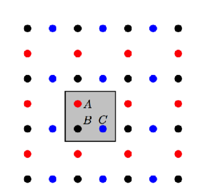
Band Degeneracies in $\pi/2-$Rotationally Invariant, Periodic Schrödinger Operators



Rachael Keller[1]

In Collaboration With:
J.L. Marzuola[2] B. Osting[3] M.I. Weinstein[4]

[1]Department of Applied Physics and Applied Mathematics, Columbia University

[2]Department of Mathematics, University of North Carolina, Chapel Hill.

[3]Department of Mathematics, University of Utah.

[4]Department of Applied Physics and Applied Mathematics and Department of Mathematics, Columbia University.

Outline

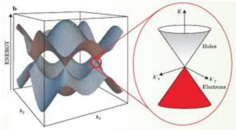
Outline

Introduction

Schrödinger operators $H_V = -\Delta + V(\mathbf{x})$ are central to the mathematical description of waves in periodic media.

Wave propagation properties are encoded in **band structure**, the collection of dispersion surfaces and associated eigenmodes.

An important feature of band structure is existence of **Dirac points**.



Main features of Dirac points:

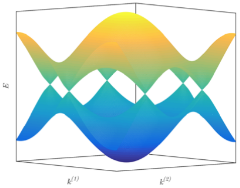
i.) Conical intersections of bands.

ii.) Wavepackets evolve according to a 2D Dirac equation.

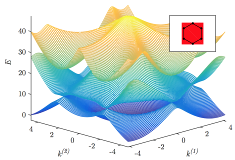
Motivating Work

Tight binding (TB) models approximate band structure of the Schrödinger operator: $H_V^\varepsilon = -\Delta + \varepsilon V(\mathbf{x}), \quad \varepsilon \nearrow \infty.$

Figure 1: Band Structures for Honeycomb Lattice Near Vertex $\mathbf{K}_\star \in \mathbb{R}^2$



(a) TB Honeycomb[1]



(b) Continuum Honeycomb

Do Dirac points from TB model persist in the continuum, $|\varepsilon| < \infty$?

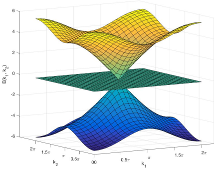
Charles Fefferman, James Lee-Thorp and Michael Weinstein showed Dirac points $\mathbf{K}_\star$ persist for honeycomb [FW12; FLTW17].

$$\mu(\mathbf{K}_\star + \kappa) - \mu(\mathbf{K}_\star) \approx \pm |\lambda_\#| \; | \; \kappa \; | \, .$$

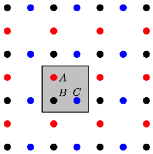
[1] PR Wallace (1947) - The band structure of graphite, Phys. Rev. (1947)

Motivating Work

Q: Do Dirac points persist for integer lattice potentials, potentials that are $\mathbb{Z}^2-$periodic, $\pi/2-$invariant?



(c) TB Lieb Bands



(d) Lieb Lattice

Specifically, in study of H_V^{ε}:

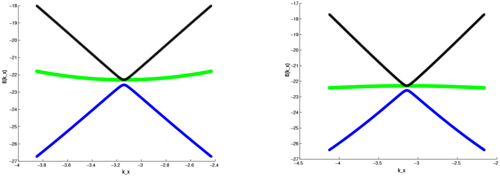
i.) Does a conical intersection of bands persist for $|\varepsilon| < \infty$?

ii.) Do wavepackets evolve according to a 2D Dirac equation?

Main Results

We show that the answer is no.

- Dispersion surfaces intersect quadratically at points $\mathbf{M}_\star$.
- Wavepackets spectrally concentrated about $\mathbf{M}_\star$ evolve in large time according to coupled 2D Schrödinger equations.



(e) $\mathbf{k} = \mathbf{M}_\star + \kappa e^{\frac{i\pi}{4}}$ (f) $\mathbf{k} = \mathbf{M}_\star + \kappa e^{\frac{i15\pi}{16}}$

Dispersion Curves for Integer Lattice Potential, $|\kappa| \ll 1$

Study the *Floquet-Bloch eigenvalue problem* on the integer lattice.

Outline

Preliminaries: Lattice Structure

- Period Lattice: $\mathbf{v} \in \Lambda = \mathbb{Z}\mathbf{v}_1 \oplus \mathbb{Z}\mathbf{v}_2$,

$$\mathbf{v}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } \mathbf{v}_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

- Dual lattice: $\mathbf{k} \in \Lambda^* = \mathbb{Z}\mathbf{k}_1 \oplus \mathbb{Z}\mathbf{k}_2$,

$$\mathbf{k}_1 = \begin{pmatrix} 2\pi \\ 0 \end{pmatrix} \text{ and } \mathbf{k}_2 = \begin{pmatrix} 0 \\ 2\pi \end{pmatrix}.$$

- Brillouin zone $\mathcal{B} \equiv [-\pi, \pi]^2$ (unit cell Λ^*)
- Define $\pi/2-$clockwise rotation matrix R:

$$R = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

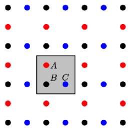


Figure 2: Shaded: Unit Cell in Λ

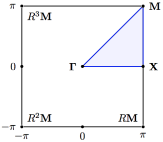


Figure 3: $\mathcal{B} \equiv [-\pi, \pi]^2$

Introduction of Floquet-Bloch Theory

Fix $\mathbf{k} \in \mathcal{B}$ and consider the Floquet-Bloch evp:

$$\begin{aligned} H_V\ \Phi(\mathbf{x}) &= \mu\ \Phi(\mathbf{x}),\ \ \mathbf{x} \in \mathbb{R}^2, \\ \Phi(\mathbf{x}+\mathbf{v}) &= e^{i\mathbf{k}\cdot\mathbf{v}}\Phi(\mathbf{x}),\ \ \mathbf{v} \in \Lambda, \end{aligned} \tag{1}$$

where $H_V \equiv -\Delta_{\mathbf{x}} + V$ and V is Λ-periodic.

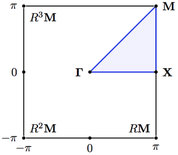


Figure 4: $\mathcal{B} = [-\pi, \pi]^2$

- Solutions Φ exist:

$$\Phi \in L^2_{\mathbf{k}} \equiv \{f \in L^2_{loc} : f(\mathbf{x}+\mathbf{v}) = e^{i\mathbf{k}\cdot\mathbf{v}} f(\mathbf{x}), \mathbf{v} \in \Lambda, \mathbf{x} \in \mathbb{R}^2\}.$$

- $\Phi \in L^2_{\mathbf{k}}$ can be written $\Phi = e^{i\mathbf{k}\cdot\mathbf{x}}\phi$, where ϕ is periodic in Λ.

Introduction of Floquet-Bloch Theory

Fix $\mathbf{k} \in \mathcal{B}$ and consider the Floquet-Bloch evp:

$$\begin{aligned} H_V\ \Phi(\mathbf{x}) &= \mu\ \Phi(\mathbf{x}),\ \ \mathbf{x} \in \mathbb{R}^2, \\ \Phi(\mathbf{x}+\mathbf{v}) &= e^{i\mathbf{k}\cdot\mathbf{v}}\Phi(\mathbf{x}),\ \ \mathbf{v} \in \Lambda, \end{aligned} \qquad (1)$$

where $H_V \equiv -\Delta_{\mathbf{x}} + V$ and V is Λ-periodic.

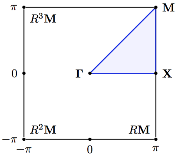


Figure 4: $\mathcal{B} = [-\pi, \pi]^2$

- Solutions Φ exist:

$$\Phi \in L^2_{\mathbf{k}} \equiv \{f \in L^2_{loc} : f(\mathbf{x}+\mathbf{v}) = e^{i\mathbf{k}\cdot\mathbf{v}} f(\mathbf{x}), \mathbf{v} \in \Lambda, \mathbf{x} \in \mathbb{R}^2\}.$$

- $\Phi \in L^2_{\mathbf{k}}$ can be written $\Phi = e^{i\mathbf{k}\cdot\mathbf{x}}\phi$, where ϕ is periodic in Λ.

