Band structure degeneracies and edge states in square lattice media and their deformations

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Abstract

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We study the spectral properties of conservative linear wave systems modeling two-dimensional periodic "bulk" media, as well as "edge" media formed by the junction of two distinct bulk media. In both scenarios, we consider the cases of (1) periodic bulk media possessing the symmetries of a square lattice, and (2) linear deformations of such media. The dissertation is divided in two parts:

In part one, we begin with a spatially infinite bulk medium modeled by the Schrödinger operator $H = \quad + V$, where the potential V is real-valued, periodic with respect to a square lattice, and invariant under the symmetry group of the square. The band structure of H is known to contain *quadratic band degeneracy points* [43, 44]; see also [8]. We prove that, under typical small linear deformations of V, each quadratic band degeneracy splits into a pair of nearby (tilted, elliptical) conical degeneracies, or *Dirac points*. Further, we show that both types of degeneracies are lifted upon the introduction of appropriate symmetry-breaking perturbations, and discuss the topology of the now non-degenerate bands.

In part two, we consider a class of Schrödinger operators, modeling either an undeformed or deformed square lattice bulk medium, perturbed by a spatially non-compact line defect commensurate with the underlying periodic bulk medium. For both cases (1) and (2), we construct *edge states*, which propagate parallel to the interface but are localized transverse to it. The edge states bifurcate from the band structure degeneracies associated with the unperturbed bulk medium; the bifurcation is controlled by *effective (homogenized) edge Hamiltonians* derived via multiple-scale analysis. In case (1), the bifurcation is governed by a matrix Schrödinger operator; in case (2), it is governed by a pair of Dirac operators. We present analytical results as well as numerical simulations, all consistent with the *bulk-edge correspondence principle* of topological physics.

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1. Introduction

A wave is a propagating disturbance which transports energy through space. Waves are ubiquitous in nature, and have motivated many of the earliest studies of classical physics. A familiar example is the appearance of ripples which spread across a body of water after a droplet has fallen onto its surface. Other examples include the longitudinal compression and rarefaction of fluids giving rise to sound, or the transverse oscillation of electric and magnetic fields which make up visible light. In fact, modern physics has revealed the presence of wave phenomena at the smallest of length scales (e.g., the quantum mechanical, wave-particle description of electrons), as well as the largest (e.g., gravitational waves emitted during a collision of supermassive black holes). Waves remain the subject of much physics and mathematics research today, and continue to inspire the work of scientists and engineers pursuing various technological advancements; see, e.g., Section 1.3.

In this dissertation, we analyze wave behavior in media which are *periodic*, or repeat in space. In such systems, their dynamics are encoded in a mathematical object known as the *band structure*, consisting of a collection of dispersion relations and associated "generalized" eigenstates. Of particular interest are the dynamics of *wavepackets*, made up by a carrier wave which oscillates on the spatial scale of the underlying periodic medium, modulated by an envelope which decays over a much larger scale. Wavepackets spectrally supported in most regions of the band structure evolve rather ordinarily: the envelope propagates at the group velocity and eventually disperses; see Section 1.2.1. However, those supported near non-generic, degenerate points within the band structure may have extremely unusual behavior. Further, these band structure degeneracies are at the heart of topological phenomena observed in spatially infinite "bulk" media (Section 1.2.2), as well as those in "edge" media formed by the junction of different bulk media. Particularly, topologically protected *edge states*, which propagate along the interface and decay into the neighboring bulk media, are stable against (possibly very large) localized perturbations to the edge (Section 1.2.3).

More specifically, the work presented in this dissertation (divided in two parts) is summarized as follows:

1. In the first part, we introduce a class of models bridging two distinct families of band structure degeneracies via the introduction of weak and nonsingular, but otherwise totally general, linear deformations to an infinite periodic square lattice medium. We show that, for deformations which break rotational

invariance, a single quadratic band degeneracy point splits into a pair of conical degeneracies, or Dirac points. An overview of the model and a summary of results is presented in Section 1.3.1.

2. In the second and final part, we introduce two classes of models of interfaces between periodic bulk media, analogous to those considered in [16]. The periodic bulk media we consider possess the symmetries of a square lattice, or are deformed versions of such media, the spectral properties of which are developed in part one. We study these models using multiple-scale analysis and provide numerous computational demonstrations of their proven and conjectured properties. An overview of the models and a summary of results is presented in Section 1.3.2.

We remark on open questions in Section 1.4 to conclude the chapter.

1.1. Physical motivation

Principal sources of motivation for the mathematical research conducted in this dissertation include studies of edge states appearing in the physics literature; we provide a brief survey below.

The integer quantum Hall effect

In two dimensions, the classical *Hall effect* is an electromagnetic phenomenon in which charge carriers in an electrical current are deflected transverse to the direction of current flow due to a uniform external magnetic field applied perpendicular to the conductor. The result is a current in the transverse direction, giving rise to a nonzero off-diagonal component of the antisymmetric electrical conductivity tensor, called the *Hall conductance*.

