The Su-Schrieffer-Heeger model

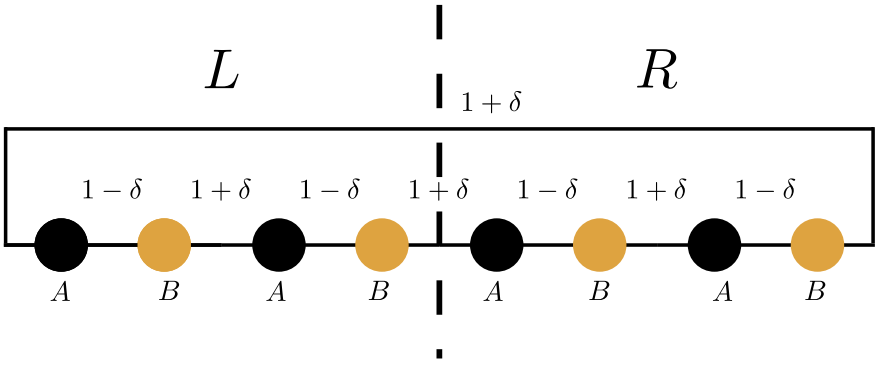

Figure 1: The SSH chain.

Consider a simple chain with two types of atoms A and B, and hoppings amplitude 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

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

labelling 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.

2) How is this spectrum changed under the transformation $-\delta \leftrightarrow \delta$? Plot the spectrum for the various values (like $\delta = +1$, $\delta = +0.2$ 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. Convince yourself that it would be hard to solve this case analytically. 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 states in the gap of the energy spectrum when we increase the system size (i.e. N) or when we tune δ from 1 to a value close to 0. Using the code written in 4), compute and plot the difference of the energy between these two states as a function of the system size. Repeat the procedure for several values of δ.

7) Comment the previous results. If these two states have any topological feature, is this expected ? Could you imagine that these two states have an energy different from zero?

8) In the fully dimerized case, i.e. when $\delta = 1$, find the analytical expression for the energy and eigenstates of these two bulk states. Show that we can always choose linear combinations where the density is zero on the leftmost A site for one state and zero on the rightmost B site for the other state. For each of these two specific linear combinations, compute the local density (i.e. the expectation value of the occupation number $\langle c^\dagger_{\alpha,j} c_{\alpha,j} \rangle$ with respect to each state).

9) Away from $\delta = 1$, numerically consider the two states in the energy gap. They are not strictly degenerate in energy in finite size. Plot the density for each of the eigenstates. Repeat the density calculations considering the linear combinations discussed in 8) (Can you justify to consider these combinations instead of the individual eigenstates?). Comment the density of these states. Why can we call them as "edge states" ?

10) To give some intuition about the topological robustness, we will see how the system react to perturbations. For that purpose, we modify each hopping term within the unit cell from $1-\delta$ to $1-\delta+r_1$ and within 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.

11) We now consider another type of perturbations by including next nearest neighbor hopping between A sites, i.e.

$$\begin{aligned} H &= \sum_j \Big[(1-\delta)\, c^\dagger_{A,j} c_{B,j} + (1+\delta)\, c^\dagger_{B,j} c_{A,j+1} \\ &\qquad + t c^\dagger_{A,j} c_{A,j+1} + \text{h.c.} \Big] \end{aligned} \tag{3}$$

where t is the next nearest neighbor amplitude. Study how the energy splitting of the edge state modes and more precisely its size dependence, is affected by this perturbation. (hint: try with e.g. $\delta = 0.5$ and $t = 0.01$). Compare to the typical disorder strength you had to apply in question 10

12) How does the situation change when adding a similar next nearest neighbor hopping between B sites (with the same amplitude t)?

13) Explain the numerical observations of questions 10, 11 and 12 using symmetry arguments.