Book of Exercises

GDR School on topology

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Contents

1 Preliminary exercises to do before the school

1.1 Tight binding model for 1d chain.

Let?s consider a chain of N identical atoms with only one orbital per atom $\phi_n(\vec{r})$, label $|\phi_n\rangle$, separated by the same distance $a/2$. We will consider the unit cell containing 2 atoms of length a, whose orbitals will be $|\phi_{2m}\rangle$ and $|\phi_{2m+1}\rangle$, with m indexing the considered cell. The reason for this 2 atoms per unit cell is that we will consider 2 different hopping integrals between the atoms of the same cell and between neighboring cells :

$$\begin{aligned}
&\langle\phi_{2m}|\,\hat{H}\,|\phi_{2m+1}\rangle = \langle\phi_{2m+1}|\,\hat{H}\,|\phi_{2m}\rangle = -t\,(1-\delta)\\
&\langle\phi_{2m}|\,\hat{H}\,|\phi_{2m-1}\rangle = \langle\phi_{2m-1}|\,\hat{H}\,|\phi_{2m}\rangle = -t\,(1+\delta)\\
&\langle\phi_{2m}|\,\hat{H}\,|\phi_{2m}\rangle = \epsilon_0\\
&\langle\phi_{2m+1}|\,\hat{H}\,|\phi_{2m+1}\rangle = \epsilon_1
\end{aligned} \tag{1}$$

All the other terms are considered null. The physical origin of this difference in hopping parameter can be an unequal distance between identical atoms (in this case $\epsilon_0 = \epsilon_1$) or just 2 different atoms per cell ($\epsilon_0 \neq \epsilon_1$). We will take the total wave function as a linear combination of the local orbital : $\Psi = \sum_m \alpha_m\,|\phi_{2m}\rangle + \beta_m\,|\phi_{2m+1}\rangle$.

We recall the Bloch theorem : in a spatially periodic system of period $\vec{T}$ the total wavefunction is decomposed in $\Psi(\vec{r}) = u(\vec{r})e^{i\vec{k}.\vec{r}}$ with $u(\vec{r}+\vec{T}) = u(\vec{r})$ a periodic function.

1. What are the limit of the Brillouin zone for a unit cell of length a ?
2. Using the periodicity of the system, calculate $\Psi(x+a)$ as a function of $\phi_{2m}(x)$ and $\phi_{2m+1}(x)$.
3. Using the block theorem, find the expression of $\Psi(x+a)$ as function of $\Psi(x)$
4. Comparing the two expressions of $\Psi(x+a)$, deduce the relation between α_{m+1} and α_m or β_{m+1} and β_m
5. Calculate the term $<\phi_{2n}|\mathcal{H}|\Psi_k>$ (ϕ_{2n} being one orbital of the first atom of the unit cell, labelled with an even index $2n$), first using the Schrödinger equation to make appear E_k, the energy of the wavefunction Ψ_k, and secondly expanding $|\Psi_k>$ to make appear the hopping integrals of the kind $\langle\phi_{2m}|\,\hat{H}\,|\phi_{2m+1}\rangle$ that we will replace by the corresponding value (see Eq. 1). By comparing the two methods, derive the first equation relating E_k, α_n, β_n, t and δ.
6. Apply the same method for the term $<\phi_{2n+1}|\mathcal{H}|\Psi_k>$ (ϕ_{2n+1} being one orbital of the second atom of the unit cell, labelled with an odd index $2n+1$) to find a second equation.
7. Using the two equations, find the two eigenvalues E_k.
8. Plot the two bands, and calculate the gap to show that it depends only on $\Delta\epsilon$ and δ, and that it vanishes when $\Delta\epsilon = \delta = 0$.

1.2 Tight binding model for 1d chain : second quantization formalism.

We will see now how to write the same system using second quantization. In second quantization, we think in term of the occupation of the sites with creation and annihilation operators that add or remove electrons on specific site. For example, the operator $c_i^\dagger$ will add an electron on the site i and $c_i^\dagger c_i$ counts the number of electron on the site i. For our 1d chain model, we can consider two sublattices : the atoms on A (corresponding to the $2m$) and the atoms on B (corresponding to $2m+1$). The previous Hamitonian can be rewritten :

$$\hat{H} = \sum_m^N \left[\epsilon_0 c_{A,m}^\dagger c_{A,m} + \epsilon_1 c_{B,m}^\dagger c_{B,m} + t(1-\delta)c_{A,m}^\dagger c_{B,m} + t(1+\delta)c_{B,m}^\dagger c_{A,m+1} + h.c.\right] \tag{6}$$

where the sum is made over N unit cells, the third term being the hopping parameter between atoms of the same unit cell and the fourth term is the hopping parameter between first neighbours of different unit cells. The $h.c.$ stands for the hermitian conjugate of these two terms so that the total Hamiltonian si hermitian. Here $h.c.$ stands for $t(1-\delta)c_{B,m}^\dagger c_{A,m} + t(1+\delta)c_{A,m+1}^\dagger c_{B,m}$ and means that hopping from A,m to B,m is the same as hopping from $B,m1$ to A,m.

9. Transform the Hamitlonian from real space to momentum space using the relations :

$$\begin{aligned} c_{A,m} &= \frac{1}{\sqrt{N}} \sum_k e^{-i\vec{k}.\vec{r}_m} c_{A,k}, \quad c^\dagger_{A,m} = \frac{1}{\sqrt{N}} \sum_k e^{i\vec{k}.\vec{r}_m} c^\dagger_{A,k} \\ c_{B,m} &= \frac{1}{\sqrt{N}} \sum_k e^{-i\vec{k}.\vec{r}_m} c_{B,k}, \quad c^\dagger_{B,m} = \frac{1}{\sqrt{N}} \sum_k e^{i\vec{k}.\vec{r}_m} c^\dagger_{B,k} \end{aligned} \tag{7}$$

and show that it can take the following form :

$$\hat{H} = \sum_k \begin{pmatrix} c^\dagger_{k,A} & c^\dagger_{k,B} \end{pmatrix} \begin{pmatrix} \epsilon_0 & t(1-\delta) + t(1+\delta)e^{ika} \\ t(1-\delta) + t(1+\delta)e^{-ika} & \epsilon_1 \end{pmatrix} \begin{pmatrix} c_{k,A} \\ c_{k,B} \end{pmatrix} \tag{8}$$

10. Rewrite the Hamiltonian matrix :

$$h = \begin{pmatrix} \epsilon_0 & t(1-\delta) + t(1+\delta)e^{ika} \\ t(1-\delta) + t(1+\delta)e^{-ika} & \epsilon_1 \end{pmatrix} \tag{16}$$

in the Pauli matrix basis and the identity, $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ and $\sigma_0 = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}$

11. Once the Hamiltonian is in the form $h = \vec{D}_k.\vec{\sigma} + \epsilon_k \sigma_0$, the eigenvalues are given by $E^\pm_k = \epsilon_k \pm |\vec{D}_k|$. Calculate the eigenvalues.

1.3 Tight binding model for 2d square lattice in second quantization

We consider now a square lattice in 2 dimension (x and y) of parameter a, with one atom per unit cell and one orbital per atom. In second-quatization, we can write the Hamiltonian :

$$\hat{H} = \sum_{m,n}^{N} \left[\epsilon_0 c^\dagger_{m,n} c_{m,n} - t c^\dagger_{m,n} c_{m+1,n} + t c^\dagger_{m,n} c_{m,n+1} + h.c. \right] \tag{19}$$

where (m,n) refers to the coordinate of the unit cell (and thus the atom) and $-t$ (t>0) the hopping parameter between first neighbour atoms.

12. Transform the Hamitlonian from real space to momentum space using the relations :

$$c_{m,n} = \frac{1}{\sqrt{N^2}} \sum_k e^{-i\vec{k}.\vec{r}_{m,n}} c_k, \quad c^\dagger_{m,n} = \frac{1}{\sqrt{N^2}} \sum_k e^{i\vec{k}.\vec{r}_{m,n}} c^\dagger_k \tag{20}$$

13. Draw the Fermi surface for $E_k < 0$, $E_k = 0$ and $E_k > 0$.

2 Introduction

2.1 Berry connection, Berry curvature and polarization

Let's consider an electronic band of a 2D system, labelled n and $|u_k^n\rangle$ the eigenfunction for this band. The electric polarization for this band is given by :

$$P_n = -\frac{e}{2\pi}\int_0^{2\pi} dk\mathcal{A}_k^n \tag{27}$$

with $\mathcal{A}_k^n$, the Berry connection, written :

$$\vec{\mathcal{A}}_k^n = i\langle u_k^n|\vec{\nabla}_k|u_k^n\rangle \tag{28}$$

The Berry curvature is defined as :

$$\vec{\Omega}^n = \vec{\nabla}_k \times \vec{\mathcal{A}}_k^n \tag{29}$$

so in 2D :

$$\Omega_{xy}^n = \partial_x\mathcal{A}_y^n - \partial_y\mathcal{A}_x^n \tag{30}$$

1. Show that adding a phase to the eigenvector $|u_k'^n\rangle = e^{i\phi_k^n}|u_k^n\rangle$ does not changes the polarization modulo the charge e.
2. Show that the Berry curvature is a gauge invariant object under this transformation.
3. how that the Berry curvature can be written as $\Omega_{xy}^n = -2\,\mathrm{Im}(\partial_x u_k^n - \partial_y u_k^n)$

2.2 Quantum spin Hall effect

We will consider the Bernevig-Hughes-Zhang model for CdTe/HgTe quantum wells for which the 4x4 Hamiltonian writes :

$$h_k = sin(k_x)\sigma_z\otimes\tau_x + sin(k_y)\sigma_0\otimes\tau_y + M_k\sigma_0\otimes\tau_z \tag{34}$$

in the basis $\left\{\left|p, m_J = \frac{3}{2}\right\rangle, \left|s, m_J = \frac{1}{2}\right\rangle, \left|p, m_J = -\frac{3}{2}\right\rangle, \left|s, m_J = -\frac{1}{2}\right\rangle\right\}$. Here $\tau_x = \sigma_x = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$, $\tau_y = \sigma_y = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}$ and $\tau_z = \sigma_z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$ are Pauli matrices (σ are the standard Pauli matrices acting on the spin basis and τ on the particule-hole basis) and $M_k = 2 - m - cos(kx) - cos(ky)$. We recall :

$$\sigma_z\otimes\tau_x = \begin{pmatrix}0 & 1 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & -1\\ 0 & 0 & -1 & 0\end{pmatrix}, \sigma_0\otimes\tau_y = \begin{pmatrix}0 & -i & 0 & 0\\ i & 0 & 0 & 0\\ 0 & 0 & 0 & -i\\ 0 & 0 & i & 0\end{pmatrix}, \sigma_0\otimes\tau_z = \begin{pmatrix}1 & 0 & 0 & 0\\ 0 & -1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & -1\end{pmatrix} \tag{35}$$

4. how that $\mathcal{T} = i\sigma_y\otimes\tau_0\mathcal{K}$, with $\mathcal{K}$ the complex conjugate operator, represents the time-reversal symmetry operator of h_k.
5. Define the inversion operator, knowing that the basis is $\left\{\left|p, m_J = \frac{3}{2}\right\rangle, \left|s, m_J = \frac{1}{2}\right\rangle, \left|p, m_J = -\frac{3}{2}\right\rangle, \left|s, m_J = -\frac{1}{2}\right\rangle\right\}$.
6. Calculate the invariant for different parameters using the Fu-Kane formula :

$$\nu = \prod_{n\in occ}\prod_{k\in TRIM}\xi_k^{2n} \tag{40}$$

   How many phases are there and what are their invariants?

7. What is the Hall conductivity of this phase? Why?
8. And the spin-hall conductivity?

2.3 Low-energy description of a Weyl semimetal

We will now consider a Weyl Hamiltonian of positive chirality, defined as:

$$\mathcal{H}_+ = +v_f \vec{k}.\vec{\sigma} \tag{41}$$

9. Show that there is no gap for this Hamiltonian. We recall (see Preliminary exercises) that if the Hamiltonian is of the form $h = \vec{D}_k.\vec{\sigma} + \epsilon_k \sigma_0$, the eigenvalues are given by $E_k^{\pm} = \epsilon_k \pm |\vec{D}_k|$.

10. Show that even under general perturbation (meaning adding terms as $\vec{b}.\vec{\sigma}$ or $b_0\sigma_0$) no gap can be induced.

11. Check that the Berry curvature takes the form of a monopole in momentum space. We recall that for an Hamiltonian of the form $h = \vec{D}_k.\vec{\sigma} + \epsilon_k\sigma_0$ (2 band hamiltonian), the Berry curvature can be derived from this equation:

$$\Omega_k^i = \frac{\epsilon^{ijl}}{2} \tilde{D}_k \left(\partial_{k_j} \tilde{D}_k \times \partial_{k_l} \tilde{D}_k \right) \tag{42}$$

with $(ijl) \equiv (xyz)$ and $\tilde{D}_k = \dfrac{\vec{D}_k}{|\vec{D}_k|}$.

