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

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A new method is developed for constructing the Hamiltonian for carriers in semiconductors in the "effective mass" approximation in the presence of external fields and deformations, which allows the symmetry requirements to be taken into account without directly using perturbation theory.

1. INTRODUCTION

THE effective-mass method used to consider the motion of carriers in a periodic lattice perturbed by external electric and magnetic fields has been derived by a number of authors (see, for example,[1,2]). This method is used for calculating the energy spectrum of carriers in semiconductors and its change during deformation,[3,4] and in the theory of scattering it leads directly to the "deformation potential" method.[5,6]

In the method the wave function Ψ, which is a solution of the Schrödinger equation

$$\hat{\mathscr{H}}\Psi = (\hat{\mathscr{H}}_0 + \hat{\mathscr{H}}_1)\,\Psi = i\hbar\partial\Psi/dt, \tag{1}$$

is written approximately as the sum of the products of smooth functions $F_i(\mathbf{r}, t)$ and Bloch functions

$$\varphi_{i\mathbf{k}_0} = u_{i\mathbf{k}_0} \exp\,[i\,(\mathbf{k}_0\mathbf{r} - Et/\hbar)],$$

which are the eigenfunctions of the operator $\hat{\mathscr{H}}_0 = -(\hbar^2/2m)\nabla^2 + V_0(r)$ at an extremum point $\mathbf{k}_0$:

$$\Psi = \sum_{i=1}^{n} F_i\varphi_i. \tag{2}$$

Here in general the band is assumed degenerate at the point $\mathbf{k}_0$ i.e., to the eigenvalue $E_{\mathbf{k}_0}$ correspond n eigenfunctions $\varphi_{i\mathbf{k}_0}$.

The method is, of course, only valid when a number of conditions are satisfied—to be explicit: for free electrons described in this approximation by plane waves, the wave vector $\mathbf{k}$, reckoned from the point $\mathbf{k}_0$, must be sufficiently small as compared with a vector of the reciprocal lattice; the external fields appearing in $\hat{\mathscr{H}}_1$ must be sufficiently smooth; if these fields depend on time, the characteristic frequencies must be small compared with the quantity $\Delta E/\hbar$, where ΔE is the distance between nearest bands.

When these conditions are satisfied, the system of differential equations determining the functions F_i has the form

$$\mathscr{D}_{ij}(\mathscr{K})\,F_j = i\hbar\,\partial F_i/\partial t. \tag{3}$$

The matrix $\mathscr{D}$, which is the Hamiltonian in the effective-mass method, depends on the operators $\mathbf{k}$, on the external electric and magnetic fields, on the deformation tensor ϵ, etc. For simplicity in what follows, we shall use a single symbol $\mathscr{K}$ for all these scalar, vector, and tensor quantities.

Various variants of perturbation theory are generally used both to prove the applicability of the effective mass method and to construct the Hamiltonian $\mathscr{D}$. To construct $\mathscr{D}(\mathscr{K})$ the calculation has to be carried to second and higher orders of perturbation. Although the constants entering into $\mathscr{D}$ can in principle also be calculated by these methods, they are in practice determined from experiment. Thus, once the validity of the effective-mass method is proved, it is not necessary to use explicitly the rather cumbersome methods of perturbation theory to calculate $\mathscr{D}(\mathscr{K})$ for each specific case, since the form of this matrix is uniquely determined by the symmetry properties.

A number of workers[7,8] have successfully used various ways of constructing $\mathscr{D}$ directly. In the present work we develop a general method of constructing the operator $\mathscr{D}(\mathscr{K})$, starting directly from the symmetry conditions and the invariance of the Schrödinger equation under time inversion.

In the first part we shall not take spin-orbit interaction into account, so as to be able to display the principles of the method more simply. In the second part[9] it will be shown how spin-orbit interaction can be accurately taken into account within the framework of this method. For clarity we shall consider several examples in the first and, especially, in the second part. Using the method we shall consider the change of the energy spectrum of carriers in semiconductors with the wurtzite and germanium structures during deformation.

Other examples are contained in the article by the author and Bir devoted to calculating the effect of deformation on the electrical properties of p and n type InSb[10] and the article by the author[11] where the energy spectrum in tellurium is calculated.

2. SYMMETRY CONDITIONS

The operator $\hat{\mathcal{H}}_0$ in (1) is invariant under all the operations of the space group characterizing the symmetry of the crystal, i.e., in particular to the operations of the wave vector group $G_{\mathbf{k}_0}$, i.e., those operations of the complete space group which move $\mathbf{k}_0$ to equivalent points differing from $\mathbf{k}_0$ by one of the reciprocal lattice vectors.

Under these operations the functions $\varphi_{i\mathbf{k}_0}$ transform linearly into one another

$$\hat{G}\varphi_i(\mathbf{r}) = \varphi_i(\hat{G}^{-1}\mathbf{r}) = G^0_{i'i}\varphi_{i'}(\mathbf{r}). \tag{4}$$

Here $G^0_{i'i}$ are the matrix elements of the representation T_0 according to which the $\varphi_i(\mathbf{r})$ transform.

For brevity we shall omit the label $\mathbf{k}_0$ on φ_i and G, here and below. The operator $\hat{\mathcal{H}}_1$ in (1) is not in general invariant under these operations.

If we apply to (1) the transformation $\hat{G}$, going from $\mathbf{r}$ to $\mathbf{r}' = \hat{G}\mathbf{r}$, then, in place of the system of equations (3), we obtain a new system

$$\mathcal{D}(\hat{G}\mathcal{H})\, F = i\hbar\partial F/\partial t. \tag{5}$$

The form of the matrix $\mathcal{D}$ depends on the choice of a definite representation, i.e., on the basis: in (3) $\mathcal{D}(\mathcal{H})$ is written in the basis $\varphi_i(\mathbf{r})$, and in (5) $\mathcal{D}(\hat{G}\mathcal{H})$ is written in the basis $\varphi_i(\hat{G}\mathbf{r}) = \hat{G}^{-1}\varphi_i(\mathbf{r})$. If $\hat{G}$ appears in the wave vector group, then, using (4), we can rewrite $\mathcal{D}(\mathcal{H})$ in the same basis as $\mathcal{D}(\hat{G}\mathcal{H})$, and then both these matrices must be identical.

Consequently,

$$G^0\mathcal{D}(\mathcal{H})\, G^{0-1} = \mathcal{D}(\hat{G}\mathcal{H}). \tag{6}$$

This equation also determines the requirements imposed on $\mathcal{D}(\mathcal{H})$ by the symmetry conditions.

The matrix $\mathcal{D}$ is of dimension $n \cdot n$. It is therefore possible to take, as the basis for constructing $\mathcal{D}$, n^2 linearly independent matrices A_l with constant coefficients, i.e., not depending on $\mathcal{H}$. Since these matrices form a complete set, any of the matrices $G^0A_lG^{0-1}$ can be expanded in terms of them, and, consequently,

$$G^0A_l\, G^{0-1} = G_{l'l}A_{l'}.$$

It is easily verified that the matrices $G_{l'l}$ of dimensions $n^2 \cdot n^2$ form a representation of the group $G_{\mathbf{k}_0}$. This representation is reducible in the general case.

The matrices A_l can be chosen so that this representation is made irreducible. Then the matrices A_{sl}, being the basis of an irreducible representation T_s of the group $G_{\mathbf{k}_0}$, transform only into one another, i.e.,

$$G^0A_{sl}\, G^{0-1} = \hat{G}A_{sl} = G^s_{l'l}\, A_{sl'}. \tag{7}$$

We label the matrices A_{sl} with two symbols here: the first gives the number of the representation, s, according to which they transform, and the second, l, the number of the matrix in the representation; l takes values from 1 to m_s, where m_s is the dimension of the representation. Clearly, $\Sigma_s m_s = n^2$.

