DOUBLE-VALUED COREPRESENTATIONS OF MAGNETIC POINT GROUPS

By A. P. Cracknell†‡ and K. C. Wong†§

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Summary

The theory of the corepresentations of non-unitary groups, which was developed by Wigner, is applied here to the determination of the double-valued corepresentations of the magnetic point groups. Complete tables are given for the double-valued corepresentations of each of the 58 magnetic point groups. A comparison is made with previous work by Dimmock and Wheeler.

I. Introduction

The idea of a "double" point group or of double-valued representations of the point groups seems to have originated with Bethe (1929) and to have been more carefully defined by Opechowski (1940). The importance of double groups in describing the behaviour of a system with half-odd-integer spin and particularly with regard to spin–orbit coupling in crystals was emphasized by Elliott (1954). Since the magnetic point groups derived by Tavger and Zaitsev (1956) have now been seen to be relevant to the description of the symmetry of many real crystals it is necessary and desirable to derive the corepresentations of these groups. Half the elements of each of these magnetic groups do not contain the operation of time inversion and are unitary elements; the other half of the elements do contain the operation of time inversion and are therefore anti-unitary. The unitary elements form a halving subgroup **H** of the magnetic group **M**. These magnetic groups **M** are therefore non-unitary, so that ordinary representation theory is not relevant to them. Dimmock and Wheeler (1962) showed how the theory developed by Wigner (1959) of the irreducible corepresentations ("coreps" for short) of non-unitary groups could be applied to the magnetic point groups. However, this work of Dimmock and Wheeler (1962) only included the character tables and not the matrix representatives themselves for **H**, the halving subgroup of the unitary elements, in each of the magnetic point groups. This means that, while their work is adequate for discussing the degeneracies of energy levels in a system with the symmetry of one of the magnetic point groups, it is rather difficult to use their results when studying wave functions that belong to a corepresentation derived from one of the degenerate representations of **H**. Complete tables including not only the character tables but also the matrix representatives themselves were given by Cracknell (1966) for the single-valued coreps of the magnetic point groups. In the present paper we now give similar tables for the double-valued coreps of the magnetic point groups. The importance of these coreps lies in the fact that the wave function of a particle, which is placed in an environment with the symmetry of one of the magnetic point groups, must belong to one of the single-valued coreps of that group if it has zero or integer spin and to one of the double-valued coreps if it has half-odd-integer spin.

† Department of Physics, University of Singapore, Singapore 10.

‡ Present address: Department of Physics, University of Essex, Colchester, Essex, England.

§ Present address: Department of Mathematics, Imperial College, London, S.W.7, England.

TABLE 1

THE DOUBLE-VALUED REPRESENTATIONS OF THE CRYSTALLOGRAPHIC POINT GROUPS

$$\omega = \exp 2\pi i/3; \qquad \varpi = \sqrt{2}+i; \qquad \theta = \frac{1}{\sqrt{2}}(1+i)$$

$1\ (C_1)$	E	$\bar{E}$
$\bar{A}$	1	-1

$\bar{1}\ (C_i)$	E	I	$\bar{E}$	$\bar{I}$
$\bar{A}_g$	1	1	-1	-1
$\bar{A}_u$	1	-1	-1	1

$2\ (C_2)$		E	C_{2z}	$\bar{E}$	$\bar{C}_{2z}$
	$m\ (C_{1h})$	E	σ_z	$\bar{E}$	$\bar{\sigma}_{2z}$
${}^1\bar{E}$	${}^1\bar{E}$	1	i	-1	$-$i
${}^2\bar{E}$	${}^2\bar{E}$	1	$-$i	-1	i

$2/m = 2 \otimes \bar{1}\quad (C_{2h} = C_2 \otimes C_i)$

$2mm\ (C_{2v})$		E	$\bar{E}$	$\sigma_x, \bar{\sigma}_x$	$\sigma_y, \bar{\sigma}_y$	$C_{2z}, \bar{C}_{2z}$
	$222\ (D_2)$	E	$\bar{E}$	$C_{2x}, \bar{C}_{2x}$	$C_{2y}, \bar{C}_{2y}$	$C_{2z}, \bar{C}_{2z}$
$\bar{E}$	$\bar{E}$	2	-2	0	0	0

$2mm\ (C_{2v})$		$P = \sigma_x$	$Q = \sigma_y$
	$222\ (D_2)$	$P = C_{2x}$	$Q = C_{2y}$
$\bar{E}$	$\bar{E}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$

$mmm = 222 \otimes \bar{1}\quad (D_{2h} = D_2 \otimes C_i)$

$4\ (C_4)$		E	C_{4z}^-	C_{2z}	$\bar{C}_{4z}^+$	$\bar{E}$	$\bar{C}_{4z}^-$	$\bar{C}_{2z}$	C_{4z}^+
	$\bar{4}\ (S_4)$	E	S_{4z}^+	C_{2z}	$\bar{S}_{4z}^-$	$\bar{E}$	$\bar{S}_{4z}^+$	$\bar{C}_{2z}$	S_{4z}^-
${}^2\bar{E}_1$	${}^2\bar{E}_1$	1	θ	i	$-\theta^*$	-1	$-\theta$	$-$i	θ^*
${}^1\bar{E}_2$	${}^1\bar{E}_2$	1	$-\theta^*$	$-$i	θ	-1	θ^*	i	$-\theta$
${}^2\bar{E}_2$	${}^2\bar{E}_2$	1	$-\theta$	i	θ^*	-1	θ	$-$i	$-\theta^*$
${}^1\bar{E}_1$	${}^1\bar{E}_1$	1	θ^*	$-$i	$-\theta$	-1	$-\theta^*$	i	θ

$4/m = 4 \otimes \bar{1}\quad (C_{4h} = C_4 \otimes C_i)$

$3\ (C_3)$	E	C_3^+	$\bar{C}_3^-$	$\bar{E}$	$\bar{C}_3^+$	C_3^-
${}^2\bar{E}$	1	$-\omega^*$	ω	-1	ω^*	$-\omega$
$\bar{A}$	1	-1	1	-1	1	-1
${}^1\bar{E}$	1	$-\omega$	ω^*	-1	ω	$-\omega^*$

$\bar{3} = 3 \otimes \bar{1}\quad (C_{3i} = C_3 \otimes C_i)$

TABLE 1 (*Continued*)

32 (D_3)		E	$\bar{E}$	C_3^+, C_3^-	$\bar{C}_3^-, \bar{C}_3^+$	$C'_{21}, \bar{C}'_{22}, C'_{23}$	$\bar{C}'_{23}, \bar{C}'_{21}, C'_{22}$
	3m (C_{3v})	E	$\bar{E}$	C_3^+, C_3^-	$\bar{C}_3^-, \bar{C}_3^+$	$\sigma_{v1}, \bar{\sigma}_{v2}, \sigma_{v3}$	$\bar{\sigma}_{v3}, \bar{\sigma}_{v1}, \sigma_{v2}$
${}^1\bar{E}$	${}^1\bar{E}$	1	−1	−1	1	i	−i
${}^2\bar{E}$	${}^2\bar{E}$	1	−1	−1	1	−i	i
$\bar{E}_1$	$\bar{E}_1$	2	−2	1	−1	0	0

32 (D_3)		$P = C_3^+$	$Q = C'_{21}$
	3m (C_{3v})	$P = C_3^+$	$Q = \sigma_{v1}$
$\bar{E}_1$	$\bar{E}_1$	$\begin{pmatrix} \frac{1}{2} & -\frac{1}{2}\sqrt{3} \\ \frac{1}{2}\sqrt{3} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$

