.
\end{equation}

The matrix $\hat{F}$ is a reflection with respect to the line $k_2 = -k_1$ and it leaves this line invariant.

Both complex conjugation and inversion result in

\begin{equation}
\omega'_1 = \overline{\omega}_1, \quad \omega'_2 = \overline{\omega}_2,
\end{equation}

and possess a unique fixed point $\vec{k} = \vec{0}$. However, their composition $V$ preserves the boundary conditions for all values of $\omega_1, \omega_2$.

To be more precise, denoting by $T$ the antiunitary operation of taking complex conjugation (or “time-reversal” in physics terminology), we have

\begin{equation}
TH(\vec{k})T^{-1} = H(-\vec{k}) = V H(\vec{k}) V^*.
\end{equation}

Equations (10), (14) and (15) show that the symmetries of the operator result in the symmetries of the dispersion relation. Those are more conveniently stated in $\vec{\xi}$ coordinates. We summarize these symmetries for the choices of $H$ that we will study in this paper.

**Corollary 1.2.** The dispersion relation of the $\Gamma$-periodic operator $H$ is invariant with respect to the dual lattice, i.e. the shifts

\begin{equation}
\vec{\xi} \mapsto \vec{\xi} + 2\pi b_1 \quad \text{and} \quad \vec{\xi} \mapsto \vec{\xi} + 2\pi b_2.
\end{equation}

If the operator $H$ is invariant with respect to rotation $R$ and time-reversal $T$, the dispersion relation $\lambda_n(\vec{\xi})$ is symmetric with respect to

- rotation by $\pi/3$ around the point $\vec{0} = (0,0)$.
- rotation by $2\pi/3$ around the points $\pm \vec{\xi}^* = \pm (0, 4\pi/3)$.

If, additionally, the operator has reflection symmetry $F$, then the symmetry groups increase to

\begin{equation}
\vec{\xi} \mapsto \vec{\xi} + 2\pi b_1 \quad \text{and} \quad \vec{\xi} \mapsto \vec{\xi} + 2\pi b_2.
\end{equation}
Figure 5. The contour plots of the two lowest bands from Fig. 4. Because of rotational symmetry, the contours are symmetric under the rotation by $2\pi/3$ around the points $(0,0)$ and $\pm \vec{\kappa}^*$. In addition, the operator has reflection symmetry and the plots are symmetric with respect to the vertical axis.

- $D_6$ around the point $\vec{0}$,
- $D_3$ around the points $\pm \vec{\kappa}^*$.

Above, $D_3$ and $D_6$ are the groups of symmetries of equilateral triangle and hexagon.

Remark 1.3. When $H$ is invariant with respect to complex conjugation, inversion symmetry of the operator does not result in any additional symmetries of the dispersion relation.

Proof. Equation (16) is simply equation (8) written in $\kappa$ coordinates.

From equations (10), (14) and (15) we know that the operator $H(\kappa)$ is unitarily equivalent to $H(\tilde{S}\kappa)$, where $S$ is the appropriate symmetry transformation. In Appendix A) the operators $\hat{R}$ and $\hat{F}$ are calculated in $\vec{\kappa}$ coordinates.

Naturally, $\hat{R}$ is just the rotation by $2\pi/3$ around the origin. Together with the involution $\kappa \mapsto -\kappa$ (i.e. rotation by $\pi$) induced by the time-reversal symmetry, this makes dispersion relation invariant with respect to rotation by $\pi/3$.

Rotation by $2\pi/3$ followed by the shift by $2\pi b_1$ is equivalent to the rotation by $2\pi/3$ around the point $\kappa^* = (0, 4\pi/3)$. Similar conclusion applies to the point $-\kappa^*$. Of course, the points $\pm \kappa^*$ are simply the points $\pm k^*$ expressed in $\vec{\kappa}$ coordinates.

Finally, reflection symmetry of the operator adds reflection symmetry to the dispersion relation resulting in the dihedral groups.

Figure 8 illustrates the results of Corollary 1.2. Here the contour plots of the two lowest bands of the dispersion relation are shown for the operator $H$ which has the reflection symmetry $F$ in addition to the (usual) rotational and time-reversal symmetries. The contours have symmetries $D_3$ and $D_6$ around the fixed points. Close to the fixed points, the contours became circular. This is also generic behaviour explained in the next lemma.

An important consequence of symmetry is a restriction on the possible local form of the dispersion relation. In particular, around a point of multiplicity two, the dispersion relation must be a circular cone (which could be degenerate).
Figure 6. Constructing multiple eigenvalues of $H(\vec{k}^*)$. Here $\omega = e^{2\pi i/3}$.

Lemma 1.4. Let $\vec{z}_0$ be one of the symmetry points, $\bar{0}$ or $\pm \vec{z}^*$. If $\lambda_n(\vec{z}_0) =: \lambda_0$ is a single eigenvalue, the dispersion relation is given locally by

$$\lambda - \lambda_0 = \alpha |\vec{z} - \vec{z}_0|^2 + \text{higher order terms}, \quad \alpha \geq 0.$$  

If $\lambda_n(\vec{z}_0) =: \lambda_0$ is a double eigenvalue, the dispersion relation is given locally by

$$(\lambda - \lambda_0)^2 = \alpha |\vec{z} - \vec{z}_0|^2 + \text{higher order terms}, \quad \alpha \geq 0.$$  

Note that $\alpha$ may be equal to zero.

Proof. We know from general theory of analytic Fredholm operators [32] that the dispersion relation is an analytic variety, i.e. given by an analytic function

$$F(\lambda, \vec{z}) = 0.$$  

Without loss of generality, consider the point $\vec{z}_0 = 0$. It is an easy special case of Hilbert-Weyl theorem on invariant functions [29] (see also [11, XII.4]), that locally around a point with rotational symmetry of order 3, the Taylor expansion for the function $F$ is

$$F(\lambda, \vec{z}) = F_0(\lambda) + F_2(\lambda)(\vec{z}_1^2 + \vec{z}_2^2) + \text{higher order terms}.$$  

The result now follows from the first terms of expansions of $F_0$ and $F_2$. Note that $\alpha$ cannot be negative since by standard perturbation theory an eigenvalue present at $\vec{z}_0$ cannot disappear. \hfill $\square$

2. Degeneracies in the spectrum

We will now give a simple proof of the presence of degeneracies in the spectrum of the operator $H(\vec{k})$ at the point $\vec{k}^*$. Similar result for the point $-\vec{k}^*$ follows from symmetry with respect to complex conjugation, see equation (15) and Corollary 1.2. Our approach is a “transplantation proof”, similar to the proofs of isospectrality of certain domains (such as the proof by Buser et al. [6] for the Gordon–Webb–Wolpert pair [13]). As in isospectrality, while the proof itself is extremely simple, it is a result of a more complicated procedure involving finding irreducible representations of the group of symmetries and performing the Band–Parzanchevski–Ben-Schach [3] quotient of the domain by a suitable representation. This procedure of “constructing the proof” is described in Appendix [3].
Consider the rhombic subdomain covering 1/3 of the hexagonal fundamental domain, shown in Fig. 6(a). Denote by $Q$ the operator having the same differential expression as $H$ and with the boundary conditions specified in Fig. 6(a).

**Theorem 2.1.** Let the self-adjoint operator $H$ be invariant under the rotation $R$ and at least one of the following: reflection $F$ or inversion $V$. Then each eigenvalue of the operator $Q$ is a double eigenvalue of the operator $H(\vec{k}^*)$ with

$$\vec{k}^* := (2\pi/3, -2\pi/3).$$

The operator $Q$ is self-adjoint.

