Effective theory of quadratic degeneracies

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We present an effective theory for the Bloch functions of a two-dimensional square lattice near a quadratic degeneracy point. The degeneracy is protected by the symmetries of the crystal, and breaking these symmetries can either open a bandgap or split the degeneracy into a pair of linear degeneracies that are continuous to Dirac points. A degeneracy of this type occurs between the second and third TM bands of a photonic crystal formed by a square lattice of dielectric rods. We show that the theory agrees with numerically computed photonic bandstructures, and yields the correct Chern numbers induced by parity breaking.

In a two-dimensional crystal with a square-lattice ($C_{4v}$) symmetry, it may happen that a pair of bands are degenerate at a point of high symmetry, such as the center (Γ) or corner (M) of the Brillouin zone. An example of this occurs in a photonic crystal formed by a square lattice of dielectric rods. As shown in Fig. 1(a), the second and third TM bands exhibit a quadratic degeneracy at the M-point. The existence of this degeneracy is independent of details such as the permittivity and radius of the rods, as long as the $C_{4v}$ symmetry is preserved. This degeneracy is of particular interest since Wang et. al. have recently shown that it can be lifted by gyromagnetic effects, which break parity and time-reversal symmetry, and that the bandgap opened in this way is populated by a one-way edge mode analogous to chiral electronic one-way edge modes were first predicted by Haldane and Raghu, who argued that they typically occur in systems possessing “Dirac points”, meaning that the modes near each degeneracy point can be described by an effective Dirac Hamiltonian. Although Dirac points have been extensively analyzed in the condensed-matter literature, there has been, to the best of our knowledge, no analogous study of these quadratic degeneracies. Since the system proposed by Wang et. al. currently appears to be the most promising for realizing electromagnetic one-way edge modes, due to its large relative bandgap, there is a present need for an effective theory of such degeneracies.

In this paper, we present an effective theory that describes the bands near a degeneracy point, based on the symmetry properties of $k$-space around that point. We show that the quadratic degeneracy in the $C_{4v}$ crystal can be regarded as a pair of linear degeneracies, analytically continuous to Dirac points, that are “pinned” to the same $k$-space point by the crystal symmetry. The quadratic degeneracy is robust against perturbations that preserve this symmetry. It can be lifted by parity and time-reversal symmetry breaking (which we will henceforth simply refer to as parity breaking.) In that case, the two bands acquire Chern numbers of ±1, in agreement with the numerical result of Wang et. al. Breaking the 90° rotational symmetry “unpins” the quadratic degeneracy point, which splits apart into two distinct linear degeneracies. The theory applies to any two-dimensional Bloch system, whether electronic or photonic, with $C_{4v}$ symmetry and a quadratic degeneracy point. In particular, we show that it accurately describes the aforementioned photonic crystal of dielectric rods for a wide range of dielectric contrasts and rod radii.

Let us consider a crystal in which two bands are degenerate at a point $\vec{k} = \vec{k}_M$, with unbroken $C_{4v}$ symmetry. We choose a pair of independent Bloch functions at $\vec{k}_M$, denoted by $u^1_M(\vec{r})$ and $u^2_M(\vec{r})$. The Bloch functions at neighboring values of $\vec{k}$ can be written as

$$u^1_k(\vec{r}) = c_{11}(\vec{k}) u^1_M(\vec{r}) + c_{12}(\vec{k}) u^2_M(\vec{r})$$
$$u^2_k(\vec{r}) = c_{21}(\vec{k}) u^1_M(\vec{r}) + c_{22}(\vec{k}) u^2_M(\vec{r}).$$

(1)

The mixing elements $c_{nm}(\vec{k})$ can be related to the mode...
frequencies, \( \omega_n(\vec{k}) \), through an eigenvalue equation

\[
H(\vec{k}) \begin{bmatrix} c_{n1}(\vec{k}) \\ c_{n2}(\vec{k}) \end{bmatrix} = \lambda_n(\vec{k}) \begin{bmatrix} c_{n1}(\vec{k}) \\ c_{n2}(\vec{k}) \end{bmatrix},
\tag{2}
\]

where the “effective Hamiltonian” \( H(\vec{k}) \) is a 2 \times 2 matrix whose eigenvalues are, by definition, \( \lambda_n(\vec{k}) \equiv \omega_n(\vec{k}) - \omega_0 \). We will not be concerned with the value of the “zero-point” frequency \( \omega_0 \). Now, suppose we alter the system that we used for defining \( u^1_M(\vec{r}) \) and \( u^2_M(\vec{r}) \), such as by breaking some of its symmetries. If the perturbation is sufficiently weak, the Bloch functions of the altered system can still be described by (1) for \( \vec{k} \sim \vec{k}_M \), with some new choice of \( c_{nm}(\vec{k}) \) and hence of \( H(\vec{k}) \).

