Corrections of the equation for the Fermi level of impurity isotropic semiconductors

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Abstract: An equation for the Fermi level of impurity isotropic semiconductors is considered when the bottom of the conduction band and the top of the valence band are at the center of the first Brillouin zone. The energy of charge carriers in the valence and conduction bands of semiconductors is considered taking into account the real positions of the top of the valence band and the bottom of the conduction band in the first Brillouin zone. A universal equation for determining the Fermi levels of impurity isotropic semiconductors is presented.

Keywords: first Brillouin zone, valence band, conduction band, Fermi level, semiconductor

The conductivity of semiconductors varies greatly with temperature, which is mainly due to the dependence of the concentration of charge carriers in semiconductors on temperature [1, 2]. Therefore, in order to understand the conductivity and many other properties of semiconductors, it is necessary to study the change of the concentration of charge carriers in semiconductors as a function of temperature. To obtain the concentration of charge carriers in semiconductors, it is necessary to know the exact position of the Fermi level, which depends on the temperature and impurities of the semiconductors. There are many methods in the literature for calculating the Fermi level and the concentration of charge carriers in semiconductors. In some literatures, the Boltzmann distribution is used instead of the Fermi-Dirac distribution [3], thus the obtained equation for the Fermi level is only suitable for non-degenerate semiconductors, but no longer suitable for degenerate semiconductors; in other literatures, although the Fermi-Dirac distribution

function is used to describe the distribution of electrons and holes along energy, various approximations to the Fermi integral are introduced [4, 5], for example, it is assumed that the top of the valence band and the bottom of the conduction band are in the center of the first Brillouin zone. Although the top of the valence band and the bottom of the conduction band are located at the extreme point of the corresponding energy band – the top of the valence band is the maximum of the valence band, and the bottom of the conduction band is the minimum of the conduction band, the extremum of the energy band is not necessarily at the center of the first Brillouin zone ($\boldsymbol{k} = \mathbf{0}$) [6, 7]. In this manuscript, we denote the vector in dark black.

When the top of the valence band and the bottom of the conduction band are at the center of the first Brillouin zone, their energies are expressed as $E_n(\mathbf{0})$,, where n is the number of the energy band.

Since the top of the valence band and the bottom of the conduction band are located at the extreme point of the corresponding energy band, near the extreme point, the energy $E_n(\boldsymbol{k})$ can be expanded to the second order in accordance with the Taylor series:

$$E_n(\boldsymbol{k}) = E_n(\mathbf{0}) + \frac{\hbar^2}{2}\sum_{\alpha}\frac{k_\alpha^2}{m_\alpha^*} \tag{1}$$

Where $\alpha = x, y, z;\ m_\alpha^* = \left[\frac{1}{\hbar^2}\left(\frac{\partial^2 E_n(\boldsymbol{k})}{\partial k_\alpha^2}\right)_{\mathbf{0}}\right]^{-1}$ – effective mass of charge carriers near the edge of the energy band.

In the case of isotropy, the isoenergetic surface in the first Brillouin zone is a sphere, and the electrons have a uniform effective mass m_-^*:

$$m_-^* = \left[\frac{1}{\hbar^2}\left(\frac{\partial^2 E_n(\boldsymbol{k})}{\partial k_x^2}\right)_{\mathbf{0}}\right]^{-1} = \left[\frac{1}{\hbar^2}\left(\frac{\partial^2 E_n(\boldsymbol{k})}{\partial k_y^2}\right)_{\mathbf{0}}\right]^{-1} = \left[\frac{1}{\hbar^2}\left(\frac{\partial^2 E_n(\boldsymbol{k})}{\partial k_z^2}\right)_{\mathbf{0}}\right]^{-1} \tag{2}$$

Similarly, holes have a uniform effective mass m_+^*. Then the energy of electrons near the bottom of the conduction band and the energy of holes near the top of the valence band have the

following forms:

$$E_c(\boldsymbol{k}) = E_- + \frac{\hbar^2}{2m_-^*}|\boldsymbol{k}|^2 \tag{3}$$

$$E_v(\boldsymbol{k}) = E_+ - \frac{\hbar^2}{2m_+^*}|\boldsymbol{k}|^2 \tag{4}$$

Where E_- – the energy of the bottom of the conduction band; E_+ – the energy of the top of the valence band.

The density of the energy state of Bloch electrons has the following form:

$$N(E) = \frac{2V}{(2\pi)^3}\oiint \frac{dS_{E(\boldsymbol{k})}}{|\nabla_{\boldsymbol{k}}E(\boldsymbol{k})|}\Big|_{E(\boldsymbol{k})=E} \tag{5}$$

Where V – the volume of semiconductor; S – isoenergy surface.