**Proof.** Let $\phi$ be an eigenfunction of the operator $Q$. To prove the theorem we will construct two eigenfunctions of the operator $H(\vec{k}^*)$.

Fill the fundamental hexagon with rotated copies of the rhombic subdomain, multiplied by $\omega = e^{2\pi i/3}$ for each rotation by $2\pi/3$, see Fig. 6(b). Because of the boundary condition along the boundary denoted by $g$, the resulting function is continuous with its first derivative. Because of the boundary condition along the boundary denoted $f$, the function satisfies the conditions on the boundary of the hexagon, see Fig. 6(c) with $\omega_1 = \omega$ and $\omega_2 = \omega^2$.

The second eigenfunction of $H(k^*)$ is now obtained by applying complex conjugate inversion (if $H$ had symmetry $V$) or reflection (if $H$ had symmetry $F$) to the constructed eigenfunction, see Fig. 6(c) and (d), correspondingly. To verify that the second eigenfunction is indeed distinct, we note that it is orthogonal to the first. Indeed, as can be seen from Fig. 6(b)-(d), the two eigenfunctions are also eigenfunctions of the unitary operator $R$ but with different eigenvalues, $\omega$ and $\bar{\omega}$, and are therefore orthogonal.

The self-adjointness of $Q$ can be obtained, for example, from the self-adjointness of $H$ restricted to the reducing subspace spanned by functions of the form of Fig. 6(b) (see, e.g., [28, Thm 7.28]).

**Corollary 2.2.** For any potential, the degenerate eigenstates of $H(\vec{k}^*)$ vanish (are suppressed) at the center of the hexagonal fundamental domain.

**Proof.** At the top left corner of the rhombic subdomain, Fig. 6(a), the boundary conditions require $g = \omega g$. This point is fixed by either the reflection or the inversion, thus both eigenfunctions have a zero there.

**2.1. Graph examples.** While the proof of Theorem 2.1 was formulated for continuous differential operators in $\mathbb{R}^2$, the method applies to other models, such as graphs, with a little adjustment. Here we explain, by example, the construction of the reduced operator $Q$. 
Example 2.3. It is easier to start with an example that has a richer structure, such as the periodic graph of Fig. 7(a). It is assumed that the black and white vertices have different potential, therefore $V$ symmetry is broken, while $R$ and $F$ symmetries are still present.

In part (b) the structure of the graph inside the dashed fundamental domain is magnified. Gray vertices outside of the fundamental domain are obtained by shifts from the corresponding vertices inside. For example, $f'_5 = \omega f_5$, therefore the operator $H$ at site 2 acts as

$$
(Hf)_2 = (f_2 - f_3) + (f_2 - f_1) + r(f_2 - \omega_2 f_3) + q_2 f_2,
$$

where we took the longer sides in the structure of Fig. 7(a) to have weight 1 and the shorter sides weight $r$ (usually, the weight is taken to be inversely proportional to length). The entire operator $H$ is

$$
H = \begin{pmatrix}
q_1 & -1 & 0 & r\overline{\omega}_1 \omega_2 & 0 & -1 \\
-1 & q_2 & -1 & 0 & -r\omega_2 & 0 \\
0 & -1 & q_1 & -1 & 0 & -r\omega_1 \\
r\omega_1 \omega_2 & 0 & -1 & q_2 & -1 & 0 \\
0 & -r\overline{\omega}_2 & 0 & -1 & q_1 & -1 \\
-1 & 0 & r\overline{\omega}_1 & 0 & -1 & q_2 \\
\end{pmatrix},
$$

where, for simplicity, the potential $q$ was made to absorb the weighted degree of its vertex.

With $q_1 = \sqrt{3}$, $q_2 = 0$ and $r = \sqrt{7}$, the eigenvalues of $H(\vec{k}^*)$, calculated numerically, are

$$
-2.5097 \quad -2.5097 \quad -1.6753 \quad 3.4074 \quad 4.2418 \quad 4.2418.
$$

To find operator $Q$ acting on the two darker vertices in Fig. 7(c), we retrace the steps of the proof of Theorem 2.1: for the gray vertices we have

$$
f_{1'} = \omega f_1, \quad f_{1''} = \overline{\omega} f_1, \quad f_{2''} = \overline{\omega} f_2
$$

by rotation and then

$$
f_{1'''} = \overline{\omega} f_{1''} = \omega f_1, \quad f_{2'''} = \overline{\omega} f_2
$$

by translation (see Fig. 2(c)). We thus get

$$
Q = \begin{pmatrix}
q_1 & -1 & 0 & 1 - \overline{\omega} - r\overline{\omega} \\
-1 & \omega & r\omega & q_2 \\
\end{pmatrix}.
$$

With the above choice of constants, the eigenvalues of $Q$ are

$$
-2.5097 \quad 4.2418
$$

which matches the double eigenvalues of $H$.

Example 2.4. We will now explain the application of our theory to the most basic example: the tight-binding approximation of graphene structure, with vertices of a discrete graph representing carbon atoms, see Fig. 8(a).

The operator $H(\vec{k})$ acts on a 2-dimensional space over vertices 1 and 2 (all other vertices of the graph are obtained by shifts). It acts as

$$
(Hf)_1 = -f_2 - f_2' - f_2'' + q_1 f_1
$$

$$
= -f_2 - \omega_1 f_2 - \omega_2 f_2 + q_1 f_1,
$$

and similarly for $(Hf)_2$. Note that the atoms are identical, hence $q_1 = q_2 = q$. When $\omega_1 = \overline{\omega}_2 = \omega$, the matrix $H$ is $q$ times identity.

The eigenproblem of the rhombic subdomain can be gleaned from Fig. 8(b). In particular, $f_1$ is forced to be zero: which can be seen from the equality $f_1 = \omega f_1 = \overline{\omega} f_1$ highlighted by the empty arrows in Fig. 8(b), or from the boundary conditions for the bottom right corner of Fig. 8(a). On the other hand, the value $f_2$ is unrestricted and $(Qf)_2 = q f_2$. The complementary eigenfunction is localized on the vertex 1.
3. Conical structure around a degeneracy

3.1. General perturbation theory. Here we list some general facts from the perturbation theory of operators depending on parameters, following \[16, 32, 14\]. Let

\[ H(r) = H_0 + (r - r_0)H_1 + O \left( |r - r_0|^2 \right) \]

be an analytic family of self-adjoint operators depending on one parameter with an isolated doubly degenerate eigenvalue \( \lambda_0 \) at \( r = r_0 \). The eigenvalue then splits into two analytic branches

\[ \lambda^\pm(r) = \lambda_0 + \lambda^\pm_1 (r - r_0) + O \left( |r - r_0|^2 \right). \]

The linear terms can be found as the eigenvalues of the \( 2 \times 2 \) matrix \( PH_1 P \), where \( P \) is the projector onto the eigenspace of \( \lambda_0 \). The corresponding eigenvectors expand as

\[ \psi^\pm(r) = \psi^\pm_0 + O \left( \frac{|r - r_0|}{|\lambda^+_1 - \lambda^-_1|} \right), \]

where \( \psi^\pm_0 \) are the eigenvectors of \( PH_1 P \) (which are in the eigenspace of \( H_0 \)). All eigenvectors are assumed to be normalized.

