A NEW METHOD OF CALCULATING THE ENERGY SPECTRUM OF CARRIERS IN SEMICONDUCTORS. II. ACCOUNT OF SPIN-ORBIT INTERACTION

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The method previously developed for constructing the Hamiltonian in the effective-mass approximation is generalized for the cases when spin-orbit interaction must be taken into account. This method is used to calculate the change of the energy spectrum when semiconductors with wurtzite or germanium lattices are deformed.

1. INTRODUCTION

In the first part of the present work,[1] a general method was developed for constructing the Hamiltonian $\mathcal{D}$ in the effective mass approximation; the method was based directly on the symmetry conditions and the invariance of the Schrödinger equation to time inversion. We shall consider how spin-orbit interaction can be accurately included in the framework of this method. We retain the notation of[1], and when referring to formulae from it we use the prefix I before the number of the formula.

To calculate $\mathcal{D}$ including spin-orbit interaction two procedures are possible: in the Hamiltonian $\hat{\mathcal{H}}$ the term describing the spin-orbit interaction for $V(\mathbf{r}) = V_0(\mathbf{r})$

$$\hat{\mathcal{H}}_{s.o.} = -(i/4m^2c^2)([\nabla V_0, \nabla]\hat{\sigma}),$$

can, on the one hand, be included in $\hat{\mathcal{H}}_1$, i.e., considered as a perturbation, since the interaction is relatively small; on the other hand, since $\hat{\mathcal{H}}_{s.o.}$ does not depend on $\mathcal{K}$ and has the same symmetry as $\hat{\mathcal{H}}_0$, this term can be immediately included in $\hat{\mathcal{H}}_0$, and only those terms describing the spin-orbit interaction which included $\mathcal{K}$ are retained in $\hat{\mathcal{H}}_1$.

In the first case the spin functions will appear in the smooth functions F_i in (I.2), and the basis functions $\varphi_{i\mathbf{k}_0}$ will, as before, depend only on the coordinates. In the second case, however, $\varphi_{i\mathbf{k}_0}$ will include functions of the spin variables, and F_i will not.

We shall consider both these methods.

2. $\hat{\mathcal{H}}_{s.o.}$ INCLUDED IN $\hat{\mathcal{H}}_1$

In this case the functions F_i depend both on the coordinates and on the spin variable α, which can take the two values $\pm 1/2$. Correspondingly, $\mathcal{D}$ depends both on the operators $\hat{\mathcal{K}}$, which act on the coordinate functions, and on the operators $\hat{\sigma}_i$, which act on the spin functions. The operator $\mathcal{D}$ can, as previously, be expressed in terms of basis matrices and written in the form (I.9), but now $f(\mathcal{K})$ will contain not only functions of the quantities k_i, H_i, ϵ_{ij}, etc., and their products, but also linear functions of $\hat{\sigma}_i$, which describe the spin-orbit splitting at the point $\mathbf{k}_0$, and functions of the products of $\hat{\sigma}_i$ and the remaining variables. In accord with (I.11) all these functions must be chosen so that they transform according to the irreducible representations of the point group $\bar{G}$, corresponding to the wave vector group $G_{\mathbf{k}_0}$. It is clear that the $\hat{\sigma}_i$ themselves transform as the components of an axial vector, and $\mathcal{D}$ must be constructed so that the terms entering in it satisfy condition (I.10). The constants C_s^{rt} for the terms containing $\hat{\sigma}_i$ are then small quantities relative to the other corresponding constants—of the order β^2, where $\beta = v/c$. Since in[1] the form of the operators appearing in $\mathcal{D}$ was nowhere precisely specified, but was denoted by the general symbol $\mathcal{K}$, it is clear that all the results of [1], in particular the formula for determining n_s taking into account the invariance to time inversion, and the methods for constructing $\mathcal{D}$, remain valid in the present case also. When determining γ in (I.18) it must be remembered that $\hat{\sigma}_i$ are odd functions, since, when changing t into $-t$ in $\hat{\mathcal{H}}$ it is necessary to change $\hat{\sigma}_i$ into $-\hat{\sigma}_i$.[2]

To construct $\mathcal{D}$ it is convenient to choose at once $F_i(\mathbf{r}, \alpha, t)$ in the form of products of coordinate functions $F_{i,\alpha}(\mathbf{r}, t)$ and spin functions α. Then the system (I.3) takes the form

$$\mathcal{D}_{ij}(\mathcal{K}) F_{j,\beta} \cdot \beta = i\hbar\alpha \partial F_{i,\alpha}/\partial t.$$

Hence we obtain the system of equations determining the coordinate functions $F_{i,\alpha}$:

$$\mathcal{D}_{i\alpha, j\beta}(\mathcal{K}') F_{j,\beta} = i\hbar \partial F_{i,\alpha}/\partial t, \quad (1)$$

where

$$\mathcal{D}_{i\alpha, j\beta}(\mathcal{K}') = \langle \alpha | \mathcal{D}_{ij}(\mathcal{K}) | \beta \rangle.$$

In $\mathcal{K}'$ in (1) the operators $\hat{\sigma}$ are, of course, not included.

If the matrices A^t_{sl} are formed by one of the methods given in [1], it is easy to set up $\mathcal{D}$ in (1). The functions $f^r_{sl}(\mathcal{K})$ in $\mathcal{D}$ are now products of functions of all the operators $\mathcal{K}'$, including unity, and the spin operators $\hat{\sigma}_r$, which are linear combinations of the Pauli operators or the unit operator, i.e.,

$$f^r_{sl}(\mathcal{K}) = f^r_{sl}(\mathcal{K}') \hat{\sigma}_r. \quad (2)$$

Therefore, if

$$\mathcal{D}(\mathcal{K}) = \sum_{t,r,s,l} C^{tr}_s A^t_{sl} f^r_{sl}(\mathcal{K}),$$

then

$$\mathcal{D}(\mathcal{K}') = \sum_{t,r,s,l} C^{tr}_s A^{tr}_{sl} f^r_{sl}(\mathcal{K}'). \quad (3)$$

Here $\mathcal{D}(\mathcal{K}')$ is expressed in terms of matrices A^{tr}_{sl} of rank $2n \cdot 2n$, which are constructed in the basis $\varphi_{i\mathbf{k}_0} \cdot \alpha$, with the matrix elements

$$A^{tr}_{sl,\, i\alpha,\, j\beta} = A^t_{sl,\, ij} \hat{\sigma}_{r\alpha\beta}. \quad (4)$$

Knowing the matrices A^t_{sl} it is possible to construct at once these matrices also, since $\hat{\sigma}_r$ is either a unit matrix or a combination of Pauli matrices determined from (2).

