Electrons in crystals – II written test

Academic year 2006/2007 – December 6, 2006

(*Time: 3 hours)*

Solve all the exercises, corresponding to a total maximum score of 36. If the score is between 33 and 36 it is considered equal to 30/30 *cum laude*, if it is between 30 and 32 it is considered equal to 30/30.

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.

Exercise 1: *Semiclassical motion in a uniform static electric field*

Consider a one-dimensionale crystal with lattice parameter a and one Bloch electron in the energy band with dispersion:

$$\mathcal{E}(k) = \mathcal{E}_1 + (\mathcal{E}_2 - \mathcal{E}_1) sin^2 \left(\frac{ka}{2} \right)$$

Consider the system in a uniform static electric field E and its motion described by the known equations of the semiclassical model.

1. Write out explicitly the expression of the dynamical effective mass as a function of the crystalline momentum k, draw the plot in the first Brillouin zone and discuss possible particular points.
2. Write out explicitly the expression of the group velocity of this electron as a function of the crystalline momentum k, draw the plot in the first Brillouin zone and discuss possible particular points.
3. Write out explicitly the expression of the temporal evolution $k(t)$ of the crystalline momentum in this case and draw the plot.
4. Write out explicitly the expression of the temporal evolution $x(t)$ of the position.
5. How much is (in seconds) the period of the orbit when $\Delta\mathcal{E} \equiv \mathcal{E}_2 - \mathcal{E}_1 = 1\ eV$, a=2Å and the applied field is $E = 0.1\ V/cm$?

Exercise 2: *Electrons in a weak periodic potential*

Consider a one-dimensional crystal with lattice parameter a and a weak periodic potential. Calculate the effect at the Brillouin zone borders, i.e., the forbidden energy gap E_g in case of:

1. a rectangular potential:
$$U(x) = \begin{cases} \mathrm{U}_0 & 0 \leq x < \frac{a}{2} \\ 0 & \frac{a}{2} \leq x < a \end{cases}$$
2. a sinusoidal potential:
$$U(x) = U_0 \; cos\left(\frac{2\pi}{a}x\right)$$

Exercise 3: Tight binding *model for s-bands*

1. Write out explicitly the s-band tight-binding $E(\mathbf{k})$ for a 3-dimensional simple-cubic (SC) lattice of spacing a, in the simplest NN approximation and neglecting the overlap integrals.
2. Draw a slice of the band in the first Brillouin zone for k_x in $(-\pi/a, \pi/a)$, $k_y = 0$, $k_z = 0$. (Make a reasonable assumption about the sign of the *hopping integral*). On the same plot, draw another slice of the band for $k_y = \pi/a$, $k_z = 0$.
3. What is the total width of the s band?
4. Write out explicitly $E(\mathbf{k})$ including also next nearest neighbor interactions but still neglecting overlap.

Consider now a one dimensional crystal, a Li-atom chain spaced by a=1 Å. In the nearest neighbor *tight binding* model the expression of the energy of the conduction band is: $E(k) = E_0 - 2\gamma cos(ka)$, with E_0=−5.39 eV with respect to the vacuum level and γ=3.25 eV.

1. Write out explicitly the electronic density of states $g(E)$ and draw a plot. (Hint: look at its symmetry!)
2. Calculate the energy needed to extract an electron from such metal (explaining your answer).