If \( H = H(k_1, k_2) \) is an analytic function of two parameters and \((0, 0)\) is the point of double multiplicity of the eigenvalue \( 0 \), the one-parameter theory is still valid in every direction \( k_1 = r \cos(\phi), \ k_2 = r \sin(\phi) \). A doubly degenerate eigenvalue is a conical point if \( \lambda^+_1 \neq \lambda^-_1 \) in every direction.

**Definition 3.1.** Let \( H(\vec{k}) \) be an analytic family of self-adjoint operators. We will say that \( H(\vec{k}) \) has a nondegenerate conical point at \( \vec{k}_0 \) with the eigenvalue \( \lambda_0 \) if \( \lambda_0 \in \sigma_g(H(\vec{k}_0)) \) is an isolated eigenvalue of geometric multiplicity 2 and in a neighborhood of \( \vec{k}_0 \), the eigenvalues are given by

\[ \lambda^\pm(\vec{k}) = \lambda_0 + (\vec{k} - \vec{k}_0) \cdot \vec{n} \pm \sqrt{Q(\vec{k}) + o(||\vec{k}||)}, \]

where \( \vec{n} \in \mathbb{R}^2 \) and \( Q(\vec{k}) \) is a positive-definite quadratic form. The point \( \vec{k}_0 \) is a fully degenerate conical point if the same is true with \( Q \equiv 0 \).

From Lemma 1.4 we know that the points of double degeneracy at \( \pm \vec{k}^* \) and \( \vec{0} \) must either be nondegenerate circular cones (in \( \kappa \) coordinates) or fully degenerate cones. It turns out that the point \( \vec{0} \) is always a fully degenerate cone; we will also derive a condition for nondegeneracy of the cone at \( \pm \vec{k}^* \). This condition is equivalent to \[3\] Cond. (4.1).
In the first order of perturbation theory, the dispersion surface (i.e. the graph of the eigenvalues as the function of parameters) is given by the solution to

\[ \det (k_1 h_1 + k_2 h_2 - \lambda) = 0, \]

where the 2 \times 2 Hermitian matrices \( h_1 \) and \( h_2 \) are given by

\[ h_1 = \Phi^* \frac{\partial H}{\partial k_1} \Phi \quad \text{and} \quad h_2 = \Phi^* \frac{\partial H}{\partial k_2} \Phi. \]

Here \( \Phi : \mathbb{R}^2 \to \mathcal{H} \) is given by the matrix \((f_1, f_2)\) formed from the orthonormal basis vectors of the degenerate eigenspace at \((0, 0)\) (the projector \( P \) onto the eigenspace is then given by \( P = \Phi \Phi^* \)).

We will now derive matrices \( h_1 \) and \( h_2 \) explicitly.

3.2. Application to graphene operators. At the singularity points \( \pm \vec{k}^* \) we are guaranteed by the construction in the proof of Theorem 2.1 (see Fig. 6(b-d)) to have two orthogonal eigenfunctions \( f_1 \) and \( f_2 \) such that

\[ Rf_1 = \omega f_1, \quad Rf_2 = \omega f_2. \]

The existence of such eigenfunctions also follows directly from representation theory, equations (39) and (44) in the Appendix. Using this basis for the eigenspace results in a simple form for the derivatives \( h_j \), \( j = 1, 2 \).

**Theorem 3.2.** In the basis \( \{ f_1, f_2 \} \) satisfying (23), the matrices \( h_1 \) and \( h_2 \) are given by

\[ h_1 = \begin{pmatrix} 0 & \alpha \\ \frac{\alpha}{\overline{\alpha}} & 0 \end{pmatrix}, \quad h_2 = \begin{pmatrix} 0 & \omega \alpha \\ \omega & 0 \end{pmatrix}, \]

where, from definition (22),

\[ \alpha = \left( f_1, \frac{\partial H}{\partial k_1} f_2 \right). \]

**Remark 3.3.** This calculation was performed in the perturbative regime (where functions \( f_1 \) and \( f_2 \) are known explicitly) in [14] and for \( \mathbb{R}^2 \) Laplacian with any symmetric \( R \) symmetric potential in [9, Prop 4.2], using explicit calculation of the derivatives \( \partial H / \partial k_j \). We give a general derivation in the spirit of the Hilbert-Weyl theory of invariant functions.

**Proof.** From Lemma 1.1 we have

\[ R \left( H(\vec{k}^* - \vec{k}) - \overline{H(\vec{k}^*)} \right) R^* = H \left( \overline{R(\vec{k}^* + \vec{k})} - H \left( \overline{R\vec{k}^*} \right) \right) = H (\vec{k}^* + \overline{R\vec{k}}) - H (\vec{k}^*), \]

where we used the fact that \( \vec{k}^* \) is a fixed point of (11). Passing to the limit, we get

\[ R \left( \partial_{\vec{k}} H \right) R^* = \partial_{\overline{R\vec{k}}} H, \]

where we by \( \partial_{\vec{k}} H \) we denote the directional derivative of \( H \) at point \( \vec{k}^* \) in the direction \( \vec{k} \).

Introduce the notation

\[ h_{\vec{k}} = k_1 h_1 + k_2 h_2 = \Phi^* \left( \partial_{\vec{k}} H \right) \Phi. \]

Conjugating equation (26) by matrix \( \Phi \) we get

\[ \rho(R)^T h_{\vec{k}} \rho(R^*)^T = h_{\overline{R\vec{k}}}, \]

where \( \rho(R^*) \) is the matrix representation of the rotation \( R^{-1} \) defined by the eigenspace span\((f_1, f_2)\), namely

\[ R^*(f_1, f_2) = (f_1, f_2) \rho(R^*)^T \]

(compare with equation (10) and other material in Appendix [15]).

---

4 This is a standard procedure in quantum mechanics or solid state physics (known as \( k \cdot p \) method in the latter); for a mathematical proof, see [14].
Figure 9. Construction of the degenerate eigenstate form the dispersion relation at \( \vec{k} = \vec{0} \).

In our choice of basis, equation (23), \( R^*(f_1, f_2) = (\overline{\omega} f_1, \omega f_2) \), therefore
\[
\rho(R^*)^T = \begin{pmatrix} \overline{\omega} & 0 \\ 0 & \omega \end{pmatrix}.
\]
Using the explicit form of the matrix \( \hat{R} \) from \( \text{(9)} \), equation (27) can be written in components as
\[
\begin{pmatrix} \omega & 0 \\ 0 & \overline{\omega} \end{pmatrix} h_1 \begin{pmatrix} \overline{\omega} & 0 \\ 0 & \omega \end{pmatrix} = -h_1 - h_2, \quad \begin{pmatrix} \omega & 0 \\ 0 & \overline{\omega} \end{pmatrix} h_2 \begin{pmatrix} \overline{\omega} & 0 \\ 0 & \omega \end{pmatrix} = h_1.
\]
It is now straightforward to check that any \( 2 \times 2 \) Hermitian matrices satisfying (28) must be of the form (24).

From expressions (24) one can explicitly calculate the shape of the dispersion relation in the first order of perturbation theory using (21). It is
\[
\lambda^2 - |\alpha|^2 |k_1 + \omega k_2|^2 = \lambda^2 - \frac{4}{3} |\alpha|^2 |x|^2 = 0,
\]
where we changed to the coordinates
\[
\vec{z} = k_1 \vec{b}_1 + k_2 \vec{b}_2,
\]
in which the dispersion relation is the circular cone with no tilt. It becomes degenerate if \( \alpha = 0 \) (this condition is equivalent to condition (4.1) of \( \text{[9]} \)). In \( \text{[14]} \), \( \alpha \) was shown to be non-zero for small potential, therefore, if the potential strength is controlled by a parameter, the cone can be degenerate only for isolated values of the parameter.