3. $\hat{\mathcal{H}}_{s.o.}$ INCLUDED IN $\hat{\mathcal{H}}_0$

The functions $\varphi_{i\alpha} = \varphi_{i\mathbf{k}_0} \cdot \alpha$ which are the basis of the matrices $\mathcal{D}(\mathcal{K}')$ in (3) transform according to the double-valued representation T', which is the direct product of the representation T_0 and the double-valued representation $T'_{1/2}$, according to which the spin functions α transform: $T' = T_0 \times T'_{1/2}$. This representation T' is in general reducible, and decomposes into the irreducible representations T'_0. If the spin-orbit splitting is sufficiently large, it is often not necessary to consider together all these representations, and it is sufficient to set up $\mathcal{D}$ only for one of the irreducible double-valued representations T'_0 corresponding to the extremum point. Of course, this matrix can also be obtained from (3); however, in the present case it is simpler to include at once $\hat{\mathcal{H}}_{s.o.}$ in $\hat{\mathcal{H}}_0$, and to choose as basis the eigen functions $\varphi'_{i\mathbf{k}_0}(\mathbf{r}, \alpha)$ of the Hamiltonian $\hat{\mathcal{H}}''_0 = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_{s.o.}$, which transform according to the representation T'_0. As before $\mathcal{D}$ can be written in the form (I.9), where $\mathcal{K}$ does not, of course, contain the operators $\hat{\sigma}$. Obviously, it is also possible to proceed when the representation $T' = T_0 \times T'_{1/2}$ is irreducible. In this case the n^2 linearly independent matrices A^t_{sl} are the basis for constructing $\mathcal{D}$, where n is the dimension of a representation T'_0. It is obvious here that Eq. (I.8) remains in force, i.e., these matrices transform according to the representations T_s contained in the product $T'_0 \times T'^*_0$. For $\chi_0(G)$ in (I.8) must now be understood the characters of the double-valued representation T'_0. If, as usual,[3] a new element $Q = C_{2\pi}$ is introduced to the group $G_{\mathbf{k}_0}$, in order to change it from a double-valued representation to a single-valued, the summation in (I.8) must be made over all the elements of this new group $G'_{\mathbf{k}_0}$, and h is to be understood as the number of elements in it. The characters of the corresponding representation of this group will be denoted below by $\chi'_0(G)$. The result of the calculations will, of course, be the same as when the double-valued representations of the group $G_{\mathbf{k}_0}$ are used. It is clear that the matrices A_{sl} and $f_{sl}(\mathcal{K})$ transform according to single-valued representations, i.e., the representations T_s of the point group $\overline{G}$, for which $Q = E$, while for the representations T'_0 we have $\chi'(Q) = -\chi'(E)$.

We now consider the additional conditions imposed on $\mathcal{D}$ in the present case by the time inversion invariance conditions. In distinction from (I.1), we now have $\hat{\mathcal{H}}^*_0 \neq \hat{\mathcal{H}}_0$, since $\hat{\mathcal{H}}_0$ now includes an imaginary term $\hat{\mathcal{H}}_{s.o.}$. In order to obtain from $\hat{\mathcal{H}}^*$ a Hamiltonian coinciding with $\hat{\mathcal{H}}$, it is now inadequate to replace H_i by $-H_i$ and k_i by $-k_i$, and it is necessary to perform a unitary transformation[2] S', so that $S' \hat{\mathcal{H}}^*_{s.o.} S'^{-1} = \hat{\mathcal{H}}_{s.o.}$, or $\hat{S}' \hat{\sigma}^*_i S'^{-1} = -\hat{\sigma}_i$; consequently $\hat{S}' = \hat{\sigma}_y$. Here, as in [1], the Hamiltonian $S\hat{\mathcal{H}}' S^{-1} = \hat{\mathcal{H}}$. Here $\hat{S}$ is the Wigner operator, $\hat{S} = \hat{S}_0 \hat{S}'$, where $\hat{S}_0$ is the complex conjugate operator. Therefore, the functions $\hat{S}\Psi'$, as well as the functions Ψ, are eigen functions of $\hat{\mathcal{H}}$, corresponding to the same eigen values E and k. The stroke denotes, as in (I.12) the replacement of H_i by $-H_i$ and of k_i by $-k_i$; the change of sign for $\hat{\sigma}_i$ in $\hat{\mathcal{H}}^*$ is now performed by the unitary transformation S'.

From the conjugate equation we again obtain the system (I.12), but now the functions $\hat{S}\varphi_{i\mathbf{k}_0}(\mathbf{r}, \alpha) = \hat{\sigma}_y \varphi^*_{i\mathbf{k}_0}(\mathbf{r}, \alpha)$ are the basis of $\mathcal{D}'^*$ in (I.12), whilst the functions $\varphi_{i\mathbf{k}_0}(\mathbf{r}, \alpha)$ are the basis of $\mathcal{D}$ in (I.3). For brevity in what follows, we shall not write out the arguments of these functions.

If a linear relationship exists between the functions $\hat{S}\varphi_i$ and φ_i, then, as previously, additional conditions are imposed on $\mathscr{D}$. According to [2] for double-valued representations such a relationship occurs in case c; in cases a and $b_{1,2}$ additional degeneracy occurs. If $\mathbf{k}_0$ and $-\mathbf{k}_0$ belong to different stars (i.e., in case b_3), then, as previously, no additional conditions, apart from (I.6), are imposed on $\mathscr{D}$.

We now consider separately all the cases when time inversion imposes new conditions on $\mathscr{D}$.

The methods of derivation are basically the same as in Sec. 3 [1]; without presenting details we emphasize only the points where there are differences.

Case c: the representations T_0' and $T_0'^*$ complex and equivalent.

1) c_1; $\mathbf{k}_0$ equivalent to $-\mathbf{k}_0$.

In this case, analogously to (I.14), the functions $\hat{S}\varphi_i$ can be expressed linearly in terms of φ_i:

$$\hat{S}\varphi_i = \hat{\sigma}_y \varphi_i^* = S_{i'i}\varphi_{i'}. \tag{5}$$

However, in distinction from (I.15) we now have $\hat{S}\hat{S} = -1$; therefore,

$$S = -S^{*-1} = -\tilde{S}. \tag{6}$$

Hence, it is apparent that in the present case $\mathscr{D}$ satisfies the relations (I.16) and (I.17), and A_{sl}^t the relation (I.19). However, since now, according to (6), $SG^*S^* = -SG^*S^{-1} = -G$, then from (I.19), instead of (I.20), we obtain

$$n_s = \frac{1}{2h} \sum_{G \in \bar{G}'_{\mathbf{k}_0}} \chi_f(G)\, [\chi_0'^2(G) - \gamma\chi_0'(G^2)]. \tag{7}$$

Consequently, for even functions ($\gamma = 1$) the quantity n_s is equal to the number of representations T_s contained in the antisymmetric product $\{T_0'^2\}$, and for odd ($\gamma = -1$) in the symmetric product $[T_0'^2]$.

2) c_2; $\mathbf{k}_0$ not equivalent to $-\mathbf{k}_0$.

In this case, analogously to (I.21a), the functions $\hat{R}\hat{S}\varphi_i$ are linearly expressed in terms of φ_i', and since $\hat{R}$ commutes with S, and $\hat{S}^2 = -1$, then $RS\varphi_i = R_{i'i}\varphi_{i'}$; but

$$R\varphi_i = -R_{i'i}^*\hat{S}\varphi_{i'}. \tag{8}$$

Now, therefore, in distinction from (I.23),

$$(R^{-1})_{ij} = -R_{ij}^{*-1} = -R_{ji}. \tag{9}$$

Consequently, $\mathscr{D}$, as previously, satisfies (I.22), and A_{sl}^t satisfies (I.24), but, since now $(R^2)_{ii} = R_{iJ}R_{Ji} = -R_{ij}R_{ji}^*$, the quantity n_s, in distinction from (I.25), is equal to

$$n_s = \frac{1}{2h} \sum_{G \in \bar{G}'_{\mathbf{k}_0}} [\chi_s(G)\,|\chi_0'(G)|^2 - \gamma\chi_s(R_0 G)\,\chi_0'(R_0 G)^2]. \tag{10}$$

Cases a and b: the representations T_0' and $T_0'^*$ real or complex non-equivalent.

1) a_1 and b_1; $\mathbf{k}_0$ equivalent to $-\mathbf{k}_0$

In these cases the functions φ_i and $\hat{S}\varphi_i$ are linearly independent and are united in a single representation. The matrix D is constructed on the basis φ_i and $\varphi_I = \hat{S}\varphi_i$, but D'^* is constructed on the basis $\bar{\varphi}_i = \hat{S}\varphi_i$ and $\bar{\varphi}_I = \hat{S}\varphi_I = \hat{S}^2\varphi_i = -\varphi_i$. Therefore, in distinction from (I.26b), now

$$\mathscr{D}_{Ji}' = -\mathscr{D}_{Ij}. \tag{11}$$

Correspondingly, instead of (I.27)

$$A_{sl,\,Ij} = -\gamma A_{sl,\,Ji}. \tag{12}$$

Therefore, for the "non-diagonal" terms n_s is now determined by (7), and for the diagonal ones, as before, by (I.8).

