QUANTUM LEVELS OF ELECTRONS IN SEMICONDUCTORS IN THE PRESENCE OF A STRONG ELECTRIC FIELD

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The energy levels of an electron moving in a periodic field of a crystal in the presence of a strong electric field are determined. The existence of a band structure, that is, of maximum and minimum values of the kinetic energy of the electron, leads to a finite motion in ordinary space, and consequently to quantization of the energy levels. The case is considered when two bands come close together. It is shown that if allowance is made for transitions from one band to the other, the energy levels corresponding to different bands can never cross.

1. ELECTRON LEVELS IN A CRYSTAL IN AN ELECTRIC FIELD

IN the presence of an external electric field, the electron levels can be obtained by solving the corresponding Schrödinger equation

$$(\hat{H}_0 - e\mathbf{Er})\psi = \varepsilon\psi, \qquad (1)$$

where $\hat{H}_0$ is the Hamiltonian of the electron in the periodic field of the crystal and $\mathbf{E}$ is the electric field intensity vector. It is more convenient, however, to go over to momentum space. To this end we expand $\psi(\mathbf{r})$ in powers of the wave functions of the electron in the crystal

$$\psi(\mathbf{r}) = \sum_n \int d\mathbf{p} e^{i\mathbf{pr}} u_n(\mathbf{p}, \mathbf{r}) c_n(\mathbf{p}). \qquad (2)$$

Here n is the number of the energy band, while the remaining notation is standard. Substituting (2) in (1), we obtain the following expression for the functions $c_n(\mathbf{p})$:

$$\varepsilon_n c_n - ie\hbar\mathbf{E}\frac{dc_n}{d\mathbf{p}} - e\mathbf{E}\sum_m{}' \mathbf{r}_{nm}c_m = \varepsilon c_n. \qquad (3)$$

In the derivation of (3) we took account of the fact that in the crystal the operator $\mathbf{r}$ has matrix elements corresponding to interband transitions (but with the same value of $\mathbf{p}$), and the intraband operator $\mathbf{r} = i\hbar\,\partial/\partial\mathbf{p}$. It is obvious that not too strong an electric field (the exact condition will be formulated later) leads to exponentially small probabilities of the transition from one phase to another, that is, in first approximation we can discard in (3) the term with r_{nm}. On the other hand, if we nonetheless take into account such transitions, then this will be done only between bands separated by a minimum energy gap.

We shall henceforth assume that there exist two bands, the gap between which is considerably smaller than the energy gaps between these bands and the remaining bands. Only these bands will be taken into account in Eq. (3), which we shall solve by quasiclassical methods. The system of equations now takes the form

$$\varepsilon_1 c_1 - ie\hbar E dc_1/dp_x - eEx_{12}c_2 = \varepsilon c_1,$$

$$\varepsilon_2 c_2 - ie\hbar E dc_2/\partial p_x - eEx_{21}c_1 = \varepsilon c_2, \qquad (4)$$

(we choose the direction of E as the x axis.)

It is convenient to introduce new functions $a_{1,2}$ such that

$$c_{1,2} = \exp\left\{\frac{i}{e\hbar E}\int^{p_x}\left(\varepsilon - \frac{\varepsilon_1+\varepsilon_2}{2}\right)dp_x'\right\}a_{1,2}. \qquad (5)$$

Then for $a_{1,2}$ we obtain

$$\tfrac{1}{2}(\varepsilon_1-\varepsilon_2)a_1 - ie\hbar E da_1/dp_x - eEx_{12}a_2 = 0,$$

$$\tfrac{1}{2}(\varepsilon_1-\varepsilon_2)a_2 + ie\hbar E da_2/dp_x + eEx_{21}a_1 = 0. \qquad (6)$$

It is easy to verify with the aid of (6) that the solutions $a_{1,2}$ have the following property:

$$|a_1|^2 + |a_2|^2 = \text{const.} \qquad (7)$$

The term in (6), describing the interband transitions, is small everywhere, except at the point in the complex plane p_x, where $\epsilon_1(p_x^{(0)}) = \epsilon_2(p_x^{(0)})$. Therefore we can neglect this term near the ground state, and we obtain

$$a_{1,2} = A_{1,2}\exp\left\{\mp\frac{i}{2e\hbar E}\int^{p_x}(\varepsilon_1-\varepsilon_2)dp_x'\right\}. \qquad (8)$$