The *integer quantum Hall effect* is a manifestation of the Hall effect in systems governed by quantum mechanics, in which the Hall conductance is quantized in integer multiples of a fundamental physical constant. It was first observed in 1980 by von Klitzing, Dorda, and Pepper [63], using an apparatus cooled to the temperature of liquid helium, allowing for the observation of a nearly ideal gas of electrons within its two-dimensional "inversion layer". (Their original objective was to measure the fine-structure constant.) Initial analysis of the phenomenon was conducted by Laughlin [46] and Thouless et al. [61] (see also [60]), who presented mathematical explanations for the observed quantization using, respectively, a gauge invariance argument and linear response theory (i.e., the Kubo formula). Later, Halperin [35] refined the argument by

(a)

(b)

Figure 1.1 – [1]Magneto-optic waveguide studied by Wang et al. [65]. (a) Out-of-plane electric field component (transverse-magnetic polarization). A source (double arrow) is located at the interface of a magnetized gyromagnetic (lower half-plane) and a regular (upper half-plane) photonic crystal. The excited edge state propagates rightward. (b) Edge state diagram. The edge state curve (red) monotonically traverses the common bulk band gap of both crystals.

Laughlin, drawing attention to the importance of current-carrying, "quasi-one-dimensional" states localized near the sample perimeter.

Notably, in 1988, Haldane [33] proposed a model which demonstrated quantized Hall conductance with net zero magnetic flux. The model, unlike those proposed earlier, did not see the band structure collapse into Landau levels, and dealt with spatially extended Floquet-Bloch eigenstates rather than localized ones.

Topological photonics

The 1988 work of Haldane further suggested a possible route for realizing quantum Hall effect-like phenomena in photonics settings. Later, in a pair of 2008 works, Haldane and Raghu [34, 54] presented a model of a photonic crystal giving rise to edge states, analogous to the 1988 Haldane model of electronic graphene. In the same year, edge states were observed by Wang et al. [65] in an experimental photonic system.

We discuss the latter in a bit more detail: The experimental set-up consisted of two crystals joined along a horizontal interface. One crystal is important: gyromagnetic (i.e., its magnetic permeability tensor has a complex off-diagonal component), a property which breaks time-reversal symmetry in the presence of an external magnetic field. This magneto-optic effect opens a gap in the photonic band structure. (We

[1]Reprinted with permission from Z. Wang, Y. D. Chong, J. D. Joannopoulos, and M. Soljačić, "Reflection-free one-way edge modes in a gyromagnetic photonic crystal," Physical Review Letters, 100(1):013905, 2008. Copyright 2008 by the American Physical Society.

note that the crystal has the symmetries of a square lattice, and that its band structure exhibits a quadratic band degeneracy when the magnetic field is turned off; see, e.g., Chapter 3. As a result, the gyromagnetic crystal acquires a nontrivial "topological phase". The second crystal is not gyromagnetic, and so remains topologically trivial, but has a common band gap with the first crystal. Hence, the system formed by the junction of both crystals has a band gap; see Figure 1.1a. Using a localized source, the authors excited an edge state wavepacket propagating rightward and decaying both leftward and into the neighboring bulk media; see Figure 1.1b.

The observations are anticipated by the bulk-edge correspondence principle, which roughly quantifies the number of edge state channels in terms of the topological information of the two bulk media which make up the interface system. In this setting, the principle predicts one family of edge stats with a dispersion curve traversing the band gap upward. (In principle, there may be others, but their dispersion curves do not traverse the band gap.) In this case, there is exactly one curve, which increases monotonically over the range of parallel quasimomenta, resulting in edge state wavepackets which are immune to leftward back-scattering.

1.2. Mathematical background

1.2.1. Waves in translation invariant media

We now introduce mathematical concepts fundamental to the discussion of our models and results.

Infinitesimal translation invariance and the Fourier transform

Consider, for example, electromagnetic waves as described by Maxwell's equations. In a vacuum (i.e., with no source charges or currents present), the components of the electric and magnetic fields are independently governed by the wave equation

$$\partial_t^2 u(x;t) = c^2 \Delta_x u(x;t); \tag{1.1}$$

with the additional constraint that the electric and magnetic fields are orthogonal, and that both are orthogonal to the direction of propagation. Here $c > 0$ is the speed of light in vacuum. Taking the Fourier transform of (1.1) in both time and space yields

$$E = E(k) \quad c|k|; \tag{1.2}$$

which relates the wave energy E (proportional to its frequency in time) to a wave vector k (with components proportional to its frequency in each spatial dimension, pointing in the direction of propagation). The functions $k \mapsto E(k)$ are called *dispersion relations*.

That the wave equation (1.1) can be recast into the dispersion relations (1.2) via the Fourier transform is a consequence of the *infinitesimal translation invariance* of the Hamiltonian operator, which governs time evolution. Since the Hamiltonian has constant coefficients, it is invariant under the change of coordinates $x' = x + x_0$, with x_0 any constant vector; equivalently, it commutes with the momentum operator $P_x = -i\partial_x$. The Fourier transform can be thought of as a change of basis operation; the new basis consists of the "generalized eigenstates" of P_x, which are the *plane waves* $x \mapsto e^{ikx}$. That is, any function $x \mapsto f(x)$ can be expressed as a linear superposition of plane waves:

$$f(x) = \frac{1}{2}\int_{\mathbb{R}} e^{ikx}\hat{f}(k)\,dk; \quad \text{where } \hat{f}(k) = \int_{\mathbb{R}} e^{-ikx} f(x)\,dx: \tag{1.3}$$

Since the constant-coefficient Hamiltonian commutes with P_x, it is therefore "diagonalized" by the same set of generalized eigenstates.

Periodicity and Floquet-Bloch (band) theory

Physical systems need not have infinitesimal translation invariance, or be translation invariant at all. However, many are naturally *periodic*, or translation invariant with respect to a regular array of points called a *lattice*. Such systems can be studied using a loose analog of Fourier analysis known as *Floquet-Bloch theory*, or *band theory*; see Section 2.1 and references cited therein. In particular, the dynamical behavior of such systems can also be studied via a set of dispersion relations and associated "generalized eigenstates" of the periodic Hamiltonian; this information is collectively known as the Hamiltonian's *band structure*.

