Mid-term assessment test of Condensed Matter Physics - January 17th 2019
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Exercise 1: Tight binding.

A square lattice with lattice constant $a = 0.1\,\text{nm}$ is formed by a unit cell containing one atom with one valence electron (see Fig. 1). The wavefunction $\phi_{1s}(\boldsymbol{r})$ of the valence electron is s-type (and real).

1. Write the expression of the resulting energy band dispersion $E(k_x, k_y)$ in the tight-binding approximation considering the contributions from the first- and second-neighbours, only. Neglect the overlap integral and assume the values of the "transfer integral" $\gamma_i \equiv \gamma(\boldsymbol{R}_i) = -\int d\boldsymbol{r}\, \phi_{1s}(\boldsymbol{r})\Delta U(\boldsymbol{r})\phi_{1s}(\boldsymbol{r} - \boldsymbol{R}_i)$ equal to $\gamma_1 = +1\,\text{eV}$ and $\gamma_2 = +0.25\,\text{eV}$ for the first- and second-neighbours, respectively. Indicate with E_s the energy level of the atomic s orbital and let $\beta = \gamma(\boldsymbol{R} = 0)$. [The numerical values of these two parameters are not needed to answer the following questions].

2. Evaluate the band amplitude (in eV) as the energy difference between the band minimum and maximum in $\boldsymbol{k}$-space.

3. Evaluate the electron effective mass m_{xx} (in kg) along the x direction at the $\Gamma = (k_x = 0, k_y = 0)$ point.

[Note that 1 eV corresponds to an energy of 1.60×10^{-19} J, and the Planck constant is $\hbar = 1.05 \times 10^{-34}$ J·s].

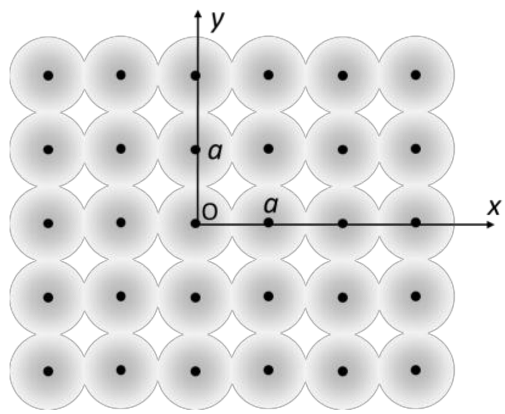

Fig. 1.

Exercise 2: Semiconductors.

Consider an intrinsic semiconductor that can be described as a two band system, with band gap $E_g = 0.75\,\text{eV}$ (assumed to be temperature independent), effective mass of the electrons in the conduction band $m_c = 0.2\,m_0$ and effective mass of the holes in the valence band $m_v = 0.3\,m_0$, where $m_0 = 9.11 \times 10^{-31}$ kg is the free electron mass. Assume the origin of the energies at the top of the valence band, ε_v, so that $\varepsilon_v = 0$ and the bottom of the conduction band is $\varepsilon_c = E_g$.

1. Calculate the density of electrons in the conduction band n_c, the density of holes in the valence band p_v, and the value of the chemical potential μ_i (in eV, the subscript i indicates that the quantity refers to the intrinsic regime) at a temperature $T = 300$ K.

[Note that 1 eV corresponds to a temperature of 1.16×10^4 K or to an energy of 1.60×10^{-19} J, the Planck constant is $\hbar = 1.05 \times 10^{-34}$ J·s, and the Boltzmann constant is $\kappa_B = 1.38 \times 10^{-23}$ J·K^{-1}].

2. Suppose now that the system is doped with a density $N_d = 5 \times 10^{20}\,\text{m}^{-3}$ of donor atoms and a density $N_a = 2 \times 10^{20}\,\text{m}^{-3}$ of acceptor atoms (each atom donates or accepts one electron). Assuming that at $T = 300$ K the system is in the predominantly extrinsic regime, and that donors and acceptors are fully ionized, calculate the density of electrons in the conduction band n_c, the density of holes in the valence band p_v, and the value of the chemical potential μ (in eV). Based on your results, show that the assumption of a predominantly extrinsic regime is consistent.

Solution of the mid-term assessment test
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Exercise 1.

1. We have

$$E(k_x,k_y)=E_s-\beta-\sum_{\boldsymbol{R}=\boldsymbol{R}_1,\boldsymbol{R}_2}\gamma(\boldsymbol{R})\,\mathrm{e}^{\mathrm{i}\,\boldsymbol{k}\cdot\boldsymbol{R}},$$

where $\boldsymbol{R}_1=(\pm a,0);\,(0,\pm a)$, $\boldsymbol{R}_2=(\pm a,\pm a)$, and $\boldsymbol{k}=(k_x,k_y)$. Then

$$E(k_x,k_y)=E_s-\beta-2\gamma_1\left[\cos(k_xa)+\cos(k_ya)\right]-4\gamma_2\cos(k_xa)\cos(k_ya).$$

2. Setting to zero the derivatives

$$\frac{\partial E}{\partial k_x}(k_x,k_y)=2\gamma_1a\sin(k_xa)+4\gamma_2a\sin(k_xa)\cos(k_ya),\qquad \frac{\partial E}{\partial k_y}(k_x,k_y)=2\gamma_1a\sin(k_ya)+4\gamma_2a\cos(k_xa)\sin(k_ya),$$

we find the minimum at $(k_x,k_y)=(0,0)$ and the maximum at $(k_x,k_y)=\left(\frac{\pi}{a},\frac{\pi}{a}\right)$. Since

$$E(\min)=E_s-\beta-4\gamma_1-4\gamma_2,\qquad E(\max)=E_s-\beta+4\gamma_1-4\gamma_2,$$

the band amplitude is $E(\max)-E(\min)=8\gamma_1=8\,\mathrm{eV}$.

3. The electron effective mass along the x axis is

$$m_{xx}=\frac{\hbar^2}{2a^2(\gamma_1+2\gamma_2)}=2.31\times10^{-30}\,\mathrm{kg}.$$

Exercise 2.

1. The gap is $E_g=1.20\times10^{-19}\,\mathrm{J}$, hence $E_g/\kappa_B=8.70\times10^3\,\mathrm{K}$. The thermal energy is $\kappa_BT=4.14\times10^{-21}\,\mathrm{J}=2.58\times10^{-2}\,\mathrm{eV}$, hence $E_g/2\kappa_BT=14.5$. The number of intrinsic carriers is

$$n_i=\frac{1}{4}\left(\frac{2\kappa_BT}{\pi\hbar^2}\right)^{3/2}(m_cm_v)^{3/4}\,\mathrm{e}^{-E_g/2\kappa_BT}=1.53\times10^{18}\,\mathrm{m}^{-3}$$

and $n_c=p_v=n_i$. The chemical potential is

$$\mu_i=\frac{E_g}{2}+\frac{3}{4}\kappa_BT\log\frac{m_v}{m_c}=0.383\,\mathrm{eV}.$$

2. The doped semiconductor is n-type, because the number of donors exceeds the number of acceptors. If the dopants are fully ionized

$$n_c\approx N_d-N_a=3\times10^{20}\,\mathrm{m}^{-3},\qquad p_v\approx\frac{n_i^2}{N_d-N_a}=7.80\times10^{15}\,\mathrm{m}^{-3}.$$

The chemical potential is

$$\mu\approx\mu_i+\kappa_BT\log\frac{N_d-N_a}{n_i}=0.519\,\mathrm{eV}.$$

Since $N_a,N_d\gg n_i$, the assumption of a predominantly extrinsic regime is consistent.