Honeycomb Schroedinger Operators in the Strong Binding Regime

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Collaborators

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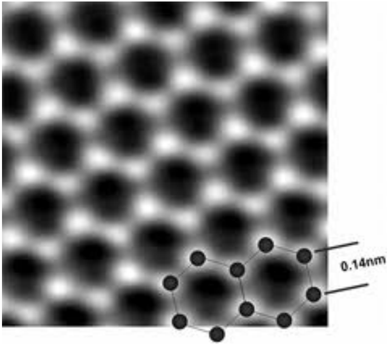
Graphene and its artificial analogues - wave properties

Graphene: Two-dimensional honeycomb arrangement of **C** atoms
$i\partial_t\psi = (\ -\Delta + V(x,y)\ )\ \psi$

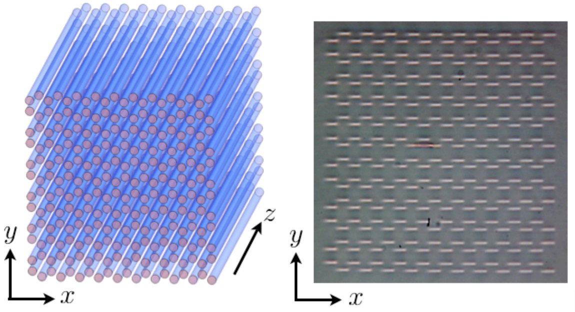


A. Geim, K. Novoselov

Artificial (photonic) graphene I.

Honeycomb arrays of optical waveguides

Paraxial Schroedinger equation (approximation to Maxwell / Helmholtz):
$i\partial_z\psi = (\ -\Delta + V(x, y)\ )\ \psi$



(a) (b)

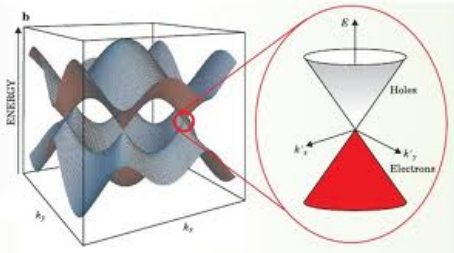
Segev, Rechtsman, Szameit *et. al.*

The propagation of waves in these two examples is approximately governed by the Schroedinger eqn, $i\partial_t\psi = H\psi$

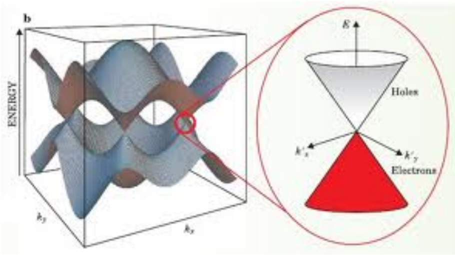
for a Hamiltonian: $H = -\Delta + V$, where V is honeycomb lattice potential

A fundamental property of wave propagation in such media is the existence of Dirac points:

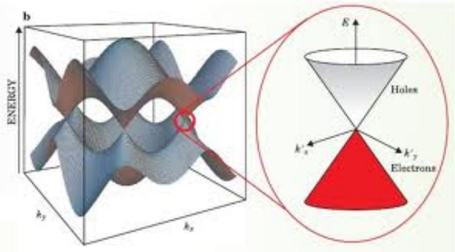
conical singularities at the intersection of adjacent dispersion surfaces.

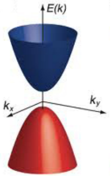


Several consequences associated with Dirac points



(1) The envelope of wave-packets (quasi-particles), spectrally localized near Dirac points, propagate like massless Fermions governed by a 2D Dirac equation.





(2) Tuning the physics:

Breaking and imposing $\mathcal{P} \circ \mathcal{T}$ symmetry causes the material to transition between "phases":

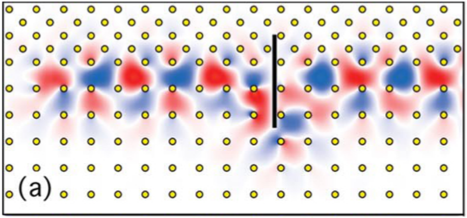
(i) conduction (no gap) $\rightleftharpoons$ insulation (gapped)

(ii) non-dispersive waves (Dirac) $\rightleftharpoons$ dispersive waves (Schrödinger)

(3) Topologically protected edge states, whose energy is concentrated along line-defects

Planar E&M structures - Haldane-Raghu (2008), Soljacic *et al* (2008)

Maxwell's equations – TM modes $-\nabla_\perp \cdot \varepsilon(\mathbf{x}_\perp)\nabla H_z = \omega^2 H_z$



Several striking features:

1) waves are propagating in only one direction.

2) when introducing the perturbation, localization at the interface persists.

3) when the propagating waves encounter the barrier, they do not reflect back or scatter into the "bulk". Rather the waves circumnavigate the barrier.

In condensed matter physics, such edge states are the hallmark of “topological insulators”.

The mechanisms for such transport are present and are being actively explored, both theoretically and experimentally, in condensed matter physics, acoustics, elasticity, mechanics,. . .

How such topologically protected edge states arise from the underlying PDEs of wave physics is a key motivation of this research.

In this talk I will focus on the properties (Dirac points *etc*) of

$$H^{\lambda} = -\Delta + \lambda^2 V(\mathbf{x}), \quad \text{where}$$

$V(\mathbf{x}) = \sum_{\mathbf{v}\in\mathbf{H}} V_0(\mathbf{x}+\mathbf{v})$, **H** = { honeycomb structure vertices }

$V_0(\mathbf{x})$ is an "atomic potential well" and

λ sufficiently large (*strong binding regime*).

