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Corepresentations of Magnetic Point Groups

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The well-established theory due to Wigner of the corepresentations of non-unitary groups is here applied to the magnetic point groups and the results are tabulated. The equivalence of the theory of the corepresentations of the grey groups to the conventional treatment of time-reversal symmetry in space groups is also considered.

§ 1. Introduction

By now the importance of the study of magnetic symmetry is well established. The magnetic groups are non-unitary and the theory originally developed by Wigner[1] of the irreducible corepresentations (or "coreps" for short) of non-unitary groups has been applied to them by Dimmock and Wheeler[2),3)] and by the present author[4] (hereafter referred to as APC I) with applications to the one-dimensional anti-ferromagnetic Kronig-Penney problem[3] and the magnetic cubic space groups[4] particularly Ia′3 and Ia3′. It seemed to be desirable, without repeating the theory here, to deduce the coreps of all the magnetic point groups and to list the results as concisely as possible.

§ 2. The magnetic point groups

The magnetic point groups were first listed by Tavger and Zaitsev.[5] If we include the non-magnetic point groups there are three types of point group, which we shall call types I, II and III by analogy with the previous work on space groups.[4] They are

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

making a total of 122 point groups altogether. A discussion of the relevance of these various types of magnetic group to the description of real crystals is given by Birss.[6]

If $\boldsymbol{G}$ is an ordinary point group (type I) then a type II point group, $\boldsymbol{M}$, is given by

$$\boldsymbol{M}=\boldsymbol{G}+R\,\boldsymbol{G}, \tag{2·1}$$

where R is the operation of time-inversion. And a type III point group, $\boldsymbol{M}$, (of which there are 58) is given by

$$\boldsymbol{M} = \boldsymbol{H} + R(\boldsymbol{G} - \boldsymbol{H}), \tag{2·2}$$

where $\boldsymbol{H}$ is a halving subgroup of $\boldsymbol{G}$. The identification of $\boldsymbol{H}$ for each of the 58 type III groups has been done by, originally, Tavger and Zaitsev,[5] Hamermesh[7] and Dimmock and Wheeler[3] and they are listed in Table I.

Table I. The Magnetic Point Groups.

The magnetic group $\boldsymbol{M}$ is given in the first column and its halving subgroup $\boldsymbol{H}$ of unitary elements is given in the second column. The same information is listed in the Schoenflies notation in the third and fourth columns, but, since this notation is singularly unsuited to the labelling of the magnetic groups, it is $\boldsymbol{G}$ rather than $\boldsymbol{M}$ which is given in the third column.

$\boldsymbol{M}$	$\boldsymbol{H}$	$\boldsymbol{G}$	$\boldsymbol{H}$
1^1	1	$C_i(S_2)$	C_1
2^1	1	C_2	C_1
m^1	1	$C_s(C_{1h})$	C_1
$2/m^1$	2	C_{2h}	C_2
$2^1/m$	m	C_{2h}	$C_s(C_{1h})$
$2^1/m^1$	1	C_{2h}	$C_i(S_2)$
22^12^1	2	$D_2(V)$	C_2
$2m^1m^1$	2	C_{2v}	C_2
2^1m^1m	m	C_{2v}	$C_s(C_{1h})$
$m^1m^1m^1$	222	$D_{2h}(V_h)$	$D_2(V)$
mmm^1	$2mm$	$D_{2h}(V_h)$	C_{2v}
m^1m^1m	$2/m$	$D_{2h}(V_h)$	C_{2h}
4^1	2	C_4	C_2
4^1	2	S_4	C_2
42^12^1	4	D_4	C_4
4^122^1	222	D_4	$D_2(V)$
$4/m^1$	4	C_{4h}	C_4
$4^1/m^1$	$\bar{4}$	C_{4h}	S_4
$4^1/m$	$2/m$	C_{4h}	C_{2h}
$4m^1m^1$	4	C_{4v}	C_4
4^1mm^1	$2mm$	C_{4v}	C_{2v}
42^1m^1	4	$D_{2d}(V_d)$	S_4
4^12m^1	222	$D_{2d}(V_d)$	$D_2(V)$
4^12^1m	$2mm$	$D_{2d}(V_d)$	C_{2v}
$4/m^1m^1m^1$	422	D_{4h}	D_4
$4/m^1mm$	$4mm$	D_{4h}	C_{4v}
$4^1/mmm$	mmm	D_{4h}	$D_{2h}(V_h)$
$4^1/m^1m^1m$	$42m$	D_{4h}	$D_{2d}(V_d)$
$4/mm^1m^1$	$4/m$	D_{4h}	C_{4h}
32^1	3	D_3	C_3
$3m^1$	3	C_{3v}	C_3
6^1	3	C_{3h}	C_3
$6m^12^1$	6	D_{3h}	C_{3h}