$\bar{3}m = 32 \otimes \bar{1}$ $(D_{3d} = D_3 \otimes C_i)$

6 (C_6)		E	C_6^+	C_3^+	$\bar{C}_2$	$\bar{C}_3^-$	$\bar{C}_6^-$	$\bar{E}$	$\bar{C}_6^+$	$\bar{C}_3^+$	C_2	C_3^-	C_6^-
	$\bar{6}$ (C_{3h})	E	S_3^-	C_3^+	$\bar{\sigma}_h$	$\bar{C}_3^-$	$\bar{S}_3^+$	$\bar{E}$	$\bar{S}_3^-$	$\bar{C}_3^+$	σ_h	C_3^-	S_3^+
${}^2\bar{E}_3$	${}^2\bar{E}_3$	1	$-i\omega$	$-\omega^*$	i	ω	$-i\omega^*$	−1	$i\omega$	ω^*	−i	$-\omega$	$i\omega^*$
${}^1\bar{E}_1$	${}^1\bar{E}_1$	1	i	−1	−i	1	i	−1	−i	1	i	−1	−i
${}^2\bar{E}_2$	${}^2\bar{E}_2$	1	$-i\omega^*$	$-\omega$	i	ω^*	$-i\omega$	−1	$i\omega^*$	ω	−i	$-\omega^*$	$i\omega$
${}^1\bar{E}_2$	${}^1\bar{E}_2$	1	$i\omega$	$-\omega^*$	−i	ω	$i\omega^*$	−1	$-i\omega$	ω^*	i	$-\omega$	$-i\omega^*$
${}^2\bar{E}_1$	${}^2\bar{E}_1$	1	−i	−1	i	1	−i	−1	i	1	−i	−1	i
${}^1\bar{E}_3$	${}^1\bar{E}_3$	1	$i\omega^*$	$-\omega$	−i	ω^*	$i\omega$	−1	$-i\omega^*$	ω	i	$-\omega^*$	$-i\omega$

$6/m = 6 \otimes \bar{1}$ $(C_{6h} = C_6 \otimes C_i)$

422 (D_4)			E	$\bar{E}$	$C_{2z}, \bar{C}_{2z}$	C_{4z}^-, C_{4z}^+	$\bar{C}_{4z}^+, \bar{C}_{4z}^-$	C_{2x}, C_{2y} $\bar{C}_{2x}, \bar{C}_{2y}$	C_{2b}, C_{2a} $\bar{C}_{2b}, \bar{C}_{2a}$
	4mm (C_{4v})		E	$\bar{E}$	$C_{2z}, \bar{C}_{2z}$	C_{4z}^-, C_{4z}^+	$\bar{C}_{4z}^+, \bar{C}_{4z}^-$	σ_x, σ_y $\bar{\sigma}_x, \bar{\sigma}_y$	σ_{db}, σ_{da} $\bar{\sigma}_{db}, \bar{\sigma}_{da}$
		$\bar{4}2m$ (D_{2d})	E	$\bar{E}$	$C_{2z}, \bar{C}_{2z}$	S_{4z}^+, S_{4z}^-	$\bar{S}_{4z}^-, \bar{S}_{4z}^+$	C_{2x}, C_{2y} $\bar{C}_{2x}, \bar{C}_{2y}$	σ_{db}, σ_{da} $\bar{\sigma}_{db}, \bar{\sigma}_{da}$
$\bar{E}_1$	$\bar{E}_1$	$\bar{E}_1$	2	−2	0	$\sqrt{2}$	$-\sqrt{2}$	0	0
$\bar{E}_2$	$\bar{E}_2$	$\bar{E}_2$	2	−2	0	$-\sqrt{2}$	$\sqrt{2}$	0	0

422 (D_4)			$P = C_{4z}^-$	$Q = C_{2x}$
	4mm (C_{4v})		$P = C_{4z}^-$	$Q = \sigma_x$
		$\bar{4}2m$ (D_{2d})	$P = S_{4z}^+$	$Q = C_{2x}$
$\bar{E}_1$	$\bar{E}_1$	$\bar{E}_1$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$
$\bar{E}_2$	$\bar{E}_2$	$\bar{E}_2$	$\frac{1}{\sqrt{2}}\begin{pmatrix} -1 & 1 \\ -1 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$

$4/mmm = 422 \otimes \bar{1}$ $(D_{4h} = D_4 \otimes C_i)$

TABLE 1 (*Continued*)

622 (D_6)			E	$\bar{E}$	$\bar{C}_3^-, \bar{C}_3^+$	C_3^+, C_3^-	$\bar{C}_2, C_2$	C_6^+, C_6^-	$\bar{C}_6^-, \bar{C}_6^+$	$C'_{21}, \bar{C}'_{23}$ $\bar{C}'_{22}, \bar{C}'_{21}$ C'_{23}, C'_{22}	$\bar{C}''_{22}, \bar{C}''_{21}$ $\bar{C}''_{23}, C''_{22}$ C''_{21}, C''_{23}
	$6mm$ (C_{6v})		E	$\bar{E}$	$\bar{C}_3^-, \bar{C}_3^+$	C_3^+, C_3^-	$\bar{C}_2, C_2$	C_6^+, C_6^-	$\bar{C}_6^-, \bar{C}_6^+$	$\sigma_{d1}, \bar{\sigma}_{d3}$ $\bar{\sigma}_{d2}, \bar{\sigma}_{d1}$ σ_{d3}, σ_{d2}	$\bar{\sigma}_{v2}, \bar{\sigma}_{v1}$ $\bar{\sigma}_{v3}, \sigma_{v2}$ σ_{v1}, σ_{v3}
		$\bar{6}2m$ (D_{3h})	E	$\bar{E}$	$\bar{C}_3^-, \bar{C}_3^+$	C_3^+, C_3^-	$\bar{\sigma}_h, \sigma_h$	S_3^-, S_3^+	$\bar{S}_3^+, \bar{S}_3^-$	$C'_{21}, \bar{C}'_{23}$ $\bar{C}'_{22}, \bar{C}'_{21}$ C'_{23}, C'_{22}	$\bar{\sigma}_{v2}, \bar{\sigma}_{v1}$ $\bar{\sigma}_{v3}, \sigma_{v2}$ σ_{v1}, σ_{v3}
$\bar{E}_1$	$\bar{E}_1$	$\bar{E}_1$	2	−2	−1	1	0	$\sqrt{3}$	$-\sqrt{3}$	0	0
$\bar{E}_2$	$\bar{E}_2$	$\bar{E}_2$	2	−2	−1	1	0	$-\sqrt{3}$	$\sqrt{3}$	0	0
$\bar{E}_3$	$\bar{E}_3$	$\bar{E}_3$	2	−2	2	−2	0	0	0	0	0

622 (D_6)	$6mm$ (C_{6v})	$\bar{6}2m$ (D_{3h})	$P = C_6^+$ $P = C_6^+$ $P = S_3^-$	$Q = C'_{21}$ $Q = \sigma_{d1}$ $Q = C'_{21}$
$\bar{E}_1$	$\bar{E}_1$	$\bar{E}_1$	$\begin{pmatrix} -\mathrm{i}\omega & 0 \\ 0 & \mathrm{i}\omega^* \end{pmatrix}$	$\begin{pmatrix} 0 & \mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}$
$\bar{E}_2$	$\bar{E}_2$	$\bar{E}_2$	$\begin{pmatrix} -\mathrm{i}\omega^* & 0 \\ 0 & \mathrm{i}\omega \end{pmatrix}$	$\begin{pmatrix} 0 & \mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}$
$\bar{E}_3$	$\bar{E}_3$	$\bar{E}_3$	$\begin{pmatrix} \mathrm{i} & 0 \\ 0 & -\mathrm{i} \end{pmatrix}$	$\begin{pmatrix} 0 & \mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}$
SU(2)	—	—	$\begin{pmatrix} e^{\mathrm{i}\pi/6} & 0 \\ 0 & e^{-\mathrm{i}\pi/6} \end{pmatrix}$	$\begin{pmatrix} 0 & -\mathrm{i} \\ -\mathrm{i} & 0 \end{pmatrix}$

