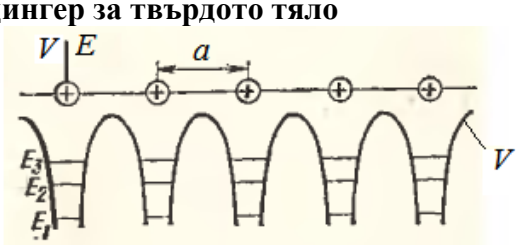
ОСНОВИ НА ЗОННАТА ТЕОРИЯ НА ТВЪРДИТЕ ТЕЛА

1. Уравнение на Шрьодингер за твърдото тяло



$$\hat{H}\psi = E\psi\,, \tag{1}$$

$$\psi = \psi(r_1, r_2 \ldots r_n, R_1, R_2 \ldots R_N)\,.$$

$$\hat{H} = \hat{T}_e + \hat{T}_z + \hat{U}_e + \hat{U}_z + \hat{U}_{ez}\,.$$

$$\hat{T}_e = \sum_i \hat{T}_i = \sum_i \left(-\frac{\hbar^2}{2m}\Delta_i \right),$$

$$\hat{T}_z = \sum_\alpha \hat{T}_\alpha = \sum_\alpha \left(-\frac{\hbar^2}{2M_\alpha}\Delta_\alpha \right),$$

$$\hat{U}_e = \frac{1}{2}\sum_i \sum_{j,i\neq j} \left(\frac{e^2}{4\pi\varepsilon_0 r_{ij}} \right),$$

$$\hat{U}_z = \hat{U}_z(R_1, R_2 \ldots R_N)\,.$$

$$\hat{U} = \hat{U}(r_1, r_2 \ldots r_n, R_1, R_2 \ldots R_N)\,.$$

2. Адиабатно приближение и валентна апроксимация

$$R_\alpha = R_{\alpha 0} = const\,.$$

$$\left[\sum_i \left(-\frac{\hbar^2}{2m}\Delta_i \right) + \frac{1}{2}\sum_i \sum_{j,i\neq j} \left(\frac{e^2}{4\pi\varepsilon_0 r_{ij}} \right) + U(r_1, r_2 \ldots r_n, R_1, R_2 \ldots R_N) \right] \psi_e = E_e \psi_e\,, \tag{2}$$

3. Едноелектронно приближение

$$U = \sum_i U_i(r_i),$$

$$\left\{ \sum_i \left(-\frac{\hbar^2}{2m}\Delta_i + \Omega_i(r_i) + U_i(r_i) \right) \right\} \psi_e = E_e \psi_e\,. \tag{3}$$

$$\hat{H}\psi_e = \left\{ \sum_i \hat{H}_i \right\} \psi_e = E_e \psi_e\,.$$

$$\hat{H}_i = -\frac{\hbar^2}{2m}\Delta_i + \Omega_i(r_i) + U_i(r_i)\,. \tag{4}$$

$$\psi_e(r_1, r_2, \ldots) = \psi_1(r_1)\psi_2(r_2)\ldots = \prod_i \psi_i(r_i)\,.$$

$$E_e = E_1 + E_2 + \ldots = \sum_i E_i\,.$$

$$\hat{H}_1\psi_1 = E_1\psi_1,\ \hat{H}_2\psi_2 = E_2\psi_2 \text{ и т.н.}$$

$$\hat{H}\psi = E\psi\,,$$

$$V(r) = U(r) + \Omega(r),$$

$$\left[-\frac{\hbar^2}{2m}\Delta + V(r)\right]\psi(r) = E\psi(r). \tag{5}$$

$$V(r) = V(r + a_n),$$
$$\psi_k(r) = e^{ikr}U_k(r),$$
$$\hat{H}\psi_k(r) = E\psi_k(r).$$