Equivalent *periodic* formulation of (1):

$$\begin{aligned} H_V(\mathbf{k})\ \phi(\mathbf{x};\mathbf{k}) &= \mu(\mathbf{k})\ \phi(\mathbf{x};\mathbf{k}) \\ \phi(\mathbf{x}+\mathbf{v};\mathbf{k}) &= \phi(\mathbf{x};\mathbf{k}),\ \ \mathbf{v} \in \Lambda, \end{aligned}$$

where $H_V(\mathbf{k}) = -(\nabla_{\mathbf{x}} + i\mathbf{k})^2\ +\ V(\mathbf{x})$ and $\mathbf{x} \in \mathbb{R}^2/\Lambda\ (\mathbb{R}^2/\mathbb{Z}^2)$.

Floquet Theory

Fix $\mathbf{k} \in \mathcal{B}$ and consider

$$\begin{aligned} H_V(\mathbf{k})\ \phi(\mathbf{x}) &= \mu\ \phi(\mathbf{x}) \\ \phi(\mathbf{x}+\mathbf{v}) &= \phi(\mathbf{x}),\ \ \mathbf{v} \in \Lambda, \end{aligned} \tag{2}$$

where $H_V(\mathbf{k}) = -(\nabla_{\mathbf{x}} + i\mathbf{k})^2\ +\ V(\mathbf{x})$.

- For each $\mathbf{k} \in \mathcal{B}$, problem (2) has a discrete set of eigenpairs:

  $$(\mu_b(\mathbf{k}), \phi_b(\mathbf{x};\mathbf{k})),\ b \in \mathbb{N},$$

  where $\{\phi_b(\mathbf{x};\mathbf{k})\}$ is complete and orthonormal in $L^2(\mathbb{R}^2/\Lambda)$, and the eigenvalues may be listed with multiplicity in order:

  $$\mu_1(\mathbf{k}) \le \mu_2(\mathbf{k}) \le \cdots \le \mu_b(\mathbf{k}) \le \cdots .$$

Floquet Theory

Fix $\mathbf{k} \in \mathcal{B}$ and consider

$$\begin{aligned} H_V(\mathbf{k})\ \phi(\mathbf{x}) &= \mu\ \phi(\mathbf{x}) \\ \phi(\mathbf{x}+\mathbf{v}) &= \phi(\mathbf{x}),\ \ \mathbf{v} \in \Lambda, \end{aligned} \tag{2}$$

where $H_V(\mathbf{k}) = -(\nabla_{\mathbf{x}} + i\mathbf{k})^2\ +\ V(\mathbf{x})$.

- For each $\mathbf{k} \in \mathcal{B}$, problem (2) has a discrete set of eigenpairs:

  $$(\mu_b(\mathbf{k}), \phi_b(\mathbf{x};\mathbf{k})), b \in \mathbb{N},$$

  where $\{\phi_b(\mathbf{x};\mathbf{k})\}$ is complete and orthonormal in $L^2(\mathbb{R}^2/\Lambda)$, and the eigenvalues may be listed with multiplicity in order:

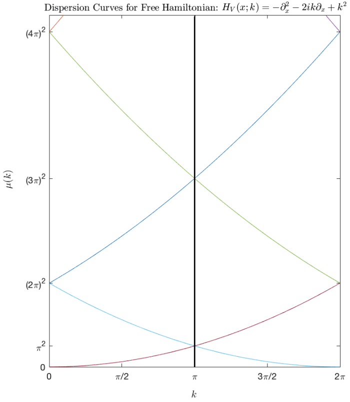
  $$\mu_1(\mathbf{k}) \leq \mu_2(\mathbf{k}) \leq \cdots \leq \mu_b(\mathbf{k}) \leq \cdots .$$

- Eigenvalues $\mu_b(\mathbf{k})$ are called the *dispersion relations* of $H_V(\mathbf{k})$;
- The collection of dispersion relations is the **band structure**. The spectrum of H_V acting in $L^2(\mathbb{R}^2)$ is:

  $$\sigma(H_V) = \mu_1(\mathcal{B}) \cup \mu_2(\mathcal{B}) \cup \cdots \cup \mu_b(\mathcal{B}) \cup \cdots .$$

Floquet-Bloch Theory in Action: 1D

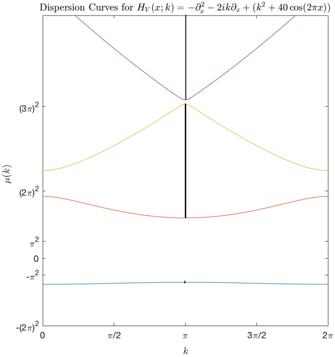
Figure 5: Band Structure $H = -d_x^2$, over $\mathcal{B} = [0, 2\pi]$, for $x \in [0, 1]$.



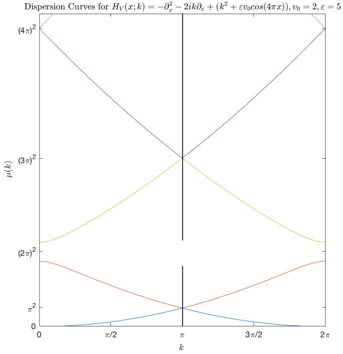
- Colored lines: Bands of $H(k) = -(d_x + ik)^2$ sweep out real intervals.
- Black line: Recover the spectrum $(0, \infty)$ of $H^{(0)} = -d_x^2$.

Floquet-Bloch Theory in Action: 1D Dirac Point

Figure 6: Band Structure H_V^{ε} over $\mathcal{B} = [0, 2\pi]$, for $x \in [0, 1]$.



(a) $\varepsilon V = 40\cos(2\pi x)$.



(b) $\varepsilon V = 10\cos(4\pi x)$.

- Left panel: Spectral gap opens for potential at across $\mathbf{k} \in \mathcal{B}$.
- Right panel: Spectral gap closes and bands intersect conically at a $k-$point. The $k-$point for which they intersect is the **Dirac point.**

Floquet-Bloch evp for $\Lambda = \mathbb{Z}^2$

Fix $\mathbf{k} \in \mathcal{B}$. Consider our Floquet-Bloch evp:

$$H_V^{\varepsilon}\ \Phi(\mathbf{x}) = \mu\ \Phi(\mathbf{x}), \mathbf{x} \in \mathbb{R}^2$$

$$\Phi(\mathbf{x}+\mathbf{v}) = e^{i\mathbf{k}\cdot\mathbf{v}}\Phi(\mathbf{x}), \quad \mathbf{v} \in \Lambda,$$

where $H_V^{\varepsilon} \equiv -\Delta_{\mathbf{x}} + \varepsilon V$ and V is **admissible**.

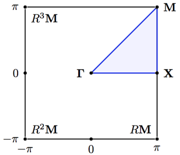


Figure 7: $\mathcal{B} = [-\pi, \pi]^2$

Definition (Admissible Potentials)

An **admissible** *potential is a smooth function* $V(\mathbf{x})$ *satisfying:*

(i.) $\mathcal{P}-$*symmetry:* $V(-\mathbf{x}) = V(\mathbf{x})$;

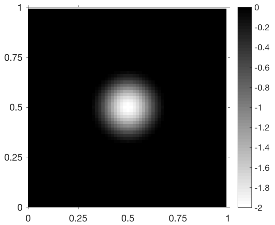
(ii.) $\mathcal{C}-$*symmetry:* $\overline{V(\mathbf{x})} = V(\mathbf{x})$;

(iii.) $\mathbb{Z}^2-$*periodicity:* $V(\mathbf{x}+\mathbf{v}) = V(\mathbf{x}), \mathbf{v} \in \mathbb{Z}^2$;

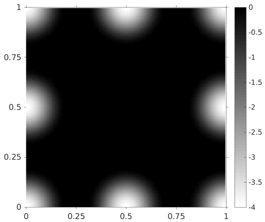
(iv.) $\pi/2-$*rotational invariance: With respect to an origin,*

$$\mathcal{R}[V](\mathbf{x}) \equiv V(R^*\mathbf{x}) = V(\mathbf{x}), \text{ for all } \mathbf{x} \in \mathbb{R}^2.$$