4. Degeneracy at \( \vec{k} = \vec{0} \)

The third fixed point of the rotation \( \hat{R} \) in the momentum space also leads to degeneracies in the spectrum. They are present even if both inversion and reflection symmetries are broken: rotation and complex conjugation are sufficient. However, the local structure of the dispersion relation is not conical, see Fig. 4 for an example.

Theorem 4.1. Let \( H \) be invariant with respect to \( R \).

- There are degeneracies at the point \( \vec{k} = \vec{0} \).
- If \( \lambda = \lambda_0 \) is such a degeneracy and has multiplicity 2, the dispersion relation is locally flat,
\[
(\lambda - \lambda_0)^2 = o(|\vec{k}|^2)
\]

Remark 4.2. The eigenvalue \( \lambda_1(\vec{0}) \) is always non-degenerate, therefore first and second bands cannot touch at \( \vec{k} = \vec{0} \).
Proof. For the first part, consider the operator $Q_0$ similar to the operator $Q$ in the Theorem 2.1 but with a slight change in the condition imposed on one side, see Fig. 9(a). Taking its eigenfunction, rotating it by $2\pi/3$ and multiplying by $\omega$ we get a function $f_1$ in the whole hexagonal domain, Fig. 9(b), which satisfies periodic boundary conditions with respect to lattice translations. The complex conjugation $f_2 = \overline{f_1}$ of the depicted function satisfies the same boundary conditions and eigenvalue equation. Thus we have two eigenfunctions, satisfying

\begin{equation}
R f_1 = \omega f_1, \quad R f_2 = \overline{\omega f_2}, \quad f_1 = \overline{f_2}, \quad f_2 = \overline{f_1}.
\end{equation}

The functions $f_1$ and $f_2$ are distinct because they are orthogonal: they are eigenfunctions of $R$ with different eigenvalues.

For the second part, the proof of Theorem 3.2 still applies so the matrices $h_1$ and $h_2$ have the form given by (24). Repeating the proof for the complex conjugation as a symmetry of $H(\vec{k})$ at $\vec{k} = \vec{0}$ we arrive to the following analogue of (27),

\begin{equation}
\rho(T) h_{\vec{k}} \rho(T^{-1}) = h_{-\vec{k}},
\end{equation}

where $T$ stands for the operator of complex conjugation (“time reversal”) and the overall complex conjugation arises because $T$ is antiunitary. By consulting (31), we find that

\[ \rho(T) = \rho(T^{-1}) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \]

From (32) and the fact that $h_{\vec{k}}$ is Hermitian, we obtain that $h_{\vec{k}}$ is necessarily diagonal (and also has trace 0). Therefore $h_{\vec{k}} \equiv 0$. \[\square\]

Remark 4.3. In a more general setting, one can get the following result. Suppose the operator $H(\vec{k}) = H(k_1, k_2)$ has the following symmetry at the point $\vec{k}_0$,

\[ H(\vec{k}_0 + \vec{k}) = H(\vec{k}_0 - \vec{k}). \]

If $\lambda_0$ is an eigenvalue of $H(\vec{k}_0)$ of multiplicity 2, it cannot be a nondegenerate conical point.

Example 4.4. Revisiting Example 2.3 and calculating the eigenvalues of $H(\vec{0})$ numerically, we get

\[ -3.8598 \quad -0.9937 \quad -0.9937 \quad 2.7257 \quad 2.7257 \quad 5.5918 \]

The corresponding operator $Q_0$ in this case can be shown to be

\[ Q_0 = \begin{pmatrix} q_1 & -1 - \omega - r\overline{\omega} \\ -1 - \omega - r\overline{\omega} & q_2 \end{pmatrix}, \]

with eigenvalues $-0.9937$ and $2.7257$.

Interestingly, in the case of Example 2.4, the graph structure is not rich enough to support the operator $Q_0$: it can be shown that the only lattice-periodic function with structure described by Fig. 9(b) must have $f_1 = f_2 = 0$.

5. Persistence of conical points

We are now going to consider whether the conical point survives when the rotational symmetry is broken by a small perturbation. We will consider two cases the perturbation retains the inversion $V$ or the reflection $F$ symmetry (all other symmetries may or may not be broken). In both cases the conical point survives. Moreover, in the second case we are able to restrict the location of the surviving point to a line in $\vec{k}$ space. Of course, if the perturbation retains both symmetries, $V$ and $F$, the stronger second result still applies.
5.1. **Keeping $V$ symmetry: Berry phase.** Let us consider the weakly broken $R$-symmetry: we add to $H$ a perturbation which is $V$-invariant but not $R$-invariant. The $F$ symmetry may or may not be preserved.

**Theorem 5.1.** Consider the perturbed operator $H_\epsilon := H + \epsilon W$, where the electric potential $W$ is $\Gamma$-periodic, real-valued and symmetric with respect to inversion $V$. Let the dispersion relation for $H$ have a nondegenerate conical point at $\vec{k}^*$. Then there exists a contour $\gamma$ around $\vec{k}^*$ in the dual $\vec{k}$ space such that for small $\epsilon$ there is a nondegenerate conical point of $H_\epsilon$ inside $\gamma$.

The tool for proving this theorem is the “Berry phase” \[4, 24\] (also known as “Pancharatnam-Berry phase” or “geometric phase”), of which we first give an informal description. Consider choosing a contour in the parameter space and tracking certain eigenvalue along this contour. The eigenvalue changes as we move along the contour, but we assume it remains simple. Now we choose the corresponding normalized eigenvector at every point of the contour. The eigenvector is defined up to a phase, and we choose it in the “most continuous fashion”. Once we completed the loop, the final eigenvector must equal the initial eigenvector up to a phase factor $e^{i\phi}$. The phase $\phi$ we call the Berry phase. The fact that it might be different from zero in the simplest form of real operator $H$ and a contour encircling a conical point has been known for a while, see \[15\] and \[1, Appendix 10.B\].

We now argue that the Berry phase of the operator $H_\epsilon(\vec{k})$ is restricted. Because of the symmetry of the perturbation $W$, the perturbed operator $H_\epsilon(\vec{k})$ will retain the symmetry $V$ for all $\vec{k}$. The operator $V$ is an antiunitary involution, i.e.

\[(33) \quad V(\alpha v) = \bar{\alpha}(V v), \quad V^2 = 1, \quad (V v, V u) = (u, v).\]

If $\psi$ is a simple eigenfunction of $H(\vec{k})$, then, after multiplication by a suitable phase,

\[(34) \quad V \psi := \psi(\vec{-x}) = \psi.\]

Indeed, because $V$ commutes with the operator $H(\vec{k})$, $\psi(\vec{-x})$ is an eigenvector with the same eigenvalue and thus equal to $e^{i\theta} \psi$ for some $\theta$. Multiplying $\psi$ by $e^{i\theta/2}$ makes it satisfy equation (34).

Condition (34) gives us a canonical way to choose the overall phase of the eigenvector, up to a sign.\[^5\] Now consider a closed path in the parameter $\vec{k}$ space. The phase acquired by a parallel section of the eigenvectors (the formal definition of the Berry phase) is restricted by condition (34): the factor must be either $+1$ or $-1$, so the phase is either $0$ or $\pi$.

On the other hand, the phase must change continuously upon a continuous deformation of the contour. Therefore, if the contour is homotopically equivalent to a point (i.e. encloses no parameter values where the eigenvalue becomes multiple), the phase must be equal to zero. But if the contour encloses a conical point, the phase is equal to $\pi$.

