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Group-Theoretical Study of the Zeeman Effect of Acceptors in Silicon and Germanium*

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Group-theoretical techniques are used to deduce the selection rules, energy splittings, and *relative intensities* of the Zeeman components of the electric dipole absorption lines $\Gamma_8 \rightarrow \Gamma_6$, $\Gamma_8 \rightarrow \Gamma_7$, and $\Gamma_8 \rightarrow \Gamma_8$ of an acceptor in a group-IV semiconductor. Results are obtained for three different orientations of the magnetic field $\vec{B}$ with respect to the crystal axes: $\vec{B} \parallel [001]$, $\vec{B} \parallel [111]$, and $\vec{B} \parallel [110]$. For a $\Gamma_8 \rightarrow \Gamma_8$ transition the relative intensities for $\vec{B} \parallel [001]$ are expressed in terms of two real parameters, which are essentially ratios of matrix elements of the electric-dipole-moment operator. The relative intensities for $\vec{B} \parallel [111]$ and $\vec{B} \parallel [110]$ depend on energy splittings as well. When terms quadratic in B are important, the relative intensities for $\vec{B} \parallel [110]$ become dependent on B. The results obtained are quite general, being based on symmetry considerations alone. They are applicable to an impurity located at a site of tetrahedral symmetry, provided that the Zeeman splitting of a given level is small in comparison with its distance from the nearest zero-field level. Our treatment proves particularly useful for studying acceptor states in group-IV semiconductors. As an example, we discuss the case of boron impurity in germanium.

I. INTRODUCTION

Several investigators have reported experimental studies of the Zeeman effect in the excitation spectra of single-hole acceptors in germanium. Fisher and Fan have studied the group-II impurities copper and zinc[1] as well as the group-III impurity boron.[2] Shenker, Swiggard, and Moore[3] have presented results for the group-II impurity beryllium. Zwerdling, Button, and Lax[4] have investigated the Zeeman effect of aluminum acceptors in silicon.

Theoretical works on this problem have been mostly devoted to perturbation calculations based on the effective-mass approximation.[5–7] The results of such calculations represent estimates for shallow acceptors only. However, a group-theoretical treatment based solely on symmetry considerations proves capable of yielding valuable information. The symmetry method does not resort to the effective-mass approximation and as such its validity is not restricted to shallow impurities. Results can be expressed in terms of a few parameters which may be adjusted to fit experiment or, in the case of shallow impurities, estimated from the effective-mass theory. The usefulness of this method for studying the Zeeman effect of acceptor states was first pointed out by Kleiner.[8] In this work we present a group-theoretical study of the Zeeman effect in the excitation spectrum of a single-hole acceptor in a group-IV semiconductor. The energy splittings and relative intensities of the Zeeman components are obtained for three crystalline orientations of the magnetic field: $\vec{B} \parallel [001]$, $\vec{B} \parallel [111]$, and $\vec{B} \parallel [110]$. We also include terms quadratic in B in the Zeeman Hamiltonian.

Zakharchenya and Rusanov[9] have presented a group-theoretical analysis of the Zeeman effect in the optical spectra of cubic crystals. A substitutional impurity in a group-IV semiconductor is located at a site of tetrahedral (T_d) symmetry. Many of the results of Zakharchenya and Rusanov for the O_h group can be simply transcribed to the case of T_d symmetry. The excitation spectrum of a single-hole acceptor involves the electric dipole transitions $\Gamma_8 \rightarrow \Gamma_6$, $\Gamma_8 \rightarrow \Gamma_7$, and $\Gamma_8 \rightarrow \Gamma_8$.[10] However, the relative intensities of the Zeeman components of a $\Gamma_8 \rightarrow \Gamma_8$ transition have not been treated in Ref. 9, while those for $\Gamma_8 \rightarrow \Gamma_6$ and $\Gamma_8 \rightarrow \Gamma_7$ have been presented only for $\vec{B} \parallel [001]$. Recently Johnston, Marlow, and Runciman[11] have considered the relative intensities for $\Gamma_8 \rightarrow \Gamma_6$ and $\Gamma_8 \rightarrow \Gamma_7$ transitions for $\vec{B} \parallel [111]$ as well as $\vec{B} \parallel [110]$. Unfortunately, contrary to the claim of the authors, their results lack generality. In fact, they are valid only for the particularly simple case of a $j=\frac{3}{2}$-like Γ_8 level (i.e., a Γ_8 level derived from $\Gamma_5 \times D^{(1/2)}$). In general, such relative intensities depend on the energy splitting of the Γ_8 level, as will be shown in the present work. We obtain the most general results for the $\Gamma_8 \rightarrow \Gamma_6$, $\Gamma_8 \rightarrow \Gamma_7$, and $\Gamma_8 \rightarrow \Gamma_8$ electric dipole transitions.

Our procedure for calculating the relative intensities of the Zeeman components is based on the method developed by Rodriguez, Fisher, and Barra[12] for stress-induced components. However, in contrast to Ref. 12, we shall not make use of any special forms for the unperturbed wave functions. The present approach ensures the complete generality of the results. In Sec. II we diagonalize the matrix representation of the Zeeman Hamiltonian in the subspace of a zero-field level of each symmetry type. The zeroth-order approximations to the wave functions of the Zeeman sublevels are obtained, as well as their symmetry classification. These results are used to deduce the selection rules (Sec. III) and the relative intensities (Sec. IV) of the Zeeman components. Section V is devoted to an application of the theory to the case of boron acceptors in germanium.

II. SPLITTING OF IMPURITY LEVELS IN A MAGNETIC FIELD

A substitutional impurity in a group-IV semiconductor finds itself at a site of tetrahedral symmetry. It is assumed that the foreign atom does not introduce any distortions that might alter this symmetry. Then an acceptor (donor) level may be visualized as a bound state of a hole (electron) of spin $\frac{1}{2}$ moving in a potential of tetrahedral symmetry (T_d). Such energy levels can be classified according to the double-valued representations of the double group $\overline{T}_d$. The characters of the single-valued and double-valued representations of $\overline{T}_d$ are shown in Tables I and II, respectively. The impurity levels of the type Γ_6 or Γ_7 are doubly degenerate, while those of the type Γ_8 have a fourfold degeneracy. The ground state of a shallow acceptor in silicon or germanium is known to be a Γ_8 level.[13]

The application of a magnetic field $\vec{B}$ introduces new terms in the Hamiltonian of the particle (hole or electron). These additional terms constitute the Zeeman Hamiltonian

$$H_z = \mp \mu_B(\vec{l} + 2\vec{s}) \cdot \vec{B} \mp \tfrac{1}{2} m \mu_B^2 [r^2 B^2 - (\vec{r} \cdot \vec{B})^2] , \quad (1)$$

where μ_B is the Bohr magneton, m the free-electron mass, $\vec{r}$ the position operator of the particle, $\vec{l}$ and $\vec{s}$ the orbital and the spin angular momenta in units of $\hbar$, respectively. The upper (lower) signs hold for a hole (electron).

The symmetry group of H_z is $\overline{C}_{\infty h}$, with the direction of the field as the symmetry axis. The magnetic field thus reduces the symmetry of the total Hamiltonian to the common subgroup of $\overline{T}_d$ and the particular $\overline{C}_{\infty h}$. For an arbitrary orientation of $\vec{B}$, this is the trivial group $\overline{C}_1$. For the crystalline orientations [001], [111], and [110] the symmetry groups are $\overline{S}_4$, $\overline{C}_3$, and $\overline{C}_{1h}$, respectively. The irreducible representations of these groups are presented in Tables III–V. The symmetry group of the system in the presence of a magnetic field is necessarily a subgroup of the Abelian group $\overline{C}_{\infty h}$, and so all its irreducible representations are one dimensional. Thus, the magnetic field removes the degeneracies of the impurity levels.

TABLE I. Character table and basis functions for the point group T_d.

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$	Basis functions
Γ_1	1	1	1	1	1	$x^2+y^2+z^2$
Γ_2	1	1	1	−1	−1	$x^4(y^2-z^2)+y^4(z^2-x^2)+z^4(x^2-y^2)$
Γ_3	2	−1	2	0	0	$\{2z^2-x^2-y^2, \sqrt{3}(x^2-y^2)\}$
Γ_4	3	0	−1	1	−1	$\{x(y^2-z^2), y(z^2-x^2), z(x^2-y^2)\}$
Γ_5	3	0	−1	−1	1	$\{x, y, z\}$

TABLE II. Character table for the double-valued representations of $\overline{T}_d$.

$\overline{T}_d$	E	$\overline{E}$	$8C_3$	$8\overline{C}_3$	$3C_2, 3\overline{C}_2$	$3(S_4, S_4^{-1})$	$3(\overline{S}_4, \overline{S}_4^{-1})$	$6\sigma_d, 6\overline{\sigma}_d$
Γ_6	2	−2	1	−1	0	$-\sqrt{2}$	$\sqrt{2}$	0
Γ_7	2	−2	1	−1	0	$\sqrt{2}$	$-\sqrt{2}$	0
Γ_8	4	−4	−1	1	0	0	0	0

To investigate how a given impurity level will split when a field is applied, we employ the first-order degenerate perturbation theory. It is assumed that the unperturbed levels are so well separated and the field so small that the splitting of each level can be treated independently. Our task then is to obtain the matrix representation of H_z in the subspace of the level in question and diagonalize it.

In order to deduce the most general form of the matrix in the subspace of a given irreducible representation of $\overline{T}_d$, we make use of the fact that H_z must retain its scalar form (Γ_1) under the coordinate transformations of the tetrahedral group. For this purpose it is convenient to classify the coefficients of various operators appearing on the right-hand side of Eq. (1) according to their transformation properties under T_d:

$$\begin{aligned} &B_x, B_y, B_z \text{ belong to } \Gamma_4 ; \\ &B^2 = B_x^2 + B_y^2 + B_z^2 \text{ belongs to } \Gamma_1 ; \\ &2B_z^2 - B_x^2 - B_y^2 , \ \sqrt{3}\,(B_x^2 - B_y^2) \text{ belong to } \Gamma_3 ; \\ &B_yB_z , \ B_zB_x, \ B_xB_y \text{ belong to } \Gamma_5 . \end{aligned} \quad (2)$$

It is important to note that the components of $\vec{B}$ are referred to the cubic axes (x, y, z) of the crys-

TABLE III. Character table for the double group $\overline{S}_4$ ($\omega = e^{i\pi/4}$).

$\overline{S}_4$	E	$\overline{E}$	C_2	$\overline{C}_2$	S_4	S_4^{-1}	$\overline{S}_4$	$\overline{S}_4^{-1}$
Γ_1	1	1	1	1	1	1	1	1
Γ_2	1	1	1	1	−1	−1	−1	−1
Γ_3	1	1	−1	−1	$-i$	i	$-i$	i
Γ_4	1	1	−1	−1	i	$-i$	i	$-i$
Γ_5	1	−1	$-i$	i	$-\omega$	ω^3	ω	$-\omega^3$
Γ_6	1	−1	i	$-i$	ω^3	$-\omega$	$-\omega^3$	ω
Γ_7	1	−1	$-i$	i	ω	$-\omega^3$	$-\omega$	ω^3
Γ_8	1	−1	i	$-i$	$-\omega^3$	ω	ω^3	$-\omega$

TABLE IV. Character table for the double group $\bar{C}_3$ ($\omega = e^{i\pi/3}$).

$\bar{C}_3$	E	$\bar{E}$	C_3	C_3^{-1}	$\bar{C}_3$	$\bar{C}_3^{-1}$
Γ_1	1	1	1	1	1	1
Γ_2	1	1	$-\omega$	ω^2	$-\omega$	ω^2
Γ_3	1	1	ω^2	$-\omega$	ω^2	$-\omega$
Γ_4	1	-1	$-\omega^2$	ω	ω^2	$-\omega$
Γ_5	1	-1	ω	$-\omega^2$.	$-\omega$	ω^2
Γ_6	1	-1	-1	-1	1	1

tal.

For a Γ_6 or Γ_7 level, the subspace is two dimensional. The representation of H_Z, being a 2×2 matrix, must be a linear combination of the unit matrix and the $j=\frac{1}{2}$ angular momentum matrices j_x, j_y, j_z. Under T_d the unit matrix transforms as Γ_1, while j_x, j_y, j_z transform as Γ_4. A comparison with (2) then leads to the most general form of the Hamiltonian matrix:

$$H_Z^{(i)} = \mu_B g^{(i)} (\vec{B}\cdot\vec{j}) + q^{(i)} B^2 , \tag{3}$$

where $i=6$, 7 corresponds to Γ_6, Γ_7. The parameters $g^{(i)}$ and $q^{(i)}$ depend on the unperturbed wave functions of the particular impurity level in question. For the usual phase convention for the eigenfunctions of j_z, we have

$$j_x = \frac{1}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad j_y = \frac{1}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad j_z = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{4}$$

The spinors

$$\varphi^{(6)}_{+1/2} = f_0(r)\,|\,\alpha\rangle , \quad \varphi^{(6)}_{-1/2} = f_0(r)\,|\,\beta\rangle \tag{5}$$

form a basis for the representation (4) [$f_0(r)$ is a normalized s function]. An alternative set of basis functions for (4) is given by

$$\varphi^{(7)}_{+1/2} = (1/\sqrt{3})\,[(X+iY)\,|\,\beta\rangle + Z\,|\,\alpha\rangle],$$
$$\varphi^{(7)}_{-1/2} = (1/\sqrt{3})\,[(X-iY)\,|\,\alpha\rangle - Z\,|\,\beta\rangle] , \tag{6}$$

where $X = xf(r)$, $Y = yf(r)$, $Z = zf(r)$ are normalized p functions. It is easy to see that the sets $\{\varphi^{(6)}_\mu\}$ and $\{\varphi^{(7)}_\mu\}$, respectively, generate the representations Γ_6 and Γ_7 of $\bar{T}_d$.

The matrix for the Zeeman Hamiltonian in the four-dimensional subspace of a Γ_8 level is necessarily a linear combination of 16 linearly independent 4×4 matrices. Starting with the $j=\frac{3}{2}$ angular momentum matrices J_x, J_y, J_z, Luttinger[14] has constructed a set of 16 linearly independent matrices, having definite transformation properties under $\bar{T}_d$:

$$\begin{aligned}
&\Gamma_1:\ 1 ;\\
&\Gamma_2:\ J_xJ_yJ_z + J_zJ_yJ_x ;\\
&\Gamma_3:\ 2J_z^2 - J_x^2 - J_y^2 , \quad \sqrt{3}\,(J_x^2 - J_y^2) ;\\
&\Gamma_4:\ J_x , J_y , J_z , J_x^3 , J_y^3 , J_z^3 ;\\
&\Gamma_5:\ \{J_y ; J_z\} \equiv U_x , \quad \{J_z ; J_x\} \equiv U_y , \quad \{J_x ; J_y\} \equiv U_z ,\\
&\qquad \{J_x ; (J_y^2 - J_z^2)\} \equiv V_x , \quad \{J_y ; (J_z^2 - J_x^2)\} \equiv V_y ,\\
&\qquad \{J_z ; (J_x^2 - J_y^2)\} \equiv V_z ,
\end{aligned} \tag{7}$$

where $\{P;\ Q\} = \frac{1}{2}(PQ+QP)$.

Combining (7) with (2) we obtain the tetrahedrally invariant forms

$$\begin{aligned}
&B^2 ,\\
&(2B_z^2 - B_x^2 - B_y^2)(2J_z^2 - J_x^2 - J_y^2)\\
&\qquad + \sqrt{3}\,(B_x^2 - B_y^2)\sqrt{3}\,(J_x^2 - J_y^2) ,\\
&B_xJ_x + B_yJ_y + B_zJ_z ,\\
&B_xJ_x^3 + B_yJ_y^3 + B_zJ_z^3 ,\\
&(B_yB_z)U_x + (B_zB_x)U_y + (B_xB_y)U_z ,\\
&(B_yB_z)V_x + (B_zB_x)V_y + (B_xB_y)V_z .
\end{aligned}$$

However, the last term changes sign under time reversal and is, therefore, incompatible with the quadratic term in the Zeeman Hamiltonian. So the most general form of the Hamiltonian matrix for a Γ_8 level can be expressed as

$$H_Z^{(8)} = \mu_B g_1'(\vec{B}\cdot\vec{J}) + \mu_B g_2'(B_xJ_x^3 + B_yJ_y^3 + B_zJ_z^3) + q_1B^2 + q_2(\vec{B}\cdot\vec{J})^2 + q_3(B_x^2J_x^2 + B_y^2J_y^2 + B_z^2J_z^2) , \tag{8}$$

where the parameters g_1', g_2', q_1, q_2, q_3 depend on the unperturbed wave functions of the level. We shall use the following representation[14] of the angular momentum matrices:

$$J_x = \frac{i}{2}\begin{bmatrix} 0 & \sqrt{3} & 0 & 0 \\ -\sqrt{3} & 0 & 2 & 0 \\ 0 & -2 & 0 & \sqrt{3} \\ 0 & 0 & -\sqrt{3} & 0 \end{bmatrix}, \quad J_y = \frac{1}{2}\begin{bmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{bmatrix}, \quad J_z = \frac{1}{2}\begin{bmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -3 \end{bmatrix}. \tag{9}$$

The functions

$$\varphi^{(8)}_{+3/2} = (1/\sqrt{2})\,(X+iY)\,|\,\alpha\rangle ,$$

$$\varphi^{(8)}_{+1/2} = (i/\sqrt{6})\,[(X+iY)\,|\,\beta\rangle - 2Z\,|\,\alpha\rangle] ,$$
$$\varphi^{(8)}_{-1/2} = (1/\sqrt{6})\,[(X-iY)\,|\,\alpha\rangle + 2Z\,|\,\beta\rangle] ,$$

TABLE V. Character table for the double group $\bar{C}_{1h}$.

