§5.4 Effective mass approximation

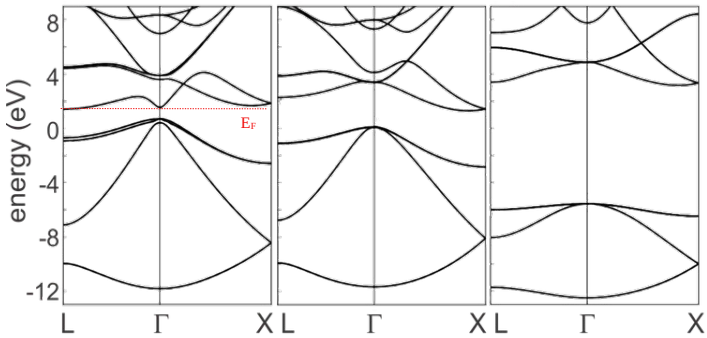

Figure 22

The effective mass approximation is useful to simplify the description of the properties of electrons in semiconductors and dielectrics. The main idea is as follows. The general Schrödinger equation looks like this:

$$\left(-\frac{\hbar^2}{2m}\Delta+V\right)\varphi=E\varphi \tag{1}$$

Here V - exact periodic potential energy for electrons. The result of solution give the energy of electrons (set of bands) $E_n(k_x,k_y,k_z)$. Here n – number of band. As example consider the calculated band structure for Ge crystal (Figure 22). Near the maximum and minimum of $E_n(k_x,k_y,k_z)$, this function can be extended into the Taylor series:

$$E_n(k_x,k_y,k_z)=E_n(k_{0x},k_{0y},k_{0z})+\sum_{\alpha}\frac{dE}{dk_\alpha}\Big|_{k_0}(k_\alpha-k_{0\alpha})+\sum_{\alpha,\beta}\frac{d^2E}{dk_\alpha dk_\beta}\Big|_{k_0}(k_\alpha-k_{0\alpha})(k_\beta-k_{0\beta})+\ldots \tag{2}$$

But in extremum point first derivative is equal to zero so:

$$E_n(k_x,k_y,k_z)=E_n(k_{0x},k_{0y},k_{0z})+\sum_{\alpha,\beta}\frac{d^2E}{dk_\alpha dk_\beta}\Big|_{k_0}(k_\alpha-k_{0\alpha})(k_\beta-k_{0\beta})+\ldots \tag{3}$$

Introduce a new parameter $m^*_{\alpha\beta}=\dfrac{\hbar^2}{2\left(\dfrac{d^2E}{dk_\alpha dk_\beta}\Big|_{k_0}\right)}$ in this case the (3) quadratic form looks like follows:

$$E_n(k_x,k_y,k_z)=E_n(k_{0x},k_{0y},k_{0z})+\sum_{\alpha,\beta}\frac{\hbar^2}{2m^*_{\alpha\beta}}(k_\alpha-k_{0\alpha})(k_\beta-k_{0\beta}) \tag{4}$$

The sum can be diagonalized:

$$E_n(k_x,k_y,k_z)=E_0+\sum_{\gamma}\frac{\hbar^2}{2m^*_\gamma}(k_\gamma-k_{0\gamma})^2 \tag{5}$$

Now this equation we can compare with corresponding equation for free electrons: $E=\dfrac{\hbar^2(k_x^2+k_y^2+k_z^2)}{2m}$ .You can see that (5) and (5.1/16) are practically coincided. For cubic crystal in minimum of energy located in Γ point and on zero level of energy (5) looks like as follows:

$$E_n(k_x,k_y,k_z)=\frac{\hbar^2(k_x^2+k_y^2+k_z^2)}{2m^*} \tag{6}$$

equations are exactly the same. There is only one difference in (6) instead of real mass we use a new parameter which have the name – effective mass of electron. It means that near of minimum or maximum of electron energy we can instead of equation (1) use much more simplest equation:

$$-\frac{\hbar^2}{2m^*}\Delta\varphi=E\varphi \tag{7}$$

without any additional periodic potential. Near the extremum of energy electrons moving like free particles but instead of real masses we need to use in this case the mathematical parameter – effective mass. All effects concerned to real potential, created by other electrons and nuclei, are hidden in effective mass of electron. But this method is well working only near the extremum of electron energy (maximum or minimum).

Do not forget that the effective mass is a mathematical object, it is a second order tensor (second derivative with respect to wave vector projections), the values of which can be negative and depend on the direction of motion of the electron. For example in Ge there are two different effective masses: the transversal m_t=0.082m and longitudinal m_t=1.59m (here m is the mass of free electron).

The tensor of effective mass can be calculated directly for tight binding model by using equation (5.3/18). This tensor is diagonal and all diagonal elements are equal:

$$m_{\alpha\beta}=\frac{\hbar A}{2a^2}\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix} \quad . \tag{8}$$