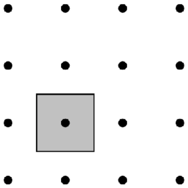
Examples of Admissible Potentials



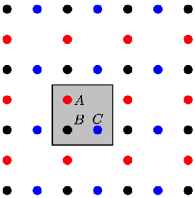
(a) V_S: Wells at Square Sites



(b) V_L: Wells at Lieb Sites



(c) Square Lattice



(d) Lieb Lattice

High Symmetry Quasi-momenta

The vertices of $\mathcal{B}$, $\mathbf{M}_\star$, are **high-symmetry** quasi-momenta.

$$\mathbf{M}_\star \in \{(\pi,\pi),(\pi,-\pi),(-\pi,-\pi),(-\pi,\pi)\}.$$

Floquet-Bloch evp:

$$H_V^\varepsilon \, \Phi(\mathbf{x}) = \mu \, \Phi(\mathbf{x}),$$
$$\Phi(\mathbf{x}+\mathbf{v}) = e^{i\mathbf{M}_\star \cdot \mathbf{v}} \Phi(\mathbf{x}), \quad \mathbf{v} \in \Lambda, \qquad (3)$$

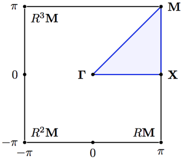


Figure 8: $\mathcal{B} = [-\pi,\pi]^2$

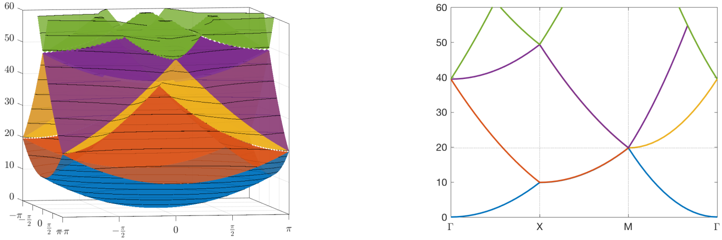
where V is admissible. Solution space:

$$L^2_{\mathbf{M}_\star} \equiv \{f \in L^2_{loc} : f(\mathbf{x}+\mathbf{v}) \;=\; e^{i\mathbf{M}_\star\cdot\mathbf{v}} \; f(\mathbf{x}),\; \mathbf{v} \in \Lambda, \mathbf{x} \in \mathbb{R}^2\}.$$

- $L^2_{\mathbf{M}_\star}$ is equivalent for all vertices $\mathbf{M}_\star$ (*high-symmetry*).
$$e^{i(\pi,\pi)\cdot(1,0)} = e^{i(\pi,-\pi)\cdot(1,0)} = \cdots.$$
$$e^{i(\pi,\pi)\cdot(0,1)} = e^{i(\pi,-\pi)\cdot(0,1)} = \cdots.$$
- Elicits a *four-fold degenerate* eval $\mu(\mathbf{M}_\star) = |\mathbf{M}_\star|^2$ for $H_V^{\varepsilon=0}$.
- Study (3) for $\mathbf{M}_\star = (\pi,\pi) \equiv \mathbf{M}$ wlog for any $\mathbf{M}_\star$.

Focus: Free Hamiltonian Lowest Eigenvalues

Figure 9: Numerical Dispersion Surfaces of $H^{(0)} = -\Delta$.



(a) Dispersion Surfaces (b) 2D Cross Section

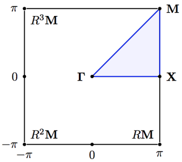
The first five dispersion surfaces are plotted over the BZ, $[-\pi, \pi]^2$.

- Four lowest bands touch at $\mu^{(0)} = |\mathbf{M}|^2 = 2\pi^2$.

  (High-symmetry quasimomenta and $\mathcal{R}-$invariance of H_V^{ε} with bc.)

Consequences of $\pi/2$−rotational invariance

Let $H_V^\varepsilon \equiv -\Delta_{\mathbf{x}} + \varepsilon V$ and V be **admissible**.



$$
\begin{aligned}
H_V^\varepsilon\ \Phi(\mathbf{x}) &= \mu\ \Phi(\mathbf{x}),\ \ \mathbf{x} \in \mathbb{R}^2, \\
\Phi(\mathbf{x}+\mathbf{v}) &= e^{i\mathbf{M}\cdot\mathbf{v}}\Phi(\mathbf{x}),\ \ \ \mathbf{v} \in \Lambda.
\end{aligned} \tag{4}
$$

Recall for a function f on $\mathbb{R}^2$: $\mathcal{R}[f](\mathbf{x}) \equiv f(R^*\mathbf{x})$.

Proposition ($L^2_{\mathbf{M}}$ Decomposition by $\mathcal{R}$)

(i) $\mathcal{R}^4 = Id$ *and is unitary on* $L^2_{\mathbf{M}}$. *Thus,*

$$\mathcal{R}^4 f = \sigma^4 f = f, \quad \sigma \equiv \{+1, -1, +i, -i\}.$$

(ii) *The operators* $\mathcal{R}$ *and* H_V *commute on* $L^2_{\mathbf{M}}$.

(iii) *If* $\Phi \in L^2_{\mathbf{M}}$ *solves* (5) *with eval* μ, $\mathcal{R}[\Phi]$ *solves* (5)*with eval* μ.

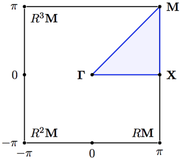
- *Hence* $\mathcal{R}^j\Phi = \sigma^j\Phi$, $j = 0, 1, 2, 3$, *solves* (5), *where* $\mathcal{R}^j\Phi \in L^2_{\mathbf{M}}$.

(iv) $\mathcal{R}$ *decomposes* $L^2_{\mathbf{M}} = L^2_{\mathbf{M},(+1)} \oplus L^2_{\mathbf{M},(-1)} \oplus L^2_{\mathbf{M},(+i)} \oplus L^2_{\mathbf{M},(-i)}$

$$L^2_{\mathbf{M},\sigma} \equiv L^2_{\mathbf{M}} \cap \{f\ |\mathcal{R}f = \sigma f\}$$

Key Properties of H_V^ε for Admissible V

Let $H_V^\varepsilon \equiv -\Delta_{\mathbf{x}} + \varepsilon V$ and V be **admissible**.



$$\begin{aligned} H_V^\varepsilon\ \Phi(\mathbf{x}) &= \mu\ \Phi(\mathbf{x}),\ \ \mathbf{x} \in \mathbb{R}^2, \\ \Phi(\mathbf{x}+\mathbf{v}) &= e^{i\mathbf{M}\cdot\mathbf{v}}\Phi(\mathbf{x}),\quad \mathbf{v} \in \Lambda. \end{aligned} \qquad (5)$$

H_V^ε is $\pi/2-$rotationally $(\mathcal{R}-)$ invariant and $\mathcal{P}\circ\mathcal{C}-$symmetric.

- $\mathcal{R}$ decomposes $L^2_{\mathbf{M}}$ by its eigenvalues $\sigma \equiv \{+1, -1, +i, -i\}$:

$$L^2_{\mathbf{M}} = L^2_{\mathbf{M},(+1)} \oplus L^2_{\mathbf{M},(-1)} \oplus L^2_{\mathbf{M},(+i)} \oplus L^2_{\mathbf{M},(-i)}.$$

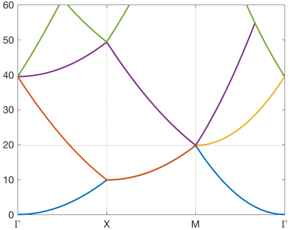
- $\mathcal{P}\circ\mathcal{C}$ symmetry of states: If $\Phi_1 \in L^2_{\mathbf{M},(+i)}, \Phi_2 \in L^2_{\mathbf{M},(-i)}$

$$\Phi_1 = \overline{\Phi_2(-\mathbf{x})} = (\mathcal{P}\circ\mathcal{C})\,[\Phi_1].$$

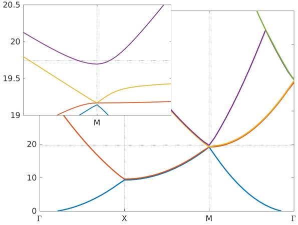
Perturbation by Admissible Potential

Perturbation by **admissible** V *splits* the 4D espace of $H^{(0)}$ into

- *one* 2-dimensional espace with eigenvalue $\mu_S^{\varepsilon} = \mu_{(\pm i)}^{\varepsilon}$ and
- *two* 1-dimensional espaces with eigenvalue $\mu_{(\pm 1)}^{\varepsilon}$.