**Lemma 5.2.** Let the self-adjoint operator $H(\vec{k})$, which analytically depends on the two parameters $\vec{k} = (k_1, k_2)$, has a nondegenerate conical point at $(0, 0)$. Let $H(\vec{k})$ commute with an antiunitary involution $V$. Then the Berry phase acquired on a contour enclosing the singularity $(0, 0)$ is $\pi$.

**Remark 5.3.** This result for a real-valued operator $H$ can be traced back at least to Herzberg and Longuet-Higgins \[15\]. Their proof is based on reducing the question using perturbation theory to a question about $2 \times 2$ matrices and computing the eigenvectors explicitly. A more general formula is derived in \[3 \text{ Sec. 3}\], from which Lemma 5.2 follows. In Appendix \[1\] we include an alternative derivation which avoids computing anything explicitly, opting instead for a more geometric explanation, which has interesting similarities to considerations of Section 5.2.

\[^5\]This choice of the eigenvector along a curve in the parameter space actually defines a parallel section of the line bundle of the eigenspaces.
From this we immediately conclude that an isolated non-degenerate conical point cannot disappear under a perturbation which preserves the above symmetry.

**Proof of Theorem 5.4.** Surround the point with a small contour $\gamma$, such that inside this contour the eigenvalue $\lambda_-(\vec{k})$ of $H_{\epsilon=0}(\vec{k})$, see [20], is simple except at $\vec{k}^\ast$. Then on contour $\gamma$ the Berry phase of the corresponding eigenfunction must be $\pi$.

For small values of $\epsilon$, the eigenvalue on the contour $\gamma$ remains simple (as a continuous function on a compact set). Therefore, the phase must change continuously, so it must remain constant. Finally, if there were no multiplicity of $\lambda_-(\vec{k})$ inside the contour, the Berry phase would be 0. The multiplicity gives rise to a nondegenerate conical point by continuity. □

5.2. **Keeping $F$ symmetry: parity exchange.** Let us now consider the weakly broken $R$-symmetry: we add to $H$ a perturbation which is $F$-invariant but not $R$-invariant. The $V$ symmetry may or may not be preserved.

**Theorem 5.4.** Consider the perturbed operator $H_\epsilon := H + \epsilon W$, where the electric potential $W$ is $\Gamma$-periodic, real-valued and symmetric with respect to inversion $F$. Let the dispersion relation for $H$ have a nondegenerate conical point at $\vec{k}^\ast$. Then for small $\epsilon$ there is a nondegenerate conical point of $H_\epsilon$ on the line $k_2 = -k_1$ modulo $2\pi$.

**Proof.** As explained in Section 1.4, $F$ remains a symmetry of the operator $H(\vec{k})$ when the quasi-momenta $\vec{k}$ satisfy $\omega_2 = \omega_1$ or, equivalently, $k_2 = -k_1$ modulo $2\pi$.

Since the subgroup generated by $F$ has two representations, trivial and alternating (i.e. $F \mapsto (-1)$), the space $\mathcal{H}(\vec{k})$ decomposes into two subspaces, even and odd, defined by

$$\mathcal{H}_{F,+} = \{ \psi \in \mathcal{H}(\vec{k}) : F \psi = \psi \} \quad \text{“even”},$$
$$\mathcal{H}_{F,-} = \{ \psi \in \mathcal{H}(\vec{k}) : F \psi = -\psi \} \quad \text{“odd”}.$$ (35)

(36)

As usual, the subspaces are orthogonal. All simple eigenvectors of $H(\vec{k})$ on the symmetry line belong to one or the other subspace. Multiple eigenspaces admit a basis consisting of vectors, each of which is either odd or even.

Now suppose we are at the special symmetry point $\vec{k}^\ast$ in the presence of rotational symmetry $R$ (i.e. $\epsilon = 0$). At the conical point we have a doubly degenerate eigenvalue with orthogonal eigenvectors described by Fig. [12](b). It can be seen directly that the sum of these eigenvectors is even and the difference is odd with respect to $F$.

Now consider the restrictions of the operator $H$ to the two subspaces $\mathcal{H}_{F,+}$ and $\mathcal{H}_{F,-}$. The above consideration shows that at the special point each restriction has a simple eigenvalue (which coincide). As we go along the line $k_2 = -k_1$, the eigenvalue of each restriction is an analytic function. These functions have an intersection at the point $k_1 = 2\pi/3$. Because the two functions form a section of the non-degenerate cone, the intersection is transversal, see Fig. [10](b). Such intersection is stable under perturbation, and therefore, when we consider small $\epsilon \neq 0$ (keeping the symmetry $F$), the intersection survives. Moreover, we know it remains on the line $k_2 = -k_1$ and the only way it can disappear is by colliding with another intersection on this line.

The intersection is a degenerate eigenvalue of the operator $H(k)$ which, for small perturbations of the original potential, must still be a non-degenerate cone.

**Appendix A. Matrices of symmetry transformations**

In this section we discuss different coordinates for the position and dual spaces and calculate the matrix $\hat{R}$ in those coordinates. The considerations are very basic, but can be useful for avoiding confusion.
There are two sets of coordinates of the position space: the rectangular Cartesian \( \vec{x} = (x_1, x_2)^T \) and coordinates with respect to the basis of the lattice-defining vectors \( \vec{a}_1, \vec{a}_2 \). The latter coordinates we will denote \( \vec{\xi} = (\xi_1, \xi_2)^T \). The connection between the two sets is

\[
\vec{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \xi_1 \vec{a}_1 + \xi_2 \vec{a}_2 = \begin{pmatrix} \sqrt{3}/2 & \sqrt{3}/2 \\ 1/2 & -1/2 \end{pmatrix} \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix} =: A \vec{\xi}.
\]

The inverse matrix \( A^{-1} \) is

\[
A^{-1} = \begin{pmatrix} 1/\sqrt{3} & 1 \\ 1/\sqrt{3} & -1 \end{pmatrix} = \begin{pmatrix} \vec{b}_1 \\ \vec{b}_2 \end{pmatrix}.
\]

The \( \vec{\xi} \) coordinates are more convenient for the description of the hexagonal lattice, while \( \vec{x} \) coordinates are slightly more convenient for the description of symmetries: for example the rotation is given by a unitary matrix. Namely, \( R\psi(\vec{x}) = \psi(M_R \vec{x}) \), where

\[
M_R = \begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}
\]

is the matrix of rotation by \( 2\pi/3 \) in the clockwise (negative) direction. As usual, to rotate the function in the positive direction, we rotate its coordinates in the negative direction.

In terms of coordinates \( \vec{\xi} \) we therefore have \( R\psi(\vec{\xi}) = \psi(A^{-1} M_R \vec{\xi}) \), where

\[
A^{-1} M_R A = \begin{pmatrix} 1 & -1 \\ -1 & 0 \end{pmatrix},
\]

which is, of course, still a rotation by \( -2\pi/3 \) in terms of the basis \( (\vec{a}_1, \vec{a}_2) \).

