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Exercises for Computational Methods in Solid State Theory
SS 2015

Exercise Set 1

(Due date: Tuesday, April 28, 2015)

Exercise 1 (**Tight binding and tetrahedron method**) (10 points)

Consider a lattice with lattice constants

$$a = 8.5381\text{Å}, \quad b = 13.273\text{Å}, \quad c = 15.912\text{Å}, \quad \alpha = 113.917°, \quad \beta = \gamma = 90° .$$

There are two lattice sites in the positions

$$\vec{s}_1 = (0, 1/4, 0), \qquad \vec{s}_2 = (1/2, 3/4, 0) .$$

This is an anisotropic triangular lattice with the tight binding Hamiltonian

$$H = \mu \sum_i c_i^\dagger c_i + \sum_{<ij>} t\left(c_i^\dagger c_j + \text{H.c.}\right) + \sum_{[ij]} t'\left(c_i^\dagger c_j + \text{H.c.}\right) \tag{1}$$

where $< ij >$ and $[ij]$ indicate summations over nearest and next-nearest neighbors, respectively. The nearest neighbour hopping is $t = 0.04957735$ eV (associated to the distance $d = 7.891$ Å) and the next nearest neighbour hopping is $t' = 0.0426178$ eV (associated to the distance $d = 8.5381$ Å). The chemical potential is $\mu = 0$.
Remark: This model Hamiltonian is obtained from the charge transfer salt κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ at $T = 20$ K.

a) Write a program that calculates the bandstructure along the path

$$M - X - \Gamma - Y - M - \Gamma$$

in the Brillouin zone where $\Gamma = (0, 0, 0)$, $X = (0.5, 0, 0)$, $Y = (0, 0.5, 0)$, and $M = (0.5, 0.5, 0)$ in reduced coordinates. Plot the bandstructure, taking into account the different lengths of the path segments in reciprocal space. If you are unsure how the lattice sites are connected by the hoppings, make a sketch.

b) Use the tetrahedron method to calculate the density of states (DOS) for the same tight binding Hamiltonian. Make sure that the DOS is properly normalized. Compare to the result of a brute force calculation of the DOS.

Remark: Please do not write parameters directly into the code. The program is intended for reuse and should be as general as possible.