Mid-term test of Condensed Matter Physics - january 14th 2022
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Exercise 1. A hexagonal lattice with lattice parameters $a = 0.45\,\mathrm{nm}$ and $c = 0.70\,\mathrm{nm}$ (see left panel of Fig. 1, where the conventional unit cell is shown and a primitive cell is highlighted with thicker lines) hosts a metallic element with outer s orbitals, contributing one electron per primitive cell. Assume that the electron states can be described within a tight-binding approximation, where only the nearest-neighbors transfer integrals in the basal plane, $\gamma_a = 0.25\,\mathrm{eV}$, and along the c axis, $\gamma_c = 0.15\,\mathrm{eV}$, should be considered. All other transfer integrals and all overlap integrals are negligible. The atomic energy of the s orbitals is $E_s = -5.15\,\mathrm{eV}$ and the tight-binding shift is $\beta = 0.35\,\mathrm{eV}$.

1. [5 points] Determine the tight-binding dispersion law $E_{\boldsymbol{k}}$, where $\boldsymbol{k} = (k_x, k_y, k_z)$ is the Bloch wave vector.

2. [8 points] Show that the minimum and maximum of the band are located at the Γ and H points of first Brillouin zone (see right panel of Fig. 1), respectively, then determine the extremal values of the band dispersion, $E_{\boldsymbol{k}}^{\max}$ and $E_{\boldsymbol{k}}^{\min}$, and the band width W.

3. [2 points] Determine the electron density n (number of conduction electrons per unit volume).

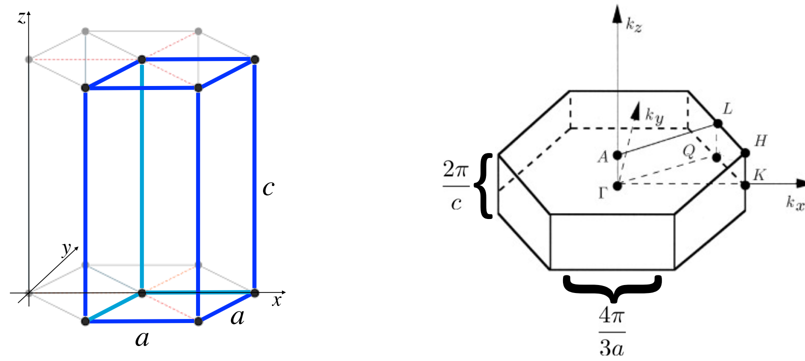

Fig. 1.

Exercise 2. An intrinsic semiconductor with direct gap is formed by a two-dimensional lattice of atoms with even valence. The electron states of the semiconductor can be described within the nearly free electron model, so that the energy vs. quasi-momentum dispersion law of the conduction and valence bands can be approximated by a parabolic expression over the entire first Brillouin zone. Let $E_g = 0.900\,\mathrm{eV}$ be the semiconductor fundamental band gap, and $m_c = 0.05\,m_0$ and $m_v = 0.10\,m_0$ be the electron and hole effective mass (m_0 is the free electron mass), respectively.

1. [5 points] Show that the energy densities of states per unit surface of the conduction and valence band, $g_c(E)$ and $g_v(E)$ respectively, are constant and determine their numerical values.

2. [5 points] Assuming that $(E_c - \mu) \gg k_B T$ and $(\mu - E_v) \gg k_B T$, where E_c is the bottom of the conduction band, E_v is the top of the valence band, and μ is the chemical potential, determine the concentration of electrons and holes, n and h, at $T = 300\,\mathrm{K}$.

3. [5 points] At the same temperature, determine the variation of the chemical potential with respect to its value at $T = 0\,\mathrm{K}$, assuming that the temperature dependence of E_c and E_v can be neglected.

[Useful constants and conversion factors: $\hbar = 1.055 \times 10^{-34}\,\mathrm{J{\cdot}s}$ (Planck's constant), $k_B = 1.381 \times 10^{-23}\,\mathrm{J{\cdot}K^{-1}}$ (Boltzmann's constant), $1\,\mathrm{eV}$ corresponds to $1.602 \times 10^{-19}\,\mathrm{J}$, the free electron mass is $m_0 = 9.109 \times 10^{-31}\,\mathrm{kg}$.].

Solution of the Mid-term test of Condensed Matter Physics - January 14th 2022
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Exercise 1.

1. Let $\boldsymbol{R}_a=(a,0,0)$, $\boldsymbol{R}_\pm=(\frac{a}{2},\pm\frac{a\sqrt{3}}{2},0)$, and $\boldsymbol{R}_c=(0,0,c)$, then we have

$$E_{\boldsymbol{k}}=E_s-\beta-\sum_{\boldsymbol{R}}\gamma(\boldsymbol{R})\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}=E_s-\beta-\gamma_a\sum_{\substack{\boldsymbol{R}=\pm\boldsymbol{R}_a,\\ \pm\boldsymbol{R}_\pm}}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}-\gamma_c\sum_{\boldsymbol{R}=\pm\boldsymbol{R}_c}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}$$

$$=E_s-\beta-2\gamma_a\left\{\cos(k_xa)+\cos\left[\frac{a}{2}(k_x+\sqrt{3}k_y)\right]+\cos\left[\frac{a}{2}(k_x-\sqrt{3}k_y)\right]\right\}-2\gamma_c\cos(k_zc)$$

$$=E_s-\beta-2\gamma_a\left[\cos(k_xa)+2\cos\left(\frac{k_xa}{2}\right)\cos\left(\frac{\sqrt{3}k_ya}{2}\right)\right]-2\gamma_c\cos(k_zc).$$