In particular, we're interested in

1. Precise characterization of the low-lying dispersion surfaces
2. Consequences for:

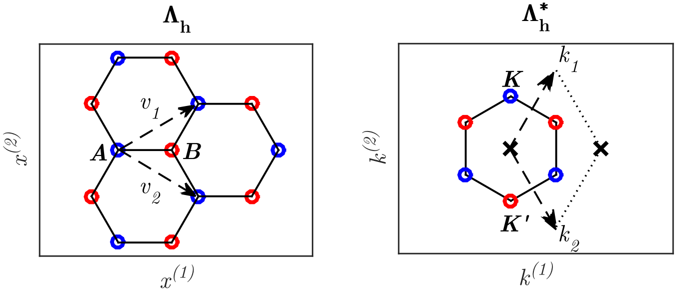
   (a) spectral gaps for $\mathcal{P}\circ\mathcal{T}-$ breaking perturbations of H^{λ} and

   (b) edge states concentrated along "rational edges"

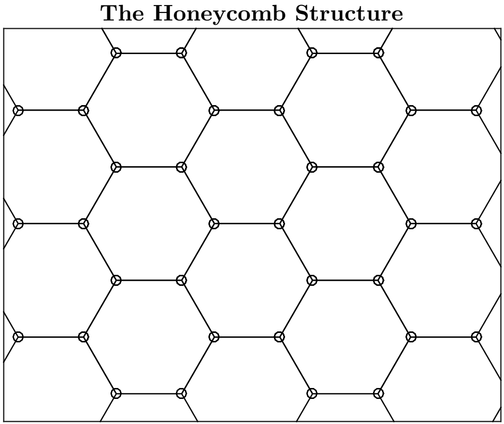
H, union of two interpenetrating triangular lattices

$$\Lambda_h = \mathbb{Z}\mathbf{v}_1 \oplus \mathbb{Z}\mathbf{v}_2$$

$$\mathbf{H} = (\mathbf{A} + \Lambda_h) \cup (\mathbf{B} + \Lambda_h)\ ,$$ Brillouin zone, $\mathcal{B}_h$



$$\mathbf{H} = (\mathbf{A} + \Lambda_h) \cup (\mathbf{B} + \Lambda_h) = \Lambda_A \cup \Lambda_B$$



Honeycomb lattice potentials

$V(\mathbf{x})$ is a honeycomb lattice potential if

1. $V(\mathbf{x})$ is Λ_h- periodic: $V(\mathbf{x}+\mathbf{v}) = V(\mathbf{x})$ for all $\mathbf{x} \in \mathbb{R}^2$ and $\mathbf{v} \in \Lambda_h$,
2. $V(\mathbf{x})$ is real,

   and with respect to some origin of coordinates:
3. $V(\mathbf{x})$ is inversion-symmetric: $V(-\mathbf{x}) = V(\mathbf{x})$ and
4. $V(\mathbf{x})$ is invariant under $2\pi/3$ rotation :

$$\mathcal{R}[V](\mathbf{x}) \equiv V(R^*\mathbf{x}) = V(\mathbf{x}),$$

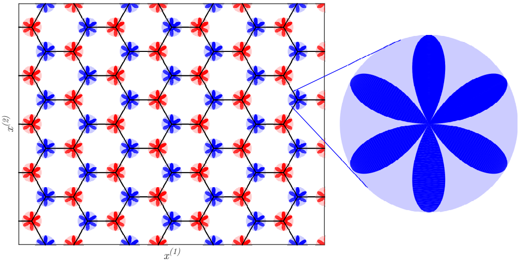
where R is a $2\pi/3$- rotation matrix .

$$(2),(3) \implies [-\Delta + V, \mathcal{P}\circ\mathcal{T}] = 0$$

$$(4) \implies [-\Delta + V, \mathcal{R}] = 0$$

Example of a honeycomb lattice potential

$V(\mathbf{x}) = \sum_{\mathbf{v}\in\mathbf{H}} V_0(\mathbf{x})$, superposition of "atomic potentials", $V_0(\mathbf{x})$

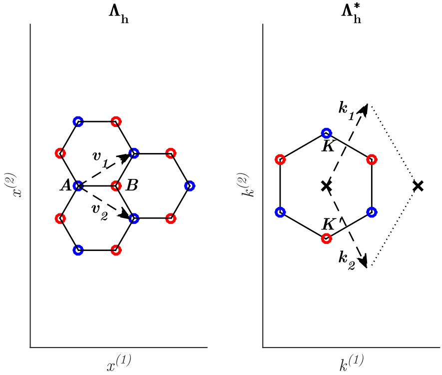


Quick review of spectral theory of $H = -\Delta + V$, where V is $\Lambda-$ periodic

For each "quasi-momentum" $\mathbf{k} \in \mathcal{B}$, seek : $u(x;\mathbf{k}) = e^{i\mathbf{k}\cdot x} p(x;\mathbf{k})$,

$$H(\mathbf{k})\ p(\mathbf{x};\mathbf{k}) \ \equiv\ \left(-\left(\nabla + i\mathbf{k}\right)^2 + V(\mathbf{x}) \right) p(\mathbf{x};\mathbf{k}) = E(\mathbf{k}) p(\mathbf{x};\mathbf{k}),$$

$$p(\mathbf{x}+\mathbf{v};\mathbf{k}) \ = \ p(\mathbf{x};\mathbf{k}), \quad \text{all} \ \ \mathbf{v} \in \Lambda, \ \ \mathbf{x} \in \mathbb{R}^2$$



The band structure

The EVP has, for each $\mathbf{k} \in \mathcal{B}$, a discrete sequence of e-values:

$$E_1(\mathbf{k}) \leq E_2(\mathbf{k}) \leq E_3(\mathbf{k}) \leq \cdots \leq E_b(\mathbf{k}) \leq \ldots$$

with $\Lambda-$ periodic eigenfunctions $p_b(\mathbf{x}; \mathbf{k}), \ b = 1, 2, 3, \ldots$

- The (Lipschitz) mappings $\mathbf{k} \in \mathcal{B} \mapsto \ E_b(\mathbf{k}), \ \ b = 1, 2, 3, \ldots$ are called **dispersion relations** of $-\Delta + V$

  Their graphs are **dispersion surfaces**.