The coordinates \( \vec{k} \) are dual to \( \vec{\xi} \) and therefore the action of \( R \) on \( \vec{k} \) is given by

\[
\hat{R} = (A^{-1} M_R A)^*,
\]

which agrees with equation (9).
Finally, one can also use Cartesian coordinates in the dual space. As mentioned before, those are
\[ \vec{z} = k_1 \vec{b}_1 + k_2 \vec{b}_2 = \begin{pmatrix} 1/\sqrt{3} & 1/\sqrt{3} \\ 1 & -1 \end{pmatrix} \begin{pmatrix} k_1 \\ k_2 \end{pmatrix} = B \begin{pmatrix} k_1 \\ k_2 \end{pmatrix}, \]
where
\[ B = \begin{pmatrix} \vec{b}_1, \vec{b}_2 \end{pmatrix} = (A^{-1})^*. \]
Therefore, in coordinates \( \vec{z} \) the action of \( R \) is given by
\[ B \hat{R} B^{-1} = M_R^*, \]
a unitary matrix. For the dual of the horizontal reflection we have
\[ \hat{F}_k = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \]
in \( k \) coordinates and
\[ \hat{F}_\kappa = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} = B \hat{F}_k B^{-1} \]
in \( \kappa \) coordinates. As before, \( \hat{F}_\kappa = (M_F)^* \), where \( M_F \) defines the horizontal reflection in the \( x \) coordinates: \( F_\psi(x) = \psi(M_F \vec{x}) \).

Appendix B. Representations and degeneracies in the spectrum

B.1. Subspace carrying a representation. Let \( H \) be a self-adjoint operator (“Hamiltonian”) acting on a separable Hilbert space \( \mathcal{H} \). Let \( S = \{ \text{Id}, S_1, \ldots \} \) be a finite group of unitary operators on \( \mathcal{H} \) which commute with \( H \) (are “symmetries” of \( H \)).

Remark B.1. It is assumed implicitly that the domain of \( H \) is invariant under the action of operators \( S \in S \). Such technical details will be omitted unless they have some importance to the task at hand.

It is well-known (see, e.g. [12]) that in the circumstances described above, there is an isotypic decomposition of \( \mathcal{H} \) into a finite orthogonal sum of subspaces each carrying copies of a representation of \( S \). More precisely,
\[ \mathcal{H} = \bigoplus_\rho \mathcal{H}_\rho, \]
where for any two vectors \( v_1, v_2 \in \mathcal{H}_\rho \), there is an isomorphism between the spaces
\[ [Sv_1] = \text{span} \{ Sv_1 : S \in S \} \quad \text{and} \quad [Sv_2] = \text{span} \{ Sv_2 : S \in S \}, \]
which preserves the group action on the spaces (i.e. commutes with all \( S \in S \)).

For each \( v \in \mathcal{H}_\rho \), the finite-dimensional subspace \([Sv]\) is an irreducible representation of \( S \): if it were reducible (i.e. had a proper subspace invariant with respect to \( S \)), there would be \( u \in [Sv] \subset \mathcal{H}_\rho \), such that \([Su]\) is a proper subspace of \([Sv]\) and therefore not isomorphic to it. The components \( \mathcal{H}_\rho \) are maximal: different components correspond to different representations. Thus \( \rho \) can be understood as labelling irreducible representations. The dimension of \([Sv]\) is called the dimension of the representation \( \rho \).

Example B.2. Let \( \mathcal{H} = L^2(\mathbb{R}) \) and \( S \) be the cyclic group of order 2 generated by the reflection \( x \mapsto -x \) or, more precisely,
\[ S : f(x) \mapsto f(-x). \]
Then \( \mathcal{H} = \mathcal{H}_{\text{even}} \oplus \mathcal{H}_{\text{odd}} \), where
\[ \mathcal{H}_{\text{even}} = \{ f \in \mathcal{H} : f(-x) = f(x) \}, \quad \mathcal{H}_{\text{odd}} = \{ f \in \mathcal{H} : f(-x) = -f(x) \}. \]
Then \( \mathcal{H}_{\text{even}} \) carries infinitely many copies of the trivial representation of \( S \):
\[ \text{Id} \mapsto (1), \quad S \mapsto (1), \]
while \( \mathcal{H}_{\text{odd}} \) carries infinitely many copies of the alternating representation of \( S \):
\[
\text{Id} \mapsto (1), \quad S \mapsto (-1).
\]
Both representations are one-dimensional. Note that the decomposition of a \( \mathcal{H}_\rho \) into irreducible copies is not unique.

Each isotypic component \( \mathcal{H}_\rho \) is invariant with respect to \( H \): either \( Hv = 0 \) or \( H \) provides the isomorphism between subspaces \([Sv]\) and \([SHv]\).

If \( H \) has discrete spectrum then the restriction of \( H \) to \( \mathcal{H}_\rho \) has eigenvalues with multiplicities divisible by the dimension of \( \rho \). Indeed, by commuting \( S \) and \( H \) we see that if \( v \) is an eigenvector of \( H \), then the entire subspace \([Sv]\) is an eigenspace of \( H \) with the same eigenvalue.

It is sometimes stated in the physics literature that if the group of symmetries of an operator has an irreducible representation \( \rho \), the operator will have eigenspaces carrying this irreducible representation; in particular, the corresponding eigenvalue will have multiplicity equal to the dimension of \( \rho \). This is not completely correct, as the isotypic component corresponding to this representation can be absent from the domain of operator, due to natural (see [3, Sec. 7.2] for an example) or artificial reasons (e.g., the operator may be restricted to another isotypic component). Thus the fundamental question in describing spectral degeneracies is finding the isotypic decomposition of the domain of the operator.

In the following sections we will describe the isotypic decomposition of the domain \( \mathcal{H}^2(\vec{k}) \) and the restriction of the operator to an isotypic component.

**B.2. Restricting the operators.** Restricting an operator to an isotypic component is the essence of the technique of “taking the quotient of an operator by a representation”, applied in [3, 22] to constructing isospectral graphs and domains (the method is itself a generalization of the so-called Sunada method [25]). We recast their method below as a description of equivariant vectors (cf. [33, Def 1.19]).

**B.2.1. \( R \) and \( F \) symmetry.** Suppose the operator \( H \) on the whole space had \( R \) and \( F \) symmetry and let us consider the special point \( K \) in the Brillouin zone \( \omega_1 = \omega_2 = \omega = e^{2\pi i/3} \). At this point, the reduced operator \( H(\vec{k}) \) is still symmetric with respect to \( R \) and \( F \).

The symmetries satisfy the relations \( R^3 = F^2 = \text{id} \) and \( FR^2 = RF \) and the symmetries group \( S \) is thus isomorphic to the symmetric group \( S_3 \). The representations are
\[
\text{(37)} \quad R \mapsto (1), \quad F \mapsto (1) \quad \text{“trivial”},
\]
\[
\text{(38)} \quad R \mapsto (1), \quad F \mapsto (-1) \quad \text{“alternating”},
\]
\[
\text{(39)} \quad R \mapsto \begin{pmatrix} \omega & 0 \\ 0 & \overline{\omega} \end{pmatrix}, \quad F \mapsto \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \text{“standard”}.
\]

An isotypic component is spanned by the vectors that transform according to a given representation. To put it formally, for a \( n \)-dimensional representation \( \rho \), we are looking to characterize \( n \)-tuples of vectors from our Hilbert space \( \mathcal{H} \) such that
\[
\text{(40)} \quad (\phi_1(Sx), \ldots, \phi_n(Sx)) = (\phi_1(x), \ldots, \phi_n(x))\rho(S)^T,
\]
for each \( S \in S \). The right-hand side should be interpreted as matrix multiplication of a \( \text{dim}(\mathcal{H}) \times n \) matrix by an \( n \times n \) matrix.

