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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 $|i, A\rangle$ ($|i, B\rangle$)

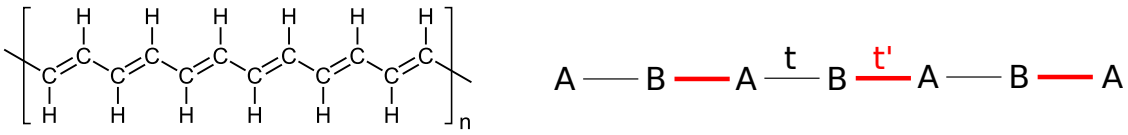


Figure 1: Left: Sketch of the polyacetylene molecule. Right: Tight-binding model of with two different jumping amplitudes t and t'. The distance between A and B atoms is denoted a.

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

Correction.

$$H = \sum_{m} \left(t \left|m, A\right\rangle \left\langle m, B\right| + t' \left|m+1, A\right\rangle \left\langle m, B\right| + \text{h.c.}\right)$$

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

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

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.

Correction.
We can inverse the Fourier transform:

$$|m,A\rangle = \frac{1}{\sqrt{N}}\sum_m \mathrm{e}^{-imak}\,|k,A\rangle$$

Thus introducing this expression in the Hamiltonian:

$$\begin{aligned} H &= \frac{t}{N}\sum_{k,k'}\underbrace{\sum_m \mathrm{e}^{-ima(k-k')}}_{=N\delta_{k,k'}}|k,A\rangle\langle k',B| + \frac{t'}{N}\sum_{k,k'}\underbrace{\sum_m \mathrm{e}^{-ia(m+1)k'}\,\mathrm{e}^{imak}}_{=N\delta_{k,k'}\,\mathrm{e}^{-iak'}}|k,A\rangle\langle k',B| \\ &= \sum_k (t + t'\,\mathrm{e}^{-iak})\,|k,A\rangle\langle k,B| + \text{h.c.} \\ &= \sum_k \begin{pmatrix} |k,A\rangle & |k,B\rangle \end{pmatrix} \begin{pmatrix} 0 & t+t'\,\mathrm{e}^{-iak} \\ t+t'\,\mathrm{e}^{iak} & 0 \end{pmatrix} \begin{pmatrix} \langle k,A| \\ \langle k,B| \end{pmatrix} \end{aligned}$$

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.

Correction.

$$H_k = \begin{pmatrix} 0 & t+t'\,\mathrm{e}^{-iak} \\ t+t'\,\mathrm{e}^{iak} & 0 \end{pmatrix} = (t+t'\cos(ka))\sigma_x + t'\sin(ka)\sigma_y = t\boldsymbol{h}_k\cdot\boldsymbol{\sigma}$$

with

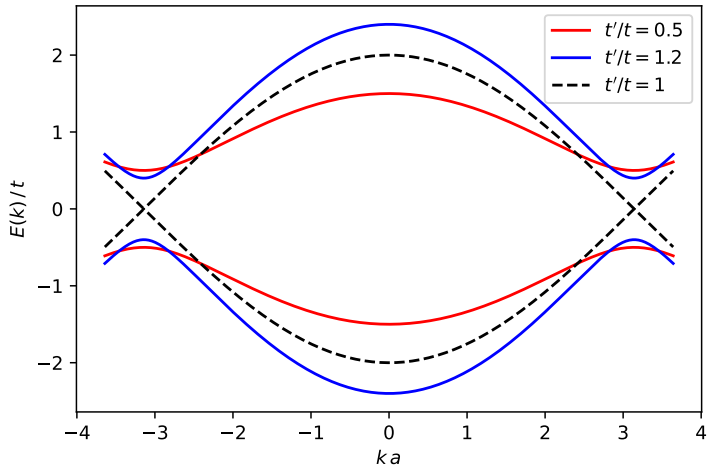
$$\boldsymbol{h}_k = \begin{pmatrix} 1+\frac{t'}{t}\cos(ka) \\ \frac{t'}{t}\sin(ka) \\ 0 \end{pmatrix}$$

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?

