Symmetry of Energy Bands in Crystals of Wurtzite Type II. Symmetry of Bands with Spin-Orbit Interaction Included

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Abstract

Double-valued representations of the space group C_{6v}^4 (wurtzite lattice) have been constructed. A variant of perturbation theory is presented, allowing the investigation of the dispersion law in the vicinity of symmetry elements taking into consideration the spin-orbit interaction. The formulae obtained here differ from those available in the literature and lead to a qualitatively different dispersion law for a number of points. A group theoretical analysis of the structure of energy bands in a wurtzite type lattice was carried out taking the spin-orbit interaction into consideration. The possibility of energy surfaces $E(\boldsymbol{k})$, where (in a proper approximation) the extremum is reached along an entire curve rather than in isolated points of $\boldsymbol{k}$ space, is demonstrated.

Introduction

A previous paper by one of the authors [1] provided a group theoretical analysis of the structure of the energy bands in crystals with a wurtzite lattice (space group C_{6v}^4) without taking the spin-orbit interaction into account. In particular, the possible positions of the zero-slope points were determined and the dispersion law near the symmetry elements was found. A similar analysis is carried out in the present study but with the spin-orbit interaction taken into account. Particular attention is paid to deriving the dispersion law in the vicinity of the symmetry elements where extrema can be located in the absence of spin-orbit interaction.

1 Construction of double-valued irreducible representations

A description of the wurtzite-type lattice with the indication of the symmetry operations may be found in [1] (Fig. 1). The scheme of the first Brillouin zone with the definition of

the symmetry points may also be found there (Fig. 2). We adhere below to all notations of Ref. [1].

The factor group of the double space group over the translation subgroup comprises 24 elements. It is easy to obtain the multiplication table for the double space group, once the multiplication table has been constructed for the double point group, by multiplying the 2×2 matrices of the representation $D_{1/2}$ [2]. For all symmetry points, the tables of the characters of the double-valued representations of the wave vector groups can be obtained directly from the tables of the characters of the corresponding point groups in a manner similar to that employed in [1] for single-valued representations. Characters of the irreducible double-valued representations for all symmetry points are presented in Tables 1 – 5.

It is easy to see that the characters of the representations Δ_9, F_3, F_4, U_5, and P_6 are periodic in $\boldsymbol{k}$-space with the period of the reciprocal lattice. The characters of Δ_7, Δ_8, B_3, B_4, P_4, and P_5 have a doubled period in the direction of the axis k_z, and a shift along it by $2\pi/t_0$ results in a pair-wise transformation of the representations one into another. We note that a similar situation is realized in a number of single-valued representations [1].

Using the characters of the irreducible representations (Tables 1 – 5) we derive, in the usual manner, the compatibility conditions for the representations at the various symmetry elements

$$\Delta_7, \Delta_8, \Delta_9 \rightarrow F_3 + F_4; \qquad \Delta_7, \Delta_8, \Delta_9 \rightarrow B_3 + B_4;$$
$$U_5 \rightarrow F_3 + F_4; \qquad U_5 \rightarrow B_3' + B_4';$$
$$P_4 \rightarrow B_3, B_3'; \qquad P_5 \rightarrow B_4, B_4'; \qquad P_6 \rightarrow B_3 + B_4, B_3' + B_4'.$$

By calculating the characters of the direct products of particular single-valued representations D of the wave vector group and the representation $D_{1/2}$, it is easy to obtain the following relations which indicate (i) into how many sublevels the original energy level splits due to the spin-orbit interaction and (ii) according to which double-valued irreducible representation the wave functions belonging to the specific sublevels transform:

$$\Delta_i \times D_{1/2} = \Delta_7 \ (i = 1, 2); \qquad \Delta_i \times D_{1/2} = \Delta_8 \ (i = 3, 4);$$
$$\Delta_5 \times D_{1/2} = \Delta_8 + \Delta_9; \qquad \Delta_6 \times D_{1/2} = \Delta_7 + \Delta_9;$$
$$F_i \times D_{1/2} = F_3 + F_4; \qquad B_i \times D_{1/2} = B_3 + B_4; \qquad B_i' \times D_{1/2} = B_3' + B_4' \ (i = 1, 2);$$
$$U_i \times D_{1/2} = U_5 \ (i = 1, 2, 3, 4);$$
$$P_i \times D_{1/2} = P_6 \ (i = 1, 2); \qquad P_3 \times D_{1/2} = P_4 + P_5 + P_6.$$

When applied to the irreducible double-valued representations, time reversal symmetry results in additional degeneracies either if the representation can be brought to a real form (case a), or if it is not equivalent to the complex conjugate representation (case b). If a complex representation is equivalent to its complex conjugate (case c), no additional degeneracy arises [3]. Using Herring's criterion [4], one can check that double-valued

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Table 1: Characters of the irreducible double-valued representations for the point Δ, where $\eta_k = \exp\left(ik_z t_0/2\right)$. The representation corresponding to the Cayley-Klein matrices is $D_{1/2} = \Delta_7$.

24		Δ_7	Δ_8	Δ_9
1	$\{\varepsilon \mid 0\}$	2	2	2
1	$\{\bar{\varepsilon} \mid 0\}$	-2	-2	-2
2	$\{\delta_6 \mid \frac{t_0}{2}\}$, $\{\bar{\delta}_6^5 \mid \frac{t_0}{2}\}$	$\sqrt{3}\,\eta_k$	$-\sqrt{3}\,\eta_k$	0
2	$\{\delta_6^2 \mid 0\}$, $\{\bar{\delta}_6^4 \mid 0\}$	1	1	-2
2	$\{\delta_6^4 \mid 0\}$, $\{\bar{\delta}_6^2 \mid 0\}$	-1	-1	2
2	$\{\delta_6^5 \mid \frac{t_0}{2}\}$, $\{\bar{\delta}_6 \mid \frac{t_0}{2}\}$	$-\sqrt{3}\,\eta_k$	$\sqrt{3}\,\eta_k$	0
2	$\{\delta_6^3 \mid \frac{t_0}{2}\}$, $\{\bar{\delta}_6^3 \mid \frac{t_0}{2}\}$	0	0	0
6	$\{\sigma_1 \mid 0\}$, $\{\sigma_2 \mid 0\}$, $\{\sigma_3 \mid 0\}$, $\{\bar{\sigma}_1 \mid 0\}$, $\{\bar{\sigma}_2 \mid 0\}$, $\{\bar{\sigma}_3 \mid 0\}$	0	0	0
6	$\{\sigma_1' \mid \frac{t_0}{2}\}$, $\{\sigma_2' \mid \frac{t_0}{2}\}$, $\{\sigma_3' \mid \frac{t_0}{2}\}$, $\{\bar{\sigma}_1' \mid \frac{t_0}{2}\}$, $\{\bar{\sigma}_2' \mid \frac{t_0}{2}\}$, $\{\bar{\sigma}_3' \mid \frac{t_0}{2}\}$	0	0	0

Table 2: Characters of the irreducible double-valued representations U_5. $D_{1/2} = U_5$.