- Energy spectrum of $-\Delta + V$ is given by the union of intervals (spectral bands) swept out by $E_b(\mathbf{k})$:

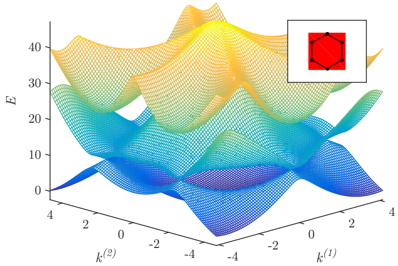
$$E_1(\mathcal{B}) \cup E_2(\mathcal{B}) \cup E_3(\mathcal{B}) \cup \ldots E_b(\mathcal{B}) \cup \ldots$$

Energy transport depends on the detailed properties of $\mathbf{k} \mapsto E_b(\mathbf{k}),\ b \geq 1$:

regularity, critical points,...

$$H = -\Delta + V,$$

$$[\,\exp(\,-i\,Ht\,)\,f\,]\,(x,t) = \sum_{b\geq 1} \int_{\mathcal{B}} \tilde{f}_b(\mathbf{k})\; e^{\,i(\,\mathbf{k}\cdot\mathbf{x} - E_b(\mathbf{k})t\,)}\; p_b(\mathbf{x};\mathbf{k})\; d\mathbf{k}$$



What is a Dirac point ?

A quasi-momentum / energy pair $(\mathbf{k}, E) = (\mathbf{K}_\star, E_D)$ such that for $\mathbf{k}$ near $\mathbf{K}_\star$ we have

$$E_\pm(\mathbf{k}) - E_D \;=\; \pm v_F \;|\mathbf{k} - \mathbf{K}_\star| \;\left(1 \;+\; \mathcal{O}(|\mathbf{k} - \mathbf{K}_\star|) \right), \quad \text{with } v_F \;>\; 0 \;\text{“Fermi velocity”}$$

For $\mathbf{k} = \mathbf{K}_\star$, $E = E_D$ is two-fold degenerate $\mathbf{K}_\star-$ pseudo-periodic eigenvalue.

More precisely,

$L^2_{\mathbf{K}_\star} -$ kernel of $H - E_D I$ (boundary cond. $\Phi(\mathbf{x} + \mathbf{v}) = e^{i\mathbf{K}_\star \cdot \mathbf{x}}\Phi(\mathbf{x})$)

$= \text{span}\{\Phi_1, \Phi_2\}$,

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

Honeycomb lattice potentials, V, and Dirac Points; Fefferman & W JAMS '12

$H^\varepsilon = -\Delta + \varepsilon V$

$V_{1,1} \ = \ \int_\Omega e^{-i(\mathbf{k}_1+\mathbf{k}_2)\cdot \mathbf{y}} \ V(\mathbf{y}) \ d\mathbf{y} \neq 0$ (non-degeneracy)

Thm 1: Generic honeycomb potentials have Dirac points at the vertices of $\mathcal{B}_h$.

(a) If ε lies outside of a possible discrete real subset, $\mathcal{C} \subset \mathbb{R}$, $H^{(\varepsilon)}$ has Dirac points at $\mathbf{k} = \mathbf{K}_\star$ at the vertices of $\mathcal{B}$:

$$E^\varepsilon_\pm(\mathbf{k}) - E^\varepsilon_\star \ \approx \ \pm v^\varepsilon_F \ |\mathbf{k} - \mathbf{K}_\star| \,, \quad \text{with} \ \ v^\varepsilon_F > 0$$

No restriction on size of ε.

(b) If $\varepsilon V_{1,1} > 0$ and small, then Dirac points occur at intersections of 1st and 2nd dispersion surfaces.

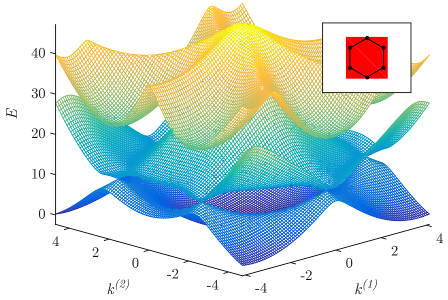
(c) If $\varepsilon V_{1,1} < 0$ and small, then Dirac points occur at intersections of 2nd and 3rd dispersion surfaces.

NOTE: For general ε we don't know which dispersion surfaces intersect.

We can display examples with "transitions" as ε varies.

3 low-lying dispersion surfaces of $-\Delta + V(\mathbf{x})$, $\mathbf{k} \in \mathcal{B}_h \;\mapsto\; E_b(\mathbf{k}),\; b = 1, 2, 3,$

$V(\mathbf{x})$ is a H.L.P. satisfying $\varepsilon V_{1,1} > 0$



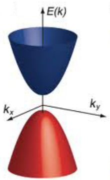
Related work on Dirac points:
Grushin (2009), Berkolaiko-Comech (arXiv: 2014)

Stability / Instability of Dirac Points

Thm 2: (Persistence)
Dirac points persist against small perturbations of $-\Delta + V_h$, which preserve $\mathcal{P} \circ \mathcal{T}$, *i.e.* one may break rotational invariance.

(…but "Dirac cones" may perturb away from the vertices of $\mathcal{B}_h$)

Thm 3: (Non-persistence)
If $\mathcal{P}$ or $\mathcal{T}$ is broken then the dispersion surfaces are smooth in a neighborhood of the vertices of $\mathcal{B}_h$.



