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On the Structure of the Electron Spectrum in Lattices of the Tellurium Type

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The general properties of the energy spectrum of an excess electron in a crystal with a lattice of the tellurium type are studied by group-theoretical methods, without resort to the approximation of weak or strong coupling. The possibility of contact between the zones in definite directions in the **k**-space is demonstrated. The effect of the spin-orbit interaction is investigated. It is shown that in semiconductors of this type there can be present two kinds of carriers of the same sign. Dispersion laws in the approximation quadratic in **k** are found on various assumptions about the location of the extrema of $E(\mathbf{k})$.

THE PROBLEM OF the energy spectrum of electrons in semiconductors is of extreme importance in the study of all the properties of semiconductors and, in particular, for the understanding of the kinetics of processes occurring in these materials. The complex structure of the electron spectrum in germanium was predicted theoretically and has been convincingly confirmed in relatively recent experiments on the cyclotron resonance.[1] There is every reason to suppose that, within the framework of the one-electron approximation, the effective mass by no means always has the properties of a tensor quality (for example, for holes in germanium[2]). Therefore it is of interest to see what information on this point can be obtained by considering the symmetry properties of the lattice.

The experiments of Shalyt obviously provide evidence that two kinds of holes are present in tellurium.[3] This is not possible in the simplified theory of the zone spectrum of tellurium recently proposed by Callen[4,5]. Moreover, the group-theoretical formula he used do not correspond to the actual structure of tellurium. Although some of the conclusions of Callen's work are also confirmed in our exact theory, the reasons for the occurrence of the effects in question are entirely different. But the considerations given by Callen on the origin of the zones do not encounter any contradictions, and we make use of them in the choice of the theoretical possibilities, which, as it will turn out, can occur.

1. METHOD OF TREATMENT

The method* we have used is based on general premises of group theory. The idea of the method is as follows: as is well known, the wave function of an electron in an ideal crystal can be written in the form $\Psi_{n\mathbf{k}} = e^{i\mathbf{k}\mathbf{r}} u_{n\mathbf{k}}$. The Schrödinger equation for the modulating factor takes the form:

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_l^2} - i\frac{\hbar^2}{m}k_l\frac{\partial}{\partial x_l} + \frac{\hbar^2 k^2}{2m} + U(\mathbf{r})\right] u_{n\mathbf{k}}(\mathbf{r}) = E_n(\mathbf{k})\, u_{n\mathbf{k}}(\mathbf{r}). \quad (1)$$

Here summation is understood over the twice repeated indices l, and $U(\mathbf{r})$ is the self-consistent periodic potential. The function $U(\mathbf{r})$ possesses definite symmetry properties. We introduce the symme-

* A more rigorous exposition of this method can be found in a paper by Seitz.[6]

try operators $\hat{G}_i$ such that $\hat{G}_i U(\mathbf{r}) = U(\mathbf{r}') = U(\mathbf{r})$, *i.e.*, such that the action of the operator $\hat{G}_i$ in the "coordinate" representation consists in taking the point r over into the point r', *i.e.*,

$$\hat{G}_i \mathbf{r} = \mathbf{r}'. \tag{2}$$

It is clear that the required properties are possessed by the operators of translation by a whole number of lattice constants (we shall denote them by $\bar{\tau}_l = \mathbf{i}_0 x_l^0 + \mathbf{j}_0 y_l^0 + \mathbf{k}_0 z_l^0$), and also by rotation and reflection operators that take one atom in a crystal cell over into the position of another atom in the same or in another cell (we shall denote such operators by $\hat{\rho}_j$).

In addition there can exist so-called "open" symmetry elements, which reduce to rotations or reflections with subsequent translations. For such operators we shall use the notation

$$\{\hat{\rho}_j | \bar{\tau}_j\}. \tag{3}$$

If we write the Schrödinger equation in primed coordinates r' and choose a new value of k' such that its components along the new axes are equal to those of the old wave vector k in Eq. (1) along the unprimed axes, then this equation will have the same form as Eq. (1):

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_l'^2} - i\frac{\hbar^2}{m}k_l\frac{\partial}{\partial x_l'} + \frac{\hbar^2 k^2}{2m} + U(\mathbf{r}')\right] u_{n\mathbf{k}}(\mathbf{r}') = E_n(k_1, k_2, k_3)\, u_{n,\mathbf{k}}(\mathbf{r}'). \tag{4}$$

Since Eqs. (1) and (4) are identical in form and possess the same transformation properties, their eigenvalues are equal. But in Eq. (4) the wave vector is written in terms of its components along the new axes, and if we write it in terms of components along the old axes we shall have from Eqs. (1) and (4):

$$E_n(k_1, k_2, k_3) = E_n(k_1', k_2', k_3'). \tag{5}$$

Let us go over to the unprimed coordinates in Eq. (4). The Laplacian operator and $U(\mathbf{r})$ are invariant with respect to our transformations. The application of the operator (3) to the coordinates gives:

$$x_l' = (\hat{\rho}_j)_{lm} x_m + x_l^0, \tag{6}$$

$$x_m = (\hat{\rho}_j^{-1})_{ml} x_l' + (\hat{\rho}_j^{-1}\bar{\tau}_j)_m. \tag{7}$$

Since $\frac{\partial}{\partial x_l'} = \frac{\partial x_i}{\partial x_l'}\frac{\partial}{\partial x_i}$, then $k_l\frac{\partial}{\partial x_l'} = k_l\frac{\partial x_i}{\partial x_l'}\frac{\partial}{\partial x_i} = k_i'\frac{\partial}{\partial x_i}$.

Consequently $k_i' = k_l\frac{\partial x_i}{\partial x_l'} = (\hat{\rho}_j^{-1})_{il} k_l$, *i.e.*, $\mathbf{k}' = (\hat{\rho}_j^{-1})\mathbf{k}$.

If we denote the Hamiltonian by $\hat{H}_{\mathbf{k}}$, then Eq. (4) in the unprimed coordinates will have the form:

$$\hat{H}_{\mathbf{k}'} u_{n\mathbf{k}}(\hat{G}_j\mathbf{r}) = E_n(k_1', k_2', k_3')\, u_{n\mathbf{k}}(\hat{G}_j\mathbf{r}). \tag{8}$$

If we understand the operators $\hat{G}_j$ to be taken in the representation with the functions $u_{n\mathbf{k}}(\mathbf{r})$ as the basis, then $u_{n\mathbf{k}}(\mathbf{r}) = \hat{G}_j u_{n\mathbf{k}}(\mathbf{r})$. Thus we have

$$\hat{H}_{\mathbf{k}'}\hat{G}_j\, u_{n\mathbf{k}}(\mathbf{r}) = E_n(\mathbf{k}')\,\hat{G}_j\, u_{n\mathbf{k}}(\mathbf{r}), \tag{9}$$

i.e., our operators do not commute:

$$\hat{G}_j\hat{H}_{\mathbf{k}} = \hat{H}_{\mathbf{k}'}\hat{G}_j. \tag{10}$$

We see that $\hat{G}_j u_{n\mathbf{k}}(\mathbf{r})$ is an eigenfunction of the Hamiltonian $\hat{H}_{\mathbf{k}'}$. But we have just seen that the eigenvalues for Eqs. (1) and (4) are the same, *i.e.*, the spectrum is symmetrical with respect to all the operators $\hat{\rho}_j$ as applied to the k-space:

$$E_n(\mathbf{k}') = E_n(\mathbf{k}), \quad \hat{G}_j u_{n\mathbf{k}}(\mathbf{r}) = u_{n\mathbf{k}'}(\mathbf{r}). \tag{11}$$

By the action of all the $\hat{\rho}_j$ on k we get in the k-space what is called the "star"[7] for the wave vector k remains invariant under the action of a cergroup of the operators $\hat{\rho}_j$, this group of operators is called the group of the wave vector k.[7] In this case there is commutability:

$$\hat{G}_j\hat{H}_{\mathbf{k}} = \hat{H}_{\mathbf{k}}\hat{G}_j. \tag{12}$$

We can now apply the general premises of group theory to the study of the electron spectrum, and,

having compiled tables of the characters of the groups of various wave vectors, find out whether the zones coincide for a given value of the wave vector (*i.e.*, whether there is degeneracy). Such degeneracy occurs if for the group in question there exist representations of dimensionality greater than unity.