8		U_5
1	$\{\varepsilon \mid 0\}$	2
1	$\{\bar{\varepsilon} \mid 0\}$	-2
2	$\{\sigma_1 \mid 0\}$, $\{\bar{\sigma}_1 \mid 0\}$	0
2	$\{\sigma_1' \mid \frac{t_0}{2}\}$, $\{\bar{\sigma}_1' \mid \frac{t_0}{2}\}$	0
2	$\{\delta_6^3 \mid \frac{t_0}{2}\}$, $\{\bar{\delta}_6^3 \mid \frac{t_0}{2}\}$	0

Table 3: Characters of the irreducible double-valued representations for the point P. $D_{1/2} = P_6$.

12		P_4	P_5	P_6
1	$\{\varepsilon \mid 0\}$	1	1	2
1	$\{\bar{\varepsilon} \mid 0\}$	-1	-1	-2
2	$\{\delta_6^2 \mid 0\}$, $\{\bar{\delta}_6^4 \mid 0\}$	-1	-1	1
2	$\{\delta_6^4 \mid 0\}$, $\{\bar{\delta}_6^2 \mid 0\}$	1	1	-1
3	$\{\sigma_1' \mid \frac{t_0}{2}\}$, $\{\sigma_2' \mid \frac{t_0}{2}\}$, $\{\sigma_3' \mid \frac{t_0}{2}\}$	$i\eta_k$	$-i\eta_k$	0
3	$\{\bar{\sigma}_1' \mid \frac{t_0}{2}\}$, $\{\bar{\sigma}_2' \mid \frac{t_0}{2}\}$, $\{\bar{\sigma}_3' \mid \frac{t_0}{2}\}$	$-i\eta_k$	$i\eta_k$	0

Table 4: Characters of the irreducible double-valued representations for the point F. $D_{1/2} = F_3 + F_4$.

4		F_3	F_4
1	$\{\varepsilon \mid 0\}$	1	1
1	$\{\bar{\varepsilon} \mid 0\}$	-1	-1
1	$\{\sigma_1 \mid 0\}$	i	$-i$
1	$\{\bar{\sigma}_1 \mid 0\}$	$-i$	i

Table 5: Characters of the irreducible double-valued representations for the point B. $D_{1/2} = B_3 + B_4$.

4		B_3	B_4
1	$\{\varepsilon \mid 0\}$	-1	-1
1	$\{\bar{\varepsilon} \mid 0\}$	-1	-1
1	$\{\sigma_1' \mid \frac{t_0}{2}\}$	$i\eta_k$	$-i\eta_k$
1	$\{\bar{\sigma}_1' \mid \frac{t_0}{2}\}$	$-i\eta_k$	$i\eta_k$

representations show the following behavior with respect to time reversal.

Case a: A_9, L_5, R_3, R_4, G.

Case b with common star: A_7, A_8, H_4, H_5, S_3, S_4 (S_3', S_4').

Case b with different stars: $\Delta_7 - \Delta_9$, U_5, $P_4 - P_6$, F_3, F_4, B_3, B_4 (B_3', B_4').

Case c: $\Gamma_7 - \Gamma_9$, M_5, $K_4 - K_6$, Σ_3, Σ_4, T_3, T_4 (T_3', T_4'), N, H_6.

It follows directly from these observations that time reversal results in additional degeneracies in the whole $k_z = \pi/t_0$ plane, similarly to the problem of spinless electrons. The only exception is the point H_6. We note that for spinless electrons the point H_3 was a similar exception. There is no additional "sticking together" of bands in any other point of the Brillouin zone.

2 Derivation of the dispersion law with spin-orbit interaction included

Recently, it has been established in a number of studies [5, 6] that a proper account for the relativistic terms is highly important in the investigation of the energy spectrum of electrons in solids, in particular in the study of the structure of energy bands. This is related to the fact that the spin-orbit interaction usually gives rise to splittings of the energy levels and a displacement of the zero-slope points from the symmetry elements, hence, to a significant change in the dispersion law in the vicinity of extrema. At the same time, the spin-orbit interaction is comparatively small in its absolute value and spin-orbit splitting in semiconductors is usually of the order of $10^{-2} - 10^{-1}$ eV, while the separation between the consecutive electron levels in the spinless problem is of the order of an electron-volt. For this reason, instead of the Dirac equation, one usually considers the equation

$$H\psi = \left[\frac{\boldsymbol{p}^2}{2m} - e\Phi - \frac{e\hbar}{4m^2c^2}(\boldsymbol{\sigma}[\boldsymbol{\nabla}\Phi \times \boldsymbol{p}]) - \frac{e\hbar^2}{8m^2c^2}\Delta\Phi - \frac{\boldsymbol{p}^4}{8m^3c^2} \right] \psi = E\psi, \qquad (1)$$

which is derived from the Dirac equation by expanding in the small parameter c^{-1} and keeping the terms up to the order c^{-2} [7]. In Eq. (1) ψ is a two-component spinor, Φ is

the electrostatic potential, $\boldsymbol{\sigma} = \sigma_x\,\boldsymbol{i} + \sigma_y\,\boldsymbol{j} + \sigma_z\,\boldsymbol{k}$. The third term on the left-hand side of Eq. (1) describes the spin-orbit interaction, the fourth is the Darwin term, and the fifth is a relativistic correction to the effective mass.

When the condition of smallness of the relativistic terms is fulfilled, the change from the Dirac equation to an approximate Eq. (1) appears expedient. Indeed, a group-theoretical analysis of the energy bands performed on the basis of the Dirac equation would indicate, for example, a non-zero slope at the points at which the slope is of higher order in the small parameter c^{-1}. However, in view of the extreme smallness of the higher relativistic corrections the changes introduced by them into the band structure will actually be negligibly small and such an approach would only result in unwarranted complications of the problem. For this reason, in the analysis of the dispersion law it is expedient to obtain results in the form of an expansion in the small parameter c^{-1} to evaluate the relative importance of individual terms.

Since Eq. (1) is an approximate one, its eigenvalues must also be sought approximately, retaining only the first non-vanishing relativistic terms ($\sim c^{-2}$). An analysis of the dispersion law in this approximation is presented below.[1]