Moving along the real axis, we have both to the left and to the right of the singular point solutions of the type (8), but with different coefficients. It follows from (7) that in this case the coefficients on the left and on the right are connected by means of the unitary matrix

$$U=\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}, \tag{9}$$

and α and δ are obviously the transmission coefficients of the waves $a_{1,2}$ respectively, that is, $|\alpha| = |\delta| = D$ is the transmission coefficient ($D < 1$), and inasmuch as the phases of α and δ are determined essentially by the phase in (8), we have on going from $p_x^{(1)}$ to $p_x^{(2)}$

$$\alpha = D\exp\left\{-\frac{i}{2e\hbar E}\int_{p_x^{(1)}}^{p_x^{(2)}}(\varepsilon_1-\varepsilon_2)\,dp_x'\right\},$$

$$\delta = D\exp\left\{\frac{i}{2e\hbar E}\int_{p_x^{(1)}}^{p_x^{(2)}}(\varepsilon_1-\varepsilon_2)\,dp_x'\right\}. \tag{10}$$

In addition, it follows from the property of unitary matrices that

$$|\alpha|^2+|\beta|^2=1,\quad |\gamma|^2+|\delta|^2=1,\quad \beta=-\gamma^*. \tag{11}$$

From this we obtain the eigenvalues of the matrix U

$$\lambda_{1,2} = D\cos\varphi \pm i(1-D^2\cos^2\varphi)^{1/2}, \tag{12}$$

$$\varphi = \frac{1}{2e\hbar E}\int_{p_x^{(1)}}^{p_x^{(2)}}(\varepsilon_1-\varepsilon_2)\,dp_x'. \tag{13}$$

We shall henceforth assume that the field is directed along one of the crystallographic axes. In this case

$$c_{1,2}(p_x+p_{x0})$$

$$=\lambda_{1,2},c_{1,2}(p_x)\exp\left\{\frac{i}{e\hbar E}\int_0^{p_{x0}}\left(\varepsilon-\frac{\varepsilon_1+\varepsilon_2}{2}\right)dp_x'\right\}, \tag{14}$$

where p_{x_0} is the component of the reciprocal-lattice vector along the x axis, and $p_x^{(2)}-p^{(1)}=p_{x_0}$. The periodicity condition $c_{1,2}(p_x+p_{x_0})=c_{1,2}(p_x)$ then leads, with account of (14) and (12), to the relation

$$\varepsilon=\frac{1}{2p_{x0}}\int_0^{p_{x0}}(\varepsilon_1+\varepsilon_2)p_x'+\hbar\omega\left(n\pm\frac{\psi}{2\pi}\right) \tag{15}$$

where n is an arbitrary integer (positive or negative)

$$\omega=2\pi eE/p_{x_0},\quad \psi=\arccos(D\cos\varphi_0),$$

$$\varphi_0=\frac{1}{2e\hbar E}\int_0^{p_{x0}}(\varepsilon_1-\varepsilon_2)\,dp_x'. \tag{16}$$

We note that ω is the frequency of the classical motion. Indeed, $dp_x/dt = eE$ or $p_x = eEt + p_0$. The period of the motion is determined from the condition $\Delta p_x = eET = p_{x_0}$, from which follows $\omega = 2\pi eE/p_{x_0}$.

We see from (15) that the energy levels will be completely determined if we know the coefficient D. Before we find D, let us investigate the general properties of (15). We first put D = 1, that is, we do not take into account the interband transitions. Then $\psi = \varphi_0$ and we obtain

$$\varepsilon=\hbar\omega n+\frac{1}{p_{x0}}\int_0^{p_{x0}}\varepsilon_{1,2}\,dp_x', \tag{17}$$

i.e., a system of equidistant levels, corresponding to the first and second bands, shifted by an amount

$$\frac{1}{p_{x0}}\int_0^{p_{x0}}(\varepsilon_1-\varepsilon_2)\,dp_x'=\bar{\varepsilon}_1-\bar{\varepsilon}_2.$$

The existence of such a quantization of the electron levels in the lattice, in the presence of an electric field, was first indicated in[1].

