EIGENVALUE APPROACH TO DISCRETE DOUBLE GROUPS OF SYMMETRY ELEMENTS

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A complete set of independent and commuting symmetry operators is defined for discrete double groups of symmetry elements. Possible sets of eigenvalues of this complete set are derived. The eigenstates are related to irreducible double valued representations. The discussion involves the double groups C'_n, S'_{2n}, C'_{nv}, C'_{nh}, D'_n, D'_{nh}, D'_{nd}, T', T'_h, T'_d, O' and O'_h.

1. *Introduction*

It has been shown recently by the author (Gołębiewski, 1970) that for any discrete point group of symmetry elements a complete set of independent and commuting "symmetry operators can be defined. The eigenvalues of this set of operators characterize the symmetry eigenfunctions" in a similar way as do the full representation matrices in the standard approach. The eigenvalue description has made it possible to introduce a new type of projection operators into the framework of the group theory of discrete point groups. In the present work we are going to extend this treatment to double groups in order to cover the double valued representations. In what follows we mean by I a reference to the previous work (Gołębiewski, 1970) in which all theorems necessary in this treatment are described in details.

2. *Properties of symmetry operators. Equivalence*

Let R_1, R_2, ..., R_h be a set of symmetry operators which make up a group G. With any symmetry operator R_t there is associated a new coordinate system. We can put

$$R_t(xyz) = (xyz)\, \boldsymbol{D}_l(R_t),\ t = 1, 2, ..., h \tag{1}$$

where $\boldsymbol{D}_l(R_t)$ is, by definition, the regular representation of the element R_t. Usually we say that $R_t = R_v$ if, and only if, $\boldsymbol{D}_l(R_t) = \boldsymbol{D}_l(R_v)$.

We adopt a similar convention for the case of double groups, putting

$$R_t(\alpha\, \beta) = (\alpha\beta)\, \boldsymbol{D}_s(R_t),\ \ t = 1,\ 2,\ ...,\ h \tag{2}$$

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where α and β are spinfunctions for spin 1/2 and its components $\pm 1/2$. We say that $R_t = R_v$ if, and only if, $\boldsymbol{D}_l(R_t) = \boldsymbol{D}_l(R_v)$ and simultaneously $\boldsymbol{D}_s(R_t) = \boldsymbol{D}_s(R_v)$.

It is customary to derive the regular matrices $\boldsymbol{D}_l(R_t)$ and $\boldsymbol{D}_s(R_t)$ with the use of the Euler transformations. However, an alternative treatment seems to be more convenient in many cases. Let Θ be, for example, the rotation angle, and let $\vec{e}$ be a unit vector parallel to the rotation axis. For clockwise rotation of the coordinate system we have then that $R_t(\Theta, \vec{e}) = \exp\left(+\frac{i}{\hbar}\,\Theta\vec{e}\cdot\vec{l}\right)$, when acting upon a function of Cartesian coordinates, and $R_t(\Theta, \vec{e}) = \exp\left(+\frac{i}{\hbar}\,\Theta\vec{e}\cdot\vec{s}\right)$, when acting upon a spin function. Acting with these operators upon the row vector (xyz) or $(\alpha\beta)$ respectively, one finds what follows:

$$C_n^k(\vec{e})\,(xyz) = (xyz)\,\{\mathbf{1}\cos x + \boldsymbol{V}(1-\cos x) + \boldsymbol{W}\sin x\} \tag{3}$$

$$C_n^k(\vec{e})\,(\alpha\beta) = (\alpha\beta)\left\{\mathbf{1}\cos\frac{x}{2} + i\sin\frac{x}{2}\,\boldsymbol{T}\right\} \tag{4}$$

$$\mathrm{i}\,(xyz) \stackrel{\text{def}}{=} -(xyz)\,;\ \mathrm{i}\,(\alpha\beta) \stackrel{\text{def}}{=} (\alpha\beta) \tag{5}$$