Let $\psi_{\boldsymbol{k}} = u_{\boldsymbol{k}}\exp(i\boldsymbol{kr})$ and $E_{\boldsymbol{k}}$ be the eigenfunctions and eigenvalues of Eq. (1) belonging to a wave vector $\boldsymbol{k}$. It is easy to show in the usual way that the eigenvalues $E_{\boldsymbol{k}+\boldsymbol{K}}$ of Eq. (1) are, at the same time, eigenvalues of the equation

$$\mathcal{H}(\boldsymbol{K})\varphi_{\boldsymbol{k},\boldsymbol{K}} = [H_0 + V_{\boldsymbol{K}}]\,\varphi_{\boldsymbol{k},\boldsymbol{K}} = E_{\boldsymbol{k}+\boldsymbol{K}}\,\varphi_{\boldsymbol{k},\boldsymbol{K}}, \qquad (2)$$

corresponding to the eigenfunctions $\varphi_{\boldsymbol{k},\boldsymbol{K}} = u_{\boldsymbol{k}+\boldsymbol{K}}\exp(i\boldsymbol{kr})$, belonging to the wave vector $\boldsymbol{k}$. Here

$$H_0 = \frac{\boldsymbol{p}^2}{2m} - e\Phi, \qquad V_{\boldsymbol{K}} = \sum_{i=1}^{5} V_i,$$

$$V_1 = V_1' + V_1'' = -\frac{e\hbar}{4m^2c^2}(\boldsymbol{\sigma}[\boldsymbol{\nabla}\Phi \times \boldsymbol{p}]) - \left[\frac{e\hbar^2}{8m^2c^2}\Delta\Phi + \frac{\boldsymbol{p}^4}{8m^3c^2}\right],$$

$$V_2 = \frac{\hbar}{m}(\boldsymbol{Kp}), \qquad V_3 = \frac{\hbar^2\boldsymbol{K}^2}{2m},$$

$$V_4 = V_4' + V_4'' = \frac{e\hbar^2}{4m^2c^2}(\boldsymbol{K}[\boldsymbol{\nabla}\Phi \times \boldsymbol{\sigma}]) - \frac{\hbar p^2\,(\boldsymbol{Kp})}{2m^3c^2},$$

$$V_5 = V_5' + V_5'' = -\frac{\hbar^2\,(\boldsymbol{Kp})^2}{2m^3c^2} - \frac{\hbar^2\,\boldsymbol{p}^2\,\boldsymbol{K}^2}{4m^3c^2}. \qquad (3)$$

From comparison of Eqs. (2) and (3) with Eq. (1) it follows that $E_{\boldsymbol{k}+\boldsymbol{K}}$ may be considered as an eigenvalue of the perturbed equation corresponding to the same value of the quasimomentum $\boldsymbol{k}$ as the eigenvalue $E_{\boldsymbol{k}}$ of the unperturbed equation. The perturbation operator $\sum_{i=2}^{5} V_i$ is invariant with respect to all translations. For this reason, $E_{\boldsymbol{k}+\boldsymbol{K}}$ can be found by standard perturbation theory. Eigenfunctions of the Hamiltonian

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[1]In principle it is an interesting question under what conditions the dispersion law, thus defined, coincides qualitatively with the exact dispersion law obtained from the Dirac equation. From the standpoint of choosing the most technically useful approach, it is also important under what conditions the approximate and exact solutions of Eq. (1) give rise to qualitatively the same results.

$\tilde{H} = H_0 + V_1$, belonging to the quasimomentum $\boldsymbol{k}$, must be chosen as the unperturbed eigenfunctions.

However, as was indicated above, our task is not finding the exact solutions of Eq. (1), but finding its eigenvalues approximately including the terms of the order $\sim c^{-2}$. For this reason it is more expedient to consider H_0 as the unperturbed Hamiltonian and $V_{\boldsymbol{K}} = \sum_{i=1}^{5} V_i$ as a perturbation. The operator $V_{\boldsymbol{K}}$ includes two independent small parameters ($K = |\boldsymbol{K}|$ and c^{-2}), in the powers of which the expansion should be performed. Accordingly, the terms of zeroth and first order in the small parameter c^{-2} must be retained. Regarding the expansion in the powers of K, we will retain the terms up to and including K^2.

Before deriving the secular equation, we note that not all the terms in the perturbation operator are equally important. The term V_1'' does not depend on $\boldsymbol{K}$ and does not include spin matrices. For this reason it may be included in H_0, which leads only to a minor modification to the eigenfunctions of H_0 and does not change their symmetry. The term V_3 provides only a global energy shift proportional to K^2. The term V_5'', after calculating its matrix elements between the eigenfunctions of H_0 belonging to the same irreducible representation of the single group, results in a matrix that is proportional to the identity matrix. For this reason the effect of V_5'' can be fully accounted for by introducing a relativistic mass correction in the term V_3. We will not consider the term V_5'' any further. Similarly, it is easy to see that V_4'' only results in a relativistic correction to the electron mass in V_2. Finally, evaluation of V_5' in first-order perturbation theory results only in a minor adjustment of the second-order correction from the operator V_2. After omitting unessential terms in Eq. (3), all significant perturbation terms may be written as

$$V_1 = -\frac{e\hbar}{4m^2c^2}(\boldsymbol{\sigma}[\boldsymbol{\nabla}\Phi \times \boldsymbol{p}]), \qquad V_2 = \frac{\hbar}{m}(\boldsymbol{K}\boldsymbol{p}),$$
$$V_3 = \frac{\hbar^2 \boldsymbol{K}^2}{2m}, \qquad V_4 = \frac{e\hbar^2}{4m^2c^2}(\boldsymbol{K}\,[\boldsymbol{\nabla}\Phi \times \boldsymbol{\sigma}]). \tag{4}$$

A version of perturbation theory proposed by Löwdin [8] is the most technically convenient to proceed with. Let a contact of several bands of a problem of spinless electrons with a Hamiltonian H_0 take place at some point $\boldsymbol{k}$. Let us denote the wave functions corresponding to this level by f_{nl} and its energy by E_n; the index l designates mutually degenerate functions. Let us denote by ψ_{ns}^0 the spinors $\binom{f_{nl}}{0} \equiv f_{nl}\alpha$ and $\binom{0}{f_{nl}} \equiv f_{nl}\beta$ constructed with all functions f_{nl}, or some of their linear combinations. Let the set of spinors ψ_{ns}^0 make up the class (A) of basis functions in the sense of Ref. [8].[2] Then, retaining in the expansion of the matrix elements the lowest-order terms including the terms of the order $\sim K^2$ and $\sim c^{-2}K^2$,[3] we obtain:

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[2]Formulae defining the dispersion law for a different choice of the class (A) are given in the Appendix.

[3]We note that, in general, this approximation does not allow us to achieve an equally small absolute inaccuracy in the expansion coefficients of the eigenvalues in the powers of K. For example, at a point of contact where the slope does not vanish for spinless electrons but vanishes when the spin-orbit interaction is included, the expansion of E in powers of K, in the immediate vicinity of the point $K = 0$, begins with the terms $\sim c^2K^2$, and the coefficient of the term $\sim c^{-2}K^2$ cannot be obtained from the approximate Eq. (1). However, the relative inaccuracy originating from such terms is small and the approximation remains sufficient.

$$\text{Det} \|U_{ns,nt} - E\delta_{st}\| = 0, \tag{5}$$

$$U_{ns,nt} = \left(\sum_{i=1}^{4} V_i\right)_{ns,nt} + (V_{12})_{ns,nt} + (V_{22})_{ns,nt} + (V_{24})_{ns,nt} + (V_{122})_{ns,nt}, \tag{6}$$

$$(V_{ij})_{ns,nt} = \sum_{\substack{mr \\ m\neq n}} \frac{(V_i)_{ns,mr}(V_j)_{mr,nt} + (V_j)_{ns,mr}(V_i)_{mr,nt}}{E - E_m}, \quad (ij = 12, 22, 24), \tag{7}$$

$$(V_{122})_{ns,nt} = \sum_{\substack{lq \\ l\neq n}} \sum_{\substack{mr \\ m\neq n}} \frac{(V_1)_{ns,lq}(V_2)_{lq,mr}(V_2)_{mr,nt} + (V_2)_{ns,lq}(V_2)_{lq,mr}(V_1)_{mr,nt} +}{}$$

$$\frac{+ (V_2)_{ns,lq}(V_1)_{lq,mr}(V_2)_{mr,nt}}{(E - E_l)(E - E_m)}. \tag{8}$$