$6/mmm = 622 \otimes \bar{1}$ $(D_{6h} = D_6 \otimes C_i)$

23 (T)	E	$\bar{E}$	$C_{2x}, \bar{C}_{2y}, \bar{C}_{2x}$ $C_{2y}, \bar{C}_{2z}, C_{2z}$	C_{31}^-, C_{34}^- $\bar{C}_{33}^-, C_{32}^-$	$\bar{C}_{31}^-, \bar{C}_{34}^-$ $C_{33}^-, \bar{C}_{32}^-$	C_{31}^+, C_{33}^+ $\bar{C}_{34}^+, \bar{C}_{32}^+$	$\bar{C}_{31}^+, \bar{C}_{33}^+$ C_{34}^+, C_{32}^+
$\bar{E}$	2	−2	0	1	−1	−1	1
$^1\bar{F}$	2	−2	0	ω	$-\omega$	$-\omega^*$	ω^*
$^2\bar{F}$	2	−2	0	ω^*	$-\omega^*$	$-\omega$	ω

TABLE 1 (*Continued*)

23 (T)	$P = C_{31}^-$	$Q = C_{2x}$	$R = \bar{C}_{2y}$
$\bar{E}$	$\begin{pmatrix} -\omega & 0 \\ 0 & -\omega^* \end{pmatrix}$	$\frac{1}{\sqrt{3}}\begin{pmatrix} \mathrm{i} & -1+\mathrm{i} \\ 1+\mathrm{i} & -\mathrm{i} \end{pmatrix}$	$\frac{1}{\sqrt{3}}\begin{pmatrix} \mathrm{i} & -\omega(1-\mathrm{i}) \\ \omega^*(1+\mathrm{i}) & -\mathrm{i} \end{pmatrix}$
${}^1\bar{F}$	$\begin{pmatrix} -\omega^* & 0 \\ 0 & -1 \end{pmatrix}$	$\frac{1}{\sqrt{3}}\begin{pmatrix} \mathrm{i} & -1+\mathrm{i} \\ 1+\mathrm{i} & -\mathrm{i} \end{pmatrix}$	$\frac{1}{\sqrt{3}}\begin{pmatrix} \mathrm{i} & -\omega(1-\mathrm{i}) \\ \omega^*(1+\mathrm{i}) & -\mathrm{i} \end{pmatrix}$
${}^2\bar{F}$	$\begin{pmatrix} -1 & 0 \\ 0 & -\omega \end{pmatrix}$	$\frac{1}{\sqrt{3}}\begin{pmatrix} \mathrm{i} & -1+\mathrm{i} \\ 1+\mathrm{i} & -\mathrm{i} \end{pmatrix}$	$\frac{1}{\sqrt{3}}\begin{pmatrix} \mathrm{i} & -\omega(1-\mathrm{i}) \\ \omega^*(1+\mathrm{i}) & -\mathrm{i} \end{pmatrix}$

$m3 = 23 \otimes \bar{1} \quad (T_h = T \otimes C_i)$

432 (O)	$\bar{4}3m$ (T_d)	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8
$\bar{E}_1$	$\bar{E}_1$	2	-2	0	1	-1	$\sqrt{2}$	$-\sqrt{2}$	0
$\bar{E}_2$	$\bar{E}_2$	2	-2	0	1	-1	$-\sqrt{2}$	$\sqrt{2}$	0
$\bar{F}$	$\bar{F}$	4	-4	0	-1	1	0	0	0

432 (O)

C_1	E
C_2	$\bar{E}$
C_3	$C_{2x}, C_{2y}, C_{2z}, \bar{C}_{2x}, \bar{C}_{2y}, \bar{C}_{2z}$
C_4	$C_{31}^-, C_{32}^-, \bar{C}_{33}^-, C_{34}^-, \bar{C}_{31}^+, C_{32}^+, C_{33}^+, C_{34}^+$
C_5	$\bar{C}_{31}^-, \bar{C}_{32}^-, C_{33}^-, \bar{C}_{34}^-, C_{31}^+, \bar{C}_{32}^+, \bar{C}_{33}^+, \bar{C}_{34}^+$
C_6	$C_{4x}^+, C_{4y}^+, C_{4z}^+, C_{4x}^-, C_{4y}^-, C_{4z}^-$
C_7	$\bar{C}_{4x}^+, \bar{C}_{4y}^+, \bar{C}_{4z}^+, \bar{C}_{4x}^-, \bar{C}_{4y}^-, \bar{C}_{4z}^-$
C_8	$C_{2a}, C_{2b}, C_{2c}, C_{2d}, C_{2e}, C_{2f}, \bar{C}_{2a}, \bar{C}_{2b}, \bar{C}_{2c}, \bar{C}_{2d}, \bar{C}_{2e}, \bar{C}_{2f}$

$\bar{4}3m$ (T_d)

C_1	E
C_2	$\bar{E}$
C_3	$C_{2x}, C_{2y}, C_{2z}, \bar{C}_{2x}, \bar{C}_{2y}, \bar{C}_{2z}$
C_4	$C_{31}^-, C_{32}^-, \bar{C}_{33}^-, C_{34}^-, \bar{C}_{31}^+, C_{32}^+, C_{33}^+, C_{34}^+$
C_5	$\bar{C}_{31}^-, \bar{C}_{32}^-, C_{33}^-, \bar{C}_{34}^-, C_{31}^+, \bar{C}_{32}^+, \bar{C}_{33}^+, \bar{C}_{34}^+$
C_6	$S_{4x}^-, S_{4y}^-, S_{4z}^-, S_{4x}^+, S_{4y}^+, S_{4z}^+$
C_7	$\bar{S}_{4x}^-, \bar{S}_{4y}^-, \bar{S}_{4z}^-, \bar{S}_{4x}^+, \bar{S}_{4y}^+, \bar{S}_{4z}^+$
C_8	$\sigma_{da}, \sigma_{db}, \sigma_{dc}, \sigma_{dd}, \sigma_{de}, \sigma_{df}, \bar{\sigma}_{da}, \bar{\sigma}_{db}, \bar{\sigma}_{dc}, \bar{\sigma}_{dd}, \bar{\sigma}_{de}, \bar{\sigma}_{df}$.

TABLE 1 (*Continued*)

432 (O)	$\bar{4}3m$ (T_d)	$P = C_{4x}^{+}$ $P = S_{4x}^{-}$	$Q = \bar{C}_{31}^{-}$ $Q = \bar{C}_{31}^{-}$	$R = C_{2b}$ $R = \sigma_{db}$
$\bar{E}_1$	$\bar{E}_1$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} -1 & \mathrm{i}\varpi^* \\ \mathrm{i}\varpi & -1 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} \mathrm{i} & \varpi^* \\ -\varpi & -\mathrm{i} \end{pmatrix}$
$\bar{E}_2$	$\bar{E}_2$	$\frac{1}{\sqrt{2}}\begin{pmatrix} -1 & -1 \\ 1 & -1 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} -1 & \mathrm{i}\varpi^* \\ \mathrm{i}\varpi & -1 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} -\mathrm{i} & -\varpi^* \\ \varpi & \mathrm{i} \end{pmatrix}$
$\bar{F}$	$\bar{F}$	$\frac{1}{\sqrt{2}}\left(\begin{array}{cc\|cc} 1 & \mathrm{i} & 0 & 0 \\ \mathrm{i} & 1 & 0 & 0 \\ \hline 0 & 0 & -1 & \mathrm{i} \\ 0 & 0 & \mathrm{i} & -1 \end{array}\right)$	$\frac{1}{4}\left(\begin{array}{c\|c} \begin{matrix} 1 & -\varpi \\ \varpi^* & 1 \end{matrix} & \sqrt{3}\begin{pmatrix} \varpi & 1 \\ -1 & \varpi^* \end{pmatrix} \\ \hline \sqrt{3}\begin{pmatrix} \varpi^* & 1 \\ -1 & \varpi \end{pmatrix} & \begin{matrix} 1 & -\varpi^* \\ \varpi & 1 \end{matrix} \end{array}\right)$	$\frac{\mathrm{i}}{4}\left(\begin{array}{c\|c} \begin{matrix} 1 & -\varpi \\ -\varpi^* & -1 \end{matrix} & \sqrt{3}\begin{pmatrix} \varpi & 1 \\ 1 & -\varpi^* \end{pmatrix} \\ \hline \sqrt{3}\begin{pmatrix} \varpi^* & 1 \\ 1 & -\varpi \end{pmatrix} & \begin{matrix} 1 & -\varpi^* \\ -\varpi & -1 \end{matrix} \end{array}\right)$
SU(2)	—	$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -\mathrm{i} \\ -\mathrm{i} & 1 \end{pmatrix}$	$\frac{1}{2}\begin{pmatrix} -1+\mathrm{i} & 1-\mathrm{i} \\ -1-\mathrm{i} & -1-\mathrm{i} \end{pmatrix}$	$\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -1-\mathrm{i} \\ 1-\mathrm{i} & 0 \end{pmatrix}$

$m3m = 432 \otimes \bar{1}$ $(O_h = O \otimes C_i)$

II. THEORY

We follow the notation of Cracknell (1966) and classify the 122 magnetic point groups into three types:

- I ordinary point groups (32)
- II "grey" point groups (32)
- III "black and white" point groups (58).