(c) Dispersion Curves for $H^{\varepsilon=0}$



(d) Dispersion Curves for $H_{V_L}^{\varepsilon=1}$

$$\text{“}4 \to 2 + 1 + 1\text{”}$$

The “sticking” of two evals is due to the $(\mathcal{P} \circ \mathcal{C})-$symmetry.

Outline

Main Theorem

Theorem (Quadratic touching of dispersion surfaces)

Let $H_V = -\Delta + V$, where V is an admissible potential. Assume:

H1) *H_V has simple ($L^2_{\mathbf{M},+i}$)-eval μ_S with efunc $\Phi_1(\mathbf{x})$.*

H2) *H_V has simple ($L^2_{\mathbf{M},-i}$)-eval μ_S with efunc $\Phi_2 = (\mathcal{P} \circ \mathcal{C})[\Phi_1]$.*

H3) *μ_S is neither an $L^2_{\mathbf{M},+1}$ nor an $L^2_{\mathbf{M},-1}$ eval of H_V.*

Then, there exist dispersion curves $\mathbf{k} \mapsto \mu_\pm(\mathbf{k})$ associated with H^ε_V, that are quadratic and $\pi/2-$invariant locally in κ about $\mathbf{M}$:

$$\mu_\pm(\mathbf{M}+\kappa) - \mu_S =$$

$$(1-\alpha)|\kappa|^2 + \mathcal{Q}_6(\kappa) \pm \sqrt{\left|\ \gamma(\kappa_1^2 - \kappa_2^2) + 2\beta\kappa_1\kappa_2\ \right|^2 + \mathcal{Q}_8(\kappa)},$$

$\mathcal{Q}_n = \mathcal{O}(|\kappa|^n)$ analytic in κ; and $\alpha = 4a^{1,1}_{1,1}, \beta = 4a^{1,2}_{1,2}, \gamma = 4a^{1,2}_{1,1}$, depend on the first partials of the ($\pm i$) estates and resolvent $\mathcal{R}_\mathbf{M}$:

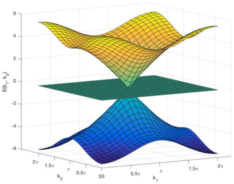
$$a^{j_1,j_2}_{l,m} = \langle \partial_{x_l}\Phi_{j_1}, \mathcal{R}_\mathbf{M}\partial_{x_m}\Phi_{j_2}\rangle,\ \ l,m,j_1,j_2 \in \{1,2\}.$$

Focus: Local Behavior about Vertices $\mathbf{M}_\star$

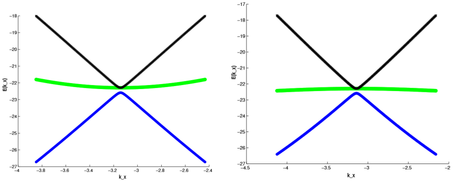
Dispersion curves quadratic and $\pi/2-$invariant:

$$\mu_\pm(\mathbf{M}_\star+\kappa)-\mu_S \approx (1-\alpha)|\kappa|^2 \pm \left| \gamma(\kappa_1^2-\kappa_2^2)+2\beta\kappa_1\kappa_2 \right|.$$

Lieb Lattice TB



Continuum Dispersion Curves



(e) $\frac{\pi}{4}-$line about $\mathbf{M}$ (f) $\frac{15\pi}{16}-$line about $\mathbf{M}$

$\alpha=4a_{1,1}^{1,1}, \beta=4a_{1,2}^{1,2}, \gamma=4a_{1,1}^{1,2}$, are given by $a_{l,m}^{j_1,j_2}=\langle \partial_{x_l}\Phi_{j_1}, \mathcal{R}_{\mathbf{M}}\partial_{x_m}\Phi_{j_2}\rangle$.

Comparison to Honeycomb

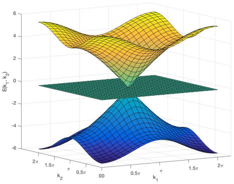
For honeycomb: Conical singularity persists for $|\varepsilon| < \infty$:

$$\mu_{\pm}(\mathbf{K}_{\star} + \kappa) - \mu(\mathbf{K}_{\star}) \approx \pm |\lambda_{\#}| \ | \ \kappa \ | \, .$$

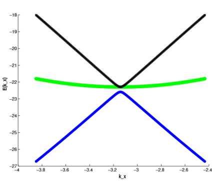
For Lieb/square: Conical singularity does *not* persist for $|\varepsilon| < \infty$.

$$\mu_{\pm}(\mathbf{M}_{\star} + \kappa) - \mu_S \approx (1 - \alpha \ )| \ \kappa \ |^2 \pm \left| \ \gamma(\kappa_1^2 - \kappa_2^2) + 2\beta\kappa_1\kappa_2 \ \right| .$$

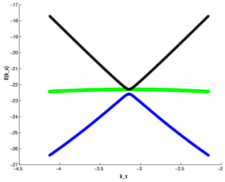
Lieb Lattice TB



Continuum Dispersion Curves



(g) $\frac{\pi}{4}$—line about **M**



(h) $\frac{15\pi}{16}$—line about **M**

Conditions for Quadratic Touching

Let V_{m_1,m_2} denote the (m_1, m_2) Fourier coefficient of V.

Theorem (Small ε behavior)

Assume $V_{11} \neq V_{00}$. For ε small, the 4D espace of $H_V^{\varepsilon=0}$ perturbs to

(i.) *A 2D eigenspace $\mathbb{X}_i \subset L^2_{\mathbf{M},i}$ and $\mathbb{X}_{-i} \subset L^2_{\mathbf{M},-i}$ with corresponding multiplicity-two eval μ_S^ε, given by:*

$$\mu_S^\varepsilon = |\mathbf{M}|^2 + \varepsilon(V_{0,0} - V_{1,1}) + \mathcal{O}(\varepsilon^2).$$

(ii.) *Two 1D espaces $\mathbb{X}_{\pm 1} \subset L^2_{\mathbf{M},\pm 1}$ with distinct evals $\mu^\varepsilon_{(\pm 1)}$, where*

$$\mu^\varepsilon_{(\pm 1)} = |\mathbf{M}|^2 + \varepsilon(V_{0,0} \pm 2V_{0,1} + V_{1,1}) + \mathcal{O}(\varepsilon^2).$$

Theorem (Generic ε behavior)

Except for a discrete set of $\varepsilon \in \mathbb{R}$, the Hamiltonian H_V^ε has two touching dispersion curves locally about the $\mathbf{M}$−point given by:

$$\mu_\pm^\varepsilon(\mathbf{M} + \kappa) - \mu_S^\varepsilon \approx (1 - \alpha^\varepsilon)|\kappa|^2 \pm \left| \gamma^\varepsilon(\kappa_1^2 - \kappa_2^2) + 2\beta^\varepsilon \kappa_1 \kappa_2 \right|.$$

Proof Sketch: Lyapunov Schmidt Reduction Analysis

Consider small perturbation $|\kappa| \ll 1$ about the $\mathbf{M}-$point:

$$\begin{cases} H_V(\mathbf{M}+\kappa)\phi = \mu(\mathbf{M}+\kappa)\phi, \\ \phi(\mathbf{x}+\mathbf{v}) = \phi(\mathbf{x}), \mathbf{v} \in \Lambda, \quad \mathbf{x} \in \mathbb{R}^2, \end{cases} \tag{6}$$

where $H_V(\mathbf{k}) = (-(\nabla_\mathbf{x} + i(\mathbf{k}))^2 + V(\mathbf{x}))$ and V is admissible.