$$\sigma(\vec{e})\,(xyz) \stackrel{\text{def}}{=} Q\,\mathrm{i}\,C_2(\vec{e})\,(xyz) = (xyz)\,(\mathbf{1}-2\boldsymbol{V}) \tag{6}$$

$$\sigma(\vec{e})\,(\alpha\beta) = -\mathrm{i}\,(\alpha\beta)\,\boldsymbol{T} \tag{7}$$

$$S(_n^k, \vec{e})\,(xyz) = C_n^k(\vec{e})\,\sigma_h(\vec{e})\,(xyz)$$

$$= (xyz)\,\{\mathbf{1}\cos x - \boldsymbol{V}(1+\cos x) + \boldsymbol{W}\sin x\} \tag{8}$$

$$(S_n^k, \vec{e})\,(\alpha\beta) = (\alpha\beta)\left\{\mathbf{1}\sin\frac{x}{2} - i\cos\frac{x}{2}\,\boldsymbol{T}\right\} \tag{9}$$

where $x = 2\pi k/n$, $Q = R(2\pi, \vec{e})$ and

$$\boldsymbol{V} = \begin{pmatrix} e_x e_x & e_x e_y & e_x e_z \\ e_y e_x & e_y e_y & e_y e_z \\ e_z e_x & e_z e_y & e_z e_z \end{pmatrix}, \quad \boldsymbol{W} = \begin{pmatrix} 0 & e_z & -e_y \\ -e_z & 0 & e_x \\ e_y & -e_x & 0 \end{pmatrix} \tag{10}$$

$$\boldsymbol{T} = \begin{pmatrix} e_z & e_x - ie_y \\ e_z + ie_y & -e_z \end{pmatrix}. \tag{11}$$

In spite of the evident simplicity of these formulae we could not find them in standard books on group theory and quantum mechanics [*e. g.* Bhagavantam, Venkatarayudu (1951), Cotton (1963), Hamermesh (1962), Heine (1960), Messiah (1962), Tinkham (1964)]. However, we did not try to trace them in the more than voluminous literature. One way or another, these are the formulae which have been used to prove all equivalence relations applied in this work.

Formulae (3) to (11) allow one, for example, to prove easily that *i*) if there is an axis $C_2' \perp C_n$ or a reflection plane $\sigma_v || C_n$, then C_n and $C_n^{n-1}Q$ belong to the same class; *ii*) if there is an axis $C_2' \perp S_n$ or a reflection plane $\sigma_v || S_n$, then S_n and $S(_n^{n-1})$ belong to the same class; *iii*) if there is an axis $C_2 || \sigma$ then σ and σQ belong to the same class.

3. *Groups C_n', S_n' and D_n'*

The case of groups C_n' and S_n' (for even n's) is trivial. We reproduce the double valued eigenvalues in Tables I and II for completness.

Tables of symmetry eigenvalues for double groups

TABLE 1

Groups C_{2n}' and S_{2n}'

C_{2n}' S_{2n}'	E_1'		E_2'		E_3'		...	E_n'		Comment
	τ_1'	τ_2'	τ_3'	τ_4'	τ_5'	τ_6'	...	τ_{2n-1}'	τ_{2n}'	
$\lambda(C_{2n})$ $\lambda(S_{2n})$	z	z^{-1}	z^3	z^{-3}	z^5	z^{-5}	...	z^{2n-1}	z^{1-2n}	$z = \exp(\pi i/2n)$; all bases are formally 1-dimensional

TABLE II

Groups C_{2n+1}'

C_{2n+1}'	A'	E_1'		E_2'		...	E_n'		Comment
	τ_1'	τ_2'	τ_3'	τ_4'	τ_5'	...	τ_{2n}'	τ_{2n+1}'	
$\lambda(C_{2n+1})$	-1	z	z^{-1}	z^3	z^{-3}	...	z^{2n-1}	z^{1-2n}	$z = \exp[\pi i/(2n+1)]$; all bases are formally 1-dimensional