M	**H**	**G**	**H**
$\bar{6}^1m2^1$	$3m$	D_{3h}	C_{3v}
$\bar{6}^1m^12$	32	D_{3h}	D_3
6^1	3	C_6	C_3
$\bar{3}^1$	3	$S_6(C_{3i})$	C_3
$\bar{3}m^1$	$\bar{3}$	D_{3d}	$S_6(C_{3i})$
$\bar{3}^1m$	$3m$	D_{3d}	C_{3v}
$\bar{3}^1m^1$	32	D_{3d}	D_3
62^12^1	6	D_6	C_6
6^122^1	32	D_6	D_3
$6/m^1$	6	C_{6h}	C_6
$6^1/m^1$	$\bar{3}$	C_{6h}	$S_6(C_{3i})$
$6^1/m$	$\bar{6}$	C_{6h}	C_{3h}
$6m^1m^1$	6	C_{6v}	C_6
6^1mm^1	$3m$	C_{6v}	C_{3v}
$6^1/mm^1m$	$\bar{6}2m$	D_{6h}	D_{3h}
$6^1/m^1m^1m$	$\bar{3}m$	D_{6h}	D_{3d}
$6/m^1m^1m^1$	622	D_{6h}	D_6
$6/m^1mm$	$6mm$	D_{6h}	C_{6v}
$6/mm^1m^1$	$6/m$	D_{6h}	C_{6h}
m^13	23	T_h	T
$\bar{4}^13m^1$	23	T_d	T
4^132^1	23	O	T
m^13m^1	432	O_h	O
m^13m	$\bar{4}3m$	O_h	T_d
$m3m^1$	$m3$	O_h	T_h.

§ 3. The coreps of the magnetic point groups

The character tables of the ordinary point groups (type I) are reproduced in many books on group theory, see, e.g. Heine.[8] The grey magnetic groups are direct product groups of $\boldsymbol{G}$ with the group $(E+R)$. The deduction of their character tables too is therefore trivial; they are tabulated by Dimmock and Wheeler.[5] This means that the only groups which need to be considered here are the 58 black and white magnetic groups (type III). We shall consider one or two examples in detail and simply tabulate the results for all the other groups. In what follows the term "magnetic group" is used to cover only type III groups, and we refer to the theory of § 4 of APC I in which the only necessary alteration is to replace $\bar{\boldsymbol{G}}^k$, $\bar{\boldsymbol{H}}^k$ and $\bar{\boldsymbol{M}}^k$ of that paper by $\boldsymbol{G}$, $\boldsymbol{H}$ and $\boldsymbol{M}$ respectively. In labelling the point-group elements we follow the notation of Altmann and Bradley[9] with the symmetry operations having the meaning that they have there but acting on the points of space instead of on the axes, but this has no important consequences here, for it only affects the labelling of some of the irreducible representations of a few of the point groups.

§ 4. An example, m^13

From Table I it can be seen that for this group the unitary subgroup $\boldsymbol{H}$ is the point group $23(T)$, whose character table is given in Table II. The

Table II. The character table of the point group $23(T)$.

	E	$3C_{2m}$	$4C_{3n}^-$	$4C_{3n}^+$
A	1	1	1	1
^1E	1	1	ω	ω^*
^2E	1	1	ω^*	ω
T	3	-1	0	0

$\omega=\exp(2\pi i/3)$.

fact that the elements of $(\boldsymbol{G}-\boldsymbol{H})$ have been multiplied by R does not affect the division of a group into classes, thus since $m3(T_h)$ has 8 classes and is a direct product group $23\times 1(T\times C_i)$ we can write

$$m^13=23+R.I.23$$
$$(=T+R.I.T). \qquad (4\cdot 1)$$

This group is a direct product of $23(T)$ and the group $(E+R.I)$, and it has 8 classes also:

E	RI
$C_{2x},\ C_{2y},\ C_{2z}$	$R\sigma_x,\ R\sigma_y,\ R\sigma_z$
$C_{31}^-,\ C_{32}^-,\ C_{33}^-,\ C_{34}^-$	$RS_{61}^+,\ RS_{62}^+,\ RS_{63}^+,\ RS_{64}^+$
$C_{31}^+,\ C_{32}^+,\ C_{33}^+,\ C_{34}^+$	$RS_{61}^-,\ RS_{62}^-,\ RS_{63}^-,\ RS_{64}^-$

If we use the theory of coreps in § 4 of APC I and choose $\boldsymbol{a}_0=R.I$ then $\bar{\boldsymbol{\Delta}}(\boldsymbol{u})=\boldsymbol{\Delta}(\boldsymbol{a}_0^{-1}\boldsymbol{u}\boldsymbol{a}_0)^*=\boldsymbol{\Delta}(\boldsymbol{u})^*$. For the reps A and T of the unitary subgroup $\boldsymbol{H}$, $\boldsymbol{\Delta}(\boldsymbol{u})$ is real so that $\boldsymbol{\Delta}(\boldsymbol{u})$ and $\boldsymbol{\Delta}(\boldsymbol{u})^*$ are equivalent and identical so that $\boldsymbol{\beta}\boldsymbol{\beta}^*=+\mathbf{1}=+\boldsymbol{\Delta}(\boldsymbol{a}_0^2)$ and the coreps of $\boldsymbol{M}$ are of the first type. $\boldsymbol{\beta}$ may be $+\mathbf{1}$ or $-\mathbf{1}$ so that we get the reps A, $\underline{A}$, T and $\underline{T}$ given in Table III. For the complex

Table III. The character table of m^13.

	E	$3C_{2m}$	$4C_{3n}^-$	$4C_{3n}^+$	RI	$3R\sigma_m$	$4RS_{6n}^+$	$4RS_{6n}^-$
A	1	1	1	1	1	1	1	1
$\underline{A}$	1	1	1	1	-1	-1	-1	-1
T	3	-1	0	0	3	-1	0	0
$\underline{T}$	3	-1	0	0	-3	1	0	0

reps ^1E and ^2E of $\boldsymbol{H}$, $\boldsymbol{\Delta}(\boldsymbol{u})$ and $\boldsymbol{\Delta}(\boldsymbol{u})^*$ are inequivalent, and the corep derived from $\boldsymbol{\Delta}(\boldsymbol{u})$ is thus of the third type so that from Eq. $(4\cdot 4)$ of APC I

$$\boldsymbol{D}(\boldsymbol{u}) = \begin{pmatrix} \boldsymbol{\Delta}(\boldsymbol{u}) & 0 \\ 0 & \bar{\boldsymbol{\Delta}}(\boldsymbol{u}) \end{pmatrix},$$

$$\boldsymbol{D}(\boldsymbol{a}_0\boldsymbol{u}) = \begin{pmatrix} 0 & \boldsymbol{\Delta}(\boldsymbol{u}) \\ \boldsymbol{\Delta}(\boldsymbol{u})^* & 0 \end{pmatrix} \tag{4·2}$$

so that from ${}^1E$ and ${}^2E$ we get the matrices shown in Table IV. These two

Table IV. Coreps of $m'3$ derived from ${}^1E$ and ${}^2E$ of 23 (T).

	$\boldsymbol{D}(\boldsymbol{u})$			$\boldsymbol{D}(\boldsymbol{a}_0\boldsymbol{u})$	
	${}^1E$	${}^2E$		${}^1E$	${}^2E$
E	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	RI	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
C_{2m}	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$R\sigma_m$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
C_{3n}^-	$\begin{pmatrix} \omega & 0 \\ 0 & \omega^* \end{pmatrix}$	$\begin{pmatrix} \omega^* & 0 \\ 0 & \omega \end{pmatrix}$	RS_{6n}^+	$\begin{pmatrix} 0 & \omega \\ \omega^* & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & \omega^* \\ \omega & 0 \end{pmatrix}$
C_{3n}^+	$\begin{pmatrix} \omega^* & 0 \\ 0 & \omega \end{pmatrix}$	$\begin{pmatrix} \omega & 0 \\ 0 & \omega^* \end{pmatrix}$	RS_{6n}^-	$\begin{pmatrix} 0 & \omega^* \\ \omega & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & \omega \\ \omega^* & 0 \end{pmatrix}$

corepresentations are equivalent and irreducible.