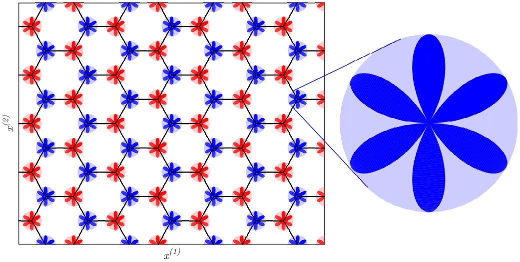
N.B. However, spectral gap may open only locally in **k** !

Dispersion surfaces may "fold over" away from the vertices $\mathbf{K}_\star$ of $\mathcal{B}_h$.

Honeycomb Schroedinger operators in the strong binding regime

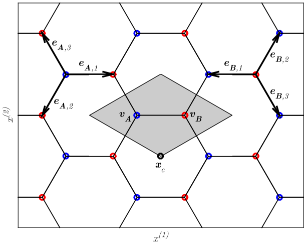
We study the continuous Schroedinger operator $-\Delta + \lambda^2 V(\mathbf{x})$, with *honeycomb lattice potential* $V(\mathbf{x})$ defined on $\mathbb{R}^2$ and $\lambda > \lambda_\star$ sufficiently large.

$V(\mathbf{x}) \;=\; \sum_{\mathbf{v}\in\mathbf{H}}\; V_0(\mathbf{x})$ superposition of "atomic potentials":



Hypotheses on atomic potential, $V_0(\mathbf{x})$ $\left[V(\mathbf{x}) = \sum_{\mathbf{v}\in\mathbf{H}} V_0(\mathbf{x}+\mathbf{v})\right]$

1. $\text{support}(V_0) \subset B_{r_0}(0)$, with $0 < r_0 < r_{critical}$, where
$$.33\,|e_{A,1}| < r_{critical} < .5\,|e_{A,1}| \quad .$$
$|e_{A,1}|$ = distance from a point in **H** to its nearest neighbor
2. $-1 \le V_0(\mathbf{x}) \le 0, \quad \mathbf{x} \in \mathbb{R}^2$
3. $V_0(-\mathbf{x}) = V_0(\mathbf{x})$
4. $V_0(\mathbf{x})$ invariant by 120° rotation about $\mathbf{x} = 0$
5. $(p_0^\lambda, E_0^\lambda)$, ground state of $-\Delta + \lambda^2 V_0$: $E_0^\lambda \le -C\lambda^2$
6. $\langle(-\Delta + \lambda^2 V_0 - E_0^\lambda)\psi, \psi\rangle \ge c_{gap}\,\|\psi\|^2$ for all $\psi \perp p_0^\lambda$ $\qquad (c_{gap} > 0)$



Floquet-Bloch spectrum of $H^\lambda = -\Delta + \lambda^2 V(\mathbf{x})$, $V(\mathbf{x}) = \sum_{\mathbf{v}\in\mathbf{H}} V_0(\mathbf{x})$

k- dependent Hamiltonian: $H^\lambda(\mathbf{k}) = -(\nabla + i\mathbf{k})^2 + \lambda^2 V(\mathbf{x})$, $\mathbf{k} \in \mathcal{B}_h$

Λ_h- periodic eigenvalues of $H^\lambda(\mathbf{k})$: $E_1^\lambda(\mathbf{k}) \leq E_2^\lambda(\mathbf{x}) \leq \cdots \leq E_b^\lambda(\mathbf{k}) \leq \cdots$

Dispersion surfaces: $\mathbf{k} \in \mathcal{B}_h \mapsto E_b^\lambda(\mathbf{k})$, b=1,2,3,...

Problem: Describe the behavior of the dispersion surfaces of H^λ, obtained from the low-lying (two lowest) eigenvalues of $H^\lambda(\mathbf{k})$:

$$\mathbf{k} \mapsto E_1^\lambda(\mathbf{k}) = E_-^\lambda(\mathbf{k}) \qquad \text{and} \qquad \mathbf{k} \mapsto E_2^\lambda(\mathbf{k}) = E_+^\lambda(\mathbf{k}),$$

for all $\lambda > \lambda_\star$ sufficiently large.

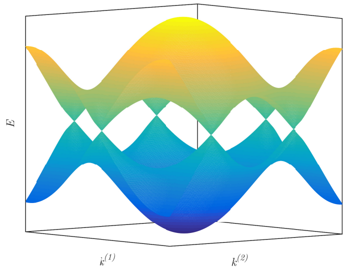
Theorem- Strong Binding Regime (Fefferman, Lee-Thorp & W. - 2016)

$$H^\lambda = -\Delta + \lambda^2 V(\mathbf{x}), \qquad V(\mathbf{x}) = \sum_{\mathbf{v}\in\mathbf{H}} V_0(\mathbf{x})$$

For <u>all</u> $\lambda > \lambda_\star$ sufficiently large, the two lowest dispersion surfaces,

$$\mathbf{k} \in \mathcal{B}_h \mapsto E_\pm^\lambda(\mathbf{k}),$$

upon rescaling, are uniformly close to the dispersion surfaces of the 2-band tight-binding model:



PR Wallace (1947) - *The band structure of graphite, Phys. Rev. (1947)*

More precisely, there exists at energy $E_D^\lambda \approx E_0^\lambda$ such that $(E_D^\lambda, \mathbf{K}_\star)$, where $\mathbf{K}_\star$ varies over the vertices of $\mathcal{B}_h$, are Dirac points.