12. Give an argument why Berry monopoles must always come in pairs within the Brillouin zone.

13. Double the Hamiltonian with a Weyl of the opposite chirality $\mathcal{H}_- = -v_f \vec{k}.\vec{\sigma}$ such that $\mathcal{H}_+ = \tau_z \otimes v_f \vec{k}.\vec{\sigma}$ where τ_z is a valley degree of freedom (or orbital degree of freedom).

14. What happens to the spectrum when we add the off-diagonal term $M\tau_x \otimes \sigma_0$?

15. Add a perturbation of the form $\tau_0 \otimes \vec{b}.\vec{\sigma} + b_0\tau_z \otimes \sigma_0$. Plot the spectrum for different values of $\dfrac{|\vec{b}|^2 - b_0^2}{M^2}$ and identify the different phases.

16. Show that $\tau_0 \otimes \vec{b}.\vec{\sigma}$ and $b_0\tau_z \otimes \sigma_0$ break time-reversal $\mathcal{T} = -i\sigma_u\mathcal{K}$ and inversion $\mathcal{I} = \tau_x$, respectively.

17. Show that it is only possible to have Weyl fermions if either, or both symmetries are broken.

2.4 Lattice model for a Weyl semimetal

Consider the three-dimensional model Hamitlonian :

$$h_k = tsin(k_x)\sigma_x + tsin(k_y)\sigma_y + (m - t\sum_{i \in xyz} cos(k_i))\sigma_z \tag{46}$$

18. Show that for $m = 2t$, the gap closes at two points, the Weyl cones, and give their position in momentum space. We recall (see Preliminary exercises) that if the Hamiltonian is of the form $h = \vec{D}_k.\vec{\sigma} + \epsilon_k\sigma_0$, the eigenvalues are given by $E_k^{\pm} = \epsilon_k \pm |\vec{D}_k|$.

19. Assuming that Pauli matrices represent a spin degree of freedom, show that this Hamiltonian breaks time-reversal symmetry $\mathcal{T} = -i\sigma_y\mathcal{K}$.

20. Fix $m = 2t$ and show that this model has a surface state, known as the Fermi arc, between the two Weyl nodes. To do this, you can check the Chern number as a function of k_z.

21. Calculate the Hall conductivity σ_{xy} of this model as a function of the Weyl node separation ΔK_W.

22. What happens when the nodes touch at the Brillouin zone boundaries ? Tip: Use how the Chern number varies as a function of k_z.

3 Topological Quantum Chemistry - Hands-on session

3.1 Bismuth

In this tutorial, we will use IrRep to classify the topology of Bi. We will use as input DFT data obtained with the Vienna *ab initio* simulation package. This data consists of the POSCAR and WAVECAR files in the current directory. The input files for VASP necessary to obtain this data can be found in the directory `inputs`.

Exercises:

- Exercise 1: Identify the space group
- Exercise 2: Calculate the irreducible representations at maximal k-points
- Exercise 3: Diagnose the topology of valence bands
- Exercise 4: Separate wave functions by inversion eigenvalues

3.1.1 Identification of the space group

Bismuth crystallizes in a rhombohedral structure. However, there exist many rhombohedral space groups. To find the space group of our material, we need the cell vectors that describe the periodicity of the lattice, and the positions of atoms within the unit cell. This is contained in the POSCAR file. We can open the POSCAR and try to identify the space group, but usually this is not a straightforward task. Instead, we can use IrRep to do it automatically:

```
irrep -onlysym > out
```

With `> out`, we have saved the output of IrRep into a file called `out`. If we open this file with a text editor, we will find:

- A description of the crystal structure parsed from DFT files (the POSCAR, in this case). We see that the cell used for the DFT calculation was a primitive cell which contains two Bi atoms.
- The name of the space group. It is the rhombohedral group R-3m (No. 166). It contains 12 symmetry operations (mod. translations).
- A list of symmetry operations. Each symmetry operation is described by giving the matrix of its rotational part, the vector of the translational part, its action on a generic **k**-point, its rotation axis, angle and whether it respects chirality or not (`inversion` tag).

3.1.2 Irreducible representations at maximal k-points

IrRep is able to calculate the traces of symmetry operations in every **k**-point. Furthermore, if the **k**-point is maximal, IrRep can identify the irreducible representation of every wave function by comparing the traces to the character tables of irreducible representations. For that, we have to run IrRep with the `-kpnames` option:

```
irrep -code=vasp -kpnames=T,GM,F,L -Ecut=50 -IBend=12 -searchcell -spinor -EF=5.2244 > out
```

Let us comment on each argument passed to the command above:

- `code` specifies the interface that should be applied. In this case, it is the interface for VASP (default).
- `kpnames` passes the labels of **k**-points. They should follow the same order as in the file of wave functions (the WAVECAR in this case).
- `Ecut` sets the plane-wave cutoff that will be used for the calculation. Coefficients of plane waves with larger energy will be discarded. Setting it to a value smaller than the cutoff considered in the DFT calculation reduces considerably the time of the calculation.

- `IBend` is the index of the last band considered for the calculation. The convergence of the last bands tends to be poor in DFT, hence it might be convenient to discard them.
- `spinor` indicates that the DFT calculation included SOC.
- `EF` is the Fermi energy. All energy levels will be given with respect to this value. If it is set to `-EF=auto`, IrRep will try to parse it from DFT data and it will set it to 0.0 if it could not find it (the case of VASP).
- `searchcell` is an important parameter. It is used to ask IrRep to determine automatically the transformation from the DFT cell to the conventional cell of the tables. The transformation can alternatively be specified via `-refUC` and `-shiftUC`.

Let us open the file `out` generated by this command and go through the output.

- First, we see the same description of the unit cell and space group that we studied above. However, we can find something that is different:

```
        |   1.0000 -1.0000 -0.0000 |
refUC = |   0.0000  1.0000 -1.0000 |    shiftUC = [-0. -0. -0.]
        |   1.0000  1.0000  1.0000 |
```

  It tells us that the transformation from the DFT cell to the conventional setting. See IrRep's documentation for more details.

- Then, we have a block for each maximal **k**-point passed to the code. The header of each block contains the coordinates of the **k**-point in both, the DFT and conventional cell. The number of symmetries in the little group is also written (mod. translations).

```
k-point   1 : [0.5 0.5 0.5] (in DFT cell)
              [0.  0.  1.5] (after cell trasformation)

number of states : 12
```

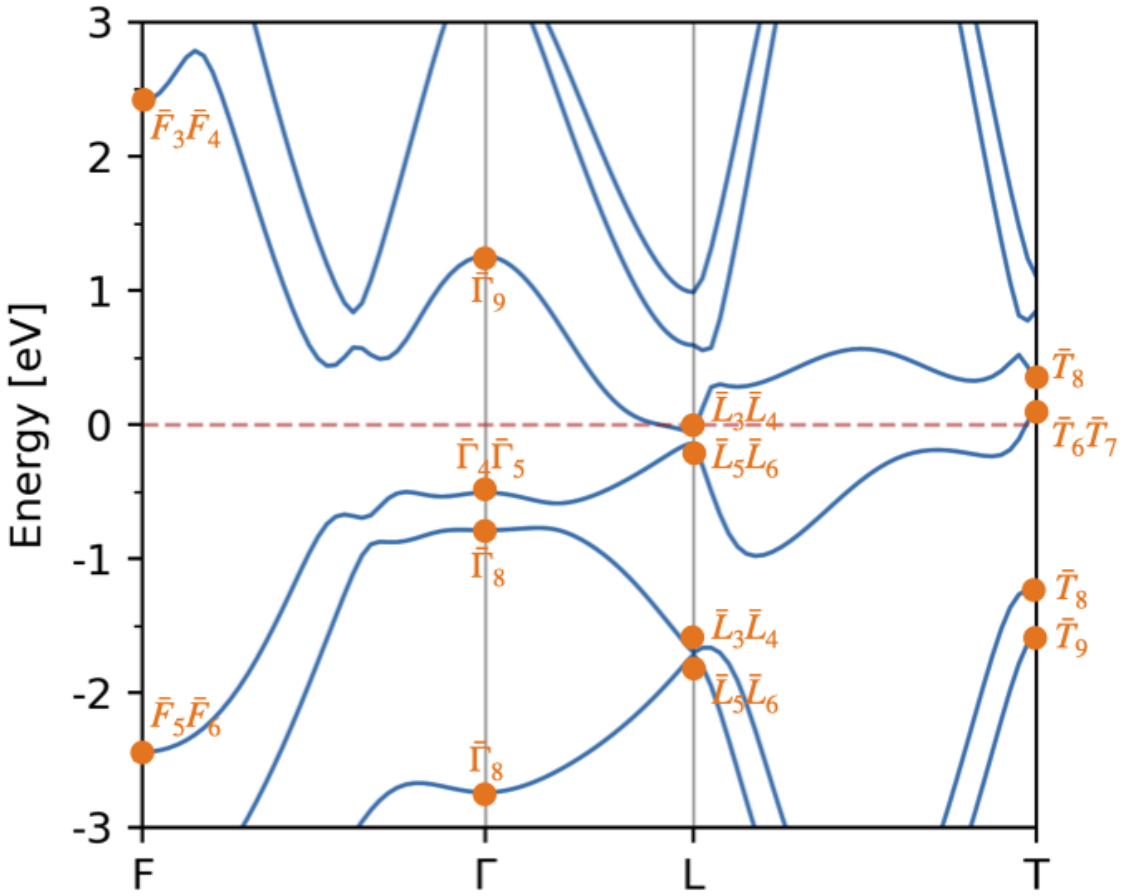
- After the header, we can find a list of **energy levels** and **irreducible representations** of identified for each one. The **traces** of symmetries in the little-group are also listed in the same row. The next row contains the traces in the conventional cell.

```
   Energy  |   degeneracy  |       irreps       | sym. operations
           |               |                    |    1        2        3        4
 -11.6046  |        2      | -T9(1.0)           |   2.0000   1.0000   1.0000  -0.0000
           |               |                    |   2.0000   1.0000   1.0000   0.0000
 -10.0391  |        2      | -T8(1.0)           |   2.0000   1.0000   1.0000   0.0000
           |               |                    |   2.0000   1.0000   1.0000  -0.0000
  -1.5692  |        2      | -T9(1.0)           |   2.0000   1.0000   1.0000  -0.0000
           |               |                    |   2.0000   1.0000   1.0000   0.0000
  -1.2288  |        2      | -T8(1.0)           |   2.0000   1.0000   1.0000   0.0000
           |               |                    |   2.0000   1.0000   1.0000  -0.0000
   0.1380  |        2      | -T6(1.0), -T7(1.0) |   2.0000  -2.0000  -2.0000   0.0000
           |               |                    |   2.0000  -2.0000  -2.0000  -0.0000
   0.2922  |        2      | -T8(1.0)           |   2.0000   1.0000   1.0000   0.0000
           |               |                    |   2.0000   1.0000   1.0000  -0.0000
```

- Finally, the gap with respect to the next set of bands (with index `IBend`+1) is given. Also the number of inversion odd Krammers pairs, if the little group contains inversion.

```
Invariant under inversion: Yes
Number of inversions-odd Kramers pairs : 3
Gap with upper bands:  0.5552250943410071
```

Once we know the irreps, we can place them on top of a band structure plot, which should be calculated via DFT.



3.1.3 Diagnosing topology of valence bands

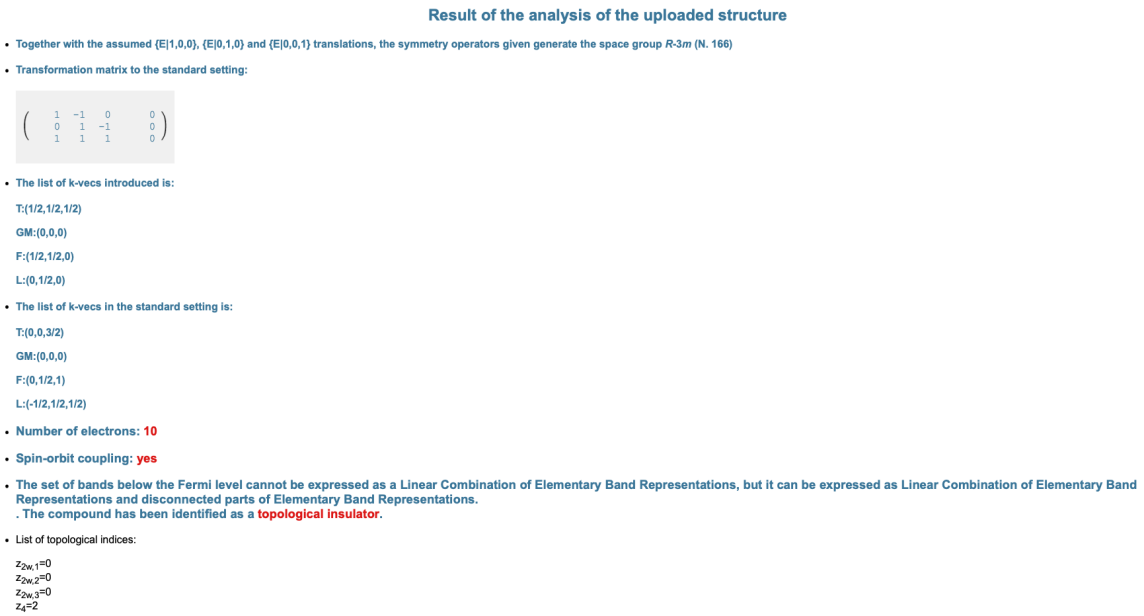
In the previous section, we have determined the irreducible representations of valence and some conduction bands. In order to classify the topology of a material, **we need to focus on its valence bands**. We can do so by **setting `-IBend` to the index of the last valence band**, which is 10 in the case of Bi:

```
irrep -code=vasp -kpnames=T,GM,F,L -Ecut=50 -IBend=10 -searchcell -spinor -EF=5.2244 > out
```

If we inspect the output saved into the file `out`, we will notice that only the lowest 10 bands (*i.e.* the valence bands) were considered for the calculation. According to the formalism of topological quantum chemistry, to show that the material is topological, it is enough to demonstrate that the irreducible representations do not match with those of a linear combination of elementary band representation. We can check this by means of the file `trace.txt` written by IrRep.