The group D_n' is generated by two operators, C_2' and C_n. Thus C_n and $C_n^{n-1}Q = C_n^{-1}$ belong to the same class. Following the definition of the almost complete set (I.2) we find the set: $X = C_2'$ and $Y = \frac{1}{2}(C_n + C_n^{n-1}Q)$. Looking for possible eigenvalues of X and Y we find that $\lambda(X) = \pm 1$, $\pm i$ and $\lambda(Y) = \cos\frac{k\pi}{n}$, where $k = 0, 1, 2, \ldots, n$, in accordance with theorems I.1 and I.2, adapted to double groups. However, the eigenvalues $\lambda(X)$ and $\lambda(Y)$ are interrelated through the condition $\lambda(Q) = \pm 1$. In particular one notices that

a) for the D_2' case: $Q = X^2 = 2Y^2 - E$,

b) for the D_3' case: $Q = X^2 = 4Y^3 - 3Y$,

c) for the D_4' case: $Q = X^2 = 8Y^4 - 8Y^2 + E$, *etc.* All the possible pairs of simultaneous eigenvalues $\lambda(X)$ and $\lambda(Y)$, which correspond to the case $\lambda(Q) = -1$, are given in Tables III and IV. By taking sets of eigenvalues which make complex conjugate pairs we can group the eigenstates into two-dimensional sets (Tables III and IV).

TABLE III

Groups D'_{2n}, $C'_{2n,v}$ and D'_{nd} for even n

D'_{2n}	$C'_{2n,v}$	D'_{nd}	E'_1		E'_2		E'_3		…	E'_n		Comment
			τ'_1	τ'_2	τ'_3	τ'_4	τ'_5	τ'_6	…	τ'_{2n-1}	τ'_{2n}	
$\lambda(C'_2)$	$\lambda(\sigma_v)$	$\lambda(C'_2)$	i	$-i$	i	$-i$	i	$-i$	…	i	$-i$	$x = \pi/2n$,
$\lambda(Y)$	$\lambda(Y)$	$\lambda(Y')$	$\cos x$		$\cos 3x$		$\cos 5x$		…	$\cos(2n-1)x$		$Y = \frac{1}{2}(C_{2n} + QC_{2n}^{2n-1})$,
												$Y' = \frac{1}{2}(S_{2n} + S_{2n}^{2n-1})$

TABLE IV

Groups D'_{2n+1} and $C'_{2n+1,v}$

D'_{2n+1}	$C_{2n+1,v}$	E'_1		E'_2		E'_3		…	E'_{n+1}		Comment
		τ'_1	τ'_2	τ'_3	τ'_4	τ'_5	τ'_6	…	τ'_{2n+1}	τ'_{2n+2}	
$\lambda(C'_2)$	$\lambda(\sigma_v)$	i	$-i$	i	$-i$	i	$-i$	…	i	$-i$	$x = \pi/(2n+1)$,
$\lambda(Y)$	$\lambda(Y)$	$\cos x$		$\cos 3x$		$\cos 5x$		…	-1	-1	$Y = \frac{1}{2}(C_{2n+1} + QC_{2n+1}^{2n})$,
											last two states never mix

4. *Groups C'_{nv}, D'_{nd} and C'_{nh}*

The group C'_{nv} is isomorphous with D'_n. It suffices to replace C'_2 by σ_v (Table III). The group D'_{nd} is isomorphous with D'_{2n} in the case of even values of n. It suffices to replace C_{2n} by S_{2n} (Table III).

Considering odd values of n we have that $D'_{nd} = D'_n \times C_i$. As $\lambda(i) = \pm 1$, all the eigenstates of Table IV have to be doubled now, once as g states and the other time as u states.