In this system, we will be interested in three different symmetry-breaking operations. Firstly, we could “shear” the lattice by rotating the basis vectors as follows:

\[
\vec{a}_1 = a (\cos \theta, \sin \theta) \\
\vec{a}_2 = a (\sin \theta, \cos \theta),
\tag{3}
\]

where \( a \) denotes the lattice constant. This breaks the symmetry under \( C_4 \) rotations and reflections about the \( x \) and \( y \) axes. Secondly, we could distort the rods by stretching them along the \( x \) or \( y \) axes—or, alternatively, stretching the lattice vectors and rescaling \( k_x \) and/or \( k_y \); this breaks the symmetry under rotations and reflections about \( y = \pm x \). Thirdly, we could break parity, which can be accomplished in a photonic crystal, e.g., using a magneto-optic effect that adds an imaginary off-diagonal term \( \mu_{xy} = i\eta \) to the permeability tensor of the rods.

The goal is to find an effective Hamiltonian that describes bands such as those in Fig. 1 including the results of the above symmetry-breaking operations. We claim that the desired Hamiltonian has the following form:

\[
H = \lambda_0 \left[ \sum_{i=1}^3 \sigma_i + \beta(\kappa_x^2 - \kappa_y^2) \sigma_1 + 2\kappa_x \kappa_y \sigma_3 + \gamma |\vec{\kappa}|^2 \right],
\tag{4}
\]

where \( \vec{\kappa} \equiv \vec{k} - \vec{k}_M \) is the \( k \)-space displacement from the degeneracy point and \( \sigma_i \) are the usual Pauli matrices. The phenomenological parameter \( \lambda_0 \) determines the frequency scale, \( \beta \) and \( \gamma \) control the relative curvatures of bands along different directions, \( \alpha_1 \) controls the relative lengths of the two lattice vectors, \( \alpha_2 \) is proportional to the parity-breaking permeability component \( \eta \), and \( \alpha_3 \) is proportional to the shear angle \( \theta \) defined in (3). This Hamiltonian is valid in the neighborhood of \( \kappa = 0 \), and we have omitted \( O(\kappa^4) \) terms which have negligible effects on the band properties in the regime of interest. Furthermore, we assume that the symmetry-breaking is weak (e.g., \( \theta \ll 1 \)), and thus retain only symmetry-breaking terms that are zeroth-order in \( \kappa \).

Before discussing the validity of the ansatz (3), let us determine its band structure and then show that it is consistent with the symmetries of the system. First, consider

\[
\lambda \pm (\vec{k}) / \lambda_0 = \gamma |\vec{\kappa}|^2 \pm \sqrt{\gamma^2 |\vec{\kappa}|^4 + (\beta^2 - 1)(\kappa_x^2 - \kappa_y^2)^2 + \alpha_2^2}.
\tag{5}
\]

Suppose we assume \( \beta = 1 \) (setting \( \beta \neq 1 \) simply distorts the bandstructure along the \( \kappa_x = \pm \kappa_y \) directions). For \( \alpha_2 = 0 \), (5) then reduces to a pair of quadratic bands \( \lambda \pm (\vec{k}) = (\pm 1)|\vec{\kappa}|^2 \), which meet at \( \vec{k} = 0 \). The parameter \( \gamma \) controls the relative curvatures of the two bands. For instance, when \( \gamma = 0 \), the bands have equal and opposite curvatures, as shown in Fig. 2(a); when \( -1 < \gamma < 0 \), the two bands curve in opposite directions but the upper band is flatter, as in Fig. 2(c). Setting \( \alpha_2 \neq 0 \) lifts the degeneracy and opens a bandgap \( \Delta \lambda = 2\lambda_0\alpha_2 \). The two bands will curve in the same direction at \( \vec{k} = 0 \), as observed in Fig. 2 of Wang et al. and in Fig. 1(b) of the
can be thought of as a vertical relative displacement of the line \( \kappa \) states from a discontinuity to a linear “dip” centered at \( \kappa \).