Furthermore, there exists $\rho_\lambda > 0$ (with $e^{-c_1\lambda} \lesssim \rho_\lambda \lesssim e^{-c_2\lambda}$) such that as $\lambda \to \infty$ (uniformly in $\mathbf{k} \in \mathcal{B}_h$):

$$\left(E_-^\lambda(\mathbf{k}) - E_D^\lambda \right) / \rho_\lambda \to -\mathcal{W}_{TB}(\mathbf{k}) \;\; \text{and} \;\; \left(E_+^\lambda(\mathbf{k}) - E_D^\lambda \right) / \rho_\lambda \to +\mathcal{W}_{TB}(\mathbf{k}) \,,$$

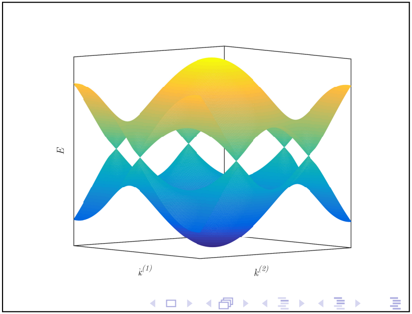
Here, $\mathcal{W}_{TB}(\mathbf{k}) \equiv \left| \, 1 + e^{i\mathbf{k}\cdot\mathbf{v}_1} + e^{i\mathbf{k}\cdot\mathbf{v}_2} \, \right|$

- On $\mathcal{B}_h$, the fn $\mathcal{W}_{TB}(\mathbf{k})$ vanishes precisely at the vertices.

- For $\mathbf{K}_\star$, any vertex of $\mathcal{B}_h$:

$$\mathcal{W}_{TB}(\mathbf{K}_\star + \boldsymbol{\kappa}) = \frac{\sqrt{3}}{2}\,|\boldsymbol{\kappa}| + \mathcal{O}(|\boldsymbol{\kappa}|^2)$$

- $v_F^\lambda = \left[\frac{\sqrt{3}}{2} + \mathcal{O}(e^{-c\lambda}) \right] \rho_\lambda$



(Th'm cont'd) Derivative bounds near and away from Dirac points

$$H^\lambda \;=\; -\Delta \;+\; \lambda^2 V(\mathbf{x}), \quad V(\mathbf{x}) = \sum_{\mathbf{v}\in\mathbf{H}} V_0(\mathbf{x}+\mathbf{v})$$

Fix β_{max}. There exists $\lambda_\star = \lambda_\star(V_0, \beta_{max})$, such that for all $\lambda > \lambda_\star$

(a) Low-lying dispersion surfaces away from Dirac points:

For all $\mathbf{k} \in \mathbb{R}^2$ such that $\mathcal{W}_{\rm TB}(\mathbf{k}) \;\geq \lambda^{-\frac{1}{4}}$:

$$\left|\, \partial_{\mathbf{k}}^{\beta} \left\{ \left(E_{\pm}^{\lambda}(\mathbf{k}) \;-\; E_{D}^{\lambda} \right) / \rho_\lambda \;-\; [\, \pm\, \mathcal{W}_{\rm TB}(\mathbf{k})\,] \right\} \right| \;\leq\; e^{-c\lambda} \;, \; |\beta| \leq \beta_{max} \;.$$

(b) Low-lying dispersion surfaces near Dirac points:

For any vertex, $\mathbf{K}_\star$, of $\mathcal{B}_h$ and all $\mathbf{k}$ satisfying $0 < |\mathbf{k} - \mathbf{K}_\star| < c_{\star\star}$:

$$\left|\, \partial_{\mathbf{k}}^{\beta} \left\{ \left(E_{\pm}^{\lambda}(\mathbf{k}) \;-\; E_{D}^{\lambda} \right) / \rho_\lambda \;-\; [\, \pm\, \mathcal{W}_{\rm TB}(\mathbf{k})\,] \right\} \right| \;\leq e^{-c\lambda}\, |\mathbf{k} - \mathbf{K}_\star|^{1-|\beta|} \;, \; |\beta| \leq \beta_{max} .$$

Two Corollaries in the strong binding regime

Corollary A:

Spectral gaps for $\mathcal{P} \circ \mathcal{T}$ breaking perturbations of $-\Delta + \lambda^2 V(\mathbf{x})$.

$$H^{\lambda,\eta} = -\Delta + \lambda^2 V(\mathbf{x}) + \eta W(\mathbf{x})$$

Corollary B:

Topologically protected edge states concentrated along rational edges

$$H^{(\lambda,\delta)} \equiv -\Delta + \lambda^2 V(\mathbf{x}) + \delta\kappa(\delta\mathfrak{K}_2 \cdot \mathbf{x}) W(\mathbf{x}).$$

[motivated by Haldane and Raghu (2008), Su-Schrieffer-Heeger (1979)]

Corollary A: Consider the perturbed honeycomb Schrödinger

$$H^{\lambda,\eta} = -\Delta + \lambda^2 V(\mathbf{x}) + \eta W(\mathbf{x}),$$

1. $W(\mathbf{x})$ is real-valued and Λ_h periodic.
2. $W(\mathbf{x})$ breaks inversion symmetry: $W(-\mathbf{x}) = -W(\mathbf{x})$
3. $$\vartheta_\sharp^\lambda \equiv \left\langle \Phi_1^\lambda, W\Phi_1^\lambda \right\rangle \neq 0,$$

Then, for all $\lambda > \lambda_\star$ sufficiently large and all $0 < \eta < \eta_\star$ sufficiently small

$$\left(E_D^\lambda - \vartheta_\sharp^\lambda \, \eta \, , \, E_D^\lambda + \vartheta_\sharp^\lambda \, \eta \right) \cap \mathrm{spec}(H^{\lambda,\eta}) = \emptyset$$

Idea of the proof:

(a) For $\mathbf{k} \in \mathcal{B}_h$, such that $|\mathbf{k} - \mathbf{K}_\star|$ small

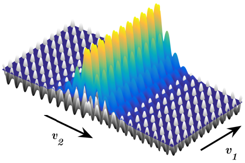
$$E_\pm^{(\lambda,\eta)}(\mathbf{k}) \approx E_D^\lambda \pm \sqrt{|v_F^\lambda|^2 \, |\mathbf{k} - \mathbf{K}_\star|^2 + (\vartheta_\sharp^\lambda)^2 \, \eta^2}$$

(b) For $\mathbf{k} \in \mathcal{B}_h$, such that $|\mathbf{k} - \mathbf{K}_\star|$ bounded away from zero, use the uniform converg. of rescaled $E_\pm^{(\lambda,0)}(\mathbf{k})$ to $\pm\mathcal{W}_{\text{TB}}(\mathbf{k})$.