Correction.
A σ matrix is the representation of a symmetry. TO find the eigenvalues, one can calculate the square of H_k: $H_k^2 = t^2||\boldsymbol{h}_k||^2\mathbb{1}$. Thus, the eigenvalues are

$$E_k = \pm t f\left(\frac{t'}{t}\right) \qquad \text{with} \qquad f_k(x) = \sqrt{1 + x^2 + 2x\cos(ka)}$$

The minimal distance between the two bands (the gap Δ) is obtained for $k = \pm\pi/a$, such that $f_k(x) = |1 - x|$.



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:

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

Correction.
h_x and h_x are real and imaginary parts of the complex $|h|\,\mathrm{e}^{i\phi_k}$, thus ϕ_k is defined but when h_x and h_y vanish *at the same time*. If this situation is possible, that means that the gap Δ vanishes, or equivalently $t' = t$.
If $t' \neq t$, then

$$H_k = t \begin{pmatrix} 0 & |h|\,\mathrm{e}^{-i\phi_k} \\ |h|\,\mathrm{e}^{i\phi_k} & 0 \end{pmatrix}$$

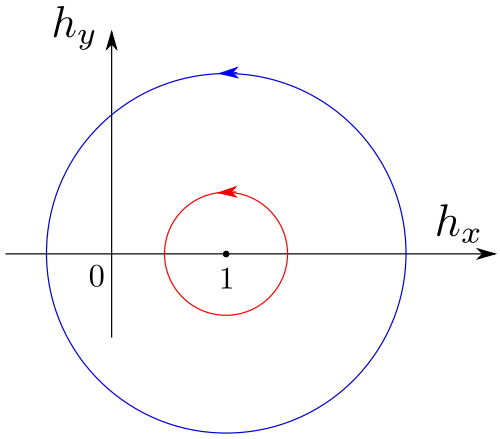
Looking for an eigenvector of H_k:

$$H_k \begin{pmatrix} u_k^A \\ u_k^B \end{pmatrix} = t|h| \begin{pmatrix} \mathrm{e}^{-i\phi_k}\, u_k^B \\ \mathrm{e}^{i\phi_k}\, u_k^A \end{pmatrix} = \pm E_k \begin{pmatrix} u_k^A \\ u_k^B \end{pmatrix}$$

If one chooses $u_k^A = 1/\sqrt{2}$, then we get $u_k^B = \frac{|h|}{\pm E_k}\,\mathrm{e}^{i\phi_k}\, u_k^A = \pm\,\mathrm{e}^{i\phi_k}/\sqrt{2}$. Finally, $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm\,\mathrm{e}^{i\phi_k} \end{pmatrix}$ is an eigenvector of H_k.

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.

Correction.



There are two cases, depending on t'/t :

- If $\frac{t'}{t} < 1$, then the circle does not wind around the origin, the phase ϕ_k comes back to its initial value.
- If $\frac{t'}{t} > 1$, then the origin is inside the loop γ, and going around this point, the phase accumulates a factor 2π.

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]

Correction.

$$\begin{aligned}
\mathcal{Z}_+ &= i \oint_{-\pi/a}^{\pi/a} \langle u_{k,+} | \boldsymbol{\partial}_k u_{k,+} \rangle \, \mathrm{d}k = \frac{i}{2} \oint_{-\pi/a}^{\pi/a} \begin{pmatrix} 1 & \mathrm{e}^{-i\phi_k} \end{pmatrix} \begin{pmatrix} 0 \\ i\partial_k \phi \, \mathrm{e}^{i\phi_k} \end{pmatrix} \mathrm{d}k \\
&= -\frac{1}{2} \underbrace{\oint_{-\pi/a}^{\pi/a} \partial_k \phi \mathrm{d}k}_{2\pi\times \text{ winding number around } 0} \\
&= \begin{cases} 0 & \text{if } \frac{t'}{t} < 1 \\ \pi & \text{if } \frac{t'}{t} > 1 \end{cases}
\end{aligned}$$

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]

[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.

Correction.
$\delta\mathbb{1}$ only shifts the bands in energy. It does not carry any topological information. The σ_z term is really different. If it does not vanish, it means that the winding number around the origin is no more well-defined. In fact, to go from 0 to π in the Bloch sphere, one can use the z component, which was forbidden is the vector only has two non-zero components h_x and h_y.

References

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