2) a_2 and b_2; $\mathbf{k}_0$ not equivalent to $-\mathbf{k}_0$

Here the functions φ_i and $\varphi_I = R_0 S\varphi_i$ are united into a single representation. The matrix $\mathscr{D}$ is also written in this basis. Then $\mathscr{D}'^*$ is written in the basis $\bar{\varphi}_i = \hat{S}\varphi_i$ and $\bar{\varphi}_I = \hat{S}\varphi_I = -R_0\varphi_i$; therefore, instead of (I.29), $\bar{\varphi}_I = (R_0R)_{i'i}\bar{\varphi}_{i'}$, and $\varphi_i = -(RR^{-1})_{i'i}\bar{\varphi}_{I'}$. Correspondingly, instead of (I.30b) and (I.31), we obtain

$$\mathscr{D}_{Ij}(\mathscr{K}) = -(RR_0^{-1})_{I'j}\mathscr{D}_{J'i'}'(\hat{R}\mathscr{K})(R_0R)_{i'i} \tag{13}$$

and

$$A_{sl,\,Ij}^t = -\gamma\,(RR_0^{-1})_{i'j}(R_0R)_{j'I}R_{l'l}^{*s}A_{sl',\,I'j'}^t. \tag{14}$$

Hence, it follows that for the "non-diagonal" elements n_s is determined from (10), while for diagonal elements (I.8) is retained.

From (I.8), (7), and (10) the formulae derived previously by Sheka [4] are obtained for determining the points of zero slope for the double-valued representations.

We shall deal briefly with the methods of constructing the basis matrices $A_{s,l}^t$ and the matrix $\mathscr{D}$ for double-valued representations.

These methods do not differ from those described in [1], Sec. 4. It is clear that each of the terms in $\mathscr{D}$ must satisfy condition (I.10). If the group $G_{\mathbf{k}_0}$ is equivalent to the point group $\bar{\bar{G}}$, the basis for A_{sl}^t can be chosen to be the eigen functions of this group, which can consist of the eigen functions of the space group $D_j^{\pm}$ with the

Table I. The distribution of $f(\mathscr{K})$ and $\varphi(J)$ over the representations Γ and K (wurtzite)

Representation Γ	Representation K	$f(\mathscr{K})$ Odd	$f(\mathscr{K})$ Even	$\varphi(J)$ For equation (15)	$\varphi(J)$ For equation (20)
Γ_1	K_1	k_z	$k_z^2;\ k_\perp^2;\ \varepsilon_{zz};\ \varepsilon_\perp;\ \sigma_+ k_- - \sigma_- k_+$	$I,\ J_z^2$	—
Γ_4		—	—	—	$J_+^3 - J_-^3$
Γ_2	K_2	σ_z	$\sigma_z k_z,\ \sigma_+ k_- + \sigma_- k_+$	J_z	J_z^3
Γ_3		—	—	—	$J_+^3 - J_-^3$
Γ_5	K_3	—	$k_+^2,\ k_-^2;\ \varepsilon_+,\ \varepsilon_-;$ $\sigma_+ k_+,\ \sigma_- k_-$	$J_+^2,\ J_-^2$	$[J_z J_+^2],\ [J_z J_-^2]$
Γ_6		$\sigma_+,\ \sigma_-$ $k_+,\ k_-$	$k_+ k_z,\ k_- k_z;\ \varepsilon_{+z},\ \varepsilon_{-z};$ $\sigma_+ k_z,\ \sigma_- k_z;\ \sigma_z k_-,\ \sigma_z k_-$	$J_+,\ J_-$ $[J_+ J_z],\ [J_- J_z]$	$[J_+ J_z^2],\ [J_- J_z^2]$

Note: $k_\pm = k_x \pm i k_y$, $J_\pm = (J_x \pm iJ_y)/\sqrt{2}$, $\varepsilon_\pm = \varepsilon_{xx} \pm 2i\,\varepsilon_{xy} - \varepsilon_{yy}$, $\varepsilon_{\pm z} = \varepsilon_{xz} \pm i\varepsilon_{yz}$, $\varepsilon_\perp = \varepsilon_{xx} + \varepsilon_{yy}$.

corresponding half-integral values of j, and the matrices A_{sl} can be chosen to be the matrices of the functions of the components of the axial vector $\varphi_{sl}(\hat{J}_i)$, which transform according to the representation T_s, constructed in this basis as was shown in Part 1, Sec. 3 of [1]. The additional conditions associated with time inversion must be included separately. In case c_1, (I.38) is now satisfied, since here also $\hat{S}^4 = 1$; consequently, $\hat{\mathscr{D}}$ can contain only even products of $f(\mathscr{K})$ and $\varphi(\hat{J})$, which do not change sign when changing the signs of k_i, H_i and J_i. In the other cases it is necessary to use the general formulae given above.

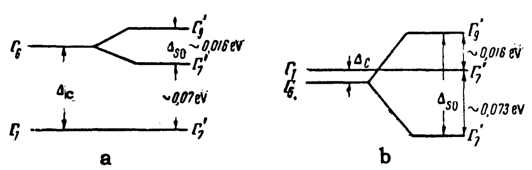
If the representation T_0' is two-dimensional, $\mathscr{D}$ can be constructed by the method discussed in Part 4, of Sec. 4 of [1]. When necessary, D can also be constructed here for a combined representation which includes several irreducible representations. However, if all these representations arise as a result of the spin-orbit splitting of one representation T_0, i.e., are contained in $T' = T_0 \times T_{1/2}$, then the first method is more convenient for their simultaneous consideration. This method is especially convenient when the double-valued representation—reducible or irreducible—arises from a two-dimensional single-valued representation, since then the construction of the matrices A_{sl} is performed in the simple way as described in Part 4 of Sec. 4[1]. The defect of the second method is the difficulty in determining the order of the coefficients C_s^{tr}. Whereas in the first method the coefficients of the first order of smallness in β^2 are determined at once (the coefficients in $f(\mathscr{K})$ containing σ_i), to do this by the second method requires as a rule additional comparison. To do this, for example, one can compare the general expressions for $\mathscr{D}$, obtained by both methods, and consider how they turn into one another for weak spin-orbit interaction, as is done, for example, in[5] (Appendix B). It is not, of course, necessary to write out in explicit form the matrices $\varphi_{sl}(J)$ for both cases.

Below we consider a number of examples where both methods are used.

4. THE EFFECT OF DEFORMATION ON THE ENERGY SPECTRUM OF WURTZITE-TYPE CRYSTALS

In[1] we considered the effect of deformation on the spectrum of wurtzite-type crystals ignoring spin-orbit interaction. The formulae obtained are valid when the splitting of the bands due to spin-orbit interaction is small in comparison with both kT and the splitting caused by the deformation.

Of the crystals in this group CdS has been studied best. By analyzing experimental data on the absorption and reflection of light in these crystals, Birman[6] and Thomas and Hopfield[7] con-



Genesis of the bands: a – according to Birman[6], b – according to Thomas and Hopfield.[7]

cluded that the extremum of the valence band in CdS lies on the Δ axis, apparently at the point Γ ($\mathbf{k} = 0$), where the wave functions at the extremum point, ignoring spin-orbit interaction, transform according to the representation Γ_6 (in the notation of[8]).

However, the representation Γ_1 also lies close to the edge of the band at a distance Δ_C from it. Owing to spin-orbit interaction, the representation Γ_6 is split into two double-valued representations Γ_7' and Γ_9', where Γ_9' corresponds to the maximum energy of the electrons, and Γ_1 goes over to Γ_7'. According to[6], the spin-orbit splitting Δ_{S0} is smaller than Δ_C but comparable with it, whereas, according to[7], Δ_{S0} is greater than Δ_C. The geneses of the bands according to[6,7] are shown schematically in the figure. We consider the effect of deformation on the spectrum of CdS for both these models. Thus, we must construct $\mathscr{D}$ simultaneously for both the representations Γ_1 and Γ_6. We first write down $\hat{\mathscr{D}}$, using the first method. The characters of the single-valued representations at the point Γ calculated by Rashba[8] are given in Table I in[1]. Both the representations Γ_1 and Γ_6 belong to case a_1; therefore, according to (I.20), there must appear in $\hat{\mathscr{D}}$ even functions of $\mathscr{K}$ which transform according to the representations $[(\Gamma_1 + \Gamma_6)^2] = 2\Gamma_1 + \Gamma_5 + \Gamma_6$, and odd functions which transform according to $\{(\Gamma_1 + \Gamma_6)^2\} = \Gamma_2 + \Gamma_6$.

