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Exercise class 6: Graphene and the Haldane model

1 Graphene and Dirac points

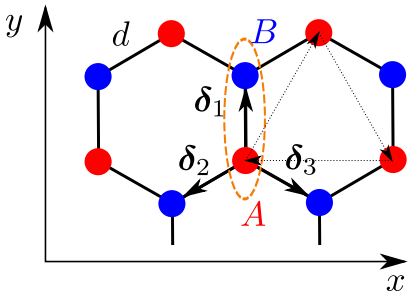


Figure 1: The geometry of the graphene lattice. The distance between atoms is d, $\boldsymbol{\delta}_i$ are the vectors linking nearest neighbors. Each link between nearest neighbors has a hopping amplitude $-t$ ($t > 0$). The on-site energies are identical, and will be taken as zero.

1. Like the SSH model, graphene also has two atoms per unit cell, so the same formalism applies. The $H_{\boldsymbol{k}}$ matrix can be written

$$H_{\boldsymbol{k}} = \begin{pmatrix} 0 & (f_{\boldsymbol{k}})^\star \\ f_{\boldsymbol{k}} & 0 \end{pmatrix}, \qquad \text{with} \qquad f_{\boldsymbol{k}} = -t \sum_j e^{i\boldsymbol{k}\cdot\boldsymbol{\delta}_i} \tag{1}$$

and where $\boldsymbol{\delta}_i$ are the vectors linking A atoms to B's nearest neighbors (see Fig. 1). Express the $\boldsymbol{\delta}_i$ and $f_{\boldsymbol{k}}$. Find and plot the associated energy spectrum.

Correction.
Some elementary geometry gives us:

$$\boldsymbol{\delta}_1 = \begin{pmatrix} 0 \\ d \end{pmatrix} \qquad \boldsymbol{\delta}_2 = \begin{pmatrix} -\frac{\sqrt{3}}{2}d \\ -\frac{d}{2} \end{pmatrix} \qquad \boldsymbol{\delta}_2 = \begin{pmatrix} +\frac{\sqrt{3}}{2}d \\ -\frac{d}{2} \end{pmatrix}$$

From this vectors, we deduce the expression of $f_{\boldsymbol{k}}$:

$$f_{\boldsymbol{k}} = -t\left(\mathrm{e}^{ik_y d} + 2\cos\left(\frac{\sqrt{3}}{2}k_x d\right)\mathrm{e}^{-ik_y d/2}\right)$$

With $E_{\boldsymbol{k}} = |f_{\boldsymbol{k}}|$, the band structure is depicted on the following figure (taken from [4]).

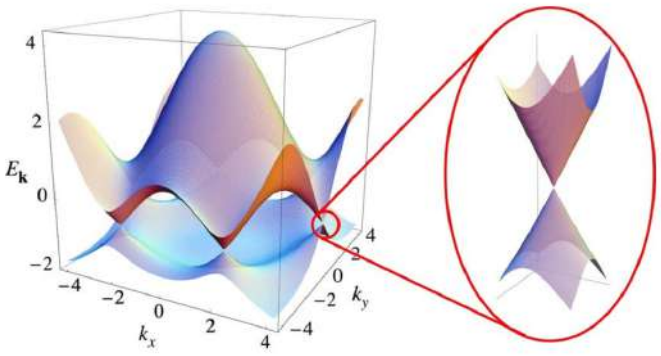


FIG. 3. (Color online) Electronic dispersion in the honeycomb lattice. Left: energy spectrum (in units of t) for finite values of t and t', with t=2.7 eV and t'=−0.2t. Right: zoom in of the energy bands close to one of the Dirac points.

2. Linearise the Hamiltonian in the vicinity of $K(\frac{4\pi}{3\sqrt{3}d}, 0)$, and show that K is a *Dirac point* for graphene (a degeneracy point in the vicinity of which the band structure is linear). As Dirac points come by pairs, there is another point $\tilde{K}$ in the Brillouin zone near which the spectrum is linear.