- Ansatz of solution for (6):

$$\mu = \mu(\mathbf{M}+\kappa) = \mu_S + \mu^{(1)};$$
$$\phi = \phi(\mathbf{x}; \mathbf{M}+\kappa) = \phi^{(0)} + \phi^{(1)};$$

$$\phi^{(0)} \in \mathrm{kernel}(H(\mathbf{M}) - \mu_S I), \quad \phi^{(1)} \perp \mathrm{kernel}(H(\mathbf{M}) - \mu_S I).$$

- Substitute ansatz into (6) and obtain system[1] $\mathcal{M}(\mu^{(1)}, \kappa)$.
- Seek $\mu^{(1)}$ satisfying

$$det[\mathcal{M}(\mu^{(1)}, \kappa)] = 0.$$

[1] Those interested can view details validating this ansatz in our paper online.

Proof Sketch: Lyapunov-Schmidt Reduction

- $\mathcal{M}$ can be decomposed into linear and higher order terms:

$$\mathcal{M}(\mu^{(1)}, \kappa) \equiv \mathcal{M}^{(0)}(\mu^{(1)}, \kappa) \; + \; \mathcal{M}^{(1)}(\mu^{(1)}, \kappa).$$

Linear-termed $\mathcal{M}^{(0)}(\mu^{(1)}, \kappa) \equiv$

$$\begin{pmatrix} \mu^{(1)} - \kappa \cdot \kappa + \langle \Phi_1, 2i\kappa \cdot \nabla \Phi_1 \rangle & \langle \Phi_1, 2i\kappa \cdot \nabla \Phi_2 \rangle \\ \langle \Phi_2, 2i\kappa \cdot \nabla \Phi_1 \rangle & \mu^{(1)} - \kappa \cdot \kappa + \langle \Phi_2, 2i\kappa \cdot \nabla \Phi_2 \rangle \end{pmatrix},$$

and $\mathcal{M}^{(1)}(\mu^{(1)}, \kappa) \equiv$

$$4 \begin{pmatrix} \langle \kappa \cdot \nabla_{\mathbf{x}} \Phi_1, \mathcal{R}_{\mathbf{M}} \left(\kappa \cdot \nabla_{\mathbf{x}} \Phi_1 \right) \rangle & \langle \kappa \cdot \nabla_{\mathbf{x}} \Phi_1, \mathcal{R}_{\mathbf{M}} \left(\kappa \cdot \nabla_{\mathbf{x}} \Phi_2 \right) \rangle \\ \langle \kappa \cdot \nabla_{\mathbf{x}} \Phi_2, \mathcal{R}_{\mathbf{M}} \left(\kappa \cdot \nabla_{\mathbf{x}} \Phi_1 \right) \rangle & \langle \kappa \cdot \nabla_{\mathbf{x}} \Phi_2, \mathcal{R}_{\mathbf{M}} \left(\kappa \cdot \nabla_{\mathbf{x}} \Phi_2 \right) \rangle \end{pmatrix} + \mathcal{O}_{2\times 2}\left(\, |\kappa|^3 + |\mu^{(1)}||\kappa| \, \right),$$

where $\mathcal{R}_{\mathbf{M}}$ is the resolvent operator associated with μ_S.

Symmetries Imply Vanishing Linear Terms

Linear-termed $\mathcal{M}^{(0)}(\mu^{(1)}, \kappa) \equiv$

$$\begin{pmatrix} \mu^{(1)} - \kappa\cdot\kappa + \langle \Phi_1, 2i\kappa\cdot\nabla\Phi_1\rangle & \langle \Phi_1, 2i\kappa\cdot\nabla\Phi_2\rangle \\ \langle \Phi_2, 2i\kappa\cdot\nabla\Phi_1\rangle & \mu^{(1)} - \kappa\cdot\kappa + \langle \Phi_2, 2i\kappa\cdot\nabla\Phi_2\rangle \end{pmatrix},$$

Proposition (Vanishing linear-in-κ terms)

If smooth functions f_1 and f_2 on $\mathbb{R}^2$ are $\mathcal{R}-$invariant,

$$\langle f_1, \nabla f_2\rangle_{L^2(\Omega)} = \mathbf{0}.$$

In particular, for $j_1, j_2 \in \{1,2\}$, $\langle \Phi_{j_1}, \nabla\Phi_{j_2}\rangle_{L^2(\Omega)} = \mathbf{0}$.

- For admissible (e.g. Lieb and square) potential:

$$\mathcal{M}^{(0)}(\mu^{(1)}, \kappa) = \begin{pmatrix} \mu^{(1)} - \kappa\cdot\kappa & 0 \\ 0 & \mu^{(1)} - \kappa\cdot\kappa \end{pmatrix},$$

and we progress to quadratic-in-κ terms.

Symmetries Imply Vanishing Linear Terms

Linear-termed $\mathcal{M}^{(0)}(\mu^{(1)}, \kappa) \equiv$

$$\begin{pmatrix} \mu^{(1)} - \kappa \cdot \kappa + \langle \Phi_1, 2i\kappa \cdot \nabla \Phi_1 \rangle & \langle \Phi_1, 2i\kappa \cdot \nabla \Phi_2 \rangle \\ \langle \Phi_2, 2i\kappa \cdot \nabla \Phi_1 \rangle & \mu^{(1)} - \kappa \cdot \kappa + \langle \Phi_2, 2i\kappa \cdot \nabla \Phi_2 \rangle \end{pmatrix},$$

Proposition (Vanishing linear-in-κ terms)

If smooth functions f_1 and f_2 on $\mathbb{R}^2$ are $\mathcal{R}-$invariant,

$$\langle f_1, \nabla f_2 \rangle_{L^2(\Omega)} = \mathbf{0}.$$

In particular, for $j_1, j_2 \in \{1, 2\}$, $\langle \Phi_{j_1}, \nabla \Phi_{j_2} \rangle_{L^2(\Omega)} = \mathbf{0}$.

- Key point of departure from honeycomb potentials:

$$\mathcal{M}_h^{(0)}(\nu; \kappa) = \begin{pmatrix} \nu & -\overline{\lambda_\#} \times (\kappa_1 + \ i\ \kappa_2) \\ -\lambda_\# \times (\kappa_1 - \ i\ \kappa_2) & \nu \end{pmatrix},$$

where $\mathcal{M}_h^{(0)}$ is the linear-in-κ matrix for honeycomb potentials.

Simplifying and Solving $\det[\mathcal{M}(\mu^{(1)}, \kappa)] = 0$

Using rotational symmetries, one can show:

$$\mathcal{M}(\mu^{(1)}, \kappa) = \begin{pmatrix} \mu^{(1)} - \kappa \cdot \kappa + \alpha\ (\kappa_1^2 + \kappa_2^2) & \gamma(\kappa_1^2 - \kappa_2^2) + 2\beta\kappa_1\kappa_2 \\ \overline{\gamma}(\kappa_1^2 - \kappa_2^2) + 2\overline{\beta}\kappa_1\kappa_2 & \mu^{(1)} - \kappa \cdot \kappa + \alpha(\kappa_1^2 + \kappa_2^2) \end{pmatrix}$$
$$+\ \mathcal{O}_{2\times 2}(\ |\kappa|^3 + |\mu^{(1)}||\kappa|\ ).$$

where $\alpha = 4a_{1,1}^{1,1}, \beta = 4a_{1,2}^{1,2}, \gamma = 4a_{1,1}^{1,2}$, are inner products

$$a_{l,m}^{j_1,j_2} = \langle \partial_{x_l}\Phi_{j_1}, \mathcal{R}_{\mathbf{M}}\partial_{x_m}\Phi_{j_2}\rangle.$$

Careful residue analysis with Rouché's Theorem yield the result:

$$\mu_\pm(\mathbf{M} + \kappa) - \mu_S =$$
$$(1-\alpha)|\kappa|^2 + \mathcal{Q}_6(\kappa) \pm \sqrt{\left|\ \gamma(\kappa_1^2 - \kappa_2^2) + 2\beta\kappa_1\kappa_2\ \right|^2\ + \mathcal{Q}_8(\kappa)}. \quad \square$$

Main Theorem

Theorem (Quadratic touching of dispersion surfaces)

Let $H_V = -\Delta + V$*, where* V *is an admissible potential. Assume:*

H1) H_V *has simple* $(L^2_{\mathbf{M},+i})$*-eval* μ_S *with efunc* $\Phi_1(\mathbf{x})$.

