Institute of Theoretical Physics
University of Cologne
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Based on problem sets by Peter Bröcker

Solid State Theory

Exercise sheet 7

This exercise sheet will be discussed on Friday, February 1st 2019.
You should hand in your solution of the exercise marked with (★)
in the mail box or email by 16:00 on Thursday January 31st 2019.

Exercise sheets online at `www.thp.uni-koeln.de/trebst/Lectures/2018-SolidState.shtml`

1 The Haldane model on the Honeycomb lattice (★)

Our goal in this exercise is to extend the tight binding model on the honeycomb lattice to one that includes complex next-nearest neighbor hoppings and to study how this affects the physics. Previously, we were only interested in finding the eigenvalues, i.e. the eigenenergies for the models we studied. Now, we will see that such an approach is insufficient to fully characterize the physical properties and that we have to work with the eigenvectors as well to extract all of the necessary information. This model, published in 1988, is very special in that it was the first model to realize a topological insulator without Landau levels. It was conceived by one of 2016's Nobel laureates, F.D.M. Haldane.
On the previous exercise sheet, we saw that the tight binding model on the honeycomb features Dirac fermions with a linear dispersion relation at special points in the Brillouin zone. The Hamiltonian we considered was simply

$$H_{\mathrm{NN}} = -t \sum_i \left(a_i^\dagger b_{i+\delta_1} + a_i^\dagger b_{i+\delta_2} + a_i^\dagger b_{i+\delta_3} \right) + \mathrm{h.c.}\,, \tag{1}$$

where he have labelled ladder operators on the two respective sublattices with a and b and their connecting vectors

$$\begin{aligned} \delta_1 &= a\ (0,1) \\ \delta_2 &= a\left(-\frac{\sqrt{3}}{2}, \frac{1}{2}\right) \\ \delta_3 &= a\left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right). \end{aligned}$$

1. Redo the tight-binding calculation and find an analytical expression for the dispersion relations of the two bands

In this exercise, we now allow the electrons to also hop to next nearest neighbors with a *complex* amplitude by multiplying the hopping strength with a phase $e^{\pm \mathrm{i}\phi}$. The extended Hamiltonian takes the form

$$H = H_{\mathrm{NN}} + H_{\mathrm{NNN}} \tag{2}$$

$$H_{\mathrm{NNN}} = -t' e^{\mathrm{i}\phi} \sum_i \left(a_i^\dagger a_{i+v_1} + a_{i+v_1}^\dagger a_{i-v_3} + a_{i-v_3}^\dagger a_i \right) \tag{3}$$

$$- t' e^{-\mathrm{i}\phi} \sum_i \left(b_i^\dagger b_{i+v_1} + b_{i+v_1}^\dagger b_{i-v_3} + b_{i-v_3}^\dagger b_i \right) + \mathrm{h.c.}\,. \tag{4}$$

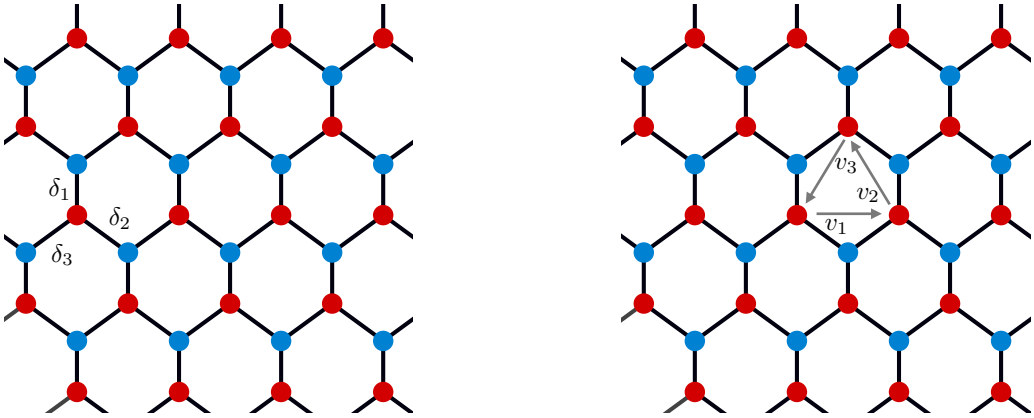

Figure 1: The honeycomb lattice with the nearest (left) and the next-nearest neighbor hopping vectors (right).

where the vectors that are used are:

$$v_1 = a\left(\sqrt{3}, 0\right)$$
$$v_2 = a\left(-\frac{\sqrt{3}}{2}, \frac{3}{2}\right)$$
$$v_3 = a\left(\frac{\sqrt{3}}{2}, -\frac{3}{2}\right) .$$

Physically, adding this phase corresponds to putting the sample into a magnetic field, thus breaking time reversal symmetry.

2. Incorporate the next nearest neighbor hopping Hamiltonian in the tight binding calculation and recalculate the dispersion relations.