Chern number is a topological quantity and cannot be our theory only describes weak symmetry-breaking, the values of \( \alpha \) the degeneracies are located at an intermediate location, so the calculation are given in the Appendix, and the result is edges, dropping to zero inside the band gap.

When \( \gamma = 0 \) and \( \beta = 1 \), this reduces to a two-dimensional Dirac Hamiltonian near each each degeneracy point (or “Dirac point”). Furthermore, \( \alpha_2 \) plays the role of a mass term, opening a bandgap \( \Delta \lambda = 2\alpha_0 \alpha_2 \). Setting \( \gamma \neq 0 \) distorts the Dirac Hamiltonian and its eigenvalue spectrum; for example, the Dirac cones in the \( \alpha_2 = 0 \) limit become tilted in \( k \)-space, as shown in Fig. 3(d). Along the line \( \kappa_y = \pm \kappa_x \), the splitting of the degeneracy point can be thought of as a vertical relative displacement of the two parabolic bands (note, however, that the bands meet only at isolated points in the full \( k \)-space.) The splitting is accompanied by a change in the density of states from a discontinuity to a linear “dip” centered at the frequency of the band degeneracy. When \( \alpha_2 \neq 0 \), the density of (TM) states is discontinuous at the band edges, dropping to zero inside the band gap.

The situation is very similar for \( \alpha_1 \neq 0 \). When \( \alpha_2 = \alpha_3 = 0 \), the degeneracy splits into two, but along the line \( \kappa_y = 0 \) (if \( \alpha_1 > 0 \)) or \( \kappa_x = 0 \) (if \( \alpha_1 < 0 \)), instead of \( \kappa_x = \pm \kappa_y \). When both \( \alpha_1 \) and \( \alpha_3 \) are nonzero, the degeneracies are located at an intermediate location, \( \kappa_{\pm} = \pm (\alpha_1^2 + \alpha_3^2)^{1/4}(\cos \phi, \sin \phi) \), where \( \tan \phi = \alpha_3/\alpha_1 \), and expanding around each point yields a Dirac-like Hamiltonian analogous to [7].

When \( \alpha_2 \neq 0 \), the bands are non-degenerate, and their Chern numbers can be calculated. The details of this calculation are given in the Appendix, and the result is that the upper and lower bands possess Chern numbers \( -\text{sgn}(\alpha_2) \) and \( \text{sgn}(\alpha_2) \) respectively, regardless of the values of \( \alpha_1 \), \( \alpha_3 \), \( \beta \), and \( \gamma \). This implies the existence of a single family of one-way edge modes\[3\], and agrees exactly with the numerical results of Wang et al.\[3\]. Although the effective Hamiltonian \[3\] is only valid near \( \kappa = 0 \), it yields the same Chern number as the actual band-structure because only the region near the broken degeneracy point provides a non-vanishing “Berry flux” contribution to the Chern number\[3\]. Furthermore, while our theory only describes weak symmetry-breaking, the Chern number is a topological quantity and cannot be altered by non-perturbative distortions (as long as the bands remain non-degenerate\[3\]), which is why it remains unchanged even in the strong parity-breaking regime explored by Wang et al. When \( \alpha_1 \) and/or \( \alpha_3 \) are non-zero, the two linear degeneracy points each contribute \( \pm 1/2 \) to the Chern number, in accordance with previous analyses of the Dirac Hamiltonian\[3\]. When \( \alpha_1 = \alpha_3 = 0 \), the Berry connection winds twice as fast around the point \( \kappa = 0 \), which provides the entire contribution of \( \pm 1 \). The dependence of the Chern number on the sign of \( \alpha_2 \) confirms that \( \alpha_2 \) controls parity breaking, since the Chern number can be shown to vanish identically when parity is unbroken.

The fully symmetric Hamiltonian \( H_0 \equiv H|_{\alpha_i=0} \) must transform under any operation \( g \in \mathcal{C}_{4v} \) as

\[
D(g)H_0(\kappa)D^{-1}(g) = H_0(g\kappa).
\]

Regardless of the values of \( \beta \), \( \gamma \), and \( \lambda_0 \), this holds if \( D(g) \) falls under \( E \), the only two-dimensional irreducible representation of \( \mathcal{C}_{4v} \). Thus, \( \pm 90^\circ \) rotations can be represented by \( \pm i\sigma_2 \), reflections about the \( \kappa_x \) (\( \kappa_y \)) axes by \( \sigma_1 \) (\( -\sigma_1 \)), and reflections about \( \kappa_{\pm} = \pm \kappa_x \) by \( \pm \sigma_3 \).