1. Open the webpage of the application ChecktopologicalMat in the Bilbao Crystallographic Server.
2. Upload the file named `trace.txt` generated by IrRep. This software will use the output of IrRep to determine if the representation of the bands passed to it matches a band representation, and it will calculate the values of space group's symmetry-indicators of topology.

You should see something like the following picture:



According to this analysis, Bi hosts a topological phase classified by a z_2, due to a double band inversion invisible to the z_2 indicator. This number indicates that **Bi is a higher-order topological insulator**. Indeed, F. Schindler *et al.* demonstrated that Bi exhibits gapless hinge modes.

3.1.4 Separating states by inversion eigenvalues

Identifying irreducible representations is not IrRep's only function. It is also able to separate wave functions based on eigenvalue of a symmetry operation. Let us take advantage of this function to corroborate the calculation of strong z_2 invariant and the z_4. For that, we have to separate wave functions in subspaces of inversion.

1. First, we have to identify the number of inversion. Open the output generated by IrRep in any of the previous steps and identify the number that labels inversion:

```
### 7

rotation : | -1   0   0 |     rotation : | -1   0   0 |
           |  0  -1   0 |       (refUC)  |  0  -1   0 |
           |  0   0  -1 |                |  0   0  -1 |
```

   Thus, **inversion is the symmetry number 7**.

2. Indicate IrRep that we want to separate the wave functions in terms of inversion, by setting `-isymsep=7`:

```
irrep -isymsep=7 -kpnames=GM,F,T,L -IBend=78 -Ecut=100 -EF=auto -code=espresso
       -prefix=out/Bi2Se3 > output
```

   IrRep will write first the traces and irreducible representations without separating them. Then, it will focus on each subspace of inversion and write the traces and irreps within each.

3. We are interested in the inversion-odd subspace. We can find the data about odd wave functions after the heading

```
#####################################################

NEXT SUBSPACE:   sym # 7 -> eigenvalue -1.000
```

After the heading, we will listed every wave function and its irrep. To corroborate the z_2 and z_4 numbers, we count the number of odd valence states at every inversion-invariant **k**-point:

	T	Γ	F	L
N_-	6	2	6	6

Since there are 3 partners for the points F and L, the number of inversion-odd wave functions is:

$$N_4 = 6 + 2 + 6 \times 3 + 6 \times 3 = 44.$$

According to Fu-Kane's formula, the strong invariant is z_2:

$$z_2 = N_- \mod 2 = 0.$$

On the other hand, the z_4 number is:

$$z_4 = N_- \mod 4 = 2.$$

3.2 Bi_2Se_3

In this tutorial, we will use IrRep to classify the topology of Bi_2Se_3. We will use as input DFT data obtained with the Quantum Espresso. The data is in the out directory. The input files for Quantum Espresso necessary to obtain this data can be found in the directory `inputs`.

Exercises:

- Exercise 1: Identify the space group
- Exercise 2: Diagnose the topology of valence bands
- Exercise 3: Separate wave functions by inversion eigenvalues

3.2.1 Identification of the space group

If we look into the input files for Quantum Espresso, we notice that the lattice vectors specified for Bi_2Se_3 belong to a rhombohedral family. However, it is not easy to guess the space group by inspecting the atomic positions. We can use IrRep for this task:

```
irrep -code=espresso -prefix=out/Bi2Se3 -onlysym > output
```

The `prefix` option should indicate the path to the `.save` directory generated by Quantum Espresso, thus it is related to the Quantum Espresso's arguments `outdir` and `prefix`. With `> out`, we have saved the output of IrRep into a file called `out`. If we open this file with a text editor, we will find:

- A description of the crystal structure parsed from DFT files. We see that the cell used for the DFT calculation was a primitive cell.

```
 ---------- CRYSTAL STRUCTURE ----------

Cell vectors in angstroms:

      Vectors of DFT cell       |      Vectors of REF. cell
a0 =  2.0715   1.1960   9.5453  |  a0 =  2.0715  -2.0715   0.0000
a1 = -2.0715   1.1960   9.5453  |  a1 =  1.1960   1.1960  -2.3920
a2 =  0.0000  -2.3920   9.5453  |  a2 =  9.5453   9.5453   9.5453

Atomic positions in direct coordinates:
```

```
Atom type |   Position in DFT cell    |   Position in REF cell
    1     |  0.6015   0.6015   0.6015 |  0.6015   0.6015   0.6015
    1     |  0.3985   0.3985   0.3985 |  0.3985   0.3985   0.3985
    2     |  0.0000   0.0000   0.0000 |  0.0000   0.0000   0.0000
    2     |  0.7885   0.7885   0.7885 |  0.7885   0.7885   0.7885
    2     |  0.2115   0.2115   0.2115 |  0.2115   0.2115   0.2115
```

- The name of the space group. It is the rhombohedral group R-3m (No. 166). It contains 12 symmetry operations (mod. translations).

```
Space group: R-3m (# 166)
Number of symmetries: 12 (mod. lattice translations)
```

- A list of symmetry operations. Each symmetry operation is described by giving the matrix of its rotational part, the vector of the translational part, its action on a generic **k**-point, its rotation axis, angle and whether it respects chirality or not (`inversion` tag).

```
 ### 3

rotation : |  0   0   1 |
           |  1   0   0 |
           |  0   1   0 |

gk = [kz, kx, ky]

spinor rot.         : | 0.500-0.866j -0.000-0.000j |
                      | 0.000-0.000j  0.500+0.866j |

translation         :  [   0.0000   0.0000   0.0000 ]

axis: [0. 0. 1.] ; angle = 2/3 $\pi$, inversion : False
```

3.2.2 Diagnosing topology of valence bands

Let us calculate the irreducible representations at maximal **k**-points for the occupied bands. For that, we need to:

- Pass the labels of the maximal **k**-points via the argument `-kpnames`. The labels should be in the same order as the k-points in the `K_POINTS` block in Quantum Espresso input (file `nscf_IrRep.in` in this tutorial).
- We need to set `-IBend` to the index of the last band we want to consider. Since the number of electrons is 78 (see output of the self-consistent Quantum Espresso calculation), the occupied band has index 78, thus we need `-IBend=78`.

```
irrep -kpnames=GM,F,T,L -IBend=78 -Ecut=100 -EF=auto -code=espresso -prefix=out/Bi2Se3 > output
```

Let us comment on the rest of arguments passed to the command above:

- `code` specifies the interface that should be applied. In this case, it is the interface for Quantum Espresso.
- `Ecut` sets the plane-wave cutoff that will be used for the calculation. Coefficients of plane waves with larger energy will be discarded. Setting it to a value smaller than the cutoff considered in the DFT calculation reduces considerably the time of the calculation.
- `EF` is the Fermi energy. All energy levels will be given with respect to this value. Here, we are asking IrRep to parse it from the DFT output.

Let us open the file `out` generated by this command and go through the output.

- First, we see the same description of the unit cell and space group that we studied above. However, we can find something that is different:

```
        |   1.0000 -1.0000  0.0000 |
refUC = |  -0.0000  1.0000 -1.0000 |    shiftUC = [-0.  0.  0.]
        |   1.0000  1.0000  1.0000 |
```

It tells us that the transformation from the DFT cell to the conventional setting. See IrRep's documentation for more details.

- Then, we have a block for each maximal **k**-point passed to the code. The header of each block contains the coordinates of the **k**-point in both, the DFT and conventional cell. The number of symmetries in the little group is also written (mod. translations).

```
k-point   2 : [ 0.5  0.5 -0. ] (in DFT cell)
              [0.  0.5 1. ] (after cell trasformation)

number of states : 80
```

After the header, we can find a list of *energy levels* and *irreducible representations* of identified for each one. The *traces* of symmetries in the little-group are also listed in the same row. The next row contains the traces in the conventional cell.

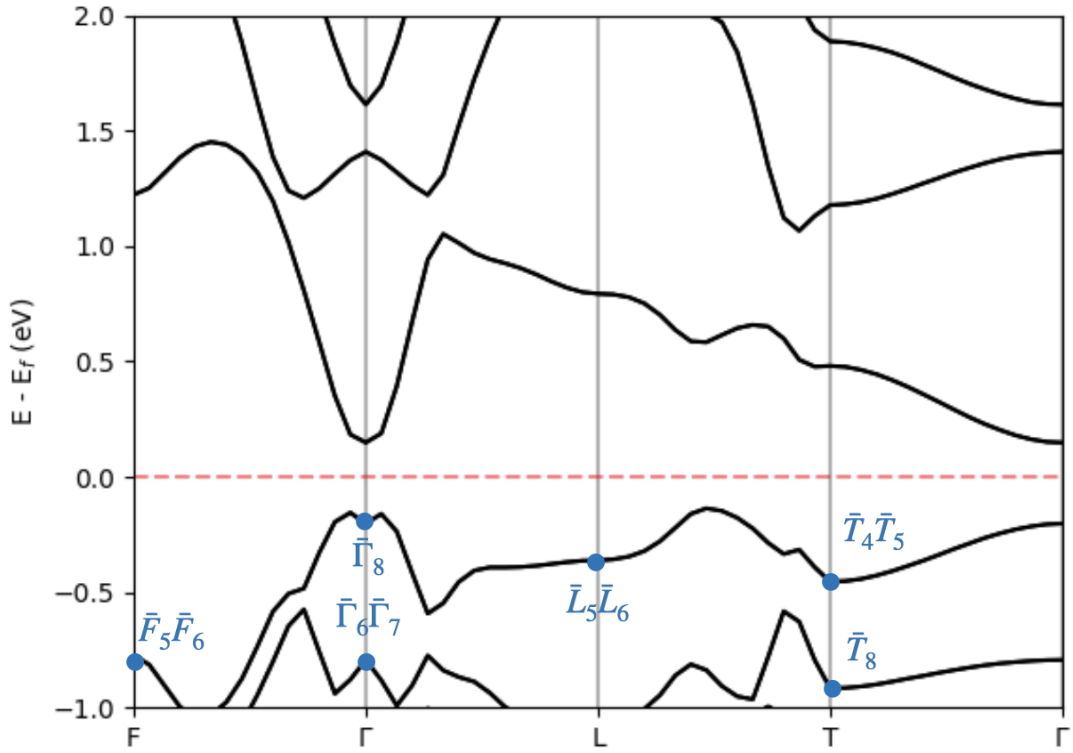
```
   Energy  |   degeneracy  |       irreps       | sym. operations
           |               |                    |    1        5        7        11
 -49.4201  |        2      | -F3(1.0), -F4(1.0) |   2.0000   0.0000   2.0000   0.0000
           |               |                    |   2.0000   0.0000   2.0000   0.0000
 -49.1098  |        2      | -F3(1.0), -F4(1.0) |   2.0000  -0.0000   2.0000  -0.0000
           |               |                    |   2.0000  -0.0000   2.0000  -0.0000
 -48.6115  |        2      | -F5(1.0), -F6(1.0) |   2.0000  -0.0000  -2.0000   0.0000
           |               |                    |   2.0000  -0.0000  -2.0000   0.0000
 -47.6185  |        2      | -F3(1.0), -F4(1.0) |   2.0000   0.0000   2.0000   0.0000
```

In this case, the form pairs due to the presence of time-reversal symmetry in the symmetry group.