3. What happens to the dispersion relation at the Dirac points as you vary ϕ from 0 to π?

4. To make further investigations easier, take the Hamiltonian matrix

$$H = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \tag{5}$$

and rewrite it in the form

$$H = \mathbf{H} \cdot \sigma \tag{6}$$

where σ is the vector of Pauli matrices and $\mathbf{H} = (H_x, H_y, H_z)$.

Having achieved this, the eigenvalues actually take the very easy form

$$\epsilon_{\pm}(\boldsymbol{k}) = \pm\sqrt{H_x^2(\boldsymbol{k}) + H_y^2(\boldsymbol{k}) + H_z^2(\boldsymbol{k})} \tag{7}$$

and one possible choice of the Bloch function of the lowest band is given as

$$u(k) = \begin{pmatrix} H_z - |\mathbf{H}| \\ H_x + \mathrm{i}H_y \end{pmatrix} . \tag{8}$$

One has to emphasize that while this is an eigenvector and represents the Bloch function in almost all of the Brillouin zone, it does not do so at one of the Dirac points, specifically K, where this function is *singular* and therefore not a valid choice for a wavefunction. One may however,

exploit the gauge freedom and multiply an arbitrary phase to the wavefunction. The singularity may be lifted by choosing this phase to be

$$e^{\mathrm{i}\varphi} = \frac{H_z + |\mathbf{H}|}{H_x + \mathrm{i}H_y} \cdot \left| \frac{H_z + |\mathbf{H}|}{H_x + \mathrm{i}H_y} \right|^{-1} . \tag{9}$$

This changes the wavefunction to

$$u'(k) = u(k)e^{\mathrm{i}\varphi} = \begin{pmatrix} -H_x + \mathrm{i}H_y \\ H_z + |\mathbf{H}| \end{pmatrix} , \tag{10}$$

which no longer has a singularity at K but instead at K'.
Now let us discuss what we can do with these eigenvectors and in particular what this has to do with topology. We define the *Berry connection* as

$$\mathbf{A} = -\mathrm{i} \langle u(\boldsymbol{k}) | \nabla | u(\boldsymbol{k}) \rangle \tag{11}$$

which tells us how the phase angle between two states that are infinitesimally close in the Brillouin zone. Now imagine that we follow our state along a closed loop and sum up the contribution of this phase difference. The resulting phase is called the *Berry phase*.

5. Show that the Berry connection transforms as

$$\mathbf{A}' = \mathbf{A} + \nabla\varphi(\boldsymbol{k}) , \tag{12}$$

when the Bloch factor transforms as

$$u'(\boldsymbol{k}) = e^{\mathrm{i}\varphi(\boldsymbol{k})} u(\boldsymbol{k}) . \tag{13}$$

In a final step, we define the *Berry curvature* as $\Omega = \nabla \times \mathbf{A}$. Note the similarity to the magnetic field and vector potential in electrodynamics! Let us now calculate the flux through the Brillouin zone, which is given as

$$\oiint_{\mathrm{BZ}} \Omega \, \mathrm{d}\boldsymbol{k} \tag{14}$$

Now proceed as follows to evaluate this integral:

6. Because the wavefunction has to be split in two parts, we have to do the same for the Berry connection. Let us call the surface parts S_1 and S_2, respectively.

7. Use Stoke's theorem to replace the surface integrals by line integrals over the Berry connection.

8. Exploiting the periodicity of the Brillouin zone, replace the boundary ∂S_2 by the boundary ∂S_1 and adjust the prefactor accordingly.

9. Now use the fact that it can be shown that the resulting integral is equal to $2\pi\, n$, where n is an integer number, also called *Chern number* in this context. Proving this result is beyond the scope of this exercise, but it holds generally for a compact manifold without boundary.

10. To evaluate the resulting expression, expand H_x, H_y and H_z around the Dirac point K and calculate the phase from (9) needed to avoid the singularity in the wave function.

11. Now set S_1 to be a circle around K with infinitesimal radius k and use the above results to conclude that the Chern number is non-vanishing.

Let us recapitulate what we have seen so far: By adding next-nearest neighbor interactions, we open a gap between the two bands of the honeycomb tight binding model. The Bloch functions that we obtain from the diagonalization procedure are not well defined on the entire Brillouin zone, but we need to introduce a phase shift to avoid a singularity at either one of the Dirac points. We then proceeded to study how the quantum phase of a state changes as we track the state around a closed loop in the Brillouin zone and found that it leads us to the concepts of Berry phases, Berry connections, Berry curvatures and Chern numbers. In particular, we find a non-trivial Chern number in this model.
In a final last part, let us study what happens if we open a gap in the energy spectrum by means of another mechanism. We replace the next-nearest neighbor hopping term H_{NNN} by a chemical potential that alternates on sublattices A and B:

$$H_{\mathrm{pot}} = \mu \sum_i \left(a_i^\dagger a_i - b_i^\dagger b_i \right) \tag{15}$$

12. Recalculate the energy spectrum and the wavefunctions. *Hint:* If you bring the Hamiltonian to the correct form, you will be able to reuse many of the previous calculations!

13. What is the Chern number in this case?