ICFP M2 - Topological theory in condensed matter

TD 1 The Su-Schrieffer-Heeger (SSH) model

Christophe Mora & Leonardo Mazza

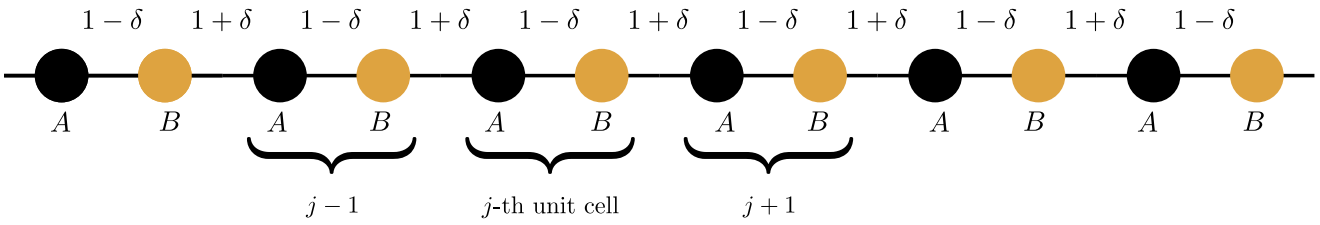

Figure 1 – The SSH chain.

Consider a simple chain with two types of atoms A and B, and hopping amplitudes between neighboring sites as shown in Fig. 1 (where $|\delta| \leq 1$). The tight binding Hamiltonian reads

$$H = \sum_j \left[(1-\delta)\, c^\dagger_{A,j} c_{B,j} + (1+\delta)\, c^\dagger_{B,j} c_{A,j+1} + \text{h.c.} \right] \tag{1}$$

Here j denotes the unit cell index and we consider N unit cells. For most of the numerical calculations, you can consider $N = 40$. We define the Fourier transform as

$$\tilde{c}_{\alpha,k} \quad = \quad \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} c_{\alpha,j}\, e^{ikj} \tag{2}$$

labeling the sites with the unit cell coordinate j from 0 to $N-1$ and the atom (or orbital) index $\alpha = A$ or B.

1) First we consider periodic boundary conditions. Using Bloch theorem, find the analytical expression for the energy spectrum and rewrite the second quantized Hamiltonian as

$$H = \sum_k \varepsilon^\pm_k\, f^\dagger_{\pm,k} f_{\pm,k} \tag{3}$$

with the two band dispersions $\varepsilon^\pm_k$ and the corresponding fermionic annihilation operators $f_{\pm,k}$.

2) How is this spectrum changed under $-\delta \leftrightarrow \delta$? Plot the spectrum for $\delta = +1$, $\delta = +0.2$ and $\delta = 0$. Comment the two cases $\delta = +1$ and $\delta = 0$.

3) Write a code to compute the energy spectrum directly from the tight binding, i.e., without using the Bloch theorem. As a sanity check, verify that you obtained the same results than the analytical result.

4) We now consider open boundary conditions. Write a code to compute the energy spectrum.

5) Plot the spectrum for various values of δ, both negative and positive. What do you observe ?

6) We want to see the fate of the two in-gap states when increasing the system size (i.e. N) or when tuning δ from 1 to a value close to 0. Using the code written in 4), compute and plot the energy difference between the two in-gap states as a function of system size. Repeat the procedure for several values of δ. Plot also the electronic density distributions of the in-gap states.

7) In the fully dimerized case, i.e. when $\delta = 1$, find the analytical expression for the energy and eigenstates of these two in-gap states.

8) Consider a semi-infinite chain and $\delta > 0$. Find analytically a zero-energy eigenstate as a geometric series. Where is it located ? Derive its localization length.

9) Consider the sublattice polarization operator $P = \sigma_3 \otimes \mathbb{1}_N$. Show that $PH_1P = -H_1$ (where H_1 is the one-particle first quantized Hamiltonian) - it is also called the chiral symmetry. Deduce from this identity that (i) eigenstates go by pairs of opposite values $\pm\varepsilon$, (ii) a single zero-energy state remains robustly tied to zero as long as this symmetry is preserved.

10) In order to gain some intuition on the topological robustness, we will see how the system reacts to perturbations. For that purpose, we modify each hopping term within the unit cell from $1-\delta$ to $1-\delta+r_1$ and between unit cells from $1+\delta$ to $1+\delta+r_2$. Here r_1 and r_2 are random numbers distributed uniformly between $-R$ and R, R being the disorder strength. Note that r_1 or r_2 are in principle different for each bond. Look at the effect on the spectrum for various values of $\delta > 0$ and R. Discuss the fate of the edge states. Take the analytical case of a semi-infinite chain and show that an exactly zero-energy state survives disorder.