Based on (5), one can obtain the density of the energy state of electrons near the bottom of the conduction band:

$$N_-(E) = \frac{V}{2\pi^2}\left(\frac{2m_-^*}{\hbar^2}\right)^{3/2}(E - E_-)^{1/2} \tag{6}$$

The density of energy states of holes near the top of the valence band:

$$N_+(E) = \frac{V}{2\pi^2}\left(\frac{2m_+^*}{\hbar^2}\right)^{3/2}(E_+ - E)^{1/2} \tag{7}$$

With a high concentration of impurities in conductors, the condition $|E - E_F| \gg k_BT$ is no longer met, thus the Fermi-Dirac distribution function is used for any conductor.

Conduction band electrons are distributed according to the function:

$$f_e(E) = \frac{1}{e^{(E-E_F)/k_BT} + 1} \tag{8}$$

Valence band holes are distributed according to the function:

$$f_h(E) = 1 - f_e(E) = \frac{1}{e^{(E_F-E)/k_BT} + 1} \tag{9}$$

Let $(E - E_-)/(k_BT) = \varepsilon_n$, $(E_F - E_-)/(k_BT) = x_n$, $(E_+ - E)/(k_BT) = \varepsilon_p$, $(E_+ - E_F)/(k_BT) = x_p$, then the concentration of the conduction band electrons and the

concentration of the valence band holes in thermal equilibrium are expressed as:

$$n = \frac{(2k_BT)^{1/2}}{\pi^2}\left(\frac{m_-^*}{\hbar^2}\right)^{3/2}\int_0^{\infty}\frac{{\varepsilon_n}^{1/2}}{e^{\varepsilon_n - x_n}+1}d\varepsilon_n \tag{10}$$

$$p = \frac{(2k_BT)^{1/2}}{\pi^2}\left(\frac{m_+^*}{\hbar^2}\right)^{3/2}\int_{-\infty}^{E_+}\frac{{\varepsilon_p}^{1/2}}{e^{\varepsilon_p - x_p}+1}d\varepsilon_p \tag{11}$$

Let in thermal equilibrium N_D – the concentration of donors, N_A – the concentration of acceptors, n_d – the concentration of conduction band electrons excited by donors, p_a – the concentration of the valence band holes excited by acceptors.

In impurity semiconductors, the electrical neutrality condition is expressed as:

$$n - n_d = p - p_a \tag{12}$$

Where

$$\begin{cases} n_d = N_D\dfrac{1}{1+2e^{(E_F-E_D)/k_BT}} \\ p_a = N_A\dfrac{1}{1+2e^{(E_A-E_F)/k_BT}} \end{cases} \tag{13}$$

Combining (10), (11), (12), (13) we obtain the equation for the Fermi level of impurity isotropic semiconductors when the top of the valence band and the bottom of the conduction band are in the center of the first Brillouin zone:

$$\frac{(2k_BT)^{1/2}}{\pi^2}\left(\frac{m_-^*}{\hbar^2}\right)^{3/2}\int_0^{\infty}\frac{{\varepsilon_n}^{1/2}}{e^{\varepsilon_n - x_n}+1}d\varepsilon_n - N_D\frac{1}{1+2e^{(E_F-E_D)/k_BT}} =$$

$$\frac{(2k_BT)^{1/2}}{\pi^2}\left(\frac{m_+^*}{\hbar^2}\right)^{3/2}\int_{-\infty}^{E_+}\frac{{\varepsilon_p}^{1/2}}{e^{\varepsilon_p - x_p}+1}d\varepsilon_p - N_A\frac{1}{1+2e^{(E_A-E_F)/k_BT}} \tag{14}$$

In practical semiconductors, the top of the valence band and the bottom of the conduction band are not necessarily at the center of the first Brillouin zone. Let the top of the valence band be at the position $\boldsymbol{k_{0v}}$ and the bottom of the conduction band at the position $\boldsymbol{k_{0c}}$. Near the extreme point $\boldsymbol{k_0}$, the energy $E_n(\boldsymbol{k})$ can be extended to the second order in accordance with the Taylor series:

$$E_n(\boldsymbol{k}) = E_n(\boldsymbol{k_0}) + \frac{\hbar^2}{2}\sum_{\alpha}\frac{(k_\alpha - k_{0\alpha})^2}{m_\alpha^{*\prime}} \tag{15}$$

Where $m_\alpha^{*\prime} = \left[\frac{1}{\hbar^2}\left(\frac{\partial^2 E_n(\boldsymbol{k})}{\partial k_\alpha^2}\right)_{\boldsymbol{k_0}}\right]^{-1}$ – corrected effective mass of charge carriers near the edge of the energy band.