The case which we have considered illustrates that some of the 58 magnetic point groups (of type III) are direct product groups. If $(\boldsymbol{G}-\boldsymbol{H})=P\,\boldsymbol{H}$ where the elements E and P form a group, then

$$\begin{aligned} \boldsymbol{M} &= \boldsymbol{H}+R(\boldsymbol{G}-\boldsymbol{H}) \\ &= \boldsymbol{H}+RP\boldsymbol{H}, \end{aligned} \tag{4·3}$$

which is still a direct product group because E and RP also form a group. However, this does not really effect any great shortening of the work because with non-unitary groups there is no simple way of getting the coreps of direct product groups like that used for the reps of unitary groups which are direct product groups. Therefore one still has to examine each of the reps $\boldsymbol{\Delta}(\boldsymbol{u})$ of the unitary subgroup $\boldsymbol{H}$ whether or not $\boldsymbol{M}$ is a direct product group.

§ 5. Tables of coreps of all 58 magnetic point groups

In Table V we identify for each magnetic point group $\boldsymbol{M}$ the unitary subgroup $\boldsymbol{H}$, the classes in the set $(\boldsymbol{G}-\boldsymbol{H})$ and the element $\boldsymbol{a}_0$ chosen in deducing the coreps of $\boldsymbol{M}$.

The elements and character table of the unitary subgroup $\boldsymbol{H}$ for any of the magnetic groups can be found by reference to the part of Table VI indicated in column two of Table V. The type of the coreps derived from the reps of $\boldsymbol{H}$ is also indicated at the right-hand side of each character table in Table VI;

Table V. The classes in $(\boldsymbol{G}-\boldsymbol{H})$.

In column three elements in the same class in $(\boldsymbol{G}-\boldsymbol{H})$ are separated by commas, the classes are separated by semicolons, each element in columns three and four is understood to be multiplied by the factor R.