Similarly $C'_{nh} = C'_n \times C_h$. Now $\lambda(\sigma_h) = \pm 1, \pm i$ and $\lambda(C_n) = \exp(i\pi k/n)$, $k = 0, 1, 2, \ldots, 2n-1$. However, $\lambda^2(\sigma_h) = \lambda^n(C_n) = \lambda(Q)$. Therefore the double valued eigenstates of C'_{nh} follow from doubling the number of eigenstates of group C'_n (Tables I and II), once with $\lambda(\sigma_h) = i$, the other time with $\lambda(\sigma_h) = -i$.

5. *The group D'_{nh}*

If n is even then $D'_{nh} = D'_n \times C_i$ and the number of eigenstates of Table IV has to be doubled, denoting the eigenstates as g states for $\lambda(i) = 1$, or u states for $\lambda(i) = -1$. In the case of odd values of n the group D'_{nh} is generated by two elements, $S_n = C_n\sigma_h$ and C'_2. We obtain thus the commuting set:

$$X = C'_2, \quad Y = \frac{1}{2}(C_n + C_n^{n-1})\sigma_n. \tag{12}$$

Let us consider the particular case of the group D_{3h}. The eigenvalues of X which correspond to $\lambda(Q) = -1$ are equal to $\pm i$. On the other hand one can prove that

$$Y^3 = \frac{3}{4} Y + \frac{1}{8} \sigma_h(E+Q). \tag{13}$$

Thus, if $\lambda(Q) = -1$, then $\lambda^3(Y) = \frac{3}{4}\lambda(Y)$ and $\lambda(Y) = 0, \frac{1}{2}\sqrt{3}, -\frac{1}{2}\sqrt{3}$. Similarly for the $\lambda(C_2') = \pm i$ case of the D_{5h} group we find that

$$Y^5 = \frac{5}{4} Y^3 - \frac{5}{16} Y + \frac{1}{32} \sigma_h(E+Q) \tag{14}$$

so that

$$\lambda^5(Y) - \frac{3}{4} \lambda^3(Y) + \frac{5}{16} \lambda(Y) = 0.$$

Possible sets of eigenvalues for any odd value of n are given in Table V. In Table V all the eigenstates which are complex conjugate have been grouped together. With this grouping the orthonormality condition (I.5) is satisfied. Therefore the description of the symmetry properties is complete and no other symmetry eigenstates do exist.

TABLE V

Groups $D'_{2n+1,h}$

$D'_{2n+1,h}$	E'_1		E'_2		E'_3		...	E'_{2n+1}		Comment
	τ'_1	τ'_2	τ'_3	τ'_4	τ'_5	τ'_6	...	τ'_{4n+1}	τ'_{4n+2}	
$\lambda(C'_2)$	i	$-i$	i	$-i$	i	$-i$	...	i	$-i$	$x = 2\pi/(2n+1)$,
$\lambda(Y)$	0	0	$\sin x$		$\sin 2x$		...	$\sin 2nx$		$Y = \frac{1}{2}(C_{2n+1} + C_{2n+1}^{2n})\, \sigma_h$

6. *Groups T' and T'_h*

Let us consider the group T' first. Similarly as in the case of the T group (I) we introduce a set of commuting and independent operators which happens to be complete:

$$X = C_3 \text{ (say } C_{3a}), \quad Y = \frac{1}{3} (C_{2x} + C_{2y} + C_{2z}). \tag{15}$$

Discussing the $\lambda(Q) = -1$ case we find that $\lambda(X) = z$, z^* and -1, where $z = \exp(i\pi/3)$. On the other hand,

$$Y^2 - \frac{1}{3} (E+Q)Y - \frac{1}{3} Q = 0. \tag{16}$$

Therefore $\lambda^2(Y) = -1/3$. All the possible sets of eigenstates are given in Table VI. In order to find the mixing properties under the action of any element of the group T' upon these eigenstates let us note that $C_{3a} Y = \frac{1}{3} (C_{3b} + C_{3c} + C_{3d})Q$ and that $R = (C_{3a} + C_{3b} +$