Correction.
Let's linearize $f_{\boldsymbol{k}}$ near the K point, so we define: $\boldsymbol{k} = \begin{pmatrix} \frac{4\pi}{3\sqrt{3}d} + q_x \\ q_y \end{pmatrix}$, then:

$$\begin{aligned} f_{\boldsymbol{k}} &= -t\left(\mathrm{e}^{iq_y d} + 2\cos\left(\frac{2\pi}{3} + \frac{\sqrt{3}}{2}q_x d\right)\mathrm{e}^{-iq_y d/2}\right) \\ &\approx -t\left(1 + iq_y d + 2\left[\left(-\frac{1}{2}\right) - \frac{\sqrt{3}}{2}\left(\frac{\sqrt{3}}{2}q_x d\right)\right]\left(1 - i\frac{q_y d}{2}\right)\right) \\ &= -\frac{3td}{2}(iq_y - q_x) \\ &= \frac{3td}{2}q^\star \end{aligned}$$

So the linearized Bloch Hamiltonian is:

$$H_{\boldsymbol{k}} = \hbar v_F \begin{pmatrix} 0 & q \\ q^\star & 0 \end{pmatrix} \qquad \text{with} \qquad v_F = \frac{3td}{2\hbar}$$

3. Using the linearized Hamiltonian, calculate the Berry connection $\boldsymbol{\mathcal{A}}_{\pm\boldsymbol{k}} = i\langle u_{\pm\boldsymbol{k}}|\boldsymbol{\nabla}_{\boldsymbol{k}} u_{\pm\boldsymbol{k}}\rangle$ in the two bands.

Correction.
The energy spectrum of the linearized Hamiltonian is very simple: $E_\pm = \pm\hbar v_F |q|$, and associated eigenvectors are:

$$u_\pm = \frac{1}{\sqrt{2}} \begin{pmatrix} \pm\, \mathrm{e}^{i\varphi_{\boldsymbol{k}}} \\ 1 \end{pmatrix} \qquad \text{with the definition} \qquad q = |q|\, \mathrm{e}^{i\varphi_{\boldsymbol{k}}}$$

And because $\partial_{\boldsymbol{k}} u_\pm = \mp \partial_{\boldsymbol{k}} \varphi_{\boldsymbol{k}} \begin{pmatrix} \mathrm{e}^{-i\varphi_{\boldsymbol{k}}} \\ 0 \end{pmatrix}$, we get the following Berry connection:

$$\boldsymbol{\mathcal{A}}_\pm = i \langle u_\pm | \partial_{\boldsymbol{k}} u_\pm \rangle = \frac{1}{2} \partial_{\boldsymbol{k}} \varphi_{\boldsymbol{k}}$$

The Berry connection is the same for the upper or lower band or a given Dirac point.

4. Calculate the Berry phase for a loop winding around a Dirac point in the lower band. What can we say about the Berry phase around the second Dirac point in $\tilde{K}$?

Correction.
The Berry phase around the Dirac point K is the line integral of the Berry connection over a circle around K. The Berry phase is thus a π factor. Calculating the Berry phase around the $\tilde{K}$ point will give: $-\pi$ which is the same physical Berry phase. The minus sign only reminds us that one can annihilate the two Dirac points by merging them (which is not always the case in other systems).

5. If the graphene sheet is under a physical stress, the lattice will be deformed and loose its 3-fold symmetry. Assume that the bonds along the y axis now have jumping amplitudes t'. Express the modified band energy.

Correction.
The new f function in the Hamiltonian is, with $\alpha = t'/t$:

$$f_{\boldsymbol{k}} = -t \left(\alpha\, \mathrm{e}^{ik_y d} + 2 \cos\left(\frac{\sqrt{3}}{2} k_x d \right) \mathrm{e}^{-ik_y d/2} \right)$$

6. In the Brillouin zone, one can follow the motion of graphene Dirac points when t' is changing. For the special value $t' = 2t$, the Dirac point is now at the position $M(0, \frac{2\pi}{3d})$. Derive the effective Hamiltonian near such a point.