As is well known,[12] the wave vector group has two types of representation: for one of them under translation by a reciprocal lattice vector $\mathbf{t}$ we have $(0\,|\,\mathbf{t})_{l'l} = e^{i\mathbf{k}_0\cdot\mathbf{t}}\delta_{l'l}$. The wave functions $\varphi_{i\mathbf{k}_0}$ transform according to these representations. For the other type of representation $(0\,|\,\mathbf{t})_{l'l} = \delta_{l'l}$. These representations of the group $G_{\mathbf{k}_0} = (g\,|\,\tau)$ coincide with the representations of the corresponding point group $\overline{\overline{G}}$ with elements $(g\,|\,0)$. The matrices A_{sl} also transform according to these representations. Knowing the representation T_0 according to which the functions $\varphi_{i\mathbf{k}_0}$ transform, the irreducible representations according to which the matrices A_{sl} transform can be established. We write (7) in expanded form:

$$A_{sl,\,ij} = G^{0-1}_{ii'}\, G^0_{j'j}\, G^s_{l'l}\, A_{sl',\,i'j'} = G^s_{l,\,ij;\,l',\,i'j'}A_{sl',\,i'j'}. \tag{7a}$$

From a well-known theorem of group theory[12,13] the number of linearly independent groups of m_s matrices transforming according to the representation T_s is n_s:

$$n_s = \frac{1}{h}\sum_{G\in\bar{G}_{\mathbf{k}_0}} G^s_{l,\,ij;\,l,\,ij} = \frac{1}{h}\sum_{G\in\bar{G}_{\mathbf{k}_0}} \chi_s(G)\,|\chi_0(G)|^2, \tag{8}$$

where χ_0 and χ_s are the characters of the representations T_0 and T_s.

The summation here is carried over all the elements of the factor group $\bar{G}_{\mathbf{k}_0}$ of the wave vector group $G_{\mathbf{k}_0}$ which contains h elements. In other words, n_s is the number of identity representations contained in the direct product $T_0 \times T_0^* \times T_s$, or, correspondingly, the number of representations T_s contained in $T_0 \times T_0^*$. If $n_s > 1$ i.e., if T_s comes in more than once in $T_0 \times T_0^*$, then several groups of linearly independent matrices A_{sl} transform according to this representation. In order to distinguish these groups, we introduce a third label, t, and shall label these matrices A^t_{sl}. Of course, the form of these matrices depends on the choice of a concrete representation T_0.

We consider below in detail the methods of constructing these matrices; meanwhile we shall assume them to be known, and shall show how then to construct $\mathcal{D}(\mathcal{K})$, satisfying condition (6) and the conditions associated with the invariance of the Schrödinger equation to time inversion.

We express $\mathcal{D}(\mathcal{K})$ in terms of the basis mattrices A^t_{sl} and write it in the form

$$\mathcal{D}(\mathcal{K}) = \sum_{t,r,s} C^{tr}_s \sum_l A^t_{sl} f^r_{sl}(\mathcal{K}). \quad (9)$$

Here $f(\mathcal{K})$ are functions of the variables k_i, H_i, ϵ_{ij}, etc., and their products, which we wish to include in $\mathcal{D}$. For example, to calculate the spectrum it is only necessary to include in $\mathcal{D}$ functions of k_i. Depending on the problem considered, we can either limit ourselves to linear or quadratic terms, or include terms of higher orders. Various functions of $\mathcal{K}$, for example k_x^2, H_x^2, ϵ_{xx}, etc., can be associated with one matrix A^t_{sl}. We distinguish these functions by an index r. The coefficients C^{tr}_s are constants of the substance. If the matrices $\sum_l A^t_{sl} f^r_{sl}(\mathcal{K})$ are Hermitian these constants are real.

Let us see how to choose $f(\mathcal{K})$ so that condition (6) is satisfied.

We substitute (9) in (6). Then, taking (7) into account and comparing terms in the independent constants C^{tr}_s in (9), we obtain

$$\sum_l \hat{G}A^t_{sl} \cdot \hat{G}f^r_{sl}(\mathcal{K}) = \sum_l A^t_{sl} f^r_{sl}(\mathcal{K}). \quad (10)$$

Analogously to (4), $\hat{G}f(\mathcal{K}) = f(\hat{G}^{-1}\mathcal{K})$ here. Equation (10) means that each of the sums over l in (9) should transform according to an identity representation. Consequently, the matrices A_{sl}, which transform according to the representation T_s, must have as multipliers the functions $f_{sl}(\mathcal{K})$, which transform according to a conjugate (equivalent) representation T_s^*, i.e., so that

$$\hat{G}f_{sl}(\mathcal{K}) = f_{sl}(G^{-1}\mathcal{K}) = G^{s*}_{l'l} f_{sl'}(\mathcal{K}) = G^{s-1}_{ll'} f_{sl'}(\mathcal{K}). \quad (11)$$

In fact, Eq. (10) follows at once from (7) and (11).

Thus, to construct $\mathcal{D}$ it is necessary to construct functions of $\mathcal{K}$, which transform according to the irreducible representations contained in the direct product $T_0 \times T_0^*$. Functions $f(\mathcal{K})$, transforming according to other representations, cannot appear in $\mathcal{D}$. In practice, the construction of such functions presents no difficulty. All the quantities $\mathcal{K}$ are scalars, the components of polar or axial vectors or tensors and their symmetrized products, and they can be expressed in terms of irreducible representations by the usual methods of group theory.[13]

We shall not linger especially on this question, and point out only one particular case: according to [6], to take account of scattering by nonpolar optical vibrations, it is necessary to include in $\mathcal{D}$ functions of the components of the vector **u**, which describes the displacement of one of the sublattices relative to the other. This vector transforms as a usual polar vector under all operations which do not interchange the sublattices, but changes sign under those operations which do interchange the sublattices. It is necessary to take this fact into account when expressing $f(u_i)$ in irreducible representations.

3. INVARIANCE UNDER TIME INVERSION

If in the original equation (1) we change t into $-t$, and then go to the conjugate equation and replace in it H_i by $-H_i$ and $\hat{k}_i$ by $-\hat{k}_i$, we obtain the equation

$$\hat{\mathcal{H}}'^*\Psi'^* = i\hbar\partial\Psi'^*/\partial t.$$

If the system of differential equations (3) follows from (1), then we obtain similarly from this equation the system

$$\mathcal{D}'^* F'^* = i\hbar\,\partial F'^*/\partial t. \quad (12)$$

The prime signifies here the replacement of k_i by $-k_i$ and H_i by $-H_i$.

The Hamiltonians $\hat{\mathcal{H}}$ and $\hat{\mathcal{H}}^*$ are in general different. For them to coincide it is necessary to change H_i into $-H_i$ and k_i into $-k_i$ in $\hat{\mathcal{H}}$.[2,14] Consequently, the wave functions Ψ'^*, as well as the functions Ψ, are eigenfunctions of $\hat{\mathcal{H}}$, corresponding to the same value of the energy and the same value of the wave vector **k**, if, of course, **k** also remains an integral of motion in the "perturbed" equation (1).

Since $\hat{\mathcal{H}}_0^* \equiv \hat{\mathcal{H}}$, the functions $\hat{S}\varphi_i = \varphi_i^*$ are the basis of Eq. (12). If these functions are linearly related to the φ_i, which are the basis of $\mathcal{D}$ in (3), then $\mathcal{D}$ and $\mathcal{D}'^*$ can be written in a single basis. Since in this case the functions Ψ and Ψ'^* coincide, the matrices $\mathcal{D}$ and $\mathcal{D}'^*$, being written in a single basis, must also exactly coincide. This requirement imposes additional conditions on $\mathcal{D}(\mathcal{K})$. As Wigner[14] has shown, there is a linear relationship between φ_i and φ_i^* when the representation T_0 is real (case a). If the representations

T_0 and T_0^* are essentially complex and non-equivalent (case b) and $\mathbf{k}_0$ and $-\mathbf{k}_0$ appear in a single star, or if these representations are complex and equivalent (case c), they must be combined into one, i.e., in this case there is additional degeneracy.