By studying how \( H(\kappa) \) transforms under \( E \), we can show that the quadratic degeneracy is protected by the crystal symmetry. Any zeroth-order term proportional to the identity matrix, when added to \( H_0 \), simply shifts the eigenvalues without opening a gap. Adding a zeroth-order term proportional to \( \sigma_1 \) (i.e. \( \alpha_1 \neq 0 \)) breaks \( \mathcal{C}_{4v} \) since, under the representation \( E \), \( \alpha \rightarrow -\alpha \) for \( 90^\circ \) rotations and reflections across \( \kappa_x = \pm \kappa_y \). Note that \( \alpha \rightarrow \alpha \) for reflections across the \( \kappa_x \) and \( \kappa_y \) axes, in agreement with our claim that \( \alpha_1 \neq 0 \) corresponds to stretching the lattice. Similarly, setting \( \alpha_2 \neq 0 \) preserves the rotational symmetries but breaks the reflection symmetries (parity). Finally, setting \( \alpha_3 \neq 0 \) preserves the reflection symmetry across \( \kappa_x = \pm \kappa_y \) but breaks the symmetry under \( 90^\circ \) rotations and reflections across \( \kappa_x = 0 \) and \( \kappa_y = 0 \).

Furthermore, the Hamiltonian cannot include terms that are first-order in \( \kappa \) if the \( \mathcal{C}_{4v} \) symmetry is unbroken or only partially broken. Such terms have the general form \( \Delta H = \sum_{i,j=1}^{3} \sum_{\kappa_{\pm}} \kappa_{i}\kappa_{j}\sigma_{i}\sigma_{j} \), and we can show that \( c_{ij} = 0 \) for all \( i,j \) as long as the system is symmetric under either rotations, reflections about the \( \kappa_x \) and \( \kappa_y \) axes, or reflections about \( \kappa_{\pm} = \pm \kappa_y \). At least one of these symmetries is preserved by each of the three “elementary” distortions discussed above. This situation may be contrasted with a triangular or honeycomb lattice, for which there is a \( \mathcal{C}_{3v} \) symmetry around each corner of the hexagonal Brillouin zone. There, one can write down an \( O(\kappa) \) Hamiltonian which transforms under a two-dimensional irreducible representation of \( \mathcal{C}_{3v} \): this is just the Dirac Hamiltonian

\[
H'(\kappa) = \lambda_0 (k_x\sigma_1 + k_y\sigma_3).
\]

In this case, a zeroth-order “mass” term proportional to \( \sigma_2 \) controls parity breaking\[3\].

We checked the validity of the ansatz \[3\] and computed the parameters \( \alpha_i \), \( \beta \), and \( \gamma \) using the MPB\[3\] and
In particular, we showed that quadratic nature of the degeneracy is protected by the $C_{4v}$ symmetry. We have also shown that the theory accurately describes the second and third TM bands of square-lattice photonic crystals near their M-point degeneracy, including the correct Chern numbers when parity is broken. On the other hand, the theory should be applicable to any electronic or photonic system possessing $C_{4v}$ symmetry and a two-fold band degeneracy; it is possible, for instance, to construct tight-binding electronic models that reduce to our effective Hamiltonian near a degeneracy point. The advantage of the present method is that it relies only on symmetry principles, and can therefore be applied to systems, such as photonic crystals, where other methods such as tight-binding are not applicable. For lattice symmetries other than $C_{4v}$, effective Hamiltonians can be constructed by finding an appropriate representation of the symmetry group.

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APPENDIX: CALCULATING THE CHERN NUMBER

In this Appendix, we describe the calculation of the Berry connection and Chern number for the bands associated with our effective Hamiltonian. We will consider the lower band $|\psi^- (\vec{k})\rangle$; the calculation for the upper band proceeds analogously.