- Finally, the gap with respect to the next set of bands (with index `IBend`+1) is given. Also the number of inversion odd Kramers pairs, if the little group contains inversion.

```
Invariant under inversion: Yes
Number of inversions-odd Kramers pairs : 18
Gap with upper bands:  1.193565132807561
```

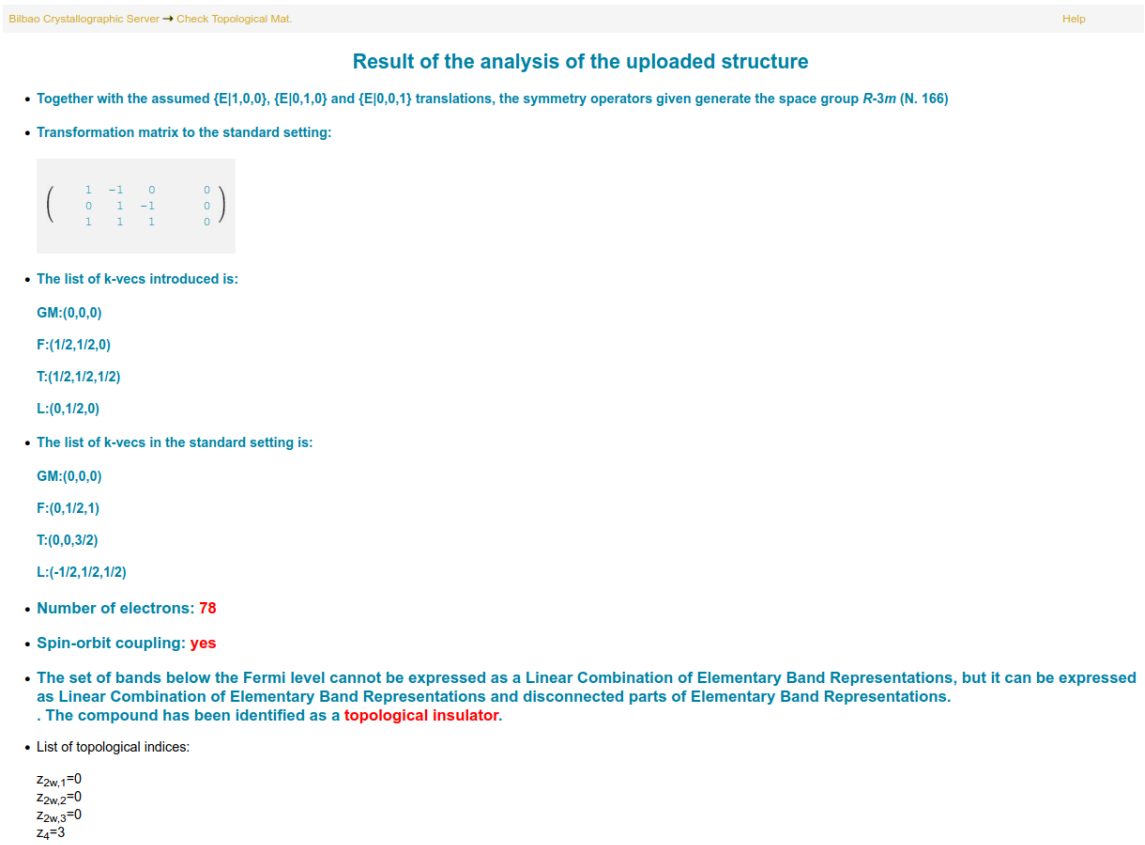
Once we know the irreps, we can place them on top of a band structure plot, which should be calculated via DFT.



If we inspect the output saved into the file `output`, we will notice that only the lowest 78 bands (*i.e.* the valence bands) were considered for the calculation. According to the formalism of topological quantum chemistry, to show that the material is topological, it is enough to demonstrate that the irreducible representations do not match with those of a linear combination of elementary band representation. We can check this by means of the file `trace.txt` written by IrRep.

1. Open the webpage of the application ChecktopologicalMat in the Bilbao Crystallographic Server.
2. Upload the file named `trace.txt` generated by IrRep. This software will use the output of IrRep to determine if the representation of the bands passed to it matches a band representation, and it will calculate the values of space group's symmetry-indicators of topology.

You should see something like the following picture:



According to this analysis, Bi hosts a topological phase classified by the following symmetry-indicators:

$$(z_{2w,1}, z_{2w,2}, z_{2w,3}, z_4) = (0, 0, 0, 3).$$

These numbers indicate that Bi_2Se_3 **is a strong-topological insulator protected by time-reversal symmetry**.

3.2.3 Separating states by inversion eigenvalues

Identifying irreducible representations is not IrRep's only function. It is also able to separate wave functions based on eigenvalue of a symmetry operation. Let us take advantage of this function to corroborate the calculation of z_2 invariant and z_4 invariants. For that, we have to separate wave functions in subspaces of inversion.

1. First, we have to identify the number of inversion. Open the output generated by IrRep in any of the previous steps and identify the number that labels inversion:

```
 ### 7

rotation : | -1   0   0 |     rotation : | -1   0   0 |
           |  0  -1   0 |       (refUC)  |  0  -1   0 |
           |  0   0  -1 |                |  0   0  -1 |
```

Thus, **inversion is the symmetry number 7**.

2. Indicate IrRep that we want to separate the wave functions in terms of inversion, by setting `-isymsep=7`:

```
irrep -isymsep=7 -kpnames=GM,F,T,L -IBend=78 -Ecut=100 -EF=auto -code=espresso
       -prefix=out/Bi2Se3 > output
```

IrRep will write first the traces and irreducible representations without separating them. Then, it will focus on each subspace of inversion and write the traces and irreps within each.

3. We are interested in the inversion-odd subspace. We can find the data about odd wave functions after the heading

```
################################################

NEXT SUBSPACE:   sym # 7 -> eigenvalue -1.000
```

After the heading, we will list every wave function and its irrep. To corroborate the z_2 and z_4 numbers, we count the number of odd valence states at every inversion-invariant **k**-point:

	Γ	F	T	L
N_-	36	38	38	38

Since there are 3 partners for the points F and L, the number of inversion-odd wave functions is:

$$N_4 = 34 + 38 \times 3 + 38 + 38 \times 3 = 300.$$

According to Fu-Kane's formula, the strong invariant is z_2:

$$z_2 = N_- \mod 2 = 0.$$

On the other hand, the z_4 number is:

$$z_4 = N_- \mod 4 = 3.$$

3.3 SnTe

In this tutorial, we will use IrRep to classify the topology of SnTe, but **we will force ourselves to use the argument** `-refUC`. This way, we will learn how to deal with the difference between DFT and conventional settings. We will use as input DFT data obtained with the Abinit. This data consists of the file `maxK_WFK` located in the current directory. The input files for Abinit necessary to obtain this data can be found in the directory `inputs`.

Exercises:

- Exercise 1: Identify the space group
- Exercise 2: Identify the transformation to the conventional cell
- Exercise 3: Calculate the irreducible representations at maximal k-points
- Exercise 4: Determine the topology of valence bands
- Exercise 5: Separate the states by inversion eigenvalues

3.3.1 Identification of the Space Group

SnTe crystallizes in a face-centered cubic structure. There exist 11 different face-centered cubic space groups. To determine the precise space group of our material, we need the cell vectors that describe the periodicity of the lattice, and the positions of atoms within the unit cell. This information is in the `maxK_WFK` file, but we cannot open and read it, as this is a binary file. Instead, we can use IrRep to extract this information:

```
irrep -onlysym -code=abinit -fWFK=maxK_WFK > out
```

With the specifications `-code=abinit` and `-fWFK=maxK_WFK`, we are telling IrRep to use the interface for Abinit and to parse the DFT data from the file `maxK_WFK`. With `> out`, we have saved the output of IrRep into a file called `out`. If we open this file with a text editor, we will find:

- A description of the crystal structure parsed from DFT files. We see that the cell used for the DFT calculation was a primitive cell which contains one Sn atom at the origin and another Te atom in the center of the cell.
- The name of the space group. It is the rhombohedral group Fm-3m (No. 225). It contains 48 symmetry operations (mod. translations).
- A list of symmetry operations. Each symmetry operation is described by giving the matrix of its rotational part, the vector of the translational part, its action on a generic **k**-point, its rotation axis, angle and whether it respects chirality or not (`inversion` tag).

3.3.2 Transformation to the Conventional Cell

IrRep is able to calculate the traces of symmetry operations in every **k**-point, also to identify the irreducible representations (irreps). For that, it needs the transformation from the DFT cell to the conventional setting in which the tables of irreps are written. As long as we set a valid `-kpnames`, IrRep will work out the transformation automatically. But, we enjoy challenges, so **let us assume that we want to use -refUC**.

In our DFT calculation, we used a primitive unit cell. This is often the case, as primitive cells include fewer atoms than centered cells, and therefore reduce the time and computational resources needed to run the calculation. On the other hand, the table of irreps is written with a conventional cell choice, which is a face-centered cell in this case. The transformation from the DFT cell's vectors ($\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$) into the face-center cube's vectors ($\mathbf{c}_1$, $\mathbf{c}_2$, $\mathbf{c}_3$) is given by:

$$\begin{pmatrix} \boldsymbol{c}_1 \\ \boldsymbol{c}_2 \\ \boldsymbol{c}_3 \end{pmatrix} = \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix} \begin{pmatrix} \boldsymbol{a}_1 \\ \boldsymbol{a}_2 \\ \boldsymbol{a}_3 \end{pmatrix}$$

We have to set `-refUC` as to pass to IrRep this transformation matrix, so we will be running IrRep with

```
-refUC=-1,1,1,1,-1,1,1,1,-1
```

For a more detailed explanation of the cell transformation, visit IrRep's documentation.

3.3.3 Irreducible Representations at Maximal k-Points

Now, we can calculate the irreps. There are 20 electrons in the unit cell, so there are 20 occupied bands. Let us set `-IBend=22` to calculate the irreps of all valence and the first 2 conduction bands:

```
irrep -kpnames=GM,X,L,W -IBend=22 -Ecut=100 -refUC=-1,1,1,1,-1,1,1,1,-1 -EF=auto
        -code=abinit -fWFK=maxK_WFK  > out
```

Let us open the file `out` generated by this command and go through the output.

- After a description of the crystal structure and space group, we have a block for each maximal **k**-point passed to the code. The header of each block contains the coordinates of the **k**-point in both, the DFT and conventional cell. The number of symmetries in the little group is also written (mod. translations).

  ```
  k-point   2 : [0.5 0.  0.5] (in DFT cell)
                [0. 1. 0.] (after cell trasformation)

  number of states : 22
  ```

  After the header, we can find a list of **energy levels** and **irreducible representations** of identified for each one. The **traces** of symmetries in the little-group are also listed in the same row. The next row contains the traces in the conventional cell.

Energy	degeneracy	irreps	sym. operations				
			1	2	3	4	21
-7.2711	2	-X6(1.0)	2.0000	0.0000	0.0000	0.0000	1.4142
			2.0000	0.0000	0.0000	0.0000	1.4142
-6.3611	2	-X8(1.0)	2.0000	-0.0000	0.0000	-0.0000	1.4142
			2.0000	-0.0000	0.0000	-0.0000	1.4142
-4.7342	2	-X8(1.0)	2.0000	0.0000	0.0000	-0.0000	1.4142
			2.0000	0.0000	0.0000	-0.0000	1.4142
-4.2995	2	-X9(1.0)	2.0000	-0.0000	0.0000	0.0000	-1.4142
			2.0000	-0.0000	0.0000	0.0000	-1.4142
1.4154	2	-X7(1.0)	2.0000	-0.0000	-0.0000	-0.0000	-1.4142
			2.0000	-0.0000	-0.0000	-0.0000	-1.4142

- Finally, the gap with respect to the next set of bands (with index `IBend`+1) is given. Also the number of inversion odd Kramers pairs, if the little group contains inversion.

```
Invariant under inversion: Yes
Number of inversions-odd Kramers pairs : 3
Gap with upper bands:  2.3747815703844037
```

Once we know the irreps, we can place them on top of a band structure plot, which should be calculated via DFT.

