Electrons in crystals
II written test
academic year 2008/2009
December 2, 2008

(*Time: 3 hours*)

Exercise 1: *Semiclassical theory of electron dynamics in presence of an electric field*

1. Consider the BCC crystal structure with lattice spacing a. Use the tight-binding method considering s-type wavefunctions, nearest-neighbor interactions only and negligible overlap to determine the band structure to derive the expression for the band structure:

$$\mathcal{E}(\mathbf{k}) = \mathcal{E}_0 - 8\gamma \cos\left(\frac{ak_x}{2}\right) \cos\left(\frac{ak_y}{2}\right) \cos\left(\frac{ak_z}{2}\right)$$

with reference to the texbook for the definition of $\gamma = \gamma(\mathbf{R}_{NN})$ and $\mathcal{E}_0$.

2. Using the above expression for the energy band, consider the application of an external electric field $\vec{E}$ costant in time and uniform in space. For an electron which is at rest ($\vec{k} = 0$) at $t = 0$, write the expression of its velocity as a function of $\vec{E}$.

3. Write the expression for the time evolution of its position $\vec{r}(t)$.

4. Specify it in the particular case of the electric field in the [110] direction. Describe and sketch the orbit.

5. Given $|\vec{E}| = 1$ V/cm and $\gamma = 1$ eV, give the numerical estimate of the amplitude of the spatial oscillation.

Exercise 2: *Semiclassical theory of electron dynamics: cyclotron orbits*

Consider the problem of a cyclotron orbit in the $k_x k_y$ plane for a nonisotropic solid with band structure ($A, B, C > 0$):

$$\mathcal{E}(\mathbf{k}) = \mathcal{E}_0 - 2[A\cos(ak_x) + B\cos(ak_y) + C\cos(ak_z)]$$

under the influence of an external uniform magnetic field along z.

1. Show that the equation for the orbit with a given energy $\mathcal{E}$ close to the minimum $\mathcal{E}_{min}$ is: $\mathcal{E} = \mathcal{E}_{min} + (Aa^2k_x^2 + Ba^2k_y^2)$.

2. Describe the rate at which $\vec{k}$ changes during that orbit when $A > B$.

3. Describe the orbit in real space.

Hint: Remember that the area of an ellipse centered at the origin: $(x^2/a^2) + (y^2/b^2) = 1$ *is* πab.

Exercise 3: *Filling of bands*

A one dimensional metal of lattice constant a has a band whose dispersion is

$$\mathcal{E}(k) = V_0 - V_1 \cos(ka) - V_2 \cos(2ka).$$

(take $V_1 > 0$, $V_2 > 0$, and $|V_2|$ sufficiently small that $\mathcal{E}(k)$ depends monotonically on k from 0 to π/a). The band is partially occupied in such a way that the Fermi wavevector is $k_F = \pi/2a$.

1. Discuss the filling of this band (what fraction of the band is occupied, and how many electrons per cell are contributed).
2. Find the effective mass m^* and the group velocity (i.e., the Fermi velocity) v_F of electrons at k_F.

Exercise 4: *Filled bands are inert*

We have shown in class that the total current carried by a completely filled band in a metal at T = 0 is zero. Show it at T $\neq$ 0. To simplify the problem, consider a 1D crystal with a single band crossing μ, and the electron system in equilibrium (Fermi-Dirac filling) at temperature T. Assume that the band energy increases monotonically as k increases from Γ to π/a and also as k decreases from Γ to $-\pi/a$.

1. First, show that under the assumption $\mathcal{E}(k) = \mathcal{E}(-k)$, the current vanishes.
2. Consider the more general case where $\mathcal{E}(k) \neq \mathcal{E}(-k)$ and show that even then, the total current vanishes.

NOTE:

- Give all the steps necessary to understand in detail the solution procedure. Answers with the final result only or with insufficient details will not be considered valid.
- When required, numerical evaluations should be given exactly with 3 significant figures, if not otherwise indicated.