H2) H_V *has simple* $(L^2_{\mathbf{M},-i})$*-eval* μ_S *with efunc* $\Phi_2 = (\mathcal{P} \circ \mathcal{C})[\Phi_1]$.

H3) μ_S *is neither an* $L^2_{\mathbf{M},+1}$ *nor an* $L^2_{\mathbf{M},-1}$ *eval of* H_V.

Then, there exist dispersion curves $\mathbf{k} \mapsto \mu_\pm(\mathbf{k})$ *associated with* H^ε_V*,that are* *quadratic* *and* $\pi/2-$*invariant* *locally in* κ *about* $\mathbf{M}$:

$$\mu_\pm(\mathbf{M} + \kappa) - \mu_S =$$

$$(1-\alpha)|\kappa|^2 + \mathcal{Q}_6(\kappa) \pm \sqrt{\left|\ \gamma(\kappa_1^2 - \kappa_2^2) + 2\beta\kappa_1\kappa_2\ \right|^2 + \mathcal{Q}_8(\kappa)},$$

$\mathcal{Q}_n = \mathcal{O}(|\kappa|^n)$ *analytic in* κ*; and* $\alpha = 4a^{1,1}_{1,1}, \beta = 4a^{1,2}_{1,2}, \gamma = 4a^{1,2}_{1,1}$*, depend on the first partials of the* $(\pm i)$ *estates and resolvent* $\mathcal{R}_\mathbf{M}$*:*

$$a^{j_1,j_2}_{l,m} = \langle \partial_{x_l}\Phi_{j_1}, \mathcal{R}_\mathbf{M}\partial_{x_m}\Phi_{j_2}\rangle,\ \ l, m, j_1, j_2 \in \{1, 2\}.$$

Corollary: Time Evolution of Wavepackets

Consider the time-dependent Schrödinger equation (TDSE):

$$i\partial_t \psi(\mathbf{x}, t) = (-\Delta_{\mathbf{x}} + V(\mathbf{x}))\psi(\mathbf{x}, t).$$

Corollary (Dynamics of Wavepackets)

Solutions to the TDSE with initial condition wavepackets:

$$\psi(\mathbf{x}, 0) = \ C_{10}(\mathbf{X})\ \Phi_1(\mathbf{x})\ +\ C_{20}(\mathbf{X})\ \Phi_2(\mathbf{x}),$$

where $\mathbf{X} \equiv \delta\mathbf{x} = (X_1, X_2)$ *and* $C_{j0}(\mathbf{X}),\ j = 1, 2$ *in Schwartz class, evolve for large time according to a coupled system of 2D Schrödinger equations* $(T = \delta^2 t,\ \mathbf{X}_1 = \delta\mathbf{x})$*:*

$$i\partial_{T=} C_p = -\Delta_{\mathbf{X}_1} C_p + 4 \sum_{q=1}^{2} \sum_{r,s=1}^{2} a_{r,s}^{p,q} \frac{\partial^2 C_q}{\partial X_{1r} \partial X_{1s}}, \quad p = 1, 2,$$

where $a_{r,s}^{p,q}$ *are the inner products from before:*

$$a_{r,s}^{p,q} = \langle \partial_{x_r} \Phi_p, \mathcal{R}_{\mathbf{M}} \partial_{x_s} \Phi_q \rangle.$$

Proof Sketch: Multiple Scale Analysis

Ansatz dependent on multiple spatial and temporal scales ($\delta \ll 1$):

$$\psi^\delta = e^{-i\mu_S t} \sum_{j\geq 0} \delta^j \; \psi_j(\mathbf{x}; \vec{\mathbf{X}}, \vec{T}),$$

where $\vec{\mathbf{X}} = (\mathbf{X}_1, \mathbf{X}_2) = (\delta\mathbf{x}, \delta^2\mathbf{x})$; $\vec{T} = (T_1, T_2) = (\delta t, \delta^2 t)$.

Hierarchy of Equations:

$$\begin{aligned}
\mathcal{O}(\delta^0): &\quad (\mu_S - H_V)\psi_0 = 0 \; ; \\
\mathcal{O}(\delta^1): &\quad (\mu_S - H_V)\psi_1 = -\left(i\partial_{T_1} + 2\, \nabla_{\mathbf{x}} \cdot \nabla_{\mathbf{X}_1}\right)\psi_0 \; ; \\
\mathcal{O}(\delta^2): &\quad (\mu_S - H_V)\psi_2 = -(i\partial_{T_2} + 2\, \nabla_{\mathbf{x}} \cdot \nabla_{\mathbf{X}_2} + \Delta_{\mathbf{X}_1})\psi_0 \\
&\qquad\qquad - (i\partial_{T_1} + 2\nabla_{\mathbf{x}} \cdot \nabla_{\mathbf{X}_1})\psi_1 \; .
\end{aligned}$$

- $\mathcal{O}(\delta^0)$ equation has solutions $\Phi_1 \in L^2_{\mathbf{M},(+i)}, \Phi_2 \in L^2_{\mathbf{M},(-i)}$.

$$\psi_0 = C_1(\vec{\mathbf{X}}, \vec{T})\Phi_1(\mathbf{x}) + C_2(\vec{\mathbf{X}}, \vec{T})\Phi_2(\mathbf{x}),$$

$C_1(\vec{\mathbf{X}}, \vec{T})$ and $C_2(\vec{\mathbf{X}}, \vec{T})$ are to be determined.

Proof Sketch: Multiple Scale Analysis

Ansatz dependent on multiple spatial and temporal scales ($\delta \ll 1$):

$$\psi^\delta = e^{-i\mu_S t} \sum_{j\geq 0} \delta^j \, \psi_j(\mathbf{x}; \vec{\mathbf{X}}, \vec{T}),$$

where $\vec{\mathbf{X}} = (\mathbf{X}_1, \mathbf{X}_2) = (\delta \mathbf{x}, \delta^2 \mathbf{x})$; $\vec{T} = (T_1, T_2) = (\delta t, \delta^2 t)$.

Hierarchy of Equations:

$$\mathcal{O}(\delta^0): \quad (\mu_S - H_V)\psi_0 = 0 \; ;$$

$$\mathcal{O}(\delta^1): \quad (\mu_S - H_V)\psi_1 = -\left(i\partial_{T_1} + 2\, \nabla_{\mathbf{x}} \cdot \nabla_{\mathbf{X}_1}\right)\psi_0 \; ;$$

$$\mathcal{O}(\delta^2): \quad (\mu_S - H_V)\psi_2 = -(i\partial_{T_2} + 2\, \nabla_{\mathbf{x}} \cdot \nabla_{\mathbf{X}_2} + \Delta_{\mathbf{X}_1})\psi_0 - (i\partial_{T_1} + 2\nabla_{\mathbf{x}} \cdot \nabla_{\mathbf{X}_1})\psi_1 \; .$$

- Key feature for admissible (Lieb/square) potential:

$$\langle \Phi_p, \nabla_{\mathbf{x}} \Phi_q \rangle = \mathbf{0}; \quad p, q = 1, 2.$$

$\mathcal{O}(\delta^1)$ problem is solvable:

$$\psi_1(\mathbf{x} + \mathbf{v}; \vec{\mathbf{X}}, \vec{T}) = 2\mathcal{R}_{\mathbf{M}} \sum_{q=1}^{2} \nabla_{\mathbf{X}_1} C_q(\mathbf{X}_1, \mathbf{X}_2, T_2) \cdot \nabla_{\mathbf{x}} \Phi_q(\mathbf{x}).$$

Proof Sketch: Multiple Scale Expansion Key Points

We have :