In addition to the functions given in Table III of[1], we now include in $\mathscr{D}$ terms with $\hat{\sigma}_i$ not dependent on $\mathbf{k}$ and linear in $\mathbf{k}$. All these functions are given in Table I. Also given are nine functions $\varphi(\hat{\mathbf{J}})$ transforming according to the representations quoted above. Using these functions, we form $\hat{\mathscr{D}}$ in accord with the requirements of Part 1 of Sec. 4[1]:

$$\begin{aligned}\hat{\mathscr{D}} = {} & \Delta_1 J_z^2 + \Delta_2 J_z \hat{\sigma}_z + \Delta_3 (\hat{\sigma}_+ J_- + J_- \hat{\sigma}_+) + B_1 k_z^2 + B_2 k_\perp^2 \\ & + B_3 (J_+^2 k_-^2 + J_-^2 k_+^2) + B_4 \hat{J}_z^2 k_z^2 + B_5 J_z^2 k_\perp^2 \\ & + B_6 k_z ([J_z J_+] k_- + [J_z J_-] k_+) + i B_7 (k_+ J_- - k_- J_+) \\ & + i (\beta_1 + \beta_3 J_z^2)(\hat{\sigma}_+ k_- - \hat{\sigma}_- k_+) + i\beta_2 (J_+^2 k_- \hat{\sigma}_- - J_-^2 k_+ \hat{\sigma}_+) \\ & + i\beta_4 \hat{\sigma}_z ([J_z J_+] k_- - [J_z J_-] k_+) + i\beta_5 k_z ([J_z J_+] \hat{\sigma}_- \\ & - [J_z J_-] \hat{\sigma}_+) + C_1 \varepsilon_{zz} + C_2 \varepsilon_\perp + C_3 J_z^2 \varepsilon_{zz} + C_4 J_z^2 \varepsilon_\perp \\ & + C_5 (J_-^2 \varepsilon_+ + J_+^2 \varepsilon_-) + C_6 ([J_z J_+] \varepsilon_{+z} + [J_z J_-] \varepsilon_{-z}). \end{aligned} \quad (15)$$

Here

$$2 [J_i J_j] = J_i J_j + J_j J_i, \qquad \varepsilon_{\pm z} = \varepsilon_{xz} \pm i\varepsilon_{yz},$$

$$\varepsilon_\pm = \varepsilon_{xx} \pm 2i\varepsilon_{xy} - \varepsilon_{yy}, \qquad \varepsilon_\perp = \varepsilon_{xx} + \varepsilon_{yy},$$

$$k_\pm = k_x \pm i k_y, \qquad k_\perp^2 = k_x^2 + k_y^2.$$

We shall not write out $\mathscr{D}$ in a general form, but consider limiting cases.

1. $\Delta_C \gg \Delta_{S0}$. In this case it is possible to ignore the representation Γ_1. Then $\hat{\mathscr{D}}$ must contain only matrices which transform according to the representations $\Gamma_6 \times \Gamma_6 = \Gamma_1 + \Gamma_2 + \Gamma_5$, i.e., 1, J_Z^2, J_+^2 and J_-^2. Since the representation Γ_6 is twofold degenerate, and the functions $f(\mathscr{K})$ were chosen in accordance with the requirements of Part 4 of Sec. 4[1], the matrices of these operators, according to (I.46), can be put, respectively, equal to I, σ_Z, σ_+, and σ_-. (In fact, this corresponds to a choice of the basis functions in the form $u_\pm = (\pm x - iy)/\sqrt{2}$.)

If we now write, in accordance with (I.4), the matrix $\mathscr{D}$ in the basis $u_-\alpha_+$, $u_+\alpha_-$, $u_+\alpha_+$, $u_-\alpha_-$, we obtain

$$\mathscr{D} = \begin{vmatrix} \lambda - \Delta_2 & F & G & I \\ F^* & \lambda - \Delta_2 & I^* & G^* \\ G^* & I^* & \lambda + \Delta_2 & 0 \\ I^* & G & 0 & \lambda + \Delta_2 \end{vmatrix}, \quad (16)$$

where $\lambda = B_1 k_Z^2 + B_2 k_\perp^2 + C_1 \epsilon_{ZZ} + C_2 \epsilon_\perp$, $F = -i\beta_2 k_+$, $G = B_3 k_+^2 + C_3 \epsilon_+$, $I = i\beta_1 k_-$, $\Delta_2 = \Delta_{S0}/2$. Here the constants β_i are of the first order of smallness with respect to β^2, and the remaining constants of zero order. If we omit the terms associated with the deformation, this matrix coincides with that obtained previously by Rashba and Sheka.[9]

The secular equation $\|\mathscr{D} - E\| = 0$ according to (16) has the form

$$\begin{aligned}(\lambda - E')^2 & [(\lambda - E' - 2\Delta_2)^2 - |F|^2] - 2(\lambda - E')[(\lambda - E' \\ & - 2\Delta_2)(|I|^2 + |G|^2) - I^* F G^* - I F^* G] \\ & + (|G|^2 - |I|^2)^2 = 0. \end{aligned} \quad (17)$$

Here $E' = E - \Delta_2$, i.e., the energy of the electrons measured relative to the edge of the valence band.

If, in this equation, of the terms proportional to β^2, only those not dependent on k are retained, its solution will be

$$\begin{aligned} E' = {} & \lambda - \Delta \pm \{\Delta^2 + B_2^2 k_\perp^4 + 2B_3 C_3 [(k_x^2 - k_y^2)(\varepsilon_{xx} - \varepsilon_{yy}) \\ & + 4\varepsilon_{xy} k_x k_y] + B_3^2 [(\varepsilon_{xx} - \varepsilon_{yy})^2 + 4\varepsilon_{xy}^2]\}. \end{aligned} \quad (18)$$

Close to the extremum, i.e., for $E' \ll \Delta_{S0}$

$$E = \lambda + 2B_3 C_3 [(k_x^2 - k_y^2)(\varepsilon_{xx} - \varepsilon_{yy}) + 4\varepsilon_{xy} k_x k_y]/\Delta_{s0}. \quad (19)$$

It follows from (18) that when Δ_{S0} exceeds both kT and the splitting of the bands due to the deformation, the deformation causes only a change of the effective masses. These changes are relatively large—of the order $C_3\epsilon/\Delta_{S0}$; comparatively large values of the piezo-resistance constants Π_{xxxx}, Π_{xxyy}, and Π_{xyxy}, can therefore be expected here; however, in distinction from the case considered in Sec. 5 of[1], these coefficients are now proportional to C_3/Δ_{S0}, i.e., they do not depend on temperature.