Formulae (5)–(8) determine the dispersion law in the vicinity of the symmetry elements. It is easy to see that they differ from those used in the literature (see, for instance, Ref. [9]) by a number of terms. First of all, Eq. (6) includes two terms proportional to K/c^2: $(V_4)_{ns,nt}$ usually considered in the literature and $(V_{12})_{ns,nt}$. Estimates show that the second term is of the same order of magnitude as the first one, or even exceeds it by an order of magnitude. However, because in practice the calculation of the coefficients in the dispersion law is not actually performed on the basis of Eqs. (6)–(8), the fundamental role in the evaluation of the importance of these two terms for the study of the $E(\boldsymbol{k})$ surfaces depends on the fact whether they result in qualitatively identical or different dispersion laws rather than on their relative magnitude.

To answer this question we note that the system of spinors ψ^0_{ns} forms the basis of a representation not only with respect to simultaneous rotations in the coordinate and spin spaces (corresponding to all operations of the double group), but also with respect to rotations in the coordinate space corresponding to the operations of the single group. The operators V_4 and V_{12} behave identically with respect to rotations of the first type, but in general they behave differently with respect to rotations of the second type. It is therefore quite natural to expect that the matrices of the operators V_4 and V_{12} will be different. Actually, an analysis of the band structure near the various symmetry points described in the next section shows that at some symmetry points the term V_{12} changes the dispersion law qualitatively, leading, for example, to the change in the position of the zero-slope points.[4]

As far as the terms $\sim K^2/c^2$ are concerned, they are defined by the matrix elements of the operators V_{24} and V_{122}. Additional terms of the same order of magnitude come from expanding the denominators of the operators V_{22} and V_{12}. When evaluating the

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[4]The origin of the additional terms becomes particularly clear if one performs the perturbation theory expansion in two steps. First, considering only the operator V_1 and using the spinors ψ^0_{ns}, one finds the spinors ψ_{ns} defining the wave functions, corresponding to the wave vector $\boldsymbol{k}$, in a first approximation in c^{-2}. Then, to find corrections to the energy of the order $\sim K$ and $\sim K/c^2$, it is necessary to calculate the matrix elements of $V_2 + V_4$ using the spinors ψ_{ns}. Calculating the matrix elements of V_4 (having the order K/c^2) using the unperturbed spinors ψ^0_{ns} results in the $(V_4)_{ns,nl}$ terms, and calculating the matrix elements of V_2 (having the order K) using the unperturbed spinors ψ^0_{ns} and the first-order corrections to them results in the terms $(V_{12})_{ns,nt}$.

energy E in the denominators of these terms, in the first of them the terms $\sim c^{-2}$ must be retained and in the second one the terms $\sim K$.

3 Dispersion law in the vicinity of various symmetry elements

Let us go on to deriving the dispersion law in the vicinity of the symmetry elements. Let us designate by X_i^j a point X in which the spinors ψ_{ns}^0 transform according to the representation X_i and the wave functions f_{nl}, through which the spinors ψ_{ns}^0 were constructed, transform according to the representation X_j.

Among the six single-valued irreducible representations for the axis Δ, four $(\Delta_1 - \Delta_4)$ are one-dimensional and two (Δ_5, Δ_6) are two-dimensional. All the points on the axis Δ, with the exclusion of the point A, are potential zero-slope points for all representations $\Delta_1 - \Delta_6$, and the slope always vanishes at the points $\Gamma_1 - \Gamma_6$.

Let f_i be a wave function transforming according to an irreducible representation Δ_i $(i = 1, 2, 3, 4)$. If $\psi_{i1}^0 = f_i \alpha$ and $\psi_{i2}^0 = f_i \beta$ are chosen as the basis spinors, and the representation $\sigma_x = \left\| \begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix} \right\|$, $\sigma_y = \left\| \begin{smallmatrix} 0 & -i \\ i & 0 \end{smallmatrix} \right\|$, $\sigma_z = \left\| \begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix} \right\|$ is chosen for the Pauli matrices, then the secular equation (5), with the terms of the order $\sim K^3$ and $\sim K^2/c^2$ included, takes the form:

$$\begin{vmatrix} (a + dK_z)K_\perp^2 + (b + gK_z)K_z^2 + hK_z - E & i\alpha K_- + i\beta K_- K_z \\ -i\alpha K_+ - i\beta K_+ K_z & (a + dK_z)K_\perp^2 + (b + gK_z)K_z^2 + hK_z - E \end{vmatrix} = 0, \tag{9}$$

where $K_\pm = K_x \pm iK_y$. Here and below the lower-case Latin letters designate the coefficients of zeroth order in the small parameter c^{-2} and the Greek letters designate the coefficients of the order c^{-2}. We will not write out the cumbersome expressions for these coefficients in terms of the matrix elements of the operators appearing in Eq. (4). Expanding Eq. (9), we arrive at the dispersion law for the points Δ_7^1, Δ_7^2, Δ_8^3, and Δ_8^4,

$$E = (a + dK_z)K_\perp^2 + (b + gK_z)K_z^2 + hK_z \pm (\alpha + \beta K_z)K_\perp,$$
$$K_\perp = \sqrt{K_x^2 + K_y^2}. \tag{10}$$

If an extremum is reached in a point k_z^0 on the axis Δ, for $\alpha = \beta = 0$, then $h = 0$ in it.[5] Then, with the spin-orbit interaction taken into account, it follows from Eq. (9) that the extremum is reached at a circle with a radius $\simeq \left| \frac{\alpha}{2a} \right|$. Its center is located at the axis Δ in the plane $k_z = k_z^0 + \frac{\alpha}{4ab} \left(\beta - \frac{\alpha d}{2a} \right)$. Near the extremum, the surfaces of constant energy form toroids. They are figures of revolution around the axis k_z of ellipses; one of the axes of which is almost parallel to the axis k_z and makes up the angle $\varphi_0 = \frac{1}{2} \arctan \left| \frac{\alpha}{a-b} \left(\frac{d}{a} - \frac{\beta}{\alpha} \right) \right|$ with it.

It follows from time reversal symmetry that $d = g = h = \beta = 0$ in the point Γ. The extremum is realized on a circle lying in the plane $k_z = 0$ with $\varphi_0 = 0$.

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[5]The constant h in Eq. (10), side by side with a non-relativistic term, contains a small relativistic correction which leads to a small displacement of the extremum along the k_z axis as compared with its position when the spin-orbit interaction is disregarded. We designate this displaced position of the extremum as k_z^0.