2. GROUPS OF SYMMETRY ELEMENTS FOR A LATTICE OF THE TELLURIUM TYPE

The space group of tellurium is D_3^6. Tellurium is a uniaxial crystal, with a structure consisting of a set of parallel chains of atoms. Within each of the infinite chains the atoms are connected by a screw axis of the third order directed along the principal axis of the crystal. The atoms of different chains are connected by simple axes of the second order and screw axes of the second order, located in planes perpendicular to the principal axis of the crystal.[8]

We adopt the following notations for the symmetry operators: $\hat{\rho}_3^1$ is the operator for a clockwise rotation around a third order screw axis, and its square $\hat{\rho}_3^2$ is the rotation in the counterclockwise direction; the operators of rotation around the second order axes are $\hat{\rho}_2^{(j)}$ (the upper index j corresponds to the number of the axis chosen); the operator for a translation along the principal axis is $\bar{\tau}_3$, and those for translations in the plane perpendicular to the principal axis are $\bar{\tau}_1$ (along the x axis) and $\bar{\tau}_2$.

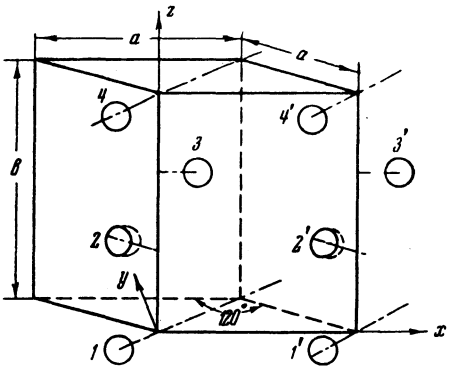

FIG. 1.

From Fig. 1, which shows the arrangement of the tellurium atoms in the crystal cell (there are three to a cell), and from Ref. 8, which gives the arrangement of the symmetry elements in the cell, we get the following expressions for the symmetry operators in the coordinate representation:

$$\hat{\rho}_3^1 = \begin{vmatrix} -1/2 & \sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{vmatrix}; \quad \hat{\rho}_3^2 = \begin{vmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{vmatrix};$$

$$\hat{\rho}_2^{(1)} = \begin{vmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{vmatrix}; \quad \hat{\rho}_2^{(2)} = \begin{vmatrix} -1/2 & \sqrt{3}/2 & 0 \\ \sqrt{3}/2 & 1/2 & 0 \\ 0 & 0 & -1 \end{vmatrix}; \quad \hat{\rho}_2^{(3)} = \begin{vmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & 1/2 & 0 \\ 0 & 0 & -1 \end{vmatrix} \tag{13a}$$

$$\bar{\tau}_1 = \mathbf{i}_0 a; \quad \bar{\tau}_2 = -\mathbf{i}_0 \frac{a}{2} + \mathbf{j}_0 \frac{\sqrt{3}}{2} a; \quad \bar{\tau}_3 = \mathbf{k}_0 b.$$

Then, according to the notation (3), the operator for a single step along a 3rd-order screw axis will be denoted by $\tilde{C}_3^1 = \{\rho_3^1 | \bar{\tau}_3/3\}$. For the unit operator we write $E = \{\varepsilon | 0\}$. We write the operators for the three 2nd-order axes in the form:

$$U_2^{(1)} = \{\hat{\rho}_2^{(1)} | \bar{\tau}_3/3\}; \quad U_2^{(2)} = \{\hat{\rho}_2^{(2)} | 0\},$$

$$U_2^{(3)} = \{\hat{\rho}_2^{(3)} | 2\bar{\tau}_3/3\}. \tag{13}$$

We have presented only the principal symmetry elements. The word "principal" is used in the sense that all the remaining symmetry operations around other axes located inside the cell (according to Ref. 8 there are 15 of them in all) reduce to rotations around these "principal" axes, multiplied by principal translations.

From the meaning of the action of the operators that have been introduced we have the following multiplication law for them:

$$\{\hat{\rho}_k \mid \bar{\tau}_k\}\cdot\{\hat{\rho}_l \mid \bar{\tau}_l\} = \{\hat{\rho}_k\hat{\rho}_l \mid \bar{\tau}_k + \hat{\rho}_k\bar{\tau}_l\}, \qquad (14)$$

i.e., in the general case the operators do not commute. After the expressions for the operators in the "coordinate" representation are found, we can find for them the multiplication table (Table 1), which will be the same in all representations, including the representation of those Bloch functions $\Psi_{n,\mathbf{k}}$ that are solutions of the Schrödinger equation in which the Hamiltonian commutes with the group of operators described above. But in this last case it can turn out that some of the translations have the effect of unit elements, and the multiplication table takes a simpler form.

TABLE I

	E	$\tilde{C}_3^1$	$\tilde{C}_3^2$	$U_2^{(1)}$	$U_2^{(2)}$	$U_2^{(3)}$	T_1	T_2	T_3
E	E	$\tilde{C}_3^1$	$\tilde{C}_3^2$	$U_2^{(1)}$	$U_2^{(2)}$	$U_2^{(3)}$	T_1	T_2	T_3
$\tilde{C}_3^1$	$\tilde{C}_3^1$	$\tilde{C}^2$	T_3	$U_2^{(3)}$	$U_2^{(1)}$	$T_3U_2^{(2)}$	$T_1^{-1}T_2^{-1}C_3^1$	$T_1\tilde{C}_3^1$	$T_3\tilde{C}_3^1$
$\tilde{C}_3^2$	$\tilde{C}_3^2$	T_3	$T_3\tilde{C}_3^1$	$T_3U_2^{(2)}$	$U_2^{(3)}$	$T_3U_2^{(1)}$	$T_2\tilde{C}_3^2$	$T_2^{-1}T_1^{-1}\tilde{C}_3^2$	$T_3\tilde{C}_3^2$
$U_2^{(1)}$	$U_2^{(1)}$	$U_2^{(2)}$	$T_3^{-1}U_2^{(3)}$	E	$\tilde{C}_3^1$	$T_3^{-1}\tilde{C}_3^2$	$T_1U_2^{(1)}$	$T_2^{-1}T_1^{-1}U_2^{(1)}$	$T_3^{-1}U_2^{(1)}$
$U_2^{(2)}$	$U_2^{(2)}$	$T_3^{-1}U_2^{(3)}$	$T_3^{-1}U_2^{(1)}$	$T_3^{-1}\tilde{C}_3^2$	E	$T_3^{-1}\tilde{C}_3^1$	$T_2U_2^{(2)}$	$T_1U_2^{(2)}$	$T_3^{-1}U_2^{(2)}$
$U_2^{(3)}$	$U_2^{(3)}$	$U_2^{(1)}$	$U_2^{(2)}$	$\tilde{C}_3^1$	$\tilde{C}^2$	E	$T_2^{-1}T_1^{-1}U_2^{(3)}$	$T_2U_2^{(3)}$	$T_3^{-1}U_2^{(3)}$

3. ON THE BRILLOUIN ZONE FOR LATTICES OF THE TELLURIUM TYPE

It is well known that the shape of the first Brillouin zone can be found from the condition

$$(\mathbf{k}/2\pi)\boldsymbol{\tau}_i = n_i \quad (n_i = 0.1). \qquad (15)$$

From Eq. (15) we have

$$\frac{\mathbf{k}}{2\pi} = n_1\frac{[\boldsymbol{\tau}_2\boldsymbol{\tau}_3]}{[\boldsymbol{\tau}_1[\boldsymbol{\tau}_2\boldsymbol{\tau}_3]]} + n_2\frac{[\boldsymbol{\tau}_3\boldsymbol{\tau}_1]}{[\boldsymbol{\tau}_1[\boldsymbol{\tau}_2\boldsymbol{\tau}_3]]} + n_3\frac{[\boldsymbol{\tau}_1\boldsymbol{\tau}_2]}{[\boldsymbol{\tau}[\boldsymbol{\tau}_{12}\boldsymbol{\tau}_3]]}. \qquad (15a)$$

Taking (13 a) into account we get

$$\frac{\mathbf{k}}{2\pi} = \frac{n_1}{a}\left(\mathbf{i}_0 + \frac{1}{\sqrt{3}}\mathbf{j}_0\right) + \frac{n_2}{a}\frac{2}{\sqrt{3}}\mathbf{j}_0 + \frac{n_3}{b}\mathbf{k}_0. \qquad (15b)$$

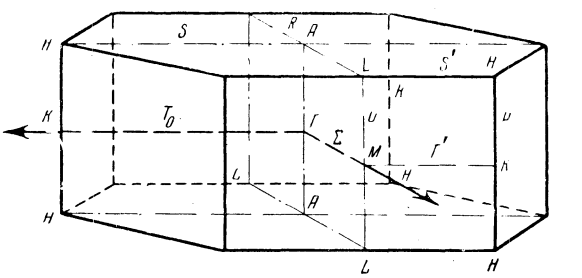

FIG. 2.