For example, let us consider the initial value problem for the Schrödinger equation

$$\begin{aligned} i\partial_t \psi(x;t) &= H\psi(x;t); \quad \text{where } H = -\partial_x^2 + V(x); \\ \psi(x;0) &= \psi_0(x); \end{aligned} \tag{1.4}$$

for a given initial state $x \mapsto \psi_0(x)$. Assume that the potential $x \mapsto V(x)$ is periodic with respect to some lattice. The band structure of H is given by the collection of Floquet-Bloch eigenpairs $(E_b(k); x \mapsto \psi_b(x;k))$

with $b \geq 1$. The eigenstate $x \mapsto \phi_b(x;k)$ is k-pseudoperiodic and $k \mapsto \phi_b(x;k)$ is periodic with respect to a dual lattice; hence, k can be taken to vary over a compact set known as the Brillouin zone B. The solution to the initial value problem (1.4) can then be expressed as

$$u(x;t) = \sum_{b \geq 1} \int_B e^{iE_b(k)t}\, \tilde{u}_{0;b}(k)\, \phi_b(x;k)\, dk; \quad \text{where} \tag{1.5}$$

$$\tilde{u}_{0;b}(k) = \int_{\mathbb{R}^n} \overline{\phi_b(x';k)}\, u_0(x')\, dx'.$$

In general, obtaining information about the solution (e.g., dispersive estimates) from the expression (1.5) requires methods from harmonic analysis. However, for initial states $x \mapsto u_0(x)$ with speci c spectral properties, one can obtain information about the dynamics by different means, which we discuss below.

Dynamics of wavepackets

Consider the set-up of the initial value problem in the previous section. For simplicity, suppose there exists $b_\star$ such that the dispersion relation $k \mapsto E_{b_\star}(k)$ is non-degenerate, that is, for all $k \in B$ and $b \neq b_\star$, assume $E_b(k) \neq E_{b_\star}(k)$. Now, fix some $k_\star$ and denote $E_\star = E_{b_\star}(k_\star)$. A wavepacket spectrally supported about $(E_\star; k_\star)$ is the solution to (1.4) arising from an initial state of the form

$$u_0(x) = a_0(\epsilon x)\, \phi_{b_\star}(x;k_\star); \tag{1.6}$$

where $x \mapsto \phi_{b_\star}(x;k_\star)$ is the Floquet-Bloch eigenstate associated with $(E_\star; k_\star)$, the slowly varying envelope function $X \mapsto a_0(X)$ is suf ciently smooth and rapidly decaying, and $\epsilon > 0$ is a small parameter; see Figure 1.2 for an example.

The initial state (1.6) is characterized by two spatial scales, represented by the variables x and $X = \epsilon x$, and it is natural to seek a solution to (1.4) with corresponding two-scale character. The solution $u(x;t)$ is given by

$$u(x;t) = e^{iE_\star t} a(\epsilon x; t)\, \phi_{b_\star}(x;k_\star) + O(\epsilon) \text{ as } \epsilon \to 0; \tag{1.7}$$

where, in terms of the slow timescale $T = \epsilon t$, the envelope modulation $X \mapsto a(X;T)$ satis es the initial

(a) (b)

Figure 1.2 – Wavepacket in (a) one, and (b) two spatial dimensions.

value problem

$$\begin{aligned} \partial_T a(X;T) &= v_g(E_?;k_?) \cdot \nabla_X a(X;T); \quad \text{where } v_g(E_?;k_?) = \nabla_k E_{b_?}(k_?); \\ a(X;0) &= a_0(X): \end{aligned} \tag{1.8}$$

This is the *transport equation*, which translates an initial state linearly in time without dispersion. The quantity $v_g(E_?;k_?)$ is known as the *group velocity* at $(E_?;k_?)$, and determines the direction and rate of transport of the wavepacket envelope on a timescale of order $O(\varepsilon^{-2})$. Expanding the $O(\varepsilon)$ correction to (1.8), one finds that the leading contribution has a similar two-scale character, where the envelope is instead governed by an equation describing its dispersion, as determined by the curvature of $E_{b_?}(k)$ at $k_?$. This multiple-scale analysis can be continued to any arbitrary, finite order in ε.

1.2.2. Band structure degeneracies

In the last section, we introduced the dynamics of wavepacket initial conditions spectrally concentrated about a generic non-degenerate point of the band structure. Their behavior (e.g., linear transport at the group velocity at first order, dispersion at the next order, etc.) has so far been nothing too unusual. However, if we instead consider degenerate points within the band structure, the wavepacket dynamics are dramatically different. The local geometry of these *band structure degeneracies*, which similarly determines the behavior of wavepackets, may be constrained by additional *point group* symmetries (e.g., invariance under rotations or reflections about a certain axis) of the underlying periodic medium. Hence, the symmetries a material

possesses directly impact the wavepacket dynamics it supports.