First, consider $\alpha_1 = \alpha_3 = 0$. We note that the eigenvectors of the effective Hamiltonian do not depend on $\gamma$ since that parameter multiplies the identity matrix. For simplicity, we set $\beta = 1$. The eigenvector corresponding to the lower band is

$$|\psi^- (\vec{k})\rangle = \frac{1}{\sqrt{2[\kappa^4 + \alpha^2 + \kappa^2 \sqrt{\kappa^4 + \alpha^2} \sin 2\phi]}} \times \left[ \begin{array}{c} -\kappa^2 \cos 2\phi + i\beta \\ \kappa^2 \sin 2\phi + \sqrt{\kappa^4 + \alpha^2} \end{array} \right], \quad (A.1)$$

regardless of the values of $\gamma$. Here, $(\kappa, \phi)$ is the cylindrical coordinate representation of $\vec{k}$. The Berry connection is

$$\vec{A}^- (\vec{k}) = \langle \psi^- (\vec{k}) | \nabla_{\vec{k}} | \psi^- (\vec{k}) \rangle = i\alpha_2 \kappa \left( \cos 2\phi \hat{k} - \sin 2\phi \hat{\phi} \right) \left( \kappa^4 + \beta^2 \sqrt{\kappa^4 + \alpha^2} \sin 2\phi \right). \quad (A.2)$$

To obtain the Chern number, we integrate the Berry connection around a loop $\kappa = \kappa_0$:

$$C^- = \frac{1}{2\pi i} \int_{\kappa=\kappa_0} d\vec{k} \cdot \vec{A}^- (\kappa) = \frac{-2\alpha_2}{\pi} \int_0^{2\pi} \frac{\kappa_0^2 \sin 2\phi d\phi}{\kappa_0^4 + \alpha_2^2 + \kappa_0^2 \sqrt{\kappa_0^4 + \alpha_2^2} \sin 2\phi}. \quad (A.3)$$

The integral can be performed via the substitution $\sin 2\phi = \tanh u$, and we obtain

$$C^- = \text{sgn}(\alpha_2) - \frac{\alpha_2}{\sqrt{\kappa_0^4 + \alpha_2^2}} \rightarrow \text{sgn}(\alpha_2) \text{ for } |\alpha_2| \ll \kappa_0^2. \quad (A.4)$$

As discussed in the text, the above result remains unchanged even when we enter the non-perturbative regime, even though our effective theory is only valid for small values of $\kappa$ and $\alpha_i$.

When $\alpha_1$ and/or $\alpha_3$ are non-zero, the band maximum at $\kappa = 0$ splits into two distinct maxima, and expanding around each maximum yields a Dirac-like Hamiltonian. For instance, when $\alpha_1 = 0$ and $\alpha_3 \neq 0$ the maxima occur at $\kappa_{\pm} = \pm(\sqrt{\alpha_3^2/2}, -\sqrt{\alpha_3^2/2})$, and the Hamiltonian near each of these points is given by (7). In terms of the variables $q_1$ and $q_2$ defined in (9), the Berry connection for the lower band is

$$\vec{A}_\pm (\vec{q}) = \pm \frac{ib}{2} \cdot \frac{\cos \phi \hat{q} + \sin \phi \hat{\phi}}{q_1^2 + b^2 \pm q \sqrt{q_1^2 + b^2} \sin \phi}, \quad (A.5)$$

where $b \equiv \alpha_2/\sqrt{\alpha_3}$, $\pm$ refers to which maximum we are expanding around, and $(q, \phi)$ is the cylindrical coordinate representation of $\vec{q}$. This Berry connection has the same form as (A.2), but winds half as quickly around each maximum point as (A.2) does around $\vec{k} = 0$. Each maximum thus contributes $\text{sgn}(\alpha_2)/2$ to the Chern number of the lower band.

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1. Z. Wang, Y. D. Chong, J. D. Joannopoulos, and M. Soljačić, Phys. Rev. Lett. 100, 013905 (2008).
2. R. E. Prange and S. M. Girvin, ed. The Quantum Hall Effect. (Springer-Verlag, New York, 1987).
3. F. D. M. Haldane and S. Raghu, Phys. Rev. Lett. 100, 013904 (2008).
4. S. Raghu and F. D. M. Haldane, cond-mat/0602501.
5. F. D. M. Haldane, Phys. Rev. Lett. 61, 2015 (1988).
6. B. Simon, Phys. Rev. Lett. 51, 2167 (1983).
7. Y. Hatsugai, Phys. Rev. Lett. 71, 3697 (1993).
8. S. G. Johnson and J. D. Joannopoulos, Opt. Express 8 173 (2001).
9. Comsol Multiphysics 3.3, COMSOL Inc. www.comsol.com