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Exercise class 5: The SSH Model

1 Tight-binding approximation in a nutshell

1. We consider a Hamiltonian of an electron in a infinite lattice. Justify that one can look for eigenfunctions of the generic form: $\psi_{n\boldsymbol{k}} = e^{i\boldsymbol{k}\cdot\boldsymbol{r}} u_{n\boldsymbol{k}}$ where $u_{n\boldsymbol{k}}$ is a periodic function in $\boldsymbol{r}$.

2. In the case of a crystal with one atom per unit cell, in the tight-binding approximation, the Hamiltonian can be written:

$$H = \sum_{\boldsymbol{R}} \varepsilon \left|\boldsymbol{R}\right\rangle \left\langle\boldsymbol{R}\right| + \sum_{\boldsymbol{R},\boldsymbol{R}'} t(\boldsymbol{R}-\boldsymbol{R}') \left|\boldsymbol{R}'\right\rangle \left\langle\boldsymbol{R}\right| . \tag{1}$$

where ε is a constant, and $t(\boldsymbol{r})$ is a function that only depends on $\boldsymbol{r}|$. Explain the meaning of this expression. Generalize it for a crystal with two atoms per unit cell.

3. In the case of one atom per unit cell, show that the Bloch state

$$\left|\boldsymbol{k}\right\rangle = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R}} \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{R}} \left|\boldsymbol{R}\right\rangle . \tag{2}$$

is an eigenstate of the Hamiltonian, and find its eigenvalue. Write the Hamiltonian in a diagonilized way.

2 The SSH model

A polyacetylene molecule is depicted on Fig. 1. Polyacetylene is a polymer with more than 10^4 acetylen units, such that a tight-binding approach is possible. Because all carbon atoms do not feel the same environment, one should differentiate two types of atoms: A and B and two jumping amplitudes t and t' (see Fig. 1). Cells are indexed by an integer i, and the orbital of an A (B) atom will be denoted $|i, A\rangle$ ($|i, B\rangle$)

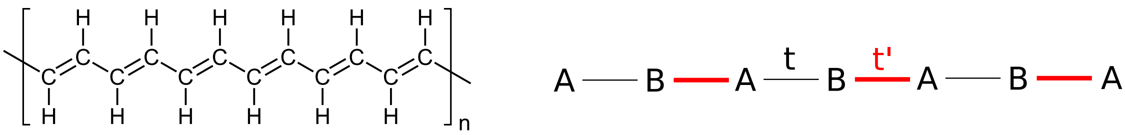

Figure 1: Left: Sketch of the polyacetylene molecule. Right: Tight-binding model of with two different jumping amplitudes t and t'. The distance between A and B atoms is denoted a.

1. Write the tight-binding Hamiltonian of the problem, assuming a vanishing on-site energy of carbon atoms.

2. To diagonalize the Hamiltonian, we go to the Bloch basis:

$$\left|\psi_k\right\rangle = u_k^A \left|k, A\right\rangle + u_k^B \left|k, B\right\rangle \qquad \text{where} \qquad \left|k, A\right\rangle = \frac{1}{\sqrt{N}} \sum_m \mathrm{e}^{imak} \left|m, A\right\rangle \tag{3}$$

Show that the Hamiltonian can be written

$$H = \sum_k \begin{pmatrix} |k, A\rangle & |k, B\rangle \end{pmatrix} \quad H_k \quad \begin{pmatrix} \langle k, A| \\ \langle k, B| \end{pmatrix} \tag{4}$$

and give the expression of the 2×2 matrix H_k.

3. This matrix can be factorized $H_k/t = \boldsymbol{h}_k \cdot \boldsymbol{\sigma}$, with $\boldsymbol{\sigma}$ the vector of the Pauli matrices. Write the 3 components h_x, h_y and h_z of this vector.

4. Find the eigenvalues $\pm E_k$ of this Hamiltonian. The following identity could be used: $(\boldsymbol{a}\cdot\boldsymbol{\sigma})(\boldsymbol{b}\cdot\boldsymbol{\sigma}) = \boldsymbol{a}\cdot\boldsymbol{b}\mathbb{1} + i(\boldsymbol{a}\times\boldsymbol{b})\cdot\boldsymbol{\sigma}$. Plot them in function of k. What is the value of the gap?

5. Let us defined the phase ϕ_k as $h_x + ih_y = |h|e^{i\phi_k}$. Give a condition for ϕ_k to be well-defined. If this condition is verified, show that the following vectors are eigenvectors of H_k:

$$|u_{k,\pm}\rangle = \begin{pmatrix} u_k^A \\ \pm u_k^B \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm\, \mathrm{e}^{i\phi_k} \end{pmatrix} \tag{5}$$

6. Because of the periodicity of the crystal, a wavevector k should give the same physical result as $k + G$ where G in a vector in the reciprocal lattice. Let γ be a path from k to $k + G$. Represent the trajectory of $h_x + ih_y$ in the plane (h_x, h_y) while k describes the path γ. Isolate two different situations in function of t'/t.

7. Because the path γ is actually a closed loop in the Brillouin zone, one can calculate the Berry phase associated to this loop, the external parameter being the wavevector k. This phase is called the *Zak phase*:

$$\mathcal{Z} = \int_k^{k+G} \mathcal{A}_k \,\mathrm{d}k = i \oint_{-\pi/a}^{\pi/a} \langle u_k | \boldsymbol{\partial}_k u_k \rangle \,\mathrm{d}k \tag{6}$$

Express $\mathcal{Z}_+$ the Zak phase for the eigenvector $u_{k,+}$ in function of φ_k. Deduce the value of the Zak phase depending on the parameter t'/t, justify that this quantity is a topological invariant. It can not be changed unless something dramatically changes in the band structure: the gap closes. Two systems with different Zak phases are in two different states of matter. Going from one to another requires going through a topological phase transition.[1]

8. In the SSH model, the H_k matrix is restricted to be a linear combination of σ_x and σ_y. If one includes a term $\delta\mathbb{1}$ does the above result changes? or a $\varepsilon\sigma_z$?[2]

References

[1] Cooper et al., Topological Bands for Ultracold Atoms (2018).

[1] This kind of phase transitions that do not involve the temperature were not anticipated by Landau and its classification. They are also called *quantum phase transitions*.

[2] This particularity of the SSH model is due to the presence of a symmetry in the system, the *chiral symmetry*. The topology of the system is protected by the presence of this symmetry. Reversely, breaking the chiral symmetry destroy the topological phases.