If $\mathbf{k}_0$ and $-\mathbf{k}_0$ do not appear in a common star, there is no additional degeneracy at the point $\mathbf{k}_0$, and $E(\mathbf{k})$ must satisfy only the usual condition following from the equality of $\hat{\mathcal{H}}$ and $\hat{\mathcal{H}}'^*$: $E(\mathbf{k}) = E(-\mathbf{k})$. Knowing the characters of the representation, it is possible, using Herring's formula,[12,15] to decide to which case this representation belongs:

$$\frac{M}{h'}\sum_{\substack{(g|\tau)^2\in G_{\mathbf{k}_0}\\ \hat{g}\mathbf{k}_0=-\mathbf{k}_0}}\chi(g|\tau)^2=\begin{cases}1 - \text{case } a,\\ 0 - \text{case } b,\\ -1 - \text{case } c.\end{cases}\tag{13}$$

Summation here is performed over the operations of the factor group of the complete space group $G' = (g|\tau)$, for which $\hat{g}\mathbf{k}_0 = -\mathbf{k}_0$; h' is the number of elements of this group, and M is the number of vectors in the star of $\mathbf{k}_0$. It is clear that the operations $(g|\tau)^2$ always appear in the wave vector group $G_{\mathbf{k}_0}$. From (13) it follows that, if $\mathbf{k}_0$ and $-\mathbf{k}_0$ appear in different stars, then we are concerned with case b. In this case, which we shall label as b_3, no additional conditions apart from (6) are imposed on $\mathcal{D}$.

We shall consider in greater detail the case when invariance to time inversion leads to additional requirements on $\mathcal{D}$.

Case a: representation T_0 real.

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

In this case

$$\hat{S}\varphi_i=\varphi_i^*=S_{i'i}\varphi_{i'}.\tag{14}$$

Since $\hat{S}\hat{S} = 1$, and S is a unitary matrix, then

$$S=S^{*-1}=\tilde{S},\tag{15}$$

where $\tilde{S}$ signifies the matrix obtained by transposing S. The matrix $\mathcal{D}'^*$ in the representation φ_i, must coincide with $\mathcal{D}$, and, consequently, taking into account (15) and the fact that $\mathcal{D}$ is Hermitian,

$$\mathcal{D}=S\mathcal{D}'^*S^{-1}=S\tilde{\mathcal{D}}'S^{-1}=(S^{-1}\mathcal{D}'S)^{\sim},\tag{16}$$

it follows from (16) and (6) that

$$(G^0S)^{-1}\mathcal{D}'(\hat{G}\mathcal{K})(G^0S)=\tilde{\mathcal{D}}(\mathcal{K}).\tag{17}$$

We substitute $\mathcal{D}$ in the form (9) into (17), remembering that $f(\mathcal{K})$ is a homogeneous function of $\mathcal{K}$, and, therefore,

$$f(\mathcal{K}')=\gamma f(\mathcal{K}),\tag{18}$$

where $\gamma = \pm 1$, depending on the "parity" of $f(\mathcal{K})$.

We then obtain equations similar to (7a)

$$\begin{aligned}A^t_{sl,ij}&=(G^0S)^{ts}_{l,ij;l',i'j'}A^t_{sl',i'j'}\\&=\gamma\,(G^0S)^*_{i'j}(G^0S)_{j'i}G^{*s}_{l'l}A^t_{sl'i'j'}.\end{aligned}\tag{19}$$

We introduce the expanded group consisting of the elements of G and GS, the matrix elements of which are defined by (7a) and (19), and find n_S:

$$\begin{aligned}n_s&=\frac{1}{2h}\sum_{G\in\bar{G}_{\mathbf{k}_0}}G^{0ts}_{l,ij;l,ij}+(G^0S)^{ts}_{l,ij;l,ij}\\&=\frac{1}{2h}\sum_{G\in\bar{G}_{\mathbf{k}_0}}\chi_s(G)\,[\chi_0^2(G)+\gamma\chi_0(G^2)].\end{aligned}\tag{20}$$

Thus, we learn that, because $\hat{G}$ and $\hat{S}$ commute, and because of (16), it follows that $SG^{*0}S^* = SG^{0*}S^{-1} = G^0$, and also that $\chi_0^*(G) = \chi_0(G)$.

Thus, in case a_1, for even functions $f(\mathcal{K})$, the number n_S is equal to the number of representations T_S contained in the symmetric product $[T_0^2]$, and for odd, in the antisymmetric one $\{T_0^2\}$.

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

In this case the functions $\hat{S}\varphi_{i\mathbf{k}_0} = \varphi^*_{i\mathbf{k}_0}$ are linearly related, not to $\varphi_{i\mathbf{k}_0}$, but to $\varphi_{i,-\mathbf{k}_0}$. However, according to (13), there are in this case in the space group operations R that turn $\mathbf{k}_0$ into $-\mathbf{k}_0$. Therefore the functions $\hat{R}\hat{S}\varphi_{i\mathbf{k}_0}(\mathbf{r}) = \varphi^*_{i\mathbf{k}_0}(R^{-1}\mathbf{r})$ can be linearly expressed in terms of $\varphi_{i\mathbf{k}_0}(\mathbf{r})$:

$$\hat{R}\hat{S}\varphi_i=R_{i'i}\varphi_{i'}.\tag{21a}$$

Since $\hat{R}$ and $\hat{S}$ commute, and $\hat{S}^2 = 1$, it follows that

$$\hat{R}\varphi_i=R^*_{i'i}\varphi_{i'}.\tag{21b}$$

In order to write the matrix $\mathcal{D}'^*$ in (13) in the same basis as $\mathcal{D}$ in (3), we apply to the original equation the transformation $\hat{R}$, translating from $\mathbf{r}$ to $\mathbf{r}' = \hat{R}\mathbf{r}$. Instead of $\mathcal{D}'^*(\mathcal{K})$ in (12), we then obtain $\mathcal{D}'^*(\hat{R}\mathcal{K})$, where the basis of this matrix will already be the functions $\varphi_i^*(\hat{R}\mathbf{r}) = \hat{R}^{-1}\hat{S}\varphi_i = (\hat{R}^{-1})_{i'i}\varphi_{i'}$. In the basis $\varphi_i(\mathbf{r})$ this matrix must coincide with $\mathcal{D}$. Consequently,

$$R^{-1}\mathcal{D}'(\hat{R}\mathcal{K})R=\mathcal{D}(\mathcal{K}).\tag{22}$$

Here the matrix of the inverse operator $\hat{R}^{-1}$ is

$$(\hat{R}^{-1})_{ij}=R^{*-1}_{ij}=R_{ji},\tag{23}$$

which follows directly from the relationship $(\hat{R}^{-1}\hat{R})_{ij} = \hat{R}^{-1*}_{il}R_{lj} = \delta_{ij}$, and the fact that R is unitary.

An expanded group can be introduced, consisting of the elements of $G_{\mathbf{k}_0}$ and R. All the elements of R can be obtained by multiplying one of the elements of R_0 by all the elements of $G_{\mathbf{k}_0}$. In fact, the product of any of the elements of R by R_0 does not change $\mathbf{k}_0$, and therefore this element of the space group RR_0 is one of the elements of G.

