Institute for Theoretical Physics
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Computational Many-Body Physics

Exercise Sheet 4

Summer Term 2018

Due date: Monday, **18th June** 2018, 2 pm

Website: www.thp.uni-koeln.de/trebst/Lectures/2018-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. By using the previously implemented lattice library you will be able to explore a vast family of example systems.

Exercise 15: Band structure calculations

In this exercise, we want to introduce the calculations of band structures in solids. To start, let us quickly recap the basis of these calculations, **tight-binding models** given in the second quantized form

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

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

$$c_j \to c_j(\vec{r}) \tag{2}$$

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

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

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

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

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 $N_{UC} \times N_{UC}$ 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 below).

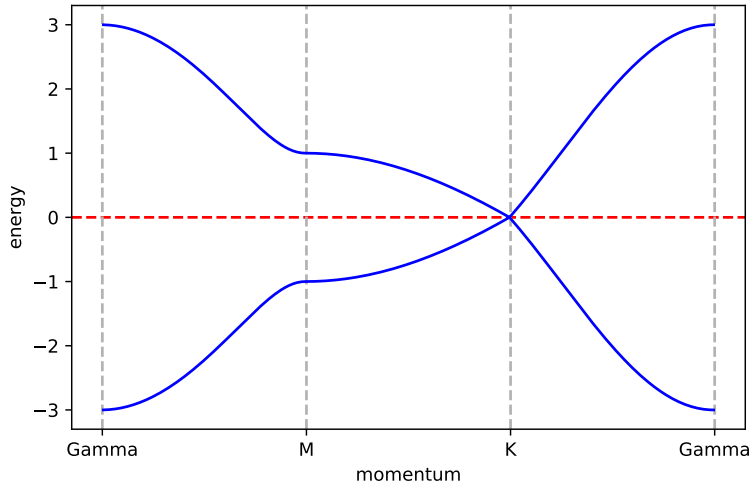


Figure 1: Band structure of the 2D honeycomb lattice hopping problem with the Fermi energy of half filling shown as a red dashed line.

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 filled up. 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. 1/2 fermions per site.

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). If you do not have such a code, you can also find the 2D lattice library on the course website.

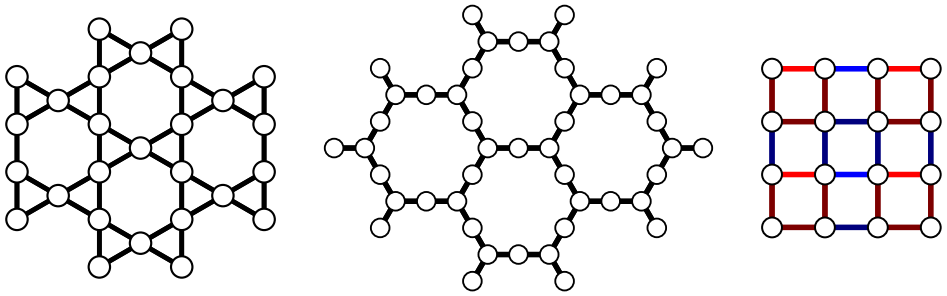
(ii) Implement the 2D honeycomb lattice (if not implemented already).

(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 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). At this point it is very helpful for debugging if you are able to generate finite lattices out of your unit cells and plot them to see if you implemented all connections correctly (Note: the plots below were actually generated with the lattice library that Jan is using).



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 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.

d) So far, the dimension of the lattice has not played a major role. Therefore it should be feasable to also extent the calculations to three-dimensional lattices like the cubic or diamond lattice. Implement a new julia type unitcell for 3 dimensional lattices and implement the diamond lattice as well as the cubic lattice. Calculate the band structures for those lattices as well following the same scheme as in previous calculations.