Thus in the approximation in which the terms up to K^3 and K^2/c^2 are included, the extremum is reached at a circle (loop) centered around the k_z axis rather than in isolated points of the Brillouin zone as was the case in all the cases studied to date. In higher approximations of perturbation theory the extrema will be located in a set of isolated points. However the saddle points between them, for weak spin-orbit coupling, should be low. Hence, the approximation based on the loop of extrema must be more useful than an approximation based on isolated extremal points.

Semiconductors with a loop of extrema must possess a number of characteristic properties related, in part, with a change in the density of states and vanishing semiclassical cyclotron frequency for a field $\boldsymbol{H}$ parallel to the axis k_z.

Let f_{il} be wave functions transforming according to an irreducible representation Δ_i $(i = 5, 6)$. Let us choose them in such a way that f_{51} and f_{52} transform into one another as $(x - iy)^2 \exp(ik_z z)$ and $(x + iy)^2 \exp(ik_z z)$, and f_{61} and f_{62} transform as $(x + iy) \exp(ik_z z)$ and $(x - iy) \exp(ik_z z)$. Then $\psi_{51}^0 = f_{52}\alpha$ and $\psi_{52}^0 = f_{51}\beta$ transform according to the representation Δ_8^5, $\psi_{61}^0 = f_{62}\alpha$ and $\psi_{62}^0 = f_{61}\beta$ transform according to Δ_7^6, and $\psi_{53}^0 = f_{51}\alpha$ and $\psi_{54}^0 = f_{52}\beta$, and $\psi_{63}^0 = f_{61}\alpha$ and $\psi_{64}^0 = f_{62}\beta$ transform according to Δ_9^5 and Δ_9^6, respectively. In this basis, the secular equation takes the form:

$$\begin{vmatrix} \theta - \lambda & i(\alpha + \beta K_z)K_+ & (a_1 + i\rho + a_2 K_z)K_+^2 & i(\gamma + \delta K_z)K_- \\ -i(\alpha + \beta K_z)K_- & \theta - \lambda & -i(\gamma + \delta K_z)K_+ & (a_1 + i\rho + a_2 K_z)K_-^2 \\ (a_1 - i\rho + a_2 K_z)K_-^2 & i(\bar\gamma + \bar\delta K_z)K_- & -\theta - \lambda & 0 \\ -i(\bar\gamma + \bar\delta K_z)K_+ & (a_1 - i\rho + a_2 K_z)K_+^2 & 0 & -\theta - \lambda \end{vmatrix} = 0,$$

(11)

where $E = \lambda + (a + dK_z)K_\perp^2 + (b + gK_z)K_z^2 + hK_z$, $\theta = \varepsilon + \varkappa K_z + \tau K_\perp^2 + \eta K_z^2$. Expanding (11), we find

$$\lambda^4 - (2\theta^2 + A_1)\lambda^2 + (2\theta A_2 + A_3)\lambda + \theta^4 + \theta^2 A_4 + \theta A_3 + A_5 = 0, \qquad (12)$$

where

$$
\begin{aligned}
A_1 &= (\alpha + \beta K_z)^2 K_\perp^2 + 2|\gamma + \delta K_z|^2 K_\perp^2 + 2[(a_1 + a_2 K_z)^2 + \rho^2]K_\perp^4, \\
A_2 &= -(\alpha + \beta K_z)^2 K_\perp^2, \\
A_3 &= -4(\alpha + \beta K_z)\operatorname{Re}[(a_1 + a_2 K_z - i\rho)(\gamma + \delta K_z)]K_\perp^4, \\
A_4 &= -(\alpha + \beta K_z)^2 K_\perp^2 + 2|\gamma + \delta K_z|^2 K_\perp^2 + 2[(a_1 + a_2 K_z)^2 + \rho^2]K_\perp^4, \qquad (13) \\
A_5 &= |\gamma + \delta K_z|^4 K_\perp^4 - 2\operatorname{Re}[(a_1 + a_2 K_z - i\rho)^2(\gamma + \delta K_z)^2]K_\perp^6 + [(a_1 + a_2 K_z)^2 + \rho^2]^2 K_\perp^8.
\end{aligned}
$$

At $K = 0$ it has two doubly degenerate roots $E = \pm\varepsilon$. The root $E = \varepsilon$ corresponds to the representation Δ_7^6 (Δ_8^5). The dispersion law for it with an accuracy up to the terms $\sim K^2$ and $\sim K/c^2$ is

$$E_{1,2} = aK_\perp^2 + bK_z^2 + hK_z + \varepsilon + \varkappa K_z \pm (\alpha + \beta K_z)K_\perp. \qquad (14a)$$

The dispersion law for the root $E = -\varepsilon$, corresponding to the representation Δ_9^6 (Δ_9^5), with an accuracy up to the terms $\sim K^3$ and $\sim K^2/c^2$ is

$$E_3 = E_4 = (a + dK_z)K_\perp^2 + (b + gK_z)K_z^2 + hK_z - \left[\varepsilon + \varkappa K_z + \left(\tau + \frac{|\gamma|^2}{2\varepsilon}\right)K_\perp^2 + \eta K_z^2\right].$$

(14b)

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At the points Γ_7^6 (Γ_8^5), Γ_9^6 (Γ_9^5), $h = d = g = a_2 = \varkappa = \rho = \beta = 0$, $\gamma = \bar{\gamma}$, $\delta = -\bar{\delta}$ due to time reversal symmetry, and the dispersion law simplifies into

$$E_{1,2} \;=\; aK_\perp^2 + bK_z^2 + \varepsilon \pm \alpha K_\perp, \tag{15a}$$

$$E_3 \;=\; E_4 = aK_\perp^2 + bK_z^2 - \left[\varepsilon + \left(\tau + \frac{\gamma^2}{2\varepsilon}\right)K_\perp^2 + \eta K_z^2\right]. \tag{15b}$$

As is seen from Eq. (15a), if $ab > 0$ the extremum for Γ_7^6 (Γ_8^5) is realized on a circle with the center at the origin of the coordinate system and the radius of $\simeq |\frac{\alpha}{2a}|$. Since K_x and K_y appear in Eq. (12) only in the combination $K_\perp$, the loop of extrema does not disintegrate into separate extrema even when this equation is solved exactly. A similar situation occurs at the points Δ_7^6 (Δ_8^5) in the vicinity of the extrema at the points Δ_6 (Δ_5).

We note that the displacement of the extremum from the k_z axis [Eqs. (14a), (14b)] is caused exclusively by the matrix elements of the operator V_{12}. For this reason it is absent if, as is usually done, only the operator V_4 is taken into account. Thus, we encounter here one of the cases when introducing the operator V_{12} changes the dispersion law qualitatively.

In all cases, the slope at the point A differs from zero in the absence of spin-orbit interaction [1], and for this reason an extremum cannot be reached in it. In view of this the investigation of the dispersion law in its vicinity is of minor interest and one can keep in the expansion less terms than at Δ and Γ.

