Tight binding model python project

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1 Introduction

In this project we used the tight binding model to calculate the band energy of a monoatomic and diatomic square lattice. The atoms used attribute one single electron. The tight binding model can be used in materials for which the electrons are "tightly bound" to the atom, so they only feel a limited amount of neighbours. This is true for the inner electrons of atoms, but it is not often a good discription of the conduction electrons themselves. In this course we learned the nearly free electron model to calculate the band structure. The tight binding model is a way to get the band structure looking at closely bound electrons.

2 Execution guidelines

The programs are written in Spyder 3.5. For the calculations we used the package Pybinding [1]. This package can only be used in Python 3.4 or newer. To correctly run our programs first set the following setting:

Tools > Preferences > Ipython Console > Graphics > Graphics Backend > Backend: "Automatic".

The squarelattice1atom.py shows the band structure for one atom per unit cell in a 2d square lattice. After running the code a new window opens. In this window it is possible to do the folowing things:

- Change the one site energy. By changing "Energy". This shifts the total band structure up or down.
- Change the hopping in the x direction by changing: "Hopping x". For a negative hopping the energy is the lowest at [0,0] so the electron will be sitting close to the atom. In this case the lattice will fall apart. For a positive hopping the energy is lower between the atoms $[\pi/a, \pi/a]$ so the electron will bind the lattice.
- Change the hopping in the y direction by changing: "Hopping y". This is the analogue to hopping in the x direction.
- The button "Lattice" opens a plot of the schematic lattice in real space together with the lattice vectors.
- The button "Unit" will open a plot of the unit cell in real space together with the lattice vectors.
- The button "Brillouin" opens a figure of the billion zone with the reciprocal lattice vectors.

The squarelattice2atom.py shows the band structure for two atoms per unit cel in a 2d square lattice. After running the code a new window opens. In this window it is possible to do the following things:

- Change on site energy of atom A by changing "Energy A".
- Change on site energy of atom B by changing "Energy B".
- Change the magnitude of the hopping by changing "hopping". The hopping between two certain atoms is calculated by scaling this "hopping" by a term dependent on the distance between the two atoms: the smaller the distance, the larger the hopping and visa versa.
- Change the x coordinate of atom B in the unit cell by changing "Location x".
- Change the y coordinate of atom B in the unit cell by changing "Location y".
- The button "Lattice" opens a plot of the schematic lattice in real space together with the lattice vectors.

[1] `http://docs.pybinding.site`

- The button "Unit" will open a plot of the unit cell in real space together with the lattice vectors.
- The button "Brillouin" opens a figure of the Brillouin zone with the reciprocal lattice vectors.