

Computational Many-Body Physics

Exercise Sheet 5

Summer Term 2021

Due date: Monday, **12th July** 2021, 10 am

Website: thp.uni-koeln.de/trebst/Lectures/2021-CompManyBody.shtml

On this week's exercise sheet we introduce the concept of **band structure calculations** and demonstrate its central role in modern condensed matter physics, e.g. in identifying topological band structures. The purpose of the exercises is to give you a practical angle on these calculations. If you have previously implemented a lattice library, you will be able to explore a vast family of example systems.

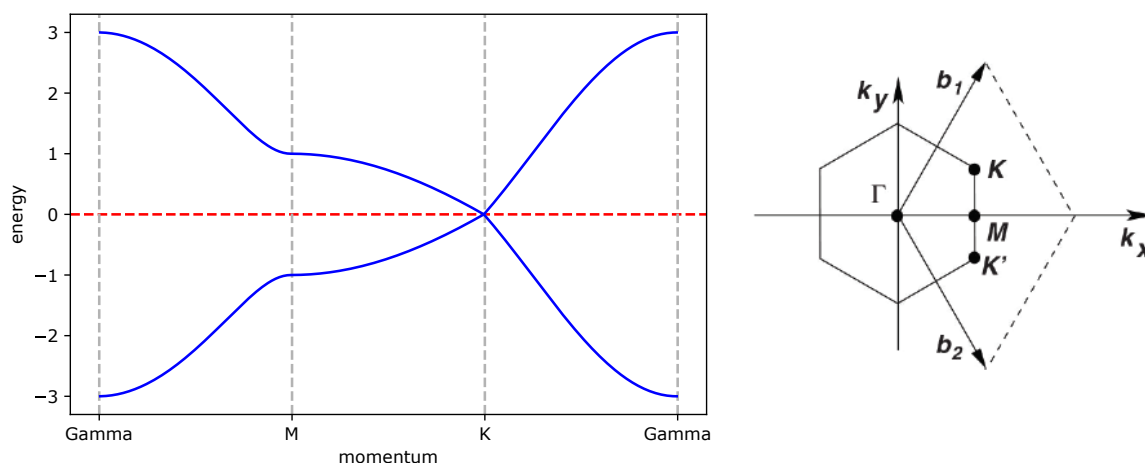


Figure 1: **Band structure of the 2D honeycomb lattice** hopping problem with the Fermi energy of half filling shown as a red dashed line (left) and the reciprocal honeycomb lattice with path in momentum space (right).

Exercise 16: Band structure calculations

Let's start with the calculation of band structures for regular solids, i.e. the spectrum of non-interacting electrons hopping on elementary lattice geometries. To do so, we quickly recap the basic idea of these calculations: We explore **tight-binding models**, which given in second quantized form, look like

$$\mathcal{H} = \sum_{\langle ij \rangle} t_{ij} c_i^\dagger c_j, \quad (1)$$

where i and j denote site indices of an underlying lattice and $\langle ij \rangle$ denotes all nearest neighbor pairs. The operators c_i^\dagger and c_j describe the creation and annihilation of fermions on sites of the lattice, respectively. Such a tight-binding model is an appropriate description of electrons in a solid whenever the electron-electron correlations can be neglected.

To solve the tight-binding model for a given lattice structure, one in general performs a two-step calculation. First, the model is rewritten in terms of position space

$$c_j \rightarrow c_j(\vec{r}) \quad (2)$$

(where j only labels an index inside the unitcell now) and then a **Fourier transformation** into momentum space is applied

$$c_{j,\vec{k}} = \sum_{\vec{r}} e^{i\vec{k}\cdot\vec{r}} c_j(\vec{r}). \quad (3)$$

If one inserts these two steps into the Hamiltonian, one finds that it turns into

$$\mathcal{H} = \frac{1}{N} \sum_{\vec{k}} \sum_{\langle ij \rangle} t_{ij} c_{i,\vec{k}}^\dagger c_{j,\vec{k}} e^{i\vec{k}\cdot\vec{\delta}_{ij}}, \quad (4)$$

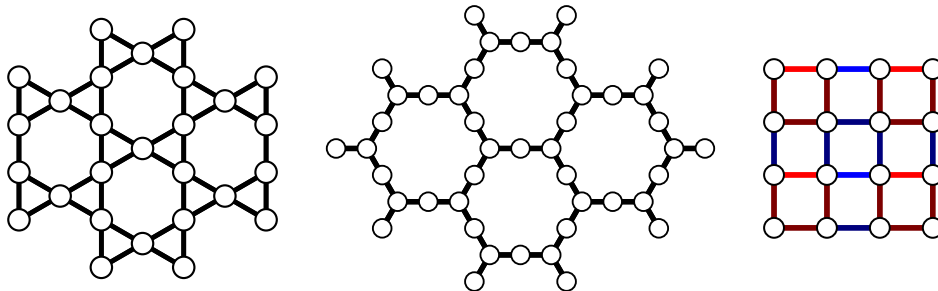
where $\vec{\delta}_{ij}$ is the vector connecting sites i and j (respecting periodic boundaries of the unit cell).