$\bar{C}_{1h}$	E	$\bar{E}$	σ_h	$\bar{\sigma}_h$
Γ_1	1	1	1	1
Γ_2	1	1	-1	-1
Γ_3	1	-1	$-i$	i
Γ_4	1	-1	i	$-i$

$$\varphi^{(8)}_{-3/2} = (i/\sqrt{2})\,(X - iY)\,|\,\beta\rangle\,, \tag{10}$$

form a basis for the representation (9). The set $\{\varphi^{(8)}_\mu\}$ also generates the irreducible representation Γ_8 of $\bar{T}_d$.

So far nothing has been said about the unperturbed wave functions of an impurity level, except that they belong to a particular irreducible representation Γ_i ($i = 6$, 7, or 8) of the group $\bar{T}_d$. Of course, they are the basis functions of the matrix $H^{(i)}_Z$ representing the Zeeman Hamiltonian. The following labeling scheme suggests itself: The unperturbed functions for a Γ_i level are denoted by $\psi^{(i)}_\mu$, where $\mu = +\frac{1}{2}$, $-\frac{1}{2}$ for $i = 6$ or 7 and $\mu = +\frac{3}{2}$, $+\frac{1}{2}$, $-\frac{1}{2}$, $-\frac{3}{2}$ for $i = 8$. A closer examination reveals that this labeling scheme has a definite meaning. By choosing the explicit forms of the angular momentum matrices, Eqs. (4) and (9), we have also chosen the matrices representing various operations of $\bar{T}_d$ for each of the irreducible representations Γ_6, Γ_7, and Γ_8. Thus we have implicitly chosen the functions $\{\psi^{(i)}_\mu\}$ in such a way that the matrix generated by them for a given operation of $\bar{T}_d$ is the same as that generated by the angular momentum eigenfunctions $\{\varphi^{(i)}_\mu\}$. In other words, $\psi^{(i)}_\mu$ and $\varphi^{(i)}_\mu$ belong to the same row of the irreducible representation Γ_i. (This is explicitly demonstrated in Appendix A.) Clearly, this particular choice of the transformation properties of $\psi^{(i)}_\mu$ does not imply any loss of generality. The labeling scheme turns out to be particularly convenient for classifying the Zeeman sublevels according to the irreducible representations of the appropriate symmetry group ($\bar{S}_4$, $\bar{C}_3$, or $\bar{C}_{1h}$). The following discussions will clarify this point.

Let the orientation of $\vec{B}$ be given by the polar angle β and the azimuthal angle α. That is, $\vec{B} = B\hat{n}$ with

$$n_x = \sin\beta\cos\alpha\,, \quad n_y = \sin\beta\sin\alpha\,, \quad n_z = \cos\beta\,.$$

Now consider a rotation of the functions $\varphi^{(i)}_\mu$ by the Euler angles (α, β, 0). The rotated functions are given by

$$\varphi'^{(6),(7)}_\mu = \sum_{\mu'} D^{(1/2)}_{\mu'\mu}(\alpha, \beta, 0)\varphi^{(6),(7)}_{\mu'}\,, \tag{11a}$$

$$\varphi'^{(8)}_\mu = \sum_{\mu'} D^{(3/2)}_{\mu'\mu}(\alpha, \beta, 0)\varphi^{(8)}_{\mu'}\,. \tag{11b}$$

Here,

$$D^{(1/2)}_{\mu'\mu}(\alpha, \beta, 0) = \langle\varphi^{(6),(7)}_{\mu'}\,|\,e^{-i\alpha\hat{J}_z}\,e^{-i\beta\hat{J}_y}\,|\,\varphi^{(6),(7)}_\mu\rangle \tag{12a}$$

and

$$D^{(3/2)}_{\mu'\mu}(\alpha, \beta, 0) = \langle\varphi^{(8)}_{\mu'}\,|\,e^{-i\alpha\hat{J}_z}\,e^{-i\beta\hat{J}_y}\,|\,\varphi^{(8)}_\mu\rangle\,, \tag{12b}$$

where $\hat{J}_z$ and $\hat{J}_y$ are angular momentum operators. The explicit forms of the matrices $D^{(1/2)}(\alpha, \beta, 0)$ and $D^{(3/2)}(\alpha, \beta, 0)$ are obtained in Appendix B. Because of the unusual phase convention for $\{\varphi^{(8)}_\mu\}$ [Eq. (10)], $D^{(3/2)}(\alpha, \beta, 0)$ turns out to be different from the $j = \frac{3}{2}$ rotation matrix available in the literature. Clearly,

$$(\hat{n}\cdot\vec{J})\,\varphi'^{(i)}_\mu = \mu\varphi'^{(i)}_\mu\,. \tag{13}$$

Let us now define

$$\psi'^{(6),(7)}_\mu = \sum_{\mu'} D^{(1/2)}_{\mu'\mu}(\alpha, \beta, 0)\,\psi^{(6),(7)}_{\mu'}\,, \tag{14a}$$

$$\psi'^{(8)}_\mu = \sum_{\mu'} D^{(3/2)}_{\mu'\mu}(\alpha, \beta, 0)\psi^{(8)}_{\mu'}\,. \tag{14b}$$

It should be noted that $\psi'^{(i)}_\mu$ is not necessarily the rotated version of $\psi^{(i)}_\mu$. Nevertheless, $\{\psi'^{(i)}_\mu\}$ transform like $\{\varphi'^{(i)}_\mu\}$ under the operations of $\bar{T}_d$. This is very convenient. $\varphi'^{(i)}_\mu$, being an eigenfunction of $\hat{n}\cdot\vec{J}$, has simple transformation properties under symmetry operations about $\vec{B}$. In fact, $\varphi'^{(i)}_\mu$ belongs to a definite double-valued representation of the appropriate symmetry group ($\bar{S}_4$, $\bar{C}_3$, or $\bar{C}_{1h}$), and so does $\psi'^{(i)}_\mu$. Thus, in the new basis $\{\psi'^{(i)}_\mu\}$ the Hamiltonian matrix $H'^{(i)}_Z$ will be composed of blocks belonging to distinct irreducible representations. This transformation necessarily accomplishes the diagonalization of $H^{(6),(7)}_Z$ and simplifies that of $H^{(8)}_Z$. At the same time one obtains the symmetry classification of the Zeeman sublevels. Let us now proceed to discuss each orientation of $\vec{B}$ separately.

A. Magnetic Field along [001]

The symmetry group of the system is $\bar{S}_4$, with four double-valued representations: Γ_5, Γ_6, Γ_7, and Γ_8 (Table III).

We have $B_x = B_y = 0$, $B_z = B$; the Zeeman Hamiltonian $H^{(i)}_Z$ [Eqs. (3) and (8)] referred to the basis $\{\psi^{(i)}_\mu\}$ is already diagonal. Splittings of the impurity levels are described below.

1. Splitting of a Γ_6 Level

The symmetry decomposition is $\Gamma_6(\bar{T}_d) = \Gamma_5 + \Gamma_6$. The energies of the Zeeman sublevels are given by

$$E^{(6)}_\mu = \mu_B g^{(6)} B\mu + q^{(6)} B^2\,, \tag{15}$$

where $\mu = +\frac{1}{2}$, $-\frac{1}{2}$. The wave function $\psi^{(6)}_{+1/2}$ belongs to Γ_5, as $\varphi^{(6)}_{+1/2}$ belongs to Γ_5. Similarly $\psi^{(6)}_{-1/2}$ belongs to Γ_6 of $\bar{S}_4$. Thus, the symmetry classification of the Zeeman sublevels can be listed as

$$+\tfrac{1}{2}(\Gamma_5)\,, \quad -\tfrac{1}{2}(\Gamma_6)\,. \tag{16}$$

2. Splitting of a Γ_7 Level

The symmetry decomposition is $\Gamma_7(\overline{T}_d)=\Gamma_7+\Gamma_8$. The energies of the Zeeman sublevels are

$$E_\mu^{(7)}=\mu_B g^{(7)}B\mu+q^{(7)}B^2, \tag{17}$$

where $\mu=+\frac{1}{2},\ -\frac{1}{2}$. The wave functions $\psi_{+1/2}^{(7)}$ and $\psi_{-1/2}^{(7)}$ have the symmetry assignments

$$+\tfrac{1}{2}(\Gamma_7)\ ,\quad -\tfrac{1}{2}(\Gamma_8)\ . \tag{18}$$

3. Splitting of a Γ_8 Level

We observe that $\Gamma_8(\overline{T}_d)=\Gamma_5+\Gamma_6+\Gamma_7+\Gamma_8$ describes the splitting. The Zeeman sublevels are

$$E_\mu^{(8)}=\mu_B(g_1'\mu+g_2'\mu^3)B+[q_1+(q_2+q_3)\mu^2]B^2\ , \tag{19}$$

where $\mu=+\frac{3}{2},\ +\frac{1}{2},\ -\frac{1}{2},\ -\frac{3}{2}$. The symmetry classification of the wave functions $\{\psi_\mu^{(8)}\}$ is given by

$$+\tfrac{3}{2}(\Gamma_6)\ ,\ +\tfrac{1}{2}(\Gamma_7)\ ,\quad -\tfrac{1}{2}(\Gamma_8)\ ,\quad -\tfrac{3}{2}(\Gamma_5)\ . \tag{20}$$

B. Magnetic Field along [111]

The symmetry group of the system is $\overline{C}_3$, with the double-valued representations Γ_4, Γ_5, and Γ_6 (Table IV).

Here $B_x=B_y=B_z=(1/\sqrt{3})B$, that is, $\alpha=\frac{1}{4}\pi$ and $\beta=\cos^{-1}(1/\sqrt{3})$. We shall use the notation

$$D^{(j)}[111]\equiv D^{(j)}[\tfrac{1}{4}\pi,\ \cos^{-1}(1/\sqrt{3}),\ 0]\ , \tag{21}$$

where $j=\frac{1}{2},\ \frac{3}{2}$.

1. Splitting of a Γ_6 Level

The symmetry decomposition is $\Gamma_6(\overline{T}_d)=\Gamma_4+\Gamma_5$. The functions

$$\psi_\mu'^{(6)}=\sum_{\mu'}D_{\mu'\mu}^{(1/2)}[111]\psi_{\mu'}^{(6)} \tag{22}$$

are such that $\psi_{+1/2}'^{(6)}$ belongs to Γ_4, while $\psi_{-1/2}'^{(6)}$ belongs to Γ_5. This follows from the transformation properties of the rotated angular momentum eigenfunctions $\varphi_{+1/2}'^{(6)}$ and $\varphi_{-1/2}'^{(6)}$, which are easily seen to belong to Γ_4 and Γ_5, respectively. The Zeeman Hamiltonian referred to the transformed basis $\{\psi_{\mu\mu}'^{(6)}\}$ is

$$H_Z'^{(6)}=D^{(1/2)\dagger}[111]H_Z^{(6)}D^{(1/2)}[111]\ .$$

As $D^{(1/2)\dagger}(\hat{n}\cdot\vec{j})D^{(1/2)}=j_z$, we find that

$$H_Z'^{(6)}=\mu_B g^{(6)}Bj_z+q^{(6)}B^2$$

is diagonal, as expected. The energies of the Zeeman sublevels are again given by Eq. (15). The wave functions $\psi_{+1/2}'^{(6)}$ and $\psi_{-1/2}'^{(6)}$ have the symmetry classification

$$+\tfrac{1}{2}(\Gamma_4),\quad -\tfrac{1}{2}(\Gamma_5)\ . \tag{23}$$

2. Splitting of a Γ_7 Level

The symmetry decomposition is $\Gamma_7(\overline{T}_d)=\Gamma_4+\Gamma_5$. The transformation

$$\psi_\mu'^{(7)}=\sum_{\mu'}D_{\mu'\mu}^{(1/2)}[111]\psi_{\mu'}^{(7)} \tag{24}$$

diagonalizes the Zeeman Hamiltonian $H_Z^{(7)}$. The energies of the sublevels are given by Eq. (17). The wave functions $\psi_{+1/2}'^{(7)}$ and $\psi_{-1/2}'^{(7)}$ have the symmetry assignment

$$+\tfrac{1}{2}(\Gamma_4),\quad -\tfrac{1}{2}(\Gamma_5)\ . \tag{25}$$

3. Splitting of a Γ_8 Level

We have $\Gamma_8(\overline{T}_d)=\Gamma_4+\Gamma_5+2\Gamma_6$. The functions

$$\psi_\mu'^{(8)}=\sum_{\mu'}D_{\mu'\mu}^{(3/2)}[111]\psi_{\mu'}^{(8)} \tag{26}$$

are such that $\psi_{+1/2}'^{(8)}$ belongs to Γ_4, $\psi_{-1/2}'^{(8)}$ belongs to Γ_5, while both $\psi_{+3/2}'^{(8)}$ and $\psi_{-3/2}'^{(8)}$ belong to Γ_6. Thus the Zeeman Hamiltonian may mix only $\psi_{+3/2}'^{(8)}$ and $\psi_{-3/2}'^{(8)}$. Let us now derive the explicit form of H_Z in the transformed basis $\{\psi_\mu'^{(8)}\}$. We first rewrite Eq. (8) as

$$H_Z^{(8)}=\mu_B g_2'B\{p(\hat{n}\cdot\vec{J})+(n_xJ_x^3+n_yJ_y^3+n_zJ_z^3)+[s_1+s_2(\hat{n}\cdot\vec{J})^2+s_3(n_x^2J_x^2+n_y^2J_y^2+n_z^2J_z^2)]B\}\ , \tag{27}$$

where

$$p\equiv(g_1'/g_2')\ ,\quad s_k\equiv q_k/\mu_B g_2'\qquad (k=1,2,3)\ . \tag{28}$$

For $\vec{B}\parallel[111]$, Eq. (27) yields

$$H_Z^{(8)}=\mu_B g_2'B\{p(\hat{n}\cdot\vec{J})+(1/\sqrt{3})(J_x^3+J_y^3+J_z^3)+[s_1+s_2(\hat{n}\cdot\vec{J})^2+\tfrac{5}{4}s_3]B\}\ . \tag{29}$$

In the basis $\{\psi_\mu'^{(8)}\}$ we obtain

$$H_Z'^{(8)}=D^{(3/2)\dagger}[111]H_Z^{(8)}D^{(3/2)}[111]=\mu_B g_2'B[pJ_z+(1/\sqrt{3})(J_x'^3+J_y'^3+J_z'^3)+(s_1+s_2J_z^2+\tfrac{5}{4}s_3)B]\ , \tag{30}$$

where

$$\vec{J}'=D^{(3/2)\dagger}[111]\vec{J}D^{(3/2)}[111]\ .$$

Explicitly,

$$J_x'=(1/\sqrt{6})J_x-(1/\sqrt{2})J_y+(1/\sqrt{3})J_z\ , \tag{31a}$$

$$J_y'=(1/\sqrt{6})J_x+(1/\sqrt{2})J_y+(1/\sqrt{3})J_z\ , \tag{31b}$$

$$J_z'=-(\sqrt{2}/\sqrt{3})J_x+(1/\sqrt{3})J_z\ . \tag{31c}$$

We obtain

$$\frac{1}{\sqrt{3}}(J_x'^3+J_y'^3+J_z'^3)=\begin{bmatrix}\frac{23}{8} & 0 & 0 & (1/\sqrt{2})i\\ 0 & \frac{13}{8} & 0 & 0\\ 0 & 0 & -\frac{13}{8} & 0\\ -(1/\sqrt{2})i & 0 & 0 & -\frac{23}{8}\end{bmatrix}\ . \tag{32}$$

Thus

$$H_Z'^{(8)} = \mu_B g_2' B \begin{bmatrix} (\frac{3}{2}p + \frac{23}{8}) + \sigma B & 0 & 0 & (1/\sqrt{2})i \\ 0 & (\frac{1}{2}p + \frac{13}{8}) + \sigma' B & 0 & 0 \\ 0 & 0 & -(\frac{1}{2}p + \frac{13}{8}) + \sigma' B & 0 \\ -(1/\sqrt{2})i & 0 & 0 & -(\frac{3}{2}p + \frac{23}{8}) + \sigma B \end{bmatrix}, \quad (33)$$

where $\sigma \equiv s_1 + \frac{9}{4}s_2 + \frac{5}{4}s_3$ and $\sigma' \equiv s_1 + \frac{1}{4}s_2 + \frac{5}{4}s_3$. It should be noted that the matrix $H_Z'^{(8)}$ has the expected form: The only nonzero off-diagonal elements are those between $\psi'^{(8)}_{+3/2}$ and $\psi'^{(8)}_{-3/2}$. The diagonalization of $H_Z'^{(8)}$ is accomplished by the unitary transformation

$$C(\gamma) = \begin{bmatrix} \frac{1}{(1+\gamma^2)^{1/2}} & 0 & 0 & \frac{i\gamma}{(1+\gamma^2)^{1/2}} \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \frac{i\gamma}{(1+\gamma^2)^{1/2}} & 0 & 0 & \frac{1}{(1+\gamma^2)^{1/2}} \end{bmatrix}, \quad (34)$$

where

$$\gamma = \sqrt{2}\ \{(\tfrac{3}{2}p + \tfrac{23}{8}) - [(\tfrac{3}{2}p + \tfrac{23}{8})^2 + \tfrac{1}{2}]^{1/2}\} . \quad (35)$$

The energies of the Zeeman sublevels are

$$E^{(8)}_{\pm 3/2} = \{\pm [(\tfrac{3}{2}p + \tfrac{23}{8})^2 + \tfrac{1}{2}]^{1/2} + (s_1 + \tfrac{9}{4}s_2 + \tfrac{5}{4}s_3)B\}\ \mu_B g_2' B , \quad (36a)$$

$$E^{(8)}_{\pm 1/2} = [\pm (\tfrac{1}{2}p + \tfrac{13}{8}) + (s_1 + \tfrac{1}{4}s_2 + \tfrac{5}{4}s_3)B]\ \mu_B g_2' B . \quad (36b)$$

The wave functions are given by

$$\Psi^{(8)}_\mu = \sum_{\mu'} C_{\mu'\mu}(\gamma)\psi'^{(8)}_{\mu'} . \quad (37)$$

Equation (37) can be rewritten as

$$\Psi^{(8)}_\mu = \sum_{\mu'} S_{\mu'\mu}(\gamma)\psi^{(8)}_{\mu'} , \quad (38)$$

where

$$S(\gamma) = D^{(3/2)}[111]C(\gamma) . \quad (39)$$

The symmetry assignments of the Zeeman sublevels are, clearly,

$$+\tfrac{3}{2}(\Gamma_6) , \quad +\tfrac{1}{2}(\Gamma_4) , \quad -\tfrac{1}{2}(\Gamma_5) , \quad -\tfrac{3}{2}(\Gamma_6) . \quad (40)$$

C. Magnetic Field along [110]

The symmetry group of the system is $\overline{C}_{1h}$, with two double-valued representations: Γ_3 and Γ_4 (Table V).

