Arnaud RAOUX (arnaud.raoux@sorbonne-universite.fr)
http://www.phys.ens.fr/~raoux/

Homework assignment: Graphene and Haldane model

1 Graphene and Dirac points

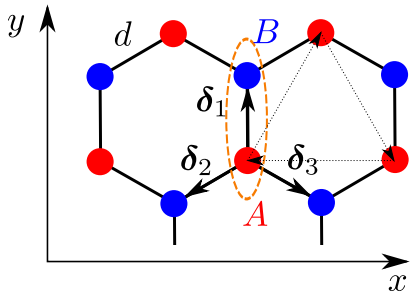

Figure 1: The geometry of the graphene lattice. The distance between atoms is d, $\boldsymbol{\delta}_i$ are the vectors linking nearest neighbors. Each link between nearest neighbors has a hopping amplitude $-t$ ($t > 0$). The on-site energies are identical, and will be taken as zero.

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.

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.

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.

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 $\tilde{K}$?

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.

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.

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?

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

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.

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

2. 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.

3. 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: $\sum_{1\le i\le 3}\sin(\boldsymbol{b}_i\cdot\boldsymbol{K}) = -\frac{3\sqrt{3}}{2}$.

4. 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.

5. 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.

6. 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.

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

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

8. 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.

9. 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.

[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 $\boldsymbol{d}$.