Although this looks similar to the initial Hamiltonian, one has performed a major step as the Hamiltonian matrix no longer is $N \times N$ dimensional but rather $N_{\text{UC}} \times N_{\text{UC}}$ dimensional for every value of \vec{k} inside the first Brillouin zone (where N_{UC} is the number of sites within one unit cell). The structure of the Hamiltonian suggests that an eigenstate of the system can be composed out of many individual periodic functions with wavevector \vec{k} which are eigenfunctions of the Hamiltonian matrix at wavevector \vec{k} .

Therefore, the system can now be solved by diagonalizing the Hamiltonian matrix for every value of \vec{k} and obtaining energies and wavefunctions from the eigenvalues and eigenvectors of this matrix. The energies obtained from the calculation will vary smoothly as one varies \vec{k} inside the first Brillouin zone and because some of them are related by symmetries it is a common approach to plot the energy values **along a path in momentum space**, resulting in a so-called band structure (see Figure 1 above).

To identify the states that the fermions occupy within the band structure, one fills electrons into the states from bottom to top until all electrons are assigned. The highest energy reached is then called the **Fermi energy**. From a technical perspective, one is concerned with the number of fermions per site which gives the location of the Fermi energy with respect to minimum and maximum of energy values. The case that we want to consider in the following is the case of **half filling**, i.e. one fermion per site (which is half of maximum number of two fermions per site if one allows for a spin degree of freedom).

- a) In the first part of this exercise, you should apply the aforementioned algorithm to compute the band structure of the honeycomb lattice tight-binding model along a suitable path within the Brillouin zone. For this purpose, proceed along the following steps:
- (i) Make sure that you have a lattice library code that utilizes unit cells (or can otherwise construct periodic lattices).
 - (ii) Implement the 2D honeycomb lattice (if not implemented already).
 - (iii) Analytically calculate the reciprocal vectors of the Bravais lattice and draw the Brillouin zone to visually determine the high-symmetry points. Connect these high-symmetry points to form a path in momentum space (which you then can save in Julia).
 - (iv) Implement a function that takes a unit cell and a path in momentum space to draw a band structure (similar to Figure 1).
 - (v) Draw the Fermi energy into your band structure depending on the given filling-fraction.
- b) Once you have a working algorithm for calculating the band structure of an arbitrary (two-dimensional) unit cell, it is straight-forward to calculate the band structures of other elementary lattices as well. So, go ahead and calculate the band structures of the lattices shown below by first identifying and implementing their unit cell and then performing the same scheme as in part a).

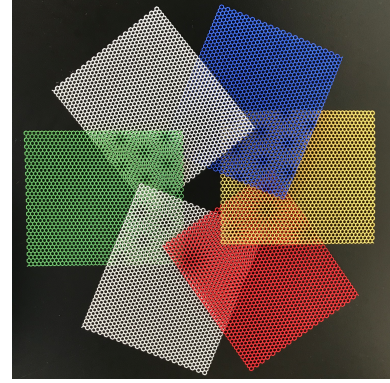


- c) In some instances, not the complete band structure is needed but only the shape and topology of the **Fermi surface**. The Fermi surface is defined as the manifold of all \vec{k} points which have an energy eigenvalue located right at the Fermi energy.

Your task is to take this definition and write a function to calculate the Fermi surface of a given unit cell and hopping parameters and filling fraction. Then, plot the Fermi surface for the two-dimensional honeycomb lattice as well as the two-dimensional square lattice and compare your findings.

Exercise 17: Moiré band structures (bonus)

In this exercise we want to go beyond elementary lattice geometries and look at the example of a **moiré lattice**. Such a moiré lattice is generated, e.g., by taking two sheets of two-dimensional lattices and twist them against one another, creating a so called moiré pattern. This pattern can also be interpreted as lattice with a (very) large unit cell. For small angles θ the unit cell can contain tens of thousands of different sites.



In similar fashion as the previous exercise we want to calculate the band structure of such moiré lattices for varying twist angles.

- a) We want to model a **twisted bilayer graphene** system, which has attracted wide-spread interest for its formation of a superconducting state when tuning to a **magic angle**. We will explore what features in the moire band structure make certain angles “magic”.

To get started, generate two honeycomb unit cells structures, which will represent the lower and upper lattice layers. Afterwards write a function which will rotate a unit cell by an angle θ . The rotation can be done simply by applying a rotation matrix to the primitive vectors and site positions, while the bonds remain the same.