Further, band structure degeneracies are nuclei of topological behavior. Perhaps most explicitly, they can be identi ed as monopoles of the *Berry curvature*, de ned as follows: Consider a single band, separated from the consecutive band by a *band gap*. The collection of all bands below the band gap de nes a ber (vector) bundle over the Brillouin zone, which is equivalent to a torus; each ber is the direct product of all Floquet-Bloch eigenspaces corresponding to each of these bands. The Berry curvature is then the curvature of a connection over this ber bundle, called the *Berry connection*, which describes the parallel transport of the bers as the quasimomentum varies over the Brillouin zone. Integrating the Berry curvature over the entire Brillouin zone results in an integer-valued topological index known as the *Chern number*. The Chern number is a topological invariant: preserved by continuous deformations of the Hamiltonian which do not close the band gap. The class of all such Hamiltonians with equal Chern number forms a connected set, identifying a *topological phase*; moving continuously between phases must require passage through the conducting phase, in which the band gap closes at a band structure degeneracy.

When two materials with differing Chern numbers are joined together, topologically protected *edge states* must propagate along the interface, as ensured by the *bulk-edge correspondence principle*, see Sections 6.2 and 6.3, and references cited therein. Moreover, band structure degeneracies play a key role in the construction of these edge states via multiple-scale analysis; a substantial insight we make use of in the second half of this dissertation.

Conical degeneracies (Dirac points)

A well-known and intensely studied family of band structure degeneracies are *Dirac points*: the (typically) right-circular conical touchings of consecutive dispersion surfaces, now known to arise in the band structures of Hamiltonians modeling two-dimensional periodic media with the symmetries of a honeycomb (hexagonal) lattice; see Figure 1.3. In a 2008 review [5], Berry and Jeffrey indicated that Dirac points have been known for nearly two centuries, dating back to an 1832 study of light in anisotropic crystals by Hamilton, in which he referred to them as “diabolical points”. In 1947, Wallace identi ed Dirac points in his discrete model of the material *graphite* [64], consisting of many layers of *graphene*, an essentially planar hexagonal arrangement of carbon atoms. Fefferman and Weinstein, in 2012, proved that Dirac points generically appear in the band structures of continuum Schrödinger operators with honeycomb lattice potentials [29].

The Wallace model is an example of a discrete, scalar *tight-binding model*, which can be used to

(a) (b)

Figure 1.3 – (a) Dispersion surfaces of the Wallace tight-binding model of graphene. (b) Blow-up in a neighborhood of a Dirac point, located at a vertex of the hexagonal Brillouin zone.

approximate the low-energy dispersion relations of an associated continuum Schrödinger operator in an asymptotic scaling regime characterized by deep potential wells, see [28]. Other examples include the one-dimensional Su-Schrieffer-Heeger (SSH) model of polyacetylene [58], the Hubbard model of electrons in a periodic potential with homogenized short-range electron-electron interactions [39], and the Haldane model [33], which exhibits a generalization of the quantum Hall effect with net zero magnetic ux; see also the discussion in Section 1.2.3. A rigorous derivation of tight-binding models from rst principles, including for magnetic systems and general (not necessarily periodic) discrete sets was presented in [56].

Dirac points are renowned for the novel wavepacket dynamics they induce; the envelope of a wavepacket spectrally supported about a Dirac point evolves according to a Dirac equation [30], which, like the wave equation, is non-dispersive and governs the dynamics of massless particles. An emergent quantity describing the envelope propagation speed is the Fermi or Dirac velocity, analogous to the speed of light in (1.2). The emergence of Berry phase, in the presence of band structure degeneracies, for semi-classically scaled wavepackets is also of interest; see, e.g., [66] and references cited therein.

In the above examples, the Dirac points are right-circular cones, however this need not be the case; in general, the cones can be tilted with elliptical cross-sections, corresponding to a broader class of Dirac operators with advection, or linear transport; see, e.g., [45, Section 5.10]. In the rst part of this dissertation, we analyze a class of models based on deformed square lattices and show that their band structures generically feature pairs of tilted, elliptical Dirac points. This result is a manifestation of the conjecture that Dirac

(a) (b) (c)

Figure 1.4 – Examples of quadratic band degeneracies: (a) One upward- and one downward-facing circular paraboloids (b) Two upward-facing circular paraboloids (c) Hyperbolic paraboloid and upward-facing circular paraboloid.

points are the generic type of band structure degeneracy encountered in the class of self-adjoint second-order periodic, elliptic operators; see, e.g., [13, Conjecture 1], which proves this conjecture in the context of Hermitian matrices depending on three parameters (e.g., those arising as Hamiltonians of two-dimensional tight-binding models).

Finally, we note that Dirac points can also arise in one-dimensional settings as linear band crossings within a one-dimensional band structure (e.g., the SSH model with equal hopping coefficients), and in higher-dimensional settings, where they are identified as two-fold Weyl points [48].

Quadratic band degeneracies

Another class of band structure degeneracies, particularly relevant for the work of this dissertation, are quadratic band degeneracies: locally quadratic touchings of two consecutive dispersion surfaces. A simple example of a quadratic band degeneracy consists of dispersion surfaces meeting at a pair of one upward- and one downward-facing circular paraboloids, but may be a pair of upward- or downward-facing circular paraboloids, or include saddle-like hyperbolic paraboloids; see Figure 1.4. The precise nature of the dispersion surfaces near the degeneracy determine the envelope dynamics of wavepackets spectrally concentrated there; in all cases, these are now governed by a matrix Schrödinger operator.

In a 2008 work by Chong, Wen, and Soljačić [8], the generic approximate character of dispersion surfaces near a quadratic degeneracy was derived using representation theory of the symmetry group of the square, the dihedral group of order eight, denoted C_{4v}. In 2018, using mathematical techniques similar to those of Fefferman-Weinstein, Keller, Marzuola, Osting, and Weinstein (Keller et al. [43, 44]) provided

a rigorous foundation for this characterization for a class of continuum Schrödinger operators with periodic, $\frac{\pi}{2}$-rotationally invariant potentials, which may possibly possess additional symmetries (i.e., the full C_{4v} symmetry group). Their work serves as a starting point for the research presented in this dissertation.