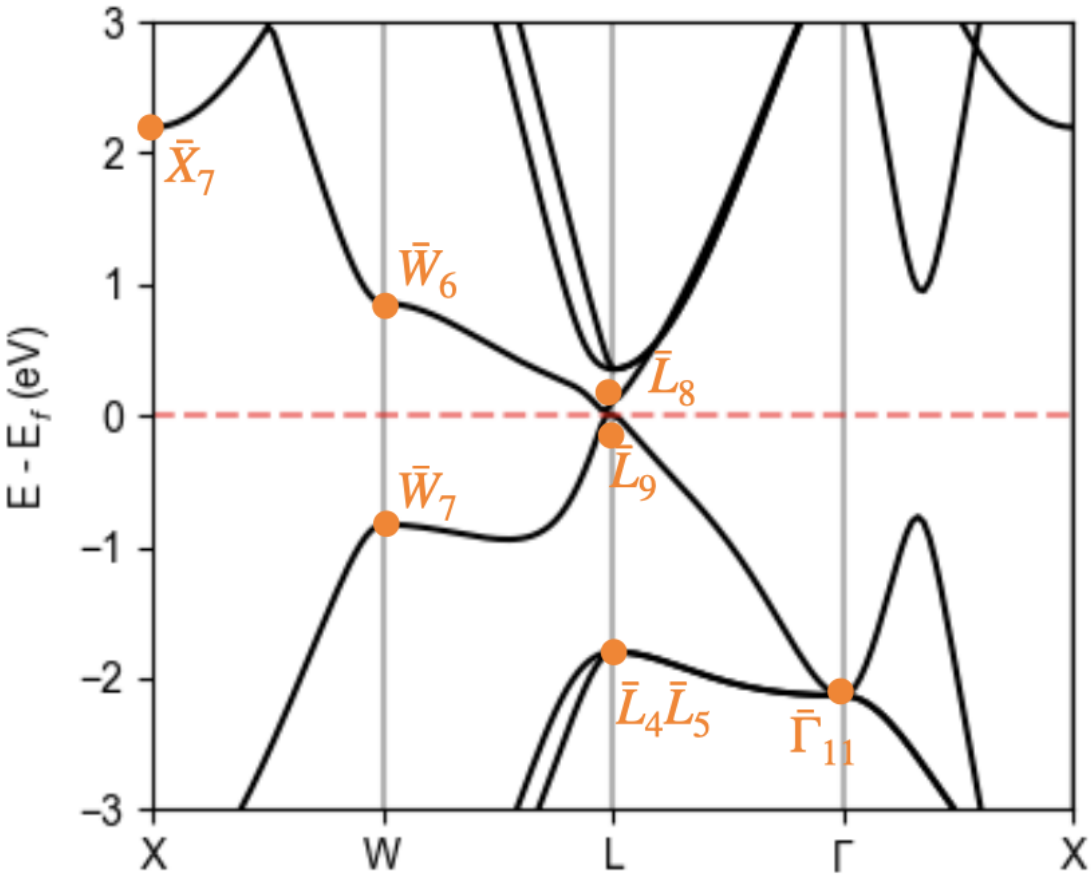


Figure 1: Band structure plot

3.3.4 Diagnosing topology of valence bands

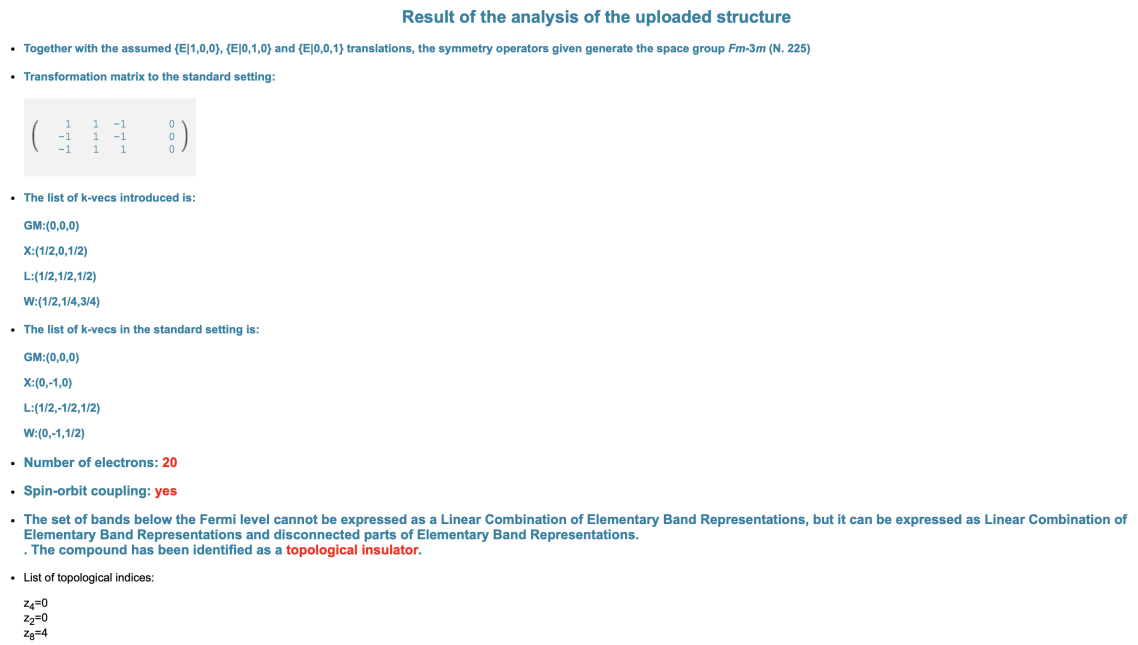
In the previous section, we have determined the irreducible representations of valence and some conduction bands. In order to classify the topology of a material, **we need to focus on its valence bands**. We can do so by **setting `-IBend` to the index of the last valence band**, which is 20 in the case of SnTe:

```
irrep -kpnames=GM,X,L,W -IBend=20 -Ecut=100 -refUC=-1,1,1,1,-1,1,1,1,-1 -EF=auto
      -code=abinit  -fWFK=maxK_WFK  > out
```

If we inspect the output saved into the file `out`, we will notice that only the lowest 10 bands (i.e. the valence bands) where considered for the calculation. According to the formalism of topological quantum chemistry, to show that the material is topological, it is enough demonstrate that the irreducible representations do not match with those of a linear combination of elementary band representation. We can check this by means of the file `trace.txt` written by IrRep.

1. Open the webpage of the application ChecktopologicalMat in the Bilbao Crystallographic Server.
2. Upload the file named `trace.txt` generated by IrRep. This software will use the output of IrRep to determine if the representation of the bands passed to it matches a band representation, and it will calculate the values of space group's symmetry-indicators of topology.

You should see something like the following picture:



According to this analysis, SnTe is a topological insulator classified by a $z_8 = 4$, which indicates that the phase hosts mirror Chern invariants, as well as glide invariants (see the work by Song *et al.*).

3.3.5 Separating states by inversion eigenvalues

Identifying irreducible representations is not IrRep's only function. It is also able to separate wave functions based on eigenvalues of a symmetry operation. Let us take advantage of this function to corroborate the calculation of strong z_2 invariant and the z_4. For that, we have to separate wave functions in subspaces of inversion.

1. First, we have to identify the number of inversion. Open the output generated by IrRep in any of the previous steps and identify the number that labels inversion:

```
### 25

rotation : | -1   0   0 |     rotation : | -1   0   0 |
           |  0  -1   0 |      (refUC)   |  0  -1   0 |
           |  0   0  -1 |                |  0   0  -1 |
```

Thus, **inversion is the symmetry number 25**.

2. Indicate IrRep that we want to separate the wave functions in terms of inversion, by setting `-isymsep=25`:

```
irrep -isymsep=25 -kpnames=GM,X,L,W -IBend=20 -Ecut=100
      -refUC=-1,1,1,1,-1,1,1,1,-1 -EF=auto -code=abinit
      -fWFK=maxK_WFK  > out
```

   Ups, it seems something went wrong... The problem is in the list of points. We are asking IrRep to separate wave functions based on their eigenvalue of inversion at W. But this point is not invariant under inversion! So, what we are trying to do does not make sense.

   We need to get rid of the point W. For that, we have to specify only the inversion invariant **k**-points via the argument `-kpoints`:

```
irrep -isymsep=25 -kpnames=GM,X,L -kpoints=1,2,3 -IBend=20
      -Ecut=100 -refUC=-1,1,1,1,-1,1,1,1,-1 -EF=auto -code=abinit
      -fWFK=maxK_WFK  > out
```

   IrRep will write first the traces and irreducible representations without separating them. Then, it will focus on each subspace of inversion and write the traces and irreps within each.

3. We are interested in the inversion-odd subspace. We can find the data about odd wave functions after the heading

```
###############################################
NEXT SUBSPACE:   sym # 25 -> eigenvalue -1.000
```

   After the heading, we will list every wave function and its irrep. To corroborate the z_2 and z_4 numbers, we count the number of odd valence states at every inversion-invariant **k**-point:

	Γ	X	L
N_-	6	6	4

   The points X and L have 4 and 3 symmetry related partners, respectively. Hence, the number of inversion-odd wave functions is:

$$N_4 = 6 + 6 \times 3 + 4 \times 4 = 40.$$

   According to Fu-Kane's formula, the strong invariant is z_2:

$$z_2 = N_- \mod 2 = 0.$$

   On the other hand, the z_4 number is:

$$z_4 = N_- \mod 4 = 0.$$

4 Homotopy

4.1 Homotopy group

Homotopy groups can be used to characterize the topology of different spaces. The most pedagogical example is to work in three-dimensional Euclidean space, denoted as $\mathbb{R}^3$. We will focus on the topology of various solid, continuous, and compact objects, which may have a varying number of holes. For instance, the topology of a sphere or the surface of a wine glass is the same, and these two objects are characterized by the same homotopy groups (as a common aspect, their surface surround a hole, but in itself the surface show no hole). Similarly, the torus, resembling a donut, will have the same homotopy group as the surface of a mug, which has a handle and thus a hole in the surface. In terminology, the hole is called the defect. The hunter rule states that $d' + r = d - 1$, with d' the dimension of the defect, r the dimension of the contour (closed path) to catch the defect and d the dimension of the space considered (here $\mathbb{R}^3$).

1. Determine the dimension of the contour required to find the number of holes in compact surfaces (sphere, torus...)
2. Represent graphically the different elemental contours that can, when combined, generate the classes of closed path for the sphere (S^2).
3. Deduce the homotopy group of the sphere, noted $\pi_r(S^2)$ with r the dimension of the contours determined previously.
4. Do the same graphical representation for the torus (T^2) and deduce its homotopy group $\pi_r(T^2)$.
5. Try to generalise the homotopy group for any number n of holes.

4.2 Magnetic skyrmions with Heisenberg spins

Magnetic skyrmions are topological objects. They are real-space spin textures, sometimes referred to as magnetic bubbles. Their main characteristic is that the magnetization at the core of the bubble is opposite to that outside the bubble. They form in ultrathin films, allowing the system to be considered two-dimensional. These structures, generally originating from the Dzyaloshinskii-Moriya interaction, cannot be continuously deformed into a homogeneous spin state across the entire surface, thus conferring them this topological property. The position of the spin on the surface is thus described by a 2D space $\mathbb{R}^2$: the plane of the thin film. They can be described by the coordinates x and y in the Cartesian coordinate system or by r and α in the polar coordinate system (see Fig. 2. The spin orientation, if we fix the amplitude of the moment $|\vec{m}| = 1$, can be described by the two spherical coordinates θ and ϕ) as represented in Fig 2 and belong to the unit sphere $\mathbb{S}^2$. The topological invariant of these bubble can thus be caught by considering the homotopy group $\pi_2(\mathbb{S}^2)$. The magnetic texture covers a portion of the sphere $\mathbb{S}^2$ as we move in the real space $\mathbb{R}^2$ of spin positions. As we can see in Fig. 3, we can then orient this surface by observing how the spins rotate as we move in a direction in $\mathbb{R}^2$:

$$dS = \vec{m}.\left(\frac{\partial \vec{m}}{\partial x} \times \frac{\partial \vec{m}}{\partial y}\right) dxdy \tag{51}$$

The topological invariant can be determined by evaluating the surface of $\mathbb{S}^2$ covered by the spins when traversing the entire surface $\mathbb{R}^2$ of the magnetic bubble. The expression is given by:

$$n = \frac{1}{4\pi} \int_S \vec{m}.\left(\frac{\partial \vec{m}}{\partial x} \times \frac{\partial \vec{m}}{\partial y}\right) dxdy \tag{52}$$

6. Show that for a homogeneous magnetization, $\vec{m}(x, y) = m\vec{u}_z$, the texture is topologically trivial : n=0.
7. In order to work on magnetic skyrmions, it is convenient to use the polar coordinate for the spin position. Writing $x = rcos(\alpha)$, $y = rsin(\alpha)$ for the $\mathbb{R}^2$ space of the spin positions, and $\vec{m} = sin(\theta)cos(\varphi)$. For centrosymmetric structure, as in our case, θ only depends on r and φ on α. We give : $\frac{\partial}{\partial x} = \frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial \alpha}{\partial x}\frac{\partial}{\partial \alpha}$
8. Show that in polar coordinate, we can write :

$$n = \frac{1}{4\pi} \int_r sin(\theta) \frac{\partial \theta}{\partial r} \partial r \int_\alpha \frac{\partial \varphi}{\partial \alpha} \partial \alpha \tag{53}$$

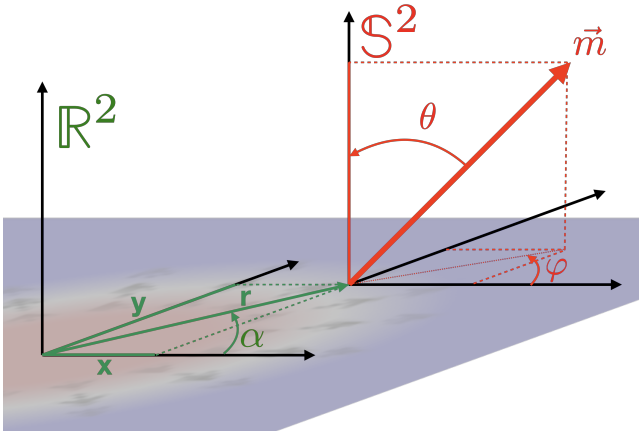


Figure 2: Representation of the different coordinates set for the magnetic skyrmions. $\mathbb{R}^2$ correspond to the position of the spin in Cartesian coordinates (x,y) or in polar coordinate (r,α). $\mathbb{S}^2$ corresponds to the spin space (2 dimension since the norm of the spin is fixed), and the direction of the magnetic moments is given by the two angles (θ,φ).