Now $B_x = B_y = (1/\sqrt{2})B$, $B_z = 0$; that is, $\alpha = \frac{1}{4}\pi$ and $\beta = \frac{1}{2}\pi$. The relevant rotation matrices are

$$D^{(j)}[110] \equiv D^{(j)}(\tfrac{1}{4}\pi, \tfrac{1}{2}\pi, 0) , \quad (41)$$

where $j = \frac{1}{2}, \frac{3}{2}$.

1. Splitting of a Γ_6 Level

The symmetry decomposition is $\Gamma_6(\overline{T}_d) = \Gamma_3 + \Gamma_4$. Let

$$\psi'^{(6)}_\mu = \sum_{\mu'} D^{(1/2)}_{\mu'\mu}[110]\psi^{(6)}_{\mu'} . \quad (42)$$

The Zeeman Hamiltonian is diagonal in the basis $\{\psi'^{(6)}_\mu\}$. $\psi'^{(6)}_{+1/2}$ belongs to Γ_3, and $\psi'^{(6)}_{-1/2}$ belongs to Γ_4. The energies of the Zeeman sublevels are again given by Eq. (15). The symmetry classification is

$$+\tfrac{1}{2}(\Gamma_3) , \quad -\tfrac{1}{2}(\Gamma_4) . \quad (43)$$

2. Splitting of a Γ_7 Level

We note that $\Gamma_7(\overline{T}_d) = \Gamma_3 + \Gamma_4$. The transformation of basis

$$\psi'^{(7)}_\mu = \sum_{\mu'} D^{(1/2)}_{\mu'\mu}[110]\psi^{(7)}_{\mu'} \quad (44)$$

diagonalizes the Zeeman Hamiltonian. $\psi'^{(7)}_{+1/2}$ belongs to Γ_4, while $\psi'^{(7)}_{-1/2}$ belongs to Γ_3. The energies of the Zeeman sublevels are given by Eq. (17). The symmetry assignments are

$$+\tfrac{1}{2}(\Gamma_4) , \quad -\tfrac{1}{2}(\Gamma_3) . \quad (45)$$

3. Splitting of a Γ_8 Level

The symmetry decomposition is $\Gamma_8(\overline{T}_d) = 2\Gamma_3 + 2\Gamma_4$. Let

$$\psi'^{(8)}_\mu = \sum_{\mu'} D^{(3/2)}_{\mu'\mu}[110]\psi^{(8)}_{\mu'} . \quad (46)$$

Then $\psi'^{(8)}_{+3/2}$ and $\psi'^{(8)}_{-1/2}$ belong to Γ_3, while $\psi'^{(8)}_{+1/2}$ and $\psi'^{(8)}_{-3/2}$ belong to Γ_4. The Zeeman Hamiltonian in the basis $\{\psi'^{(8)}_\mu\}$ will, therefore, be composed of two uncoupled 2×2 blocks. Let us now derive this matrix. For $\vec{B} \parallel [110]$, Eq. (27) gives

$$H^{(8)}_Z = \mu_B g_2' B\{p(\hat{n}\cdot\vec{J}) + (1/\sqrt{2})(J_x^3 + J_y^3) + [s_1 + s_2(\hat{n}\cdot\vec{J})^2 + \tfrac{1}{2}s_3(\tfrac{15}{4} - J_z^2)]B\} . \quad (47)$$

In the transformed basis, this becomes

$$H_Z'^{(8)} = D^{(3/2)\dagger}[110]H^{(8)}_Z D^{(3/2)}[110] = \mu_B g_2' B\{pJ_z + (1/\sqrt{2})(J_x'^3 + J_y'^3) + [s_1 + s_2 J_z^2 + \tfrac{1}{2}s_3(\tfrac{15}{4} - J_z'^2)]B\} , \quad (48)$$

where

$$\vec{J}' = D^{(3/2)\dagger}[110]\vec{J} D^{(3/2)}[110] .$$

Explicitly, we have

$$J'_x = -(1/\sqrt{2})(J_y - J_z)\,, \tag{49a}$$

$$J'_y = (1/\sqrt{2})(J_y + J_z)\,, \tag{49b}$$

$$J'_z = -J_x\,. \tag{49c}$$

We obtain

$$(1/\sqrt{2})(J'^3_x + J'^3_y) = \begin{bmatrix} 3 & 0 & \frac{3}{8}\sqrt{3} & 0 \\ 0 & \frac{5}{4} & 0 & -\frac{3}{8}\sqrt{3} \\ \frac{3}{8}\sqrt{3} & 0 & -\frac{5}{4} & 0 \\ 0 & -\frac{3}{8}\sqrt{3} & 0 & -3 \end{bmatrix}. \tag{50}$$

Thus

$$H'^{(8)}_z = \mu_B g'_2 B \begin{bmatrix} (\frac{3}{2}p+3)+\rho B & 0 & \frac{1}{8}\sqrt{3}(3+2s_3B) & 0 \\ 0 & (\frac{1}{2}p+\frac{5}{4})+\rho' B & 0 & -\frac{1}{8}\sqrt{3}(3-2s_3B) \\ \frac{1}{8}\sqrt{3}(3+2s_3B) & 0 & -(\frac{1}{2}p+\frac{5}{4})+\rho' B & 0 \\ 0 & -\frac{1}{8}\sqrt{3}(3-2s_3B) & 0 & -(\frac{3}{2}p+3)+\rho B \end{bmatrix}, \tag{51}$$

where $\rho \equiv s_1 + \frac{9}{4}s_2 + \frac{3}{2}s_3$, and $\rho' \equiv s_1 + \frac{1}{4}s_2 + s_3$. Clearly, this matrix has the expected simple form. The diagonalization of $H'^{(8)}_z$ is accomplished by the unitary transformation

$$C(\delta_1,\delta_2) = \begin{bmatrix} \frac{1}{(1+\delta_1^2)^{1/2}} & 0 & \frac{\delta_1}{(1+\delta_1^2)^{1/2}} & 0 \\ 0 & \frac{1}{(1+\delta_2^2)^{1/2}} & 0 & \frac{-\delta_2}{(1+\delta_2^2)^{1/2}} \\ \frac{-\delta_1}{(1+\delta_1^2)^{1/2}} & 0 & \frac{1}{(1+\delta_1^2)^{1/2}} & 0 \\ 0 & \frac{\delta_2}{(1+\delta_2^2)^{1/2}} & 0 & \frac{1}{(1+\delta_2^2)^{1/2}} \end{bmatrix}. \tag{52}$$

Here

$$\delta_1 = \frac{-\Delta_+ + [\Delta_+^2 - \frac{3}{64}(3+2s_3B)^2]^{1/2}}{\frac{1}{8}\sqrt{3}(3+2s_3B)}, \tag{53a}$$

$$\delta_2 = \frac{-\Delta_- + [\Delta_-^2 - \frac{3}{64}(3-2s_3B)^2]^{1/2}}{\frac{1}{8}\sqrt{3}(3-2s_3B)}, \tag{53b}$$

where

$$\Delta_\pm = \{([p+\tfrac{17}{8}] \pm [s_2 + \tfrac{1}{4}s_3]B)^2 + \tfrac{3}{64}(3 \pm 2s_3B)^2\}^{1/2}\,. \tag{54}$$

It is interesting to note that δ_1 and δ_2 are functions of B. This field dependence of the wave functions is a consequence of the quadratic terms in the Zeeman Hamiltonian. If $s_2 = s_3 = 0$, then $\delta_1 = \delta_2 = \delta$ is field independent:

$$\delta = (8/3\sqrt{3})\{(p+\tfrac{17}{8}) - [(p+\tfrac{17}{8})^2 + \tfrac{27}{64}]^{1/2}\}\,. \tag{55}$$

The energies of the Zeeman sublevels are

$$E^{(8)}_{+3/2} = \mu_B g'_2 B\{\Delta_+ + (\tfrac{1}{2}p+\tfrac{7}{8}) + [s_1 + \tfrac{5}{4}(s_2+s_3)]B\}\,, \tag{56a}$$

$$E^{(8)}_{+1/2} = \mu_B g'_2 B\{\Delta_- - (\tfrac{1}{2}p+\tfrac{7}{8}) + [s_1 + \tfrac{5}{4}(s_2+s_3)]B\}\,, \tag{56b}$$

$$E^{(8)}_{-1/2} = \mu_B g'_2 B\{-\Delta_+ + (\tfrac{1}{2}p+\tfrac{7}{8}) + [s_1 + \tfrac{5}{4}(s_2+s_3)]B\}\,, \tag{56c}$$

$$E^{(8)}_{-3/2} = \mu_B g'_2 B\{-\Delta_- - (\tfrac{1}{2}p+\tfrac{7}{8}) + [s_1 + \tfrac{5}{4}(s_2+s_3)]B\}\,. \tag{56d}$$

The wave functions of the sublevels are

$$\Psi^{(8)}_\mu = \sum_{\mu'} C_{\mu'\mu}(\delta_1,\delta_2)\psi'^{(8)}_{\mu'}\,. \tag{57}$$

This can be written as

$$\Psi^{(8)}_\mu = \sum_{\mu'} S_{\mu'\mu}(\delta_1,\delta_2)\psi^{(8)}_{\mu'}\,, \tag{58}$$

where

$$S(\delta_1,\delta_2) = D^{(3/2)}[110]C(\delta_1,\delta_2)\,. \tag{59}$$

The symmetry assignments of the sublevels are

$$+\tfrac{3}{2}(\Gamma_3)\,,\quad +\tfrac{1}{2}(\Gamma_4)\,,\quad -\tfrac{1}{2}(\Gamma_3)\,,\quad -\tfrac{3}{2}(\Gamma_4)\,. \tag{60}$$

III. SELECTION RULES FOR ELECTRIC-DIPOLE TRANSITIONS

Let us consider the transition of a system from the state $\chi^{(i)}_\mu$ to the state $\chi^{(k)}_{\mu'}$, induced by the electric vector of some incident radiation. The transition probability is proportional to the square of the magnitude of the matrix element

$$M_{\mu'\mu} = \langle \chi^{(k)}_{\mu'} | \hat{\epsilon}\cdot\vec{Q} | \chi^{(i)}_\mu \rangle\,, \tag{61}$$

where $\vec{Q}$ is the electric-dipole-moment operator of the system, and the unit vector $\hat{\epsilon}$ describes the polarization of the incident radiation. The wave functions $\chi^{(i)}_\mu$ and $\chi^{(k)}_{\mu'}$, respectively, belong to the irreducible representations Γ_i and Γ_k of the sym-

TABLE VI. Symmetry classification of the components of $\vec{Q}$ ($\hat{z}' \parallel \vec{B}$).

Group	$Q_{z'}$ ($\epsilon_\parallel$)	$Q_{x'}+iQ_{y'}$ (ϵ_+)	$Q_{x'}-iQ_{y'}$ (ϵ_-)
$\bar{S}_4$	Γ_2	Γ_3	Γ_4
$\bar{C}_3$	Γ_1	Γ_2	Γ_3
$\bar{C}_{1h}$	Γ_2	Γ_1	Γ_1

metry group of the system. Let us suppose that the operator $\hat{\epsilon}\cdot\vec{Q}$ belongs to the irreducible representation Γ_j. Then the well-known orthogonality theorem tells us that $M_{\mu'\mu}$ is zero unless Γ_k is contained in $\Gamma_j \times \Gamma_i$. Thus radiation of polarization $\hat{\epsilon}$ may induce the transition $\mu \rightarrow \mu'$ if and only if $\Gamma_j \times \Gamma_i$ contains Γ_k. This allows us to deduce the selection rules from the character table of the symmetry group.

In the absence of the magnetic field the symmetry of the system under consideration is $\bar{T}_d$. The impurity levels are classified according to the double-valued representations Γ_6, Γ_7, and Γ_8. The components of $\vec{Q}$ belong to the single-valued representation Γ_5. We note that $\Gamma_5\times\Gamma_6=\Gamma_7+\Gamma_8$, $\Gamma_5\times\Gamma_7=\Gamma_6+\Gamma_8$, and $\Gamma_5\times\Gamma_8=\Gamma_6+\Gamma_7+2\Gamma_8$. Thus the allowed electric dipole transitions are $\Gamma_6 \leftrightarrow \Gamma_7$, $\Gamma_6\leftrightarrow\Gamma_8$, $\Gamma_7\leftrightarrow\Gamma_8$, and $\Gamma_8\leftrightarrow\Gamma_8$. As the ground state of an acceptor is a Γ_8 level, the excitation spectrum consists of lines of three types: $\Gamma_8\rightarrow\Gamma_6$, $\Gamma_8\rightarrow\Gamma_7$, and $\Gamma_8\rightarrow\Gamma_8$. We now proceed to deduce the selection rules for the Zeeman components of such lines.

In Sec. II we have already obtained the symmetry classification of the Zeeman sublevels according to the irreducible representations of the appropriate symmetry group ($\bar{S}_4$, $\bar{C}_3$, or $\bar{C}_{1h}$ depending on the orientation of $\vec{B}$). To determine the selection rules for transitions between the Zeeman substates belonging to two different impurity levels, we only need to classify the components of $\vec{Q}$ according to the irreducible representations of the groups $\bar{S}_4$, $\bar{C}_3$, and $\bar{C}_{1h}$. This classification is presented in Table VI. The right-handed coordinate system (x', y', z') is chosen with the z' axis along $\vec{B}$. Thus $Q_{z'}$ determines the selection rules for longitudinal polarization ($\hat{\epsilon}_\parallel=\hat{z}'$). $Q_{x'}+iQ_{y'}$ corresponds to the left-circular polarization $[\hat{\epsilon}_+=(1/\sqrt{2})\times(\hat{x}'+i\hat{y}')]$, while $Q_{x'}-iQ_{y'}$ corresponds to the right-circular polarization $[\hat{\epsilon}_-=(1/\sqrt{2})(\hat{x}'-i\hat{y}')]$. Using Table VI and the character Tables III–V we obtain the desired selection rules.

Tables VII–IX present the selection rules for the Zeeman components for $\vec{B}\parallel[001]$, $\vec{B}\parallel[111]$, and $\vec{B}\parallel[110]$, respectively. The components are those of the zero-field transitions $\Gamma_8\rightarrow\Gamma_6$, $\Gamma_8\rightarrow\Gamma_7$, and $\Gamma_8\rightarrow\Gamma_8$. In each table, a nonzero entry indicates an allowed electric dipole transition and specifies the polarization that may induce it. Note that, for $\vec{B}\parallel[110]$, the absence of any rotational symmetry precludes the specification of a definite circular polarization for $\hat{\epsilon}\perp\vec{B}$.

TABLE VII. Selection rules for the Zeeman components with $\vec{B}\parallel[001]$.