Table II. Characters of the double-valued representations for the point Δ (wurtzite)

Number of elements	Elements of the class	Δ_7'	Δ_8'	Δ_9'
1	$(\varepsilon\|0)$	2	2	2
1	$(\bar{\varepsilon}\|0)$	−2	−2	−2
2	$\left(\delta_6, \bar{\delta}_6^5 \middle\| \frac{t_0}{2}\right)$	$\sqrt{3}\,\eta_k$	$-\sqrt{3}\,\eta_k$	0
2	$(\delta_6^2, \bar{\delta}_6^4\|0)$	1	1	−2
2	$(\delta_6^4, \bar{\delta}_6^2\|0)$	−1	−1	2
2	$\left(\delta_6^5, \bar{\delta}_6 \middle\| \frac{t_0}{2}\right)$	$-\sqrt{3}\,\eta_k$	$\sqrt{3}\,\eta_k$	0
2	$\left(\delta_6^3, \bar{\delta}_6^3 \middle\| \frac{t_0}{2}\right)$	0	0	0
6	$(\sigma_1, \sigma_2, \sigma_3\|0)$, $(\bar{\sigma}_1, \bar{\sigma}_2, \bar{\sigma}_3\|0)$	0	0	0
6	$\left(\sigma_1', \sigma_2', \sigma_3' \middle\| \frac{t_0}{2}\right)$, $\left(\bar{\sigma}_1', \bar{\sigma}_2', \bar{\sigma}_3' \middle\| \frac{t_0}{2}\right)$	0	0	0

Note: $\eta_k = \exp\{ik_{z0}t_0/2\}$; for the point Γ the quantity $\eta_k = 1$.

2. $\Delta_{s0} \gg \Delta_c$. In this case we can consider only the two split-off half-integral representations Γ_9' and Γ_7'. The corresponding expression for $\mathscr{D}$ can be obtained from (15); it is, however, more convenient here to use the second method, and to consider only these two representations. In Table II are given the characters of the double-valued representations at the point Δ, calculated by Rashba and Sheka.[9]*

The representations Γ_9' and Γ_7' belong to case c_1, and therefore, according to (7), $\mathscr{D}$ contains even functions of $\mathscr{K}$ which transform according to the representations $\{(\Gamma_7' + \Gamma_9')^2\} = 2\Gamma_1 + \Gamma_5 + \Gamma_6$, and odd functions which transform according to $[(\Gamma_7' + \Gamma_9')^2] = 2\Gamma_2 + \Gamma_3 + \Gamma_4 + \Gamma_5 + \Gamma_6$. These functions can be chosen from Table I. In the same table are given sixteen corresponding functions $\varphi(\mathbf{J})$ that transform according to these representations. Here, as shown above, can appear in $\mathscr{D}$ in case c_1 products only of even functions of $\mathscr{K}$ and $\mathbf{J}$, or only of odd.

We construct $\hat{\mathscr{D}}$ following Part 1 of Sec. 4 of [1]:

$$\mathscr{D} = \delta_1 J_z'^2 + B_1 k_z^2 + B_2 k_\perp^2 + \frac{2B_3}{\sqrt{3}}(J_+^2 k_-^2 + J_-^2 k_+^2) + B_4 J_z'^2 k_z^2 + B_5 J_z'^2 k_\perp^2 + \sqrt{\frac{2}{3}} B_6 J_z k_z ([J_z J_+] k_- + [J_z J_-] k_+) + i\sqrt{\frac{2}{3}} B_7 (J_+ k_- - J_- k_+) + i\sqrt{\frac{2}{3}} \beta_1 ([J_z''^2 J_+] k_- - [J_z''^2 J_-] k_+) + C_1 \varepsilon_{zz} + C_2 \varepsilon_\perp + \frac{2}{\sqrt{3}} C_3 (J_+^2 \varepsilon_- + J_-^2 \varepsilon_+) + C_4 J_z'^2 \varepsilon_{zz} + C_5 J_z'^2 \varepsilon_\perp + \sqrt{\frac{2}{3}} C_6 ([J_z J_+] \varepsilon_{-z} - [J_z J_-] \varepsilon_{z+}). \quad (20)$$

Here

$$J_z'^2 = \frac{1}{2}\left(\frac{9}{4} - J_z^2\right), \qquad J_z''^2 = \frac{5}{4} - J_z^2,$$
$$2\,[J_i J_k] = J_i J_k + J_k J_i.$$

This choice of the numerical coefficients in (20) is made with the aim of obtaining a matrix $\mathscr{D}$ closest to (16), to simplify the comparison of the two cases. The constants B_i and C_i in (16) and (20) are not, of course, identical. In the approximation of weak spin-orbit coupling, these constants can be expressed in terms of one another by the use, for example, of the method mentioned above due to Luttinger.[5]

We shall not make such a comparison, but only point out that from (15) and (20) it follows at once that all the constants B_i and C_i in (20) are of zero order in β^2. Only the constant β_1 for the cubic term in J_i is of the first order of smallness in β^2. Of course, the remaining constants can also include contributions of the same order. The complete set of functions Y_m^j with $j = 3/2$ are the basis for $\mathscr{D}$. Therefore the actual choice of the representation for $\varphi(\mathbf{J})$ can be arbitrary here. The corresponding matrices are given, for example, in,[10] p. 171. In the representation $Y_{-1/2}^{3/2}$, $Y_{+1/2}^{3/2}$, $Y_{+3/2}^{3/2}$, $Y_{-3/2}^{3/2}$, the matrix $\mathscr{D}$ takes the form

$$\mathscr{D} = \begin{vmatrix} \lambda + \theta & F & G & I + H \\ F^* & \lambda + \theta & I^* - H^* & G^* \\ G^* & I - H & \lambda & 0 \\ I^* + H^* & G & 0 & \lambda \end{vmatrix}, \quad (21)$$

where

$$\lambda = B_1 k_z^2 + B_2 k_\perp^2 + C_1 \varepsilon_{zz} + C_2 \varepsilon_\perp,$$
$$\theta = \delta_1 + B_4 k_z^2 + B_5 k_\perp^2 + C_4 \varepsilon_{zz} + C_5 \varepsilon_\perp,$$
$$F = -\frac{2}{\sqrt{3}} i (B_7 + \beta_1) k_+, \qquad G = B_3 k_+^2 + C_3 \varepsilon_+,$$
$$I = i B_7 k_-, \qquad H = B_6 k_- k_z + C_6 \varepsilon_{-z}.$$

*Throughout the tables of the groups the following notation is used for the operators: δ – rotation, ρ – reflection rotation, σ – reflection.

The secular equation $\| \mathcal{D} - E \| = 0$ has the form

$$(\lambda - E)^2 [(\lambda + \theta - E)^2 - |F|^2] - 2(\lambda - E) \times [(\lambda + \theta - E)(|I|^2 + |H|^2 + |G|^2) - FG^*I^* - F^*GI] + |G|^4 - 2|G_\perp|^2(|I|^2 - |H|^2) + (I^2 - H^2)(I^{*2} - H^{*2}) = 0. \quad (22)$$

It is not difficult to verify that here, just as in (17), k_x and k_y appear in the terms not containing ϵ only in the combination $k_\perp^2 = k_x^2 + k_y^2$. This means that in the undeformed crystal the extremum in the lowest band Γ_7', is in both cases a ring—with $k_\perp$ = const. However, in distinction from (17), the term in (20) linear in k is not small, since it arises, not due to the spin-orbit interaction, but as a result of the interaction of the two bands Γ_1 and Γ_6. Therefore the extremum can be far from the point $\mathbf{k} = 0$, where terms of the fourth order in k, not included in (20), play an important part.

In the uppermost band Γ_9', which corresponds to the minimum energy of holes, the extremum is at the point $\mathbf{k} = 0$. Close to this point for $E(\mathbf{k}, \epsilon) \ll \delta_1$ we have

$$E = \lambda + \frac{B_7^2}{\delta}\left\{k_\perp^2 + \frac{4C_3}{\sqrt{3}\,\delta}[(k_x^2 - k_y^2)(\varepsilon_{xx} - \varepsilon_{yy}) + 4k_xk_y\varepsilon_{xy}]\right\} + \frac{2}{\delta}\{B_3C_3[(k_x^2 - k_y^2)(\varepsilon_{xx} - \varepsilon_{yy}) + 4k_xk_y\varepsilon_{xy}] + B_6C_6(k_xk_z\varepsilon_{xz} + k_yk_z\varepsilon_{yz})\}. \quad (23)$$

Here we neglect terms of the order β^2k, and also ignore the splitting of the bands caused by the deformation and proportional to ϵk, since this splitting leads to effects of higher order in ϵ. It can be expected that the coefficient B_7^2/δ in (23) greatly exceeds B_2. In this case the principal contribution to $m_\perp^* = \hbar^2/2(B_2 + B_7^2/\delta)$ is provided by the interaction of the bands Γ_6 and Γ_1, and the change of the corresponding effective masses under deformation in the plane xy is basically determined by the first term in (23) proportional to $B_7^2C_3/\delta^2$.