If k varies over the range $-\pi \leq \mathbf{k}\boldsymbol{\tau} \leq \pi$, then

$$\mathbf{k}_1^{gr} = \pm\frac{\pi}{a}\left(\mathbf{i}_0 + \frac{1}{\sqrt{3}}\mathbf{j}_0\right), \quad \mathbf{k}_2^{gr} = \pm\frac{2}{a}\frac{\pi}{\sqrt{3}}\mathbf{j}_0;$$
$$\mathbf{k}_3^{gr} = \mathbf{k}^{gr} - \mathbf{k}_2^{gr} = \pm\frac{\pi}{a}\left(\mathbf{i}_0 - \frac{1}{\sqrt{3}}\mathbf{j}_0\right); \qquad (16)$$
$$\mathbf{k}_4^{gr} = \pm\frac{\pi}{b}\mathbf{k}_0.$$

TABLE II

Designation of special point	Components of wave vector along axes	Designation of special point	Components of wave vector along axes
Γ	0, 0, 0	T'	k_x, $2\pi/\sqrt{3}\,a$, 0
A	0, 0, π/b	S'	k_x, $2\pi/\sqrt{3}\,a$, π/b
K	$4\pi/3a$, 0, 0	Λ	0, 0, k_z
H	$4\pi/3a$, 0, π/b	P	$4\pi/3a$, 0, k_z
M	$2\pi/\sqrt{3}\,a$, 0, 0	T_0	k_x, 0, 0
L	$2\pi/\sqrt{3}\,a$, 0, π/b		

Thus the first Brillouin zone has the shape of a hexagonal prism. We adopt the usual[9,10] designations for the special points. Table 2 shows the values of the wave vector corresponding to the special points, in terms of components along the axes.

4. CONSTRUCTION OF TABLES OF CHARACTERISTICS FOR GROUPS BELONGING TO WAVE VECTORS

If we choose as basis functions the oscillating Bloch factors $u_{n\mathbf{k}}(\mathbf{r})$, then all translations will act as unit elements, *i.e.*, with respect to this basis the group will be isomorphic to D_3 and we can make use of well known results.[11] Thus for the point $\Gamma(\mathbf{k}=0)$ two-fold degeneracy is possible (because the group has a representation of the second order), *i.e.*, at this point some of the zones come together in pairs. If for the point A we take as basis functions the $u_{n\mathbf{k}_A}(\mathbf{r})$, then we shall have:

$$U_2^{(i)}\hat{H}_{\mathbf{k}_A} = \hat{H}_{-\mathbf{k}_A}U_2^{(i)}; \quad \widetilde{C}_3^1\hat{H}_{\mathbf{k}_A} = \hat{H}_{\mathbf{k}_A}\widetilde{C}_3^1. \quad (17)$$

But since $\mathbf{k}_A$ and $-\mathbf{k}_A$ differ by $2\pi/b$, and we are using the concept of the reduced wave vector, we can also include all the $U_1^{(i)}$ in the group of the wave vector, along with $\widetilde{C}_3^1$ and $\widetilde{C}_3^2$. The table of characters for the Bloch oscillating factor $u_{n,\mathbf{k}_A}$ will be the same as for $u_{n,0}$.

Similar results are also obtained for the points K and H. Thus there can be contacts between zones at the points Γ, A, K, H. For the points L, M, T_0, T', S the group of the wave vectors will be E and $U_2^{(1)}$. This is the point group C_2,[11] and since here the multiplicity of the representations does not exceed unity, there is no degeneracy at these points. For the points Λ and P the group of the wave vector is E, $\widetilde{C}_3^1$, $\widetilde{C}_3^2$, *i.e.*, a group isomorphic to C_3.[11]

In the case in which the symmetry elements include "open" ones (screw axes, slip planes), the space group is not a simple product of a point group by a group of translations, and the groups for which the $\Psi_{n,\mathbf{k}}$ are taken as basis are not isomorphic to the corresponding point groups. (For example, this occurs for the case of the hexagonal close-packed lattice D_{6h}^4 and for the germanium lattice[9,10] D_h^7). For the point Γ we have $\Psi_{n,0} = u_{n,0}$; the results obtained can also be referred to the new basis. For the point A we have $\psi_{n,\mathbf{k}_A} = e^{i\pi/b}u_{n,\mathbf{k}_A}$. In this case

$$(\widetilde{C}_3^1)^3\psi_{n,\mathbf{k}_A} = \{\varepsilon|\overline{\tau}_3\}\psi_{n,\mathbf{k}_A} = -\psi_{n,\mathbf{k}_A}.$$

We write $\{\varepsilon|\overline{\tau}_3\} = T_3$. Now $(T_3)^2 = E$ (where E is the unit element). But $\{\varepsilon|\overline{\tau}_1\}$ and $\{\varepsilon|\tau_2\}$ act as unit elements, *i.e.*, the multiplication table takes a simplified form. We can now divide the elements into classes, using the following property:

$$A_i^{-1}BA_i = C_i. \quad (18)$$

If A_i runs through all the elements of the group, then B and all the C_i obtained by this operation belong to one class. It is not hard to verify that there are six classes (we shall denote them by K_j):

$$K_1 = E; \quad K_2 = T_3; \quad K_3 = \widetilde{C}_3^1, T_3\widetilde{C}_3^2;$$

$$K_4 = \widetilde{C}_3^2, T_3\widetilde{C}_3^1;$$

$$K_5 = U_2^1, T_3U_2^{(2)}, T_3U_2^{(3)}; \quad K_6 = T_3U_2^{(1)}, U_2^{(2)}, U_2^{(3)}.$$

Thus we shall have six representations. To find their dimensionalities we make use of the fact that

$n = \Sigma m_i^2$ where m_i is the dimensionality of the ith representation and n is the number of elements in the group. We get four one-dimensional representations and two with two dimensions. To construct the table of characters we use the following theorem[12]

$$(h_i\chi_i^{(d)}/\chi_E^{(d)})\cdot(h_j\chi_j^{(d)}/\chi_E^{(d)}) = \sum_l a_{ijl}h_l\chi_l^{(d)}/\chi_E^{(d)}. \tag{19}$$

Here h_i is the number of elements in the ith class, and $\chi_i^{(d)}$ is the character of the elements of the ith class in the representation d. The coefficient a_{ijl} is the number of times the class K_l is contained in the products of all elements of the class K_i by all elements of the class K_j. Since the multiplication table of the elements is known, we can find the coefficients a_{ijl} and get the system of equations for the $\chi_j^{(d)}$. By solving this system we get Table 3. In this table we must take the last three representations, where the action of T_3 is equivalent to multiplication by -1. The first three representations relate to $u_{n,\mathbf{k}_A}$. From Table 3 it follows that $\Psi_{n,\mathbf{k}_A}$ that we have determined the degree of degeneracy at the point A correctly. Similar results are obtained for the points K and H, because

$$T_1\psi_{n,\mathbf{k}_H} = \omega^2\psi_{n,\mathbf{k}_H};\quad T_2\psi_{n,\mathbf{k}_H} = \omega^2\psi_{n,\mathbf{k}_H};$$
$$T_1T_2\psi_{n,\mathbf{k}_H} = \omega\psi_{n,\mathbf{k}_H};\quad \omega = e^{i2\pi/3}, \tag{20}$$

i.e., the elements T_1T_2, T_1 and T_2 commute with all the elements of the group, and inclusion of them in the groups of the wave vectors for the points K and H would lead to a trivial tripling of the number of representations obtained (Table 3), by multiplying the characters already found by 1, ω, ω^2. Such considerations show that the results for the points K are similar to those for the point Γ.