TABLE V

Group T'

T'	E'		G'				Comment
	τ_1'	τ_2'	τ_3'	τ_4'	τ_5'	τ_6'	
$\lambda(C_3)$	z	z^*	-1	z	-1	z^*	$z = \exp(\pi i/3)$,
$\lambda(Y)$	$i/\sqrt{3}$	$-i/\sqrt{3}$	$i/\sqrt{3}$	$-i/\sqrt{3}$	$-i/\sqrt{3}$	$i/\sqrt{3}$	$Y = \frac{1}{3}(C_{2x}+C_{2y}+C_{2z})$

$+C_{3c}+C_{3d})Q$ does obviously commute with any element $W \in T'$. Therefore $[W, R] = 0$, where $R = C_3(3Y+Q)$. It follows from theorem I.3 that only eigenstates which have equal $\lambda(R)$ can be mixed together. Let us denote by $x(\tau_i)$ the eigenvalue $\lambda(R)$ which corresponds to the state τ_i'. Then $x(\tau_1') = x(\tau_2') = -2$, $x(\tau_3') = x(\tau_4') = 1-i\sqrt{3}$, $x(\tau_5') = x(\tau_6') = 1+i\sqrt{3}$. The irreducible basis sets cannot be larger then than the following ones: (τ_1', τ_2'), (τ_3', τ_4') and (τ_5', τ_6'). However, with this subdivision the orthonormality condition (I.5) is already satisfied. Therefore no further division into smaller basis sets is possible. There is, however, a physical equivalence of states τ_3' and τ_5', and τ_4' and τ_6'.

7. *Groups O', T_d' and O_h'*

Let us start with group O'. Adopting the complete set of commuting and independent operators of group O (I) to the requirements of a double group we obtain the set:

$$X = C_{4z}, \quad Y = \frac{1}{4}\{C_{4x}+C_{4y}+C_{4x}^3Q+C_{4y}^3Q\} \tag{17}$$

and a subsidiary commuting operator Z, where

$$Z = \frac{1}{4}\{C_{2x}+C_{2y}+C_{2x}Q+C_{2y}Q\}. \tag{18}$$

However

$$Z^2 = \frac{1}{4}(E+Q)(E+C_{4z}^2). \tag{19}$$

Therefore, if $\lambda(Q) = -1$, then $\lambda(Z) = 0$. The double valued eigenvalues of C_{4z} are equal to z, z^*, $-z$ and $-z^*$, where $z = \exp(i\pi/4)$. Passing to the eigenvalue problem for Y let us note that

$$4Y^2 = Z+E+(C_{4z}+C_{4z}^3Q)Y. \tag{20}$$

Replacing operators by their eigenvalues we find the equation to be satisfied by $\lambda(Y)$. All the possible sets of eigenvalues are listed in Table VII. The subdivision into basis sets, given in Table VII, follows from the following three requirements: *i*) equality of characters for a basis, $\chi(C_{4z}) = \chi(Y)$, *ii*) equivalence of eigenstates with complex conjugate eigenvalues, *iii*) the orthonormality condition (I.5).

TABLE VII

Groups T_d' and O'

T_d'	O'	E_1'		E_2'		G'				Comment
		τ_1'	τ_2'	τ_3'	τ_4'	τ_5'	τ_6'	τ_7'	τ_8'	
$\lambda(S_{4z})$	$\lambda(C_{4z})$	z	z^*	$-z$	$-z^*$	z	z^*	$-z$	$-z^*$	$z = \exp(\pi i/4)$, $x = 1/\sqrt{2}$,
$\lambda(Y')$	$\lambda(Y)$	x	x	$-x$	$-x$	$-x/2$	$-x/2$	$x/2$	$x/2$	$Y = \frac{1}{4}\{C_{4x}+C_{\bar{4}y}+QC_{4x}^3+QC_{4y}^3\}$, $Y' = \frac{1}{4}\{S_{4x}+S_{4y}+S(^3_{4x})+S(^3_{4y})\}$

The possible sets of eigenvalues in the case of the T_d' group follow from the isomorphism of groups O' and T_d' (Table VII).

