Goethe-Universität Frankfurt
Fachbereich Physik

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Einführung in die Theoretische Festkörperphysik

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Exercise 10

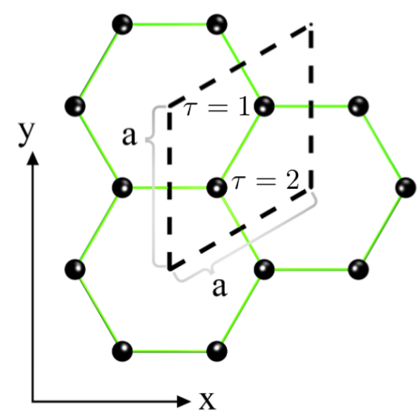
(Due date: 20.01.2020)

Problem 1 (**Fermi statistic at room temperature**) (5 points)

The Fermi temperature of copper is approximately 81000 K. Calcuate the fraction of thermally excitable conducting electrons, i.e. those electrons, whose energy at room temperature (300 K) is larger than $E_F - 2k_BT$ (E_F is the Fermi energy).

Hint: Consider the conducting electrons to be a free electron gas. You can use the expression for the density of states from the script. The exercise can be solved via integration by parts if you assume the dericative of the Fermi function to be a delta function (due to the small temperature).

Problem 2 (**Electronic Properties in the honeycomb lattice**) (10 points)



Consider a crystal that orders in a 2D honeycomb lattice. The unit cell of the crystal (shown in the figure) contains two atoms in the basis, which has to be reflected in the tight-binding model Hamiltonian:

$$H = \sum_{\tau\vec{R}} \varepsilon_0 |\tau\vec{R}\rangle\langle\tau\vec{R}| + \sum_{\tau\tau'}\sum_{\vec{R}\vec{R}'} t^{\tau\tau'}_{\vec{R}\vec{R}'} |\tau\vec{R}\rangle\langle\tau'\vec{R}'| \tag{1}$$

where $\tau = 1, 2$ runs over the basis atoms and a single orbital per atom is assumed. The Wannier functions $|\tau\vec{R}\rangle$ are orthogonal: $\langle\tau\vec{R}|\tau'\vec{R}'\rangle = \delta_{\vec{R}\vec{R}'}\delta_{\tau\tau'}$.

a) Calculate the dispersion relation for the crystal considering only the nearest-neighbor hopping matrix elements t. Use the coordinate system shown in the figure.
(*Hint:* You may use the Bloch-like functions

$$|\tau\vec{k}\rangle = \frac{1}{\sqrt{N}}\sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}}|\tau\vec{R}\rangle$$

as an ansatz. Calculate $H|\tau''\vec{k}\rangle$ and diagonalize the resulting 2×2 matrix to determine the energy dispersion in terms of $\vec{k}$.)

b) Sketch the bandstructure along the path from $\Gamma = (0,0)$ to $K = (\frac{2\pi}{\sqrt{3}a}, \frac{2\pi}{3a})$ setting $\varepsilon_0 = 0$ and $t = 1$.

c) Numerically calculate the density of states and the Fermi surface.