2. The extrema of the band are located at the simultaneous solutions of the three equations

$$\sin(k_xa)+\sin\left(\frac{k_xa}{2}\right)\cos\left(\frac{\sqrt{3}k_ya}{2}\right)=0,\qquad \cos\left(\frac{k_xa}{2}\right)\sin\left(\frac{\sqrt{3}k_ya}{2}\right)=0,\qquad \sin(k_zc)=0.$$

The last equation has two inequivalent solutions $k_z=0,\frac{\pi}{c}$. The first two equations have the three inequivalent solutions $k_x=0$, $k_y=0$ (center Γ of the basal hexagonal first Brillouin zone); $k_x=0$, $k_y=\frac{2\sqrt{3}\pi}{3a}$ (equivalent under point-group symmetry transformations to the midpoint Q of the side of the basal hexagonal first Brillouin zone in the right panel of Fig. 1); $k_x=\frac{4\pi}{3a}$, $k_y=0$ (corner K of the basal hexagonal first Brillouin zone). All other extremal points are equivalent to the above, either under translation by a reciprocal lattice vector, or under point-group symmetry transformations of the hexagonal lattice.

The direct calculations shows that the minimum of the band is located at $k_x=k_y=k_z=0$ (Γ point), where $E^{\min}_{\boldsymbol{k}}=E_s-\beta-6\gamma_a-2\gamma_c=-7.30\,\mathrm{eV}$; the maximum is located at $k_x=\frac{4\pi}{3a}$, $k_y=0$, $k_z=\frac{\pi}{c}$ (H point), where $E^{\max}_{\boldsymbol{k}}=E_s-\beta+3\gamma_a+2\gamma_c=-4.45\,\mathrm{eV}$. All other inequivalent extremal points are saddle points of the band dispersion. The bandwidth is $W=E^{\max}_{\boldsymbol{k}}-E^{\min}_{\boldsymbol{k}}=9\gamma_a+4\gamma_c=2.85\,\mathrm{eV}$.

3. The volume of the primitive cell is $v=\frac{\sqrt{3}}{2}a^2c$, and there is one conduction electron per primitive cell, so the conduction electron density is

$$n=\frac{1}{v}=\frac{2\sqrt{3}}{3\,a^2c}=8.146\times10^{27}\,\mathrm{m}^{-3}.$$

Exercise 2.

1. The number of states within the k-space surface element $2\pi k\,\mathrm{d}k$ is given by $\mathrm{d}N^{2D} = 2\times 2\pi k\,\mathrm{d}k/(2\pi/L)^2 = \frac{L^2}{\pi}k\,\mathrm{d}k$, where the spin degeneracy is taken into account, $(2\pi/L)^2$ is the k-space surface per permitted k value and L^2 is the surface of the two-dimensional crystal. Given that $E = \frac{\hbar^2 k^2}{2m}$ and $\mathrm{d}k = \frac{1}{2\hbar}\sqrt{\frac{2m}{E}}\,\mathrm{d}E$ one gets the energy density of states for the conduction band

$$\frac{1}{L^2}\frac{\mathrm{d}N_c^{2D}}{\mathrm{d}E} = g_c(E) = \frac{m_c}{\pi\hbar^2} = 2.089\times 10^{17}\,\mathrm{eV}^{-1}\cdot\mathrm{m}^{-2}.$$

Similarly, one gets the energy density of states for the valence band

$$\frac{1}{L^2}\frac{\mathrm{d}N_v^{2D}}{\mathrm{d}E} = g_v(E) = \frac{m_v}{\pi\hbar^2} = 4.178\times 10^{17}\,\mathrm{eV}^{-1}\cdot\mathrm{m}^{-2}.$$

2. The electron concentration is given by

$$n(T) = \int_{E_c}^{+\infty}\mathrm{d}E\,g_c(E)\frac{1}{\mathrm{e}^{\beta(E-\mu)}+1} \approx \frac{m_c}{\pi\hbar^2}k_B T\,\mathrm{e}^{-\beta(E_c-\mu)},$$

where $\beta = 1/(k_B T)$. Similarly, one finds for the hole concentration

$$h(T) = \int_{-\infty}^{E_v}\mathrm{d}E\,g_v(E)\frac{1}{\mathrm{e}^{\beta(\mu-E)}+1} \approx \frac{m_v}{\pi\hbar^2}k_B T\,\mathrm{e}^{-\beta(\mu-E_v)}.$$

Since the semiconductor is intrinsic, from the law of mass action we obtain

$$n(T) = h(T) = \sqrt{n(T)\,h(T)} = k_B T\,\frac{\sqrt{m_c\,m_v}}{\pi\hbar^2}\,\mathrm{e}^{-\beta E_g/2} = 2.105\times 10^{8}\,\mathrm{m}^{-2}.$$

3. From

$$\frac{n(T)}{h(T)} = 1 = \frac{m_c}{m_v}\,\mathrm{e}^{\beta(2\mu-E_c-E_v)}$$

we obtain

$$\mu(T) = \frac{1}{2}(E_c+E_v) + \frac{1}{2}k_B T\log\frac{m_v}{m_c}.$$

Hence,

$$\mu(T) - \mu(0) = \frac{1}{2}k_B T\log\frac{m_v}{m_c} = 8.96\,\mathrm{meV}.$$