$\boldsymbol{M}$	$\boldsymbol{VI}$	Classes in $(\boldsymbol{G}-\boldsymbol{H})$	$\boldsymbol{a}_0$
1^1	a	I	I
2^1	a	C_{2z}	C_{2z}
m^1	a	σ_z	σ_z
$2/m^1$	b	$I\ ;\ \sigma_z$	I
$2^1/m$	b	$I\ ;\ C_{2z}$	I
$2^1/m^1$	b	$C_{2z}\ ;\ \sigma_z$	C_{2z}
22^12^1	b	$C_{2x}\ ;\ C_{2y}$	C_{2x}
$2m^1m^1$	b	$\sigma_x\ ;\ \sigma_y$	σ_x
2^1m^1m	b	$C_{2z}\ ;\ \sigma_x$	C_{2z}
$m^1m^1m^1$	c	$I\ ;\ \sigma_x\ ;\ \sigma_y\ ;\ \sigma_z$	I
mmm^1	c	$C_{2x}\ ;\ C_{2y}\ ;\ I\ ;\ \sigma_z$	I
m^1m^1m	c	$C_{2x}\ ;\ C_{2y}\ ;\ \sigma_x\ ;\ \sigma_y$	C_{2x}
4^1	b	$C_{4z}^+\ ;\ C_{4z}^-$	C_{4z}^+
$\bar{4}^1$	b	$S_{4z}^-\ ;\ S_{4z}^+$	S_{4z}^-
42^12^1	e	$C_{2x},\ C_{2y}\ ;\ C_{2a},\ C_{2b}$	C_{2x}
4^122^1	c	$C_{4z}^+,\ C_{4z}^-\ ;\ C_{2a},\ C_{2b}$	C_{2a}
$4/m^1$	e	$I\ ;\ S_{4z}^-\ ;\ \sigma_z\ ;\ S_{4z}^+$	I
$4^1/m^1$	e	$I\ ;\ C_{4z}^+\ ;\ \sigma_z\ ;\ C_{4z}^-$	I
$4^1/m$	c	$C_{4z}^+\ ;\ C_{4z}^-\ ;\ S_{4z}^+\ ;\ S_{4z}^+$	C_{4z}^+
$4m^1m^1$	e	$\sigma_x,\ \sigma_y\ ;\ \sigma_{da},\ \sigma_{db}$	σ_x
4^1mm^1	c	$C_{4z}^+,\ C_{4z}^-\ ;\ \sigma_{da},\ \sigma_{db}$	σ_{da}
42^1m^1	e	$C_{2x},\ C_{2y}\ ;\ \sigma_{da},\ \sigma_{db}$	C_{2x}
$\bar{4}^12m^1$	c	$S_{4z}^-,\ S_{4z}^+\ ;\ \sigma_{da},\ \sigma_{db}$	σ_{da}
$\bar{4}^12^1m$	c	$S_{4z}^-,\ S_{4z}^+\ ;\ C_{2a},\ C_{2b}$	C_{2a}
$4/m^1m^1m^1$	g	$I\ ;\ \sigma_z\ ;\ S_{4z}^-,\ S_{4z}^+\ ;\ \sigma_x,\ \sigma_y\ ;\ \sigma_{da},\ \sigma_{db}$	I
$4/m^1mm$	g	$I\ ;\ \sigma_z\ ;\ S_{4z}^-,\ S_{4z}^+\ ;\ C_{2x},\ C_{2y}\ ;\ C_{2a},\ C_{2b}$	I
$4^1/mmm$	d	$C_{4z}^+,\ C_{4z}^-\ ;\ C_{2a},\ C_{2b}\ ;\ S_{4z}^-,\ S_{4z}^+\ ;\ \sigma_{da},\ \sigma_{db}$	C_{2a}
$4^1/m^1m^1m$	g	$I\ ;\ \sigma_z\ ;\ C_{4z}^+,\ C_{4z}^-\ ;\ \sigma_x,\ \sigma_y\ ;\ \sigma_{da},\ \sigma_{db}$	I
$4/mm^1m^1$	f	$C_{2x},\ C_{2y}\ ;\ C_{2a},\ C_{2b}\ ;\ \sigma_x,\ \sigma_y\ ;\ \sigma_{da},\ \sigma_{db}$	C_{2x}
32^1	h	$C_{21}',\ C_{22}',\ C_{23}'$	C_{21}'
$3m^1$	h	$\sigma_{d1},\ \sigma_{d2},\ \sigma_{d3}$	σ_{d1}
6^1	h	$I\ ;\ S_6^-\ ;\ S_6^+$	I
$\bar{6}m^12^1$	l	$C_{21}',\ C_{22}',\ C_{23}',\ \sigma_{d1},\ \sigma_{d2},\ \sigma_{d3}$	C_{21}'
$\bar{6}^1m2^1$	j	$\sigma_z\ ;\ S_6^-,\ S_6^+\ ;\ C_{21}',\ C_{22}',\ C_{23}'$	σ_z
$\bar{6}^1m^12$	j	$\sigma_z\ ;\ S_6^-,\ S_6^+\ ;\ \sigma_{d1},\ \sigma_{d2}\ \sigma_{d3}$	σ_z
6^1	h	$C_6^+\ ;\ C_6^-\ ;\ C_2$	C_2
$\bar{3}^1$	h	$I\ ;\ S_6^-\ ;\ S_6^+$	I
$3m^1$	i	$C_{21}',\ C_{22}',\ C_{23}'\ ;\ \sigma_{d1},\ \sigma_{d2}\ \sigma_{d3}$	C_{21}'
$\bar{3}^1m$	j	$I\ ;\ S_6^-,\ S_6^+\ ;\ C_{21}',\ C_{22}',\ C_{23}'$	I
$\bar{3}^1m^1$	j	$I\ ;\ S_6^-,\ S_6^+\ ;\ \sigma_{d1},\ \sigma_{d2},\ \sigma_{d3}$	I