For the levels $A_7^1 - A_8^3$ ($A_7^2 - A_8^4$) the dispersion law is

$$E = aK_\perp^2 + bK_z^2 \pm hK_z \pm \alpha K_\perp; \tag{16}$$

in Eq. (16) the non-relativistic terms up to the quadratic and the relativistic terms up to the linear terms in K are taken into account.

For the levels originating from A_5 and A_6, the dispersion law takes the form

$$E = \pm\varepsilon \pm hK_z. \tag{17}$$

This takes into account only nonrelativistic terms proportional to K and K-independent nonrelativistic terms; each of the levels is doubly degenerate in this approximation. Thus, from two mutually degenerate levels A_5 and A_6 two fourfold degenerate levels ($A_7^6 - A_8^5$ and $A_9^6 - A_9^5$) arise.

Let us pass to the consideration of the dispersion law in the vicinity of the vertical edges of the Brillouin zone. In the absence of spin-orbit interaction, the points P_1 and P_2 are potential zero-slope points. If we choose the basis spinors as $\psi_{i1} = f_i\alpha$ and $\psi_{i2} = f_i\beta$ ($i = 1, 2$), the secular equation (including the terms $\sim K^3$ and K^2/c^2) takes the form

$$\begin{vmatrix} -\lambda & i(\alpha + \beta K_z)K_- + i\gamma K_+^2 \\ -i(\alpha + \beta K_z)K_+ - i\gamma K_-^2 & -\lambda \end{vmatrix} = 0, \tag{18a}$$

$$E = \lambda + (a + dK_z)K_\perp^2 + (b + gK_z)K_z^2 + hK_z + l(K_+^3 + K_-^3).$$

Solving it, we arrive at

$$E = (a + dK_z)K_\perp^2 + (b + gK_z)K_z^2 + hK_z + l(K_+^3 + K_-^3) \pm |(\alpha + \beta K_z)K_- + \gamma K_+^2|. \tag{18b}$$

Let an extremum be located at the point P_1 (P_2) in the absence of spin-orbit interaction; at this point $h = 0$. If we restrict ourselves to the terms $\sim K^2$ and $\sim K/c^2$ in (18b), we arrive at a loop of extrema—a circle with a radius of $|\alpha/2a|$. Introducing the terms $\sim K^3$ and $\sim K^2/c^2$ leads to the disintegration of the loop of extrema. Six zero-slope points of $E(\boldsymbol{K})$ are positioned on rays which make up the angles $\varphi_n = \pi n/3$ with the axis k_x. Three of these points are extremal points, and the other three are saddle points. These two groups of points are displaced to the opposite sides with respect to the circle with a radius of $|\alpha/2a|$ by a distance $\sim c^{-4}$. The height of the barriers separating them is of the order of $\sim c^{-6}$

At the points K_6^1 and K_6^2, $d = g = h = \beta = 0$.

At P_3 the slope always differs from zero [1] and for this reason an extremum cannot be reached at this point. In the presence of spin-orbit interaction, the secular equation takes the form

$$
\begin{vmatrix}
\varepsilon - \lambda & 0 & pK_- & 0 \\
0 & \varepsilon - \lambda & 0 & pK_+ \\
pK_+ & 0 & -\varepsilon - \lambda & i\alpha \\
0 & pK_- & -i\alpha & -\varepsilon - \lambda
\end{vmatrix} = 0,
\tag{19}
$$

with $E = \lambda + (aK_\perp^2 + bK_z^2 + dK_z)$. In Eq. (19) the non-relativistic terms proportional to K and K-independent relativistic terms are taken into account. The basis is chosen as in the secular equation (11). Expanding Eq. (19) and restricting in the solutions to a quadratic expansion in powers of K, we obtain

$$
\begin{aligned}
E_1 &= E_2 = aK_\perp^2 + bK_z^2 + dK_z + \varepsilon + \frac{p^2 K_\perp^2}{2\varepsilon - \alpha}, \\
E_{3,4} &= aK_\perp^2 + bK_z^2 + dK_z - \varepsilon \pm \alpha - \frac{p^2 K_\perp^2}{2\varepsilon \mp \alpha}.
\end{aligned}
\tag{20}
$$

We note that, according to Eq. (20), the curvature of the parabolas $E(K_\perp)$ is of the order $\sim c^2$.

At the point K_3, $d = 0$.

The functions f_1 and f_2, which transform according the representations H_1 and H_2, are mutually degenerate and can be chosen as $f_2 = \{\delta_2 | \frac{t_0}{2}\} \bar{f}_1$ because they belong to the case b with respect to time reversal symmetry. Let us choose functions f_{31} and f_{32} transforming according to H_3 in such a way that they transform as $(x + iy) \exp(\pi i z/t_0)$ and $(x - iy) \exp(\pi i z/t_0)$ under the operations of the wave vector group. Since H_3 pertains to the case c, the phase can be chosen in such a way that $\psi_2 = \{\delta_2 | \frac{t_0}{2}\} \bar{\psi}_1$.

At H_1 and H_2 the slope differs from zero. For the corresponding states, let us select $\psi_{11}^0 = f_1 \alpha$, $\psi_{12}^0 = f_1 \beta$, $\psi_{21}^0 = f_2 \alpha$, and $\psi_{22}^0 = f_2 \beta$ as the basis spinors. Then we arrive at the following secular equation, including the terms $\sim K^2$ and $\sim K/c^2$

$$
\begin{vmatrix}
dK_z - \lambda & i\alpha K_+ & \varepsilon & 0 \\
-i\alpha K_- & dK_z - \lambda & 0 & -\varepsilon \\
\varepsilon & 0 & -dK_z - \lambda & i\alpha K_+ \\
0 & -\bar{\varepsilon} & -i\alpha K_- & -dK_z - \lambda
\end{vmatrix} = 0;
\tag{21}
$$

here $E = \lambda + (aK_\perp^2 + bK_z^2)$. It reduces to a biquadratic equation. At $K = 0$ the roots $E = \pm|\varepsilon|$ of Eq. (21) are doubly degenerate and belong to the representation H_6. The

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dispersion law is

$$E = aK_\perp^2 + bK_z^2 \pm (d^2K_z^2 + |\varepsilon|^2 + \alpha^2K_\perp^2 \pm 2\alpha dK_\perp K_z)^{1/2}. \tag{22}$$

As is seen from Eq. (22), and in accordance with the general requirements of symmetry, the double degeneracy persists at the edge P ($K_\perp = 0$) and in the plane $k_z = \pi/t_0$ ($K_z = 0$) and is lifted in all other directions.

