Exercise-sheet 3 (November 9, 2015)

1 In-class exercises

1.1 Tight-binding approximation

Consider a linear lattice of atoms which are well separated such that their atomic orbitals have only small overlaps. In such a situation, the electronic states are fairly well represented by localized atomic orbitals ψ_n, for which

$$H_{\rm at}(R)\psi_n(r-R) = \epsilon_n \psi_n(r-R), \tag{1}$$

where the atomic Hamiltonian ($H_{\rm at}$) is given by

$$H_{\rm at}(R) = \frac{p^2}{2m} + V_{\rm at}(r-R), \tag{2}$$

with $V_{\rm at}$ the atomic potential.

Let us consider a single-particle Hamiltonian for an electron in the lattice which combines all the potential of the atoms as follows

$$H = \frac{p^2}{2m} + \sum_R V_{\rm at}(r-R) = H_{\rm at}(R) + \Delta V(r-R) \tag{3}$$

(a) Approximate the extended Bloch function with the function

$$\psi_k(r) = \sum_R e^{ikR}\phi(r-R), \tag{4}$$

with $\phi(r) = \sum_n b_n \psi_n(r)$, where the $\psi_n(r)$ are a set of localized atomic wave functions. Find an expression for determining the b_n constants.

(b) Find the dispersion relation for an s-band arising from a single atomic s-level.

1.2 Tight-binding model on a honeycomb lattice

(a) Compute the dispersion relation for the tight-binding model on a honeycomb lattice of lattice constant a.

(b) Give an approximate expression for the dispersion close to the point $K = (\frac{2\pi}{3a}, \frac{2\pi}{3\sqrt{3}a})$.

2 Homework - due date: November 16, 2015 (25 points).

2.1 Linear chain with next-nearest neighbor hopping

Consider a linear chain of atoms with first- and second-neighbor hopping amplitudes t_1 and t_2, respectively.

(a) Determine the tight-binding band structure of the chain.

(b) What's the number of minima of the dispersion?

(c) Compute the DOS for $t_1 = 1/2$ and $t_2 = -t_1$.

2.2 Tight-binding model on a kagomé lattice

(a) Find the dispersion relation for the tight-binding model on a kagomé lattice of lattice constant a.

(b) Plot the band structure of the model along the path $\Gamma - K - M - \Gamma$ with $\Gamma = (0, 0)$, $K = \frac{\pi}{a}(\frac{1}{3}, \frac{1}{\sqrt{3}})$ and $M = \frac{\pi}{a}(\frac{2}{3}, 0)$ in reciprocal space.