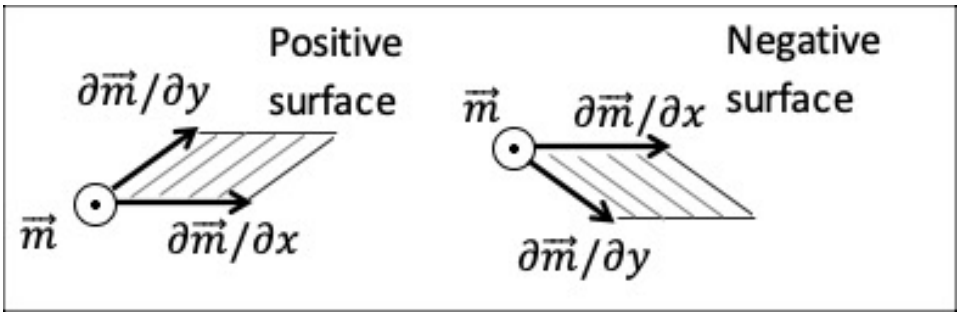


Figure 3: Two different orientations of the surface depending on the corss product $\frac{\partial\vec{m}}{\partial x} \times \frac{\partial\vec{m}}{\partial y}$: positive or negative.

9. Using this last equation, determine the topological number for the 8 configuration in Fig. 4.

10. Magnetic textures having the same topological number are equivalent : they can be continuously deformed fomr one to another. For the equivalent textures of Fig. 4, determine a possible transformation.

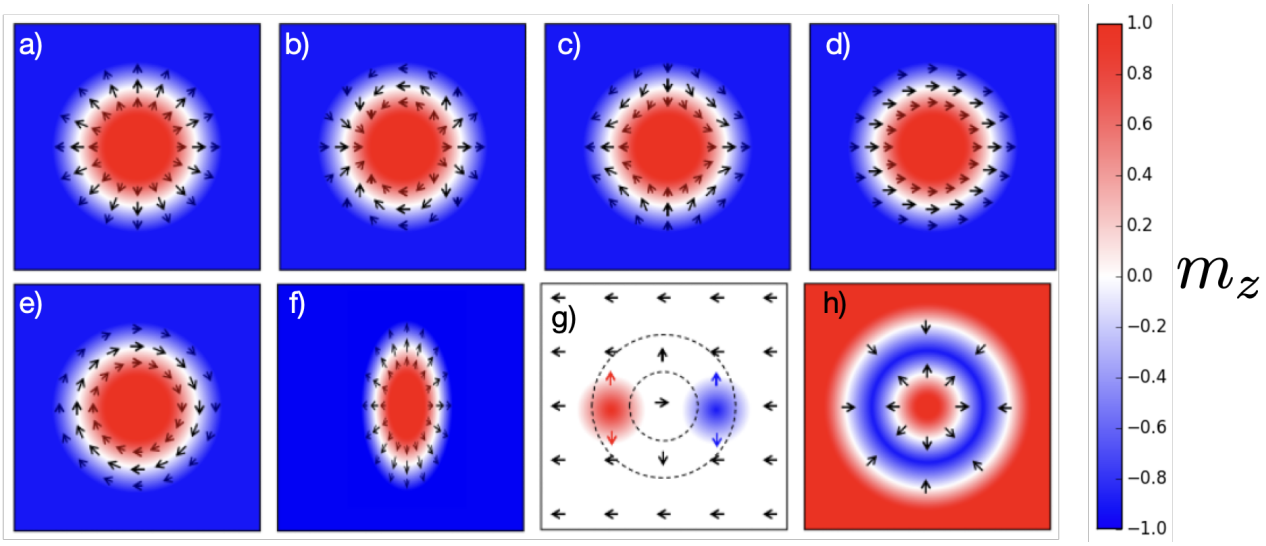


Figure 4: Different spin configuration on the 2D $\mathbb{R}^2$ space. Spin is represented by the black arrow for in-plane components (m_x and m_y) and by the color for m_z component : red is for $m_z = +1$, white for $m_z = 0$ and blue for $m_z = -1$ as shown in the colorbar.

5 Topological Magnons

5.1 First neighbour interaction

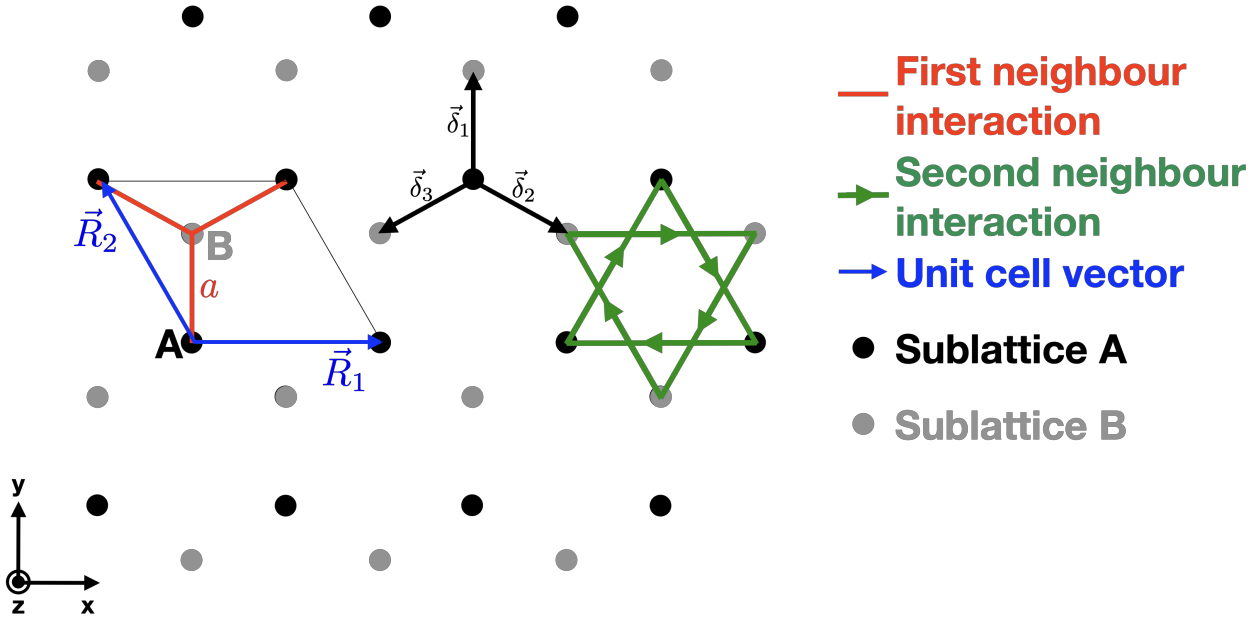


Figure 5: Honeycomb lattice in the Cartesian basis ($\vec{x}$,$\vec{y}$) .

In this exercise we shall see how interacting magnetic moments can lead to nontrivial topology in the low energy excitation spectrum. Consider the honeycomb lattice represented in Fig. 5, with a nearest neighbour distance a (we can conveniently take a= 1) with moments (spin S) on the vertices coupled via ferromagnetic Heisenberg exchange :

$$H = -J \sum_{<i,j>} \hat{S}_i . \hat{S}_j \tag{56}$$

with J>0 for ferromagnetic interaction and <i,j> stands for each pair of first neighbour spins. The exact ground state is :

$$|\Psi\rangle_{GS} = |\uparrow\uparrow ... \uparrow\rangle \tag{57}$$

To study the excitations of this ground state, the magnons, we need to express the Hamiltonian in terms of the non-Hermitian spin ladder operators S^+ and S^-. We remind that $S^+ = S^x + iS^y$ and $S^- = S^x - iS^y$.

1. Show that the Hamiltonian can then be rewritten as :

$$H = -J \sum_{<i,j>} S_i^z S_j^z + \frac{1}{2} \left(S_i^+ S_j^- + S_i^- S_j^+ \right) \tag{58}$$

The honeycomb lattice is comprised of 2 sublattices, denoted A and B at positions (0,0) and (0,a) in the Cartesian basis ($\vec{x}$,$\vec{y}$) respectively. The basic vectors of the elementary lattice are given by $\vec{R}_1 = (\sqrt{3}a, 0)$ and $\vec{R}_2 = (-\frac{\sqrt{3}}{2}a, \frac{3}{2}a)$ in the Cartesian basis ($\vec{x}$,$\vec{y}$) as represented in Fig. 5.

2. Verify that this is an eigenstate and compute the energy E_{GS} of this ground state.

3. Rewrite the Hamiltonian in terms of the creation and annihilation operators (of magnons) $a_i^\dagger$ and a_i, knowing that $S^+ = \sqrt{2S} a_i^\dagger$, $S^- = \sqrt{2S} a_i$, and $S^z = S - a_i^\dagger a_i$ and keep only the linear terms.

4. Rewrite the Hamiltonian in terms of the creation and annihilation operators on each sublattice in momentum space, namely $a^\dagger_{\vec{k}A}$, $a_{\vec{k}A}$, $a^\dagger_{\vec{k}B}$ and $a_{\vec{k}B}$. Show that it can take the form :

$$H = E_{GS} + H_{SW} \; with \; H_{SW} = JS \sum_k \begin{pmatrix} a^\dagger_{\vec{k}A} & a^\dagger_{\vec{k}B} \end{pmatrix} \begin{pmatrix} 3 & \gamma_{\vec{k}} \\ \gamma^*_{\vec{k}} & 3 \end{pmatrix} \begin{pmatrix} a_{\vec{k}A} \\ a_{\vec{k}B} \end{pmatrix} \tag{59}$$

5. Calculate the dispersion relation.

6. Show that on the K point of the reciprocal space defined by $\vec{K} = (\frac{4\pi}{3\sqrt{3}a}, 0) = \frac{2\pi}{a}(\frac{2}{3\sqrt{3}}, 0)$ (there are actually 6 equivalent K points in the Brillouin Zone), $\left|\gamma_{\vec{k}}\right| = 0$. This is a Dirac point and the spectrum is the magnon analogue of graphene. Perform a first-order Taylor expansion in k around $\vec{K}$.

5.2 Second neighbour interaction

Now we add a Dzyaloshinskii-Moriya (DMI) exchange coupling acting between second neighbours as indicated in the Fig. 5. The arrows in the figure indicate the orientation of the cross product. This coupling is symmetry-allowed and naturally arises to leading order in the superexchange when spin-orbit is included. In other words, this coupling is relevant to materials. The ferromagnetic ground state is stable to the presence of DMI. It is straightforward to see that the state written above is exact even in the presence of DMI. Now, the total Hamiltonian is written :

$$H = -J \sum_{<i,j>} \hat{S}_i . \hat{S}_j + D \sum_{<i,j>2} \vec{z} . \left(\hat{S}_i \times \hat{S}_j \right) \tag{60}$$

where $< i, j > 2$ stands for all bond between second neighbour, meaning between sites belonging to the same sublattice.

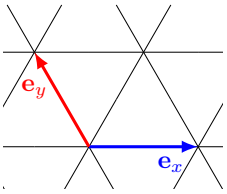
7. Using the same methodology as before, show that the DMI Hamiltonian $H_{DMI} = D \sum_{<i,j>2} \vec{z} . \left(\hat{S}_i \times \hat{S}_j \right)$ can be rewritten in the same form as the celebrated Haldane model, where ϕ needs to be determined:

$$H_{DMI} = D \sum_k \begin{pmatrix} a^\dagger_{\vec{k}A} & a^\dagger_{\vec{k}B} \end{pmatrix} \begin{pmatrix} \sum_{\mu=1}^{3} cos(\vec{k}.\vec{\eta}_\mu - \phi) & 0 \\ 0 & \sum_{\mu=1}^{3} cos(\vec{k}.\vec{\eta}_\mu + \phi) \end{pmatrix} \begin{pmatrix} a_{\vec{k}A} \\ a_{\vec{k}B} \end{pmatrix} \tag{61}$$

6 Topological magnetic order

6.1 Schwinger boson mean-field theory

We consider antiferromagnetic interactions between nearest neighboring spins $S = 1/2$ on a triangular lattice: $\hat{H} = \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$. Basis vectors $\mathbf{e}_x$ and $\mathbf{e}_y$ are:



Despite the simplicity of $\hat{H}$, no exact expression of the ground state is known. Its nature has remained controversial and has led to the proposal of resonating valence bond. Here we use the Schwinger boson mean-field theory to handle this problem, that we detail step by step in this exercise.

We construct an equivalent model with bosonic particles (different from the Holstein Primakoff transformation used in spin-wave theory, but in a similar spirit) possessing a local $U(1)$ gauge symmetry. $a^\dagger_{\sigma i}$ is the creation operator of a boson of spin $\sigma = \pm 1/2$ on lattice site i. We can then define $n_\uparrow = a^\dagger_{\uparrow i} a_{\uparrow i}$ as the number of spin up on site i. We also give the commutation relation $\left[a^\dagger_{\uparrow i}, a_{\uparrow j}\right] = \delta_{ij}$

$$S^+_i = a^\dagger_{\uparrow i} a_{\downarrow i}, \qquad S^-_i = a^\dagger_{\downarrow i} a_{\uparrow i}, \qquad S^z_i = \frac{1}{2}\left(a^\dagger_{\uparrow i} a_{\uparrow i} - a^\dagger_{\downarrow i} a_{\downarrow i}\right) \tag{62}$$

1. What is the number of possible states on a site i for the spin model with S=1/2 ? And for the bosonic model ? What is the constraint on site i insuring that both models have the same Hilbert space ?