The type I groups are simply the ordinary point groups, so that they are unitary groups and the theory of corepresentations is not relevant to them. The character tables of these groups are given in many books (see, for instance, Heine 1960), and matrix representatives are given by Altmann and Bradley (1963). The grey magnetic point groups (type II) are direct product groups of one of the ordinary point groups $\mathbf{G}$ with the group $(E+R)$, where E is the identity and R is the operation of time inversion. The "black and white" (or type III) magnetic point groups $\mathbf{M}$ can be defined by

$$\mathbf{M} = \mathbf{H} + R(\mathbf{G}-\mathbf{H}), \tag{2.1}$$

where $\mathbf{H}$ is a halving subgroup of $\mathbf{G}$. The identification of $\mathbf{H}$ for each of the 58 type III groups was originally done by Tavger and Zaitsev (1956).

The theory of the deduction of the irreducible corepresentations of magnetic groups as developed by Wigner (1959) and Dimmock and Wheeler (1962) is neatly summarized in Section 4 of a paper by Cracknell (1965) (hereafter referred to as APC I), in which the only necessary alteration is to replace $\overline{\mathbf{G}}^{\mathbf{k}}$, $\overline{\mathbf{H}}^{\mathbf{k}}$, and $\overline{\mathbf{M}}^{\mathbf{k}}$ of that paper by $\mathbf{G}$, $\mathbf{H}$, and $\mathbf{M}$ respectively. It is assumed that the irreducible representations ("reps") $\boldsymbol{\Delta}(\mathbf{u})$ of the subgroup $\mathbf{H}$ of unitary elements are known already, where $\mathbf{u}$ is any member of $\mathbf{H}$. The coreps of $\mathbf{M}$ derived from $\boldsymbol{\Delta}(\mathbf{u})$ will then follow one of three cases depending on the relationship between $\boldsymbol{\Delta}(\mathbf{u})$ and $\overline{\boldsymbol{\Delta}}(\mathbf{u})$, where

$$\overline{\boldsymbol{\Delta}}(\mathbf{u}) = \boldsymbol{\Delta}(\mathbf{a}_0^{-1}\,\mathbf{u}\mathbf{a}_0)^*, \tag{2.2}$$

$\mathbf{a}_0$ being any (fixed) member of the set $R(\mathbf{G}-\mathbf{H})$. If $\overline{\boldsymbol{\Delta}}(\mathbf{u})$ is equivalent to $\boldsymbol{\Delta}(\mathbf{u})$ then it is possible to write

$$\overline{\boldsymbol{\Delta}}(\mathbf{u}) = \boldsymbol{\beta}^{-1}\,\boldsymbol{\Delta}(\mathbf{u})\,\boldsymbol{\beta}. \tag{2.3}$$

If $\boldsymbol{\beta\beta}^* = +\boldsymbol{\Delta}(\mathbf{a}_0^2)$ the corep of $\mathbf{M}$ derived from $\boldsymbol{\Delta}(\mathbf{u})$ belongs to case 1 and is given by equation (4.2) of APC I, but if $\boldsymbol{\beta\beta}^* = -\boldsymbol{\Delta}(\mathbf{a}_0^2)$ then the corep belongs to case 2 and is given by equation (4.3) of APC I. If $\overline{\boldsymbol{\Delta}}(\mathbf{u})$ is not equivalent to $\boldsymbol{\Delta}(\mathbf{u})$ then the corep of $\mathbf{M}$ derived from $\boldsymbol{\Delta}(\mathbf{u})$ belongs to case 3 and is given by equation (4.4) of APC I.

III. The Coreps of the Grey Magnetic Point Groups

Since the grey magnetic point groups are direct product groups, their single-valued corepresentations can easily be deduced using the theory that we have mentioned together with the complete set of matrix representatives given by Altmann and Bradley (1963). For each of these 32 grey groups we can choose $\mathbf{a}_0$ to be the element R, the operation of time inversion itself; this means that, from equation (2.2), $\overline{\boldsymbol{\Delta}}(\mathbf{u}) = \boldsymbol{\Delta}(\mathbf{a}_0^{-1}\,\mathbf{u}\mathbf{a}_0)^* = \boldsymbol{\Delta}(\mathbf{u})^*$. It can be seen from the work of Altmann and Bradley that for the degenerate single-valued reps of the point groups it is always possible to choose $\boldsymbol{\Delta}(\mathbf{u})$ to be real, so that, for degenerate reps and for the real non-degenerate reps of any ordinary point group $\mathbf{G}$, $\overline{\boldsymbol{\Delta}}(\mathbf{u})$ is not only equivalent but also identical to $\boldsymbol{\Delta}(\mathbf{u})$ so that of necessity $\boldsymbol{\beta} = \pm\mathbf{1}$ and $\boldsymbol{\beta\beta}^* = +\mathbf{1}$. For complex non-degenerate reps of $\mathbf{G}$, $\overline{\boldsymbol{\Delta}}(\mathbf{u}) = \boldsymbol{\Delta}(\mathbf{u})^*$ and is therefore inequivalent to $\boldsymbol{\Delta}(\mathbf{u})$. For single-valued reps of $\mathbf{G}$, which are used in connection with entities having zero or integer spin, then $\boldsymbol{\Delta}(\mathbf{a}_0^2) = \boldsymbol{\Delta}(R^2) = +\mathbf{1}$ (see Wigner 1959). Therefore, for any grey group $\mathbf{G}+R\mathbf{G}$ there will be two coreps derived from $\boldsymbol{\Delta}(\mathbf{u})$ and given by equation (4.2) of APC I with $\boldsymbol{\beta} = \pm\mathbf{1}$ for each degenerate or real non-degenerate rep $\boldsymbol{\Delta}(\mathbf{u})$ of $\mathbf{G}$; and there will be one corep given by equation (4.4) of APC I derived from each complex non-degenerate rep $\boldsymbol{\Delta}(\mathbf{u})$ of $\mathbf{G}$. It is therefore possible to write down the single-valued coreps of any grey point group without much trouble.