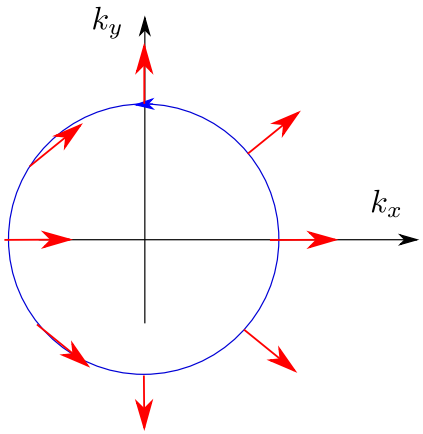
Correction.
Now the development should be done near the M point, that is to write $\boldsymbol{k} = \begin{pmatrix} q_x \\ \frac{2\pi}{3d} + q_y \end{pmatrix}$, then:

$$\begin{aligned}
f_{\boldsymbol{k}} &= -t \left(2\, \mathrm{e}^{2\pi/3}\, \mathrm{e}^{iq_y d} + 2 \cos\left(\frac{\sqrt{3}}{2} q_x d \right) \mathrm{e}^{-\pi/3}\, \mathrm{e}^{-iq_y d/2} \right) \\
&\approx -t \left\{ 2\, \mathrm{e}^{2\pi/3} (1 + iq_y d) + 2 \left[1 - \frac{1}{2} \left(\frac{\sqrt{3}}{2} q_x d \right)^2 \right] \mathrm{e}^{-\pi/3} \left(1 - i \frac{q_y d}{2} \right) \right\} \\
&= -t \left(2\, \mathrm{e}^{2\pi/3} + 2i\, \mathrm{e}^{2\pi/3}\, q_y d + 2\, \mathrm{e}^{-\pi/3} - \mathrm{e}^{-\pi/3} \frac{3}{4} q_x^2 d^2 - i\, \mathrm{e}^{-\pi/3}\, q_y d \right) \\
&= -3\, \mathrm{e}^{2\pi/3}\, t \left(\frac{q_x^2 d^2}{4} + iq_y d \right)
\end{aligned}$$

The spectrum has a very different structure now. It is still linear in the k_y direction, but *quadratic* in the k_x direction.

7. Let γ be a circle winding around the M point in the $k_x - k_y$ plane. Plot the orientation of the linearized $f(\boldsymbol{k})$, for different points on γ (by associating the complex number $f(\boldsymbol{k})$ and the 2D vector $(\Re e(f), \Im m(f))$). What is the Berry phase associated to this Dirac point?

Correction.



The angle between the vector (in red) and the horizontal axis while $k/|k|$ is describing the unit circle, follows $0 \to \frac{\pi}{2} \to 0 \to -\frac{\pi}{2} \to 0$. So the vector does not describe S^1. The winding number and the Berry phase vanish.

8. Describe the system if $t' > 2t$.

Correction.
The two former Dirac point have merged, and the geometrical structure seems trivial is $t' = 2t$. If $t' > 2t$, then a gap opens (allowed by the disappearance of the Dirac cones). The insulating phase is trivial.

2 The Haldane model

If one applies a perpendicular magnetic field on graphene, it will acquire a non-zero Chern number but the time-reversal symmetry (TRS) of the system will be broken.

Haldane suggested a modified model that preserves TRS but exhibits nonetheless a topological phase transition. He added a "local magnetic field" that acts in opposite ways on the two sublattices, such that the global magnetic field vanishes. Let us modify the graphene model as follow:

- We add a staggered potential on the lattice: $+M$ for A sites and $-M$ for B's.
- For a $A - A$ link in the clockwise loop, we add a $t_2 e^{i\varphi}$ hopping amplitude (depicted on Fig 1).
- For a $B - B$ link in the clockwise loop, we add a $t_2 e^{-i\varphi}$ hopping amplitude.

9. Write down the real-space Hamiltonian of this model.

10. Calculate the Bloch Hamiltonian in reciprocal space $H(\boldsymbol{k})$, and put it in the form: $H(\boldsymbol{k}) = \varepsilon_0(\boldsymbol{k})\mathbb{1} + \boldsymbol{d}(\boldsymbol{k}) \cdot \boldsymbol{\sigma}$. Show in particular that

$$d_z(\boldsymbol{k}) = M - 2t_2 \sin\varphi \sum_{1 \le i \le 3} \sin(\boldsymbol{k} \cdot \boldsymbol{b}_i) \tag{2}$$

where $\boldsymbol{b}_1$, $\boldsymbol{b}_2$ and $\boldsymbol{b}_3$ are the vectors linking A and A sites in the clockwise direction.