$\bar{T}_d$		Γ_8			
	$\bar{S}_4$	$+\frac{3}{2}(\Gamma_6)$	$+\frac{1}{2}(\Gamma_7)$	$-\frac{1}{2}(\Gamma_8)$	$-\frac{3}{2}(\Gamma_5)$
Γ_6	$+\frac{1}{2}(\Gamma_5)$	ϵ_-	$\epsilon_\parallel$	ϵ_+	0
	$-\frac{1}{2}(\Gamma_6)$	0	ϵ_-	$\epsilon_\parallel$	ϵ_+
Γ_7	$+\frac{1}{2}(\Gamma_7)$	ϵ_+	0	ϵ_-	$\epsilon_\parallel$
	$-\frac{1}{2}(\Gamma_8)$	$\epsilon_\parallel$	ϵ_+	0	ϵ_-
Γ_8	$+\frac{3}{2}(\Gamma_6)$	0	ϵ_-	$\epsilon_\parallel$	ϵ_+
	$+\frac{1}{2}(\Gamma_7)$	ϵ_+	0	ϵ_-	$\epsilon_\parallel$
	$-\frac{1}{2}(\Gamma_8)$	$\epsilon_\parallel$	ϵ_+	0	ϵ_-
	$-\frac{3}{2}(\Gamma_5)$	ϵ_-	$\epsilon_\parallel$	ϵ_+	0

Tables VII–IX provide a simple means for checking our calculation of relative intensities of the Zeeman components, presented in Sec. IV.

IV. RELATIVE INTENSITIES OF ZEEMAN COMPONENTS

The relative intensities of the Zeeman components of an impurity absorption line $\Gamma_i\rightarrow\Gamma_k$, induced by the polarization $\hat{\epsilon}$, can be obtained from the transition probabilities $|\hat{\epsilon}\cdot\vec{M}_{\nu\mu}^{(i\rightarrow k)}|^2$, where

$$\vec{M}_{\nu\mu}^{(i\rightarrow k)}=\langle\Theta_\nu^{(k)}|\vec{Q}|\Psi_\mu^{(i)}\rangle\ . \tag{62}$$

Here $\vec{Q}$ is the electric-dipole-moment operator. The wave functions $\Psi_\mu^{(i)}$ and $\Theta_\nu^{(k)}$ represent the Zeeman sublevels of the initial and the final impurity levels, respectively. The zeroth-order approximation to these wave functions are given by appropriate linear combinations of the unperturbed wave functions:

$$\Psi_\mu^{(i)}=\sum_{\mu'} S_{\mu'\mu}\,\psi_{\mu'}^{(i)}\ , \tag{63a}$$

$$\Theta_\nu^{(k)}=\sum_{\nu'} S'_{\nu'\nu}\,\theta_{\nu'}^{(k)}\ , \tag{63b}$$

TABLE VIII. Selection rules for the Zeeman components with $\vec{B}\parallel[111]$.

$\bar{T}_d$		Γ_8			
	$\bar{C}_3$	$+\frac{3}{2}(\Gamma_6)$	$+\frac{1}{2}(\Gamma_4)$	$-\frac{1}{2}(\Gamma_5)$	$-\frac{3}{2}(\Gamma_6)$
Γ_6	$+\frac{1}{2}(\Gamma_4)$	ϵ_-	$\epsilon_\parallel$	ϵ_+	ϵ_-
	$-\frac{1}{2}(\Gamma_5)$	ϵ_+	ϵ_-	$\epsilon_\parallel$	ϵ_+
Γ_7	$+\frac{1}{2}(\Gamma_4)$	ϵ_-	$\epsilon_\parallel$	ϵ_+	ϵ_-
	$-\frac{1}{2}(\Gamma_5)$	ϵ_+	ϵ_-	$\epsilon_\parallel$	ϵ_+
Γ_8	$+\frac{3}{2}(\Gamma_6)$	$\epsilon_\parallel$	ϵ_+	ϵ_-	$\epsilon_\parallel$
	$+\frac{1}{2}(\Gamma_4)$	ϵ_-	$\epsilon_\parallel$	ϵ_+	ϵ_-
	$-\frac{1}{2}(\Gamma_5)$	ϵ_+	ϵ_-	$\epsilon_\parallel$	ϵ_+
	$-\frac{3}{2}(\Gamma_6)$	$\epsilon_\parallel$	ϵ_+	ϵ_-	$\epsilon_\parallel$

TABLE IX. Selection rules for the Zeeman components with $\vec{B} \parallel [110]$.

$\bar{T}_d$		Γ_8			
	$\bar{C}_{1h}$	$+\frac{3}{2}(\Gamma_3)$	$+\frac{1}{2}(\Gamma_4)$	$-\frac{1}{2}(\Gamma_3)$	$-\frac{3}{2}(\Gamma_4)$
Γ_6	$+\frac{1}{2}(\Gamma_3)$	ϵ_+, ϵ_-	$\epsilon_\parallel$	ϵ_+, ϵ_-	$\epsilon_\parallel$
	$-\frac{1}{2}(\Gamma_4)$	$\epsilon_\parallel$	ϵ_+, ϵ_-	$\epsilon_\parallel$	ϵ_+, ϵ_-
Γ_7	$+\frac{1}{2}(\Gamma_4)$	$\epsilon_\parallel$	ϵ_+, ϵ_-	$\epsilon_\parallel$	ϵ_+, ϵ_-
	$-\frac{1}{2}(\Gamma_3)$	ϵ_+, ϵ_-	$\epsilon_\parallel$	ϵ_+, ϵ_-	$\epsilon_\parallel$
Γ_8	$+\frac{3}{2}(\Gamma_3)$	ϵ_+, ϵ_-	$\epsilon_\parallel$	ϵ_+, ϵ_-	$\epsilon_\parallel$
	$+\frac{1}{2}(\Gamma_4)$	$\epsilon_\parallel$	ϵ_+, ϵ_-	$\epsilon_\parallel$	ϵ_+, ϵ_-
	$-\frac{1}{2}(\Gamma_3)$	ϵ_+, ϵ_-	$\epsilon_\parallel$	ϵ_+, ϵ_-	$\epsilon_\parallel$
	$-\frac{3}{2}(\Gamma_4)$	$\epsilon_\parallel$	ϵ_+, ϵ_-	$\epsilon_\parallel$	ϵ_+, ϵ_-

where $\{\psi_\mu^{(i)}\}$ and $\{\theta_\nu^{(k)}\}$ are the unperturbed wave functions of the respective impurity levels. Thus, we can write

$$\vec{M}_{\nu\mu}^{(i\to k)} = (S'^{\dagger}\vec{Q}^{(i\to k)}S)_{\nu\mu} , \tag{64}$$

where

$$\vec{Q}_{\nu\mu}^{(i\to k)} = \langle \theta_\nu^{(k)} | \vec{Q} | \psi_\mu^{(i)} \rangle . \tag{65}$$

It should be noted that the matrices S and S' contain the effect of the magnetic field, whereas the matrices $\vec{Q}^{(i\to k)}$ are field independent. The forms of S and S' have been obtained in Sec. II. The task in hand then is to derive the matrices $\vec{Q}^{(i\to k)}$. We shall address ourselves to the transitions $\Gamma_8 \to \Gamma_6$, $\Gamma_8 \to \Gamma_7$, and $\Gamma_8 \to \Gamma_8$ only.

Let us recall that the components of $\vec{Q}$ belong to Γ_5 of $\bar{T}_d$. We note that

$$\Gamma_5 \times \Gamma_8 = \Gamma_6 + \Gamma_7 + 2\Gamma_8 \tag{66}$$

contains Γ_6 only once. So, according to the "generalized Wigner–Eckart theorem" developed by Koster,[15] $\vec{Q}^{(8\to 6)}$ is proportional to a known matrix. Thus, we have

$$\langle \theta_\nu^{(6)} | \vec{Q} | \psi_\mu^{(8)} \rangle \propto \langle \varphi_\nu^{(6)} | \vec{Q} | \varphi_\mu^{(8)} \rangle , \tag{67}$$

where $\{\varphi_\nu^{(6)}\}$ and $\{\varphi_\mu^{(8)}\}$ are the angular momentum eigenfunctions given in Eqs. (5) and (10). It is easy to derive the matrix $[\langle \varphi_\nu^{(6)} | \vec{Q} | \varphi_\mu^{(8)} \rangle]$; this is done in Appendix C. The proportionality (67) then yields

$$\vec{Q}^{(8\to 6)} = D_0 \begin{bmatrix} \sqrt{3}\,(\hat{x}+i\hat{y}) & -2i\hat{z} & (\hat{x}-i\hat{y}) & 0 \\ 0 & i(\hat{x}+i\hat{y}) & 2\hat{z} & i\sqrt{3}\,(\hat{x}-i\hat{y}) \end{bmatrix} , \tag{68}$$

where D_0 is a complex parameter that can be determined by calculating one nonzero matrix element with the actual unperturbed wave functions $\theta_\nu^{(6)}$ and $\psi_\mu^{(8)}$.

From Eq. (66) we find that Γ_7 appears only once in the direct product $\Gamma_5 \times \Gamma_8$. Thus, $\vec{Q}^{(8\to 7)}$ is proportional to a known matrix.[15] This allows us to write

$$\langle \theta_\nu^{(7)} | \vec{Q} | \psi_\mu^{(8)} \rangle \propto \langle \varphi_\nu^{(7)} | \vec{Q} | \varphi_\mu^{(8)} \rangle , \tag{69}$$

where $\{\varphi_\nu^{(7)}\}$ are those of Eq. (6). The matrix $[\langle \varphi_\nu^{(7)} | \vec{Q} | \varphi_\mu^{(8)} \rangle]$ is deduced in Appendix C. We obtain

$$\vec{Q}^{(8\to 7)} = D_0' \begin{bmatrix} -(\hat{x}-i\hat{y}) & 0 & \sqrt{3}(\hat{x}+i\hat{y}) & 2i\hat{z} \\ -2\hat{z} & i\sqrt{3}\,(\hat{x}-i\hat{y}) & 0 & -i(\hat{x}+i\hat{y}) \end{bmatrix} , \tag{70}$$

where D_0' is a complex parameter that can be obtained by calculating one nonzero matrix element with the actual unperturbed wave functions.

For a $\Gamma_8 \to \Gamma_8$ transition, we observe that Γ_8 appears *twice* in the direct product $\Gamma_5 \times \Gamma_8$, and so each of the matrices Q_x, Q_y, and Q_z is a linear combination of *two* known matrices.[15] The most general form of $\vec{Q}^{(8\to 8)}$ can be obtained from a simple symmetry argument. Each component, being a 4×4 matrix, must be expressible as a linear combination of the 16 matrices listed in (7). However, the matrices $\vec{Q}^{(8\to 8)}$ are referred to the two sets of functions $\{\theta_\nu^{(8)}\}$ and $\{\psi_\mu^{(8)}\}$, both generating the same irreducible representation Γ_8. So the matrices Q_x, Q_y, Q_z will retain the transformation properties (Γ_5) of the operators Q_x, Q_y, Q_z. Now there are only two sets of matrices (U_x, U_y, U_z) and (V_x, V_y, V_z) in (7) that belong to Γ_5. Thus we can write

$$\vec{Q}^{(8\to 8)} = -(2/\sqrt{3})(D+D')\vec{U} - (4i/\sqrt{3})D'\vec{V} . \tag{71}$$

The nomenclature of the two complex parameters that multiply $\vec{U}$ and $\vec{V}$ is chosen to conform to the notations of Rodriguez, Fisher, and Barra.[12] Clearly, D and D' can be determined by calculating two suitable matrix elements with the actual unperturbed wave functions.

It should be noted that Eqs. (68), (70), and (71) were obtained by Rodriguez *et al.*[12] by making explicit use of specific forms for the unperturbed wave functions. However, the functions chosen by them are not the most general permitted by symmetry. (See Appendix D.) The derivation presented above clearly establishes the complete generality of the results.

We shall now proceed to calculate the relative intensities of the Zeeman components. Strictly speaking, we are going to calculate only the relative values of transition probabilities. In order to obtain the relative intensity of a given component, the relative transition probability has to be multiplied by the energy of the particular transition as well as the fractional population of the initial sublevel. If the Zeeman splittings are sufficiently small so that the factors $(E_\nu^{(k)} - E_\mu^{(8)})$ may be approximated by the energy of the zero-field transition, and if all the initial sublevels may be assumed to be equally populated, then the relative intensity would become identical with the relative transition probability. It is with this fact in mind that we use the terminology "relative intensity" to mean the relative transition probability that we actually calculate. The three different orientations of $\vec{B}$ are treated separately.

A. Magnetic Field along [001]

This is the simplest case; both $\underset{\sim}{S}$ and S' are unit matrices. The transition matrix $\vec{M}^{(i\to k)}$ is the same as the matrix $\vec{Q}^{(i\to k)}$. The components will be denoted by $Q_x[001]$, $Q_y[001]$, and $Q_z[001]$. We write them explicitly for each type of transition:

Case (i) $\Gamma_8 \to \Gamma_6$:

$$Q_x[001] = D_0\begin{bmatrix} \sqrt{3} & 0 & 1 & 0 \\ 0 & i & 0 & i\sqrt{3} \end{bmatrix}, \quad Q_y[001] = D_0\begin{bmatrix} i\sqrt{3} & 0 & -i & 0 \\ 0 & -1 & 0 & \sqrt{3} \end{bmatrix}, \quad Q_z[001] = D_0\begin{bmatrix} 0 & -2i & 0 & 0 \\ 0 & 0 & 2 & 0 \end{bmatrix};$$

Case (ii) $\Gamma_8 \to \Gamma_7$:

$$Q_x[001] = D_0'\begin{bmatrix} -1 & 0 & \sqrt{3} & 0 \\ 0 & i\sqrt{3} & 0 & -i \end{bmatrix}, \quad Q_y[001] = D_0'\begin{bmatrix} i & 0 & i\sqrt{3} & 0 \\ 0 & \sqrt{3} & 0 & 1 \end{bmatrix}, \quad Q_z[001] = D_0'\begin{bmatrix} 0 & 0 & 0 & 2i \\ -2 & 0 & 0 & 0 \end{bmatrix};$$

Case (iii) $\Gamma_8 \to \Gamma_8$:

$$Q_x[001] = \begin{bmatrix} 0 & -(D+2D') & 0 & \sqrt{3}D' \\ -D & 0 & \sqrt{3}D' & 0 \\ 0 & -\sqrt{3}D' & 0 & D \\ -\sqrt{3}D' & 0 & (D+2D') & 0 \end{bmatrix},$$

$$Q_y[001] = \begin{bmatrix} 0 & -i(D+2D') & 0 & -i\sqrt{3}D' \\ iD & 0 & i\sqrt{3}D' & 0 \\ 0 & i\sqrt{3}D' & 0 & iD \\ -i\sqrt{3}D' & 0 & -i(D+2D') & 0 \end{bmatrix},$$

$$Q_z[001] = \begin{bmatrix} 0 & 0 & -i(D-D') & 0 \\ 0 & 0 & 0 & -i(D+3D') \\ i(D+3D') & 0 & 0 & 0 \\ 0 & i(D-D') & 0 & 0 \end{bmatrix}.$$

For each polarization the transition probability for a given Zeeman component is proportional to the absolute square of the corresponding element of the appropriate transition matrix. The matrix $Q_x[001] + iQ_y[001]$ corresponds to the left-circular polarization (ϵ_+) in the Faraday configuration, while $Q_x[001] - iQ_y[001]$ corresponds to the right-circular polarization (ϵ_-); the relative intensities of the allowed Zeeman components are presented in Table X. The matrix $Q_z[001]$ corresponds to linear polarization ($\epsilon_\parallel$) parallel to $\vec{B}$, whereas $Q_x[001]$ or $Q_y[001]$ corresponds to linear polariza-

TABLE X. Relative intensities of the Zeeman components in the Faraday configuration with $\vec{B} \parallel [001]$ (circular polarization).

Zero-field transition	Components ϵ_+	ϵ_-	Relative intensity
$\Gamma_8 \to \Gamma_6$	$-\frac{3}{2} \to -\frac{1}{2}$	$+\frac{3}{2} \to +\frac{1}{2}$	$\frac{3}{4}$
	$-\frac{1}{2} \to +\frac{1}{2}$	$-\frac{1}{2} \to -\frac{1}{2}$	$\frac{1}{4}$
$\Gamma_8 \to \Gamma_7$	$+\frac{3}{2} \to +\frac{1}{2}$	$-\frac{3}{2} \to -\frac{1}{2}$	$\frac{1}{4}$
	$+\frac{1}{2} \to -\frac{1}{2}$	$-\frac{1}{2} \to +\frac{1}{2}$	$\frac{3}{4}$
$\Gamma_8 \to \Gamma_8$	$+\frac{3}{2} \to +\frac{1}{2}$	$-\frac{3}{2} \to -\frac{1}{2}$	$\frac{1}{2} - \frac{3}{8}u + \frac{1}{2}v$
	$+\frac{1}{2} \to -\frac{1}{2}$	$-\frac{1}{2} \to +\frac{1}{2}$	$\frac{3}{8}u$
	$-\frac{1}{2} \to -\frac{3}{2}$	$+\frac{1}{2} \to +\frac{3}{2}$	$\frac{1}{2} - \frac{3}{8}u - \frac{1}{2}v$
	$-\frac{3}{2} \to +\frac{3}{2}$	$+\frac{3}{2} \to -\frac{3}{2}$	$\frac{3}{8}u$

tion ($\epsilon_\perp$) perpendicular to $\vec{B}$; the relative intensities are presented in Table XI. The parameters u and v that appear in the relative intensities of the Zeeman components of a $\Gamma_8 \to \Gamma_8$ transition were introduced by Rodriguez *et al.*[12] They are discussed below.