We note that, in distinction from (19), a large change of the effective mass and, consequently, of the conductivity also, can occur not only under deformations ϵ_{xx}, ϵ_{yy}, and ϵ_{xy}, but, as seen from (23), also under deformation ϵ_{xz} and ϵ_{yz}.

By the use of Table I it is also easy to construct the operator $\mathcal{D}$ for an arbitrary point on the Δ axis, where an extremum can also exist. At these points time inversion imposes no additional conditions on $\mathcal{D}$, and in it there can appear products of any even and odd functions of $\mathcal{K}$ and $\mathbf{J}$ which transform according to conjugate (equivalent) representations.

We shall not linger on this, but consider the spectrum at the point H_3, where there is also a point of zero slope in wurtzite.

3. Spectrum for the representation H_3. To construct $\mathcal{D}$ we use the first method. The characters of the single-valued representations at the point H are given in Table II of [1]. As shown in [1], the representation H_3 belongs to the case a_2, and, according to (I.25), there can appear in $\mathcal{D}$ odd functions transforming according to the representations Γ_2 and Γ_5, and even functions transforming according to Γ_1 and Γ_6.

These functions are given in Table I. The matrices A_{sl} can be chosen according to (I.46). The basis of these matrices will be denoted as φ_1, φ_2.

$$\mathcal{D} = A_1[B_1k_z^2 + B_2k_\perp^2 + i\beta_1(\hat{\sigma}_+k_- - \hat{\sigma}_-k_+) + C_1\varepsilon_{zz} + C_2\varepsilon_\perp] + A_2\Delta\hat{\sigma}_z + A_{31}[B_3k_zk_+ + C_3\varepsilon_{+z} + i\beta_2\hat{\sigma}_zk_+ + i\beta_3\hat{\sigma}_+k_z] + A_{32}[B_3k_zk_- + C_3\varepsilon_{-z} - i\beta_2\hat{\sigma}_zk_- - i\beta_3\hat{\sigma}_-k_z]. \quad (24)$$

In the basis $(\varphi_1\alpha_+, \varphi_2\alpha_-, \varphi_1\alpha_-, \varphi_2\alpha_+)$ the matrix $\mathcal{D}$ is

$$\mathcal{D} = \begin{vmatrix} \lambda + \Delta & F & G & I + H \\ F^* & \lambda + \Delta & I^* - H^* & G^* \\ G^* & I - H & \lambda - \Delta & 0 \\ I^* + H^* & G & 0 & \lambda - \Delta \end{vmatrix}, \quad (25)$$

where

$$\lambda = B_1k_z^2 + B_2k_\perp^2 + C_1\varepsilon_{zz} + C_2\varepsilon_\perp,$$
$$I = B_3k_zk_+ + C_3\varepsilon_{z+}, \qquad H = i\beta_2k_+,$$
$$F = i\beta_3k_z, \qquad G = i\beta_1k_-.$$

When the terms proportional to ϵ are ignored, this matrix agrees with that obtained previously in [9]. In form (25) is similar to (21), and the secular equation $\| \mathcal{D} - E \| = 0$ is similar to (22). Of course, the explicit form of the matrix elements in (25) and (21) is different. If, of the terms proportional to β^2 in $\mathcal{D}$, we retain only those independent of k, the solution of the secular equation is of the form

$$E = \lambda \pm \{\Delta + B_3^2k_\perp^2k_z^2 + 2B_3C_3(\varepsilon_{xz}k_xk_z + \varepsilon_{yz}k_yk_z) + B_3^2(\varepsilon_{xz}^2 + \varepsilon_{yz}^2)\}^{1/2}. \quad (26)$$

Close to the extremum point for $E' \ll \Delta$

$$E' = E - \Delta = \lambda \pm (B_3C_3/\Delta)(k_xk_z\varepsilon_{xz} + k_yk_z\varepsilon_{yz}). \quad (27)$$

Thus, in distinction from (23) and (19), a significant change of the effective masses occurs here only for deformations ϵ_{xz} and ϵ_{yz}, and large values of the constants $\Pi_{xzxz} = \Pi_{yzyz}$ can be expected.

Consequently, the study of the effects of piezoresistance in these crystals can serve as one of

Table III. Characters of the irreducible representations for the point Γ (germanium)

Number of elements	Elements of the class	Single-valued $\Gamma_1^\pm$	$\Gamma_2^\pm$	$\Gamma_{12}^\pm$	$\Gamma_{15}^\pm$	$\Gamma_{25}^\pm$	Double-valued $\Gamma_6'^\pm$	$\Gamma_7'^\pm$	$\Gamma_9'^\pm$
1	$(\varepsilon\|0)$	1	1	2	3	3	2	2	4
1	$(\bar{\varepsilon}\|0)$						—2	—2	—4
6	$(\delta_4^2\|0)$, $(\bar{\delta}_4^2\|0)$	1	1	2	—1	—1	0	0	0
6	$(\delta_4\|\tau)$, $(\delta_4^3\|\tau)$	1	—1	0	1	—1	$\sqrt{2}$	$-\sqrt{2}$	0
6	$(\delta_4\|\tau)$, $(\bar{\delta}_4^3\|\tau)$						$-\sqrt{2}$	$\sqrt{2}$	0
12	$(\delta_2\|\tau)$, $(\bar{\delta}_2\|\tau)$	1	—1	0	—1	1	0	0	0
8	$(\delta_3\|0)$, $(\delta_3^2\|0)$	1	1	—1	0	0	1	1	—1
8	$(\bar{\delta}_3\|0)$, $(\bar{\delta}_3^2\|0)$						—1	—1	1
48	$(i\|\tau)\times z$	$\pm\chi(z)$							

the methods for determining the positions of the extremum points.

5. THE CHANGE OF THE ENERGY SPECTRUM DUE TO DEFORMATION IN LATTICES OF THE GERMANIUM TYPE

We shall not consider here the spectrum at all the points of zero slope where there are degenerate representations, but limit ourselves to two of them only: the points Γ at the center of the Brillouin zone, and X at its edge on the [001] axis.

1) The point Γ. The characters of the single-valued and double-valued representations of Γ are given in Table III.[11] At this point there are three pairs of degenerate single-valued representations. Two of them, $\Gamma_{15}^\pm$ and $\Gamma_{25}^\pm$, are threefold degenerate (without spin); due to spin-orbit interaction, these representations break up, respectively, into $\Gamma_6^\pm + \Gamma_8^\pm$ and $\Gamma_7^\pm + \Gamma_8^\pm$. To construct the spectrum for the fourfold degenerate representations $\Gamma_8^\pm$, derived from $\Gamma_{15}^\pm$ or $\Gamma_{25}^\pm$, it is more convenient to use the second method. The functions $f(\mathscr{K})$ and $\varphi(\mathbf{J})$ transforming according to the corresponding representations Γ are given in Table IV. Since the representations $\Gamma_8^\pm$ belong to case c_1, then there appear in $\mathscr{D}$, according to Sec. 3, only products of even functions which transform according to the representations $\{\Gamma_8^{\pm 2}\} = \Gamma_1^+ + \Gamma_{12}^+ + \Gamma_{25}^+$, and odd functions which transform according to $[\Gamma_8^{\pm 2}] = \Gamma_2^+ + 2\Gamma_{15}^+ + \Gamma_{25}^+$.