5. THE DOUBLE-VALUED GROUPS FOR TELLURIUM

For the construction of the double-valued representations, which give the transformations of spinors, we can use the artifice proposed by Bethe.[13] For the case in which the $u_{n,\mathbf{k}}$ are taken as the basis, the groups in question are isomorphic to certain point groups, so that we can use the double-valued groups obtained for the latter.[11] If the $\Psi_{n,\mathbf{k}}$ are taken as the basis, we must introduce the following consideration. We shall assume that

$$(\hat{\rho}_3^1)^3 = \delta;\quad (\hat{\rho}_2^{(i)})^2 = \delta,\quad (\delta)^2 = \varepsilon.$$

Then

$$(\tilde{C}_3^1)^3 = \{\delta \mid \bar{\tau}_3\};\quad (\tilde{C}_3^1)^6 = \{\varepsilon \mid 2\bar{\tau}_3\};$$
$$(U_2^{(i)})^2 = \{\delta \mid 0\};\quad (U_2^{(i)})^4 = \{\varepsilon \mid 0\}. \tag{21}$$

TABLE III

	K_1	K_2	K_3	K_4	K	K_6
A_1''	1	1	1	1	1	1
A_2''	1	1	1	1	−1	−1
A_3''	2	2	−1	−1	0	0
A_1	1	−1	−1	1	1	−1
A_2	1	−1	−1	1	−1	1
A_3	2	−2	1	−1	0	0

TABLE IV

Таблица 4

	E	T_3	$Q=\{\delta\mid 0\}$	QT_3	$\tilde{C}_3^1$ $T_3\tilde{C}_3^2$	$T_3\tilde{C}_3^2$ $\tilde{C}_3^1$	$T_3\tilde{C}_3^2$ $Q\tilde{C}_3^1$	$\tilde{C}_3^1$ $Q\tilde{C}_3^2$	$U_2^{(1)}$ $T_3U_2^{(2)}$ $T_3U_2^{(3)}$	$QU_2^{(1)}$ $QT_3U_2^{(2)}$ $QT_3U_2^{(3)}$	$T_3U_2^{(1)}$ $U_2^{(2)}$ $U_2^{(3)}$	$QT_3U_2^{(1)}$ $T_3U_2^{(2)}$ $T_3U_2^{(3)}$
A_1'	1	−1	−1	1	1	1	−1	−1	i	$-i$	$-i$	i
A_2'	1	−1	−1	1	1	1	−1	−1	$-i$	i	i	$-i$
A_3'	2	−2	−2	2	−1	−1	1	1	0	0	0	0

But the relations (21) are insufficient for the construction of the complete multiplication table of the elements, which is necessary for the determination of the characters. In the Appendix it is shown that it suffices to know any two non-trivial multiplication rules, whereupon all the others can be found. Using the relation (18) and the law of multiplication of the elements, we can divide the elements into classes and use the theorem (19) to find the characters. In this connection it must be noted that our operators have the same action on the coordinates as before, although they act differently on the spinors (*cf.* Appendix). By these considerations we get Table 4. For the points H the results are similar to those obtained previously.

6. GENERAL PROPERTIES OF THE ZONE STRUCTURE

Using the results that have been obtained, we consider the problem of contacts between the zones. What happens with the two-dimensional representation Γ_3 if we place ourselves at the point Λ? Using the table of characters for the groups of these wave vectors, we reduce Γ_3 into irreducible representations of the group of Λ (*i.e.*, we reduce the representation E of the group D_3 in terms of representations of the group C_3).[3] We have:

$$\Gamma_3 = \Lambda_2 + \Lambda_3. \tag{22}$$

Since Λ_1 and Λ_2 are complex conjugate representations, they belong to a large number of pairs of complex conjugate functions. But because of the symmetry with respect to time inversion [11, 14] any pair of complex conjugate functions belongs to a single energy level, *i.e.*, in the absence of a magnetic field we will have contacts of the zones along the entire z axis in the k space. This conclusion is also valid for points of the type P. Along all other directions in the k space the degeneracy is removed, and there is no contact of zones (apart from the possibility of an accidental degeneracy). If we take into account the spin-orbit interaction, these results are somewhat changed. As is well known,[15] the operator for the spin-orbit interaction has the form:

$$(\hbar / 4m^2c^2)\,[\nabla U\,(\mathbf{r})\,\hat{p}]\,\hat{\sigma}. \tag{23}$$

In the case of degeneracy we seek the ψ-function in the form:

$$u = a_1 u_1 S_{1/2} + a_2 u_1 S_{-1/2} + a_3 u_2 S_{1/2} + a_4 u_2 S_{-1/2}, \tag{24}$$

where u will transform according to the representation $A \times D_{1/2}$, if u_1 and u_2 transform according to the representation A and the "free" spinor $(S_{1/2}, S_{-1/2})$ according to $D_{1/2}$. To find out whether the degeneracy is removed, we must reduce $A \times D_{1/2}$ into irreducible double-valued representations of the symmetry group of the given Hamiltonian. The characters for $D_{1/2}$ can be found by taking the traces of the matrices $\begin{vmatrix} \alpha & \beta \\ \gamma & \delta \end{vmatrix}$, which give the transformations of the "free" spinors.[11] We have

$$\hat{\rho}_3^1 = \begin{vmatrix} e^{i\pi/3} & 0 \\ 0 & e^{i\pi/3} \end{vmatrix}; \qquad \hat{\rho}_2^{(1)} = \begin{vmatrix} 0 & i \\ i & 0 \end{vmatrix} \text{ etc.} \tag{25}$$

i.e., $\chi(\hat{\rho}_3^1) = 1$, $\chi(\hat{\rho}_3^2) = -1$, $\chi(\hat{\rho}_2^{(i)}) = 0$.

After some simple algebraic transformations, we get:

$$\begin{aligned} \Gamma_3 \times D_{1/2} &= \Gamma_1' + \Gamma_2' + \Gamma_3'; \\ K_3 \times D_{1/2} &= K_1' + K_2' + K_3', \\ A_3 \times D_{1/2} &= A_1' + A_2' + A_3'; \\ H_3 \times D_{1/2} &= H_1' + H_2' + H_3'. \end{aligned} \tag{26}$$

We recall that Γ_3 and K_3 are identical to E in the group D_3, and Γ_3' and K_3' are identical to E_2' in the group D_3'; Γ_1' and Γ_2', K_1' and K_2' are identical with E' in the group D_3' (*cf.* Ref. 11).

Since in all of the equations (26) the two first primed double-valued representations are complex conjugates, they can be combined into one. Thus, at the points Γ, A, K, H the two-fold degeneracy is removed. Furthermore,

$$\Lambda_2 \times D_{1/2} = \Lambda_1' + \Lambda_3' \text{ and } \Lambda_3 \times D_{1/2} = \Lambda_1' + \Lambda_2'. \tag{27}$$

Here Λ_2' and Λ_3' are conjugates, arose from a single level, and therefore can be united in a single representation of doubled dimensionality (in virtue of the symmetry of the spinors with respect to time reversal[16, 17]). Thus in this case also the two-fold degeneracy is removed.

Thus, if we neglect the spin-orbit interaction, among the infinite set of zones there are pairs of zones that are in contact with each other along the directions in the k space that have been indicated above. Although one cannot draw a unique conclusion as to whether contact occurs between the two last valence p zones in tellurium, there is such a possibility. According to Callen, these p zones are in general contact along all directions in the k

space, which excludes the possibility of the presence of two kinds of holes in tellurium. From the above considerations it follows that the contact occurs only along certain directions in the k space, and then the dispersion law $E(\mathbf{k})$ can be different in the two p zones, *i.e.*, the effective masses of the carriers in these zones can be different. A choice between the existing possibilities can be made either by comparison with experiment, or else by resorting to Callen's idea about the origin of the zones in tellurium,[4] assuming that his arguments provide evidence in favor of overlapping of the p zones (but not their complete contact). If in zeroth approximation the edges of the valence zones coincide, then they have their extrema in common, and they necessarily lie on the lines of contact or near them. As we have seen, the spin-orbit interaction removes the degeneracy, and the lower edges of the zones do not coincide, *i.e.*, as the temperature rises there will be an increase of the relative number of those current carriers that are in the state corresponding to the energetically higher zone. If the holes in the lower zone have different effective masses from those in the upper zone, then at low temperatures these holes alone will play an effective part in processes; but at higher temperatures, when the numbers of carriers of the two kinds is approximately the same, the course of a process can be mainly determined by the properties of the other holes. Just such properties in tellurium are proposed by Shalyt for one of the possible explanations of his experiments.[3]

The results are valid for arbitrary values of the wave vector k [we agree to reckon k from the point of the extremum for $E(\mathbf{k})$]. To be more specific, let us obtain in analytic form the dispersion law $E(\mathbf{k})$ in the approximation quadratic in k, for various particular assumptions about the locations of the extrema.

7. THE DISPERSION LAW FOR LOCATION OF THE EXTREMA AT THE POINTS Γ, *A*, *K*, *H*

We assume that an extremum occurs at one of these points. For the non-degenerate case (representations of types A_1 and A_2 in the notation of Ref. 11) the dispersion law has the form:[2]

$$E = D_{jj}^{\alpha\beta} k^\alpha k^\beta, \tag{28}$$

where $D_{jj}^{\alpha\beta} = \frac{\hbar^2}{2m}\delta_{\alpha\beta} + \frac{\hbar^2}{m^2}\sum_i \frac{p_{ji}^\alpha p_{ij}^\beta}{E_j(\mathbf{k}_0) - E_i(\mathbf{k}_0)}$,

$$p_{ji}^\alpha = -i\hbar \int u_{j,\mathbf{k}_0} \frac{\partial}{\partial_\alpha} u_{i,\mathbf{k}_0}\, d\tau,$$

and $\mathbf{k}_0$ is the point around which the resolution is carried out. This is the equation of an ellipsoid. It is not hard to see that this will be an ellipsoid of revolution around the z axis, because from the symmetry properties of the spectrum it follows that $E(\mathbf{k}) = E(\mathbf{k}')$ if $\mathbf{k}' = \hat{\rho}_3^{\frac{1}{2}}\mathbf{k}$. For the point Γ this will be a single ellipsoid (Fig. 3, *a*); for the points *A*, *K*, *H* the pictures are more peculiar, and are shown in Fig. 3, *b*, *c*, *d*.

