Condensed Matter Physics I
II partial written test
academic year
December 19, 2013

(*Time: 3 hours*)

Exercise : *Free electrons in a 2D "empty" square lattice*

Consider a hypothetical 2D metal in a square lattice with lattice constant a.

1. Give the expression of the radius of the Fermi circle if we have in general x electrons per atom. (In general consider x as a fractional number. This is possible in alloys or using dopants, considering the *average* number of electrons per primitive unit cell.)

2. Let us study what would the Fermi circle look like. Depending on the value of x it can span multiple Brillouin zones. Although x can be non integer, if we restrict ourselves to simple monatomic lattice, then we can have only integer values of x. For a number of electrons per atom equal to:

   (a) 1
   (b) 2
   (c) 3
   (d) 4

   you are asked (for each case):
   (i) to specify whether the first Brillouin zone is totally filled or not;
   (ii) to specify which are the partially filled Brillouin zones;
   (iii) to make a plot of the Fermi circle in the each partially filled Brillouin zone.

Exercise : *Tight binding*

Consider a one-dimensional chain of atoms.

1. Which is the general form of a *Bloch sum* made of atomic orbitals ϕ centered on sites $\{\mathrm{R}\}$?

2. Consider in particular a chain of N atoms spaced by a and with a gaussian atomic wavefunction $\phi(x)$ on each atom. Assume periodic boundary conditions. Show that the *Bloch sum* for this particular system is of the form:

$$\psi_k(x) = \frac{1}{\sqrt{N}} \sum_n e^{ikna} \phi(x - na).$$

   Show that this $\psi_k(x)$ indeed satisfies the Bloch theorem.

3. Show that $\psi_k(x)$ is correctly normalized provided a certain assumption is made. What is the assumption?

4. Make a plot of $\psi_k(x)$ for $k = 0$, $k = 0.25\pi/a$ and $k = 0.5\pi/a$.

Exercise : *Semi-classical model of the electron dynamics and Bloch oscillations*

Consider the semi-classical model of the electron dynamics. We focus on the one-dimensional tight-binding model with the dispersion relation $E(k) = -2t\cos(ka)$, where t is the nearest neighbor hopping constant and a the lattice constant (for simplicity we consider only one band).

1. Consider an applied uniform electric field E. Calculate analytically $k(t)$ and $x(t)$. Show that E does not accelerate the electrons but lets them oscillate around some fixed position.

2. Give the expression of the amplitude of the oscillations in real space as a function of the applied electric field E.

3. Give the expression of the period of the oscillations as a function of the applied electric field E and calculate how big a field must be applied in Cu in order that a cycle can finish before the electron scatters. Consider for Cu a relaxation time τ of 21×10^{-14} sec and a lattice spacing of 0.361 nm.

4. For "normal" electric fields and typical relaxation times, in which case we could observe Bloch oscillations? *(Hint: Which other parameter of the physical system does enter in the expression of the period of oscillations?)*

5. We now add a small damping term, so that the rate of change of the quasi-momentum is given by
$$\hbar\dot{k} = F_{ext} - \frac{m\dot{r}}{\tau}$$
where τ is the relaxation time. Which is $k(t)$? Can this damping term lead to a vanishing of the oscillations and thus to a stationary solution?

6. What would the corresponding condition be and how would the stationary solution look like?

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.