62^12^1	l	$C_{21}', C_{22}', C_{23}'$; $C_{21}'', C_{22}'', C_{23}''$	$C_{21}{}^1$
6^122^1	j	C_2 ; C_6^+, C_6^- ; $C_{21}'', C_{22}'', C_{23}''$	C_2
$6/m^1$	l	I ; S_3^- ; S_3^+ ; S_6^- ; S_6^+ ; σ_h	I
$6^1/m^1$	i	C_6^+ ; C_6^- ; C_2 ; S_3^+ ; S_3^- ; σ_h	C_2
$6^1/m$	l	I ; S_6^- ; S_6^+ ; C_2 ; C_6^+ ; C_6^-	I
$6m^1m^1$	l	$\sigma_{d1}, \sigma_{d2}, \sigma_{d3}$; $\sigma_{v1}, \sigma_{v2}, \sigma_{v3}$	σ_{d1}
6^1mm^1	j	C_2 ; C_6^+, C_6^- ; $\sigma_{v1}, \sigma_{v2}, \sigma_{v3}$	C_2
$6^1/mm^1m$	n	I ; C_2 ; S_6^+, S_6^- ; C_6^+, C_6^- ; $\sigma_{d1}, \sigma_{d2}, \sigma_{d3}$; $C_{21}'', C_{22}'', C_{23}''$	I
$6^1/m^1m^1m$	k	C_2 ; σ_h ; C_6^+, C_6^- ; S_3^-, S_3^+ ; $C_{21}'', C_{22}''\ C_{23}''$; $\sigma_{v1}, \sigma_{v2}, \sigma_{v3}$	C_2
$6/m^1m^1m^1$	n	I ; σ_h ; S_6^+, S_6^- ; S_3^+, S_3^- ; $\sigma_{d1}, \sigma_{d2}, \sigma_{d3}$; $\sigma_{v1}, \sigma_{v2}, \sigma_{v3}$	I
$6/m^1mm$	n	I ; σ_h ; S_6^+, S_6^- ; S_3^+, S_3^- ; $C_{21}', C_{22}'\ C_{23}'$; $C_{21}'', C_{22}'', C_{23}''$	I
$6/mm^1m^1$	m	$C_{21}', C_{22}', C_{23}'$; $C_{21}'', C_{22}'', C_{23}''$; $\sigma_{d1}, \sigma_{d2}, \sigma_{d3}$; $\sigma_{v1}, \sigma_{v2}, \sigma_{v3}$	$C_{21}{}^1$
m^13	o	I ; $\sigma_x, \sigma_y, \sigma_z$; $S_{61}^-, S_{62}^-, S_{63}^-, S_{64}^-$; $S_{61}^+, S_{62}^+, S_{63}^+, S_{64}^+$	I
4^13m^1	o	$\sigma_{da}, \sigma_{db}, \sigma_{dc}, \sigma_{dd}, \sigma_{de}, \sigma_{df}$; $S_{4x}^+, S_{4y}^+, S_{4z}^+, S_{4x}^-, S_{4y}^-, S_{4z}^-$	σ_{da}
4^132^1	o	$C_{2a}, C_{2b}, C_{2c}, C_{2d}, C_{2e}, C_{2f}$; $C_{4x}^+, C_{4y}^+, C_{4z}^+, C_{4x}^-, C_{4y}^-, C_{4z}^-$	C_{2a}
m^13m^1	q	I ; $S_{61}^+, S_{62}^+, S_{63}^+, S_{64}^+, S_{61}^-, S_{62}^-, S_{63}^-, S_{64}^-$; $\sigma_x, \sigma_y, \sigma_z$; $\sigma_{da}, \sigma_{db}, \sigma_{dc}, \sigma_{dd}, \sigma_{de}, \sigma_{df}$; $S_{4x}^+, S_{4y}^+, S_{4z}^+, S_{4x}^-, S_{4y}^-, S_{4z}^-$	I
m^13m	q	I ; $S_{61}^+, S_{62}^+, S_{63}^+, S_{64}^+, S_{61}^-, S_{62}^-, S_{63}^-, S_{64}^-$; $\sigma_x, \sigma_y, \sigma_z$; $C_{2a}, C_{2b}, C_{2c}, C_{2d}, C_{2e}, C_{2f}$; $C_{4x}^+, C_{4y}^+, C_{4z}^+, C_{4x}^-, C_{4y}^-, C_{4z}^-$	I
$m3m^1$	p	$C_{2a}, C_{2b}, C_{2c}, C_{2d}, C_{2e}, C_{2f}$; $C_{4x}^+, C_{4y}^+, C_{4z}^+, C_{4x}^-, C_{4y}^-, C_{4z}^-$; $\sigma_{da}, \sigma_{db}, \sigma_{dc}, \sigma_{dd}, \sigma_{de}, \sigma_{df}$; $S_{4x}^-, S_{4y}^-, S_{4z}^-, S_{4x}^+, S_{4y}^+, S_{4z}^+$	C_{2a}

although this is independent of the choice of $\boldsymbol{a}_0$, the actual $\boldsymbol{a}_0$ chosen in deducing this is indicated in the last column of Table V. Table VII lists matrices for those cases where reps of the unitary subgroup $\boldsymbol{H}$ are degenerate. These tables contain all the information which it is necessary to have available in order to write down the coreps of any magnetic point group instantly.