The point H_3 is a point of zero slope. Let us select the spinors $\psi_{31}^0 = f_{32}\alpha$, $\psi_{32}^0 = f_{31}\beta$, $\psi_{33}^0 = f_{31}\alpha$, $\psi_{34}^0 = f_{32}\beta$ as the basis spinors for the levels arising from H_3. Then we arrive at the following secular equation, including the terms of $\sim K^2/c^2$:

$$\begin{vmatrix} \theta - \lambda & i\beta K_z K_+ & fK_z K_- + i\mu K_- + i\rho K_+^2 & i\gamma K_- + \delta K_z K_- + i\nu K_+^2 \\ -i\beta K_z K_- & \theta - \lambda & -i\gamma K_+ - \delta K_z K_+ - i\nu K_-^2 & fK_z K_+ + i\mu K_+ + i\rho K_-^2 \\ fK_z K_+ - i\mu K_+ - i\rho K_-^2 & i\gamma K_- - \delta K_z K_- + i\nu K_+^2 & -\theta - \lambda & i\alpha K_z \\ -i\gamma K_+ + \delta K_z K_+ - i\nu K_-^2 & fK_z K_- - i\mu K_- - i\rho K_+^2 & -i\alpha K_z & -\theta - \lambda \end{vmatrix} = 0, \tag{23}$$

here $E = \lambda + aK_\perp^2 + bK_z^2$, $\theta = \varepsilon + \tau K_\perp^2 + \eta K_z^2$. Expanding Eq. (23), we find:

$$\lambda^4 - (2\theta + A_1)\lambda^2 + (2\theta A_2 + A_3)\lambda + \theta^4 + \theta^2 A_4 + \theta A_5 + A_6 = 0, \tag{24}$$

where

$$\begin{aligned}
A_1 &= (\alpha^2 + \beta^2 K_\perp^2)K_z^2 + 2f^2 K_z^2 K_\perp^2 \\
&\quad + 2[(\mu^2 + \gamma^2)K_\perp^2 + (\rho^2 + \nu^2)K_\perp^4 + (\rho\mu + \nu\gamma)(K_+^3 + K_-^3) + \delta^2 K_z^2 K_\perp^2], \\
A_2 &= (\alpha^2 - \beta^2 K_\perp^2)K_z^2, \\
A_3 &= -2\alpha K_z^2[2(\gamma f - \delta\mu)K_\perp^2 + (\nu f - \delta\rho)(K_+^3 + K_-^3)] \\
&\quad - 2\beta K_z^2[(\gamma f - \delta\mu)(K_+^3 + K_-^3) + 2(\nu f - \delta\rho)K_\perp^4], \\
A_4 &= 2f^2 K_z^2 K_\perp^2 - (\alpha^2 + \beta^2 K_\perp^2)K_z^2 \\
&\quad + 2[(\mu^2 + \gamma^2)K_\perp^2 + (\mu\rho + \gamma\nu)(K_+^3 + K_-^3) + (\rho^2 + \nu^2)K_\perp^4 + \delta^2 K_z^2 K_\perp^2], \\
A_5 &= 2\alpha K_z^2[2(\gamma f - \delta\mu)K_\perp^2 + (\nu f - \delta\rho)(K_+^3 + K_-^3) \\
&\quad - 2\beta K_z^2(\gamma f - \delta\mu)(K_+^3 + K_-^3) + 2(\nu f - \delta\rho)K_\perp^4], \\
A_6 &= -\alpha\beta K_z[(\gamma^2 + \nu^2 K_\perp^2 + \delta^2 K_z^2)(K_+^3 + K_-^3) + 4\gamma\nu K_\perp^4] \\
&\quad - \alpha\beta K_z^2[(\mu^2 + \rho^2 K_\perp^2 + f^2 K_z^2)(K_+^3 + K_-^3) + 4\mu\rho K_\perp^4] \\
&\quad + \alpha^2\beta^2 K_z^4 K_\perp^2 + |(\mu K_- + \rho K_+^2)^2 + f^2 K_z^2 K_\perp^2|^2 + |(\gamma K_- + \nu K_+^2)^2 + \delta^2 K_z^2 K_\perp^2|^2 \\
&\quad + 2\,\mathrm{Re}\{(fK_z K_- + i\mu K_- + i\rho K_+^2)(fK_z K_+ + i\mu K_+ + i\rho K_-^2) \\
&\quad \times (\delta K_z K_- - i\gamma K_- - i\nu K_+^2)(\delta K_z K_+ - i\gamma K_+ - i\nu K_-^2)\}. \tag{25}
\end{aligned}$$

Solving Eq. (24) approximately, we arrive at

$$\begin{aligned}
E_{1,2} &= aK_\perp^2 + bK_z^2 - \varepsilon \pm \alpha K_z, \tag{26a} \\
E_{3,4} &= aK_\perp^2 + bK_z^2 + \varepsilon + \left(\tau + \frac{\gamma^2 + \mu^2}{2\varepsilon}\right)K_\perp^2 + \eta K_z^2 \pm \beta K_z K_\perp. \tag{26b}
\end{aligned}$$

In Eq. (26a) the terms of the order $\sim K^2$ and $\sim K/c^2$ are taken into account, and in Eq. (26b) the terms of the order $\sim K^2$ and $\sim K^2/c^2$ are accounted for.

The roots E_1 and E_2 belong to the representations H_4 and H_5, whereas E_3 and E_4 belong to the representation H_6. Let the extremum be reached at H_3 in the nonrelativistic approximation. Then, within the accuracy of Eq. (26), the constant energy

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surfaces for E_1 and E_2 of Eq. (26a) are ellipsoids of revolution around the k_z axis; they are displaced along the axis k_z in the opposite directions by $|\alpha/2b|$. The constant energy surfaces for E_3 and E_4 are fourth-order self-intersecting surfaces. Each of them is obtained by rotating an ellipse around the k_z axis, where one of the ellipse's axes is almost parallel to k_z and makes a small angle $\varphi_0 \simeq \frac{1}{2}\arctan|\beta/(a-b)|$ with it. In a reasonable approximation this angle can be neglected and one can assume $E_3 \simeq E_4$. Hence, in this case the spin-orbit interaction simplifies the dispersion law in close vicinity of the extrema. If the spin-orbit splitting is of the order of $0.01 - 0.1$ eV, then the angular dependencies of various effects will be comparatively simple at low temperatures and may be interpreted in terms of elliptical constant energy surfaces. On the other hand, at high temperatures the angular dependencies are expected to show more complexities and must be interpreted in the framework of the dispersion law of Eq. (26) of Ref. [1].

With spin-orbit interaction disregarded, time reversal symmetry results in a double degeneracy in all points of the general position G in the $k_z = \pi/t_0$ plane, while the eigenfunctions f_1 and f_2 can always be chosen in such a way that $f_2 = \{\delta_2|\frac{t_0}{2}\}\bar{f}_1$. The secular equation has the form

$$\begin{vmatrix} \gamma + dK_z - \lambda & \alpha - i\beta & \delta + gK_z & 0 \\ \alpha + i\beta & -\gamma + dK_z - \lambda & 0 & -\delta + gK_z \\ \bar{\delta} + \bar{g}K_z & 0 & -\gamma - dK_z - \lambda & \alpha - i\beta \\ 0 & -\bar{\delta} + \bar{g}K_z & \alpha + i\beta & \gamma - dK_z - \lambda \end{vmatrix} = 0, \quad (27)$$

where $E = \lambda + aK_x + bK_y$. Eq. (27) accounts for K-independent relativistic terms and non-relativistic terms proportional to K; the basis is chosen in the same way as in Eq. (21). Expanding Eq. (27), we arrive at a biquadratic equation with the roots

$$\lambda^2 = [\alpha^2 + \beta^2 + \gamma^2 + |\delta|^2] + (d^2 + |g|)^2)K_z^2 \mp K_z\sqrt{[2\gamma d + \delta\bar{g} + \bar{\delta}g]^2 + 4(\alpha^2 + \beta^2)(d^2 + |g|^2)}. \quad (28)$$

The dispersion law in the vicinity of the points R, S (S'), and L can be obtained from Eq. (28) by setting some parameters equal to zero, namely:

$$\text{Point } R: \quad a = \beta = \gamma = \delta = 0, \quad (29a)$$

$$\text{Point } S \ (S'): \quad b = g = \alpha = 0, \quad (29b)$$

$$\text{Point } L: \quad a = b = g = \alpha = \beta = \gamma = \delta = 0. \quad (29c)$$

As is seen from Eqs. (28) and (29), a zero slope in the points G, R, S (S'), and L is "vanishingly improbable".