11. Deduce the band energy. To which condition the gap closes? In the plane $(\sin\phi, M)$ plot the location of gapless phases. It separates the space in different gapped regions. You could use the following relation: $\sum_{1\leq i\leq 3}\sin(\boldsymbol{b}_i\cdot\boldsymbol{K}) = -\frac{3\sqrt{3}}{2}$.

12. One can show that the Chern number can be calculated as a simple sum:[1]

$$\nu = \frac{1}{4\pi}\int_{\mathrm{FBZ}}\frac{\boldsymbol{d}\cdot(\partial_{k_x}\boldsymbol{d}\times\partial_{k_y}\boldsymbol{d})}{d^3}\mathrm{d}k_x\mathrm{d}k_y = \sum_{\boldsymbol{k}=K,K'}\mathrm{sign}(\boldsymbol{d}(\boldsymbol{k})\cdot\boldsymbol{n}(\boldsymbol{k})) \tag{3}$$

where $\boldsymbol{n}(\boldsymbol{K}) = \boldsymbol{e}_z$ and $\boldsymbol{n}(\tilde{\boldsymbol{K}}) = -\boldsymbol{e}_z$. Calculate the Chern numbers for the different insulating phases.

13. Let us now consider the interface at $y = 0$ between two insulating phases of the Haldane model. Justify that the gap of the band structure is $2|\Delta|$, where $\Delta(y) = d_z(K)$, and represent Δ as a function of y.

14. Assuming that the Bloch Hamiltonian is not modified significantly away from the K point at the transition, we focus on a low-energy approximation of the Hamiltonian around $\boldsymbol{k} = K + \boldsymbol{q}$. Find the expression of $H_1(\boldsymbol{q})$ the linearized Hamiltonian.

15. Show that in real space, it corresponds to:

$$H_1 = -i\hbar v_F(\partial_x\sigma_x + \partial_y\sigma_y) + \Delta(y)\sigma_z. \tag{4}$$

16. Verify that

$$\psi_{q_x}(x,y) \propto e^{iq_x x}e^{\frac{1}{\hbar v_F}\int_0^y\Delta(y')\mathrm{d}y'}\begin{pmatrix}1\\1\end{pmatrix} \tag{5}$$

is a spinor eigenfunction of the Hamiltonian, and calculate the associated eigenvalue.

17. Justify the *edge* state denomination by plotting $|\psi|^2$ as a function of y. Determine the group velocity of such a state. Justify that this edge state is chiral.

References

[1] Carpentier, Topology of Bands in Solids: From Insulators to Dirac Matter, Séminaire Poincaré XVIII (2014).

[2] Cayssol, Introduction to Dirac materials and topological insulators, C.R. Physique 14 (2013) 760.

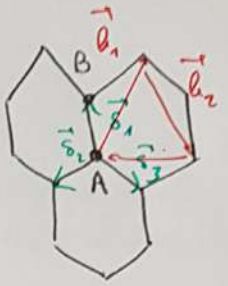
[3] Haldane, Model for a Quantum Hall Effect without Landau Levels: Condensed-Matter Realization of the Parity Anomaly, Phys. Rev. Lett. **61** 2015 (1988).

[4] Castro Neto et al., "The electronic properties of graphene," Rev. Mod. Phys. **81**, 109 (2009).

[1] This equality yields because a Chern number is a wrapping number that counts how many times does the surface traced by $\boldsymbol{d}$ wrap around the origin when $\boldsymbol{k}$ varies in the FBZ. It is then equal to the *Brouwer* degree of $\boldsymbol{d}$.