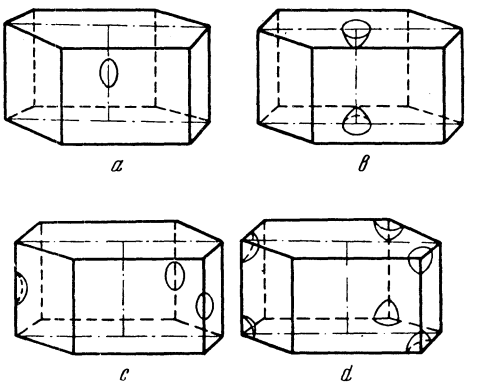

FIG. 3.

Of more interest is the case of two-fold degenerate states (representations of type E in the notation of Ref. 11), for which the dispersion law is determined by the equation:[2]

$$\begin{vmatrix} D_{11}^{\alpha\beta}k^\alpha k^\beta - E & D_{12}^{\alpha\beta}k^\alpha k^\beta \\ D_{21}^{\alpha\beta}k^\alpha k^\beta & D_{22}^{\alpha\beta}k^\alpha k^\beta - E \end{vmatrix} = 0. \tag{29}$$

The coefficients D are determined in a way similar to that shown in Eq. (28). All told there are 24 unknown coefficients. We can reduce this number, knowing the law of transformation of u_1 and u_2 under the action of the symmetry operators. Obviously:

$$\widetilde{C}_3^1 u_1 = (\widetilde{C}_3^1)_{11} u_1 + (\widetilde{C}_3^1)_{12} u_2;$$
$$\widetilde{C}_3^1 u_2 = (\widetilde{C}_3^1)_{21} u_1 + (\widetilde{C}_3^1)_{22} u_2$$

and similarly for the operators $\widetilde{C}_3^2$, $U_2^{(1)}$, $U_2^{(2)}$, $U_2^{(3)}$. We must find the two-rowed matrices corresponding to these operators in the representation of the Bloch oscillating factors u_1 and u_2. For this it suffices to use the operator multiplication law obtained in the coordinate representation, but valid in any representation, and the orthogonality rules for matrix elements[11]

$$\sum_G G_{ik}^\alpha (G_{lm}^\beta)^* = (p/f_\alpha)\,\delta_{\alpha\beta}\delta_{il}\delta_{km}. \tag{30}$$

Here α and β are indices labelling irreducible representations, f_α is the dimensionality of representa-

tion α, p is the number of elements in the group, and G^{α}_{jk} are the elements of the matrix corresponding to the element G in the representation α. In this way one can show that u_1 and u_2 transform like x and y under the action of the operators of the group D_3 in the case in which the first 2nd order axis makes the angle φ with the x axis, *i.e.*,

$$E=\begin{vmatrix}1&0\\0&1\end{vmatrix};\quad \tilde{C}^1_3=\begin{vmatrix}1/2&\sqrt{3}/2\\-\sqrt{3}/2&1/2\end{vmatrix};\qquad U^{(1)}_2=\begin{vmatrix}\cos 2\varphi&\sin 2\varphi\\-\sin 2\varphi&\cos 2\varphi\end{vmatrix}\quad etc. \tag{31}$$

Using the law of transformation of the functions under the action of the operators of the group D_3, one can verify that:

$$p^z_{1a}=p^z_{2a}=p^z_{1b}=p^z_{2b}=0;$$
$$p^y_{1a}=p^y_{2a}=p^x_{1b}=p^y_{2b}=0;$$
$$p^z_{11'}=p^z_{22'}=0;\quad p^x_{12'}=p^x_{21'}=p^y_{11'}=p^y_{22'}=0;$$
$$p^x_{1a}=p^y_{2a};\quad p^x_{2b}=-p^x_{1b};\quad p^z_{12'}=-p^z_{21'}; \tag{32}$$
$$p^x_{11'}=-p^x_{22'}=-p^y_{12'}=-p^y_{21'}.$$

Here the index a labels functions transforming according to the representation A_1, the index b those belonging to the representation A_2; the indices 1 and 1′, 2 and 2′, and also l and l' label functions transforming by various two-rowed representations E. We get the dispersion law in the form:

$$\begin{vmatrix}-A_1k_x^2-Ak_yk_z+A_3k_z^2+A_2(k_x^2+k_y^2)-E & -A_1k_xk_y-Ak_xk_z\\ -A_1k_xk_y-Ak_xk_z & -A_1k_y^2+Ak_yk_z+A_3k_z^2+A_2(k_x^2+k_y^2)-E\end{vmatrix}=0;$$

$$A_1=\frac{\hbar^2}{m^2}\sum_a\frac{|p^x_{1a}|^2}{E_a-E}-\frac{\hbar^2}{m^2}\sum_b\frac{|p^y_{1b}|^2}{E_b-E};\quad A_3=\frac{\hbar^2}{2m}-\frac{\hbar^2}{m^2}\sum_l\frac{|p^z_{12'}|^2}{E_l-E};$$
$$A_2=\frac{\hbar^2}{2m}-\frac{\hbar^2}{m^2}\sum_l\frac{|p^x_{11'}|}{E_l-E}-\frac{\hbar^2}{m^2}\sum_b\frac{|p^y_{1b}|^2}{E_b-E}; \tag{33}$$
$$A=\frac{\hbar^2}{m^2}\sum_l\frac{p^y_{12'}p^z_{2'1}+p^z_{12'}p^y_{2'1}}{E_l-E}.$$

Solving the quadratic equation for E, we get:

$$E=A_3k_z^2+\left(A_2-\frac{A_1}{2}\right)(k_x^2+k_y^2)\pm\left[\frac{A_1^2}{4}(k_x^2+k_y^2)^2+A^2k_z^2(k_x^2+k_y^2)-AA_1(k_y^2-3k_x^2)k_yk_z\right]^{1/2}. \tag{34}$$

It is not hard to see that the radicand is equal to

$$\left|\frac{A_1}{2}(k_x+ik_y)^2+iAk_z(k_x-ik_y)\right|^2,$$

i.e., it is always positive, and consequently E is real.

In addition the solution is invariant with respect to $\hat{\rho}^{(1)}_2$, since the action of this operator reduces to the replacements $k_y\to -k_y$, $k_z\to -k_z$, and with respect to $\hat{\rho}^1_3$, since this results in multiplying k_x+ik_y by $\omega=e^{i2\pi/3}$ and k_x-ik_y by $\omega^2=e^{i4\pi/3}$. Thus our spectrum satisfies the needed requirements of symmetry and reality. Keeping in mind that

$$k_x=k\sin\vartheta\cos\varphi,\quad k_y=k\sin\vartheta\sin\varphi,$$
$$k_z=k\cos\vartheta,$$

we rewrite Eq. 34 in the form:

$$E=k^2\left\{A_3\cos^2\vartheta+\left(A_2-\frac{A_1}{2}\right)\sin^2\vartheta\pm\right.$$
$$\left.\pm\left[\sin^2\vartheta\left(\frac{A_1^2}{4}\sin^2\vartheta+A^2\cos^2\vartheta-A_1A\sin\vartheta\cos\vartheta\cos 3\varphi\right)\right]^{1/2}\right\}. \tag{35}$$

Let us investigate the place of contact of the zones

for the case in which the radicand vanishes.

First case:

$$\sin^2\vartheta = 0,$$

i.e., there will be contact of the zones along the z axis, as follows from our earlier general arguments.