- $\psi_0 = C_1(\vec{\mathbf{X}}, \vec{T})\Phi_1(\mathbf{x}) + C_2(\vec{\mathbf{X}}, \vec{T})\Phi_2(\mathbf{x});$
- $\psi_1(\mathbf{x}+\mathbf{v}; \vec{\mathbf{X}}, \vec{T}) = 2\mathcal{R}_{\mathbf{M}} \sum_{q=1}^{2} \nabla_{\mathbf{X}_1} C_q(\mathbf{X}_1, \mathbf{X}_2, T_2) \cdot \nabla_{\mathbf{x}} \Phi_q(\mathbf{x}).$

$$\mathcal{O}(\delta^2): \quad (\mu_S - H_V)\psi_2 = -(i\partial_{T_2} + 2\nabla_{\mathbf{x}} \cdot \nabla_{\mathbf{X}_2} + \Delta_{\mathbf{X}_1})\psi_0 - (i\partial_{T_1} + 2\nabla_{\mathbf{x}} \cdot \nabla_{\mathbf{X}_1})\psi_1 \ .$$

- Solvability for $\mathcal{O}(\delta^2)$ problem leads to the result:

$$i\partial_T C_p = -\Delta_{\mathbf{X}_1} C_p + 4 \sum_{q=1}^{2} \sum_{r,s=1}^{2} a_{r,s}^{p,q} \frac{\partial^2 C_q}{\partial X_{1r} \partial X_{1s}}, \quad p = 1, 2,$$

where $a_{r,s}^{p,q}$ are the inner products from before:

$$a_{r,s}^{p,q} = \langle \partial_{x_r} \Phi_p, \mathcal{R}_{\mathbf{M}} \partial_{x_s} \Phi_q \rangle.$$

Outline

Summary: Integer Lattice "Schrödinger Point"

Conical singularity does not exist/persist for finite potential.

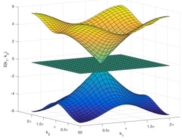
- **Quadratic**, $\pi/2-$invariant touching of dispersion surfaces

$$\mu_{\pm}(\mathbf{M}+\kappa) - \mu_S \approx (1-\alpha)|\kappa|^2 \pm \left| \gamma(\kappa_1^2 - \kappa_2^2) + 2\beta\kappa_1\kappa_2 \right|.$$

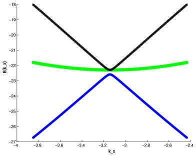
- Evolution of spectrally-concentrated wavepackets are governed by 2D **Schrödinger** equation on scales $T = \delta^2 t$ and $\mathbf{X} = \delta\mathbf{x}$:

$$i\partial_T C_p = -\Delta_{\mathbf{X}} C_p + 4 \sum_{q=1}^{2} \sum_{r,s=1}^{2} a_{r,s}^{p,q} \frac{\partial^2 C_q}{\partial X_r \partial X_s}, \quad p = 1, 2.$$

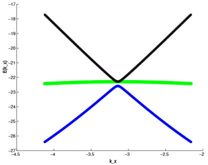
TB Dispersion Lieb



Dispersion Curves for Admissible Potential Near **M**



(i) $\mathbf{k} = \mathbf{M}_\star + \kappa e^{\frac{i\pi}{4}}$



(j) $\mathbf{k} = \mathbf{M}_\star + \kappa e^{\frac{i15\pi}{16}}$

Summary: Integer Lattice "Schrödinger Point"

Conical singularity does not exist/persist for finite potential.

- **Quadratic**, $\pi/2-$invariant touching of dispersion surfaces

$$\mu_{\pm}(\mathbf{M}+\kappa)-\mu_S \approx (1-\alpha)|\kappa|^2 \pm \left|\ \gamma(\kappa_1^2-\kappa_2^2)+2\beta\kappa_1\kappa_2\ \right|.$$

- Evolution of spectrally-concentrated wavepackets are governed by 2D **Schrödinger** equation on scales $T=\delta^2 t$ and $\mathbf{X}=\delta\mathbf{x}$:

$$i\partial_T C_p = -\Delta_{\mathbf{X}} C_p + 4\sum_{q=1}^{2}\sum_{r,s=1}^{2} a_{r,s}^{p,q}\,\frac{\partial^2 C_q}{\partial X_r \partial X_s},\ \ p=1,2.$$

Honeycomb potentials: Conical singularity persists

$$\mu_{\pm}(\mathbf{K}_\star+\kappa)-\mu(\mathbf{K}_\star)\approx \pm|\lambda_\#|\ \mid\kappa\mid.$$

Wavepackets governed by 2D Dirac equation[2], $T=\delta t$ and $\mathbf{X}=\delta\mathbf{x}$

$$\partial_T C_1(\mathbf{X},T)=\lambda_\#(\partial_{X_1}+i\partial_{X_2})C_2(\mathbf{X},T),$$
$$\partial_T C_2(\mathbf{X},T)=\lambda_\#(\partial_{X_1}-i\partial_{X_2})C_1(\mathbf{X},T).$$

[2] [FW14]

Summary: Integer Lattice "Schrödinger Point"

Conical singularity does not exist/persist for finite potential.

- **Quadratic**, $\pi/2-$invariant touching of dispersion surfaces

$$\mu_\pm(\mathbf{M}+\kappa) - \mu_S \approx (1-\alpha)|\kappa|^2 \pm \left|\ \gamma(\kappa_1^2 - \kappa_2^2) + 2\beta\kappa_1\kappa_2\ \right|.$$

Corollary (Additional symmetries imply vanishing of terms.)

Assume hypotheses of Theorem 4. Assume further that with respect to the origin of coordinates, $\mathbf{x}_c = 0$, *we have, in addition, that* V *is reflection invariant in the following sense:* $V(x_1, x_2) = V(x_2, x_1)$. *Then,*

$$\mu_\pm(\mathbf{M}+\kappa)-\mu_S = (1-\alpha)|\kappa|^2 + \mathcal{Q}_6(\kappa) \pm \sqrt{\left|\ 2\beta\kappa_1\kappa_2\ \right|^2 + \ \mathcal{Q}_8(\kappa)}\ . \tag{7}$$

Outline

Acknowledgments

We thank the US National Science Foundation and Simons Foundation for supporting this research.

Thanks to Mikael Rechtsman and Charles Fefferman for very stimulating discussions! Mikael Rechtsman also provided very helpful advice on numerical spectral calculations.

Thank you!

This research was supported in part by US National Science Foundation Graduate Research Fellowship Grant No. DGE-1144155 and DGE 16-44869 (RTK); Grants DMS-1312874 and NSF CAREER Grant DMS-1352353 (JLM); DMS 16-19755 (BO); DMS-1412560, DMS-1620418 and NSF RNMS Grant #11-07444 (Ki-Net) (RTK&MIW), and a Simons Foundation Math + X Investigator Award #376319 (MIW).

COLUMBIA | ENGINEERING
The Fu Foundation School of Engineering and Applied Science

References

C. L. Fefferman, J. P. Lee-Thorp, and M. I. Weinstein. "Honeycomb Schrödinger operators in the strong binding regime". *Commun. Pure Appl. Math. arXiv preprint arXiv:1610.04930* (2017). DOI: https://doi.org/10.1002%2Fcpa.21735.

C. L. Fefferman and M. I. Weinstein. "Honeycomb Lattice Potentials and Dirac Points". *J. Amer. Math. Soc.* 25.4 (2012), pp. 1169–1220. DOI: 10.1090/s0894-0347-2012-00745-0.

C. L. Fefferman and M. I. Weinstein. "Wave packets in honeycomb structures and two-dimensional Dirac equations". *Communications in Mathematical Physics* 326.1 (2014), pp. 251–286. DOI: 10.1007/s00220-013-1847-2.

D Guzmán-Silva, C Mejía-Cortés, M. Bandres, M. Rechtsman, S Weimann, S Nolte, M Segev, A Szameit, and R. Vicencio. "Experimental observation of bulk and edge transport in photonic Lieb lattices". *New Journal of Physics* 16.6 (2014), p. 063061. DOI: 10.1088/1367-2630/16/6/063061.

P. Kuchment. "An overview of periodic elliptic operators". *Bulletin of the American Mathematical Society* 53.3 (2016), pp. 343–414. DOI: 10.1090/bull/1528.