The functions φ_i and $\varphi_I = \hat{S}\varphi_i$ are the basis of this expanded group. For $\hat{G}$ the only matrix elements different from zero are G_{ij} and $G_{IJ} = G_i^{*j}$, but for $\hat{R}$, only R_{iJ} [$= R_{ij}$ in the notation of Eq. (21)] and $R_{Ij} = R_{ij}^*$ are non-zero. For the matrix products, for example in (22), the usual laws of multiplication are then valid, but summation must be made over all intermediate indices and i and I. Thus $\mathcal{D}_{IJ} = \mathcal{D}_{ij}^*$. Similarly in (23), as for usual operators, $(\hat{R}^{-1})_{iJ} = R_{iJ} = R_{Ji}^* = R_{ji}$.

If $\mathcal{D}$ is expressed in terms of the matrices A_{sl}^t according to (9), and A_{sl}^t and f_{sl}^r are chosen so that they transform according to the irreducible representations of the point group, corresponding to the expanded group G, $R - T_s'$, and (9) is substituted in (22), we obtain in analogy to (7a)

$$A_{slij}^t = R_{l,ij;l',i'j'}^{ts} A_{sl'i'j'}^t = \gamma R_{j'i} R_{i'j}^* R_{l'l}^{*s} A_{sl'i'j'}^t. \quad (24)$$

Thus we learn from (18) and from the fact that $\mathcal{D}$ is Hermitian that

$$\sum_l A_{lij}^* f_l'^* (\hat{R}\mathcal{K}) = \gamma \sum_l A_{lji} f_l (\hat{R}\mathcal{K}).$$

When calculating n_s it is necessary to sum the characters over all the elements of the expanded group (G and $R = R_0G$):

$$n_s = \frac{1}{2h}\Big[\sum_{G\in\bar{G}_{\mathbf{k}_0}} G_{l,ij;l,ij}^{ts} + \sum_{R\in R_0\bar{G}_{\mathbf{k}_0}} R_{l,ij;l,ij}^{ts}\Big]$$

$$= \frac{1}{2h}\sum_{G\in\bar{G}_{\mathbf{k}_0}} \chi_s(G)\,|\chi_0(G)|^2 + \gamma\chi_s(R_0G)\,\chi_0[(R_0G)^2]. \quad (25)$$

Here $(\hat{R}^2)_{ii} = R_{iJ}R_{Ji} = R_{ij}R_{ji}^*$.

Cases b and c: representations T_0 and T_0^* complex.

1) b_1 and c_1; $\mathbf{k}_0$ equivalent to $-\mathbf{k}_0$.

In these cases there is additional degeneracy at the point $\mathbf{k}_0$, and the functions φ_i and $\varphi_I = \hat{S}\varphi_i = \varphi_i^*$ are linearly independent and are united into a single representation. Under all the operations of $G_{\mathbf{k}_0}$ the "diagonal" parts of the matrix $\mathcal{D}$ — $\mathcal{D}_{ij}$ and $\mathcal{D}_{IJ}$ —, and the "non-diagonal" parts— $\mathcal{D}_{iJ}$ and $\mathcal{D}_{Ij}$ —each transform into themselves. Of course, the matrix elements between the same functions must be equivalent, both in the matrix $\mathcal{D}$, constructed in the basis φ_i, φ_I, and in $\mathcal{D}'^*$, constructed in the basis $\bar{\varphi}_i = \hat{S}\varphi_i = \varphi_I$ and $\bar{\varphi}_I = \hat{S}\varphi_I = S^2\varphi_i = \varphi_i$. Therefore

$$\mathcal{D}_{ij}'^* = \mathcal{D}_{ji}' = \mathcal{D}_{IJ}, \quad (26a)$$

$$\mathcal{D}_{Ij}'^* = \mathcal{D}_{jI}' = \mathcal{D}_{iJ}. \quad (26b)$$

These conditions do not impose additional limitations on any of the "diagonal" parts of $\mathcal{D}$, and the number of groups of matrices A_{sl}^t with a non-zero diagonal part n_s is defined by the general equation (8). As regards the "non-diagonal" parts, it follows from (26b), (18), and (9) that

$$A_{slIj} = \gamma A_{slJi}. \quad (27)$$

It is, therefore, also possible here to introduce an expanded group G, GS. Then the effect of the operator $\hat{G}$ on the matrix elements A_{slij} is determined by (7a), and the elements of (GS) are, according to (7a) and (27),

$$A_{slIj}^t = (GS)_{l,Ij;l',I'j'}^{ts} A_{sl'I'j'}^t = \gamma G_{J'I}^{0*} G_{i'j}^0 G_{l'l}^{*s} A_{sl'I'j'}^t. \quad (28)$$

Since $G_{JI}^{0*} = G_{ji}^0$, it follows from (28) and (7a) that for the "non-diagonal" parts n_s is determined in this case also by (20).

2) b_2 and c_2; $\mathbf{k}_0$ not equivalent to $-\mathbf{k}_0$.

In this case also there is additional degeneracy. In the space group there is an operation R converting $\mathbf{k}_0$ into $-\mathbf{k}_0$, and the functions referring to the same point $\mathbf{k}_0$, i.e., φ_i and $\varphi_I = \hat{R}_0\hat{S}\varphi_i = \varphi_i^*(\hat{R}_0^{-1}\mathbf{r})$, where R_0 is one of the operations of R, are united in a single representation. If $\mathcal{D}$ is written in the basis φ_i, φ_I, then $\mathcal{D}'^*$ is in the basis $S\varphi_i$ and $S\varphi_I = \hat{R}_0\varphi_i$.

In order to write $\mathcal{D}'^*$ in the same basis as $\mathcal{D}$, we apply, as in case a_2, a transformation R. Then, instead of $\mathcal{D}'^*(\mathcal{K})$, we obtain $\mathcal{D}'^*(R\mathcal{K})$ in the basis

$$\bar{\varphi}_i = \hat{R}^{-1}\hat{S}\varphi_i = (R_0R)^{-1}\varphi_I,$$

$$\bar{\varphi}_I = R^{-1}S\varphi_I = S^2R_0R^{-1}\varphi_i = R_0R^{-1}\varphi_i.$$

The functions $\varphi_i(\mathbf{r})$ and $\hat{R}\varphi_i^*(\mathbf{r})$ here are linearly independent and are not expressible in terms of one another, but the operation R_0R appears in the group $G_{\mathbf{k}_0}$, and, therefore,

$$\varphi_I = (R_0R)_{i'i}\bar{\varphi}_{i'}, \quad \varphi_i = (RR_0^{-1})_{i'i}\bar{\varphi}_{I'}. \quad (29)$$

Of course, the matrix (R_0R) cannot here be considered as the product of two matrices R_0 and R, which in general do not exist separately.

It follows from (29) that

$$\mathcal{D}_{ij} = (R_0R)_{i'i}\mathcal{D}_{I'J'}'^*(\hat{R}\mathcal{K})(RR_0^{-1})_{j'j}, \quad (30a)$$

$$\mathcal{D}_{Ij} = (R_0R)_{i'i}\mathcal{D}_{i'J'}'^*(\hat{R}\mathcal{K})(RR_0^{-1})_{j'j} = (RR_0^{-1})_{j'j}\mathcal{D}_{J'i'}'(\hat{R}\mathcal{K})(R_0R)_{i'i}. \quad (30b)$$

These conditions do not impose additional limitations on any of the "diagonal" parts of $\mathcal{D}$, and the corresponding value of n_s, as above, is determined by (11). For the "non-diagonal" parts we have, according to (30b), (18), and (7):

$$A_{slij}^t = R_{lIj;l'I'j'}^{ts} A_{sl',I'j'}^t = \gamma(RR_0^{-1})_{i'j}(R_0R)_{j'i} R_{l'l}^{*s} A_{sl'I'j'}^t. \quad (31)$$

If the expanded group G and $R = R_0G$ is introduced, then it follows from (10) and (31) that in this case n_s for the "non-diagonal" parts is determined by (25).