Edge states

Solutions $\psi(\mathbf{x}, t) = e^{-iEt}\Psi(\mathbf{x})$ of a wave equation (Schroedinger, Maxwell,. . .) which are

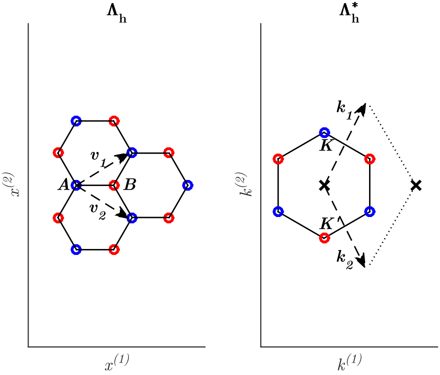
- propagating (plane-wave like) parallel to a line-defect ("edge")
- localized transverse to the edge.



- *Dirac pts provide a mechanism for producing protected edge states*

Edge States in Honeycomb Structures

Recall

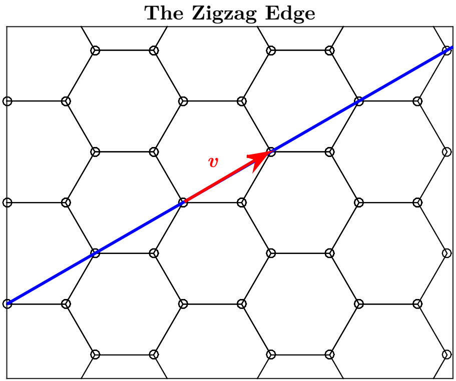


$\mathbf{k}_m \cdot \mathbf{v}_n = 2\pi\delta_{mn},$

$\mathcal{B}$

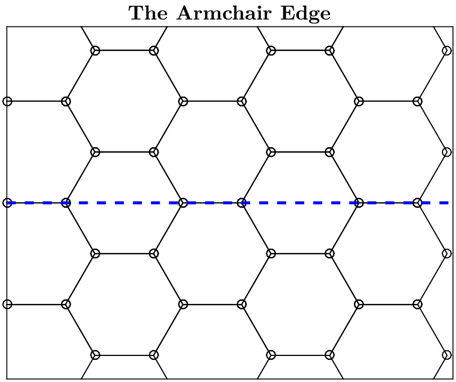
The Zigzag Edge

- $\mathfrak{v}_1 = \mathbf{v}_1$, $\mathfrak{v}_2 = \mathbf{v}_2$, $\mathfrak{K}_1 = \mathbf{k}_1$ and $\mathfrak{K}_2 = \mathbf{k}_2$; $\mathfrak{K}_m \cdot \mathfrak{v}_n = 2\pi\delta_{mn}$



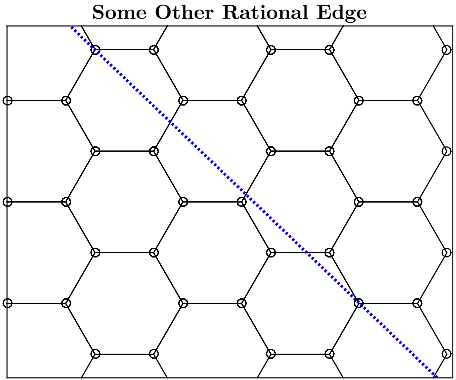
The Armchair Edge

- $\mathfrak{v}_1 = \mathbf{v}_1 + \mathbf{v}_2, \mathfrak{v}_2 = \mathbf{v}_2,\ \mathfrak{K}_1 = \mathbf{k}_1,\ \mathfrak{K}_2 = \mathbf{k}_2 - \mathbf{k}_1;\ \mathfrak{K}_m \cdot \mathfrak{v}_n = 2\pi\delta_{mn}$



General rational edge

- $$\mathfrak{v}_1 = a_1\mathbf{v}_1 + b_1\mathbf{v}_2, \quad a_1, b_1 \in \mathbb{Z}, \quad (a_1, b_1) = 1, \quad \mathfrak{v}_2, \ \mathfrak{K}_1, \ \mathfrak{K}_2$$
  $$\mathfrak{K}_m \cdot \mathfrak{v}_n = 2\pi\delta_{mn}, \quad m, n = 1, 2$$



$\mathfrak{v}_1 = -\mathbf{v}_1 + 4\mathbf{v}_2$

Motivating work on edge states - quantum and electromagnetic

Planar E&M:

Haldane & Raghu PRL '08, Raghu-Haldane Phys Rev A, '08
Photonic realization of quantum-Hall type one-way edge states

Wang, Chong, Joannopoulos & Soljacic PRL '08
Reflection free one-way edge modes in a gyromagnetic photonic crystal

1D Quantum and E&M:
Array of dimers (double-wells) w/ domain-wall induced phase shift

Su, Schrieffer & Heeger PRL '79, *Soliton in polyacetelene*

Fefferman, Lee-Thorp & W. : PNAS, '14, Memoirs AMS - 2016
Topologically protected states in 1D continuum systems

$$H^\delta = -\Delta + V(\mathbf{x}) + \delta\kappa(\delta\mathfrak{K}_2 \cdot \mathbf{x})\, W(\mathbf{x}), \quad \kappa(\zeta) \sim \tanh(\zeta)$$