Haldane Model

1) Real-space Hamiltonian :



$$H = \sum_i M_i |A,i\rangle\langle A,i| - M|B,i\rangle\langle B,i| \quad (1)$$

$$+ \sum_{\langle i,j\rangle} t\,|A,i\rangle\langle B,j| + h.c \quad (2)$$

$$+ \sum_{\langle\langle i,j\rangle\rangle} t_2 e^{i\gamma}\,|A,i\rangle\langle A,j| + h.c. \quad (3)$$

$$+ \sum_{\langle\langle i,j\rangle\rangle} t_2 e^{-i\gamma}\,|B,i\rangle\langle B,j| + h.c. \quad (4)$$

↻ means for links 

2) One can change the basis that is use to write down H. Because H only has local interactions between atoms, the use of Bloch states really simplifies the expression of H. This choice would not be as clear in a long interaction model.

$$|\vec{k},A\rangle = \frac{1}{\sqrt{N}} \sum_{\vec{R}_i} e^{i\vec{k}\cdot\vec{R}_i} |A,\vec{R}_i\rangle$$

$$|\vec{k},B\rangle = \frac{1}{\sqrt{N}} \sum_{\vec{R}_i} e^{i\vec{k}(\vec{R}_i+\vec{\delta}_1)} |B,\vec{R}_i\rangle$$

$$(1) \to \sum_k M\,|\vec{k},A\rangle\langle\vec{k},A| - M\,|\vec{k},B\rangle\langle\vec{k},B|$$

$$(2) \to \sum_k f(\vec{k})\,|\vec{k},A\rangle\langle\vec{k},B| + h.c. \quad \text{where } f(\vec{k}) = t\sum_i e^{i\vec{k}\cdot\vec{\delta}_i}$$

(same expression as graphene).

$$(3) \to \sum_{\vec{k}} e^{i\phi} g(\vec{k})\,|\vec{k},A\rangle\langle\vec{k},A| + h.c. \quad \text{where } g(\vec{k}) = t_2 \sum_{1\le i\le 3} e^{i\vec{k}\cdot\vec{b}_i}$$

$$(4) \to \sum_k e^{-i\phi} g(\vec{k})\,|\vec{k},B\rangle\langle\vec{k},B| + h.c.$$

We can thus write

$$H = \sum_k \begin{pmatrix} \langle\vec{k},A| & \langle\vec{k},B| \end{pmatrix} H_{\vec{k}} \begin{pmatrix} |\vec{k},A\rangle \\ |\vec{k},B\rangle \end{pmatrix}.$$

where

$$H_{\vec{k}} = \begin{pmatrix} M + 2\mathrm{Re}(e^{i\phi}g) & f \\ f^* & -M + 2\mathrm{Re}(e^{-i\phi}g) \end{pmatrix}$$

• With the expression $H_k = \varepsilon_0 \mathbb{1} + \vec{d}(\vec{k}) \cdot \vec{\sigma}$, we can identify :

→ $\varepsilon_0 = \frac{H_{k,AA} + H_{k,BB}}{2} = \frac{t_2}{2}\left[e^{i\phi}\sum e^{i\vec{b}_i\cdot\vec{k}} + e^{-i\phi}\sum e^{-i\vec{b}_i\cdot\vec{k}} + e^{-i\phi}\sum e^{i\vec{b}_i\cdot\vec{k}} + e^{i\phi}\sum e^{-i\vec{b}_i\cdot\vec{k}} \right]$

$2\cos\phi \sum e^{i\vec{b}_i\cdot\vec{k}}$ $\qquad$ $2\cos\phi \sum e^{-i\vec{b}_i\cdot\vec{k}}$

$4\cos\phi \sum_i \cos(\vec{b}_i\cdot\vec{k})$.

$\Rightarrow \varepsilon_0 = 2t_2 \cos\phi \sum_i \cos(\vec{b}_i\cdot\vec{k})$.

→ By the same reasoning,

$d_3 = \frac{H_{k,AA} - H_{k,BB}}{2} = M - 2t_2 \sin\phi \sum_i \sin(\vec{b}_i\cdot\vec{k})$.

→ $d_x = \mathrm{Re}\, f(k)$ and $d_y = \mathrm{Im}\, f(k)$ as in graphene.