Therefore $\mathscr{D}$ will have the form

$$\hat{\mathscr{D}} = B_1k^2 + B_2(J_1k_2 + J_2k_1) + B_3([J_xJ_y]k_xk_y + [J_xJ_z]k_xk_z + [J_yJ_z]k_yk_z) + C_1\varepsilon + C_2(J_1\varepsilon_2 + J_2\varepsilon_1) + C_3([J_xJ_y]\varepsilon_{xy} + [J_xJ_z]\varepsilon_{xz} + [J_yJ_z]\varepsilon_{yz}), \quad (28)$$

where $R_1 = R_X^2 + \omega R_Y^2 + \omega^2 R_Z^2$, $R_2 = R_1^*$ ($R_i^2 \to J_i^2$, k_i^2 or ϵ_{ii} and $\omega = e^{2\pi i/3}$).

As is well known, the wave functions in germanium and silicon at the extremum point of the valence band transform according to the representation Γ_{25}^+, where the upper of the split-off representations is $-\Gamma_8^+$. Thus (28) describes the

Table IV. The distribution of $f(\mathscr{K})$ and $\varphi(J)$ over the representations Γ (germanium)

Representation	$f(k)$	$f(\varepsilon)$	$f(\sigma)$	$f(\sigma, k)$	$\varphi(J)$ Odd	$\varphi(J)$ Even
Γ_1^+	k^2	ε	—	—	—	I
Γ_1^-	—	—	—	$k_x\sigma_x + k_y\sigma_y + k_z\sigma_z$	—	—
Γ_2^+	—	—	—	—	$J_xJ_yJ_z + J_zJ_yJ_x$	—
Γ_2^-	—	—	—	—	—	—
Γ_{12}^+	k_1, k_2	$\varepsilon_1, \varepsilon_2$	—	—	—	J_1, J_2
Γ_{12}^-	—	—	—	$(k\sigma)_1, (k\sigma)_2$	—	—
Γ_{15}^+	—	—	$\sigma_x, \sigma_y, \sigma_z$	—	$J_x, J_y, J_z, J_x^3, J_y^3, J_z^3$	—
Γ_{15}^-	k_x, k_y, k_z	—	—	$\{k_x\sigma_y\}, \{k_y\sigma_z\}, \{k_x\sigma_z\}$	—	—
Γ_{25}^+	k_xk_y, k_xk_z, k_yk_z	$\varepsilon_{xy}, \varepsilon_{xz}, \varepsilon_{yz}$	—	—	V_x, V_y, V_z	$[J_xJ_y], [J_xJ_z], [J_yJ_z]$
Γ_{25}^-	—	—	—	$[k_x\sigma_y], [k_x\sigma_z], [k_y\sigma_z]$	—	—

Note: $R_1 = R_x + \omega R_y + \omega^2 R_z$, $R_2 = R_1^*$, and $R_i \to k_i^2, \varepsilon_{ii}, k_i\sigma_i, J_i^2$, $\omega = e^{2\pi i/3}$, $V_x = [J_x(J_y^2 - J_z^2)]$ etc.

Table V. Characters of the representations for the point X (germanium)

Number of elements	Elements of the class	$\chi_{1,2}$	$\chi_{3,4}$	Number of elements	Elements of the class	$\chi_{1,2}$	$\chi_{3,4}$
1	$(\varepsilon \mid 0)$	2	2	2	$(\sigma_{xy}, \sigma_{x\bar{y}} \mid t)$	∓ 2	0
1	$(\varepsilon \mid t)$	−2	−2	2	$(i \mid \tau, \tau+t)$	0	0
1	$(\delta_{2z} \mid 0)$	2	−2	2	$(\sigma_z \mid \tau, \tau+t)$	0	0
1	$(\delta_{2z} \mid t)$	−2	2	4	$(\delta_{4z}, \delta_{4z}^{-1} \mid \tau, \tau+t)$	0	0
4	$(\rho_{4z}, \rho_{4z}^{-1} \mid 0, t)$	0	0	4	$(\sigma_x, \sigma_y \mid \tau, \tau+t)$	0	0
4	$(\delta_{2x}, \delta_{2y} \mid 0, t)$	0	0	2	$(\delta_{2xy} \mid \tau), (\delta_{2x\bar{y}} \mid \tau+t)$	0	± 2
2	$(\sigma_{xy}, \sigma_{x\bar{y}} \mid 0)$	± 2	0	2	$(\delta_{2x\bar{y}} \mid \tau), (\delta_{2xy} \mid \tau+t)$	0	∓ 2

spectrum obtaining in these crystals. Ignoring terms proportional to ϵ, for germanium $\hat{\mathscr{D}}$ in operator form has been given in [5], where all the coefficients B_i are of zero order in β^2; it is not difficult to show that this is also true for the coefficients C_i. The change of the energy spectrum of p germanium under deformation has been considered in detail in [12], where the matrix $\mathscr{D}$ was obtained with the aid of perturbation theory (equation (13)). The same results are, of course, obtained from (28). We shall not, therefore, consider this question in detail here. We merely establish the correspondence between the coefficients in (28) and in [12]

$$B_1 = {}^1/_4\,(4A - 9B), \qquad B_2 = B,$$
$$B_3 = 2/\sqrt{3}D, \qquad C_1 = {}^1/_4\,(4a - 9b), \tag{29}$$
$$C_2 = b, \qquad C_3 = 2/\sqrt{3}d.$$

We now consider the spectrum for the twofold degenerate representation $\Gamma_{12}^{\pm}$. Taking into account spin-orbit interaction, this representation goes over to $\Gamma_8^{\pm}$, i.e., in principle $\mathscr{D}$ is also given here by expression (28). But now some of the coefficients are of order β^2. It is better, therefore, to use the first method: $\mathscr{D}$ will contain even functions of $\mathscr{K}$ transforming according to $[\Gamma_{12}^{\pm 2}] = \Gamma_1^+ + \Gamma_{12}^+$, and odd ones transforming according to $\{\Gamma_{12}^{\pm 2}\} = \Gamma_2^+$.

It is apparent that $\mathscr{D}$ contains no terms of order β^2 which do not depend on **k** or are linear in **k**. Quadratic terms of this order we shall ignore. Then $\hat{\mathscr{D}}$ is

$$\hat{\mathscr{D}} = B_1 k^2 + B_2\,(J_1 k_2 + J_2 k_1) + C_1 \varepsilon + C_2\,(J_1 \varepsilon_2 + J_2 \varepsilon_1). \tag{30}$$

Since this representation is two-dimensional, the matrices J_1 and J_2 in accordance with (I.46) can be chosen to be equal to σ_+ and σ_-. Hence,

$$E = B_1 k^2 + C_1 \varepsilon \pm \Big\{ B_2 \Big(k^4 - 3 \sum_{i>j} k_i^2 k_j^2 \Big) + B_2 C_2 \Big(3 \sum_i k_i^2 \varepsilon_{ii} - k^2 \varepsilon \Big) + {}^1/_2 C_2 \sum_{i>j} (\varepsilon_{ii} - \varepsilon_{jj})^2 \Big\}^{1/2} \tag{31}$$

This differs from Eqs. (14)—(17) of [12] only in the absence of terms containing the constants D and d. Therefore, according to [13], in this case the piezo-resistance coefficients Π_{1111} and Π_{1122} will be large, but the coefficient Π_{1212} will be small. It is interesting that for the representation $\Gamma_{12}^{\pm}$ in the undeformed crystal the degeneracy is not lifted along the [111] axes, where the term in B_2 in (31) goes to zero.