From (11), (20), and (25) are obtained the formulae, previously derived by Rashba, [8] for determining the points of zero slope, i.e., those points where no terms linear in k appear in $\mathcal{D}$, i.e., where, for the corresponding representations T_s, $n_s = 0$ for $\gamma = -1$.

4. CONSTRUCTION OF THE MATRIX $\mathcal{D}$

The definite form of the matrix A^t_{sl} is determined by the choice of a definite representation T_0 according to which the basis functions transform. The more detailed methods of constructing them depends on the properties of this representation. We shall consider these methods.

1. The wave vector group $G_{\mathbf{k}_0}$ equivalent to the point group. As is well known, [12] in a number of cases the matrix elements of the representation T_0 — $(g \mid \tau_g)_{ij}$ — can be expressed as the products of matrix elements of the corresponding representation of the point group $\bar{\bar{G}}$ — $(g \mid 0)_{ij}$ and $e^{-ik_0\tau_g}$:

$$G_{ij} = \bar{\bar{G}}_{ij} e^{-i\mathbf{k}_0\tau_g}. \tag{32}$$

For this to be so, it is necessary that (32) satisfy the multiplication law of elements of the wave vector group, i.e., that

$$[(\alpha \mid \boldsymbol{\tau}_\alpha)(\beta \mid \boldsymbol{\tau}_\beta)]_{ij} = (\alpha\beta)_{ij} e^{-i\mathbf{k}_0(\tau_\alpha + \tau_\beta)} = (\alpha\beta \mid \hat{\alpha}\boldsymbol{\tau}_\beta + \boldsymbol{\tau}_\alpha) = (\alpha\beta)_{ij} e^{-i\mathbf{k}_0(\hat{\alpha}\tau_\beta + \tau_\alpha)}.$$

This condition is satisfied when

$$\psi_{\alpha\beta} = \exp\{-i\mathbf{k}_0(\hat{\alpha}\boldsymbol{\tau}_\beta = \boldsymbol{\tau}_\beta)\} \equiv 1$$

for all the operations of $G_{\mathbf{k}_0}$, which occurs for all points $\mathbf{k}_0$ lying inside the Brillouin zone and often also for points on the surface. In these conditions the factor group $\bar{G}_{\mathbf{k}_0}$ is isomorphous with the point group $\bar{G}$. Thus, to satisfy (6) it is necessary and sufficient according to (32) that

$$\bar{\bar{G}}_0 \mathcal{D}(\mathcal{K}) \bar{\bar{G}}_0^{-1} = \mathcal{D}(\hat{G}\mathcal{K}) \tag{33}$$

and, therefore, as the basis of $\mathcal{D}$, the eigenfunctions u_i of the point group $\bar{\bar{G}}$ can be chosen, which transform according to the representation $\bar{T}_0$. Since any point group is a sub-group of the complete space group, the functions u_i can consist of the eigenfunctions $Y^{j\pm}_m$ of any of the representations of the complete space group D which contain $\bar{T}_0$:

$$u_i = a^i_{j,m\pm} Y^{j\pm}_m. \tag{34}$$

If the representation $\bar{T}_0$ is irreducible, then only spherical functions $Y^{j\pm}_m$ with one value of j appear in the u_i in (34). For the matrices A^t_{sl} we can thus use the well-known matrices of the components of the axial vector J_i and their products — $\varphi^t_{s,l}(J_i)$, constructed from the corresponding basis functions u_i. The matrices $\varphi^t_{sl}(\mathbf{J})$ transform under the operations of $\bar{\bar{G}}$ just as the operator $\varphi^t_{sl}(\hat{\mathbf{J}})$. In fact, the matrix elements $\varphi^t_{sl}(\hat{\mathbf{J}})$ are non-zero only in the case when they are invariant under the operations $\bar{\bar{G}}$. Consequently,

$$\bar{\bar{G}}^0 \varphi^t_{sl}(\mathbf{J}) \bar{\bar{G}}^{0-1} = \varphi^t_{sl}(\hat{G}^{-1}\mathbf{J}) = G^s_{l'l}\varphi^t_{sl'}(\mathbf{J}), \tag{35}$$

which agrees with (7). Therefore, in the present case it is necessary to construct the operator

$$\hat{\mathcal{D}} = \sum_{t,r,s} C^{t,r}_s \sum_l \varphi^t_{sl}(\hat{\mathbf{J}}) f^r_{sl}(\mathcal{K}), \tag{36}$$

invariant under the operations G, i.e., satisfying the condition

$$\sum_l \varphi^t_{s,l}(\hat{G}\hat{\mathbf{J}}) f^r_{sl}(\hat{G}\mathcal{K}) = \sum_l \varphi^t_{sl}(\hat{\mathbf{J}}) f^r_{sl}(\mathcal{K}), \tag{37}$$

and its matrix constructed in the basis u_i will then satisfy condition (10).

Now, according to (11), $\varphi_{sl}(\hat{\mathbf{J}})$ and $f(\mathcal{K})$ must transform according to conjugate (equivalent) representations. The construction of these functions and of the operator $\mathcal{D}$ itself is very simple. The construction of the matrices $\varphi_{sl}(\mathbf{J})$ is more complicated.

The general number of linearly independent matrices $\varphi^t_{sl}(\mathbf{J})$ in the space of the functions $Y^{j\pm}_m$ is $(2j+1)^2$, while the number of linearly independent matrices in the space u_i is equal to the square of the dimensions of the representation T_0 — n^2_s, and n_s matrices from them transform according to each of the representations T_s, where n_s is given by equation (8). Applying the usual methods of group theory, [12] it can at once be established in which of the representations $D^\pm_j$ a given representation $\bar{T}_0$ is contained. Of course, j must be taken as small as possible; then the actual breaking up of this representation into irreducible representations, i.e., the determination of $a^i_{j,m}$ in (34) and the construction of the corresponding matrices $\varphi(\mathbf{J})$, becomes simplest. If $n < 2j+1$, then some of the $(2j+1)^2$ matrices $\varphi(\mathbf{J})$ either become zero or linearly dependent. Therefore, if a greater number of the group of matrices transform according to the representation T_s than given by (8), the "superfluous" matrices must not be included in $\mathcal{D}$. If $n = 2j+1$, i.e., the representation $\bar{T}_0$ coincides with $D^\pm_j$, then the matrices $\varphi(\mathbf{J})$ can be taken in any representation with the given j. In this case the method described here coincides with Luttinger's method. [7]

If there are two representations T_{01} and T_{02} for which the moduli of the characters coincide, then the same $f(\mathscr{K})$ appear in $\mathscr{D}(\mathscr{K})$ according to (8). It is not, however, obvious whether the determinants $\|\mathscr{D}(\mathscr{K})\|$ are always the same for both representations. For two-dimensional representations the equality of the determinants follows from the method of constructing $\mathscr{D}$ described below. It is apparent from (6) that the determinants are also equal if the representations T_{01} and T_{02} differ only in parity, and also in the more general case when the group $G'' = Ge^{-i\pi\delta G}$, where $e^{-i\pi\delta G} = \chi_{01}(G)/\chi_{02}(G)$, is isomorphous with the group G. In these cases it is sufficient to construct $\mathscr{D}$ only for that representation T_{0i} which is contained in $D_j^{\pm}$ with the minimum j.