2. Verify that with this constraint, we still have the correct value for $\mathbf{S}^2 = S(S+1)$. We remind that $S^+ = S^x + iS^y$ and $S^- = S^x - iS^y$.

3. Simply replacing bosons by Abrikosov fermions in Eq. (62) gives another spin representation. Show that the gauge symmetry is a local $SU(2)$ one.

4. We define the operator $\hat{A}_{ij}$, defined on the (oriented) link $i-j$ of the lattice by: $\hat{A}_{ij} = \frac{1}{2}\left(a_{\uparrow i} a_{\downarrow j} - a_{\downarrow i} a_{\uparrow j}\right)$ such that $\mathbf{S}_i \cdot \mathbf{S}_j = \frac{1}{4} - 2\hat{A}^\dagger_{ij}\hat{A}_{ij}$ We include a Lagrange multiplier λ_i and consider the mean-field Hamiltonian:

$$H_{MF} = \sum_{\langle i,j \rangle} \left(\frac{1}{4} - 2\alpha_{ij}\hat{A}^\dagger_{ij} - 2\alpha^*_{ij}\hat{A}_{ij} + 2|\alpha_{ij}|^2\right) + \sum_i \lambda_i (1 - \hat{n}_i). \tag{64}$$

   Show that H_{MF} can be written under the form of $H_{MF} = v^\dagger M v + \epsilon_0$, with $v^\dagger = (a^\dagger_{\uparrow 1}, \ldots, a^\dagger_{\uparrow N_s}, a_{\downarrow 1}, \ldots, a_{\downarrow N_s})$, M a $2N_s \times 2N_s$ matrix and ϵ_0 a constant.

5. To express the Hamiltonian in the diagonal form $\hat{H}_{MF} = \sum_{j\sigma} \epsilon_j \tilde{a}^\dagger_{\sigma j}\tilde{a}_{\sigma j} + \tilde{\epsilon}_0$, a Bogoliubov transformation is required (different from a unitary tranformation) (skip this question if you know the transformation). Let $\tilde{M}$ be the diagonal matrix with coefficients ϵ_i and J the matrix $J = \begin{pmatrix} 1_{N_s} & 0 \\ 0 & -1_{N_s} \end{pmatrix}$.

   We define $\tilde{v}^\dagger = (\tilde{a}^\dagger_{\uparrow 1}, \ldots, \tilde{a}^\dagger_{\uparrow N_s}, \tilde{a}_{\downarrow 1}, \ldots, \tilde{a}_{\downarrow N_s})$ and the $\tilde{a}_{\sigma j}$ are bosonic operators characterized by a matrix P such that $v = P\tilde{v}$. Show that the operators $\tilde{a}_{\sigma j}$ have bosonic commutation relations as long as the matrix P obeys $PJP^\dagger = J$.

   The commutation relations must be fulfilled together with condition that $P^\dagger M P = \tilde{M}$ is diagonal (this is not a standard matrix diagonalization, since P is not unitary). Show that the energies ϵ_j are the eigenvalues of JM, times ± 1.

6. What are the condition on ϵ_j to have a well defined ground state ? What is the ground state in terms of the tilde operators ? What is the ground state energy E_0 in terms of ϵ_0 and ϵ_j ? In terms of $\tilde{\epsilon}_0$?

7. Any link (i,j) can be sent on any other one (k,l) by some lattice symmetry. We consider an Ansatz such that the physical observables are invariant by such transformations Find a simple argument to prove that this does not imply that all α_{ij} are equal. Show that a lattice symmetry X must have the same effect as a gauge transformation G on the Ansatz.

8. We chose the following Ansatz and admit that it respects all lattice symmetries: $\alpha_{ii+x} = \alpha_{ii+y} = \alpha_{ii-x-y} = \alpha$ with α a real positive number. Using a Fourier transformation, H_{MF} rewrites:

$$\sum_{\mathbf{q}} \phi^\dagger_{\mathbf{q}} M_{\mathbf{q}}(\alpha,\lambda)\phi_{\mathbf{q}} + \ N_s\epsilon_0(\alpha,\lambda), \qquad \phi_{\mathbf{q}} = \begin{pmatrix} a_{\uparrow\mathbf{q}} \\ (a_{\downarrow-\mathbf{q}})^\dagger \end{pmatrix}, \qquad a_{\sigma\mathbf{q}} = \frac{1}{\sqrt{N_s}}\sum_i a_{\sigma i} e^{-i\mathbf{q}\cdot\mathbf{r}_i}, \tag{65}$$

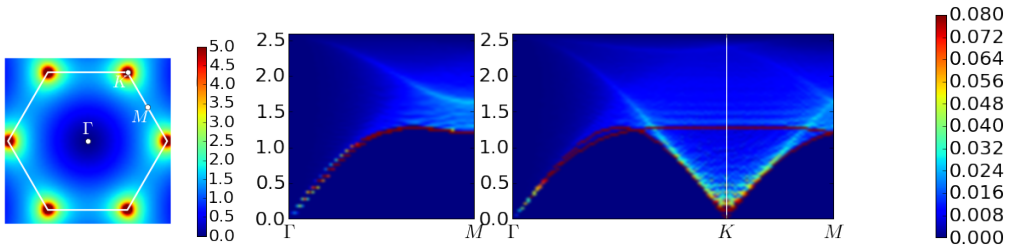
where $\mathbf{r}_i$ the position of the i'th site, $M_{\mathbf{q}}(\alpha,\lambda)$ is a 2×2 matrix, and

$$\epsilon_0(\alpha,\lambda) = N_s\left(\frac{3}{4} + 6\alpha^2 + 2\lambda\right), \qquad M_{\mathbf{q}}(\alpha,\lambda) = \begin{pmatrix} -\lambda & -\alpha f_{\mathbf{q}} \\ -\alpha f^*_{\mathbf{q}} & -\lambda \end{pmatrix}$$

$$f^{\triangle}_{\mathbf{q}} = 2i(\sin(\mathbf{q}\cdot\mathbf{e}_x) + \sin(\mathbf{q}\cdot\mathbf{e}_y) - \sin(\mathbf{q}\cdot(\mathbf{e}_y+\mathbf{e}_x))).$$

The Bogoliubov transformation seen previously defines new operators $\tilde{a}_{\uparrow\mathbf{q}}$ and $\tilde{a}_{\downarrow\mathbf{q}}$. What is the ground state in terms of the $\tilde{a}_{\mathbf{q}}$ operators ? Find the dispersion relation (the eigenenergies $\epsilon_{\uparrow k}$ and $\epsilon_{\downarrow k}$) as a function of λ and α. Give the ground state energy.

9. We give the (numerical) result of the self-consistency conditions: $\lambda = -1.282$ and $\alpha = 0.4936$. In this frame, we can calculate the dynamical structure factor $S(\mathbf{q},\omega)$ which is the space-time Fourier transform of spin-spin correlation functions $\langle \mathbf{S}(i,t)\cdot\mathbf{S}(i=0,t=0)\rangle$ and the static (equal time) structure factor $S(\mathbf{q}) = \int_0^\infty \frac{d\omega}{2\pi} S(\mathbf{q},\omega)$:



What is the static structure factor of the classical ground state (where the spin is a classical vector) ? Compare it to the SBMFT result.

10. The zero gap (apart from finite size effects)) indicates a Bose-Einstein condensation, or equivalently, a long-range spin order (Bragg peaks). If no gap had been obtained, what would have been the phase of the ground state ?

6.2 Representation of spins by Majorana fermions

Majorana Fermions

We represent spins $S = 1/2$ on sites j of a lattice by three Majorana fermions per site, $\hat{\rho}^x_j$, $\hat{\rho}^y_j$ and $\hat{\rho}^z_j$:

$$\hat{S}^\alpha_j = -\frac{i}{4}\epsilon^{\alpha\beta\gamma}\hat{\rho}^\beta_j\hat{\rho}^\gamma_j. \tag{66}$$

1. What are the anticommutators of the Majorana fermions ?
2. What is the dimension of the spin Hilbert space ? And of the space of Majorana fermions ?
3. Write a Heisenberg Hamiltonian $\hat{H} = \sum_{\langle j,l\rangle} J_{jl}\hat{\mathbf{S}}_j\cdot\hat{\mathbf{S}}_l$ in terms of these fermions.
4. We now perform a mean-field approximation with the constraint of a spin rotational invariant mean-field Hamiltonian $\hat{H}_{MF}$. What are the operators that are quadratic in Majorana fermions ? Write $\hat{H}_{MF}$.

5. What is the gauge symmetry ? What is the invariance gauge group ?

6. On a square lattice with first neighbor interactions, what are the Ansatze respecting the translational symmetries ? And on a triangular lattice ?

7. We have designed our theory to respect lattice translational and spin rotational symmetry. But are all the symmetries of the initial spin Hamiltonian respected ?

7 Topological superconductors

Chiral superconductors in two dimensions. In this problem, we calculate the Chern number to show that chiral pairing of electronic bands in two dimensions can lead to topological superconductivity, and we interpret the result using the winding of the pairing function on the Fermi surface. We will consider the following Hamiltonian in two dimensions:

$$\hat{H} = \sum_{\mathbf{k}\in \mathrm{BZ}} (\varepsilon_{\mathbf{k}} - \mu) c^\dagger_{\mathbf{k}} c_{\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{k}\in \mathrm{BZ}} \left(\Delta_{\mathbf{k}} c^\dagger_{\mathbf{k}} c^\dagger_{-\mathbf{k}} + \Delta^*_{\mathbf{k}} c_{-\mathbf{k}} c_{\mathbf{k}} \right), \tag{67}$$

where $c_{\mathbf{k}}$ and $c^\dagger_{\mathbf{k}}$ annihilate and create, respectively, an electron at momentum $\mathbf{k} = (k_x, k_y)$, while $\Delta_{\mathbf{k}}$ is the pairing function. We assume for simplicity that the kinetic energy $\varepsilon_{\mathbf{k}}$ is an even function of $\mathbf{k}$.

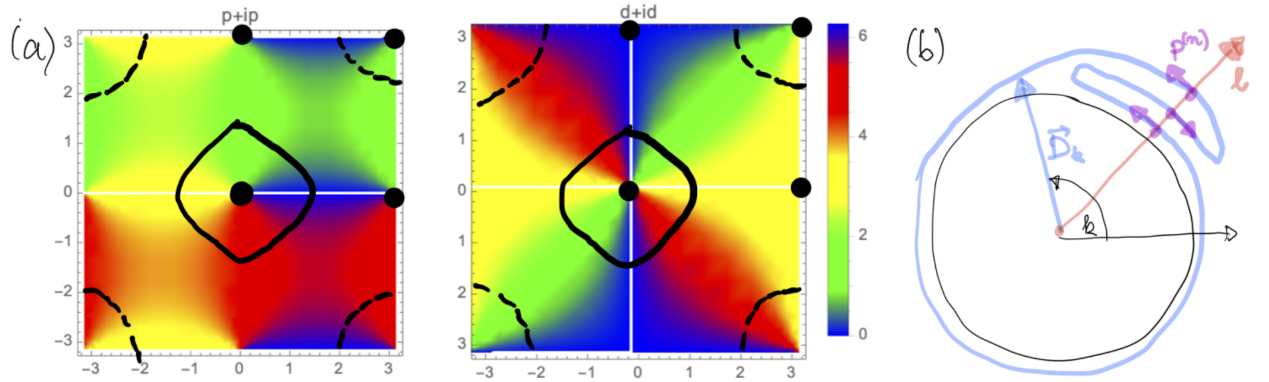


Figure 6: (a) Phase of the pairing function throughout the Brillouin Zone (BZ) for two cases of pairing. The Fermi surface of the normal state changes with chemical potential (examples are full vs. dashed black line). Note the vortices in the phase at high-symmetry momenta (black dots). (b) Illustration of the simple algebraic method to calculate how many times a surface (here, blue line) covers a hyper-sphere (here, a circle which represents the BZ in one dimension). One only needs to find intersection points with a ray (red) and properly count the orientations (direction of purple vectors). For a 2x2 Hamiltonian in two dimensions, the Chern number simply counts how many times a three-dimensional vector $\vec{D}(\vec{k})$ covers a sphere as $\vec{k}$ varies through the BZ.