Other work

Finally, we mention a recent study by Drouot and Lyman [15] which studies several other classes of band structure degeneracies arising in three-dimensional crystals. In the same article, Drouot and Lyman also developed a general framework encompassing the approach of Fefferman-Weinstein [26] for extending results on eigenvalue multiplicity in the weak potential limit to the non-perturbative regime.

1.2.3. Edge states

In the previous section, we introduced features arising in the spectral analysis of Hamiltonians modeling spatially in nite, translation invariant continuum "bulk" media. These bulk Hamiltonians support only spatially extended, plane wave-like Floquet-Bloch eigenstates and therefore have purely absolutely continuous spectrum; an initially localized state spreads out and decays in amplitude. We now turn to "edge" media formed by the junction of two bulk media along an interface. Such media are no longer fully translation invariant, and may (or may not) give rise to additional, qualitatively different eigenstates. A conceptually simple interface one may consider is that between a given bulk medium and the vacuum. These models give rise to so-called "surface states" introduced by Tamm in 1932 [53] and Shockley in 1939 [57]; see also the remarks in [24].

In the context of two-dimensional materials, an edge state is a time-harmonic solution of a conservative wave system which propagates plane wave-like parallel to and is localized transverse to a line defect, or edge, separating distinct bulk media. In particular, edge states can be made to appear when the asymptotic bulk media possess different topological indices; such topologically protected states are central to energy transport phenomena in topological condensed matter physics and other elds; we discuss speci c examples below.

Topological physics

The eld of "topological" condensed matter physics originated from the 1980 observation of the integer quantum Hall effect by von Klitzing et al. [63] and the theoretical framework proposed by Thouless et al.

[61] shortly thereafter. Many new directions have since emerged: For example, motivated by an insight by Haldane [33], Kane and Mele showed that a sheet of graphene exhibits a quantum spin-Hall effect within an energy gap at low temperatures [41]; this was an early realization of a topological insulator, made possible by recent advancements in graphene manufacturing. Another example was the inception of topological photonics, owing to predictions by Haldane and Raghu [34, 54], who demonstrated that analogues to the quantum Hall edge currents can occur in photonic crystals; see, e.g., the review [50]. The idea was first realized in Wang et al. [65]. For some further discussion, see Section 1.1 and references cited therein.

Edge states in honeycomb lattice media

The numerous studies of two-dimensional topological materials (either in experiment, numerics, or via tight-binding models) have attracted interest in realizing topologically protected edge states in the setting of continuum PDE models. The first such work was in 2016 by Fefferman, Lee-Thorp, and Weinstein [25], in which they studied a family of Schrödinger operators with honeycomb lattice potentials perturbed by a slowly varying "edge potential" modeling a spatially unbounded line defect. Similarly constructed models have since been widely considered (see the citations in Section 1.3.2); we make use of the construction here as well. The edge states they derive are first approximated through a formal multiple-scale analysis argument, making use of the slow variation of the structure transverse to the line defect. At leading order, these have a wavepacket-like character consisting of a plane wave-like Floquet-Bloch eigenstate modulated by an envelope which slowly decays transverse to the edge. Further, they show that the envelope is described by a topologically protected zero-energy bound state of a Dirac operator with a domain wall term; one such bound state always exists.

Crucial to their landmark work is the strategy used to extend the approximate edge states obtained via formal multiple-scale analysis to genuine eigenstates. The direct approach involves deriving an equation for the remainder, and analyzing it separately in terms of "near" and "far" Floquet-Bloch components. This technique was first used by the same authors two years prior in a one-dimensional continuum dimer model [21], later expanded into a book [26]. Shortly after, it was successfully extended to PDEs modeling photonic graphene analogs [47].

The analysis of edge states has since advanced significantly. For example, Drouot and Weinstein [16] consider a broader class of honeycomb models which include both spatial inversion and time-reversal symmetry breaking. They obtain a very strong result which characterizes the resolvent of the edge Hamiltonian

(a) (b)

Figure 1.5 – (a) Square lattice potential constructed as the sum of $\mathbb{Z}^2$ translates of a compactly-supported potential well. (b) Band structure of the Schrödinger operator H_V (1.18) near a quadratic band degeneracy point $(E_S; M)$. The local dispersion surfaces are approximately described by the eigenvalues of $\mathbb{R}^2 \ni \xi \mapsto H_e^M(\xi)$ (1.10), where $\xi = k - M$; see Theorem 3.2 and Remark 3.3.

within a band gap, after an appropriate re-scaling, in terms of the resolvent of a Dirac operator, implying that all edge states in honeycomb structures arise via the multiple-scale framework. Similar resolvent convergence results have also been obtained for sharply terminated honeycomb structures [31], see also [19, 20]. The edge states arising in this context arise, in the high contrast limit, from a one-dimensional flat band of an associated tight-binding model. These are not topologically protected and their existence depends sensitively on the orientation of the truncation.

1.3. Overview of models and results

1.3.1. Band structure degeneracies in deformed square lattice media

We consider a model of a two-dimensional, spatially in nite "bulk" medium possessing the symmetries of a square lattice. Speci cally, we consider the Schrödinger operator

$$H_V = -\Delta_x + V(x); \tag{1.9}$$

where the potential $\mathbb{R}^2 \ni x \mapsto V(x)$ is real-valued, periodic with respect to the lattice $\Lambda = \mathbb{Z}^2$, and invariant under the symmetry group of the square. We call such potentials *square lattice potentials*; see De nition 3.2 and the example in Figure 1.5a.