The additional requirements associated with invariance to time inversion imply that the part of the terms for which, according to (20) or (25) $n_s = 0$, is excluded from $\mathscr{D}$ in the corresponding cases. In case a_1 it is also possible to use directly relation (16), since

$$S\varphi^*(\mathbf{J})S^{-1} = SS\varphi(\mathbf{J}^*)S^{-1}S^{-1} = \varphi(\mathbf{J}^*) = \gamma'\varphi(\mathbf{J}), \quad (38)$$

where $\varphi(\mathbf{J}^*)$ is the matrix of the operator $\varphi(\hat{\mathbf{J}}^*)$, the complex conjugate of $Q(\hat{\mathbf{J}})$. Here $\gamma' = \pm 1$, depending on the parity of $\varphi(\hat{\mathbf{J}})$. It therefore follows from (16) that in case a_1 there can appear in $\mathscr{D}$ in (36) only even products with $\gamma\gamma' = 1$, i.e., those not changing sign on replacing k_i, H_i and J_i by $-k_i$, $-H_i$ and $-J_i$. In the other cases this simple rule is not, of course, valid.

2. Unifying several representations. In some cases, for example, when it is necessary to take account of the effect of the nearest zones, and also in cases $b_{1,2}$ and $c_{1,2}$, when complex representations are combined, it is necessary to construct $\mathscr{D}$ for the reducible representation T_0 which contains several irreducible representations T_{0i}. If the group $G_{\mathbf{k}_0}$ is equivalent, in the sense given above, to the point group $\overline{\overline{G}}$, then $\mathscr{D}$ can be constructed analogously. If all the irreducible representations are contained in the same representation $D_j^{\pm}$, then their basis functions can be constructed from $Y_m^{j\pm}$ with the same j, and, as above, for the matrices A_{sl}^t can be taken the matrices $\varphi_{sl}^t(\mathbf{J})$, constructed from the corresponding basis functions.

If the irreducible representations T_{0i} are contained in different representations $D_j^{\pm}$ with j differing by not more than unity, then, depending on the parity of these representations, it is simplest to choose as these matrices the matrices of either the axial vector $\mathbf{J}$ or the polar vector $\mathbf{A}$.[13] If T_0 contains, for example, two representations T_{01} and T_{02} of dimensions n_1 and n_2, then in all there are $(n_1+n_2)^2$ non-zero linearly independent matrices. Of these $2n_1n_2$ matrices transform according to the irreducible representations contained in $T_{01} \times T_{02}^* + T_{01}^* \times T_{02}$, and have only non-zero "interband" matrix elements. For the remaining $n_1^2 + n_2^2$ matrices, which transform according to the representations contained in $|T_{01}|^2 + |T_{02}|^2$, the intraband matrix elements are non-zero. As regards the conditions imposed by invariance under time inversion, in obtaining the equations of Sec. 2 we have nowhere supposed that the representation T_0 is irreducible, and all these equations therefore remain in force.

When combining two complex representations in cases $b_{1,2}$ and $c_{1,2}$, it is also necessary to take into account the additional conditions (26a) and (30a) imposed on the "diagonal" parts of the matrix $\mathscr{D}$.

3. The group $G_{\mathbf{k}_0}$ not equivalent to the point group. In this case, when the quantity $\psi_{\alpha\beta}$ is not equal to unity for all $G_{\mathbf{k}_0}$, the quantities G_{ij} cannot be represented in the form (32), and the factor group $\overline{G}_{\mathbf{k}_0}$ of the space group $\underline{\underline{G}}_{\mathbf{k}_0}$ contains more elements than the point group $\overline{\overline{G}}$. This case, which is more complicated, can occur at separate points on the zone surface; then there is usually degeneracy at such a point. In the case of twofold degeneracy, $\mathscr{D}$ can be immediately constructed by the method described in the following section. For higher degeneracy $\mathscr{D}$ can be constructed as follows.

We reduce the symmetry of the group $G_{\mathbf{k}_0}$ by excluding elements with non-primitive translations, so that the new group $\tilde{G}_{\mathbf{k}_0}$ becomes equivalent to the point group. In this group the representation T_0 can be reducible, and breaks down into irreducible representations $\tilde{T}_{0i}$. By combining these representations it is possible by the method given above to construct a matrix $\tilde{\mathscr{D}}$, satisfying Eq. (6) for the operations $\tilde{G}$. On increasing the symmetry, i.e., going from $\tilde{G}_{\mathbf{k}_0}$ to $G_{\mathbf{k}_0}$, the form of $\mathscr{D}$ can change only due to some of the constants C_s^{tr} becoming zero and some of them becoming equal. If, using relation (8), n_s is found for both groups, and $\mathscr{D}$ and $\tilde{\mathscr{D}}$ are written in the general form (9) without explicitly writing out the matrices A_{sl}^t, then, by comparing these expressions, it is usually possible to establish at once which of the constants become zero or equal on going from $\tilde{\mathscr{D}}$ to $\mathscr{D}$, and, simultaneously, to find $\mathscr{D}$. To simplify the calculations it is, of course, necessary to choose the group $\tilde{G}_{\mathbf{k}_0}$ so that the symmetry remains the maximum possible.

4. Twofold degeneracy. In the case of twofold degeneracy at the point $\mathbf{k}_0$, both the determinant $\|\mathscr{D} - E\|$ and the matrix $\mathscr{D}$ can be constructed

without using concrete basis functions. From (6) follows the obvious identity

$$\|\mathcal{D}(\mathcal{K})-E\|=\|\mathcal{D}(\hat{G}\mathcal{K})-E\|, \tag{39}$$

i.e., the determinant $\|\mathcal{D}(\mathcal{K})-E\|$ must be invariant to the operations $\hat{G}$. We write the matrix $\mathcal{D}-E$ in the form

$$\mathcal{D}-E=\begin{vmatrix} a_0+a_1-E & a_{12} \\ a_{12}^* & a_0-a_1-E \end{vmatrix}. \tag{40}$$

Then

$$\|\mathcal{D}-E\|=(E-a_0)^2-a_1^2-|a_{12}|^2. \tag{41}$$

Here we have formally replaced all operators in a_i by numbers. We remember that only symmetrized products of operators appear in $\mathcal{D}$. It is clear from (39) that only functions $f(\mathcal{K})$ appear in a_0 which are invariant to $\hat{G}$, i.e., transform according to an identity representation, but in $a_2=a_1^2+|a_{12}|^2$ there appear only quadratic invariants of $f(\mathcal{K})$, which transform according to non-identity representations. These invariants can be constructed uniquely. Since in the direct product $T_s \times T_{s'}$ an identity representation is contained only once if $s=s'$, and not at all if $s \neq s'$, only products of $f(\mathcal{K})$ can appear in a_2 which transform according to the same representation —one product for each irreducible representation T_s for which n_s is non-zero according to (8), (20), or (25). These formulae therefore uniquely determine $\|\mathcal{D}-E\|$.

For two-dimensional representations T_0 the product $T_0 \times T_0^*$ breaks down either into four one-dimensional irreducible representations or into two one-dimensional, including the identity T_1, and one two-dimensional.

In the first case, when all the representations T_s are one-dimensional,

$$a_0=\sum_r C_1^r f_1^r(\mathcal{K}), \qquad a_2=\sum_{r,s=2,3,4}|C_s^r f_s^r(\mathcal{K})|^2. \tag{42}$$

It is apparent that $\mathcal{D}$ can be chosen in any form satisfying (42) and the condition that it be Hermitian.