2) The point X. In conclusion, in order to illustrate the ways of constructing $\mathscr{D}$ in cases when the wave vector group is not equivalent to the point group, we consider the point X. The characters of the representations in this group are given in

Table VI. Characters of the representations of the groups $D_{2d}I$ and D_{2d}

Number of elements	Elements of the class	$A_1^{\pm}$ / A_1	$A_2^{\pm}$ / A_2	$B_1^{\pm}$ / B_1	$B_2^{\pm}$ / B_2	$E^{\pm}$ / E
1	ε	1	1	1	1	2
1	δ_{2z}	1	1	1	1	−2
2	$\rho_{4z}, \rho_{4z}^{-1}$	1	1	−1	−1	0
2	δ_{2x}, δ_{2y}	1	−1	1	−1	0
2	$\sigma_{xy}, \sigma_{x\bar{y}}$	1	−1	−1	1	0
8	$i \times z$ (only for $D_{2d}I$)	$\pm\chi(z)$				

Table VII. The distribution of $f(\mathscr{H})$ and $\varphi(J)$ over the representations $D_{2d}I$ and D_{2d}

Representation		$f(k, \varepsilon, \sigma)$	$\varphi(J)$
$D_{2d}I$	D_{2d}		
A_1^+	A_1	$k_z^2, k_\perp^2, \varepsilon_{zz}, \varepsilon_\perp$	I
A_1^-		$\sigma_z k_z, \sigma_x k_x + \sigma_y k_y$	
A_2^+	A_2	σ_z	J_z
A_2^-		$\sigma_x k_y - \sigma_y k_x$	
B_1^+	B_1	$k_x^2 - k_y^2, \varepsilon_{xx} - \varepsilon_{yy}$	$J_x^2 - J_y^2$
B_1^-		$\sigma_x k_x - \sigma_y k_y$	
B_2^+	B_2	$k_x k_y, \varepsilon_{xy}$	$\{J_x J_y\}$
B_2^-		$k_z, \sigma_x k_y + \sigma_y k_x$	
E^+	E	$k_x k_z, k_y k_z; \varepsilon_{xz}, \varepsilon_{yz}; \sigma_x, \sigma_y$	—
E^-		$k_x, k_y; \sigma_z k_x, \sigma_z k_y; \sigma_x k_z, \sigma_y k_z$	

Table V.[11] The point X is the point of zero slope for the representations $X_{3,4}$. These representations belong to the case a_1, and for them there appear in $\mathscr{D}$ even functions which transform according to the representations $\overline{\overline{X}}$, coinciding with the representations of the corresponding point group $\overline{\overline{X}} = D_{2d}I$, appearing in $[\overline{\overline{X}}{}^2_{3,4}] = A_1^+ + B_1^- + B_2^+$, and odd functions transforming according to $\{X^2_{3,4}\} = A_2^-$.

The characters of the representations of the group $D_{2d}I$ are given in Table VI, and the distribution of $f(\mathscr{H})$ over these representations in Table VII.

Then

$$\mathscr{D} = A_1\lambda + iA_3\beta_1(\hat{\sigma}_x k_x - \hat{\sigma}_y k_y) + A_4(B_3 k_x k_y + C_3\varepsilon_{xy}), \quad (32)$$

where $\lambda = B_1 k_z^2 + B_2 k_\perp^2 + C_1\epsilon_{zz} + C_2\epsilon_\perp$.

In the case considered, since the representations $X_{3,4}$ are two-dimensional, according to (I.43) the matrix $A_1 = 1$, and A_3 and A_4 can be chosen to be, respectively, σ_x and σ_y.

For comparison, we write down $\hat{\mathscr{D}}$, using the general method given in Part 3 of Sec. 4 of [1]. By excluding the element (i/τ) we obtain, in place of the group X, the point group D_{2d}, of which the characters of the representations are given in Table VI. The representations $X_{3,4}$ go over into E; therefore $\mathscr{D}$ contains $f(\mathscr{H})$ and $\varphi(J)$, transforming according to $E \times E = A_1 + A_2 + B_1 + B_2$.

We take these functions from Table VII, where the correspondence of the representations of the point group $D_{2d}I$ and the group D_{2d} is shown. We at once include in $\mathscr{D}$ only those $f(\mathscr{H})$ which appear in (28), and then obtain

$$\hat{\mathscr{D}} = \lambda + i\beta_1(\hat{J}_x^2 - \hat{J}_y^2)(\hat{\sigma}_x k_x - \hat{\sigma}_y k_y) + 2[J_x J_y](B_3 k_x k_y + C_3\varepsilon_{xy}). \quad (32a)$$

The matrices $J_x^2 - J_y^2$ and $2[J_x J_y] = J_x J_y + J_y J_x$ in the representation $u_\pm = (1/\sqrt{2})(\mp x - iy)$ are once again equal to σ_x and σ_y.

The solution of the equation $\| \mathscr{D} - E \| = 0$ has the form

$$E(k, \varepsilon) = \lambda \pm \{(B_3 k_x k_y + C_3\varepsilon_{xy})^2 + \beta_1^2 k_\perp^2\}^{1/2}, \quad (33)$$

i.e., the twofold degeneracy is retained. Close to the extremum in the undeformed crystal the surfaces of constant energy have the form of a torus:

$$E(k) = B_1 k_z^2 + B_2(k_\perp \pm k_\perp^0)^2, \quad (34)$$

where $k_\perp^0 = \beta_1/2B_2$. As Rashba[14] showed, semiconductors with bands of this type have a number of interesting peculiarities. For large k terms with β_1^2 can be neglected. Then

$$E(k, \varepsilon) = \lambda \pm (B_3 k_x k_y + C_3\varepsilon_{xy}). \quad (35)$$

Here the surfaces of constant energy are ellipsoids, where deformation causes splitting of the band at k = 0, i.e., the relative displacement of these ellipsoids. Large changes of resistance under shear deformations can, therefore, be expected. In addition, due to the relative displacement of the extrema situated at non-equivalent points of the star k_0, i.e., on the axes x, y, and z, there will be large effects also for the deformations ϵ_{xx}, ϵ_{yy} and ϵ_{zz}.

As is well known, the extrema in n-Si are disposed along the [100] axes, but in the interior of the zone. Thus, there should be observed only effects associated with the displacement of the extrema, and shears ϵ_{xy}, ϵ_{xz}, and ϵ_{yz} should not cause resistance changes. Experimentally the value of the constant $\frac{1}{2}(\Pi_{1111} - \Pi_{1212})$ in n-Si is, in fact, approximately eight times larger than Π_{1212}.[15]

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[1] G. E. Pikus, JETP **41**, 1258 (1961), Soviet Phys. JETP **41**, 898 (1962).

[2] E. Wigner, Nachr. Akad. Wiss. Göttingen, Math.-Physik. Kl. **5**, 546 (1932).

[3] L. D. Landau and E. M. Lifshitz, Quantum Mechanics, Pergamon Press, 1958, Chap. 12.

[4] V. I. Sheka, FTT **2**, 1211 (1960), Soviet Physics - Solid State **2**, 1096 (1960).

[5] J. M. Luttinger, Phys. Rev. **102**, 1030 (1956).

[6] J. L. Birman, Phys. Rev. **114**, 1490 (1959).

[7] D. G. Thomas and J. J. Hopfield, Phys. Rev. **116**, 573 (1959); Thomas, Hopfield and Power, Phys. Rev. **119**, 570 (1960).

[8] É. I. Rashba, FTT **1**, 407 (1959), Soviet Physics - Solid State **1**, 368 (1959).

[9] É. I. Rashba and V. I. Sheka, FTT **1**, 162 (1959), Soviet Physics - Solid State **1**, 143 (1959).

[10] L. I. Schiff, Quantum Mechanics, McGraw-Hill, N. Y., 1955.

[11] W. Döring and V. Zehler, Ann. Physik **13**, 214 (1953); V. Żehler, Ann. Physik **13**, 229 (1953).

[12] G. E. Pikus and G. L. Bir, FTT **1**, 1642 (1959), Soviet Physics - Solid State **1**, 1502 (1960).

[13] G. E. Pikus and G. L. Bir, FTT **1**, 1828 (1959), Soviet Physics - Solid State **1**, 1675 (1960).

[14] É. I. Rashba, FTT **2**, 1224 (1960); Soviet Physics - Solid State **2**, 1109 (1960); I. I. Boĭko and É. I. Rashba, FTT **2**, 1874 (1960); Soviet Physics - Solid State **2**, 1692 (1961).

[15] C. Smith, Phys. Rev. **94**, 42 (1954).

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