We turn now to the consideration of the coreps derived from the double-valued reps of the grey point groups. In Table 1 we give the character tables for the double-valued representations of the ordinary point groups, together with the matrix representatives for degenerate reps. The notation used for the symmetry elements of these groups follows that of Altmann and Bradley (1963), with the exception that rather than use a separate notation for tetragonal groups they are regarded as subgroups of the cubic groups; our operations are active instead of passive. In Table 1 the matrices are given only for the generating elements of each group; the matrices for the other elements must be found by using Table 2. The generating relations given in Table 2 enable the complete group multiplication table of the double point group to be evaluated if necessary. Only half the elements of each double point group are given in Table 2; the other elements can be found using the fact that if X has matrix representative $P^{\alpha}\,Q^{\beta}\,R^{\gamma}$ then $\overline{X}$ must have matrix representative $-P^{\alpha}\,Q^{\beta}\,R^{\gamma}$. For completeness, in order to identify the point-group elements in terms of the unitary

TABLE 2

THE MATRICES FOR DEGENERATE DOUBLE-VALUED REPS OF THE POINT GROUPS

E is the identity matrix in the appropriate number of dimensions; the matrices P, Q, and R are identified for each group in Table 1

$2mm$ (C_{2v})	222 (D_2)	Matrix
E	E	E
σ_x	C_{2x}	P
σ_y	C_{2y}	Q
C_{2z}	C_{2z}	PQ

$P^4 = E,\ Q^4 = E,\ QP = P^3Q,\ Q^2 = P^2$

32 (D_3)	$3m$ (C_{3v})	Matrix
E	E	E
C_3^+	C_3^+	P
C_3^-	C_3^-	P^5
C'_{21}	σ_{v1}	Q
C'_{22}	σ_{v2}	P^5Q
C'_{23}	σ_{v3}	P^4Q

$P^6 = E,\ Q^4 = E,\ Q^2 = P^3,\ QP = P^5Q$

422 (D_4)	$4mm$ (C_{4v})	$\bar{4}2m$ (D_{2d})	Matrix
E	E	E	E
C_{4z}^-	C_{4z}^-	S_{4z}^+	P
C_{2z}	C_{2z}	C_{2z}	P^2
C_{4z}^+	C_{4z}^+	S_{4z}^-	P^7
C_{2x}	σ_x	C_{2x}	Q
C_{2y}	σ_y	C_{2y}	P^2Q
C_{2a}	σ_{da}	σ_{da}	P^3Q
C_{2b}	σ_{db}	σ_{db}	PQ

$P^8 = E,\ Q^4 = E,\ Q^2 = P^4,\ QP = P^7Q$

unimodular matrices of SU(2) used in the initial derivation of the double point groups, the matrices of SU(2) corresponding to the generating elements of 432 (O) and 622 (D_6) are also given in Table 1. All the other point groups are very simply related to one or other of these two point groups, so that their matrices in SU(2) can easily be found.

To obtain the double-valued coreps of each of these 32 grey groups $\mathbf{G}+R\mathbf{G}$, we still have $\overline{\mathbf{\Delta}}(\mathbf{u}) = \mathbf{\Delta}(\mathbf{u})^*$, since R can be chosen as $\mathbf{a}_0$. But now, since double-valued reps are used in connection with entities having half-odd-integer spin, we have $\mathbf{\Delta}(\mathbf{a}_0^2) = \mathbf{\Delta}(R^2) = -\mathbf{1}$ (see Wigner 1959). It is then fairly straightforward to see how the coreps of a grey group are obtained from the double-valued reps of an ordinary point group. This is conveniently summarized in Table 3 together with the values

TABLE 2 (*Continued*)

$622\ (D_6)$	$6mm\ (C_{6v})$	$\bar{6}2m\ (D_{3h})$	Matrix
E	E	E	E
C_6^+	C_6^+	S_3^-	P
C_3^+	C_3^+	C_3^+	P^2
C_2	C_2	σ_h	P^9
C_3^-	C_3^-	C_3^-	P^{10}
C_6^-	C_6^-	S_3^+	P^{11}
C'_{21}	σ_{d1}	C'_{21}	Q
C'_{22}	σ_{d2}	C'_{22}	$P^{10}Q$
C'_{23}	σ_{d3}	C'_{23}	P^8Q
C''_{21}	σ_{v1}	σ_{v1}	P^9Q
C''_{22}	σ_{v2}	σ_{v2}	P^7Q
C''_{23}	σ_{v3}	σ_{v3}	$P^{11}Q$

$P^{12} = E,\ Q^4 = E,\ Q^2 = P^6,\ QP = P^{11}Q$

$23\ (T)$	Matrix
E	E
C_{2x}	Q
C_{2y}	P^3R
C_{2z}	P^3QR
C_{31}^-	P
C_{32}^-	PR
C_{33}^-	P^4QR
C_{34}^-	PQ
C_{31}^+	P^2
C_{32}^+	P^2Q
C_{33}^+	P^5R
C_{34}^+	P^2QR

$P^6 = E,\ Q^4 = E,\ R^4 = E,$
$P^3 = Q^2 = R^2,\ QP = PR,$
$RP = PQR,\ RQ = P^3QR$

of matrix $\boldsymbol{\beta}$ where relevant, where the entry in the second column indicates whether the corep belongs to case 1, case 2, or case 3. Except in the case of degenerate reps $\Delta(\mathbf{u})$ with real characters but with some matrices complex, the coreps can be written down immediately using Table 3 and the matrices $\Delta(\mathbf{u})$. For this one remaining case the characters of $\Delta(\mathbf{u})$ and $\overline{\Delta}(\mathbf{u})$ must be the same, so that the coreps derived from $\Delta(\mathbf{u})$ must belong to either case 1 or case 2; which of these actually happens can be found by determining $\boldsymbol{\beta}$ by inspection of $\Delta(\mathbf{u})$ and $\overline{\Delta}(\mathbf{u})$. Alternatively, one can use the test given by Dimmock and Wheeler (1962; equation (21)) or Bradley and Davies (personal communication 1966) to determine whether the corep derived from $\Delta(\mathbf{u})$

TABLE 2 (*Continued*)

432 (O)	$\bar{4}3m$ (T_d)	Matrix	432 (O)	$\bar{4}3m$ (T_d)	Matrix
E	E	E	C_{4x}^+	S_{4x}^-	P
C_{2x}	C_{2x}	P^2	C_{4y}^+	S_{4y}^-	P^3Q^2
C_{2y}	C_{2y}	P^5QR	C_{4z}^+	S_{4z}^-	P^6R
C_{2z}	C_{2z}	P^7QR	C_{4x}^-	S_{4x}^+	P^7
C_{31}^-	C_{31}^-	P^4Q	C_{4y}^-	S_{4y}^+	P^2Q^2R
C_{32}^-	C_{32}^-	P^6Q	C_{4z}^-	S_{4z}^+	P^5Q
C_{33}^-	C_{33}^-	PR	C_{2a}	σ_{da}	P^3Q
C_{34}^-	C_{34}^-	P^7R	C_{2b}	σ_{db}	R
C_{31}^+	C_{31}^+	Q^2	C_{2c}	σ_{dc}	PQ^2
C_{32}^+	C_{32}^+	PQ^2R	C_{2d}	σ_{dd}	P^6QR
C_{33}^+	C_{33}^+	P^3Q^2R	C_{2e}	σ_{de}	P^4Q^2R
C_{34}^+	C_{34}^+	P^2Q^2	C_{2f}	σ_{df}	P^4QR

$P^8 = E,\ Q^3 = E,\ R^4 = E,\ R^2 = P^4,\ QP = P^6Q^2R,\ QP^2 = P^3R,\ QP^4 = P^4Q,\ Q^2P = P^3Q,$
$RP = P^6Q^2,\ RP^2 = PQ,\ RQ = Q^2R$

belongs to case 1 or case 2; however, this does not achieve very much saving of effort if one actually wishes to write down the matrices in the coreps because $\boldsymbol{\beta}$ has to be found.

As an example we can consider the grey point group 2221′, which is derived from 222 (D_2); in Table 4 we list $\boldsymbol{\Delta}(\mathbf{u})$ and $\overline{\boldsymbol{\Delta}}(\mathbf{u})$ for the rep E. By inspection it can easily be seen that $\boldsymbol{\beta}$ must be the matrix $\begin{pmatrix} 0 & +1 \\ -1 & 0 \end{pmatrix}$ so that $\boldsymbol{\beta\beta}^* = -\mathbf{1} = +\boldsymbol{\Delta}(\mathbf{a}_0^2)$, since this is a double-valued rep of $\mathbf{G}$ and $\mathbf{a}_0 = R$. The corep of the grey group $\mathbf{G}+R\mathbf{G}$ derived from the rep E of $\mathbf{G}$ can thus be written down using equation (4.2) of APC I and the value of $\boldsymbol{\beta}$ that we have just found.