It is noted that, for each polarization, the sum of the transition probabilities is given by

$$N = 4|D+D'|^2 + 16|D'|^2 .$$

Thus the intensity of the zero-field transition can be normalized to N. In other words, we can keep N fixed. The parameter u is then defined by the equations

$$|D+D'|^2 + 8|D'|^2 = \tfrac{1}{4}N(1+u) , \qquad (72)$$

$$|D+D'|^2 = \tfrac{1}{4}N(1-u) . \qquad (73)$$

It is easy to see that

$$0 \le u \le 1 . \qquad (74)$$

The parameter v is introduced by

$$|D|^2 = \tfrac{1}{4}N(1 - \tfrac{3}{4}u + v) . \qquad (75)$$

Using Eqs. (72), (73), and (75) we find that

$$|D+2D'|^2 = \tfrac{1}{4}N(1 - \tfrac{3}{4}u - v) ,$$

$$|D-D'|^2 = \tfrac{1}{4}N(1+2v) ,$$

and

$$|D+3D'|^2 = \tfrac{1}{4}N(1-2v) .$$

Therefore, it is necessary to restrict v to the common range of the inequalities:

$$-\tfrac{1}{2} \le v \le \tfrac{1}{2} , \quad -(1-\tfrac{3}{4}u) \le v \le (1-\tfrac{3}{4}u) . \qquad (76)$$

The fact that the relative intensities of the components of a $\Gamma_8 \to \Gamma_8$ transition can be expressed in terms of two real parameters is not at all surprising: It is clear from Eq. (71) that ratios of the transition-matrix elements depend only on the ratio of D' and $(D+D')$, that is, on only one complex parameter. It is particularly interesting to note that u and v have been defined in such a way that either $u=0$ or $u=1$ requires $v=0$. This is quite appropriate, because $u=0$ implies $D'=0$, while $u=1$ implies $D+D'=0$. In either case, Eq. (71) shows that the relative intensities are known numbers, independent of any parameter.

B. Magnetic Field along [111]

In this case, the matrix S is given by Eq. (39):

$$S(\gamma) = D^{(3/2)}[111]C(\gamma) .$$

The matrix $C(\gamma)$ is given in Eq. (34), and

$$D^{(3/2)}[111] = \frac{1}{2}\begin{bmatrix} (1/\sqrt{2})a^3\omega^3 & -ia\omega^3 & -b\omega^3 & (i/\sqrt{2})b^3\omega^3 \\ -ia\omega & b\omega & -ia\omega & -b\omega \\ -b\omega^* & -ia\omega^* & b\omega^* & -ia\omega^* \\ (i/\sqrt{2})b^3\omega^{*3} & -b\omega^{*3} & -ia\omega^{*3} & (1/\sqrt{2})a^3\omega^{*3} \end{bmatrix} ,$$

where

$$a \equiv [(\sqrt{3}+1)/\sqrt{3}]^{1/2} ,$$

$$b \equiv [(\sqrt{3}-1)/\sqrt{3}]^{1/2} ,$$

and

$$\omega \equiv e^{-i\pi/8} .$$

For either a $\Gamma_8 \to \Gamma_6$ or $\Gamma_8 \to \Gamma_7$ transition the matrix S' is the rotation matrix

$$D^{(1/2)}[111] = \frac{1}{\sqrt{2}}\begin{bmatrix} a\omega & -b\omega \\ b\omega^* & a\omega^* \end{bmatrix} .$$

For a $\Gamma_8 \to \Gamma_8$ transition, $S' = S(\gamma')$. Note that the parameter γ for a given Γ_8 level has been defined in Eq. (35). Here we are using γ to represent the value of this parameter for the initial level, and γ' for the final level.

The derivation of the transition matrices $\vec{M}^{(8\to k)}$ is now an exercise in matrix multiplication. In writing the results we shall use the rotated coordinate system

$$\hat{x}' = (1/\sqrt{6})(\hat{x}+\hat{y}-2\hat{z}) ,$$

$$\hat{y}' = (1/\sqrt{2})(-\hat{x}+\hat{y}) ,$$

$$\hat{z}' = (1/\sqrt{3})(\hat{x}+\hat{y}+\hat{z}) ,$$

so that $\hat{z}' \parallel \vec{B}$. For each type of transition, $\vec{Q}[111]$ will denote the transition matrix $\vec{M}$:

TABLE XI. Relative intensities of the Zeeman components in the Voigt configuration with $\vec{B} \parallel [001]$.

Zero-field transition	Longitudinal polarization ($\epsilon_{\parallel}$) Components	Longitudinal polarization ($\epsilon_{\parallel}$) Relative intensity	Transverse polarization ($\epsilon_{\perp}$) Components	Transverse polarization ($\epsilon_{\perp}$) Relative intensity
$\Gamma_8 \rightarrow \Gamma_6$	$\pm\frac{1}{2} \rightarrow \pm\frac{1}{2}$	$\frac{1}{2}$	$\mp\frac{3}{2} \rightarrow \mp\frac{1}{2}$ $\mp\frac{1}{2} \rightarrow \pm\frac{1}{2}$	$\frac{3}{8}$ $\frac{1}{8}$
$\Gamma_8 \rightarrow \Gamma_7$	$\pm\frac{3}{2} \rightarrow \mp\frac{1}{2}$	$\frac{1}{2}$	$\pm\frac{3}{2} \rightarrow \pm\frac{1}{2}$ $\pm\frac{1}{2} \rightarrow \mp\frac{1}{2}$	$\frac{1}{8}$ $\frac{3}{8}$
	$\pm\frac{3}{2} \rightarrow \mp\frac{1}{2}$	$\frac{1}{4} - \frac{1}{2}v$	$\pm\frac{3}{2} \rightarrow \pm\frac{1}{2}$ $\pm\frac{1}{2} \rightarrow \mp\frac{1}{2}$	$\frac{1}{4} - \frac{3}{16}u + \frac{1}{4}v$ $\frac{3}{16}u$
$\Gamma_8 \rightarrow \Gamma_8$				
	$\pm\frac{1}{2} \rightarrow \mp\frac{3}{2}$	$\frac{1}{4} + \frac{1}{2}v$	$\mp\frac{1}{2} \rightarrow \mp\frac{3}{2}$ $\mp\frac{3}{2} \rightarrow \pm\frac{3}{2}$	$\frac{1}{4} - \frac{3}{16}u - \frac{1}{4}v$ $\frac{3}{16}u$

Case (i) $\Gamma_8 \rightarrow \Gamma_6$:

$$Q_{x'}[111] = D_0 \begin{bmatrix} \frac{\sqrt{3}}{(1+\gamma^2)^{1/2}} & 0 & 1 & \frac{i\sqrt{3}\gamma}{(1+\gamma^2)^{1/2}} \\ \frac{-\sqrt{3}\gamma}{(1+\gamma^2)^{1/2}} & i & 0 & \frac{i\sqrt{3}}{(1+\gamma^2)^{1/2}} \end{bmatrix},$$

$$Q_{y'}[111] = D_0 \begin{bmatrix} \frac{i\sqrt{3}}{(1+\gamma^2)^{1/2}} & 0 & -i & \frac{-\sqrt{3}\gamma}{(1+\gamma^2)^{1/2}} \\ \frac{i\sqrt{3}\gamma}{(1+\gamma^2)^{1/2}} & -1 & 0 & \frac{\sqrt{3}}{(1+\gamma^2)^{1/2}} \end{bmatrix}, \quad Q_{z'}[111] = D_0 \begin{bmatrix} 0 & -2i & 0 & 0 \\ 0 & 0 & 2 & 0 \end{bmatrix};$$

Case (ii) $\Gamma_8 \rightarrow \Gamma_7$:

$$Q_{x'}[111] = \frac{D_0'}{\sqrt{3}} \begin{bmatrix} \frac{i(2\sqrt{2}\gamma-1)}{(1+\gamma^2)^{1/2}} & 0 & i\sqrt{3} & \frac{(2\sqrt{2}+\gamma)}{(1+\gamma^2)^{1/2}} \\ \frac{-i(2\sqrt{2}+\gamma)}{(1+\gamma^2)^{1/2}} & -\sqrt{3} & 0 & \frac{(2\sqrt{2}\gamma-1)}{(1+\gamma^2)^{1/2}} \end{bmatrix},$$

$$Q_{y'}[111] = \frac{D_0'}{\sqrt{3}} \begin{bmatrix} \frac{-(2\sqrt{2}\gamma-1)}{(1+\gamma^2)^{1/2}} & 0 & -\sqrt{3} & \frac{i(2\sqrt{2}+\gamma)}{(1+\gamma^2)^{1/2}} \\ \frac{-(2\sqrt{2}+\gamma)}{(1+\gamma^2)^{1/2}} & -i\sqrt{3} & 0 & \frac{-i(2\sqrt{2}\gamma-1)}{(1+\gamma^2)^{1/2}} \end{bmatrix}, \quad Q_{z'}[111] = D_0' \begin{bmatrix} 0 & 2 & 0 & 0 \\ 0 & 0 & -2i & 0 \end{bmatrix};$$

Case (iii) $\Gamma_8 \rightarrow \Gamma_8$:

$$Q_{x'}[111] = \frac{1}{\sqrt{3}} \begin{bmatrix} 0 & \frac{i[(\sqrt{2}\gamma'+1)D+(2\sqrt{2}\gamma'-1)D']}{(1+\gamma'^2)^{1/2}} & \frac{[(\gamma'-\sqrt{2})D-(\gamma'+2\sqrt{2})D']}{(1+\gamma'^2)^{1/2}} & 0 \\ \frac{-i[(\sqrt{2}\gamma+1)D+3D']}{(1+\gamma^2)^{1/2}} & 0 & i2\sqrt{3}D' & \frac{[(\gamma-\sqrt{2})D+3\gamma D']}{(1+\gamma^2)^{1/2}} \\ \frac{[(\gamma-\sqrt{2})D+3\gamma D']}{(1+\gamma^2)^{1/2}} & i2\sqrt{3}D' & 0 & \frac{-i[(\sqrt{2}\gamma+1)D+3D']}{(1+\gamma^2)^{1/2}} \\ 0 & \frac{[(\gamma'-\sqrt{2})D-(\gamma'+2\sqrt{2})D']}{(1+\gamma'^2)^{1/2}} & \frac{i[(\sqrt{2}\gamma'+1)D+(2\sqrt{2}\gamma'-1)D']}{(1+\gamma'^2)^{1/2}} & 0 \end{bmatrix}$$

$$
Q_{\gamma'}[111]=\frac{1}{\sqrt{3}}\begin{bmatrix} 0 & \frac{[(\sqrt{2}\gamma'+1)D+(2\sqrt{2}\gamma'-1)D']}{(1+\gamma'^2)^{1/2}} & \frac{i[(\gamma'-\sqrt{2})D-(\gamma'+2\sqrt{2})D']}{(1+\gamma'^2)^{1/2}} & 0 \\ \frac{[(\sqrt{2}\gamma+1)D+3D']}{(1+\gamma^2)^{1/2}} & 0 & 2\sqrt{3}D' & \frac{i[(\gamma-\sqrt{2})D+3\gamma D']}{(1+\gamma^2)^{1/2}} \\ \frac{-i[(\gamma-\sqrt{2})D+3\gamma D']}{(1+\gamma^2)^{1/2}} & -2\sqrt{3}D' & 0 & \frac{-[(\sqrt{2}\gamma+1)D+3D']}{(1+\gamma^2)^{1/2}} \\ 0 & \frac{-i[(\gamma'-\sqrt{2})D-(\gamma'+2\sqrt{2})D']}{(1+\gamma'^2)^{1/2}} & \frac{-[(\sqrt{2}\gamma'+1)D+(2\sqrt{2}\gamma'-1)D']}{(1+\gamma'^2)^{1/2}} & 0 \end{bmatrix},
$$

$$
Q_{\epsilon'}[111]=\begin{bmatrix} \frac{-[(\gamma'\gamma+1)D+\lambda(\gamma',\gamma)D']}{[(1+\gamma'^2)(1+\gamma^2)]^{1/2}} & 0 & 0 & \frac{i[(\gamma'-\gamma)D+\tau(\gamma',\gamma)D']}{[(1+\gamma'^2)(1+\gamma^2)]^{1/2}} \\ 0 & (D+D') & 0 & 0 \\ 0 & 0 & (D+D') & 0 \\ \frac{i[(\gamma'-\gamma)D+\tau(\gamma',\gamma)D']}{[(1+\gamma'^2)(1+\gamma^2)]^{1/2}} & 0 & 0 & \frac{-[(\gamma'\gamma+1)D+\lambda(\gamma',\gamma)D']}{[(1+\gamma'^2)(1+\gamma^2)]^{1/2}} \end{bmatrix}.
$$

In the last matrix we have introduced

$$\lambda(\gamma',\gamma)\equiv(\gamma'\gamma+1)-2\sqrt{2}(\gamma'-\gamma),$$

$$\tau(\gamma',\gamma)\equiv(\gamma'-\gamma)+2\sqrt{2}(\gamma'\gamma+1).$$

The relative intensities for transverse circular polarizations are presented in Table XII, while those for linear polarizations are given in Tables XIII A and XIII B. It is interesting to note that the relative intensities of the Zeeman components of $\Gamma_8\to\Gamma_6$ and $\Gamma_8\to\Gamma_7$ reduce to the simple results of Johnston *et al.*[11] if we let $\gamma=0$; this, however, corresponds to the trivial case of a $j=\frac{3}{2}$-like Γ_8 level.

C. Magnetic Field along [110]

Here the matrix S is given by Eq. (59):

$$S(\delta_1,\delta_2)=D^{(3/2)}[110]C(\delta_1,\delta_2).$$

The matrix $C(\delta_1,\delta_2)$ is given in Eq. (52), and

$$
D^{(3/2)}[110]=\frac{1}{2\sqrt{2}}\begin{bmatrix} \omega^3 & -i\sqrt{3}\,\omega^3 & -\sqrt{3}\,\omega^3 & i\omega^3 \\ -i\sqrt{3}\,\omega & -\omega & -i\omega & -\sqrt{3}\,\omega \\ -\sqrt{3}\,\omega^* & -i\omega^* & -\omega^* & -i\sqrt{3}\,\omega^* \\ i\omega^{*3} & -\sqrt{3}\,\omega^{*3} & -i\sqrt{3}\,\omega^{*3} & \omega^{*3} \end{bmatrix},
$$

TABLE XII. Relative intensities of the Zeeman components in the Faraday configuration with $\vec{B}\parallel[111]$ (circular polarization).

Zero-field transition	Component ϵ_+	ϵ_-	Relative intensity
	$+\frac{3}{2}\to-\frac{1}{2}$	$-\frac{3}{2}\to+\frac{1}{2}$	$\frac{3}{4}[\gamma^2/(1+\gamma^2)]$
$\Gamma_8\to\Gamma_6$	$-\frac{1}{2}\to+\frac{1}{2}$	$+\frac{1}{2}\to-\frac{1}{2}$	$\frac{1}{4}$
	$-\frac{3}{2}\to-\frac{1}{2}$	$+\frac{3}{2}\to+\frac{1}{2}$	$\frac{3}{4}[1/(1+\gamma^2)]$
	$+\frac{3}{2}\to-\frac{1}{2}$	$-\frac{3}{2}\to+\frac{1}{2}$	$\frac{1}{12}[(2\sqrt{2}+\gamma)^2/(1+\gamma^2)]$
$\Gamma_8\to\Gamma_7$	$-\frac{1}{2}\to+\frac{1}{2}$	$+\frac{1}{2}\to-\frac{1}{2}$	$\frac{1}{4}$
	$-\frac{3}{2}\to-\frac{1}{2}$	$+\frac{3}{2}\to+\frac{1}{2}$	$\frac{1}{12}[(2\sqrt{2}\gamma-1)^2/(1+\gamma^2)]$
	$+\frac{3}{2}\to-\frac{1}{2}$	$-\frac{3}{2}\to+\frac{1}{2}$	$\frac{1}{6}[(\gamma-\sqrt{2})^2+3(\sqrt{2}\gamma-\frac{1}{2})u-(2\gamma^2-\sqrt{2}\gamma-2)v]/(1+\gamma^2)$
	$+\frac{1}{2}\to+\frac{3}{2}$	$-\frac{1}{2}\to-\frac{3}{2}$	$\frac{1}{6}[(\sqrt{2}\gamma'+1)^2-3\gamma'(\frac{1}{2}\gamma'+\sqrt{2})u-(2\gamma'^2-\sqrt{2}\gamma'-2)v]/(1+\gamma'^2)$
$\Gamma_8\to\Gamma_8$	$+\frac{1}{2}\to-\frac{3}{2}$	$-\frac{1}{2}\to+\frac{3}{2}$	$\frac{1}{6}[(\gamma'-\sqrt{2})^2+3(\sqrt{2}\gamma'-\frac{1}{2})u+(2\gamma'^2-\sqrt{2}\gamma'-2)v]/(1+\gamma'^2)$
	$-\frac{1}{2}\to+\frac{1}{2}$	$+\frac{1}{2}\to-\frac{1}{2}$	$\frac{1}{2}u$
	$-\frac{3}{2}\to-\frac{1}{2}$	$+\frac{3}{2}\to+\frac{1}{2}$	$\frac{1}{6}[(\sqrt{2}\gamma+1)^2-3\gamma(\frac{1}{2}\gamma+\sqrt{2})u+(2\gamma^2-\sqrt{2}\gamma-2)v]/(1+\gamma^2)$

TABLE XIII. Relative intensities of the Zeeman components in the Voigt configuration with $\vec{B} \parallel [111]$.