7.1 Bogoliubov-de Gennes (BdG) bands for arbitrary pairing

1. Knowing the commutation relation for fermions $\{c_{\mathbf{k}}, c^\dagger_{\mathbf{k}'}\} = \delta_{\mathbf{k},\mathbf{k}'}$, and noticing that $\sum_{\mathbf{k}} (\varepsilon_{\mathbf{k}} - \mu) c^\dagger_{\mathbf{k}} c_{\mathbf{k}} = \sum_{\mathbf{k}} (\varepsilon_{-\mathbf{k}} - \mu) c^\dagger_{-\mathbf{k}} c_{-\mathbf{k}}$, show that the we can write the Hamiltonian of Eq. 67 :

$$\hat{H} = \frac{1}{2} \sum_{\mathbf{k}\in \mathrm{BZ}} \psi^\dagger_{\mathbf{k}} H_{\mathbf{k}} \psi_{\mathbf{k}} + \text{const} \tag{68}$$

with $\psi_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}} \\ c^\dagger_{-\mathbf{k}} \end{pmatrix}$ and the 2x2 Bogoliubov-de Gennes (BdG) Hamiltonian matrix $H_{\mathbf{k}} = \begin{pmatrix} \varepsilon_{\mathbf{k}} - \mu & \Delta_{\mathbf{k}} \\ \Delta^*_{\mathbf{k}} & -(\varepsilon_{-\mathbf{k}} - \mu) \end{pmatrix}$.

2. Rewrite the Hamiltonian matrix in the Pauli matrix basis, $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ and $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, so that 2x2 Bogoliubov-de Gennes (BdG) Hamiltonian matrix $H_{\mathbf{k}}$ reads $H_{\mathbf{k}} = \vec{D}_{\mathbf{k}} \cdot \vec{\sigma}$.

3. Deduce the band energies $E_{\mathbf{k},\pm}$ from the BdG Hamiltonian matrix $H_{\mathbf{k}}$. If you want to avoid the diagonalization, you can use that the eigenvalues of a matrix of the form $\vec{M} \cdot \vec{\sigma}$ are given by $E_\pm = \pm |\vec{M}|$.

7.2 Four chiral pairings

For the following we will consider a two dimensional square lattice with only nearest-neighbour hopping, giving the kinetic energy $\varepsilon_{\mathbf{k}} = -t(\cos(k_x) + \cos(k_y))$, with $t > 0$ a fixed constant (hopping parameter). We define the lattice constant as unit of length (a=1). We use the Brillouin zone : $k_x \in]-\pi, \pi]$, $k_y \in]-\pi, \pi]$. We then introduce four separate models by also fixing the pairing function $\Delta_{\mathbf{k}}$ as one of four different possibilities[1]:

$$\begin{aligned} \Delta_{\mathbf{k}}^{1\pm} &= \Delta_0(\sin(k_x) \pm i\sin(k_y)) \\ \Delta_{\mathbf{k}}^{2\pm} &= \Delta_0(\cos(k_x) - \cos(k_y)) \pm i\sin(k_x)\sin(k_y) \end{aligned} \tag{74}$$

which are called "$p \pm ip$" and "$d \pm id$'", respectively. We fix the prefactor $\Delta_0 = 1$, making the maximum pairing amplitude the unit of energy: μ and t are in units of Δ_0. In the following we consider μ as a variable parameter that defines a phase diagram.

4. For the first model "$p + ip$", with $\Delta_{\mathbf{k}} = \Delta_{\mathbf{k}}^{1\pm}$, find the conditions for μ and $\mathbf{k}$ so that the gap closes, meaning that there is a point in the band dispersion where $E_{\mathbf{k},\pm} = 0$.

5. Deduce from the previous question that in the phase diagram defined by changing value of $\frac{\mu}{t}$, for the "$p + ip$" there are 4 gapped phases separated by the gap-closing points.

6. For the second model "$d+id$", with $\Delta_{\mathbf{k}} = \Delta_{\mathbf{k}}^{2\pm}$, the conditions for μ and $\mathbf{k}$ so that the gap closes, meaning that there is a point in the band dispersion where $E_{\mathbf{k},\pm} = 0$.

7. Deduce from the previous question that there are 3 gapped phases for the "$d + id$" depending on the value of $\frac{\mu}{t}$.

7.3 Chern number

The BdG Hamiltonians $H_{\mathbf{k}}$ in a gapped phase are in class D due to lack of time-reversal symmetry. Being in two dimensions, they are characterized by the Chern number Ch. This Chern number for our special case of two (BdG) bands has a geometrical interpretation: as the momentum $\mathbf{k} = (k_x, k_y)$ covers the entire first Brillouin zone, the endpoint of the 3-dimensional vector $\vec{D}_{\mathbf{k}} = (D_x(\mathbf{k}), D_y(\mathbf{k}), D_z(\mathbf{k}))$ sweeps out a closed surface, so that Ch equals the number of times this surface wraps around the origin $(0,0,0)$. You will calculate Ch geometrically (without integrals) for each gapped phase of each chiral SC model. Indeed, we determine the wrapping of $\vec{D}_{\mathbf{k}}$ around the origin by counting how many times the surface $\vec{D}_{\mathbf{k}}$, $\mathbf{k} \in$ BZ intersects the radial line going from the origin out to infinity along the x-axis, $\vec{l}(a) \equiv (a, 0, 0)$, $a \in [0, +\infty)$. Each time there is an intersection, i.e., there is a solution $(a^{(n)}, \mathbf{k}_x^{(n)}, \mathbf{k}_y^{(n)})$, labeled by n, of the equation $\vec{D}_{\mathbf{k}} \equiv \vec{l}(a)$, we have a contribution to the wrapping number Ch, but each intersection contributes $p^{(n)} = +1\,(-1)$ if the line intersects the surface from its inside (outside) so as to guarantee that we do not overcount local folds in the surface as wrappings around the origin (see Fig. 6c). The value of $p^{(n)} = \pm 1$ depends simply on whether the local normal to the surface is parallel (antiparallel) to the line $\vec{l}(a^{(n)})$. Since we have $\vec{l}(a^{(n)}) = \vec{D}(\mathbf{k}^{(n)})$, the $p^{(n)} = \text{sgn}\left[\vec{D}_{\mathbf{k}} \cdot \left(\partial_{k_x}\vec{D}_{\mathbf{k}} \times \partial_{k_y}\vec{D}_{\mathbf{k}}\right)\right]$ evaluated at $\mathbf{k} = \mathbf{k}^{(n)}$.

To summarize what we just said, let us consider one gapped phase of one model. The geometrical formula for its Chern number is $Ch = \sum_n p^{(n)}$, where one defines $p^{(n)} = \text{sgn}\left[\vec{D}_{\mathbf{k}} \cdot \left(\partial_{k_x}\vec{D}_{\mathbf{k}} \times \partial_{k_y}\vec{D}_{\mathbf{k}}\right)\right]\Big|_{\mathbf{k}=\mathbf{k}^{(n)}}$, and the values of momenta $\mathbf{k}^{(n)}$, indexed by n, are all the solutions to the "intersection equation" $\vec{D}_{\mathbf{k}} \equiv \vec{l}(a)$, where one defines the ray $\vec{l}(a) \equiv (a, 0, 0)$ with $a \in [0, +\infty[$, while $\mathbf{k}$ is in the first BZ.

[1] A reinterpretation of $H_{\mathbf{k}}$ occurs at this moment. The derivation of the BdG matrix $H_{\mathbf{k}}$ in the previous section started from effectively spinless single band ($c_{\mathbf{k}}^\dagger$), and in such a case, due to anticommutation $\{c_{\mathbf{k}}^\dagger, c_{-\mathbf{k}}^\dagger\} = 0$ the pairing function $\Delta_{\mathbf{k}}$ can only be odd in $\mathbf{k}$ (or it vanishes), consistent with the "$p \pm ip$". However, the exact same form of the BdG matrix $H_{\mathbf{k}}$ is obtained starting from a spinfull problem with spin-singlet pairing, i.e., when the spinor $\psi_{\mathbf{k}} \equiv (c_{\mathbf{k}\uparrow}, c_{-\mathbf{k}\downarrow}^\dagger)^T$, and the pairing function then is purely even in $\mathbf{k}$ (consistent with the "$d \pm id$"). So starting from this point in the exercise, we are using the same form of 2x2 matrix $H_{\mathbf{k}}$ with either an even or odd pairing function, but we should be aware that these describe two different many-body Hamiltonians $\hat{H}$. The careful reader may notice that in the spinfull case the $H_{\mathbf{k}}$ should actually be a 4x4 matrix, since we have two spin orientations $(\uparrow, \downarrow)$ and we also have electrons and holes for them. Indeed, but due to the fact that $\hat{H}$ preserves the spin along z-axis (there is no spin-orbit coupling nor triplet pairing), its 4x4 $H_{\mathbf{k}}$ reduces to two separate 2x2 blocks. Actually, the Chern number you calculate for your 2x2 $H_{\mathbf{k}}$ will be the same as the Chern number obtained from the other 2x2 block, so in case of the "$d \pm id$" the total Chern number of the system is double the one you find.

7.3.1 "$p+ip$" model

8. Calculate the term $\vec{D}_{\mathbf{k}} \cdot \left(\partial_{k_x}\vec{D}_{\mathbf{k}} \times \partial_{k_y}\vec{D}_{\mathbf{k}}\right)$ for the "$p+ip$" case with $\Delta_{\mathbf{k}}^{1\pm}$ (see Eq.74). Simplify this expression knowing that $\vec{D}_{\mathbf{k}^{(n)}}$ has only an $x-$component by definition ($\vec{D}_{\mathbf{k}=\mathbf{k}^{(n)}} \equiv \vec{l}(a)$).

9. For each gapped phase obtained for the "$p+ip$" (corresponding to different range of μ), find that only zero or one value of $\mathbf{k}$ satisfy the condition $\vec{D}_{\mathbf{k}=\mathbf{k}^{(n)}} \equiv \vec{l}(a)$. To help you, we recall that for $-2t < \mu < 0$ the Fermi surface is a pocket around the Γ point, while for $0 < \mu < 2t$ it is a pocket around the M point (at (π, π)), see illustration in Fig.6.

10. Deduce the Chern number for all gapped phases in this model.

7.3.2 "$d+id$" model

9. Calculate the term $\vec{D}_{\mathbf{k}} \cdot \left(\partial_{k_x}\vec{D}_{\mathbf{k}} \times \partial_{k_y}\vec{D}_{\mathbf{k}}\right)$ for the "$d+id$" case with $\Delta_{\mathbf{k}}^{2\pm}$ (see Eq.74). Simplify this expression knowing that $\vec{D}_{\mathbf{k}^{(n)}}$ has only an $x-$component by definition ($\vec{D}_{\mathbf{k}=\mathbf{k}^{(n)}} \equiv \vec{l}(a)$)

10. For each gapped phase obtained for the "$d+id$" (corresponding to different ranges of μ), find that only zero or two values of $\mathbf{k}$ satisfy the condition $\vec{D}_{\mathbf{k}=\mathbf{k}^{(n)}} \equiv \vec{l}(a)$. To help you, we recall that for $-2t < \mu < 0$ the Fermi surface is a pocket around the Γ point, while for $0 < \mu < 2t$ it is a pocket around the M point (at (π, π)), see illustration in Fig.6. .

11. Deduce the Chern number for all gapped phases in this model.

7.4 Winding vs. the Chern number

Consider the complex phase, $\varphi_{\mathbf{k}}$, of the pairing function, $\exp(i\varphi_{\mathbf{k}}) = \frac{\Delta_{\mathbf{k}}}{|\Delta_{\mathbf{k}}|}$. It's winding on the Fermi surface is

$$W = \frac{1}{L_{FS}} \oint_{FS} \mathrm{d}\vec{k} \cdot \nabla_{\vec{k}} \varphi(\vec{k}), \tag{79}$$

with L_{FS} the length of the Fermi surface contour of the metal. The Fermi surface contour varies continuously with μ, even as μ changes so much as to pass between different gapped phases. We can pick any value of μ inside a given gapped phase to calculate the W of that gapped phase, since W is topological. However, there is no value of μ that can simplify the Fermi surface shape and the integral in any of the gapped phases. This makes the calculation of W complicated. To progress, we can use the topological nature of W to deform the FS slightly, but we mustn't leave the gapped phase, which is ensured if the Fermi surface remains to be a pocket around the high-symmetry point where it was, and we do not deform it so much to enclose any other high symmetry points. More formally, we could use Stokes theorem to prove that the contour integral does not depend on the shape of the contour as long as the contour doesn't cross a singularity (a vortex) in the phase (such vortices occur exactly at the high-symmetry points, see Fig. 6). Hence, we can deform the FS pocket into a circle and the expression can be simplified. With a circle, we have $W = \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}\theta \partial_\theta \varphi(\mathbf{k}(\theta))$, where θ is the polar angle (in k space) around the high-symmetry point on which the FS is centered, i.e., $\mathbf{k} = \mathbf{\Gamma} + \mathbf{k_F}(\mathbf{cos}\theta, \mathbf{sin}\theta)$ for $-2t < \mu < 0$ or $\mathbf{k} = \mathbf{M} + \mathbf{k_F}(\mathbf{cos}\theta, \mathbf{sin}\theta)$ for $0 < \mu < 2t$.

12. Calculate W for each gapped phase of the "$p+ip$" model. To do so, consider k_F small enough to expand the expressions to lowest non-zero order in k_F. Then confirm that $Ch = W$ if the FS contour around the Γ pocket is taken counter-clockwise.

13. Calculate W for each gapped phase of the "$d+id$" model, with the same method.