3) For such a Bloch Hamiltonian, the band structure is given by :

$$E_\pm(\vec{k}) = \varepsilon_0 \pm \|\vec{d}\|$$

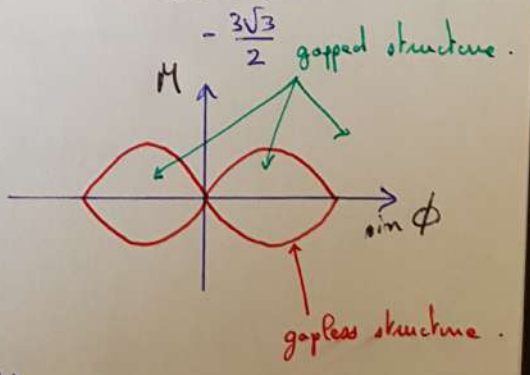
The gap closes in for a given $\vec{k}$, $d_x = d_y = d_3 = 0$. d_x and d_y are the same as graphene. The only points where $d_x(\vec{k}) = d_y(\vec{k})$ are the Dirac points K and $\tilde{K}$.

At $K\left(\frac{4\pi}{3\sqrt{3}a}, 0\right)$, we have $d_3(K) = M - 2t_2 \sin\phi \underbrace{\sum_{i\in\{1,2,3\}} \sin(\vec{b}_i\cdot\vec{K})}_{-\frac{3\sqrt{3}}{2}}$

Thus

$$d_3(K) = M + 3\sqrt{3}\, t_2 \sin\phi$$

The gap closes if $\sin\phi = -\frac{M}{3\sqrt{3}t_2}$



⇒ The structure is gapless only on the red line of the plane $M - \phi$.

Note that if $M \leq 3\sqrt{3}\, t_2$, then $d_3(K)\, d_3(\tilde{K}) \leq 0$.

but if $M > 3\sqrt{3}t_2$, then $d_3(K)\, d_3(\tilde{K}) > 0$.

⇒ We anticipate with this note that $M \gtrless 3\sqrt{3}t_2$ will be phases with different topology.

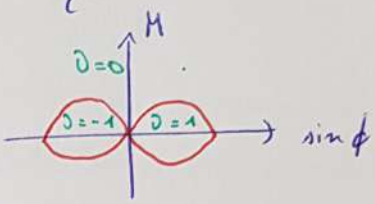
4) We use the expression of the Chern number given in the book.

- If $M > 3\sqrt{3}\,t_2$, then $d_3(k)\,d_3(\tilde{k}) > 0 \Rightarrow \nu = \frac{1}{2}(1-1) = 0$.
  This phase is topologically trivial.

- If $M < 3\sqrt{3}\,t_2$ and $\sin\phi > 0$, $\begin{matrix} d_3(k) > 0 \\ d_3(\tilde{k}) < 0 \end{matrix} \Rightarrow \nu = \frac{1}{2}(1+1) = 1$.

  $M < 3\sqrt{3}\,t_2$ and $\sin\phi < 0$, $\begin{matrix} d_3(k) < 0 \\ d_3(\tilde{k}) > 0 \end{matrix} \Rightarrow \nu = \frac{1}{2}(-1-1) = -1$.

We can complete the diagram ------->



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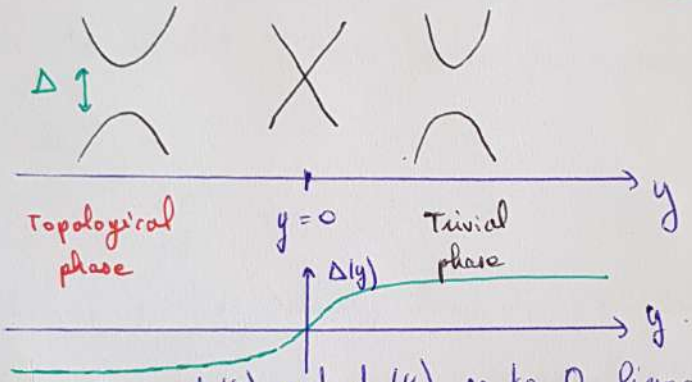


The gap is always at k and $\tilde{k}$
Then
$\Delta = \frac{1}{2}E(k) = 2\,d_z(k)$.