Zero-field transition	Components	Relative intensity
		A. Longitudinal polarization ($\epsilon_{\parallel}$)
$\Gamma_8 \to \Gamma_6$	$\pm\frac{1}{2} \to \pm\frac{1}{2}$	$\frac{1}{2}$
$\Gamma_8 \to \Gamma_7$	$\pm\frac{1}{2} \to \pm\frac{1}{2}$	$\frac{1}{2}$
	$\pm\frac{3}{2} \to \pm\frac{3}{2}$	$\frac{1}{4}[(\gamma'\gamma+1)^2(1-u)+2(\gamma'-\gamma)^2u+2\sqrt{2}(\gamma'\gamma+1)(\gamma'-\gamma)v]/[(1+\gamma'^2)(1+\gamma^2)]$
$\Gamma_8 \to \Gamma_8$	$\pm\frac{3}{2} \to \mp\frac{3}{2}$	$\frac{1}{4}[(\gamma'-\gamma)^2(1-u)+2(\gamma'\gamma+1)^2u-2\sqrt{2}(\gamma'\gamma+1)(\gamma'-\gamma)v]/[(1+\gamma'^2)(1+\gamma^2)]$
	$\pm\frac{1}{2} \to \pm\frac{1}{2}$	$\frac{1}{4}(1-u)$
		B. Transverse polarization ($\epsilon_{\perp}$)
	$\pm\frac{3}{2} \to \mp\frac{1}{2}$	$\frac{3}{8}[\gamma^2/(1+\gamma^2)]$
$\Gamma_8 \to \Gamma_6$	$\mp\frac{1}{2} \to \pm\frac{1}{2}$	$\frac{1}{8}$
	$\mp\frac{3}{2} \to \mp\frac{1}{2}$	$\frac{3}{8}[1/(1+\gamma^2)]$
	$\pm\frac{3}{2} \to \mp\frac{1}{2}$	$\frac{1}{24}[(2\sqrt{2}+\gamma)^2/(1+\gamma^2)]$
$\Gamma_8 \to \Gamma_7$	$\mp\frac{1}{2} \to \pm\frac{1}{2}$	$\frac{1}{8}$
	$\mp\frac{3}{2} \to \mp\frac{1}{2}$	$\frac{1}{24}[(2\sqrt{2}\,\gamma-1)^2/(1+\gamma^2)]$
	$\pm\frac{3}{2} \to \mp\frac{1}{2}$	$\frac{1}{12}[(\gamma-\sqrt{2})^2+3(\sqrt{2}\,\gamma-\frac{1}{2})u-(2\gamma^2-\sqrt{2}\,\gamma-2)v]/(1+\gamma^2)$
	$\pm\frac{1}{2} \to \pm\frac{3}{2}$	$\frac{1}{12}[(\sqrt{2}\,\gamma'+1)^2-3\gamma'(\frac{1}{2}\gamma'+\sqrt{2})u-(2\gamma'^2-\sqrt{2}\,\gamma'-2)v]/(1+\gamma'^2)$
$\Gamma_8 \to \Gamma_8$	$\pm\frac{1}{2} \to \mp\frac{3}{2}$	$\frac{1}{12}[(\gamma'-\sqrt{2})^2+3(\sqrt{2}\,\gamma'-\frac{1}{2})u+(2\gamma'^2-\sqrt{2}\,\gamma'-2)v]/(1+\gamma'^2)$
	$\mp\frac{1}{2} \to \pm\frac{1}{2}$	$\frac{1}{4}u$
	$\mp\frac{3}{2} \to \mp\frac{1}{2}$	$\frac{1}{12}[(\sqrt{2}\,\gamma+1)^2-3\gamma(\frac{1}{2}\gamma+\sqrt{2})u+(2\gamma^2-\sqrt{2}\,\gamma-2)v]/(1+\gamma^2)$

where $\omega = e^{-i\pi/8}$.

For either a $\Gamma_8 \to \Gamma_6$ or $\Gamma_8 \to \Gamma_7$ transition the matrix S' is the rotation matrix

$$D^{(1/2)}[110] = \frac{1}{\sqrt{2}} \begin{bmatrix} \omega & -\omega \\ \omega^* & \omega^* \end{bmatrix} .$$

For a $\Gamma_8 \to \Gamma_8$ transition $S' = S(\delta_1', \delta_2')$, where the primed parameters refer to the final Γ_8 level.

We shall write the components of the transition matrix $\vec{Q}[110]$ for each type of transition in the rotated coordinate system

$$\hat{x}' = -\hat{z} ,$$

$$\hat{y}' = (1/\sqrt{2})(-\hat{x}+\hat{y}) ,$$

$$\hat{z}' = (1/\sqrt{2})(\hat{x}+\hat{y}) ;$$

Case (i) $\Gamma_8 \to \Gamma_6$:

$$Q_{x'}[110] = D_0 \begin{bmatrix} \frac{(\sqrt{3}-\delta_1)}{(1+\delta_1^2)^{1/2}} & 0 & \frac{(\sqrt{3}\,\delta_1+1)}{(1+\delta_1^2)^{1/2}} & 0 \\ 0 & \frac{i(\sqrt{3}\,\delta_2+1)}{(1+\delta_2^2)^{1/2}} & 0 & \frac{i(\sqrt{3}-\delta_2)}{(1+\delta_2^2)^{1/2}} \end{bmatrix} ,$$

$$Q_{y'}[110] = D_0 \begin{bmatrix} \frac{i(\sqrt{3}+\delta_1)}{(1+\delta_1^2)^{1/2}} & 0 & \frac{i(\sqrt{3}\,\delta_1-1)}{(1+\delta_1^2)^{1/2}} & 0 \\ 0 & \frac{(\sqrt{3}\,\delta_2-1)}{(1+\delta_2^2)^{1/2}} & 0 & \frac{(\sqrt{3}+\delta_2)}{(1+\delta_2^2)^{1/2}} \end{bmatrix} ,$$

$$Q_{z'}[110] = D_0 \begin{bmatrix} 0 & \frac{-2i}{(1+\delta_2^2)^{1/2}} & 0 & \frac{2i\delta_2}{(1+\delta_2^2)^{1/2}} \\ \frac{-2\delta_1}{(1+\delta_1^2)^{1/2}} & 0 & \frac{2}{(1+\delta_1^2)^{1/2}} & 0 \end{bmatrix} ;$$

Case (ii) $\Gamma_8 \rightarrow \Gamma_7$:

$$Q_{x'}[110] = D_0' \begin{bmatrix} 0 & \frac{(\delta_2 - \sqrt{3})}{(1+\delta_2^2)^{1/2}} & 0 & \frac{(\sqrt{3}\,\delta_2 + 1)}{(1+\delta_2^2)^{1/2}} \\ \frac{-i(\sqrt{3}\,\delta_1 + 1)}{(1+\delta_1^2)^{1/2}} & 0 & \frac{-i(\delta_1 - \sqrt{3})}{(1+\delta_1^2)^{1/2}} & 0 \end{bmatrix} ,$$

$$Q_{y'}[110] = D_0' \begin{bmatrix} 0 & \frac{2i\delta_2}{(1+\delta_2^2)^{1/2}} & 0 & \frac{2i}{(1+\delta_2^2)^{1/2}} \\ \frac{-2}{(1+\delta_1^2)^{1/2}} & 0 & \frac{-2\delta_1}{(1+\delta_1^2)^{1/2}} & 0 \end{bmatrix} ,$$

$$Q_{z'}[110] = D_0' \begin{bmatrix} \frac{i(\sqrt{3}\,\delta_1 - 1)}{(1+\delta_1^2)^{1/2}} & 0 & \frac{-i(\delta_1 + \sqrt{3})}{(1+\delta_1^2)^{1/2}} & 0 \\ 0 & \frac{-(\delta_2 + \sqrt{3})}{(1+\delta_2^2)^{1/2}} & 0 & \frac{(\sqrt{3}\,\delta_2 - 1)}{(1+\delta_2^2)^{1/2}} \end{bmatrix} ;$$

Case (iii) $\Gamma_8 \rightarrow \Gamma_8$:

$$Q_{x'}[110] = \tfrac{1}{2} \begin{bmatrix} \frac{h_1(\delta_1, \delta_1')D + h_2(\delta_1, \delta_1')D'}{H(\delta_1, \delta_1')} & 0 & \frac{h_3(\delta_1, \delta_1')D + h_4(\delta_1, \delta_1')D'}{H(\delta_1, \delta_1')} & 0 \\ 0 & \frac{-[h_1(\delta_2', \delta_2)D + h_2(\delta_2', \delta_2)D']}{H(\delta_2', \delta_2)} & 0 & \frac{h_3(\delta_2', \delta_2)D + h_5(\delta_2', \delta_2)D'}{H(\delta_2', \delta_2)} \\ \frac{h_3(\delta_1', \delta_1)D + h_5(\delta_1', \delta_1)D'}{H(\delta_1', \delta_1)} & 0 & \frac{-[h_1(\delta_1', \delta_1)D + h_2(\delta_1', \delta_1)D']}{H(\delta_1', \delta_1)} & 0 \\ 0 & \frac{h_3(\delta_2, \delta_2')D + h_4(\delta_2, \delta_2')D'}{H(\delta_2, \delta_2')} & 0 & \frac{h_1(\delta_2, \delta_2')D + h_2(\delta_2, \delta_2')D'}{H(\delta_2, \delta_2')} \end{bmatrix} ,$$

$$Q_{y'}[110] = \frac{-i}{2} \begin{bmatrix} \frac{-[2(\delta_1 - \delta_1')D + h_6(\delta_1, \delta_1')D']}{H(\delta_1, \delta_1')} & 0 & \frac{2(1 + \delta_1\delta_1')D + h_7(\delta_1, \delta_1')D'}{H(\delta_1, \delta_1')} & 0 \\ 0 & \frac{2(\delta_2 - \delta_2')D + h_8(\delta_2, \delta_2')D'}{H(\delta_2, \delta_2')} & 0 & \frac{2(1 + \delta_2\delta_2')D + h_9(\delta_2, \delta_2')D'}{H(\delta_2, \delta_2')} \\ \frac{-[2(1 + \delta_1\delta_1')D + h_9(\delta_1, \delta_1')D']}{H(\delta_1, \delta_1')} & 0 & \frac{-[2(\delta_1 - \delta_1')D + h_8(\delta_1, \delta_1')D']}{H(\delta_1, \delta_1')} & 0 \\ 0 & \frac{-[2(1 + \delta_2\delta_2')D + h_7(\delta_2, \delta_2')D']}{H(\delta_2, \delta_2')} & 0 & \frac{2(\delta_2 - \delta_2')D + h_6(\delta_2, \delta_2')D'}{H(\delta_2, \delta_2')} \end{bmatrix} ,$$

$$Q_{z'}[110] = \frac{i}{2} \begin{bmatrix} 0 & \frac{2(1 + \delta_1'\delta_2)D + h_7(\delta_1', \delta_2)D'}{H(\delta_1', \delta_2)} & 0 & \frac{2(\delta_1' - \delta_2)D + h_8(\delta_1', \delta_2)D'}{H(\delta_1', \delta_2)} \\ \frac{-[2(1 + \delta_2'\delta_1)D + h_9(\delta_2', \delta_1)D']}{H(\delta_2', \delta_1)} & 0 & \frac{2(\delta_2' - \delta_1)D + h_6(\delta_2', \delta_1)D'}{H(\delta_2', \delta_1)} & 0 \\ 0 & \frac{2(\delta_1' - \delta_2)D + h_8(\delta_1', \delta_2)D'}{H(\delta_1', \delta_2)} & 0 & \frac{-[2(1 + \delta_1'\delta_2)D + h_9(\delta_1', \delta_2)D']}{H(\delta_1', \delta_2)} \\ \frac{2(\delta_2' - \delta_1)D + h_8(\delta_2', \delta_1)D'}{H(\delta_2', \delta_1)} & 0 & \frac{2(1 + \delta_2'\delta_1)D + h_7(\delta_2', \delta_1)D'}{H(\delta_2', \delta_1)} & 0 \end{bmatrix} .$$

The functions that appear in the transition matrices for $\Gamma_8 \rightarrow \Gamma_8$ are defined by

$$H(x, y) = [(1 + x^2)(1 + y^2)]^{1/2} ,$$

$$h_1(x, y) = \sqrt{3}\,(1 - xy) + (x + y) ,$$

$$h_2(x, y) = \sqrt{3}\,(1 - xy) + (5x - 3y) ,$$

$$h_3(x, y) = \sqrt{3}\,(x+y) - (1 - xy)\ ,$$

$$h_4(x, y) = \sqrt{3}\,(x+y) - (5 + 3xy)\ ,$$

$$h_5(x, y) = \sqrt{3}\,(x+y) + (3 + 5xy)\ ,$$

$$h_6(x, y) = \sqrt{3}\,(1 + 3xy) + (x - 3y)\ ,$$

$$h_7(x, y) = (1 + 3xy) - \sqrt{3}\,(x - 3y)\ ,$$

$$h_8(x, y) = \sqrt{3}\,(3 + xy) + (3x - y)\ ,$$

$$h_9(x, y) = (3 + xy) - \sqrt{3}\,(3x - y)\ .$$

The results for $\vec{B} \parallel [110]$ have a special feature: The Zeeman components for polarization perpendicular to the field do not have any characteristic circular polarization. This is a consequence of the absence of high rotational symmetry about the field direction. The relative intensities for linear polarization along [110], [$\bar{1}$10], and [00$\bar{1}$] are presented in Tables XIV A, XIV B, and XIV C, respectively. In tabulating the relative intensities for $\Gamma_8 \to \Gamma_8$, the following functions have been used:

$$F(x, y) = [16(1 + x^2)(1 + y^2)]^{-1}\ , \tag{77}$$

$$f_1(x, y) = (1 - xy) + \sqrt{3}\,(x - 3y)\ , \tag{78}$$

$$f_2(x, y) = (x + y) + \sqrt{3}\,(3 + xy)\ , \tag{79}$$

$$f_3(x, y) = (x + y) - \sqrt{3}\,(1 + 3xy)\ , \tag{80}$$

$$f_4(x, y) = (x + y) + \sqrt{3}\,(1 - xy)\ , \tag{81}$$

$$f_5(x, y) = (1 - xy) - \sqrt{3}\,(x + y)\ . \tag{82}$$

Note that, in each table, the Zeeman components $\mu \to \mu'$ and $-\mu \to -\mu'$ are listed next to each other; they have equal intensities for the linear Zeeman effect ($\delta_1 = \delta_2$, $\delta_1' = \delta_2'$). Also, the relative intensities of the Zeeman components of $\Gamma_8 \to \Gamma_6$ and $\Gamma_8 \to \Gamma_7$ reduce to the simple results of Johnston *et al.*[11] if we let $\delta_1 = \delta_2 = 0$; this again corresponds to the special case of a $j = \frac{3}{2}$-like Γ_8 level.

In general, the relative intensities for $\vec{B} \parallel [110]$ are functions of B. This field dependence results from the quadratic terms in the Zeeman Hamiltonian.

V. AN EXAMPLE: BORON IMPURITY IN GERMANIUM

We shall now briefly discuss the recent experimental work of Soepangkat *et al.*[16] on the Zeeman effect of boron acceptors in germanium. Measurements have been carried out in the Voigt configuration with $\vec{B} \parallel [001]$, using linearly polarized radiation. The prominent D line[17] of the excitation spectrum splits into four components for polarization parallel to $\vec{B}(\epsilon_\parallel)$ *or* perpendicular to $\vec{B}(\epsilon_\perp)$. The present theory, for a $\Gamma_8 \to \Gamma_8$ transition, predicts (see Table XI) four components for $\epsilon_\parallel$ and eight different components for $\epsilon_\perp$. Of the latter, four are of equal intensity ($= \frac{3}{16}u$), while the remaining four occur in pairs of equal intensity. Lin-Chung and Wallis[7] have calculated the relative intensities and g factors for shallow acceptors in germanium, by using the effective-mass wave functions of Mendelson and James.[18] Their results indicate that the parameter u is small ($\simeq \frac{1}{6}$). This suggests that the four components of equal intensity for $\epsilon_\perp$ are sufficiently weak to escape detection.