Second case:

$$\frac{A_1^2}{4}\sin^2\vartheta + A^2\cos^2\vartheta - AA_1\sin\vartheta\cos\vartheta\cos 3\varphi = 0.$$

For $\vartheta \neq \pi/2$ we get:

$$\tan^2\vartheta = 2\frac{A}{A_1}[\cos 3\varphi \pm (\cos^2 3\varphi - 1)^{1/2}]. \quad (36)$$

For contact of the zones it is necessary that the solution (36) be real, *i.e.*, $\cos 3\varphi = \pm 1$. Consequently, the solutions (36) will be:

$$\varphi_{extr} = 0,\quad 2\pi/3,\quad 4\pi/3;\ \tan(\vartheta_{extr}) = 2A/A_1,$$

$$\varphi_{extr} = \pi/3,\quad \pi,\quad 5\pi/3;\ \tan(\vartheta_{extr}) = -2A/A_1. \quad (37)$$

Along these directions an additional contact of the zones will occur. This is an accidental degeneracy occurring only in the approximation quadratic in k. Let us denote the angle-dependent factor in Eq. (35) by $m^{\pm}(\vartheta, \varphi)$ (the signs ± correspond to the sign of the root). According to Eq. (35) we have two kinds of carriers of the same sign, with masses m^+ and m^- which are already not tensor quantities. A change of sign of m^+ or m^- for certain values of ϑ φ would mean that we obtained a resolution near a point of inflection, which in the present work is in general of no interest. Therefore we shall assume that the parameters A, A_1, A_2, A_3 are such that this case does not occur. For the points A, K, H we get exactly similar results, with the single exception that at these points there will appear a characteristic pattern of repetition, analogous to the situation shown for nondegenerate states in Fig. 3, $a-d$.

8. THE DISPERSION LAW FOR EXTREMA AT THE POINTS Λ, P

It was shown in Sec. 4 that in this case the group of the wave vector isiisomorphic to C_3. Then:

$$u_1^* = u_2;\quad \tilde{C}_3^1 u_1 = \omega u_1;\quad \tilde{C}_3^1 u_2 = \omega^2 u_2.$$

For these points

$$\int u_j^*(\partial/\partial x \pm i\partial/\partial y)\, u_j d\tau = 0,$$

because $u_j u_j^*$ is invariant with respect to C_3^1 and $(\partial/\partial x \pm i\partial/\partial y)$ is multiplied by ω or ω^2. In a similar way we get:

$$\int u_1^*(\partial/\partial x + i\partial/\partial y)\, u_{2'}\, d\tau = \int u_2^*(\partial/\partial x - i\partial/\partial y)\, u_{1'}\, d\tau = 0.$$

Proceeding in the same way, one can verify that

$$p_{11'}^x = p_{11'}^y = p_{22'}^x = p_{22'}^y = p_{12'}^z = p_{2'1}^z = 0;\quad p_{1a}^z = p_{2a}^z = 0;$$
$$p_{21'}^x = ip_{21'}^y;\quad p_{12'}^x = -ip_{12'}^y;\quad p_{1a}^x = ip_{1a}^y;\quad p_{2a}^x = -ip_{2a}^y;\quad p_{11'}^z = -(p_{22'}^z)^*. \quad (38)$$

Here the index a is affixed to functions that transform according to the representation Λ_1 (*i.e.*, for which the operation C_3^1 amounts to a factor ω). By a procedure like that of Sec. 1, we get the dispersion equation:

$$\begin{vmatrix} A(k_x^2 + k_y^2) + Bk_z^2 - E & A_{12}(k_x + ik_y)^2 + B_{12}k_z(k_x - ik_y) \\ A_{12}(k_x - ik_y)^2 + B_{12}^*(k_z + ik_y) & A(k_x^2 + k_y^2) + Bk_z^2 - E \end{vmatrix} = 0, \quad (39)$$

where

$$A = \frac{\hbar^2}{2m} - \frac{\hbar^2}{m^2}\sum_a \frac{|p_{1a}^x|^2}{E_a - E} - \frac{\hbar^2}{m^2}\sum_j \frac{|p_{12'}^x|^2}{E_j - E};\quad A_{12} = \frac{\hbar^2}{m^2}\sum_a \frac{|p_{1a}^x|^2}{E_a - E};$$

$$B = \frac{\hbar^2}{2m} - \frac{\hbar^2}{m^2}\sum_j \frac{|p_{11'}^z|^2}{E_j - E};$$

$$B_{12} = -\frac{\hbar^2}{m^2}\sum_j \frac{p_{12'}^x p_{2'2}^z + p_{1'2}^x p_{11'}^z}{E_j - E} = B_{12}' + iB_{12}''.$$

In the problem of the contact of zones we get analogous results, the only difference being that now

$$\tan(\vartheta_{\text{extr}}) = -|B_{12}|/A_{12},$$

$$\cos 3\varphi_{\text{extr}} = \pm B''_{12}/|B_{12}|.$$

The dispersion law depends on five parameters and has the form:

$$E = Bk_z^2 + A(k_x^2+k_y^2) \pm [A_{12}^2(k_x^2+k_y^2)^2 + |B_{12}|^2 k_z^2(k_x^2+k_y^2) + 2\,\mathrm{Re}(A_{12}B_{12}^* k_z(k_x+ik_y)^3)]^{1/2}. \quad (40)$$

9. THE SPIN-ORBIT INTERACTION

The Schrödinger equation for an "excess" electron in the crystal, including relativistic effects, if we neglect the displacement of the entire spectrum by amounts of the order of $(v/c)^2$ times the separation between zones, has the form:

$$\left\{H_{\mathbf{k}} + \frac{\hbar^2}{4m^2c^2}[\nabla U(\mathbf{r})\,\mathbf{k}]\,\hat{\sigma} + \frac{\hbar}{4m^2c^2}[\nabla U(\mathbf{r})\,\hat{p}]\,\hat{\sigma}\right\} u_{n\mathbf{k}}(\mathbf{r}) = E_n(\mathbf{k})\,u_{n\mathbf{k}}(\mathbf{r}). \quad (41)$$

We introduce the spin functions $S_{1/2} = \begin{pmatrix}1\\0\end{pmatrix}$ and $S_{-1/2} = \begin{pmatrix}0\\1\end{pmatrix}$; then:

$$[\nabla U\mathbf{k}]\,\hat{\sigma}S_{1/2} = S_{1/2}\left(\frac{\partial U}{\partial x}k_y - \frac{\partial U}{\partial y}k_x\right) + S_{-1/2}\left[-ik_z\left(\frac{\partial U}{\partial x} + i\frac{\partial U}{\partial y}\right) + i\frac{\partial U}{\partial z}(k_x+ik_y)\right],$$
$$[\nabla U\mathbf{k}]\,\hat{\sigma}S_{-1/2} = -S_{-1/2}\left(\frac{\partial U}{\partial x}k_y - \frac{\partial U}{\partial y}k_x\right) + S_{1/2}\left[ikz\left(\frac{\partial U}{\partial x} - i\frac{\partial U}{\partial y}\right) - i\frac{\partial U}{\partial z}(k_x-ik_y)\right]. \quad (42)$$

The action of $[\nabla U\hat{p}]\hat{\sigma}$ is similar, but k_i must be replaced by $-i\hbar\partial/\partial x_i = \hat{p}_i$.

In order that there be an extremum at the point $\mathbf{k}_0$, we must have:

$$\int u_j^* \nabla u_{j'} d\tau = 0, \quad (s', j'|[\nabla U\mathbf{k}]\,\hat{\sigma}\,|s, j) = 0. \quad (43)$$

The second of the conditions (43) is automatically fulfilled in crystals with a center of inversion.[18] In our case it is not fulfilled. This means that the extremum is displaced from the point $\mathbf{k}_0$. For degenerate states we shall seek the function in the form:

$$u = a_1u_1S_{1/2} + a_2u_2S_{1/2} + a_3u_1S_{-1/2} + a_4u_2S_{-1/2}. \quad (44)$$

A. The points Γ, A, K, H.

A consideration of the selection rules of the matrix elements of the operators $[\nabla U\mathbf{k}]\hat{\sigma}$ and $[\nabla U\hat{p}]\hat{\sigma}$ for the two-rowed representations of the points Γ, A, K, H enables us to obtain the dispersion law in the form of the vanishing of the determinant

$$\|\alpha_{ik}\| = 0;$$

$$\begin{aligned}
\alpha_{11} &= -A_1k_x^2 - Ak_yk_z + \gamma k_y - E'; & \alpha_{12} &= -A_1k_xk_y - Ak_xk_z - \gamma k_x + i\varkappa,\\
\alpha_{13} &= i\gamma k_z; & \alpha_{14} &= -\gamma k_z; & \alpha_{21} &= -A_1k_xk_y - Ak_xk_z - \gamma k_x - i\varkappa,\\
\alpha_{22} &= -A_1k_y^2 + Ak_zk_y - \gamma k_y - E', & \alpha_{23} &= -\gamma k_z, & \alpha_{24} &= -i\gamma k_z;\\
\alpha_{31} &= -i\gamma k_z, & \alpha_{32} &= -\gamma k_z, & \alpha_{33} &= -A_1k_x^2 - Ak_yk_z - \gamma k_y - E',\\
\alpha_{34} &= -A_1k_xk_y - Ak_xk_z - \gamma k_x - i\varkappa; & \alpha_{41} &= -\gamma k_z, & \alpha_{42} &= i\gamma k_z,\\
\alpha_{43} &= -A_1k_yk_x - Ak_xk_z - \gamma k_x + i\varkappa, & \alpha_{44} &= -A_1k_y^2 + Ak_yk_z + \gamma k_y - E'.
\end{aligned} \quad (45)$$