If all the $f_s^r(\mathcal{K})$ are chosen real, then $\mathcal{D}$ can, for example, be written in the form

$$\mathcal{D}=\sum_{r,s} C_s^r A_s f_s^r(\mathcal{K}), \tag{43}$$

where $A_1=I$, and A_2, A_3, and A_4 are the Pauli matrices σ_x, σ_y, and σ_z. We note that, irrespective of the choice of basis, we have $\mathrm{Sp}\,A_s=0$ for any matrix A_s transforming according to the one-dimensional non-identity representation. In fact, $\mathrm{Sp}\,(G^0 A_s G^{0-1})=\mathrm{Sp}\,A_s$. On the other hand, for the one-dimensional representations $GA_s=e^{i\varphi G}A_{s'}$, and, consequently, $\mathrm{Sp}\,\hat{G}A_s=e^{i\varphi G}\,\mathrm{Sp}\,A_s$. Since for non-identity representations all the $e^{i\varphi G}$ cannot be equal to unity, for them $\mathrm{Sp}\,A_s=0$. Therefore A_s can always be represented as the sum of Pauli matrices, and by unitary transformations they can be brought to the form described above. This does not, of course, mean that the corresponding matrices transform as spin operators.

In the second case, when one of the representations, T_3, is two-dimensional, the $f_{3l}^r(\mathcal{K})$ transforming according to this representation can always be chosen so that $f_{32}^r(\mathcal{K})=f_{31}^{r*}(\mathcal{K})$ and $|f_{31}^r(\mathcal{K})|^2$ is invariant under G. Then

$$a_2=\sum_r |C_2^r f_2^r(\mathcal{K})|^2+|C_3^r f_{31}^r(\mathcal{K})|^2. \tag{44}$$

If here $f_2^r(\mathcal{K})$ is real, then $\mathcal{D}$ can be expressed in the form

$$\mathcal{D}=\sum_{r,s,l} C_s^r A_{sl} f_{sl}^r(\mathcal{K}), \tag{45}$$

where

$$A_1=I=\begin{vmatrix}1&0\\0&1\end{vmatrix},\quad A_2=\sigma_z=\begin{vmatrix}1&0\\0&-1\end{vmatrix},\quad A_{31}=\sigma_+=\begin{vmatrix}0&1\\0&0\end{vmatrix},$$
$$A_{32}=\sigma_-=\begin{vmatrix}0&0\\1&0\end{vmatrix}. \tag{46}$$

Of course, all the $f_{3l}^r(\mathcal{K})$ with equal indices l must transform according to the same representation, i.e., according to the representation T_s, for which all the matrix elements coincide and not only the characters.

With the choice of $f_{sl}^r(\mathcal{K})$ and the matrices A_{sl} given above, the operator $\mathcal{D}$ satisfies both condition (39) and the requirement that it be Hermitian. The method proposed here for constructing $\mathcal{D}$ for twofold degenerate representations is the most simple. This method is close to that used by Rashba.[8]

In conclusion we consider a concrete example.

5. THE EFFECT OF DEFORMATION ON THE ENERGY SPECTRUM OF CARRIERS IN WURTZITE TYPE CRYSTALS

The space group of wurtzite C_{6v}^4 has been investigated in detail by Rashba.[8] He has constructed the wave vector group for the various points and calculated the spectrum at these points. For degenerate representations the possible points of zero slope in wurtzite are: a) for the representations Δ_5 and Δ_6, all the points on the Δ axis apart from A; b) for the representations P_3, the point H (in the notation of [8]). We consider the change of the spectrum for the corresponding representations under deformation.

Table I*. Characters of the representations for the point Δ

Number of elements	Elements of the class	Δ_1	Δ_2	Δ_3	Δ_4	Δ_5	Δ_6
1	$(\varepsilon \mid 0)$	1	1	1	1	2	2
2	$(\delta_6 \mid {}^1/_2\, t_0),\ (\delta_6^{-1} \mid {}^1/_2\, t_0)$	η_k	η_k	$-\eta_k$	$-\eta_k$	$-\eta_k$	η_k
2	$(\delta_3 \mid 0),\ (\delta_3^{-1} \mid 0)$	1	1	1	1	-1	-1
1	$(\delta_2 \mid {}^1/_2\, t_0)$	η_k	η_k	$-\eta_k$	$-\eta_k$	$2\eta_k$	$-2\eta_k$
3	$(\sigma_1 \mid 0),\ (\sigma_2 \mid 0),\ (\sigma_3 \mid 0)$	1	-1	1	-1	0	0
3	$(\sigma_1' \mid {}^1/_2\, t_0),\ (\sigma_2' \mid {}^1/_2\, t_0),\ (\sigma_3' \mid {}^1/_2\, t_0)$	η_k	$-\eta_k$	$-\eta_k$	η_k	0	0

*$\eta_k = \exp(ik_z t_0/2)$. For the point Γ the quantity $\eta_k = 1$.

1) The point Δ. The characters of the representations at the points Δ calculated by Rashba are given in Table I.

The twofold representations Δ_5 and Δ_6 belong to the case b_3 and, consequently, according to (8), there can appear in $\mathscr{D}$ matrices A_{sl} and $f(\mathscr{K})$, which transform according to the representations $\Delta_5 \times \Delta_5^* = \Delta_6 \times \Delta_6^* = \Gamma_1 + \Gamma_2 + \Gamma_5$.

The functions $f(\mathscr{K})$, transforming according to these representations, are given in Table III. We limit ourselves here to terms quadratic in **k** and linear in ϵ. The matrices mentioned transform according to these representations. We choose the functions $f(\mathscr{K})$ in accordance with the requirements of Sec. 3, item 4, taking in particular (44) into account. Therefore, according to (45),

$$\mathscr{D} = A_1 (B_0 k_z + B_1 k_z^2 + B_2 k_\perp^2 + C_1 \varepsilon_{zz} + C_2 \varepsilon_\perp) + B_3 (A_{31} k_+^2 + A_{32} k_-^2) + C_3 (A_{31} \varepsilon_+ + A_{32} \varepsilon_-). \quad (47)$$

Here

$$k_\pm = k_x \pm i k_y, \quad k_\perp^2 = k_x^2 + k_y^2,$$
$$\varepsilon_\pm = \varepsilon_{xx} \pm 2i\varepsilon_{xy} - \varepsilon_{yy}, \quad \varepsilon_\perp = \varepsilon_{xx} + \varepsilon_{yy},$$

B_i and C_i are constants of the substance and the matrices A_{sl} are given by (46).

For the representations Γ_5 and Γ_6, which belong to case a_1, there can, according to (20), only appear in $\mathscr{D}$ even functions of $\mathscr{K}$, which transform according to $[\Gamma_{5,6}^2] = \Gamma_1 + \Gamma_5$ (and odd functions transforming according to $\{\Gamma_{5,6}^2\} = \Gamma_2$). Therefore, at this point $B_0 = 0$. In addition, the point of zero slope can be any of the points Δ. At these points, according to (47), the solution of the secular equation $\| \mathscr{D} - E \| = 0$ has the form

$$E(k, \varepsilon) = \lambda \pm \{B_3^2 k_\perp^4 + 2B_3 C_3 [(\varepsilon_{xx} - \varepsilon_{yy})(k_x^2 - k_y^2) + 4\varepsilon_{xy} k_x k_y] + C_3^2 [(\varepsilon_{xx} - \varepsilon_{yy})^2 + 4\varepsilon_{xy}^2]\}^{1/2}, \quad (48)$$

where

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

The splitting of the terms at **k** = 0 is

$$\delta E_0 = 2 \mid C_3 \mid [(\varepsilon_{xx} - \varepsilon_{yy})^2 + 4\varepsilon_{xy}^2]^{1/2}. \quad (49)$$

Close to the extremum, i.e., for $E(k) \ll \delta E_0$, the surfaces of constant energy have the form of ellipsoids:

$$E_{1,2} = \pm \frac{\delta E_0}{2} + \lambda \pm \frac{2C_3 B_3}{\delta E_0} [(k_x^2 - k_y^2)(\varepsilon_{xx} - \varepsilon_{yy}) + 4k_x k_y \varepsilon_{xy}]. \quad (50)$$

For large k, when $E(k) \gg \delta E_0$,

$$E = \lambda \pm \mid B_3 \mid k_\perp^2 \pm \frac{B_3 C_3}{|B_3| \, k_\perp^2} [(\varepsilon_{xx} - \varepsilon_{yy})(k_x^2 - k_y^2) + 4\varepsilon_{xy} k_x k_y]. \quad (51)$$

Therefore, according to [16], large values of the piezoresistance coefficients, $\Pi_{xxxx} = \Pi_{yyyy}$, $\Pi_{xxyy} = \Pi_{yyxx}$, and Π_{xyxy}, can be expected here —these constants being proportional to C_3/kT. Of course, all these formulae are valid only in the case when the splitting of the bands δE_0 caused by the deformation exceeds the spin-orbit splitting.