In [43, 44], it was shown that the band structure of H_V contains quadratic band degeneracies; these are the energy-quasimomentum pairs $(E_S; M)$ at which two consecutive dispersion surfaces touch quadratically. The quasimomentum $M = [\ ;\ ]^T$ at which these degeneracies occur, together with its rotational equivalents, are high-symmetry points located at the four vertices of the square Brillouin zone; see Figure 3.2. More speci cally, in an energy-quasimomentum neighborhood $(E_S; M)$, the band structure of H_V is approximated by an effective Hamiltonian with Fourier symbol

$$H_e^M(\ ) = (1\quad {}_0)j\ \ j^2\ {}_0\quad {}_1(\quad {}_1)\ {}_1\quad {}_2(\quad {}_3)\ {}_2: \tag{1.10}$$

Here, $= k\quad M$ is a quasimomentum displacement from M, the emergent parameters $_2 \in \mathbb{R}$, $0\quad `\quad 2$, are de ned in terms of two eigenstates spanning the two-dimensional Floquet-Bloch eigenspace associated with $(E_S; M)$, and $_`$, $0\quad `\quad 2$, are the Pauli matrices; see Section 2.2. The effective Hamiltonian provides a blow-up of a small energy-quasimomentum neighborhood $(E_S; M)$ within the band structure of H_V. In particular, $E\ (M + \ )\quad E_S\quad "(\ )$, where

$$"(\ ) = (1\quad {}_0)j\ \ j^2\quad \sqrt{{}_1^2(\quad {}_1)^2 + {}_2^2(\quad {}_3)^2} \tag{1.11}$$

are the two eigenvalues of $H_e^M(\ )$; see Figure 1.5b.

Our point of departure is a square lattice medium modeled by H_V as in (1.18), with a quadratic band degeneracy at $(E_S; M)$. We then consider the $T\mathbb{Z}^2$-periodic, deformed Schrödinger operator

$$H_{V\ T^{\ 1}} = \quad {}_x + V(T^{\ 1}x); \tag{1.12}$$

where T is an invertible linear transformation of $\mathbb{R}^2$. The deformed Schrödinger operator $H_{V\ T^{\ 1}}$ models a periodic medium with fundamental cell distorted as prescribed by T; see Figure 1.6a. Our analysis proceeds by rst transforming the Schrödinger operator $H_{V\ T^{\ 1}}$, using the change of variables $y = T^{\ 1}x$, into the "pushforward" operator

$$T\ H_V\quad r\ \ {}_y\ \ (T^T T)^{\ 1} r\ {}_y + V(y); \tag{1.13}$$

which is again $\mathbb{Z}^2$-periodic; this xes the fundamental cells of both $\mathbb{R}^2 =$ and $\mathbb{R}^2 =$ (i.e., the Brillouin zone) to be independent of T. Since T is invertible, $(T^T T)^{\ 1}$ is positive de nite, and so $T\ H_V$ remains

(a) (b)

Figure 1.6 – (a) Periodic potential obtained via linear deformation T of the square lattice potential in Figure 1.5a (b) Band structure of the $\mathbb{Z}^2$-periodic operator $T^{-1} H_V$ (1.13) near $(E_S; M)$; compare with Figure 1.5b. The local dispersion surfaces are approximately described by the eigenvalues of $H_e^M(\ ;\ _0;\ )$ (1.15), where $= k \quad M$ and $_0$, are defined in (4.16); see Theorem 4.3 and Remark 4.4. Here, $j \ j \ 6= 0$, so the dispersion surfaces contain a pair of tilted, elliptical Dirac points; see Theorem 4.5, as well as Figure 1.7.

elliptic. Further, since $T^T T$ is real symmetric, we have the parameterization

$$I \quad (T^T T)^{\ 1} = \ _0 I + \ _1 \ _1 + \ _3 \ _3; \tag{1.14}$$

for some $_0, \ _1, \ _3 \ 2$ R. For convenience, we write $= (\ _1; \ _3)$. If $j \ j = 0$, then T must be an orthogonal transformation composed with a nonzero scaling; we call T a pure dilation In particular, pure dilations do not break the rotational symmetry of H_V.

To determine the effect of a small deformation on the band structure near (E_S, M), we implement a Schur complement/Lyapunov-Schmidt reduction strategy, identifying the band structure near (E_S, M) with an eigenvalue problem for an approximate effective Hamiltonian. The effective Hamiltonian has the same general structure of (1.10), perturbing as

$$\begin{aligned} H_e^M(\ ;\ _0;\ ) = (\ _0 \ _0 + (1 \quad _0) j \ j^2) \ _0 \\ + (\ _1 \ _1 \quad _1 \quad _1 \ ) \ _1 + (\ _2 \ _3 \quad _2 \quad _3 \ ) \ _2 : \end{aligned} \tag{1.15}$$

The real parameters $\ , 0 \ \ ` \ 2$, are again defined in terms of the Floquet-Bloch eigenstates spanning the eigenspace of H_V at $(E_S; M)$. Note that there is no $_3$ contribution to (1.15) since the linear deforma-

(a) (b)