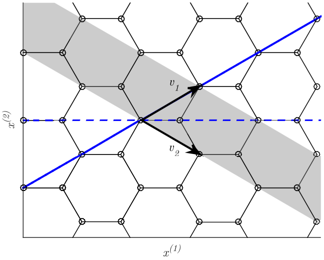
H^δ has a translation invariance, $\mathbf{x} \to \mathbf{x} + \mathfrak{v}_1$

and an associated *parallel quasi-momentum*, $k_\parallel$

Eigenvalue problem for a $\mathfrak{v}_1-$ edge state

$$H^\delta \Psi = E\,\Psi, \quad \Psi(\mathbf{x} + \mathfrak{v}_1) = e^{ik_\parallel}\Psi(\mathbf{x}), \quad \Psi(\mathbf{x}) \to 0, \ |\mathbf{x}\cdot\mathfrak{K}_2| \to \infty$$

Equivalently, $H^\delta\Psi = E\Psi, \ \Psi \in L^2_{k_\parallel}(\Sigma), \ \Sigma = \mathbb{R}^2/\mathbb{Z}\mathfrak{v}_1$.

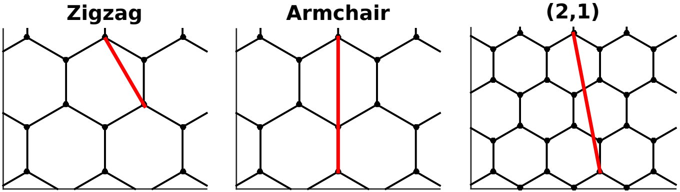


The spectral no-fold condition: - Local directional spectral gap $\implies$ full directional gap

Note that if $f(\mathbf{x}+\mathfrak{v}_1) = e^{ik_{\|}} f(\mathbf{x})$, $k_{\|} = \mathbf{K}\cdot\mathfrak{v}_1$
and is localized transverse to $\mathbb{R}\mathfrak{v}_1$ then

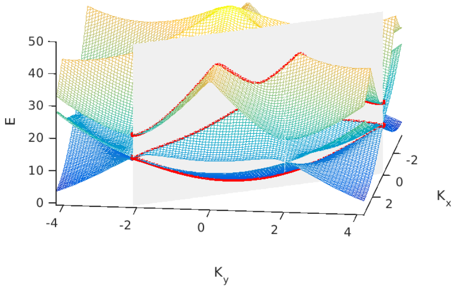
$$f(\mathbf{x}) \; = \; \sum_{b\geq 1}\int_0^1 \widetilde{f}_b(\lambda)\Phi_b(\mathbf{x};\mathbf{K}+\lambda\mathfrak{K}_2)d\lambda$$

That is we take a superposition of all Bloch modes, which are consistent with $k_{\|}-$ pseudo-periodicity: $H\,\Phi_b(\mathbf{x};\mathbf{K}+\lambda\mathfrak{K}_2) \; = \; E_b(\mathbf{K}+\lambda\mathfrak{K}_2)\;)\Phi_b(\mathbf{x};\mathbf{K}+\lambda\mathfrak{K}_2)$

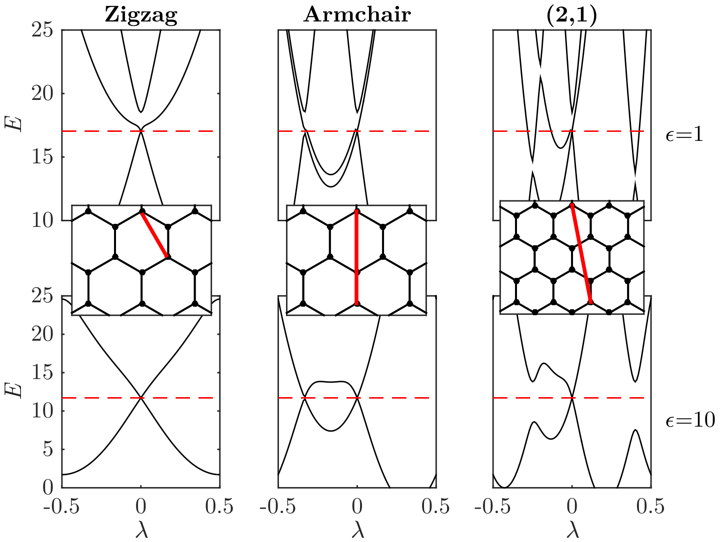


Thus we must understand the slice of the band structure consisting of the union of the graphs of:

$$\lambda \mapsto E_b(\mathbf{K} + \lambda \mathfrak{K}_2), \quad |\lambda| \leq 1/2, \quad b \geq 1.$$



Band structure slices of $-\Delta + \epsilon V_h$: from low to high contrast $\rightarrow$ TB



Theorem (Fefferman, Lee-Thorp & W., Annals of PDE 2016)

General conditions for existence of topologically protected edge states -

$$H^\delta \ = -\Delta + V(\mathbf{x}) \ + \ \delta\kappa(\delta\, \mathfrak{K}_2 \cdot \mathbf{x}) \ W(\mathbf{x}).$$

- Fix a rational edge, $\mathbb{R}\mathfrak{v}_1$
- Assume $-\Delta + V$ satisfies spectral no-fold condition (for $\mathbb{R}\mathfrak{v}_1$)