Table VI. The representation $\boldsymbol{D}(\boldsymbol{u})$ of the unitary subgroup $\boldsymbol{H}$ of $\boldsymbol{M}$, and the corepresentations of $\boldsymbol{M}$, (integral spin).

(a)

$\bar{1}^1$	2^1	m^1	E	$\bar{1}^1$	2^1	m^1
A	A	A	1	1	1	1

(b)

	$2^1/m$			E	σ_z		$2^1/m$		
		$2^1/m^1$		E	I			$2^1/m^1$	
$2/m^1$			22^12^1	E	C_{2z}	$2/m^1$			22^12^1
A	A'	A_g	A	1	1	1	1	1	1
B	A''	A_u	B	1	−1				

$2m^1m^1$		4^1	$\bar{4}^1$	E	C_{2z}	$2m^1m^1$		4^1	$\bar{4}^1$
	2^1m^1m			E	σ_y		2^1m^1m		
A	A'	A	A	1	1	1	1	1	1
B	A''	B	B	1	−1				

(c)

$m^1m^1m^1$			4^122^1	E	C_{2x}	C_{2y}	C_{2z}	$m^1m^1m^1$	4^122^1
	mmm^1			E	C_{2z}	σ_y	σ_x	mmm^1	
		m^1m^1m		E	C_{2z}	I	σ_z	m^1m^1m	
A	A_1	A_g	A	1	1	1	1	1	1
B_3	A_2	A_u	B_3	1	1	−1	−1	1	3
B_2	B_1	B_g	B_2	1	−1	1	−1	1	3
B_1	B_2	B_u	B_1	1	−1	−1	1	1	1

		$\bar{4}^12m^1$		E	C_{2x}	C_{2y}	C_{2z}			$\bar{4}^12m^1$
	4^1mm^1		$\bar{4}^12^1m$	E	σ_x	σ_y	C_{2z}		4^1mm^1	$\bar{4}^12^1m$
$4^1/m$				E	C_{2z}	I	σ_z	$4^1/m$		
A_g	A_1	A	A_1	1	1	1	1	1	1	1
A_u	B_2	B_3	B_2	1	1	−1	−1	1	3	3
B_g	B_1	B_2	B_1	1	−1	1	−1	1	3	3
B_u	A_2	B_1	A_2	1	−1	−1	1	1	1	1

(d)

$4^1/mmm$	E	C_{2x}	C_{2y}	C_{2z}	I	σ_x	σ_y	σ_z	$4^1/mmm$
A_g	1	1	1	1	1	1	1	1	1
B_{3g}	1	1	−1	−1	1	1	−1	−1	3
B_{2g}	1	−1	1	−1	1	−1	1	−1	3
B_{1g}	1	−1	−1	1	1	−1	−1	1	1
A_u	1	1	1	1	−1	−1	−1	−1	1
B_{3u}	1	1	−1	−1	−1	−1	1	1	3
B_{2u}	1	−1	1	−1	−1	1	−1	1	3
B_{1u}	1	−1	−1	1	−1	1	1	−1	1

(e)

42^12^1	$4/m^1$		E	C_{4z}^+	C_{2z}	C_{4z}^-	42^12^1	$4/m^1$	
		$4^1/m^1$	E	S_{4z}^-	C_{2z}	S_{4z}^+			$4^1/m^1$
A	A	A	1	1	1	1	1	1	1
B	B	B	1	-1	1	-1	1	1	1
^1E	^1E	^1E	1	i	-1	$-i$	1	3	3
^2E	^2E	^2E	1	$-i$	-1	i	1	3	3

$4m^1m^1$		E	C_{4z}^+	C_{2z}	C_{4z}^-	$4m^1m^1$	
	$\bar{4}2^1m^1$	E	S_{4z}^-	C_{2z}	S_{4z}^+		$\bar{4}2^1m^1$
A	A	1	1	1	1	1	1
B	B	1	-1	1	-1	1	1
^1E	^1E	1	i	-1	$-i$	1	1
^2E	^2E	1	$-i$	-1	i	1	1