A detailed comparison between the present theory and the experimental data[16] leads to four possible assignments of quantum numbers to the Zeeman sublevels for the D line. If it is assumed that the larger calculated g factors[7] have the correct sign, then the values of the principal g factors obtained experimentally are

$$g_{1/2} = -1.53 \pm 0.09\ ,\quad g_{3/2} = 0.03 \pm 0.04$$

for the ground state, and

$$g_{1/2} = -6.14 \pm 0.13\ ,\quad g_{3/2} = 0.07 \pm 0.03$$

for the excited state. The principal g factors for $\vec{B} \parallel [001]$ are defined by

$$2\mu\,\mu_B\, g_\mu B = E_\mu^{(8)} - E_{-\mu}^{(8)}\ . \tag{83}$$

From Eq. (19) we find that

$$g_{1/2} = g_1' + \tfrac{1}{4} g_2'\ ,\quad g_{3/2} = g_1' + \tfrac{9}{4} g_2'\ .$$

Thus,

$$g_1' = g_{1/2} - \tfrac{1}{8}(g_{3/2} - g_{1/2})\ , \tag{84a}$$

$$g_2' = \tfrac{1}{2}(g_{3/2} - g_{1/2})\ . \tag{84b}$$

For the D line under consideration, we obtain

$$g_1' = -1.73 \pm 0.11\ ,\quad g_2' = 0.78 \pm 0.07$$

for the ground state, and

$$g_1' = -6.92 \pm 0.15\ ,\quad g_2' = 3.11 \pm 0.08$$

for the excited state. This gives the ratios

$$p \equiv (g_1'/g_2')_{\text{ground}} = -2.22^{+0.30}_{-0.34}\ ,$$

$$p' \equiv (g_1'/g_2')_{\text{excited}} = -2.23 \pm 0.11\ .$$

From Eq. (35) we calculate the parameters γ and γ' that characterize the relative intensities of the components for $\vec{B} \parallel [111]$:

$$\gamma = -1.83^{+0.83}_{-1.23}\ ,\quad \gamma' = -1.87 \pm 0.36\ . \tag{85}$$

Let us recall that for *linear* Zeeman effect $\delta_1 = \delta_2 = \delta$ and $\delta_1' = \delta_2' = \delta'$; the relative intensities for $\vec{B} \parallel [110]$ are characterized by the parameters δ and δ'. Using Eq. (55) we obtain

$$\delta = -1.16^{+0.43}_{-0.71}\ ,\quad \delta' = -1.17 \pm 0.21\ . \tag{86}$$

The uncertainties in the values of the parameters, shown in Eqs. (85) and (86), are large. However, Eqs. (36a) and (36b) and (56a)–(56d) reveal that these parameters are directly related to the energy splittings for $\vec{B} \parallel [111]$ and $\vec{B} \parallel [110]$, respectively, and should be determined experimentally. The relevant experiments are in progress.

TABLE XIV. Relative intensities of the Zeeman components in the Voigt configuration with $\vec{B} \parallel [110]$.

Zero-field transition	Components	Relative intensity
		A. Longitudinal polarization ($\epsilon_{\parallel}$)
$\Gamma_8 \to \Gamma_6$	$+\frac{3}{2} \to -\frac{1}{2}$	$\frac{1}{2}[\delta_1^2/(1+\delta_1^2)]$
	$-\frac{3}{2} \to +\frac{1}{2}$	$\frac{1}{2}[\delta_2^2/(1+\delta_2^2)]$
	$+\frac{1}{2} \to +\frac{1}{2}$	$\frac{1}{2}[1/(1+\delta_2^2)]$
	$-\frac{1}{2} \to -\frac{1}{2}$	$\frac{1}{2}[1/(1+\delta_1^2)]$
$\Gamma_8 \to \Gamma_7$	$+\frac{3}{2} \to +\frac{1}{2}$	$\frac{1}{8}[(\sqrt{3}\,\delta_1-1)^2/(1+\delta_1^2)]$
	$-\frac{3}{2} \to -\frac{1}{2}$	$\frac{1}{8}[(\sqrt{3}\,\delta_2-1)^2/(1+\delta_2^2)]$
	$+\frac{1}{2} \to -\frac{1}{2}$	$\frac{1}{8}[(\delta_2+\sqrt{3})^2/(1+\delta_2^2)]$
	$-\frac{1}{2} \to +\frac{1}{2}$	$\frac{1}{8}[(\delta_1+\sqrt{3})^2/(1+\delta_1^2)]$
$\Gamma_8 \to \Gamma_8$	$+\frac{3}{2} \to +\frac{1}{2}$	$F(\delta_1, \delta_2')[4(1+\delta_1\delta_2')^2(1-u)+\frac{1}{4}f_1^2(\delta_1, \delta_2')u-2(1+\delta_1\delta_2')f_1(\delta_1, \delta_2')v]$
	$-\frac{3}{2} \to -\frac{1}{2}$	$F(\delta_2, \delta_1')[4(1+\delta_2\delta_1')^2(1-u)+\frac{1}{4}f_1^2(\delta_2, \delta_1')u-2(1+\delta_2\delta_1')f_1(\delta_2, \delta_1')v]$
	$+\frac{3}{2} \to -\frac{3}{2}$	$F(\delta_1, \delta_2')[4(\delta_1-\delta_2')^2(1-u)+\frac{1}{4}f_2^2(\delta_1, \delta_2')u+2(\delta_1-\delta_2')f_2(\delta_1, \delta_2')v]$
	$-\frac{3}{2} \to +\frac{3}{2}$	$F(\delta_2, \delta_1')[4(\delta_2-\delta_1')^2(1-u)+\frac{1}{4}f_2^2(\delta_2, \delta_1')u+2(\delta_2-\delta_1')f_2(\delta_2, \delta_1')v]$
	$+\frac{1}{2} \to +\frac{3}{2}$	$F(\delta_1', \delta_2)[4(1+\delta_1'\delta_2)^2(1-u)+\frac{1}{4}f_1^2(\delta_1', \delta_2)u+2(1+\delta_1'\delta_2)f_1(\delta_1', \delta_2)v]$
	$-\frac{1}{2} \to -\frac{3}{2}$	$F(\delta_2', \delta_1)[4(1+\delta_2'\delta_1)^2(1-u)+\frac{1}{4}f_1^2(\delta_2', \delta_1)u+2(1+\delta_2'\delta_1)f_1(\delta_2', \delta_1)v]$
	$+\frac{1}{2} \to -\frac{1}{2}$	$F(\delta_2, \delta_1')[4(\delta_2-\delta_1')^2(1-u)+\frac{1}{4}f_3^2(\delta_2, \delta_1')u-2(\delta_2-\delta_1')f_3(\delta_2, \delta_1')v]$
	$-\frac{1}{2} \to +\frac{1}{2}$	$F(\delta_1, \delta_2')[4(\delta_1-\delta_2')^2(1-u)+\frac{1}{4}f_3^2(\delta_1, \delta_2')u-2(\delta_1-\delta_2')f_3(\delta_1, \delta_2')v]$
		B. Transverse polarization ($\epsilon_{\perp}$) of radiation propagating along $[00\bar{1}]$
$\Gamma_8 \to \Gamma_6$	$+\frac{3}{2} \to +\frac{1}{2}$	$\frac{1}{8}[(\delta_1+\sqrt{3})^2/(1+\delta_1^2)]$
	$-\frac{3}{2} \to -\frac{1}{2}$	$\frac{1}{8}[(\delta_2+\sqrt{3})^2/(1+\delta_2^2)]$
	$+\frac{1}{2} \to -\frac{1}{2}$	$\frac{1}{8}[(\sqrt{3}\delta_2-1)^2/(1+\delta_2^2)]$
	$-\frac{1}{2} \to +\frac{1}{2}$	$\frac{1}{8}[(\sqrt{3}\,\delta_1-1)^2/(1+\delta_1^2)]$
$\Gamma_8 \to \Gamma_7$	$+\frac{3}{2} \to -\frac{1}{2}$	$\frac{1}{2}[1/(1+\delta_1^2)]$
	$-\frac{3}{2} \to +\frac{1}{2}$	$\frac{1}{2}[1/(1+\delta_2^2)]$
	$+\frac{1}{2} \to +\frac{1}{2}$	$\frac{1}{2}[\delta_2^2/(1+\delta_2^2)]$
	$-\frac{1}{2} \to -\frac{1}{2}$	$\frac{1}{2}[\delta_1^2/(1+\delta_1^2)]$
$\Gamma_8 \to \Gamma_8$	$+\frac{3}{2} \to +\frac{3}{2}$	$F(\delta_1, \delta_1')[4(\delta_1-\delta_1')^2(1-u)+\frac{1}{4}f_3^2(\delta_1, \delta_1')u+2(\delta_1-\delta_1')f_3(\delta_1, \delta_1')v]$
	$-\frac{3}{2} \to -\frac{3}{2}$	$F(\delta_2, \delta_2')[4(\delta_2-\delta_2')^2(1-u)+\frac{1}{4}f_3^2(\delta_2, \delta_2')u+2(\delta_2-\delta_2')f_3(\delta_2, \delta_2')v]$
	$+\frac{3}{2} \to -\frac{1}{2}$	$F(\delta_1', \delta_1)[4(1+\delta_1'\delta_1)^2(1-u)+\frac{1}{4}f_1^2(\delta_1', \delta_1)u-2(1+\delta_1'\delta_1)f_1(\delta_1', \delta_1)v]$
	$-\frac{3}{2} \to +\frac{1}{2}$	$F(\delta_2', \delta_2)[4(1+\delta_2'\delta_2)^2(1-u)+\frac{1}{4}f_1^2(\delta_2', \delta_2)u-2(1+\delta_2'\delta_2)f_1(\delta_2', \delta_2)v]$
	$+\frac{1}{2} \to +\frac{1}{2}$	$F(\delta_2, \delta_2')[4(\delta_2-\delta_2')^2(1-u)+\frac{1}{4}f_2^2(\delta_2, \delta_2')u-2(\delta_2-\delta_2')f_2(\delta_2, \delta_2')v]$
	$-\frac{1}{2} \to -\frac{1}{2}$	$F(\delta_1, \delta_1')[4(\delta_1-\delta_1')^2(1-u)+\frac{1}{4}f_2^2(\delta_1, \delta_1')u-2(\delta_1-\delta_1')f_2(\delta_1, \delta_1')v]$
	$+\frac{1}{2} \to -\frac{3}{2}$	$F(\delta_2, \delta_2')[4(1+\delta_2\delta_2')^2(1-u)+\frac{1}{4}f_1^2(\delta_2, \delta_2')u+2(1+\delta_2\delta_2')f_1(\delta_2, \delta_2')v]$
	$-\frac{1}{2} \to +\frac{3}{2}$	$F(\delta_1, \delta_1')[4(1+\delta_1\delta_1')^2(1-u)+\frac{1}{4}f_1^2(\delta_1, \delta_1')u+2(1+\delta_1\delta_1')f_1(\delta_1, \delta_1')v]$

TABLE XIV. (*Continued*)

Zero-field Transition	Component	Relative intensity
	C. Transverse polarization ($\epsilon_\perp$) of radiation propagating along [$\bar{1}$10]	
	$+\frac{3}{2}\to+\frac{1}{2}$	$\frac{1}{8}[(\delta_1-\sqrt{3})^2/(1+\delta_1^2)]$
$\Gamma_8\to\Gamma_6$	$-\frac{3}{2}\to-\frac{1}{2}$	$\frac{1}{8}[(\delta_2-\sqrt{3})^2/(1+\delta_2^2)]$
	$+\frac{1}{2}\to-\frac{1}{2}$	$\frac{1}{8}[(\sqrt{3}\,\delta_2+1)^2/(1+\delta_2^2)]$
	$-\frac{1}{2}\to+\frac{1}{2}$	$\frac{1}{8}[(\sqrt{3}\,\delta_1+1)^2/(1+\delta_1^2)]$
	$+\frac{3}{2}\to-\frac{1}{2}$	$\frac{1}{8}[(\sqrt{3}\,\delta_1+1)^2/(1+\delta_1^2)]$
$\Gamma_8\to\Gamma_7$	$-\frac{3}{2}\to+\frac{1}{2}$	$\frac{1}{8}[(\sqrt{3}\,\delta_2+1)^2/(1+\delta_2^2)]$
	$+\frac{1}{2}\to+\frac{1}{2}$	$\frac{1}{8}[(\delta_2-\sqrt{3})^2/(1+\delta_2^2)]$
	$-\frac{1}{2}\to-\frac{1}{2}$	$\frac{1}{8}[(\delta_1-\sqrt{3})^2/(1+\delta_1^2)]$
	$+\frac{3}{2}\to+\frac{3}{2}$	$F(\delta_1,\delta_1')[f_4^2(\delta_1,\delta_1')(1-u)+4(\delta_1-\delta_1')^2u-4(\delta_1-\delta_1')f_4(\delta_1,\delta_1')v]$
	$-\frac{3}{2}\to-\frac{3}{2}$	$F(\delta_2,\delta_2')[f_4^2(\delta_2,\delta_2')(1-u)+4(\delta_2-\delta_2')^2u-4(\delta_2-\delta_2')f_4(\delta_2,\delta_2')v]$
	$+\frac{3}{2}\to-\frac{1}{2}$	$F(\delta_1,\delta_1')[f_5^2(\delta_1,\delta_1')(1-u)+4(1+\delta_1\delta_1')^2u+4(1+\delta_1\delta_1')f_5(\delta_1,\delta_1')v]$
	$-\frac{3}{2}\to+\frac{1}{2}$	$F(\delta_2,\delta_2')[f_5^2(\delta_2,\delta_2')(1-u)+4(1+\delta_2\delta_2')^2u+4(1+\delta_2\delta_2')f_5(\delta_2,\delta_2')v]$
$\Gamma_8\to\Gamma_8$	$+\frac{1}{2}\to+\frac{1}{2}$	$F(\delta_2,\delta_2')[f_4^2(\delta_2,\delta_2')(1-u)+4(\delta_2-\delta_2')^2u+4(\delta_2-\delta_2')f_4(\delta_2,\delta_2')v]$
	$-\frac{1}{2}\to-\frac{1}{2}$	$F(\delta_1,\delta_1')[f_4^2(\delta_1,\delta_1')(1-u)+4(\delta_1-\delta_1')^2u+4(\delta_1-\delta_1')f_4(\delta_1,\delta_1')v]$
	$+\frac{1}{2}\to-\frac{3}{2}$	$F(\delta_2,\delta_2')[f_5^2(\delta_2,\delta_2')(1-u)+4(1+\delta_2\delta_2')^2u-4(1+\delta_2\delta_2')f_5(\delta_2,\delta_2')v]$
	$-\frac{1}{2}\to+\frac{3}{2}$	$F(\delta_1,\delta_1')[f_5^2(\delta_1,\delta_1')(1-u)+4(1+\delta_1\delta_1')^2u-4(1+\delta_1\delta_1')f_5(\delta_1,\delta_1')v]$

Our theory provides the framework for a complete analysis of the experimental data for all three crystalline orientations of the field. Such an analysis is expected to yield more accurate values for the g factors. It should be noted that the parameters u and v that appear in the relative intensities of the Zeeman components can be independently determined from an investigation of the stress-induced components.[12]

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APPENDIX A

Our objective here is to show that $\psi_\mu^{(i)}$ and $\varphi_\mu^{(i)}$ belong to the same row of the irreducible representation Γ_i ($i=6-8$).

Comparing Eqs. (1) and (3) for linear terms in $\vec{B}$ we find that

$$\langle\psi_\mu^{(i)}|(\vec{1}+2\vec{s})|\psi_\nu^{(i)}\rangle=g^{(i)}\langle\varphi_\mu^{(i)}|\vec{J}|\varphi_\nu^{(i)}\rangle \tag{A1}$$

for $i=6$, 7.

The operators l_x+2s_x, l_y+2s_y, l_z+2s_z belong to Γ_4 of $\overline{T}_d$, that is,

$$P_R(l_k+2s_k)P_R^{-1}=\textstyle\sum_j\Gamma_{jk}^{(4)}(R)(l_j+2s_j)\,, \tag{A2}$$

where k, $j=x$, y, z; P_R is the Hilbert-space operator corresponding to the operation R of $\overline{T}_d$, and $\Gamma^{(4)}(R)$ is the matrix representation of P_R in the subspace of Γ_4. Similarly,

$$P_R\hat{J}_kP_R^{-1}=\textstyle\sum_j\Gamma_{jk}^{(4)}(R)\hat{J}_j\,. \tag{A3}$$

Combining (A1)–(A3) we obtain

$$\langle\psi_\mu^{(i)}|P_R(l_k+2s_k)P_R^{-1}|\psi_\nu^{(i)}\rangle=g^{(i)}\langle\varphi_\mu^{(i)}|P_R\hat{J}_kP_R^{-1}|\varphi_\nu^{(i)}\rangle\,. \tag{A4}$$

Now,

$$P_R|\varphi_\mu^{(i)}\rangle=\sum_{\mu'}\Gamma_{\mu'\mu}^{(i)}|\varphi_{\mu'}^{(i)}\rangle\,. \tag{A5}$$

Substituting (A5) in (A4) and using (A1), we have

$$\langle\psi_\mu^{(i)}|P_R(l_k+2s_k)P_R^{-1}|\psi_\nu^{(i)}\rangle=\sum_{\mu',\nu'}\Gamma_{\mu\mu'}^{(i)}(R)\,\langle\psi_{\mu'}^{(i)}|(l_k+2s_k)|\psi_{\nu'}^{(i)}\rangle\,\Gamma_{\nu'\nu}^{(i)\dagger}(R)\,.$$

Thus

$$P_R|\psi_\mu^{(i)}\rangle=\sum_{\mu'}\Gamma^{(i)}_{\mu'\mu}(R)|\psi^{(i)}_{\mu'}\rangle \ . \qquad (A6)$$

Comparison of (A5) and (A6) demonstrates that $\psi_\mu^{(i)}$ and $\varphi_\mu^{(i)}$ belong to the same row of Γ_i ($i=6$, 7), that is,

$$\langle\psi_\mu^{(i)}|P_R|\psi_{\mu'}^{(i)}\rangle=\langle\varphi_\mu^{(i)}|P_R|\varphi_{\mu'}^{(i)}\rangle \ . \qquad (A7)$$

In an exactly similar manner, Eq. (A7) can be established for $i=8$, starting with

$$\langle\psi_\mu^{(8)}|(l_k+2s_k)|\psi_\nu^{(8)}\rangle=\langle\varphi_\mu^{(8)}|g_1'\hat{J}_k+g_2'\hat{J}_k^3|\varphi_\nu^{(8)}\rangle$$

and noting that $\hat{J}_x^3$, $\hat{J}_y^3$, $\hat{J}_z^3$ belong to Γ_4.