1. For all $k_\parallel \approx \mathbf{K} \cdot \mathfrak{v}_1$, the edge state EVP:

   $$H^\delta \Psi = E\Psi, \quad \Psi \in L^2_{k_\parallel}(\Sigma)$$

   has a branch of eigenpairs $\delta \mapsto (\Psi^\delta, E^\delta)$ which bifurcates from the Dirac point:

   $$\Psi^\delta(\mathbf{x}) \ \approx_{H^2_{k_\parallel}} \ \alpha_{\star,+}(\delta\mathfrak{K}_2 \cdot \mathbf{x})\Phi_+(\mathbf{x}) + \alpha_{\star,-}(\delta\mathfrak{K}_2 \cdot \mathbf{x})\Phi_-(\mathbf{x})$$

   $$E^\delta = E_\star \ + \ \mathcal{O}(\delta^2).$$

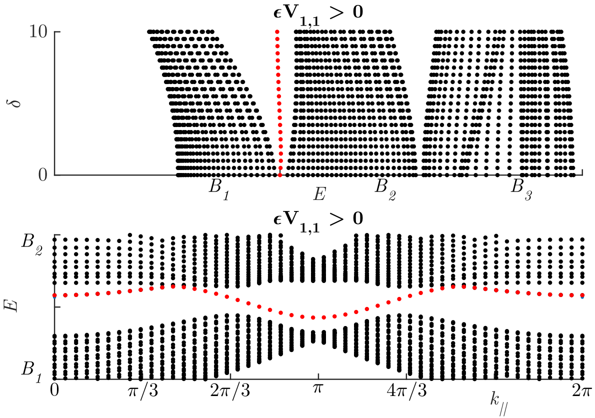
2. $\alpha_\star(\zeta)$ is a 0-energy eigenstate of the Dirac operator

   $$\mathcal{D} \equiv i\lambda_\sharp \sigma_3 \frac{\partial}{\partial\zeta} \ + \ \vartheta_\sharp \kappa(\zeta)\sigma_1$$

   $$\mathcal{D}\alpha_\star = 0, \ \alpha_\star \in L^2(\mathbb{R}_\zeta)$$

Edge state bifurcation in $H^{\delta} = -\Delta + V(\mathbf{x}) + \delta\kappa(\delta\, \mathfrak{K}_2 \cdot \mathbf{x})\, W(\mathbf{x})$

E vs. δ ($k_{\parallel}$ fixed) and E vs. $k_{\parallel}$ (δ fixed)



Bifurcation of transverse-localized states from the continuous spectrum of states which are spatially extended.

Robustness (topological stability):

The bifurcation of Thm 5 is seeded by

"protected" (rigid) zero mode of a Dirac operator, $\mathcal{D}$

$$\Psi^\delta(\mathbf{x}) \approx_{H^2_{k_\parallel}} \alpha_{\star,+}(\delta\mathfrak{K}_2 \cdot \mathbf{x})\Phi_+(\mathbf{x}) + \alpha_{\star,-}(\delta\mathfrak{K}_2 \cdot \mathbf{x})\Phi_-(\mathbf{x})$$

$$\mathcal{D}\alpha_\star(\zeta) \equiv \left(i\lambda_\sharp\sigma_3 \frac{\partial}{\partial\zeta} + \vartheta_\sharp\kappa(\zeta)\sigma_1 \right) \alpha_\star(\zeta) = 0 \,, \quad \lambda_\sharp\vartheta_\sharp \neq 0$$

For arbitrary domain walls, $\kappa(\zeta) \to \pm\kappa_\infty$, $\mathcal{D}$ has a zero-eigenvalue.

In particular, the branch of edge states persists

even when $\kappa(\zeta)$ is perturbed by a large (but localized) perturbation.

Cases in which *spectral no-fold condition* can be proved for $H^\lambda = -\Delta + \lambda^2 V$

$\Longrightarrow$ *Thm*: Existence of protected edge states in two asymptotic regimes

1. Low contrast honeycomb structures $\lambda^2 V_{1,1} > 0$ and sufficiently small

   Protected edge states along ZIGZAG edges,
   (but not, e.g., Armchair edges)

2. High-contrast honeycomb structures

   $V(\mathbf{x}) = \sum_{\mathbf{v} \in \mathbf{H}} V_0(\mathbf{x} + \mathbf{v}), \ \ \lambda > \lambda_\star$ sufficiently large

   Protected edge states along "ANY" rational edge,
   i.e. $\mathfrak{v}_{a_1,a_2} = a_1 \mathbf{v}_1 + a_2 \mathbf{v}_2, \ \ a_1, a_2$ relatively prime integers

   Given, $\mathfrak{v}_{a_1,a_2}$, there exists $\lambda_\star(\mathfrak{v}_{a_1,a_2})$, such that for all $\lambda > \lambda_\star$
   there exist protected edge states.

   Spectral no-fold condition follows from our strong binding analysis

   Theorem: Uniform conv. of scaled (low-lying) dispersion surfaces:

$$\left(E^\lambda_\pm(\mathbf{k}) - E^\lambda_\star\right) / \rho_\lambda \longrightarrow \pm \left|\mathcal{W}_{TB}(\mathbf{k})\right| , \quad \lambda \uparrow$$

What if spectral no-fold hypothesis fails for the $\mathfrak{v}_1$ edge?

Conjecture: (based on formal asymptotic analysis and numerical evidence):

There exist meta-stable states:
long-lived states, whose energy is concentrated on the $\mathfrak{v}_1-$ edge,
which eventually radiate their energy into the bulk.

A mathematical theory of such *protected edge "quasi-modes"*

is an interesting open challenge.

Open problem:
Irrational edges - Do irrational edge states exist?

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2. F-W, *Wave packets in honeycomb structures and 2D Dirac equations*, Commun. Math. Phys. 326, 251–286, (2014)
3. F-L-W, *Topologically protected states in one-dimensional continuous systems and Dirac points*, PNAS (2014)
4. F-L-W, *Edge states in honeycomb structures*, Annals of PDE (2016)
5. F-L-W, *Bifurcations of edge states – topologically protected and non-protected – in continuous 2D honeycomb structures* , 2D Materials, 3 (2016)
6. F-L-W, *Topologically protected states in one-dimensional systems*, Memoirs of the AMS (2016-17), to appear
7. F-L-W, *Honeycomb Schroedinger operators in the strong binding regime*, submitted (2016)