LMU München
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Lehrstuhl für Theoretische Nanophysik
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4. Exercise Sheet TA1: Theoretical Solid State Physics

To be discussed on Friday, November 15, 2013.

Exercise 1: Electrons in a weak periodic potential

Consider the point W ($\boldsymbol{k}_W = (2\pi/a)(1, \frac{1}{2}, 0)$) in the first Brillouin zone of the fcc structure shown (see Fig. 1).

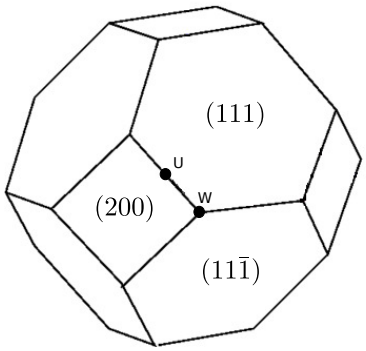

Figure 1: First Brillouin zone of the fcc lattice.

Here three Bragg planes $((200), (111), (11\bar{1}))$ meet and accordingly the free electron energies

$$\begin{aligned}
\epsilon_1^0 &= \frac{\hbar^2}{2m}k^2, \\
\epsilon_2^0 &= \frac{\hbar^2}{2m}(\boldsymbol{k} - \frac{2\pi}{a}(1,1,1))^2, \\
\epsilon_3^0 &= \frac{\hbar^2}{2m}(\boldsymbol{k} - \frac{2\pi}{a}(1,1,\bar{1}))^2, \\
\epsilon_4^0 &= \frac{\hbar^2}{2m}(\boldsymbol{k} - \frac{2\pi}{a}(2,0,0))^2
\end{aligned} \tag{1}$$

are degenerate when $\boldsymbol{k} = \boldsymbol{k}_W$ and equal to $\epsilon_W = \hbar^2\boldsymbol{k}_W^2/2m$.

a. Show that in a region of k-space near W, the first-order energies are given by solutions to

$$\begin{bmatrix} \epsilon_1^0 - \epsilon & U_1 & U_1 & U_2 \\ U_1 & \epsilon_2^0 - \epsilon & U_2 & U_1 \\ U_1 & U_2 & \epsilon_3^0 - \epsilon & U_1 \\ U_2 & U_1 & U_1 & \epsilon_4^0 - \epsilon \end{bmatrix} = 0$$

where $U_2 = U_{200}, U_1 = U_{111} = U_{11\bar{1}}$, and that at W the roots are

$$\epsilon = \epsilon_W - U_2 \text{ (twice)}, \ \epsilon = \epsilon_W + U_2 \pm 2U_1.$$

b. Using a similar method, show that the energies at the point U ($\boldsymbol{k}_U = (2\pi/a)(1, \frac{1}{4}, \frac{1}{4})$) are

$$\epsilon = \epsilon_U - U_2, \ \epsilon = \epsilon_U + \frac{1}{2}U_2 \pm \frac{1}{2}(U_2^2 + 8U_1^2)^{1/2},$$

where $\epsilon_U = \hbar^2 \boldsymbol{k}_U^2 / 2m$.

Exercise 2: Bandstructure of the triangular lattice

The unit cell of the triangular lattice is defined via the primitive vectors

$$\boldsymbol{a}_1 = \hat{\boldsymbol{x}}, \ \boldsymbol{a}_2 = \frac{\hat{\boldsymbol{x}}}{2} + \frac{\sqrt{3}}{2}\hat{\boldsymbol{y}}$$

where $\hat{\boldsymbol{x}}$ and $\hat{\boldsymbol{y}}$ are unit vectors in the direction of the coordinate axes.

a. Compute the basis vectors of the reciprocal lattice.

b. Sketch the reciprocal lattice and draw the first three Brillouin zones.

c. Determine the Fermi surface from your sketch for the electron densities $\frac{N}{V} = 1, 2, 3$.
Hint: Draw a circle with radius corresponding to each of the three densities in your sketch.

d. Draw the points $K = (2\pi/3, 2\pi/\sqrt{3})$ and $M = (0, 2\pi/\sqrt{3})$ into the sketch.

Now the bandstructure for free electrons between $\Gamma = (0, 0)$ and the points K and M shall be computed. For that purpose the $\boldsymbol{k}$ vectors need to be folded into the first Brillouin zone via translations about reciprocal lattice vectors $\boldsymbol{K}$.

e. Give a general expression for the energy bands between Γ and X that only depends on expansion coefficients of the reciprocal lattice vectors in the basis computed above and a continuous parameter κ.

f. Compute and sketch the three lowest lying bands with the help of the solution from (b). Additionally show how often degenerate the band is and which translations led to it.

Now the influence of a (weak) periodic potential

$$V(x) = \sum_n v_n e^{iK_n x} \tag{2}$$

on the bands shall be studied.

g. First, show that

$$\langle k'|V|k\rangle = \sum_n v_n \delta_{k', k+K_n}, \tag{3}$$

where $|k\rangle$ are states of the free electrons.

h. With the help of first order (degenerate) perturbation theory compute the influence of the periodic potential on the twofold degenerate band (between Γ and M) from above.