In the case of isotropy, the isoenergy surface in the first Brillouin zone is a sphere, and the electrons have a uniform effective mass $m_-^{*\prime}$:

$$m_-^{*\prime} = \left[\frac{1}{\hbar^2}\left(\frac{\partial^2 E_n(\boldsymbol{k})}{\partial k_x^2}\right)_{\boldsymbol{k_0}}\right]^{-1} = \left[\frac{1}{\hbar^2}\left(\frac{\partial^2 E_n(\boldsymbol{k})}{\partial k_y^2}\right)_{\boldsymbol{k_0}}\right]^{-1} = \left[\frac{1}{\hbar^2}\left(\frac{\partial^2 E_n(\boldsymbol{k})}{\partial k_z^2}\right)_{\boldsymbol{k_0}}\right]^{-1} \tag{16}$$

Similarly, holes have a uniform effective mass $m_+^{*\prime}$. Then the corrected energy of electrons near the bottom of the conduction band and the corrected energy of holes near the top of the valence band have the following forms:

$$E_c(\boldsymbol{k})' = E_- + \frac{\hbar^2}{2m_-^{*\prime}}|\boldsymbol{k} - \boldsymbol{k_{0c}}|^2 \tag{17}$$

$$E_v(\boldsymbol{k})' = E_+ - \frac{\hbar^2}{2m_+^{*\prime}}|\boldsymbol{k} - \boldsymbol{k_{0v}}|^2 \tag{18}$$

According to (5), the corrected density of energy states of electrons near the bottom of the conduction band is:

$$N_-(E)' = \frac{m_-^{*\prime 1/2}V}{\hbar\pi^2}\cdot\frac{|m_-^{*\prime}\nabla_{\boldsymbol{k}}E/\hbar^2 + \boldsymbol{k_{0c}}|}{[2(E-E_-)]^{1/2}} \tag{19}$$

The corrected density of energy states of holes near the top of the valence band is:

$$N_+(E)' = \frac{m_+^{*\prime 1/2}V}{\hbar\pi^2}\cdot\frac{|\boldsymbol{k_{0v}} - m_+^{*\prime}\nabla_{\boldsymbol{k}}E/\hbar^2|}{[2(E_+-E)]^{1/2}} \tag{20}$$

The corrected concentration of the conduction band electrons and the corrected concentration of the valence band holes in thermal equilibrium are expressed as:

$$n' = \left(\frac{m_-^{*\prime}}{2k_BT\hbar^2\pi^4}\right)^{1/2}\int_0^{\infty}\frac{|m_-^{*\prime}k_BT\nabla_{\boldsymbol{k}}\varepsilon_n/\hbar^2 + \boldsymbol{k_{0c}}|}{{\varepsilon_n}^{1/2}}\frac{1}{e^{\varepsilon_n - x_n}+1}d\varepsilon_n \tag{21}$$

$$p' = \left(\frac{m_+^{*\prime}}{2k_BT\hbar^2\pi^4}\right)^{1/2} \int_0^\infty \frac{\left|m_+^{*\prime}k_BT\nabla_{\boldsymbol{k}}\varepsilon_p/\hbar^2 + \boldsymbol{k}_{0v}\right|}{{\varepsilon_p}^{1/2}} \frac{1}{e^{\varepsilon_p - x_p}+1} d\varepsilon_p \quad (22)$$

Thus, a universal equation for determining the Fermi levels of impurity isotropic semiconductors is obtained:

$$\left(\frac{m_-^{*\prime}}{2k_BT\hbar^2\pi^4}\right)^{1/2} \int_0^\infty \frac{\left|m_-^{*\prime}k_BT\nabla_{\boldsymbol{k}}\varepsilon_n/\hbar^2 + \boldsymbol{k}_{0c}\right|}{{\varepsilon_n}^{1/2}} \frac{1}{e^{\varepsilon_n - x_n}+1} d\varepsilon_n - N_D \frac{1}{1+2e^{(E_F-E_D)/k_BT}} =$$

$$\left(\frac{m_+^{*\prime}}{2k_BT\hbar^2\pi^4}\right)^{1/2} \int_0^\infty \frac{\left|m_+^{*\prime}k_BT\nabla_{\boldsymbol{k}}\varepsilon_p/\hbar^2 + \boldsymbol{k}_{0v}\right|}{{\varepsilon_p}^{1/2}} \frac{1}{e^{\varepsilon_p - x_p}+1} d\varepsilon_p - N_A \frac{1}{1+2e^{(E_A-E_F)/k_BT}} \quad (23)$$

In comparison with equation (14), in equation (23) a new quantity $\nabla_{\boldsymbol{k}}\varepsilon_n$ appears, which like the effective mass depends on the structure of the energy band.

Conflicts of Interest: The authors declare no conflict of interest.

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