It is, of course, the 2-dimensional standard representation that we are interested in. But as a simpler example, we consider the alternating representation first (trivial representation being too simple). We start with the fundamental domain of the action of group \( S \) on the hexagon, shaded and numbered 1 in Fig. 11(b). We put an arbitrary function \( \psi \) in this domain. The operation \( F \) reflects it into subdomain 6, while the representation tells us we need to multiply it by \(-1\), see
The operation $R$ rotates it into subdomain 3, while the representation tells us we need to multiply it by 1. Continuing in this manner we populate the entire domain by copies of $\psi$, Fig. 11(b). We remark that in subdomains 2, 4 and 6 the function $\psi$ has actually been flipped (indicated by arrows).

To reduce the problem to the fundamental domain, we remember that the function schematically drawn in Fig. 11(b) has to satisfy the (external) boundary conditions and has to be continuously differentiable across the internal boundaries of the subdomains. The latter are simple: $\psi$ has to be zero on the long sides of the subdomain. Denoting the boundary values of $\psi$ by $f$ and $g$ on the short sides, we rotate this by $2\pi/3$, Fig. 11(c), compare it with the boundary conditions on the hexagon, Fig. 2(c) and observe that the ratio of $g$ and $f$ must be equal to $\omega_2/\omega_1 = \omega^2 = \overline{\omega}$. This fixes the boundary conditions for the short sides, Fig. 11(d). The arrows are added to indicate orientation.

In Fig. 11(e) we show the result of the analogous computation for the trivial representation. The only difference is that the subdomains 2, 4 and 6 get (flipped) function $\psi$ with no minus sign and the long sides of the fundamental subdomain get Neumann conditions.

To find the quotient of the operator by the standard representation, we need to consider a pair of functions, therefore we use two copies of the hexagon. In Fig. 12(a) we put the pair $(\psi, \xi)$ into the subdomains 1 and 1' correspondingly. Then we populate other subdomains by mapping the functions by the symmetry operators and transforming them by the corresponding representation. For example, horizontal reflection maps subdomains $(1,1')$ into subdomains $(6,6')$, where we should...
Figure 12. Constructing the isotypic component corresponding to the standard representation (a-b). The 2-vector functions are represented by two copies of the domain. Finding the boundary conditions imposed on the functions \( \psi \) and \( \xi \) (c-d). We find the boundary conditions on the copy of \( \xi \) which is located in subdomain 6 of the first component (it is, of course, equivalent to finding the conditions on the “original” copy of \( \xi \)).

Finally, we choose a subdomain of the pair of hexagons that fully describes the functions in the whole hexagons. One can choose the pair \((1, 1')\) of the subdomains, or the pair 1 and 6, or the part of the first domain shown by dashed lines in Fig. 12(c). This step is essentially choosing the “fundamental domain” of the action of group and representation on the pair of hexagons.

The latter choice gives the cleanest result. The relations between \( f \) and \( g \), \( h \) and \( k \) and the values on the two dotted lines are worked out by comparing Fig. 12 with Fig. 2(c) and using continuity properties of \( \xi \). The result is shown in Fig. 12(d). This is the origin of the operator \( Q \) used in the proof of Theorem 2.1.

Some remarks are in order. The function in the second hexagon, Fig. 12(b) is just a reflection of the function in the first one. It’s easy to see that that the two functions are orthogonal. They are also orthogonal to any function from the isotypic component of the alternating representation, Fig. 11(b), or the trivial representation. Together, the functions from trivial, alternating and two components of the standard representation span the entire space \( \mathcal{H}(\vec{k}) \).

B.2.2. \( R \) and \( V \) symmetry. On the face of it, the group generated by \( R \) and \( V \) is the group of rotations by \( \pi/3 \), which is abelian and therefore has one-dimensional representations only. However,
Figure 13. The isotypic decomposition corresponding to the symmetries $R$ and $V$. Component (a) corresponds to the 1-dimensional representation, component (b), consisting of two parts, corresponds to the 2-dimensional representation.

The symmetry relevant to us, as explained in section 1.4, is $V$ combined with complex conjugation, $\overline{V}$. Since the action of $\overline{V}$ on a function $\phi$ is given by
\begin{equation}
(\overline{V}\phi)(x) = \overline{\phi(Vx)},
\end{equation}
the definition of equivariant vectors, equation (40), has to be modified to
\begin{equation}
(\overline{\phi_1(Vx)},...,\overline{\phi_n(Vx)}) = (\phi_1(x),...,\phi_n(x))\rho(T).
\end{equation}
This shows that the representation of $V$ must be an antiunitary operator — complex conjugation followed by the multiplication by a unitary matrix. Representations combining unitary and antiunitary operators have been fully classified by Wigner [30, Chap. 26] (see also [5] for a summary of the method), who called them “corepresentations”. In short, one looks at the representation of the unitary subgroup (in our case, the cyclic group of rotations $R$) and, from them, follows a simple prescription to construct all corepresentations.

In this case, there are two corepresentations,
\begin{align}
R &: z \mapsto z, & \overline{V} &: z \mapsto \overline{z}, \\
R &: (z_1, z_2) \mapsto (\omega z_1, \overline{\omega z_2}), & \overline{V} &: (z_1, z_2) \mapsto (\overline{z_2}, \overline{z_1}).
\end{align}

The isotypic components corresponding to the above representations are shown in Fig. 13. Note that the component of Fig. 13(a) should be understood as all functions that, up to a multiplication by a unitary constant, have the prescribed form. The subcomponents of Fig. 13(b) are related by the operation $\overline{V}$: inversion plus complex conjugation.

The components are mutually orthogonal and span the whole space. The latter statement can be understood from the following example. Representing the functions on the hexagonal domains as 6-dimensional vectors with entries corresponding to the subdomains starting with the lowest one and ordered counter-clockwise, we can expand the real function supported in the first subdomain as follows,
\begin{equation}
(f, 0, 0, 0, 0, 0) = \frac{1}{6} (f, \overline{f}, f, \overline{f}, f, \overline{f}) - \frac{i}{6} (if, i\overline{f}, if, i\overline{f}, if, i\overline{f}) \\
+ \frac{1}{3} (f, 0, \omega f, 0, \overline{\omega f}, 0) + \frac{\omega}{3} (\overline{\omega f}, 0, \omega f, 0, f, 0),
\end{equation}
Above, the complex conjugation on $f$ was added only to highlight the correspondence with Fig. 13 note that the first two vectors both belong to the first isotypic component.

As before, the doubly degenerate eigenvalues come from the component corresponding to the 2-dimensional representation. We choose as the fundamental domain the first two triangles of the
Figure 14. The isotypic decomposition of the space $\mathcal{H}(\pm \vec{k}^*)$ in the presence of symmetries $R$ and $F_V$. All components correspond to 1-dimensional representations.

first component. The boundary conditions can be worked out exactly as in section 4.2.1 and the result is, remarkably, identical.

B.2.3. $R$ and $F_V$ symmetry. In this section we investigate what happens if the operator is symmetric with respect to rotation $R$ and vertical reflection $F_V$, but not horizontal reflection $F$ or inversion $V$.

In the dual space and $k$ coordinates, the vertical reflection acts as the matrix

$$\hat{F}_V = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

and therefore preserves the line $k_2 = k_1$. The special points $\pm \vec{k}^*$ are not on this line and therefore do not benefit from the “pure” symmetry $F_V$. However, the vertical reflection followed by complex conjugation, denoted by $\overline{F}_V$, preserves the line $k_1 = -k_2$ and, therefore, the special points $\pm \vec{k}^*$. The group generated by $R$ and $\overline{F}_R$ is $S_3$, yet we should be looking at corepresentations, of which there are three, all one-dimensional,

$$\begin{align*}
R &: z \mapsto \omega z, \\
\overline{F}_V &: z \mapsto \overline{z}.
\end{align*}$$

The corresponding isotypic decomposition is shown in Fig. 14.

