Exercise 1 - Nearly free electrons (2 points)

Consider a weak potential $V(x) = V_0 \cos(\frac{2\pi}{a}x)$ in one dimension. Calculate the dispersion $\epsilon(k)$ for the lowest energy band in the nearly free electron approximation. Determine the size of the energy gap between first and second band at $k = \pm\frac{\pi}{a}$. What is the Fermi energy if the first band is fully occupied with electrons?

Exercise 2 - Tight binding model in one and two dimensions (4 points)

(a) Calculate the energy bands for tight binding electrons in one dimension for the next-nearest neighbour model defined by having only these nonzero ovelaps and matrix elements of the Hamiltonian:

$$\begin{aligned} \langle i \mid j \rangle &= \delta_{i,j} \\ \langle i|H|i \pm 1\rangle &= -t_1 \\ \langle i|H|i \pm 2\rangle &= -t_2 \\ \langle i|H|i\rangle &= E_0 \end{aligned} \tag{1}$$

Assume $t_2 = 0.5t_1$. What is the Fermi energy for the half-filled case?

(b) The tight binding model can be extended to two dimensions as well. We use a similar notation for the states as in the one dimensional case: $|i_x, i_x\rangle$ denotes the atomic orbital at the site with x-position i_x and y-position i_y.

Calculate the energy bands for tight binding electrons in two dimensions for the nearest neighbour model that is defined in the following way:

$$\begin{aligned} \langle i_x, i_y \mid j_x, j_y\rangle &= \delta_{i_x,j_x}\delta_{i_y,j_y} \\ \langle i_x, i_y|H|i_x \pm 1, i_y\rangle &= -t \\ \langle i_x, i_y|H|i_x, i_y \pm 1\rangle &= -t \\ \langle i_x, i_y|H|j_x, j_y\rangle &= \delta_{i,j}\, E_0 \end{aligned} \tag{2}$$

What is the Fermi energy for the half-filled case?

Solutions due on the 13th of May 2013