Here

$$i\varkappa = \frac{\hbar}{4m^2c^2}\int u_1^*\left(\frac{\partial U}{\partial y}\hat{p}_x - \frac{\partial U}{\partial x}\hat{p}_y\right)u_2\,d\tau;$$

$$\gamma = \frac{\hbar^2}{4m^2c^2}\int u_1^*\frac{\partial U}{\partial x}u_1\,d\tau.$$

For $\mathbf{k} = 0$ the determinant breaks up into two:

$$\begin{vmatrix} E & -i\varkappa \\ i\varkappa & E\end{vmatrix} = 0, \quad \begin{vmatrix} E & i\varkappa \\ -i\varkappa & E\end{vmatrix} = 0, \quad (46)$$

i.e., at the point $\mathbf{k} = 0$, $E = \pm|\varkappa|$ and there is a splitting; therefore we can rewrite Eq. (45), using as basis functions those that satisfy Eq. (46):

for $E = -|\varkappa|$

$$u_1' = 2^{-1/2}(u_1 + iu_2)S_{1/2};\quad u_1'' = 2^{-1/2}(u_1 - iu_2)S_{-1/2},$$

for $E = |\varkappa|$

$$u'_{II} = 2^{-1/2}(u_1 - iu_2)\,S_{1/2};\quad u''_{II} = 2^{-1/2}(u_1 + iu_2)\,S_{-1/2}.$$

This corresponds to a canonical transformation by means of the operator $\hat{A}$:

$$\hat{A} = \begin{vmatrix} 1 & i & 0 & 0 \\ 0 & 0 & 1 & -i \\ 1 & -i & 0 & 0 \\ 0 & 0 & 1 & i \end{vmatrix} \tag{47}$$

Transforming the determinant (45) and expanding it, we get the equation:

$$(E'^2 - \varkappa^2 - |d|^2)^2 = 4k_z^2\gamma^2\,[(E' - |\varkappa|)^2 + A^2(k_x^2 + k_y^2)^2], \tag{48}$$

where

$$|d|^2 = \frac{A_1^2}{4}(k_x^2 + k_y^2)^2 + (A^2k_z^2 + \gamma^2)(k_x^2 + k_y^2) - AA_1(k_y^2 - 3k_x^2)\,k_yk_z,$$
$$E' = E - A_3k_z^2 - \left(A_2 - \frac{A_1}{2}\right)(k_x^2 + k_y^2). \tag{49}$$

First case:

For $A_ik^2 \gg \gamma k$, $A_ik^2 \gg |\varkappa|$ we get $E' = \pm |d|$, which is the same as Eq. (34).

Second case:

If $\gamma k \ll |\varkappa|$, $A_ik^2 \ll |\varkappa|$, where A_i is the largest of the parameters, then for $k_z \sim \gamma/A_i$ we have: $A_ik^2 \sim \gamma^2/A_i$, *i.e.*, the terms γk and A_ik^2 are of the same order of smallness. But $\gamma^2/A_i \ll |\varkappa|$, *i.e.*, the off-diagonal terms in the determinant are small in comparison with $2|\varkappa|$, and therefore we can neglect them and solve the two 2nd order determinants

$$\begin{vmatrix} -|\varkappa| - E' & 2ik_z\gamma \\ -2ik_z\gamma & -|\varkappa| - E' \end{vmatrix} = 0, \qquad \begin{vmatrix} |\varkappa| - E' & 0 \\ 0 & |\varkappa| - E' \end{vmatrix} = 0. \tag{50}$$

independently. As the equipotential surfaces we have two ellipsoids of revolution, with their centers displaced along the k_z axis by $4\gamma/A_3$:

$$E_{1,2} = |\varkappa| - 2\gamma^2/A_3 + (A_2 - A_1/2)(k_x^2 + k_y^2) + A_3(k_z \pm \gamma/A_3)^2. \tag{51}$$

Thus, in agreement with the general conclusions of Sec. 6, the effective masses of the carriers at low temperatures are different from their values for high temperatures. The points *A*, *H*, *K* differ in showing a characteristic repetition pattern, analogous to the situation shown in Fig. 3, *a*–*d*. For nondegenerate states of type A_1 or type A_2 (Ref. 11) we have not obtained any significant results, because in this case all the matrix elements of the spin-orbit interaction operator are zero.

B. Points of Types Λ and P

By a similar argument we get the secular equation

$$\|\beta_{ik}\| = 0;$$
$$\beta_{11} = \varkappa - E',\quad \beta_{12} = ik_z\delta,\quad \beta_{13} = i\gamma(k_x - - ik_y),$$
$$\beta_{14} = A_{12}(k_x + ik_y)^2 + B_{12}k_z(k_x - ik_y) + i\delta(k_x - ik_y),$$
$$\beta_{21} = -ik_z\delta_{14},\quad \beta_{22} = \varkappa - E',\quad \beta_{24} = i\tilde{\gamma}(k_x + ik_y),$$
$$\beta_{23} = A_{12}^*(k_x - ik_y)^2 + B_{12}^*k_z(k_x + ik_y) + i\delta^*(k_x + ik_y),$$
$$\beta_{31} = i\gamma(k_x + ik_y),\quad \beta_{33} = -\varkappa - E',\quad \beta_{34} = 0,$$
$$\beta_{32} = A_{12}(k_x + ik_y)^2 + B_{12}k_z(k_x - ik_y) - i\delta(k_x - ik_y),$$
$$\beta_{41} = A_{12}^*(k_x - ik_y)^2 + B_{12}^*k_z(k_x + ik_y) - i\delta^*(k_x + ik_y),$$
$$\beta_{42} = -i\gamma(k_x - ik_y),\quad \beta_{43} = 0,\quad \beta_{44} = -\varkappa - E'. \tag{52}$$

Here

$$E' = E - Bk_z^2 + A(k_x^2 + k_y^2);\quad \varkappa = \frac{\hbar}{4m^2c^2}\int u_1^*\left(\frac{\partial U}{\partial x}\hat{p}_y - \frac{\partial U}{\partial y}\hat{p}_x\right)u_1\,d\tau;$$
$$\delta = \frac{\hbar^2}{4m^2c^2}\int u_1^*\left(\frac{\partial U}{\partial x} - i\frac{\partial U}{\partial y}\right)u_2\,d\tau;\quad \gamma = \frac{\hbar^2}{4m^2c^2}\int u_1^*u_1\frac{\partial U}{\partial z}\,d\tau.$$

For $E \gg |\varkappa|$ we get the results already known from Sec. 2. For the opposite case $E \ll |\varkappa|$ we can solve independently two 2nd-order determinants; *i.e.*, we get

$$E_1 = |\varkappa| - \frac{|\delta|^2}{B} + A(k_x^2 + k_y^2) + B\left(k_z \pm \frac{|\delta|}{B}\right)^2;$$
$$E_2 = -|\varkappa| + A(k_x^2 + k_y^2) + Bk_z^2. \qquad (53)$$

(We note that γ and $\varkappa$ are real, and δ is an imaginary quantity.)

The interpretation of the results goes just as in case *A*. For the one-dimensional representations of type Λ_1 the inclusion of the spin-orbit interaction does not lead to any new results, since all the matrix elements are zero.

C. Other Cases of Location of the Extrema

For all points other than Γ, *A*, *K*, *H*, Λ, *P* there exist only one-dimensional representations, *i.e.*, at such points the zones are not in contact, and thus the dispersion law has the form (28), *i.e.*, the equipotential surfaces will be ellipsoids. A special feature is that because of the symmetry of the spectrum with respect to D_3 in the k space the number of extremal points is increased by multiplication and can be as large as six (if they do not lie on any symmetry element). For points of type *T* there will be three ellipsoids of revolution; for points *S* there will be repetition like that shown in Fig. 3, *a*–*d*. For points of type Σ we have six ellipsoids of revolution, etc.