At some value of E it may turn out that $\bar{\epsilon}_1-\bar{\epsilon}_2=\hbar\omega k$, where k is some number. This means crossing of levels of different bands, since the level of one band with given n corresponds to the same value of the energy of a different band, but shifted in number. If we now turn to the exact expressions for the levels, we find that the energies of both bands differ by an amount $\hbar\omega\psi/\pi$. It is clear from the expression for ψ that when D = 1 we actually can make $\psi = k\pi$ (in this case $\psi = \varphi_0$), which is just what we designate as level crossing. On the other hand, if we assume that D < 1, then ψ is never equal to $k\pi$. More accurately, $|\cos\psi| \leq D$ and when $\cos\psi = -D$ we have

$$\psi=k\pi+(1-D^2)^{1/2}=k\pi+R.$$

Therefore the minimum distance between the energy levels is

$$\hbar\omega R/\pi,\qquad R=(1-D^2)^{1/2}. \tag{18}$$

The value of R is obviously the coefficient of transition from one band to the other ($R \ll 1$).

We now proceed to calculate D and R, i.e., to solve the system (6). To this end, it is necessary to find the dependence of $x_{12}(x_{21})$ on p_x. Since the origin from which p_x is measured is immaterial, we place it at the point where $\epsilon_1-\epsilon_2$ is minimal and equal to Δ. If we use perturbation theory in the vicinity of $p_x = 0$ and take only the two bands in question into account, then

$$\varepsilon_{1,2}={}^1\!/_2[\varepsilon_1(0)+\varepsilon_2(0)]$$

$$\pm[\Delta^2/4+p_x^2|p_{12}(0)|^2/m^2]^{1/2}, \tag{19}$$

where $p_{12}^{(0)}$ is the matrix element of the momentum operator between the states with $p_x = 0$.

It is further obvious that $x_{12} = p_{12}/im(\epsilon_1 - \epsilon_2)$, and we must relate p_{12} with $p_{12}^{(0)}$. However, in second order perturbation theory, we have

$$\frac{1}{2}\frac{\partial^2\varepsilon_1}{\partial p_x^2}=\frac{1}{m^2}\frac{|p_{12}|^2}{\varepsilon_1-\varepsilon_2}.$$

Substituting here (19) and using the connection between x_{12} and p_{12}, we obtain finally

$$x_{12}=\frac{\Delta p_{12}(0)}{im}\left[\Delta^2+\frac{4p_x^2|p_{12}(0)|^2}{m^2}\right]^{-1}. \tag{20}$$

Generally speaking $p_{12}(0)$ can have a certain phase, but it is clear from the form of (6) that by redesignating $a_{1,2}$ we can readily get rid of it. Therefore we shall henceforth take $p_{12}(0)$ to be a real quantity. It is also natural to introduce the notation

$$\frac{p_{12}(0)}{m\sqrt{\Delta}}=\frac{1}{(2m^*)^{1/2}},\quad \tau=\frac{2p_xp_{12}(0)}{m\Delta},$$

$$\mu=\frac{m\Delta^2}{2eE\hbar p_{12}(0)}=\frac{\Delta^{3/2}(2m^*)^{1/2}}{2e\hbar E}$$

(then m^* is the effective mass near the gap). Substituting all this in (6) we have after elementary transformations

$$\begin{aligned}&\frac{da_1}{d\tau}+\frac{i\mu}{2}(1+\tau^2)^{1/2}a_1-\frac{1}{2}\frac{a_2}{1+\tau^2}=0.\\&\frac{da_2}{d\tau}-\frac{i\mu}{2}(1+\tau^2)^{1/2}a_2+\frac{1}{2}\frac{a_1}{1+\tau^2}=0.\end{aligned} \tag{21}$$

The system (21) coincides with that which arises in the theory of inelastic collisions and has been solved in a paper by one of the authors and Chaplik[2], where it was found that

$$R=(1-D^2)^{1/2}=e^{-\pi\mu/2}=\exp\left\{-\frac{\pi\Delta^{3/2}(2m^*)^{1/2}}{2e\hbar E}\right\} \tag{22}$$

This solves completely the problem of finding the energy levels.

We note that the results obtained in the present paper can apparently be used in semiconductor theory.

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[1] Chynoweth, Wannier, Logan, and Thomas, Phys. Rev. Lett. **5**, 57 (1960).

[2] A. M. Dykhne and A. V. Chaplik, JETP **43**, 889 (1962), Soviet Phys. JETP **16**, 631 (1963).

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