APPENDIX B

Here we shall derive the rotation matrices $D^{(1/2)}(\alpha,\beta,\gamma)$ and $D^{(3/2)}(\alpha,\beta,\gamma)$.

The operator

$$\hat{R}(\alpha,\beta,\gamma)=e^{-i\alpha\hat{J}_z}e^{-i\beta\hat{J}_y}e^{-i\gamma\hat{J}_z}$$

rotates the contour of a function by the Eulerian angles (α, β, γ). The rotation matrices are defined by

$$D^{(j)}_{\mu'\mu}(\alpha,\beta,\gamma)\equiv\langle j\mu'|\hat{R}(\alpha,\beta,\gamma)|j\mu\rangle \ ,$$

where

$$\hat{J}^2|j\mu\rangle=j(j+1)|j\mu\rangle$$

and

$$\hat{J}_z|j\mu\rangle=\mu|j\mu\rangle \ .$$

Thus, we have

$$D^{(j)}_{\mu'\mu}(\alpha,\beta,\gamma)=e^{-i\mu'\alpha}d^{(j)}_{\mu'\mu}(\beta)e^{-i\mu\gamma} \ , \qquad (B1)$$

where

$$d^{(j)}_{\mu'\mu}(\beta)\equiv\langle j\mu'|e^{-i\beta\hat{J}_y}|j\mu\rangle \ .$$

The point to be noted is that the matrix $d^{(j)}(\beta)$ depends on the phase convention for the functions $|j\mu\rangle$. Using Sylvester's formula[19] we obtain

$$d^{(j)}(\beta)=\sum_{\mu=-j}^{j}e^{-i\mu\beta}\prod_{\mu'\neq\mu}\frac{\mu'-\hat{J}_y}{\mu'-\mu} \ . \qquad (B2)$$

For $j=\frac{1}{2}$, Eq. (B2) yields

$$d^{(1/2)}(\beta)=\cos(\tfrac{1}{2}\beta)-2i[\sin(\tfrac{1}{2}\beta)]j_y \ . \qquad (B3)$$

By using the matrix j_y of Eq. (4) we obtain the rotation matrix $D^{(1/2)}(\alpha,\beta,\gamma)$, suitable for the phase convention of $\{\varphi_\mu^{(6)}\}$ and $\{\varphi_\mu^{(7)}\}$.

For $j=\frac{3}{2}$, Eq. (B2) gives

$$\begin{aligned}d^{(3/2)}(\beta)=&\tfrac{1}{8}[-\cos(\tfrac{3}{2}\beta)+9\cos(\tfrac{1}{2}\beta)]\\&+i\tfrac{1}{4}[\tfrac{1}{3}\sin(\tfrac{3}{2}\beta)-9\sin(\tfrac{1}{2}\beta)]J_y\\&+\tfrac{1}{2}[\cos(\tfrac{3}{2}\beta)-\cos(\tfrac{1}{2}\beta)]J_y^2\\&+i[-\tfrac{1}{3}\sin(\tfrac{3}{2}\beta)+\sin(\tfrac{1}{2}\beta)]J_y^3 \ . \qquad (B4)\end{aligned}$$

By using the matrix J_y of Eq. (9) we obtain the rotation matrix $D^{(3/2)}(\alpha,\beta,\gamma)$ suitable for the phase convention of $\{\varphi_\mu^{(8)}\}$.

APPENDIX C

The matrices $[\langle\varphi_\nu^{(6)}|\vec{Q}|\varphi_\mu^{(8)}\rangle]$ and $[\langle\varphi_\nu^{(7)}|\vec{Q}|\varphi_\mu^{(8)}\rangle]$ will be derived here.

$\vec{Q}|\varphi_\mu^{(8)}\rangle$ involves the spatial functions $\vec{Q}X$, $\vec{Q}Y$, and $\vec{Q}Z$; the nine functions can be projected onto various irreducible representations of T_d:

Γ_1: $\kappa_0=Q_xX+Q_yY+Q_zZ$;

Γ_3: $\kappa_1=2Q_zZ-Q_xX-Q_yY$, $\kappa_2=\sqrt{3}(Q_xX-Q_yY)$;

Γ_4: $\kappa_\xi=\frac{1}{2}(Q_yZ-Q_zY)$, $\kappa_\eta=\frac{1}{2}(Q_zX-Q_xZ)$, $\kappa_\zeta=\frac{1}{2}(Q_xY-Q_yX)$;

Γ_5: $\kappa_x=\frac{1}{2}(Q_yZ+Q_zY)$, $\kappa_y=\frac{1}{2}(Q_zX+Q_xZ)$, $\kappa_z=\frac{1}{2}(Q_xY+Q_yX)$.

The spatial part of $\varphi_\nu^{(6)}$ is $f_0(r)$, belonging to Γ_1. This forms a nonvanishing scalar product with κ_0 only. Thus, the only nonzero matrix elements $\langle\varphi_\nu^{(6)}|\vec{Q}|\varphi_\mu^{(8)}\rangle$ are those proportional to

$$\int f_0(r)Q_xX\,d\vec{r}=\int f_0(r)Q_yY\,d\vec{r}=\int f_0(r)Q_zZ\,d\vec{r} \ .$$

It is now easy to deduce $\langle\varphi_\nu^{(6)}|\vec{Q}|\varphi_\mu^{(8)}\rangle$ in a straightforward manner. For example,

$$\begin{aligned}\langle\varphi_{+1/2}^{(6)}|\vec{Q}|\varphi_{+3/2}^{(8)}\rangle&=(1/\sqrt{2})\int f_0(r)\vec{Q}(X+iY)\,d\vec{r}\\&=(1/\sqrt{2})(\hat{x}+i\hat{y})\int f_0(r)Q_xX\,d\vec{r} \ .\end{aligned}$$

We obtain

$$[\langle\varphi_\nu^{(6)}|\vec{Q}|\varphi_\mu^{(8)}\rangle]=d_0\begin{bmatrix}\sqrt{3}(\hat{x}+i\hat{y}) & -2i\hat{z} & (\hat{x}-i\hat{y}) & 0\\ 0 & i(\hat{x}+i\hat{y}) & 2\hat{z} & i\sqrt{3}(\hat{x}-i\hat{y})\end{bmatrix} \ ,$$

where $d_0=(1/\sqrt{6})\int f_0(r)Q_xX\,d\vec{r}$.

The spatial parts of $\varphi_\nu^{(7)}$ contain X, Y, Z. These form nonvanishing scalar products with κ_x, κ_y, κ_z, respectively. Thus, the only nonzero matrix elements $\langle\varphi_\nu^{(7)}|\vec{Q}|\varphi_\mu^{(8)}\rangle$ are those proportional to

$$\int XQ_yZ\,d\vec{r}=\int XQ_zY\,d\vec{r}=\int YQ_zX\,d\vec{r}=\int YQ_xZ\,d\vec{r}$$

$$=\int ZQ_xY\,d\vec{r}=\int ZQ_yX\,d\vec{r} \ .$$

Now the matrix elements can be calculated easily. For example,

$$\begin{aligned}\langle\varphi_{+1/2}^{(7)}|\vec{Q}|\varphi_{+3/2}^{(8)}\rangle&=(1/\sqrt{6})\int Z\vec{Q}(X+iY)\,d\vec{r}\\&=(1/\sqrt{6})(\hat{y}+i\hat{x})\int ZQ_xY\,d\vec{r} \ .\end{aligned}$$

We obtain

$$[\langle\varphi_\nu^{(7)}|\vec{Q}|\varphi_\mu^{(8)}\rangle]=d_0'\begin{bmatrix}-(\hat{x}-i\hat{y}) & 0 & \sqrt{3}(\hat{x}+i\hat{y}) & 2i\hat{z}\\ -2\hat{z} & i\sqrt{3}(\hat{x}-i\hat{y}) & 0 & -i(\hat{x}+i\hat{y})\end{bmatrix},$$

where

$$d_0'=-(i/\sqrt{6})\int XQ_yZ\,d\vec{r}\ .$$

APPENDIX D

Here we shall present the most general symmetry forms for the impurity wave functions $\{\psi_\mu^{(i)}\}$ $(i=6-8)$.

We first note that the spinors $\{|\alpha\rangle, |\beta\rangle\}$ generate the representation Γ_6. In general, $\psi_\mu^{(i)}$ is a linear combination of products of these spinors with spatial functions. The spatial functions, however, can be classified according to the single-valued irreducible representations of $\overline{T}_d$. Let us define the following functions of x, y, z by specifying their transformation properties *under* T_d:

Γ_1: f transforms as

$$x^2+y^2+z^2\ ;$$

Γ_2: g transforms as

$$x^4(y^2-z^2)+y^4(z^2-x^2)+z^4(x^2-y^2)\ ;$$

Γ_3: $\{w_1, w_2\}$ transform as

$$\{2z^2-x^2-y^2,\ \sqrt{3}(x^2-y^2)\}\ ;$$

Γ_4: $\{\xi, \eta, \zeta\}$ transform as the x, y, z components of an axial vector;

Γ_5: $\{X', Y', Z'\}$ transform as the x, y, z components of a polar vector.

The functions are assumed to be real and normalized. The products of these functions with $\{|\alpha\rangle, |\beta\rangle\}$ generate double-valued representations of $\overline{T}_d$ according to the following scheme:

$$\Gamma_1\times\Gamma_6=\Gamma_6\ ,\qquad \Gamma_2\times\Gamma_6=\Gamma_7\ ,\qquad \Gamma_3\times\Gamma_6=\Gamma_8\ ,$$

$$\Gamma_4\times\Gamma_6=\Gamma_6+\Gamma_8\ ,\qquad \Gamma_5\times\Gamma_6=\Gamma_7+\Gamma_8\ .$$

Thus, there are two types of Γ_6 functions, two types of Γ_7 functions, and three types of Γ_8 functions, each type being derived from a distinct single-valued representation. The most general form of $\psi_\mu^{(i)}$ is then a linear combination of functions of these distinct types. We obtain

$$\psi_\mu^{(i)}=a^{(i)}\Phi_\mu^{(i)}+b^{(i)}\Lambda_\mu^{(i)}+c^{(i)}\chi_\mu^{(i)}\ , \qquad \text{(D1)}$$

where $c^{(6)}=c^{(7)}\equiv 0$ and

$$\Phi_{+1/2}^{(6)}=f|\alpha\rangle\ ,\quad \Phi_{-1/2}^{(6)}=f|\beta\rangle\ ;$$
$$\Lambda_{+1/2}^{(6)}=(1/\sqrt{3})[(\xi+i\eta)|\beta\rangle+\zeta|\alpha\rangle]\ ,$$
$$\Lambda_{-1/2}^{(6)}=(1/\sqrt{3})[(\xi-i\eta)|\alpha\rangle-\zeta|\beta\rangle]\ ;$$
$$\Phi_{+1/2}^{(7)}=(1/\sqrt{3})[(X'+iY')|\beta\rangle+Z'|\alpha\rangle]\ ,$$
$$\Phi_{-1/2}^{(7)}=(1/\sqrt{3})[(X'-iY')|\alpha\rangle-Z'|\beta\rangle]\ ;$$
$$\Lambda_{+1/2}^{(7)}=g|\alpha\rangle\ ,\quad \Lambda_{-1/2}^{(7)}=g|\beta\rangle\ ;$$
$$\Phi_{+3/2}^{(8)}=(1/\sqrt{2})(X'+iY')|\alpha\rangle\ ,$$
$$\Phi_{+1/2}^{(8)}=(i/\sqrt{6})[(X'+iY')|\beta\rangle-2Z'|\alpha\rangle]\ ,$$
$$\Phi_{-1/2}^{(8)}=(1/\sqrt{6})[(X'-iY')|\alpha\rangle+2Z'|\beta\rangle]\ ,$$
$$\Phi_{-3/2}^{(8)}=(i/\sqrt{2})(X'-iY')|\beta\rangle\ ;$$
$$\Lambda_{+3/2}^{(8)}=-(1/\sqrt{6})[(\xi-i\eta)|\alpha\rangle+2\zeta|\beta\rangle]\ ,$$
$$\Lambda_{+1/2}^{(8)}=(i/\sqrt{2})(\xi-i\eta)|\beta\rangle\ ,$$
$$\Lambda_{-1/2}^{(8)}=(1/\sqrt{2})(\xi+i\eta)|\alpha\rangle\ ,$$
$$\Lambda_{-3/2}^{(8)}=-(i/\sqrt{6})[(\xi+i\eta)|\beta\rangle-2\zeta|\alpha\rangle]\ ;$$
$$\chi_{+3/2}^{(8)}=w_1|\beta\rangle\ ,\quad \chi_{+1/2}^{(8)}=-iw_2|\alpha\rangle\ ,$$
$$\chi_{-1/2}^{(8)}=w_2|\beta\rangle\ ,\quad \chi_{-3/2}^{(8)}=-iw_1|\alpha\rangle\ .$$

It should be noted that the functions $\Phi_\mu^{(i)}$, $\Lambda_\mu^{(i)}$, and $\chi_\mu^{(i)}$ are orthogonal to one another, and belong to the same row of Γ_i. The angular momentum eigenfunctions $\{\varphi_\mu^{(i)}\}$ represent a special case of $\{\Phi_\mu^{(i)}\}$.

The forms of $\{\psi_\mu^{(i)}\}$ used in Ref. 12 correspond to the restrictive assumption $b^{(6)}=a^{(7)}=c^{(8)}=0$.

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their $6S_4$. Notice, however, that we have not followed this reference in the character tables for $\overline{S}_4$, $\overline{C}_3$, and $\overline{C}_{1h}$. In fact, the character table for $\overline{S}_4$ is incorrect in this reference.

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Linewidths and Two-Electron Processes in Spin-Flip Raman Scattering from CdS and ZnSe

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We present inelastic-light-scattering data and analyses for spin-flip scattering from conduction electrons in CdS and ZnSe. Cross sections, linewidths, and line shapes are studied as functions of magnetic field, temperature, scattering angle, and donor concentration. Both free-conduction-electron spin-flip processes and spin-flip processes involving conduction electrons bound to shallow donors are observed. These processes exhibit different selection rules and temperature dependences; the free-electron spin-flip processes exhibit only α_{ij} scattering in which $i \neq j$ and i or $j \parallel \vec{H}$ as expected, while the bound-electron spin-flip processes also exhibit strong α_{xx} and α_{yy} scattering (z is the [0001] optic axis), in agreement with the selection rules calculated for shallow donors at C_{3v} Cd sites by Thomas and Hopfield. For right-angle scattering, the free-electron linewidth increases from $0.05\,\text{cm}^{-1}$ (half-width at half-height) at 2 °K to about 4 cm^{-1} at ~ 150 °K in both ZnSe and CdS. This broadening is not due to a decrease in spin lifetime, but rather to a spin diffusion, as directly confirmed by the angular dependence of the spin-flip linewidth. The linewidth is observed to vary as q^2, where q is the momentum transfer in the light-scattering process. Bound-electron scattering exhibits a linewidth which is independent of scattering angle and nearly independent of temperature over the 2–150 °K range. The spin-diffusion model is thus not applicable to bound-electron scattering. The double spin-flip process observed involves two interacting electrons with an apparent attractive energy of 0.25 ± 0.05 cm^{-1}. Selection rules, relative cross sections, field dependence, and binding energy of the double spin-flip transition are discussed. At sufficiently high input powers ($\gtrsim 3$ MW/cm^2) the CdS single spin-flip scattering becomes stimulated, resulting in a tunable, visible, spin-flip laser.

I. INTRODUCTION

In an earlier paper[1] we reported spin-flip scattering from free conduction electrons in the wide-gap semiconductors CdS and ZnSe. Reference 1 emphasized the determination of selection rules, gyromagnetic ratios (g values), and absolute scattering cross section and indicated the existence of anomalous linewidths. In the present work[2] we have systematically studied the spin-flip line shapes, the dependence of linewidth upon temperature, magnetic field, and scattering angle, and change in selection rules as the sample temperature is reduced below the exciton binding energy. We have examined scattering cross sections as functions of several parameters (temperature, field, laser power, laser frequency, donor concentration); and finally, we have studied a new two-electron scattering process involving simultaneous spin-flip scattering of two electrons bound to nearby donors. The latter process is highly resonant, involves a total spin change of $\Delta S = \pm 2$, and exhibits a spin-spin interaction energy of 0.03–0.04 meV (0.2–0.3 cm^{-1}).

In Sec. II we present line-shape and linewidth measurements as functions of temperature, field, and scattering angle. In Sec. III we present temperature and field dependences of cross sections and briefly mention the observation of stimulated spin-flip scattering in CdS. In Sec. IV the selection rules at different temperatures are discussed. Section V is concerned with the double spin-flip process, including its selection rules, resonant cross sections, and dependence upon donor concentrations.

The basic theory of spin-flip scattering is at