CONCLUSION

In presenting our results we would like to remark that on the basis of the experimental data existing at present, according to which the effective masses of the holes are different for high and low temperatures, one can draw the conclusion that for hole-type tellurium the case of zones in contact is realized and the extrema are located at some or other of the points Γ, *A*, *H*, *K*, Λ, *P*. This same case is also obviously realized for electron-type tellurium.[5] The results found are valid for arbitrary lattices with space groups D_3^{1-7}, *i.e.*, also for selenium. The whole question comes down to just where the extrema are located, and whether the last valence zones are in contact. The positions of the extrema can be found either by numerical calculations, which despite all their elaborateness cannot at present pretend to great accuracy, or by comparison with experiment of the conclusions that follow from the various possible forms of the spectrum. The latter approach appears the more promising, and in this way the writer has been able to obtain expressions for the magnetic susceptibility coefficient[19] and for the cyclotron resonance frequency.

In conclusion the writer considers it his duty to thank Prof. A. I. Ansel'm for a discussion of the results and for his constant interest in the work.

APPENDIX

For the ordinary point groups we have:

$$\hat{\rho}_3^1 \hat{\rho}_2^{(1)} = \hat{\rho}_2^{(3)}, \quad \hat{\rho}_3^1 \hat{\rho}_2^{(2)} = \hat{\rho}_2^{(1)}.$$

From geometrical considerations it is clear that these rules must be satisfied with accuracy up to a multiplication by δ, so that we must have one of the four possibilities

$$\hat{\rho}_3^1 \hat{\rho}_2^{(1)} = \delta\hat{\rho}_2^{(3)}, \quad \hat{\rho}_3^1 \hat{\rho}_2^{(2)} = \delta\hat{\rho}_2^{(1)}, \qquad (I)$$
$$\hat{\rho}_3^1 \hat{\rho}_2^{(1)} = \delta\hat{\rho}_2^{(3)}, \quad \hat{\rho}_3^1 \hat{\rho}_2^{(2)} = \hat{\rho}_2^{(1)}, \qquad (II)$$
$$\hat{\rho}_3^1 \hat{\rho}_2^{(1)} = \hat{\rho}_2^{(3)}, \quad \hat{\rho}_3^1 \hat{\rho}_2^{(2)} = \delta\rho_2^{(1)}, \qquad (III)$$
$$\hat{\rho}_3^1 \hat{\rho}_2^{(1)} = \hat{\rho}_2^{(3)}, \quad \hat{\rho}_3^1 \hat{\rho}_2^{(2)} = \hat{\rho}_2^{(1)}. \qquad (IV)$$

For case I: $\hat{\rho}_3^1 = \hat{\rho}_2^{(3)}\hat{\rho}_2^{(1)} = \hat{\rho}_2^{(1)}\hat{\rho}_2^{(2)}$, or, multiplying Eq. (I) by $\delta\hat{\rho}_3^1$ on the left, we get:

$$\hat{\rho}_3^1 \hat{\rho}_2^{(3)} = (\hat{\rho}_3^1)^{-1}\hat{\rho}_2^{(1)}, \quad i.e., \quad (\hat{\rho}_2^{(1)}\hat{\rho}_2^{(2)})^{-1}\cdot\hat{\rho}_2^{(1)} = \delta\hat{\rho}_2^{(2)}.$$

Thus we have:

$$\hat{\rho}_3^1 \hat{\rho}_2^{(3)} = \delta\hat{\rho}_2^{(2)}. \qquad (1)$$

Taking the reciprocals of (I) and (1), we have:

$$\hat{\rho}_2^1 \hat{\rho}_3^2 = \hat{\rho}_2^{(3)}; \quad \hat{\rho}_2^{(2)}\hat{\rho}_3^2 = \hat{\rho}_2^{(1)}; \quad \hat{\rho}_2^{(3)}\hat{\rho}_3^2 = \hat{\rho}_2^{(2)}. \qquad (2)$$

Multiplying Eq. (2) by $\hat{\rho}_3^1$ on the right, we get:

$$\hat{\rho}_2^{(3)}\hat{\rho}_3^1 = \delta\rho_2^{(1)}; \quad \hat{\rho}_2^{(1)}\hat{\rho}_3^1 = \delta\rho_2^{(2)}; \quad \hat{\rho}_2^{(2)}\hat{\rho}_3^1 = \delta\hat{\rho}_2^{(3)}. \qquad (3)$$

Taking the reciprocals of (3), we have:

$$\hat{\rho}_3^2 \hat{\rho}_2^{(3)} = \hat{\rho}_2^{(1)}; \quad \hat{\rho}_3^2 \hat{\rho}_2^{(1)} = \hat{\rho}_2^{(2)}; \quad \hat{\rho}_3^2 \hat{\rho}_2^{(2)} = \hat{\rho}_2^{(3)}. \qquad (4)$$

Multiplying Eqs. (I) and (1) on the right by $\hat{\rho}_2^{(1)}$, $\hat{\rho}_2^{(2)}$, $\hat{\rho}_2^{(3)}$ respectively, we get:

$$\hat{\rho}_2^{(3)}\hat{\rho}_2^{(1)} = \hat{\rho}_3^1; \quad \hat{\rho}_2^{(1)}\hat{\rho}_2^{(2)} = \hat{\rho}_3^1; \quad \hat{\rho}_2^{(2)}\hat{\rho}_2^{(3)} = \hat{\rho}_3^1. \quad (5)$$

Taking the reciprocals of (5), we see that:

$$\hat{\rho}_2^{(1)}\hat{\rho}_2^{(3)} = \delta\hat{\rho}_3^2; \quad \hat{\rho}_2^{(2)}\hat{\rho}_2^{(1)} = \delta\hat{\rho}_3^2; \quad \hat{\rho}_2^{(3)}\hat{\rho}_2^{(2)} = \delta\hat{\rho}_3^2. \quad (6)$$

It is not hard to verify that with these rules of multiplication $\hat{\rho}_2^{(1-3)}$ go into one class, and $\delta\hat{\rho}_2^{(1-3)}$ into another class, and in addition $\hat{\rho}_3^1$ and $\delta\hat{\rho}_3^2$ form one class and $\delta\hat{\rho}_3^1$ and $\hat{\rho}_3^2$ another. For the cases (II) – (IV) this would not occur, and therefore they are not realized.

The fulfillment of the conditions mentioned above is necessary. In fact: $\delta\hat{\rho}_3^2$ and $\hat{\rho}_3^1$ must go into one class, since there is an element that changes the direction of the 3rd order screw axis into its opposite; $\hat{\rho}_2^{(j)}$ and $\delta\hat{\rho}_2^{(i)}$ cannot go into a single class, because there is no element in the group that takes one 2nd order axis over into the other and at the same time changes the direction of the axis into its opposite. It is well known that the elements $\{\hat{\rho}_l|\bar{\tau}_l\}$ and $\{\hat{\rho}_m|\bar{\tau}_m\}$ belong to one class, if there is an element $\{\hat{\rho}_k|\bar{\tau}_k\}$ such that the relation

$$\{\hat{\rho}_k|\bar{\tau}_k\}\cdot\{\hat{\rho}_l|\bar{\tau}_l\} = \{\hat{\rho}_m|\bar{\tau}_m\}\cdot\{\hat{\rho}_k|\bar{\tau}_k\}. \quad (7)$$

holds.

Recalling that our operators act on the coordinates as before, we get the following limitations on $\bar{\tau}_m$ and $\bar{\tau}_l$:

$$\bar{\tau}_k + \hat{\rho}_k\bar{\tau}_l = \bar{\tau}_m + \hat{\rho}_m\bar{\tau}_k. \quad (8)$$

Taking, for example, $\hat{\rho}_l = \hat{\rho}_3^1$, $\hat{\rho}_m = \delta\hat{\rho}_3^2$ and noting that the action of δ on $\bar{\tau}$ is equivalent to multiplication by a unit element and that these rotations are conjugate by the use of $\hat{\rho}_2^{(i)}$, we shall have: $\hat{\rho}_2^{(i)}\tau_l = \tau_m$, or $\tau_l = -\bar{\tau}_m$. Thus there go into one class the elements

$$\{\hat{\rho}_3^1|\bar{\tau}_3/3\} \text{ and } \{\varepsilon|-\bar{\tau}_3\}\cdot\{\delta\hat{\rho}_3^2|2\bar{\tau}_3/3\},$$

and into the other class

$$\{\varepsilon|\bar{\tau}_3\}\cdot\{\hat{\rho}_3^1|\tau_3/3\} \text{ and } \{\delta\hat{\rho}_3^2|2\bar{\tau}_3/3\}.$$

Carrying through a similar consideration, we get 12 classes. Knowing the multiplication law of the elements, we find that of the classes, and, using Ref. 19, we find the table of characters (Table 4).

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