In Table 5 we give the information that enables those coreps of the grey groups derived from degenerate double-valued reps of the point groups to be written down. In Table 5, $\boldsymbol{\Delta}(\mathbf{u})$ is listed in the second column; the third column indicates which type of corep of $\mathbf{G}+R\mathbf{G}$ is derived from that rep of $\mathbf{G}$; and the last column gives $\boldsymbol{\beta}$ for those cases in which it exists. In the third column the number 1, 2, or 3 indicates that the corep of $\mathbf{G}+R\mathbf{G}$ derived from that rep of $\mathbf{G}$ belongs to case 1, case 2, or case 3; the actual matrices will then be given respectively by equation (4.2), equation (4.3), or equation (4.4) of APC I.

This completes the derivation of the double-valued coreps of the grey groups; the rules for all forms of $\boldsymbol{\Delta}(\mathbf{u})$ except one have been given in Table 3, and for this one exception the coreps can be found by using Table 5.

IV. THE COREPS OF THE BLACK AND WHITE MAGNETIC POINT GROUPS

In this section we shall be concerned with the double-valued coreps of the 58 type III magnetic point groups defined by equation (2.1). We shall follow the identification of $\mathbf{H}$ and of the classes in ($\mathbf{G}-\mathbf{H}$) given in Tables I and V of Cracknell

(1966);† the notation used for the symmetry elements of these groups again follows that of Altmann and Bradley (1963), with the exception that rather than use a separate notation for tetragonal groups they are regarded as subgroups of the cubic groups and our operations are active instead of passive.

TABLE 3

RULES FOR CONSTRUCTING DOUBLE-VALUED COREPS OF GREY GROUPS

$\Delta(\mathbf{u})$	Corep	Equation of APC I	$\boldsymbol{\beta}$
Non-degenerate, complex	3	(4.4)	—
Non-degenerate, real	2	(4.3)	± 1
Degenerate, some characters complex	3	(4.4)	—
Degenerate, characters real, all matrices real	2	(4.3)	± 1
Degenerate, characters real, some matrices complex	Case 1 or case 2; determine by inspection		

TABLE 4

$2221'$, $\Delta(\mathbf{u})$, AND $\bar{\Delta}(\mathbf{u})$ FOR $\bar{E}$ OF 222 (D_2)

$\mathbf{u}$	$\Delta(\mathbf{u})$	$\bar{\Delta}(\mathbf{u})$
E	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
C_{2x}	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$
C_{2y}	$\begin{pmatrix} 0 & \mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -\mathrm{i} \\ -\mathrm{i} & 0 \end{pmatrix}$
C_{2z}	$\begin{pmatrix} \mathrm{i} & 0 \\ 0 & -\mathrm{i} \end{pmatrix}$	$\begin{pmatrix} -\mathrm{i} & 0 \\ 0 & \mathrm{i} \end{pmatrix}$

The theory outlined in Section II can be applied to these groups, and by way of illustration we consider the magnetic point group $4'22'$. From APC I we can see that $\mathbf{H}$ is the point group 222 (D_2) and that the elements of $\mathbf{H}$ and $R(\mathbf{G}-\mathbf{H})$ are

$$\mathbf{H}: \quad E, \bar{E}, C_{2x}, \bar{C}_{2x}, C_{2y}, \bar{C}_{2y}, C_{2z}, \bar{C}_{2z} \tag{4.1}$$

and

$$R(\mathbf{G}-\mathbf{H}): \quad RC_{4z}^{-}, R\bar{C}_{4z}^{-}, RC_{4z}^{+}, R\bar{C}_{4z}^{+}, RC_{2a}, R\bar{C}_{2a}, RC_{2b}, R\bar{C}_{2b}. \tag{4.2}$$

† There is an error in Table V of Cracknell (1966). The line for the point group $\bar{6}'$ should read

$\bar{6}'$ $\quad h \quad$ $\sigma_h; S_3^-; S_3^+ \quad$ σ_h

It does not matter which of the elements in $R(\mathbf{G}-\mathbf{H})$ is chosen as $\mathbf{a}_0$, except that once $\mathbf{a}_0$ is chosen it should not be altered; in fact, we choose RC_{2a} as $\mathbf{a}_0$ so that

TABLE 5

THE DEGENERATE DOUBLE-VALUED COREPS OF THE GREY GROUPS

$$\rho = \pm\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

(Direct product groups are not included)

G	Rep of **G**	Corep of **M**	**β**
$2mm$ (C_{2v})	$\bar{E}$	1	ρ
222 (D_2)	$\bar{E}$	1	ρ
32 (D_3)	$\bar{E}$	1	ρ
$3m$ (C_{3v})	$\bar{E}$	1	ρ
422 (D_4)	$\bar{E}_1, \bar{E}_2$	1	ρ
$4mm$ (C_{4v})	$\bar{E}_1, \bar{E}_2$	1	ρ
$\bar{4}2m$ (D_{2d})	$\bar{E}_1, \bar{E}_2$	1	ρ
622 (D_6)	$\bar{E}_1, \bar{E}_2, \bar{E}_3$	1	ρ
$6mm$ (C_{6v})	$\bar{E}_1, \bar{E}_2, \bar{E}_3$	1	ρ
$\bar{6}2m$ (D_{3h})	$\bar{E}_1, \bar{E}_2, \bar{E}_3$	1	ρ
23 (T)	$\bar{E}$	1	ρ
	${}^1\bar{F}, {}^2\bar{F}$	3	—
432 (O)	$\bar{E}_1, \bar{E}_2$	1	ρ
	$\bar{F}$	1	$\left(\begin{array}{c\|c} \rho & 0 \\ \hline 0 & \rho \end{array}\right)$
$\bar{4}3m$ (T_d)	$\bar{E}_1, \bar{E}_2$	1	ρ
	$\bar{F}$	1	$\left(\begin{array}{c\|c} \rho & 0 \\ \hline 0 & \rho \end{array}\right)$

TABLE 6

$\mathbf{\Delta}(\mathbf{u})$ AND $\bar{\mathbf{\Delta}}(\mathbf{u})$ FOR $4'22'$

u	$\mathbf{\Delta}(\mathbf{u})$	$\bar{\mathbf{\Delta}}(\mathbf{u})$
E	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
C_{2x}	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & \mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}$
C_{2y}	$\begin{pmatrix} 0 & \mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$
C_{2z}	$\begin{pmatrix} \mathrm{i} & 0 \\ 0 & -\mathrm{i} \end{pmatrix}$	$\begin{pmatrix} \mathrm{i} & 0 \\ 0 & -\mathrm{i} \end{pmatrix}$

$\bar{\mathbf{\Delta}}(\mathbf{u}) = \mathbf{\Delta}\{(RC_{2a})^{-1}\,\mathbf{u}\,RC_{2a}\}^* = \mathbf{\Delta}(\bar{C}_{2a}\,\mathbf{u}\,C_{2a})^*$, since R commutes with all the point-group operations. The generating relations given in Table 2 can be used to evaluate products of the form $\bar{C}_{2a}\,\mathbf{u}\,C_{2a}$, so that the matrices for each of the elements of **H** in the reps $\mathbf{\Delta}(\mathbf{u})$ and $\bar{\mathbf{\Delta}}(\mathbf{u})$ can be found from Tables 1 and 2; these matrices are listed in Table 6. The matrices for $\bar{E}$, $\bar{C}_{2x}$, $\bar{C}_{2y}$, and $\bar{C}_{2z}$ are not listed, since they are given by $\mathbf{\Delta}(\bar{X}) = -\mathbf{\Delta}(X)$ where X is any point-group operation. $\mathbf{\Delta}(\mathbf{u})$ and $\bar{\mathbf{\Delta}}(\mathbf{u})$, although they are obviously not identical, are nevertheless equivalent since their characters are the same; we can therefore find $\boldsymbol{\beta}$ from

$$\bar{\mathbf{\Delta}}(\mathbf{u}) = \boldsymbol{\beta}^{-1}\,\mathbf{\Delta}(\mathbf{u})\,\boldsymbol{\beta} \tag{2.3}$$

for all $\mathbf{u}$. It is fairly easy to show that

$$\boldsymbol{\beta} = \pm\frac{1}{\sqrt{2}}\begin{pmatrix} 1-\mathrm{i} & 0 \\ 0 & 1+\mathrm{i} \end{pmatrix}, \tag{4.3}$$

and, therefore,

$$\boldsymbol{\beta\beta}^* = +\mathbf{1}. \tag{4.4}$$

But $$\mathbf{\Delta}(\mathbf{a}_0^2) = \mathbf{\Delta}\{(RC_{2a})^2\} = \mathbf{\Delta}(R^2\bar{E}) = \mathbf{\Delta}(R^2)\,\mathbf{\Delta}(\bar{E}) = +\mathbf{1},$$

so that $$\boldsymbol{\beta\beta}^* = +\mathbf{\Delta}(\mathbf{a}_0^2) \tag{4.5}$$

and the corep of $4'22'$ derived from the double-valued rep $\bar{E}$ of 222 (D_2) belongs to case 1, and its matrices can be found using equation (4.2) of APC I and the value of $\boldsymbol{\beta}$ given in equation (4.3) above.

