Condensed matter physics 2013
Solutions to exercise 12

Discussion: 10. Dec. 2013

Problem 45

All directions in the (x, y)-plane are equivalent, so we can choose $\vec{B} = (B, 0, 0)$. Using $\vec{v} = \frac{1}{\hbar}\vec{\nabla}_{\vec{k}} E(\vec{k})$ for the group velocity leads to the component j of the velocity, $v_j = \hbar k_j / m_j$, which allows us to write the semi-classical equation of motion as a set of three coupled differential equations:

$$\frac{dk_x}{dt} = 0 \tag{1}$$

$$\frac{dk_y}{dt} = \frac{-ek_z B}{m_l} \tag{2}$$

$$\frac{dk_z}{dt} = \frac{ek_y B}{m_t} \tag{3}$$

The first equation simply states that the momentum does not change with time, i.e. it is constant. Inserting the Ansatz $k_j = k_{j,0} \mathrm{e}^{-i\omega_c t}$ into the equations (2) and (3) leads to the algebraic equation system

$$\begin{pmatrix} i\omega_c & -\frac{eB}{m_l} \\ \frac{eB}{m_t} & i\omega_c \end{pmatrix} \begin{pmatrix} k_{y,0} \\ k_{z,0} \end{pmatrix} = 0 \tag{4}$$

This system of equations has a solution if the determinant of the matrix to the left is zero, which leads to the quadratic equation $-\omega_c^2 + \frac{e^2 B^2}{m_t m_l} = 0$ and to the result required on the problem sheet.

* Problem 46

The metal Gallium has the configuration [Ar] $3d^{10}$ $4s^2$ $4p^1$ and Arsenic [Ar] $3d^{10}$ $4s^2$ $4p^3$. Only the p-orbitals contribute significantly to the delocalized states, so we obtain one electron from each Ga atom and three from the As atoms. Gallium and arsenic form the III-V compound semiconductor GaAs which crystallizes in the zincblende structure, which contains 4 Ga atoms and 4 As atoms in the unit cell (p. 1.25, Fig. 1.26). From this we would conclude that an even number of electrons per unit cell have to be filled into the bands. This suggests that GaAs is an insulator (see script p. 6.39). Though this picture does not account for band overlaps, electron-electron interactions, and other effects, we find in nature that GaAs has indeed a band-gap. GaAs is an important semiconductor in industry and in research laboratories.

* Problem 47

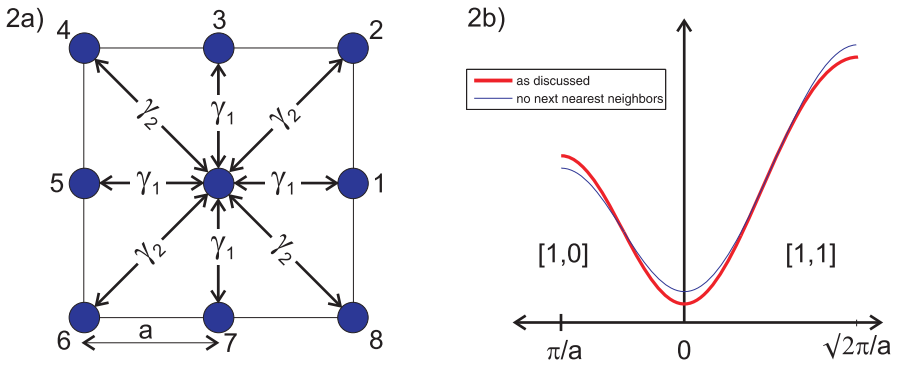
a) The width of the band is determined by γ, usually by the one due to the nearest neighbors. In the example considered in part b), the width is $\sim 2\gamma_1$.