As $O_h' = O' \times C_i$, there are twice as many eigenstates as in the case of the O' group, once with $\lambda(\mathrm{i}) = 1$, the other time with $\lambda(\mathrm{i}) = -1$.

8. *Projection operators and illustration*

Similarly as in the case of the ordinary symmetry point groups (I) we can easily construct projection operators which project a given function into a given τ_i' eigenstate. Considering for example, selected eigenstates of the O' group we find, in accordance with Table VII, the operators:

$$P(E_1', a) = P(\tau_1') = \text{const}\,(C_{4z}-z)\left(Y^2-\frac{1}{8}\right)\left(Y+\sqrt{\frac{1}{2}}\right) \qquad (21)$$

$$P(E_2', a) = P(\tau_3') = \text{const}\,(C_{4z}+z)\left(Y^2-\frac{1}{8}\right)\left(Y-\sqrt{\frac{1}{2}}\right) \qquad (22)$$

$$P(G', a) = P(\tau_5') = \text{const}\,(C_{4z}-z)\left(Y^2-\frac{1}{2}\right)\left(Y-\frac{1}{4}\sqrt{2}\right). \qquad (23)$$

We recall that the standard approach to projection operators would require knowledge of the action of all 48 elements of the O' group and of all the matrices which form an irreducible representation of the O' group. Thus the simplification is significant.

Let us consider a simple example of d orbitals and the group O'. One finds easily with the use of Eqs (3) and (4), that

$$Y\overset{+}{d}_1 = -\frac{1}{4}\sqrt{2}\,\overset{+}{d}_1 - \frac{i}{2}\,\overset{-}{d}_{xy}, \qquad Y\overset{-}{d}_1 = -\frac{1}{4}\sqrt{2}\,\overset{-}{d}_1,$$

$$Y\overset{-}{d}_{-1} = -\frac{1}{4}\sqrt{2}\,\overset{-}{d}_{-1} + \frac{i}{2}\,\overset{+}{d}_{xy}, \qquad Y\overset{+}{d}_{-1} = -\frac{1}{4}\sqrt{2}\,\overset{+}{d}_{-1},$$

$$Y\overset{+}{d}_{xy} = -\frac{i}{2}\,\overset{-}{d}_{-1}, \qquad Y\overset{-}{d}_{xy} = \frac{i}{2}\,\overset{+}{d}_1,$$

$$Y\overset{+}{d}_{x^2-y^2} = \frac{\sqrt{2}}{4}\,\overset{+}{d}_{x^2-y^2}, \qquad Y\overset{-}{d}_{x^2-{}^2y} = \frac{\sqrt{2}}{4}\,\overset{-}{d}_{x^2-y^2},$$

$$Y\overset{+}{d}_0 = -\frac{\sqrt{2}}{4}\,\overset{+}{d}_0, \qquad Y\overset{-}{d}_0 = -\frac{\sqrt{2}}{4}\,\overset{-}{d}_0,$$

and that $C_{4z}\overset{+}{d}_1 = -z^*\overset{+}{d}_1$, $C_{4z}\overset{-}{d}_1 = z\overset{-}{d}_1$, $C_{4z}\overset{+}{d}_{xy} = -z\overset{+}{d}_{xy}$, $C_{4z}\overset{-}{d}_{-1} = -z\overset{-}{d}_{-1}$, $C_{4z}\overset{+}{d}_{-1} = z^*\overset{+}{d}_{-1}$, $C_{4z}\overset{-}{d}_{xy} = -z^*\overset{-}{d}_{xy}$, $C_{4z}\overset{+}{d}_{x^2-y^2} = -z\overset{+}{d}_{x^2-y^2}$, $C_{4z}\overset{-}{d}_{x^2-y^2} = -z^*\overset{-}{d}_{x^2-y^2}$, $C_{4z}\overset{+}{d}_0 = z\overset{+}{d}_0$, $C_{4z}\overset{-}{d}_0 = z^*\overset{-}{d}_0$.