Figure 1.7 – Local band structure of the operator H_V (1.13) near the two emergent Dirac points (a) $(E_D(\ _0;\ );\ D\ (\ _0;\ ))$ and (b) $(E_D(\ _0;\ );\ D^+(\ _0;\ ))$ pictured in Figure 1.6b. The dispersion surfaces are approximately described by the eigenvalues (a) of $7!\ T\ H_e^D\ (\ )$ (1.17), where $=\ k\ \ D\ (\ _0;\ )$, and (b) $7!\ T\ H_e^{D^+}(\ )$, where $=\ k\ \ D^+(\ _0;\ )$; see Theorem 4.2 and Remark 4.4, which provide a general characterization of Dirac points.

tion preserves symmetry under spatial inversion and complex conjugation. Theorem 4.3 implies that, under suitable non-degeneracy assumptions on H_V, the band structure of H_V near $(E_S;\ M\ )$ consists of two dispersion surfaces which are approximately given by the graphs of the two eigenvalue maps of $H_e^M(\ ;\ _0;\ )$, defined by

$$"\ (\ ;\ _0;\ )\quad _0\ _0 + (1\quad _0)j\ \ j^2\quad \sqrt{(\ _1\ _1\quad _1\quad _1\ )^2 + (\ _2\ _3\quad _2\quad _3\ )^2}: \tag{1.16}$$

Hence, except in the case of a pure dilation (i.e., $j\ \ j = 0$), the band structure perturbs to one which, for $j\ \ j$ sufficiently small, has a local energy gap about E_S; see Figure 1.6b.

The expression for $H_e^M(\ ;\ _0;\ )$ in (1.15) suggests (and Theorem 4.5 establishes) that, for $_0$, $j\ \ j$ small and $j\ \ j \neq 0$, the quadratic band degeneracy point $(E_S;\ M\ )$ splits into two nearby degeneracies $(E_D(\ _0;\ );\ D\ (\ _0;\ ))$ with quasimomenta $D\ (\ _0;\ )$ approximately determined by the vanishing of off-diagonal entries of $H_e^M(\ ;\ _0;\ )$. In general, $D\ (\ _0;\ )$ is located at the inversion of $D^+(\ _0;\ )$ with respect to M: $D\ (\ _0;\ ) = 2M\ \ D^+(\ _0;\ )$.

Notably, the emergent degeneracies $(E_D(\ _0;\ );\ D\ (\ _0;\ ))$ are Dirac points; see Section 4.1. By Theorem 4.2, the generic local character of the band structure about each twofold degeneracy is a tilted elliptical cone with upper and lower branches; see Figure 1.6b. In terms of the quasimomentum displacement $q = k\ \ D$ from a Dirac point, the effective Hamiltonians governing the dynamics of wavepackets spec-

(a) (b)

Figure 1.8 – Non-degenerate dispersion surfaces of perturbed effective Hamiltonians (a) about a quadratic band degeneracy point, and (b) one of two Dirac points. Compare (a) with Figure 1.5b and (b) with Figure 1.7b.

trally supported near $(E_D; D)$ are Dirac Hamiltonians with Fourier symbols

$$T\,H_e^{D^+}(q) = (\ {}^{+}_{0}\ q)\,I + (\ {}^{+}_{1}\ q)\ {}_1 + (\ {}^{+}_{2}\ q)\ {}_2 \quad \text{and} \quad T\,H_e^{D^-}(q) = \ \ T\,H_e^{D^+}(q): \qquad (1.17)$$

For special classes of deformations (e.g., deforming the fundamental cell from a square to a rhombus, or compressing it along a coordinate axis), the motion of the Dirac point quasimomenta during the deformation $(\ {}_0;\ ) \mathrel{7!} D\ \ (\ {}_0;\ )$ is constrained to directions of preserved symmetry; see Section 4.3.3.

In Section 6.1, we further consider how the band structure near each type of degeneracy (i.e. quadratic band degeneracies and Dirac points) changes under a small (i.e., $\ $) breaking of symmetries: (i) spatial inversion (parity) symmetry, or (ii) complex conjugation (time-reversal) symmetry. This leads to more general effective Hamiltonians depending on $\ $, which now include contributions from $\ {}_3$.

1.3.2. Edge states in square lattice and deformed square lattice media

Our models of edge media are built up in three steps:

1. Periodic bulk media with PC symmetry and band structure degeneracies,
2. Periodic bulk media with PC symmetry-breaking perturbations, which “gap” degeneracies,
3. Edge media which slowly interpolate, across a line defect, between two distinct periodic bulk media with PC symmetry-breaking perturbations.

A schematic of this construction is presented in Figure 1.9 for square lattice media, and in Figure 1.10 for their deformed versions.

Periodic bulk media with band structure degeneracies

Our fundamental bulk Hamiltonian is the Schrödinger operator

$$H_{bulk} = H_V \quad {}_x + V(x): \tag{1.18}$$

The spectral theory of $H_{bulk} = H_V$ acting in $L^2(R^2)$ is given by its Floquet-Bloch band structure, see Section 2.1.1. In [43, 44], it was shown that the band structure of a Schrödinger operator with a square lattice potential exhibits quadratic band degeneracies $(E_?; k_?) = (E_S; M)$; see Figure 1.9a. The high-symmetry quasimomentum $M = [\ ;\ ]^T$ and its rotational equivalents make up the four vertices of the Brillouin zone $B = [\ ;\ ]\ [\ ;\ ]$.