At a point of the general position N in the $k_z = 0$ plane, it is possible to choose $\bar{f} = \{\delta_2|\frac{t_0}{2}\}f$, and the roots of the secular equation are

$$E = aK_x^2 + bK_y^2 + dK_xK_y + fK_z^2 + gK_x + hK_y \pm \sqrt{\alpha^2 K_z^2 + |\varepsilon + \beta K_x + \gamma K_y|^2}; \quad (30)$$

generally, the coefficients ε, β and γ are complex numbers. If in the absence of spin-orbit interaction the extremum is reached in the $k_z = 0$ plane, it will stay in this plane for both roots of Eq. (30).

The dispersion law in the vicinity of the points Σ, T (T'), and M can be obtained from Eq. (30) by setting a number of parameters equal to zero

$$\text{Point } \Sigma: \quad d = g = \alpha = 0, \ \varepsilon = \bar{\varepsilon}, \ \beta = -\bar{\beta}, \ \gamma = \bar{\gamma}, \tag{31a}$$

$$\text{Point } T \ (T'): \quad d = h = \alpha = 0, \ \varepsilon = -\bar{\varepsilon}, \ \beta = -\bar{\beta}, \ \gamma = \bar{\gamma}, \tag{31b}$$

$$\text{Point } M: \quad d = g = h = \alpha = \epsilon = 0, \ \beta = -\bar{\beta}, \ \gamma = \bar{\gamma}. \tag{31c}$$

According to Eqs. (30), (31a), and (31b), if disregarding the spin-orbit interaction the extremum is reached on the axis Σ or T (T'), then the extrema of both surfaces of Eq. (30) will stay on this very axis. If the extremum is reached at the point M, which becomes non-analytical when spin-orbit interaction is taken into account, the extremum is displaced from this point. Then, a pair of zero-slope points arises at each of the axes Σ and T, one pair being extrema and the second saddle points.

Near the points F and B, respectively, we arrive at the following dispersion laws

$$E = aK_x^2 + bK_y^2 + dK_yK_z + fK_z^2 + gK_y + hK_z \pm \sqrt{|\alpha|^2 K_x^2 + (\varepsilon + \beta K_y + \gamma K_z)^2}, \tag{32}$$

$$E = aK_x^2 + bK_y^2 + dK_xK_z + fK_z^2 + gK_x + hK_z \pm \sqrt{|\alpha|^2 K_y^2 + (\varepsilon + \beta K_x + \gamma K_z)^2}. \tag{33}$$

In both these cases, the extrema stay in the symmetry planes.

The dispersion law at the point U reads

$$E = aK_x^2 + bK_y^2 + fK_z^2 + hK_z \pm \sqrt{\alpha^2 K_x^2 + \beta^2 K_y^2}. \tag{34}$$

If $h = 0$, Eq. (34) turns into the dispersion law for the point M.

Appendix

The formulae of Sec. 2 allow finding the expansion of E in powers of K which is valid in a relatively wide range of energies, broadly similar to the expansion range in the problem without spin-orbit interaction. This range may significantly exceed the magnitude of the spin-orbit interaction.

In a number of cases, for strong spin-orbit interaction, it is sufficient to obtain an expansion that is valid in close vicinity of the extremum. In this case the equations can be simplified.

Let us expand a reducible representation spanned by spinors ψ^0_{ns} into irreducible representations which we presume to be nonequivalent. Let $\psi^0_{n\lambda r}$ be spinors forming a basis of an irreducible representation. Let us choose this set of spinors for the class (A) of functions in the sense of Ref. [8]. Then the secular equation takes the form

$$\text{Det } \|U_{n\lambda r, n\lambda s} - E\delta_{rs}\| = 0, \tag{A.1}$$

where

$$U_{n\lambda r, n\lambda s} = \left(\sum_{i=1}^4 V_i \right)_{n\lambda r, n\lambda s} + (V_{12})_{n\lambda r, n\lambda s} + (V_{22})_{n\lambda r, n\lambda s} + (V_{24})_{n\lambda r, n\lambda s} + (V_{122})_{n\lambda r, n\lambda s} + \dots \tag{A.2}$$

Matrix elements of the operators V_{ij} ($ij = 12, 22, 24$) and V_{122} are defined by formulae similar to Eqs. (7) and (8). However, in the current case the summation over intermediate states is performed over all eigenfunctions of the unperturbed Hamiltonian except the spinors $\psi^0_{n\lambda s}$ with the same value of λ, in particular, over the spinors $\psi^0_{n\mu s}$ with $\mu \neq \lambda$. Thus the terms of the order $\sim c^{-2}$ may appear in the denominators. When deriving Eq. (A.2) the contributions of the order c^0 and c^{-2} were included in the terms linear in K and the contributions of the order c^2 and c^0 in the terms quadratic in K. Formulae for higher-order terms of the expansion can easily be written out.

The significant difference between Eq. (A.2) and Eq. (6) must be emphasized. In Eq. (A.2) the matrix elements V_{24} and V_{122} are generally of zeroth order in the parameter c^{-2} as a consequence of the appearance of small denominators ($\sim c^{-2}$). In the terms of higher orders in K the large parameter c^2 appears in increasing powers which significantly affects the convergence of the expansion. Furthermore, the formulae for the coefficients at higher powers of K become cumbersome. For this reason, in the cases when the representation formed by the spinors ψ^0_{ns} is reducible, using the formulae (A.1)–(A.2) is expedient and makes the calculation significantly easier (due to the lower order of the secular equation) if it is possible to keep only a small number of terms of the expansion. For example, this is the case when analyzing the displacement of the extremum from an element of symmetry due to the spin-orbit interaction, by taking into account the non-relativistic quadratic terms and relativistic K-linear terms. In other cases using the formulae of Sec. 2 is more convenient.

Note added in proof. We have become aware that Kane (E. O. Kane, J. Phys. Chem. Solids, **1**, 249, 1957; **8**, 38, 1959), when calculating the shape of the valence band of InSb, took into account the perturbation operator corresponding to our V_{12}. However, because Kane considered only one specific case in which V_{12} results only in a numerical change in the parameters, he has not established that the term V_{12} can change the dispersion law qualitatively.

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