M Niță, B Ostahie, and A Aldea. "Spectral and transport properties of the two-dimensional Lieb lattice". *Physical Review B* 87.12 (2013), p. 125428. DOI: 10.1103/physrevb.87.125428.

C. Weeks and M. Franz. "Topological insulators on the Lieb and perovskite lattices". *Physical Review B* 82.8 (2010), p. 085310. DOI: 10.1103/physrevb.82.085310.

Characterization for ε Small Behavior

Let V_{m_1,m_2} denotes the (m_1, m_2) Fourier coefficient of V.

Proposition (Small ε behavior)

For ε sufficiently small, the 4D eigenspace of $H^{\varepsilon=0}$ perturbs to one 2D and two 1D eigenspaces that are characterized:

- *A multiplicity-two eval μ_S^ε is of geometric multiplicity 2, with a 2D eigenspace $\mathbb{X}_i \subset L^2_{\mathbf{M},i}$ and $\mathbb{X}_{-i} \subset L^2_{\mathbf{M},-i}$, and is given by:*

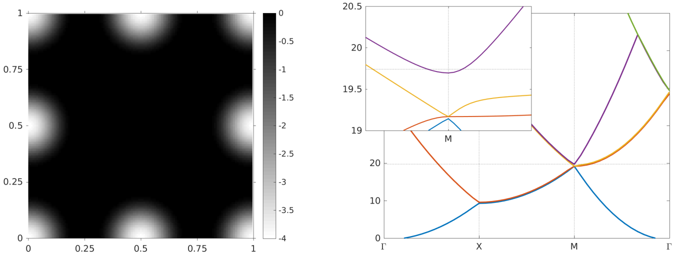
$$\mu_S^\varepsilon = |\mathbf{M}|^2 + \varepsilon(V_{0,0} - V_{1,1}) + \mathcal{O}(\varepsilon^2). \tag{8}$$

- *The distinct evals $\mu_{(+1)}^\varepsilon$ and $\mu_{(-1)}^\varepsilon$ are of geometric multiplicity 1, with 1D espaces $\mathbb{X}_{\pm 1} \subset L^2_{\mathbf{M},\pm 1}$, given by:*

$$\mu_{(\pm 1)}^\varepsilon = |\mathbf{M}|^2 + \varepsilon(V_{0,0} \pm 2V_{0,1} + V_{1,1}) + \mathcal{O}(\varepsilon^2). \tag{9}$$

Example of Ordering for Small Amplitude Potential

Figure 10: Eigenvalue ordering, up to $\mathcal{O}(\varepsilon)$: $\mu^{\varepsilon}_{-1} < \mu^{\varepsilon}_{+i} = \mu^{\varepsilon}_{-i} < \mu^{\varepsilon}_{1}$.



(a) Plot of Potential V_L (b) Dispersion curves for $H^{\varepsilon=1}_{V_L}$

Fourier coefficients, $V_{m,n}$

m/n	0	1
0	0.2242	0.0681
1	0.0681	-0.0620

Predicted dispersion relation $\mu(\mathbf{k}), \mathbf{k} = \mathbf{M} + \kappa$

$$\mu^{\varepsilon}_{-1}(\mathbf{k}) \approx (V_{0,0} - 2V_{0,1} + V_{1,1})\,\varepsilon \qquad \approx 0.0260\,\varepsilon$$

$$\mu^{\varepsilon}_{\pm i}(\mathbf{k}) \approx (V_{0,0} - V_{1,1})\,\varepsilon \qquad \approx 0.2862\,\varepsilon$$

$$\mu^{\varepsilon}_{+1}(\mathbf{k}) \approx (V_{0,0} + 2V_{0,1} + V_{1,1})\,\varepsilon \qquad \approx 0.2985\,\varepsilon$$

Physical Motivation: Lieb lattice

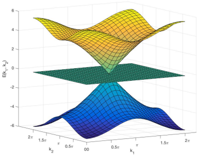
- Schrödinger operator: $H_{\varepsilon V} = -\Delta + \varepsilon V(\mathbf{x}),\ \varepsilon \in \mathbb{R}$.
- Tight-binding model ($\varepsilon \nearrow \infty$) approximates low-lying modes
- TB model for the Lieb lattice, $\mathbb{Z}^2$ lattice with 3 atomic sites, is

The TB model approximates the band structure of lattices by superimposing potential wells centered at each atomic site.

$$\begin{pmatrix} \Psi_B^{(m,n)} + \Psi_B^{(m,n+1)} \\ \Psi_A^{(m,n)} + \Psi_C^{(m,n)} + \Psi_C^{(m-1,n)} + \Psi_A^{(m,n-1)} \\ \Psi_B^{(m,n)} + \Psi_B^{(m+1,n)} \end{pmatrix} = E \begin{pmatrix} \Psi_A^{(m,n)} \\ \Psi_B^{(m,n)} \\ \Psi_C^{(m,n)} \end{pmatrix}.$$

This system has band structure (Figure **??**):

$$E_0(\mathbf{k}) = 0,\ \ E_{\pm}(k_1, k_2) = \pm\sqrt{4 + 2\cos k_1 + 2\cos k_2}.$$



Physical Motivation: Lieb lattice

- Schrödinger operator: $H_{\varepsilon V} = -\Delta + \varepsilon V(\mathbf{x}),\ \varepsilon \in \mathbb{R}$.
- Tight-binding model ($\varepsilon \nearrow \infty$) approximates low-lying modes
- TB model for the Lieb lattice, $\mathbb{Z}^2$ lattice with 3 atomic sites, is

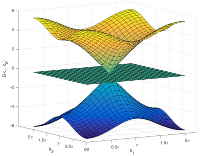
The TB model approximates the band structure of lattices by superimposing potential wells centered at each atomic site.

$$\begin{pmatrix} \Psi_B^{(m,n)} + \Psi_B^{(m,n+1)} \\ \Psi_A^{(m,n)} + \Psi_C^{(m,n)} + \Psi_C^{(m-1,n)} + \Psi_A^{(m,n-1)} \\ \Psi_B^{(m,n)} + \Psi_B^{(m+1,n)} \end{pmatrix} = E \begin{pmatrix} \Psi_A^{(m,n)} \\ \Psi_B^{(m,n)} \\ \Psi_C^{(m,n)} \end{pmatrix}.$$

This system has band structure (Figure **??**):

$$E_0(\mathbf{k}) = 0,\ \ E_\pm(k_1, k_2) = \pm\sqrt{4 + 2\cos k_1 + 2\cos k_2}.$$

- Does the three-band intersection persist for finite-depth potential wells?
- Does the conical behavior persist for finite-depth potential wells? (Do we have a Dirac Point?)

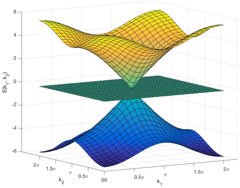


Questions and Answers

Questions:

- Does the three-band intersection persist for finite-depth potential wells?
- Does the conical behavior persist for finite-depth potential wells? (Dirac point?)

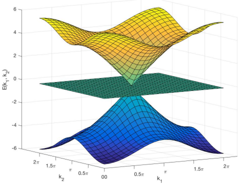
TB Dispersion Curves Lieb



Questions and Answers

<u>Questions:</u>

TB Dispersion Curves Lieb

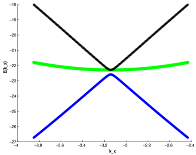


- Does the three-band intersection persist for finite-depth potential wells?
- Does the conical behavior persist for finite-depth potential wells? (Dirac point?)

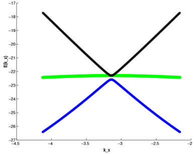
We show that the answer is <u>no</u> to all questions.

i. The three-band flat + conical behavior <u>does not</u> persist.

ii. Instead of conically, bands intersect with <u>mixed-signature</u>:



(e) $\theta = \frac{\pi}{4}$



(f) $\theta = \frac{15\pi}{16}$

Dispersion curves along $\mathbf{k} = \mathbf{M} \pm \lambda_0(\cos\theta, \sin\theta)^T$, $\lambda_0 \in \mathbb{R}$.