In conclusion, a typical problem with these symmetries is not expected have any conical points in its dispersion relation. According to Theorem 4.1 there will still be generic degeneracies at the point $\vec{0}$ but those are not conical.

Appendix C. Perturbation around degenerate point with $F$ symmetry

It is interesting to calculate the matrices $H_1, H_2$ if the degenerate eigenspace has $F$ symmetry. Suppose the basis is chosen such that

$$Ff_1 = f_1, \quad Ff_2 = -f_2.$$ 

This can be done at the special point $K$ if the operator has $R$ symmetry; in section 5.2 we showed that this situation survives even if we weakly break the symmetry $R$.

---

6i.e. one without “accidental” degeneracies; it must be mentioned that the physically intuitive claim that “accidental” degeneracies do not happen generically remains, to a large extent, mathematically unproven; the best result in this direction is by Zelditch [33].
In this case, equation (27) becomes

\[ (1 \ 0 \\
0 \ -1) \ h_{\vec{k}} \ \left( \begin{array}{cc} 1 & 0 \\
0 & -1 \end{array} \right) = h_{\hat{F}\vec{k}}, \quad \hat{F} = \begin{pmatrix} 0 & -1 \\
-1 & 0 \end{pmatrix}. \]

It is easiest to evaluate \( h_{\vec{k}} \) in the direction \( \vec{k}_e = (1, -1)^T \), which is an eigenvector of \( \hat{F} \) with eigenvalue 1, and in the direction \( \vec{k}_o = (1, 1)^T \), which is an eigenvector of \( \hat{F} \) with eigenvalue \(-1\). Remembering that \( h_{-\vec{k}} = h_{\vec{k}} \), we get

\[ (51) \ h_{\vec{k}_e} = \begin{pmatrix} a & 0 \\
0 & c \end{pmatrix}, \quad h_{\vec{k}_o} = \begin{pmatrix} 0 & b \\
b & 0 \end{pmatrix}. \]

In particular, the trace of the derivative matrix in the direction perpendicular to the symmetry line \( k_2 = -k_1 \) is zero and thus the cone can only be tilted in the direction of the symmetry line. If \( R \) symmetry is present, there is no tilt, as mentioned above.

The above picture, where the derivative matrix is diagonal in the direction preserving a symmetry, and has zeros on the diagonal in the orthogonal direction, can be generalized to other space symmetries.

**Proposition C.1.** Let \( H(\vec{k}) \) be an operator depending on quasi-momenta \( \vec{k} \). Assume that at point \( K \) it has a unitary \( \mathbb{C} \)-linear symmetry \( S \) whose eigenspaces we denote \( X_j, j = 1, \ldots \). Consider the basis of the dual \( \vec{k} \)-space, which consists of the eigenvectors of \( \hat{S} = S^* \). If the vector \( \vec{e} \) corresponds to eigenvalue 1 then

\[ \partial_{\vec{e}} H X_j \subset X_j, \quad \text{for all } j. \]

If the vector \( \vec{k} \) corresponds to eigenvalue other than 1 then

\[ \partial_{\vec{k}} H X_j \perp X_j, \quad \text{for all } j. \]

**Appendix D. Berry phase around a conical point**

Here, for completeness, we give a proof of the fact that the Berry phase around a nondegenerate conical point is \( \pi \), which has been formulated as Lemma 5.2. The proof is geometrical in nature and avoids the direct computation used in the original articles [15, 4].

Presence of the antiunitary symmetry \( V \) which squares to \(-1\) allows us to choose special bases for eigenspaces. We will be using the following lemma.

**Lemma D.1.** Let \( A \) be an antiunitary involution on a separable Hilbert space \( X \). Then

1. there is an orthonormal basis \( \{f_j\} \) of vectors such that

\[ Af_j = f_j. \]

2. if \( \dim(X) = 2 \), there exists a basis \( \{\psi, A\psi\} \).

**Proof.** To prove the first part, we start with an arbitrary basis \( \{\psi_j\} \). Then the vectors

\[ f_j^+ = \psi_j + A\psi_j, \quad \text{and} \quad f_j^- = i(\psi_j - A\psi_j) \]

both satisfy \( Af = f \) and have the vector \( \psi_j \) in their span. Therefore, the set \( \{f_j^+, f_j^-\} \) spans the whole space and can be made into a orthonormal basis by applying the Gram-Schmidt process. This preserves property (52) since all coefficients arising in the process are real:

\[ (f, f') = (Af, Af') = (f, f') \in \mathbb{R}. \]

To get the second part from the first we start with the orthonormal basis \( \{f_1, f_2\} \) satisfying (52) and then take

\[ \psi = (f_1 + if_2)/\sqrt{2}, \quad A\psi = (f_1 - if_2)/\sqrt{2}, \]

which can be checked to be orthonormal. \( \square \)
Now we are in the position to prove Lemma 5.2.

**Proof of Lemma 5.2.** Representing the parameters around the location of the conical point in polar form we will study the limiting eigenvectors

\[ \psi^0_\pm(\theta) = \lim_{r \to 0} \psi^\pm(r, \theta), \]

where \( \psi^- \) and \( \psi^+ \) are the eigenvectors of the lower and upper branches of the cone, correspondingly. We normalize these eigenvectors and fix the phase to have

\[ V\psi^\pm = \psi^\pm. \]

Because the cone is nondegenerate (and thus \( |\lambda_1^+(\theta) - \lambda_1^-(\theta)| > 0 \)), the limit exists and is continuous in \( \theta \), see equation (19).

The functions \( \psi^0_-(\theta) \) have a curious property: since the section of the cone by a vertical plane is two intersecting lines, Fig. 15, the vector \( \psi^0_+(\theta + \pi) \) is the same as \( \sigma_1 \psi^0_-(\theta) \), where \( \sigma_1 = \pm 1 \).

We expand \( \psi^0_\pm \) in a fixed basis of eigenvectors at the conical point, which we can choose to be of the form \( \{ \phi, V\phi \} \),

\[ \psi^\pm = \alpha^\pm(\theta)\phi + \beta^\pm(\theta)V\phi. \]

From condition (54) we immediately get \( \beta^\pm = \overline{\alpha^\pm} \). On the other hand, the vectors \( \psi^0_+ \) and \( \psi^0_- \) are orthogonal, leading to the condition

\[ \overline{\alpha^+}\alpha^- + \overline{\alpha^-}\alpha^+ = 0 \quad \text{or} \quad \alpha^+\alpha^- \in i\mathbb{R}. \]

From normalization of \( \psi^0_\pm \), we conclude that \( \alpha^- = i\alpha^+\sigma_2 \), where \( \sigma_2 = \pm 1 \). We therefore get

\[ \alpha^+(\theta + \pi) = \alpha^-(\theta)\sigma_1 = i\alpha^+(\theta)\sigma_1\sigma_2, \]

and, therefore,

\[ \alpha^+(\theta + 2\pi) = (i\sigma_1\sigma_2)^2\alpha^+(\theta) = -\alpha^+(\theta). \]

\[ \square \]

We remark that in the proof above, the overall sign \( \sigma_1\sigma_2 \) determines the direction of rotation of the vectors \( \psi^0_\pm(\theta) \) in the two-dimensional space.

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