This example illustrates how the double-valued coreps of all the 58 black and white (type III) magnetic point groups can be derived. The results are collected into Table 7. Columns 1 and 2 of Table 7 give **M** and **H** respectively; the actual identification of the elements and classes in **H** and $R(\mathbf{G}-\mathbf{H})$ can be done using Tables V and VI of Cracknell (1966). In column 3 of Table 7 we identify the element that has been chosen as $\mathbf{a}_0$, $\mathbf{a}_0$ being R times the entry in column 3. The coreps obtained in the end do not depend on the choice of $\mathbf{a}_0$ (Wigner 1959), although some of the details of the working will depend on $\mathbf{a}_0$. Column 4 lists the double-valued reps of **H**, column 5 indicates to which case the corep of **M** derived from that rep of **H** belongs, and column 6 gives $\boldsymbol{\beta}$ for those cases in which it exists. In column 5 the number 1, 2, or 3 indicates that the corep of **M** derived from that rep of **H** belongs to case 1, case 2, or case 3; the actual matrices will then be given respectively by equation (4.2), equation (4.3), or equation (4.4) of APC I.

V. Discussion

We have already mentioned that the earlier work of Dimmock and Wheeler (1962, 1964) on the coreps of magnetic point groups did not include either $\boldsymbol{\beta}$ or the matrix representatives for the halving subgroup of unitary elements in the type II or type III magnetic groups. The work of Cracknell (1966) on the single-valued coreps of magnetic point groups did not explicitly give $\boldsymbol{\beta}$ either, although it did give the matrix representatives $\mathbf{\Delta}(\mathbf{u})$. For the single-valued reps in that work the matrix representatives chosen were all real, so that in nearly every case $\bar{\mathbf{\Delta}}(\mathbf{u})$ is not only equivalent but also identical to $\mathbf{\Delta}(\mathbf{u})$ and, therefore, $\boldsymbol{\beta}$ is equal to $\pm\mathbf{1}$. There are three

TABLE 7

THE DOUBLE-VALUED COREPS OF THE 58 TYPE III MAGNETIC GROUPS

$$\alpha = \pm 1; \quad \epsilon = \pm\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}; \quad \rho = \pm\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}; \quad \sigma = \pm\frac{1}{\sqrt{2}}\begin{pmatrix}1-\mathrm{i} & 0\\ 0 & 1+\mathrm{i}\end{pmatrix}$$

$$\chi = \pm\frac{1}{2\sqrt{6}}\begin{pmatrix}(\sqrt{3}+1)+\mathrm{i}(\sqrt{3}-1) & 4\mathrm{i}\\ 4\mathrm{i} & (\sqrt{3}+1)-\mathrm{i}(\sqrt{3}-1)\end{pmatrix}$$

$$\psi = \pm\begin{pmatrix}0 & 1 & 0 & 0\\ -1 & 0 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & -1 & 0\end{pmatrix}$$

(1) M	(2) H	(3) $R^{-1}\mathbf{a}_0$	(4) Rep of **H**	(5) Corep of **M**	(6) $\boldsymbol{\beta}$
$\bar{1}'$	$1\ (C_1)$	I	$\bar{A}$	2	α
$2'$	$1\ (C_1)$	C_{2z}	$\bar{A}$	1	α
m'	$1\ (C_1)$	σ_z	$\bar{A}$	1	α
$2/m'$	$2\ (C_2)$	I	${}^1\bar{E}, {}^2\bar{E}$	3	—
$2'/m$	$m\ (C_{1h})$	I	${}^1\bar{E}, {}^2\bar{E}$	3	—
$2'/m'$	$\bar{1}\ (C_i)$	C_{2z}	$\bar{A}_g, \bar{A}_u$	1	α
$22'2'$	$2\ (C_2)$	C_{2x}	${}^1\bar{E}, {}^2\bar{E}$	1	α
$2m'm'$	$2\ (C_2)$	σ_x	${}^1\bar{E}, {}^2\bar{E}$	1	α
$2'm'm$	$m\ (C_{1h})$†	C_{2z}	${}^1\bar{E}, {}^2\bar{E}$	1	α
$m'm'm'$	$222\ (D_2)$	I	$\bar{E}$	1	ρ
mmm'	$2mm\ (C_{2v})$	I	$\bar{E}$	1	ρ
$m'm'm$	$2/m\ (C_{2h})$	C_{2x}	${}^1\bar{E}_g, {}^2\bar{E}_g, {}^1\bar{E}_u, {}^2\bar{E}_u$	1	α
$4'$	$2\ (C_2)$	C_{4z}^{+}	${}^1\bar{E}, {}^2\bar{E}$	3	—
$\bar{4}'$	$2\ (C_2)$	S_{4z}^{-}	${}^1\bar{E}, {}^2\bar{E}$	3	—
$42'2'$	$4\ (C_4)$	C_{2x}	${}^2\bar{E}_1, {}^1\bar{E}_2, {}^2\bar{E}_2, {}^1\bar{E}_1$	1	α
$4'22'$	$222\ (D_2)$	C_{2a}	$\bar{E}$	1	σ
$4/m'$	$4\ (C_4)$	I	${}^2\bar{E}_1, {}^1\bar{E}_2, {}^2\bar{E}_2, {}^1\bar{E}_1$	3	—
$4'/m'$	$\bar{4}\ (S_4)$	I	${}^2\bar{E}_1, {}^1\bar{E}_2, {}^2\bar{E}_2, {}^1\bar{E}_1$	3	—
$4'/m$	$2/m\ (C_{2h})$	C_{4z}^{+}	${}^1\bar{E}_g, {}^2\bar{E}_g, {}^1\bar{E}_u, {}^2\bar{E}_u$	3	—
$4m'm'$	$4\ (C_4)$	σ_x	${}^2\bar{E}_1, {}^1\bar{E}_2, {}^2\bar{E}_2, {}^1\bar{E}_1$	1	α
$4'mm'$	$2mm\ (C_{2v})$	σ_{da}	$\bar{E}$	1	σ
$\bar{4}2'm'$	$\bar{4}\ (S_4)$	C_{2x}	${}^2\bar{E}_1, {}^1\bar{E}_2, {}^2\bar{E}_2, {}^1\bar{E}_1$	1	α
$\bar{4}'2m'$	$222\ (D_2)$	σ_{da}	$\bar{E}$	1	σ
$\bar{4}'2'm$	$2mm\ (C_{2v})$	C_{2a}	$\bar{E}$	1	σ
$4/m'm'm'$	$422\ (D_4)$	I	$\bar{E}_1, \bar{E}_2$	1	ρ
$4/m'mm$	$4mm\ (C_{4v})$	I	$\bar{E}_1, \bar{E}_2$	1	ρ
$4'/mmm$	$mmm\ (D_{2h})$	C_{2a}	$\bar{E}_g, \bar{E}_u$	1	σ
$4'/m'm'm$	$\bar{4}2m\ (D_{2d})$	I	$\bar{E}_1, \bar{E}_2$	1	ρ
$4/mm'm'$	$4/m\ (C_{4h})$	C_{2x}	${}^2\bar{E}_{1g}, {}^1\bar{E}_{2g}, {}^2\bar{E}_{2g}, {}^1\bar{E}_{1g}$	1	α
			${}^2\bar{E}_{1u}, {}^1\bar{E}_{2u}, {}^2\bar{E}_{2u}, {}^1\bar{E}_{1u}$	1	α
$32'$	$3\ (C_3)$	C_{21}'	${}^2\bar{E}, \bar{A}, {}^1\bar{E}$	1	α
$3m'$	$3\ (C_3)$	σ_{d1}	${}^2\bar{E}, \bar{A}, {}^1\bar{E}$	1	α
$\bar{6}'$	$3\ (C_3)$	σ_h	${}^2\bar{E}, {}^1\bar{E}$	3	—
			$\bar{A}$	1	α

† The elements of **H** are E, $\bar{E}$, σ_y, and $\bar{\sigma}_y$ instead of the E, $\bar{E}$, σ_z, and $\bar{\sigma}_z$ used in Table 1 for $m\ (C_{1h})$.