In [7], we studied small deformations of H_V given by

$$H_{bulk} = H_{V\ T^{\ 1}} \quad {}_x + V(T^{\ 1}x); \tag{1.19}$$

where T is a real, invertible $2 \quad 2$ matrix close to the identity. The bulk Hamiltonian $H_{bulk} = H_{V\ T^{\ 1}}$ is periodic with respect to $= \ TZ^2$, and may not have any of the point group symmetries of H_V. We proved that, for generic T, the quadratic band degeneracy point $(E_S; M)$ splits into two conical degeneracies, or Dirac points $(E_?; k_?) = (E_D; D)$ at quasimomenta D inversion symmetric about M; see Figure 1.10a. That twofold degeneracies persist under deformation is a consequence of the invariance of $H_{V\ T}$ under PC as defined in (2.20).

Band structure degeneracies gapped via symmetry breaking

We consider two "insulating" periodic media, to be later joined across an interface, which are perturbations of the bulk medium by a magnetic term. These are modeled by the Hamiltonians

$$H^{;}_{bulk} = H_{bulk} \quad {}^{r}W_1 : \tag{1.20}$$

Here, > 0 is small. The operator W_1 is self-adjoint, -periodic, and commutes with P, but anticommutes with C. The scaling parameter $r = 1, 2$ depends on the local character of the dispersion surfaces of H_{bulk} about the relevant degeneracy: $r = 2$ for a quadratic band degeneracy, $r = 1$ for conical degeneracies.

Remark 1.1. (Scaling.) Suppose the dispersion relations have the local behavior $|E(k) \quad E_?| \; | \; k \quad k_?|^r$ in a quasimomentum neighborhood of the H_{bulk} band structure degeneracy $(E_?; k_?)$. Then, the dispersive (diffractive) effect on a wavepacket spectrally concentrated in a quasimomentum disk of radius about $k_?$ will be order one on the timescale $t_{disp} = O(\; ^r)$. In (1.20), and later in (1.21), the amplitude of the perturbation to H_{bulk} is chosen to balance dispersion on the timescale t_{disp}.

Since W_1 breaks the PC symmetry of H_{bulk}, the band structure degeneracies gap, or separate, yielding smooth, locally non-degenerate dispersion surfaces and a local band gap $(E_?; k_?)$; see Figure 1.9b and Figure 1.10b.

If the dispersion surfaces of $H^{;}_{bulk}$ are non-degenerate across the full Brillouin zone, one can associate integer-valued topological indices, the rst Chern numbers, to the collection of bands below the band gap. For C-invariant perturbations of H_{bulk}, the Chern number is zero, and for C-breaking perturbations of H_{bulk}, it is nonzero. Our models use C-breaking perturbations resulting in Chern numbers $+1$ and 1; see the discussion in Section 6.2.

Interpolating between gapped bulk media across a line defect

Finally, choose a vector $r_{edge} \; ^2$. The line Rv_{edge} divides R^2 into two half-spaces. We next introduce a class of edge Hamiltonians, periodic with respect to $Z v_{edge}$, which slowly interpolate between $H^{;}_{bulk}$ and $H^{+;}_{bulk}$ across Rv_{edge}. Speci cally,

$$H_{edge} = H_{bulk} + \; ^r W_{edge}; \tag{1.21}$$

where W_{edge} is a spatially non-compact and slowly varying interpolation between W_1 transverse to Rv_{edge} via a domain wall with an $O(\; ^1)$ length scale; see Figure 1.9c and Figure 1.10c. The edge Hamiltonian H_{edge} has a two-scale structure, arising from the $O(1)$ scale of the lattice and the $O(\; ^1)$ scale of the domain wall perturbation. Analogous edge Hamiltonians have been introduced in the context of 2D honeycomb media [34, 54, 23, 25, 47, 16] and in 1D dislocated media [22, 27, 14, 11]. For studies involving square lattice media with sharp interfaces, see, e.g., [52].

By the choice of v_{edge}, H_{edge} is invariant under translations by elements of Zv_{edge}. Consequently, its spectral properties as an operator on $L^2(R^2)$ can be resolved into those of its restriction onto ber subspaces $L^2_k(R^2/Zv_{edge})$, for $k \in [\quad ; \quad]$ (see Section 2.1.2), which are pseudoperiodic with wavenumber k parallel to the edge Rv_{edge} and square integrable transverse to the edge. Since H_{edge} is invariant under translations in Zv_{edge}, edge states arise as solutions of a family of Floquet-Bloch eigenvalue problems parameterized by a scalar parallel quasimomentum; see Section 2.1.2. These states are represented in an edge state diagram, see Figures 1.11 - 1.12. This edge state diagram displays a gap between two bands of continuous spectrum, arising from the non-degenerate dispersion surfaces of the asymptotic Hamiltonians H_{bulk}, as well as branches of eigenvalues corresponding to edge state eigenfunctions.

(a) (Left) Square lattice bulk medium, modeled by $H_{bulk} = H_V$ (1.18). (Right) Blow-up of its band structure near a quadratic band degeneracy point $(E_?; k_?) = (E_S; M)$.

(b) (Left) Asymptotic square lattice media, modeled by $H_{bulk}^{;}$ (1.20). (Right) C-breaking perturbation induces a band gap near $(E_?; k_?)$. The two asymptotic media acquire distinct nonzero topological indices (Chern numbers).

(c) (Left) Square lattice edge medium, modeled by H_{edge} (1.21), which interpolates between $H_{bulk}^{;}$ transverse to Rv_{edge}. Here, $v_{edge} = [0; 1]^T$. (Right) The band gap is traversed by two edge state eigenvalue curves, arising from the eigenvalue curves of a matrix Schrödinger operator.

Figure 1.9 – Square lattice media and spectra near energy $E_? = E_S$.