2) The point H. The characters of the representations at the points P are given in Table II. The twofold degenerate representation H_3 belongs to the case a_2. To construct $\mathscr{D}$ according to (25), it is necessary to construct $f(\mathscr{K})$ which transform according to the irreducible representations of the expanded group G, R, containing the elements G_H and $G_H R_0$. This group coincides with the group Γ, and we have already constructed the corresponding functions (Table III). Substituting in (25) the values of the corresponding characters from Tables I and II, we find that there can appear in $\mathscr{D}$ odd

Table II*. Characters of the representations for the point **P**

Number of elements	Elements of the class	P_1	P_2	P_3
1	$(\varepsilon \mid 0)$	1	1	2
2	$(\delta_3 \mid 0),\ (\delta_3^{-1} \mid 0)$	1	1	-1
3	$(\sigma_1' \mid {}^1/_2\, t_0),\ (\sigma_2' \mid {}^1/_2\, t_0),\ (\sigma_3' \mid {}^1/_2\, t_0)$	η_k	$-\eta_k$	0

*For the point H the quantity $\eta_k = i$, and for the point K the quantity $\eta_k = 1$.

Table III*. The distribution of $f(\mathscr{K})$ and A_{sl} over the irreducible representations Γ and K

Representation Γ	Representation K	$f(\mathscr{K})$ odd	$f(\mathscr{K})$ even	A_{sl}
Γ_1	K_1	k_z	k_z^2; $k_\perp^2$; ε_{zz}; $\varepsilon_\perp$	A_1
Γ_4		—	—	
Γ_2	K_2	—	—	A_2
Γ_3		—	—	
Γ_5	K_3	—	k_+^2, k_-^2; $\varepsilon_+, \varepsilon_-$	A_{31}, A_{32}
Γ_6		k_+, k_-	$k_+ k_z$, $k_- k_z$; ε_{+z}, ε_{-z}	

*$k_\pm = k_x \pm ik_y$, $k_\perp^2 = k_x^2 + k_y^2$, $\varepsilon_\pm = \varepsilon_{xx} \pm 2i\varepsilon_{xy} - \varepsilon_{yy}$, $\varepsilon_\perp = \varepsilon_{xx} + \varepsilon_{yy}$, $\varepsilon_{\pm z} = \varepsilon_{xz} \pm i\varepsilon_{yz}$.

functions transforming according to the representations Γ_2 and Γ_5, and even functions transforming according to Γ_1 and Γ_6. We emphasize that the matrix $\mathscr{D}$ must be invariant to the operations of the point group K corresponding to the group H, and there must appear in $\mathscr{D}$ products of $f_{sl}(\mathscr{K})$ and A_{sl}, which transform according to the equivalent representations of the group K appearing in $H_3H_3^*$, i.e., K_1, K_2, and K_3. These functions can transform according to different representations of the group Γ, since two representations Γ_i correspond to each representation K_i, as is seen from Table III.

We construct $\mathscr{D}$ using the functions from Table III:

$$\mathscr{D} = A_1(B_1k_z^2 + B_2k_\perp^2 + C_1\varepsilon_{zz} + C_2\varepsilon_\perp) + B_3(A_{31}k_+ + A_{32}k_-)k_z + C_3(A_{31}\varepsilon_{+z} + A_{32}\varepsilon_{-z}), \quad (52)$$

where $\epsilon_{\pm z} = \epsilon_{xz} \pm i\epsilon_{yz}$, and the matrices A_{sl} are given by (46). Solving the secular equation $\|\mathscr{D} - E\| = 0$ we have

$$E(k, \varepsilon) = \lambda \pm \{B_3^2k_\perp^2k_z^2 + 2B_3C_3(k_x\varepsilon_{xz} + k_y\varepsilon_{yz})k_z + C_3^2(\varepsilon_{xz}^2 + \varepsilon_{yz}^2)\}^{1/2}, \quad (53)$$

where λ is given by (48).

Consequently, the splitting of the bands at $\mathbf{k} = 0$ is

$$\delta E_0 = 2|C_3|(\varepsilon_{xz}^2 + \varepsilon_{yz}^2)^{1/2}. \quad (54)$$

The spectrum close to the extremum for small values of k is:

$$E_{1,2} = \pm\frac{\delta E_0}{2} + \lambda \pm \frac{2B_3C_3}{\delta E_0}(k_xk_z\varepsilon_{xz} + k_yk_z\varepsilon_{yz}). \quad (55)$$

The spectrum for large k is:

$$E = \lambda \pm |B_3k_\perp k_z| \pm \frac{B_3C_3}{|B_3k_\perp k_z|}(\varepsilon_{xz}k_xk_z + \varepsilon_{yz}k_yk_z). \quad (56)$$

Therefore, according to [16], there will be large piezoresistance coefficients $\Pi_{xzxz} = \Pi_{yzyz}$.

It is curious here that for any deformation all the extrema at different points of the star H are displaced equally, as is seen from (49). This means that no effects arise associated with the displacement of the extrema relative to one another, as are observed, for example, in n-Ge and n-Si.[17]

[1] S. I. Pekar, Issledovaniya po Élektronnoĭ Teorii Kristallov (Studies in the Electronic Theory of Crystals), Gostekhizdat 1951, p. 26.

[2] J. M. Luttinger and W. Kohn, Phys. Rev. **97**, 869 (1955).

[3] E. N. Adams, Phys. Rev. **96**, 803 (1954).

[4] G. E. Pikus and G. L. Bir, FTT **1**, 154 and 1642 (1959), Soviet Phys.-Solid State **1**, 136 (1959) and 1502 (1960).

[5] J. Bardeen and W. Shockley, Phys. Rev. **80**, 72 (1950).

[6] G. E. Pikus, ZhTF **28**, 2390 (1958), Soviet Phys.-Tech. Phys. **3**, 2194 (1959). G. L. Bir and G. E. Pikus, FTT **2**, 2287 (1960), Soviet Phys.-Solid State **2**, 2039 (1961).

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

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

[9] G. E. Pikus, JETP **41**, 1507 (1961), Soviet Phys. JETP, in press.

[10] G. L. Bir and G. E. Pikus, FTT **3**, 3058 (1961), Soviet Phys.-Solid State **3**, in press.

[11] G. E. Pikus, FTT **3**, 2819 (1961), Soviet Phys.-Solid State **3**, in press.

[12] G. L. Lyubarskii, Teoriya Grupp i ee Primenenie v Fizike (Group Theory and its Application in Physics), Gostekhizdat 1957.

[13] L. D. Landau and E. M. Lifshitz, Quantum Mechanics, Pergamon, 1958, Chap. XII.

[14] E. Wigner, Gött. Nachr. **5**, 546 (1932).

[15] C. Herring, Phys. Rev. **52**, 361 (1937).

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

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

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