We see that spinorbitals $\overset{-}{d}_1, \overset{+}{d}_{-1}, \overset{+}{d}_{x^2-y^2}, \overset{-}{d}_{x^2-y^2}, \overset{+}{d}_0$ and $\overset{-}{d}_0$ are already eigenfunctions of C_{4z} and Y. In accordance with Table VII

$$\overset{-}{d}_1 \in \tau_5' = G'(a), \qquad \overset{+}{d}_{-1} \in \tau_6' = G'(b),$$
$$\overset{+}{d}_0 \in \tau_5' = G'(a), \qquad \overset{-}{d}_0 \in \tau_6' = G'(b),$$
$$\overset{+}{d}_{x^2-y^2} \in \tau_7' = G'(c), \quad \overset{-}{d}_{x^2-y^2} \in \tau_8' = G'(c).$$

The remaining eigenfunctions are obtained with the use of projection operators:

$$P(E_2', a)\overset{-}{d}_{-1} = \text{const}\cdot\sqrt{\frac{2}{3}}\left\{\overset{-}{d}_{-1} - \frac{i}{\sqrt{2}}\overset{+}{d}_{xy}\right\} \in E_2'(a),$$

$$P(E_2', b)\overset{+}{d}_1 = \text{const}\cdot\sqrt{\frac{2}{3}}\left\{\overset{+}{d}_1 + \frac{i}{\sqrt{2}}\overset{-}{d}_{xy}\right\} \in E_2'(b),$$

$$P(G', c)\overset{-}{d}_{-1} = \text{const}\cdot\frac{1}{\sqrt{3}}\{\overset{-}{d}_{-1} + \sqrt{2}\, i\overset{+}{d}_{xy}\} \in G'(c),$$

$$P(G', d)\overset{+}{d}_1 = \text{const}\cdot\sqrt{\frac{1}{3}}\{\overset{+}{d}_1 - \sqrt{2}\, i\overset{-}{d}_{xy}\} \in G'(d).$$

Thus in the spin-orbit coupling theory of d-electrons in an octahedral force field $\overset{-}{d}_1$ interacts with $\overset{+}{d}_0$, $\overset{+}{d}_{-1}$ with $\overset{-}{d}_0$, $\sqrt{\frac{2}{3}}\left\{d_{-1} - \frac{i}{\sqrt{2}}d_{xy}\right\}$ is in its final form, *etc.* The same set of functions can be also conveniently used in calculations of the magnetic susceptibility (Ballhausen 1962, Gołębiewski 1969).

REFERENCES

Ballhausen, C. J., *Introduction to Ligand Field Theory*, p. 118, 144, New York, San Francisco, Toronto, London 1962.

Bhagavantam, S., Venkatarayudu, T., *Theory of Groups and Its Application to Physical Problems*, Waltair 1948.

Cotton, F. A., *Chemical Application of Group Theory*, New York, London 1963.

Gołębiewski, A., *Molecular Phys.*, (1970) (in print).

Gołębiewski, *Chemia kwantowa związków nieorganicznych*, p. 440, Warsaw 1969 (in Polish).

Hamermesh, M., *Group Theory and Its Application to Physical Problems*, London, Paris 1962.

Heine, V., *Group Theory in Quantum Mechanics*, London, Oxford, New York, Pa is 1960.

Messiah, A., *Quantum Mechanics*, Amsterdam 1962.

Tinkham, M., *Group Theory and Quantum Mechanics*, New York, San Francisco, Toronto, London 1964.