Use your code to create a plot containing both lattices placed on top of each other for various different angles. How does the moiré superlattice qualitatively change when you go to small twist angles?

Now let’s concentrate on a series of angles that allow us to form a **periodic moire structure with a unit cell**. This series of angles is given by

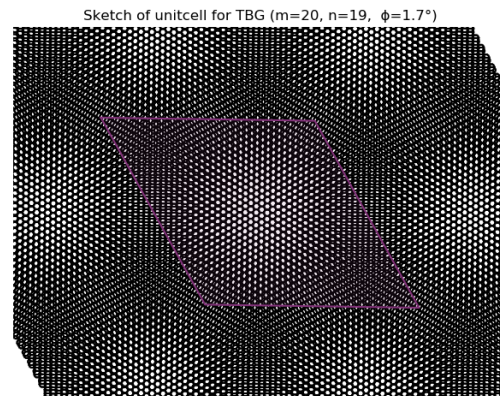
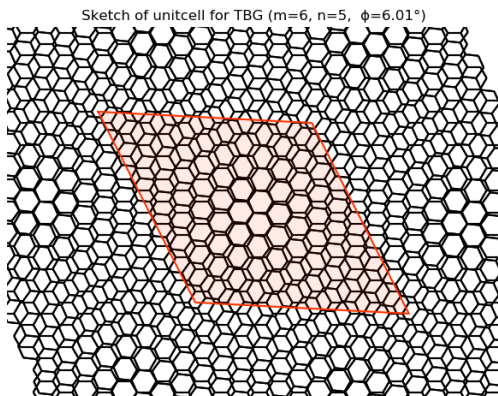
$$\cos(\theta_{m,n}) = \frac{1}{2} \frac{m^2 + n^2 + 4mn}{m^2 + n^2 mn}, \quad (5)$$

where the integers m and n define a commensurate twisting of an upper layer site $\mathbf{R}_u = m\mathbf{a}_1 + n\mathbf{a}_2$ onto a lower lattice site $\mathbf{R}_l = n\mathbf{a}_1 + m\mathbf{a}_2$.

From this one can determine the moiré lattice vectors using

$$\mathbf{a}_{1,M} = m\mathbf{a}_1 + n\mathbf{a}_2, \quad \mathbf{a}_{2,M} = R(60^\circ)\mathbf{a}_{1,M}, \quad (6)$$

with $R(60^\circ)$ being the rotation matrix.



- b) Let's consider as **example** the moiré unit cell for $m = 8$ and $n = 7$. First, calculate the lattice vectors for this choice of m and n . We now want to determine the basis sites of the moiré unit cell. To do so, generate two honeycomb sheets each with a linear size of $L = 20$. It is important that the unit cell is completely covered by the two lattices, else we will be missing some sites.

Iterate over all sites of the two lattices and add them to the unit cell structure, if they are inside the unit cell area (see the examples on the lower left). You can check this by expressing the site position as a linear combination of the moiré lattice vectors $\mathbf{R} = m'\mathbf{a}_{1,M} + n'\mathbf{a}_{2,M}$, a site is inside the unit cell if $|m'| < 0.5$ and $|n'| < 0.5$

At the same time we want to add new label to the site containing the position in the z-axis, since we actually have a 3D structure. We assume that the two lattice have a constant distance $d_0 = 2.46$. For this example assign all sites in the lower lattice a Z value of $-d_0/2$ and the upper sheet a value of $d_0/2$. Determine all sites inside the unit cell (you should find 676 sites).

- c) Perform the same construction as in the example above for all $m \in [2, 20]$ and $n = m - 1$. Determine the number of sites in the unit cell and plot this number against the angle θ .
- d) The final thing we are missing are the bonds of the unit cell. In general, all sites can be connected to each other, but we will introduce a cut-off length for the connection. All bonds which connect sites beyond the distance of $l_{max} = 5$ will be ignored. Here the unit of length is in term of the nearest neighbor distance $NN = |R_{1,M} - R_{2,M}|$.

Find all valid bonds and add them to the unit cell (in this example you should find 71776 different bonds). Do not forget to factor in z-axis into the distance between two sites.

Now we have constructed the moiré lattice and we can start calculating the **band structure**. The tight-binding Hamiltonian with all hopping amplitudes is given by

$$\mathcal{H} = \sum_{ij} t_{ij} c_i^\dagger c_j. \quad (7)$$

Note that we now sum over all pairs of sites and not only the nearest neighbours.

The distance dependent **hopping amplitudes** are given as:

$$t(r) = V_{pp\pi}(r) \left(1 - \left(\frac{r \cdot e_z}{r}\right)^2\right)^2 + V_{pp\sigma}(r) \left(\frac{r \cdot e_z}{r}\right)^2 \quad (8)$$

with

$$V_{pp\pi}(r) = V_{pp\pi}(r)^0 e^{r - a_0/\delta_0} \quad (9)$$

$$V_{pp\sigma}(r) = V_{pp\sigma}(r)^0 e^{r - d_0/\delta_0}, \quad (10)$$

where δ_0 is a decay length and $a_0 = a/\sqrt{3}$ is the intra layer nearest neighbours distance.