TABLE 7 (*Continued*)

(1) M	(2) H	(3) $R^{-1}\mathbf{a}_0$	(4) Rep of **H**	(5) Corep of **M**	(6) $\boldsymbol{\beta}$
$\bar{6}m'2'$	$\bar{6}$ (C_{3h})	C'_{21}	${}^2\bar{E}_3, {}^1\bar{E}_1, {}^2\bar{E}_2, {}^1\bar{E}_2, {}^2\bar{E}_1, {}^1\bar{E}_3$	1	α
$\bar{6}'m2'$	$3m$ (C_{3v})	σ_h	${}^1\bar{E}, {}^2\bar{E}$	1	α
			$\bar{E}_1$	1	ϵ
$\bar{6}'m'2$	32 (D_3)	σ_h	${}^1\bar{E}, {}^2\bar{E}$	1	α
			$\bar{E}_1$	1	ϵ
$6'$	3 (C_3)	C_2	${}^2\bar{E}, {}^1\bar{E}$	3	—
			$\bar{A}$	1	α
$\bar{3}'$	3 (C_3)	I	${}^2\bar{E}, {}^1\bar{E}$	3	—
			$\bar{A}$	2	α
$\bar{3}m'$	$\bar{3}$ (C_{3i})	C'_{21}	${}^2\bar{E}_g, \bar{A}_g, {}^1\bar{E}_g$	1	α
			${}^2\bar{E}_u, \bar{A}_u, {}^1\bar{E}_u$	1	α
$\bar{3}'m$	$3m$ (C_{3v})	I	${}^1\bar{E}, {}^2\bar{E}$	3	—
			$\bar{E}_1$	1	ρ
$\bar{3}'m'$	32 (D_3)	I	${}^1\bar{E}, {}^2\bar{E}$	3	—
			$\bar{E}_1$	1	ρ
$62'2'$	6 (C_6)	C'_{21}	${}^2\bar{E}_3, {}^1\bar{E}_1, {}^2\bar{E}_2, {}^1\bar{E}_2, {}^2\bar{E}_1, {}^1\bar{E}_3$	1	α
$6'22'$	32 (D_3)	C_2	${}^1\bar{E}, {}^2\bar{E}$	1	α
			$\bar{E}_1$	1	ϵ
$6/m'$	6 (C_6)	I	${}^2\bar{E}_3, {}^1\bar{E}_1, {}^2\bar{E}_2, {}^1\bar{E}_2, {}^2\bar{E}_1, {}^1\bar{E}_3$	3	—
$6'/m'$	$\bar{3}$ (C_{3i})	C_2	${}^2\bar{E}_g, {}^1\bar{E}_g, {}^2\bar{E}_u, {}^1\bar{E}_u$	3	—
			$\bar{A}_g, \bar{A}_u$	1	α
$6'/m$	$\bar{6}$ (C_{3h})	I	${}^2\bar{E}_3, {}^1\bar{E}_1, {}^2\bar{E}_2, {}^1\bar{E}_2, {}^2\bar{E}_1, {}^1\bar{E}_3$	3	—
$6m'm'$	6 (C_6)	σ_{d1}	${}^2\bar{E}_3, {}^1\bar{E}_1, {}^2\bar{E}_2, {}^1\bar{E}_2, {}^2\bar{E}_1, {}^1\bar{E}_3$	1	α
$6'mm'$	$3m$ (C_{3v})	C_2	${}^1\bar{E}, {}^2\bar{E}$	1	α
			$\bar{E}_1$	1	ϵ
$6'/mm'm$	$\bar{6}2m$ (D_{3h})	I	$\bar{E}_1, \bar{E}_2, \bar{E}_3$	1	ρ
$6'/m'm'm$	$\bar{3}m$ (D_{3d})	C_2	${}^1\bar{E}_g, {}^2\bar{E}_g, {}^1\bar{E}_u, {}^2\bar{E}_u$	1	α
			$\bar{E}_{1g}, \bar{E}_{1u}$	1	ϵ
$6/m'm'm'$	622 (D_6)	I	$\bar{E}_1, \bar{E}_2, \bar{E}_3$	1	ρ
$6/m'mm$	$6mm$ (C_{6v})	I	$\bar{E}_1, \bar{E}_2, \bar{E}_3$	1	ρ
$6/mm'm'$	$6/m$ (C_{6h})	C'_{21}	${}^2\bar{E}_{3g}, {}^1\bar{E}_{1g}, {}^2\bar{E}_{2g}$	1	α
			${}^1\bar{E}_{2g}, {}^2\bar{E}_{1g}, {}^1\bar{E}_{3g}$	1	α
			${}^2\bar{E}_{3u}, {}^1\bar{E}_{1u}, {}^2\bar{E}_{2u}$	1	α
			${}^1\bar{E}_{2u}, {}^2\bar{E}_{1u}, {}^1\bar{E}_{3u}$	1	α
$m'3$	23 (T)	I	$\bar{E}$	1	ρ
			${}^1\bar{F}, {}^2\bar{F}$	3	—
$\bar{4}'3m'$	23 (T)	σ_{da}	$\bar{E}, {}^1\bar{F}, {}^2\bar{F}$	1	χ
$4'32'$	23 (T)	C_{2a}	$\bar{E}, {}^1\bar{F}, {}^2\bar{F}$	1	χ
$m'3m'$	432 (O)	I	$\bar{E}_1, \bar{E}_2$	1	ρ
			$\bar{F}$	1	ψ
$m'3m$	$\bar{4}3m$ (T_d)	I	$\bar{E}_1, \bar{E}_2$	1	ρ
			$\bar{F}$	1	ψ
$m3m'$	$m3$ (T_h)	C_{2a}	$\bar{E}_g, {}^1\bar{F}_g, {}^2\bar{F}_g$	1	χ
			$\bar{E}_u, {}^1\bar{F}_u, {}^2\bar{F}_u$	1	χ

exceptions; for the reps T of $\bar{4}'3m'$, T of $4'32'$, and T_g and T_u of $m3m'$ $\bar{\mathbf{\Delta}}(\mathbf{u})$ and $\mathbf{\Delta}(\mathbf{u})$ are equivalent but not identical, and $\boldsymbol{\beta}$ is equal to $\pm\begin{pmatrix}0 & 1 & 0\\ 1 & 0 & 0\\ 0 & 0 & -1\end{pmatrix}$.

With regard to the grey groups Dimmock and Wheeler (1962) state that all double-valued reps with real characters and of dimension greater than 1 belong to case 1, that is, they follow equation (4.2) of APC I. This statement, which is perfectly true, is not present in their later work (Dimmock and Wheeler 1964), and there is no indication in this later work of how the coreps derived from degenerate reps with real characters but with some complex matrices may be found. In fact, they do belong to case 1 and can be found using equation (4.2) of APC I and the values of $\boldsymbol{\beta}$ given in Table 5 of the present paper.

We would like to draw attention to the following error in the work of Cracknell (1966) on the single-valued coreps of the magnetic point groups. In Table VI of that work the reps B of $4'$, B of $\bar{4}'$, and B_g and B_u of $4'/m$ do not lead to coreps belonging to case 1, as stated there, but to coreps belonging to case 2 which can be found using equation (4.3) of APC I.

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