b) Since the γ's usually lead to a reduction of the energy (binding), we use a positive number and a negative sign for emphasis. Each term in equation (3) of the problem sheet has a phase of the form $\vec{k}\vec{R} = \begin{pmatrix} k_x \\ k_y \end{pmatrix} \begin{pmatrix} R_x \\ R_y \end{pmatrix}$, where R_x and R_y are the x and y components of the lattice vector $\vec{R}$ pointing to the neighboring atoms. For example, for the nearest atom to the right (number 1 in figure 2a), $R_x = a$ and $R_y = 0$. The tight binding energy then reads (see figure for geometry):

$$\begin{aligned}\epsilon &= \epsilon_0 \quad -\gamma_1(\overbrace{e^{ik_x a}}^{\text{atom 1}} + \overbrace{e^{ik_y a}}^{\text{atom 3}} + \overbrace{e^{-ik_x a}}^{\text{atom 5}} + \overbrace{e^{-ik_y a}}^{\text{atom 7}}) \\ &\quad\quad -\gamma_2(\overbrace{e^{i(k_x+k_y)a}}^{\text{atom 2}} + \overbrace{e^{i(-k_x+k_y)a}}^{\text{atom 4}} + \overbrace{e^{i(-k_x-k_y)a}}^{\text{atom 6}} + \overbrace{e^{i(k_x-k_y)a}}^{\text{atom 8}}) \\ &= \epsilon_0 \quad -2\gamma_1[\cos(k_x a) + \cos(k_y a)] - 2\gamma_2[\cos([k_x + k_y]a) + \cos([k_x - k_y]a)]\end{aligned}$$

In the last step the terms labeled 'atom 1' and 'atom 5', 3 and 7, 2 and 6, and 4 and 8 are combined to the respective cosine terms on the last line.

In the $[1,0]$ direction, i.e. $k_x \equiv k$ and $k_y = 0$, one finds $\epsilon = \epsilon_0 - 2\gamma_1[1 + \cos(ka)] - 4\gamma_2 \cos(ka)$. In this case, k runs from $-\pi/a$ to π/a. In the $[1,1]$ direction, i.e. $k_x = k_y = \frac{1}{\sqrt{2}}k$ one finds $\epsilon = \epsilon_0 - 4\gamma_1 \cos(\frac{1}{\sqrt{2}}ka) - 2\gamma_2[1 + \cos(\sqrt{2}ka)]$, and $k \in [-\frac{\sqrt{2}\pi}{a}, \frac{\sqrt{2}\pi}{a}]$ (the Brillouin zone boundary is reached in its diagonal). The corresponding curves are plotted in figure 2b), with arbitrary energy units and $\gamma_1 = 10\gamma_2$.



MATLAB tutorial: the following code was used to plot the red curve in figure 2b):

```
a=1; gamma1=1; gamma2=0.1;
k=-pi/a:0.01:pi*sqrt(2)/a;
ind=find(k>=0);
E(ind)=-4*gamma1*cos(k(ind)*a/sqrt(2))-2*gamma2*(1+cos(sqrt(2)*k(ind)*a));
ind=find(k<0);
E(ind)=-2*gamma1*(1+cos(k(ind)*a))-4*gamma2*cos(k(ind)*a);
plot(k,E)
```

Problem 48

a) The time scale on which the electron is moving through k-space is given in equation (1) of the problem sheet. Starting at $k = 0$, the k-vector reaches the Brillouin zone boundary at π/a after $\Delta t = \pi\hbar/(aeF)$.

b) The oscillation frequency is given by $\omega = \frac{eFa}{\hbar}$ and $\nu = \omega/2\pi$. The amplitude is $A = \frac{\epsilon}{2eF}$. Plugging-in the numbers yields $\nu = 24\,\text{THz}$ and $A = 0.5\,\text{nm}$. However, how does one apply an electrical field to a metal (and not to the leads) without large currents and heating? A better experiment is to use a semiconductor with highly conducting contacts. For example, the electrical breakdown in Si occurs at $F \approx 30\,\text{MV/m}$, which yields $\nu = 0.73\,\text{THz}$ and $A = 17\,\text{nm}$.

c) The Drude scattering time in silver (largest scattering time in metals) at $273\,\text{K}$ is $4 \times 10^{-14}\,\text{s}$ (Ashcroft and Mermin. p.10), which would roughly correspond to the above Bloch oscillation time ν^{-1}. A scattering event changes the k-vector randomly and in average over many scattering events to $k = 0$. Therefore, Bloch oscillations do not occur when the scattering times are smaller than the Bloch oscillation time, which is the case for most materials.