- e) Calculate all the different hopping amplitudes using $\delta_0 = 0.184\sqrt{3}$, $V_{pp\pi}(r)^0 = -2.7$, and $V_{pp\sigma}(r)^0 = 0, 48$.

- f) Since you have now calculated the hopping amplitudes, you can calculate the bands in the same way as for the previous exercise. Calculate the bonds for the path $K \rightarrow \Gamma \rightarrow M \rightarrow K'$ and plot the spectrum. Describe what you can see.

In actual experiments there is a **corrugation effect** between the two lattice sheets causing a varying distance depending on the type of stacking. Now the lattices distance varies between d_{AA} and d_{AB} , with the periodicity of moiré unit cell as

$$d(\mathbf{R}) = d_0 + 2d_1 \sum_{i=1}^3 \cos\left(2\pi \frac{\mathbf{R} \cdot \mathbf{C}_i}{|\mathbf{C}_i|^2}\right). \quad (11)$$

Here d_0 and d_1 are based on the layer distance at AA and AB

$$d_0 = \frac{1}{3}(d_{AA} + 2d_{AB}), \quad d_1 = \frac{1}{9}(d_{AA} - d_{AB}). \quad (12)$$

Additionally \mathbf{C}_i are the so called corrugation spanning vectors, defined as

$$\mathbf{C}_1 = \frac{1}{2}(\mathbf{a}_{1,M} + \mathbf{a}_{2,M}), \quad \mathbf{C}_2 = R(60^\circ)\mathbf{C}_1, \quad \mathbf{C}_3 = R(120^\circ)\mathbf{C}_1. \quad (13)$$

g) Now, using a $d_{AA} = 4.12$ and $d_{AB} = 2.46$ for the corrugation, redo the previous steps and determine the new sites and bonds. Calculate the new band structure and compare it to the previous band structure.

h) Currently the evaluated unit cell is still too small to see the most interesting feature in the band structure – the emergence of a **flat band**. So redo your calculation and try to increase m as much as possible.

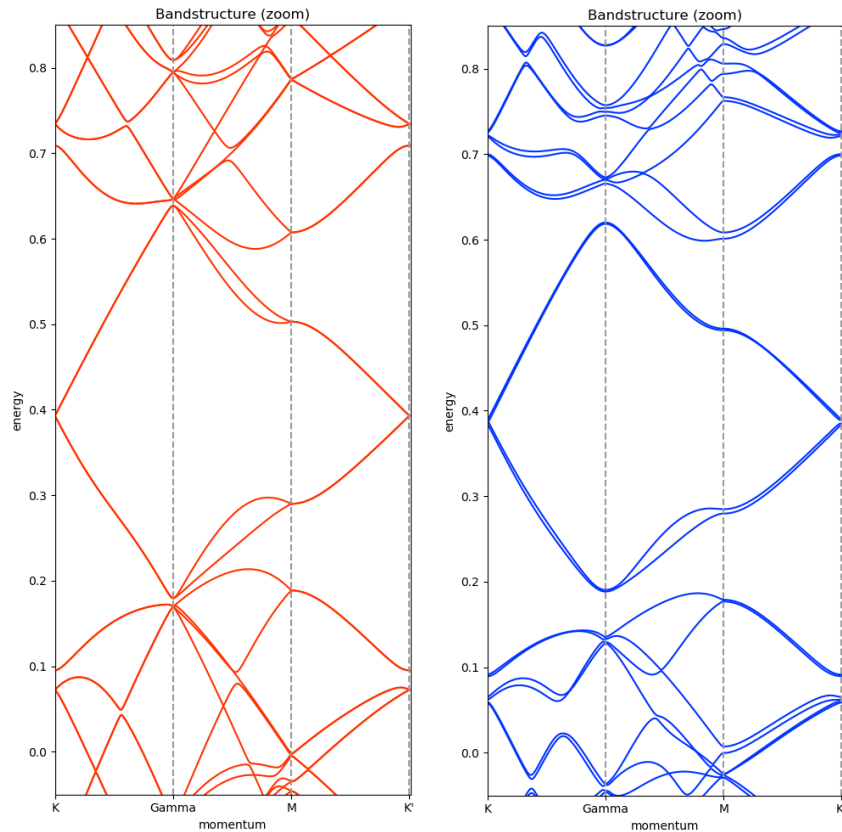


Figure 2: **Low-energy feature in the band structure** of the moiré lattice for $m = 8$ and $n = 7$. The left structure is without corrugation in the lattice, while the right structure is subjected to corrugation.