Condensed Matter Physics I
II partial written test
academic year 2017/2018
January 15, 2018

(*Time: 2 hours*)

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.

Exercise 1: Tight-binding

Consider a simple cubic lattice with lattice spacing a and one s orbital per site, only nearest-neighbor interactions and neglect overlap. The expression of the tight binding s-band is:

$$E(\mathbf{k}) = E_{1s} - \beta - 2\,\gamma\,(cos\;k_x a + cos\;k_y a + cos\;k_z a)$$

where $\beta = -\int \phi_{1s}(\mathbf{r})\,\Delta U(\mathbf{r})\,\phi_{1s}(\mathbf{r})\,d\mathbf{r}$ and $\gamma = -\int \phi_{1s}(\mathbf{r})\,\Delta U(\mathbf{r})\,\phi_{1s}(\mathbf{r}-\mathbf{R})\,d\mathbf{r}$; $\mathbf{R}$ are Bravais lattice vectors joining the nearest-neighbour sites to the origin, and $\gamma > 0$.
The high-symmetry points in the first Brillouin zone are labelled as:
$\Gamma = (0,0,0)$, $X = \frac{\pi}{a}(1,0,0)$, $M = \frac{\pi}{a}(1,1,0)$ and $R = \frac{\pi}{a}(1,1,1)$.

1. Write explicitly which are the $\mathbf{k}$ points for the (i) minimum and (ii) maximum of the band and indicate the corresponding energy values.
2. Plot $E(\mathbf{k})$ along R-Γ-X (use the same scale along the axis representing $\mathbf{k}$).
3. Write explicitly which are the saddle $\mathbf{k}$ points. Justify clearly your answer (otherwise it will not be considered valid)
4. Write explicitly the expression of the density of states $g(E)$ around the minimum of the band in terms of the parameters of the band.
5. Write the expression of the Bloch sums $\psi_{1s,\mathbf{k}}(\mathbf{r})$ corresponding to the (i) minimum and (ii) maximum of the band and describe how they look like on the different lattice sites.

Exercise 2: Semiconductors

The band gaps of Silicon is 1.1 eV and its relative dielectric constant is 11.9. Assume the effective masses at the band edges around the gap are isotropic, roughly t he same, and are roughly .5 of the bare electron mass.

1. Estimate the conduction electron concentration for intrinsic (undoped) Silicon at room temperature. *(You can use equations form the textbook, but justify their validity)*

2. Calculate the donor level in case of doping with As.

3. Make a rough estimate of the maximum concentration of ionized monovalent impurities that will still allow for the intrinsic behavior.

4. A direct gap semiconductor is doped to produce a density of 10^{23} electrons/m^3. Calculate the hole density at room temperature given that the gap is 1.0 eV, and the effective mass of carries in the conduction and valence band are 0.25 and 0.4 electron masses respectively.

Exercise 3: Metals and insulators

1. Diamond, which has 8 atoms in a fcc (conventional cubic) unit cell with a basis, is an electrical insulator, whereas silicon and germanium, which have similar structures, are semiconductors. Why?