6) Near $y = 0$, $d_1(k)$ and $d_2(k)$ go to 0 linearly as in graphene. We assume that the Hamiltonian is not much modified near $y = 0$, such that

$$H_{\vec{k}} \simeq H(\vec{q}) = \underbrace{\hbar v_F (q_x \sigma_x + q_y \sigma_y)}_{\text{graphene.}} + \underbrace{\Delta(y)\,\sigma_z}_{d_3(k)} + \underbrace{\varepsilon_0 \mathbb{1}}_{\text{which we forget in the following.}}$$

7) Going from real space to momentum space, $\partial_x \longleftrightarrow i q_x$.
This justifies the expression

$$H_1 = -i\hbar v_F (\partial_x \sigma_x + \partial_y \sigma_y) + \Delta(y)\,\sigma_z$$

8) Let us calculate $H\psi_{q_x}$:

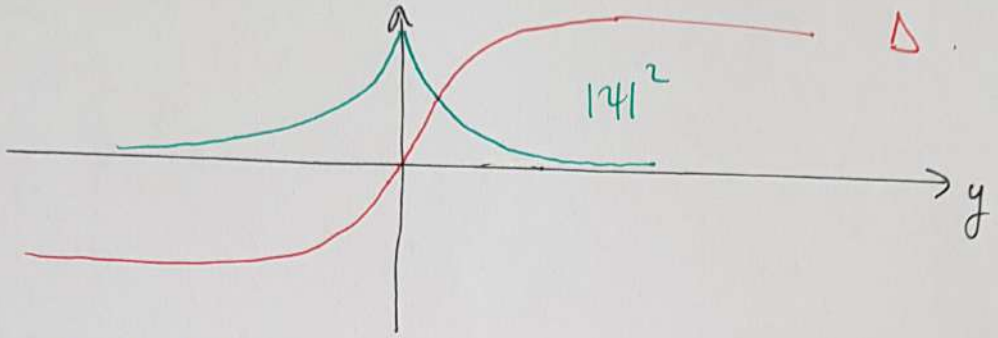
$$-i\hbar v_F \begin{pmatrix} 0 & \partial_x - i\partial_y \\ \partial_x + i\partial_y & 0 \end{pmatrix} \psi_{q_x} + \begin{pmatrix} \Delta & 0 \\ 0 & -\Delta \end{pmatrix} \psi_{q_x} = \begin{pmatrix} -i\hbar v_F \left(i q_x - i \frac{\Delta(y)}{\hbar v_F} \right) + \Delta \\ -i\hbar v_F \left(i q_x + i \frac{\Delta(y)}{\hbar v_F} \right) - \Delta \end{pmatrix} e^{i q_x x} e^{\frac{1}{i\hbar v_F}\int_{y_0}^{y} \Delta\, dy'}$$

$$= \begin{pmatrix} \hbar v_F q_x - \Delta + \Delta \\ \hbar v_F q_x + \Delta - \Delta \end{pmatrix} e^{i q_x x} e^{\frac{1}{i\hbar v_F}\int \Delta\, dy'} = \hbar v_F q_x \psi_{q_x}.$$

Finally, ψ_{q_x} is a (spinor) eigenfunction of H_1, of eigenvalue $\hbar v_f q_x$

$$H_1 \psi_{q_x} = \hbar v_f q_x \psi_{q_x}.$$

g)



$|\psi|^2$ is localized at the interface $y=0$, it decreases exponentially if $y \neq 0$. ψ_{q_x} is thus an edge state, contrary to bulk states that are delocalized over all the crystal (Bloch states for example).

Group velocity:

$$\vec{v}_g = \frac{1}{\hbar} \frac{dE}{d\vec{q}} = +v_f \vec{e}_x.$$

ψ_{q_x} has a positive velocity along $\vec{e}_x$, parallel to the interface $y=0$.

If Δ were going from positive to negative values, ψ_{q_x} would move along the $-\vec{e}_x$ direction.

$\Rightarrow$ ψ_{q_x} is a chiral edge state.