4. Енергетичен спектър на електроните в кристала

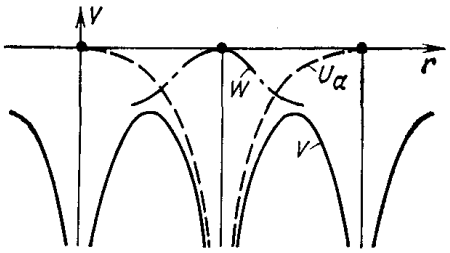
$$\left[-\frac{\hbar^2}{2m}\Delta + U_a(r)\right]\psi_a(r) = E_a\psi_a(r), \tag{6}$$

$$\hat{H}_a = -\frac{\hbar^2}{2m}\Delta + U_a(r)$$

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta + V(r)$$

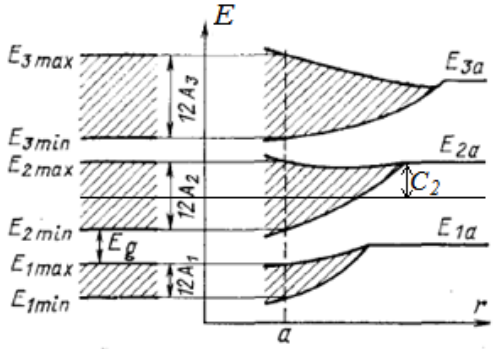
$$\hat{H} = \hat{H}_a + W(r).$$

$$W(r) = V(r) - U_a(r). \tag{7}$$



$$E = E_a + D(\sum_g e^{ikq}).$$

$$E = E_a + C + 2A(\cos k_x a + \cos k_y a + \cos k_z a). \tag{8}$$



$$E_{max} = E_a + C + 6A, \quad E_{min} = E_a + C - 6A, \quad E_{max} - E_{min} = 12A,$$
$$E(k) = E(-k).$$
$$N = \frac{V}{a^3} = \frac{1}{64.10^{-24}} \approx 10^{22} cm^{-3}.$$

5. Квазиимпулс

$$E = \frac{p^2}{2m}, \quad \lambda = \frac{h}{p} = \frac{h}{mv}, \quad k = \frac{2\pi}{\lambda}, \quad p = \hbar k, \quad E = \frac{\hbar^2 k^2}{2m},$$

като $\hbar = h/2\pi$ е квантът на действието.

$$E(p) = E(-p).$$

6. Зони на Брилуен

$$k_i = \frac{2\pi}{L_i} n_j, \quad i = x, y, z; \quad j = 1, 2, 3,$$

$$E(k_i) = E(k_i + n\frac{2\pi}{a_i}), \tag{9}$$

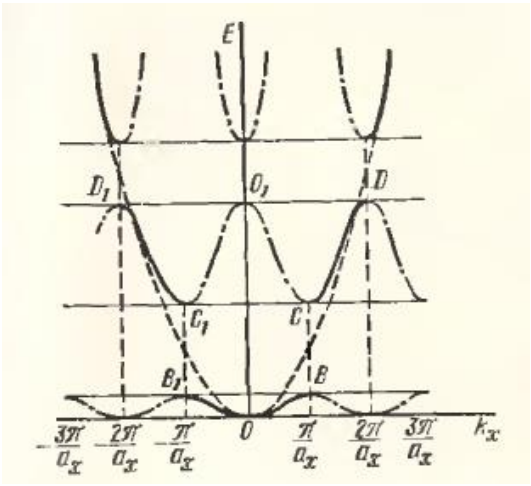
$$-\frac{\pi}{a_i} \le k_i < \frac{\pi}{a_i},$$

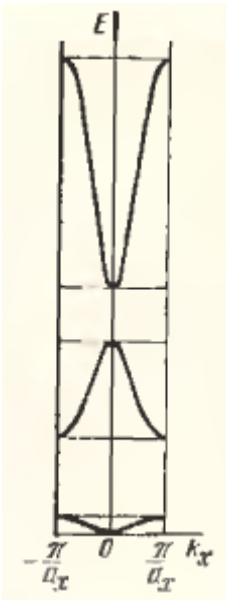
Втората зона на Брилуен

$$-\frac{2\pi}{a_i} \le k_i < -\frac{\pi}{a_i} \qquad \text{и} \qquad \frac{\pi}{a_i} \le k_i < \frac{2\pi}{a_i}.$$

Третата зона на Брилуен

$$-\frac{3\pi}{a_i} \le k_i < -\frac{2\pi}{a_i} \qquad \text{и} \qquad \frac{2\pi}{a_i} \le k_i < \frac{3\pi}{a_i}.$$





$$E(k) = const.$$