(f)

$4/mm^1m^1$	E	C_{4z}^+	C_{2z}	C_{4z}^-	I	S_{4z}^-	σ_z	S_{4z}^+	$4/mm^1m^1$
A_g	1	1	1	1	1	1	1	1	1
B_g	1	-1	1	-1	1	-1	1	-1	1
^1E_g	1	i	-1	$-i$	1	i	-1	$-i$	1
^2E_g	1	$-i$	-1	i	1	$-i$	-1	i	1
A_u	1	1	1	1	-1	-1	-1	-1	1
B_u	1	-1	1	-1	-1	1	-1	1	1
^1E_u	1	i	-1	$-i$	-1	$-i$	1	i	1
^2E_u	1	$-i$	-1	i	-1	i	1	$-i$	1

(g)

$4/m^1m^1m^1$			E	C_{2z}	$C_{4z}^{\pm}$	$C_{2x,y}$	$C_{2a,b}$	$4/m^1m^1m^1$		
	$4/m^1mm$		E	C_{2z}	$C_{4z}^{\pm}$	$\sigma_{x,y}$	$\sigma_{da,b}$		$4/m^1mm$	
		$4^1/m^1m^1m$	E	C_{2z}	$S_{4z}^{\pm}$	$C_{2x,y}$	$\sigma_{da,b}$			$4^1/m^1m^1m$
A_1	A_1	A_1	1	1	1	1	1	1	1	1
A_2	A_2	A_2	1	1	1	-1	-1	1	1	1
B_1	B_1	B_1	1	1	-1	1	-1	1	1	1
B_2	B_2	B_2	1	1	-1	-1	1	1	1	1
E	E	E	2	-2	0	0	0	1	1	1

(h)

32^1	$3m^1$	$\bar{6}^1$	6^1	$\bar{3}^1$	E	C_3^+	C_3^-	32^1	$3m^1$	$\bar{6}^1$	6^1	$\bar{3}^1$
A	A	A	A	A	1	1	1	1	1	1	1	1
${}^1E$	${}^1E$	${}^1E$	${}^1E$	${}^1E$	1	ω	ω^*	1	1	3	3	3
${}^2E$	${}^2E$	${}^2E$	${}^2E$	${}^2E$	1	ω^*	ω	1	1	3	3	3

(i)

$\bar{3}m^1$	$6^1/m^1$	E	C_3^+	C_3^-	I	S_6^-	S_6^+	$\bar{3}m^1$	$6^1/m^1$
A_g	A_g	1	1	1	1	1	1	1	1
${}^1E_g$	${}^1E_g$	1	ω	ω^*	1	ω	ω^*	1	3
${}^2E_g$	${}^2E_g$	1	ω^*	ω	1	ω^*	ω	1	3
A_u	A_u	1	1	1	-1	-1	-1	1	1
${}^1E_u$	${}^1E_u$	1	ω	ω^*	-1	$-\omega$	$-\omega^*$	1	3
${}^2E_u$	${}^2E_u$	1	ω^*	ω	-1	$-\omega^*$	$-\omega$	1	3

(j)

$\bar{6}^1m2^1$		3^1m			6^1mm^1	E	$C_3\pm$	$\sigma_{d1,\,2,\,3}$	$\bar{6}^1m2^1$	3^1m	6^1mm^1
	$\bar{6}^1m^12$		$\bar{3}^1m^1$	6^122^1		E	$C_3\pm$	$C'_{21,\,2,\,3}$	$\bar{6}^1m^12$	$\bar{3}^1m^1$	6^122^1
A^1	A_1	A^1	A_1	A_1	A^1	1	1	1	1	1	1
A_2	A_2	A_2	A_2	A_2	A_2	1	1	-1	1	1	1
E	E	E	E	E	E	2	-1	0	1	1	1

(k)

$6^1/m^1m^1m$	E	$C_3\pm$	$C'_{21,\,2,3}$	I	$S_6\mp$	$\sigma_{d1,\,2,\,3}$	$6^1/m^1m^1m$
A_{1g}	1	1	1	1	1	1	1
A_{2g}	1	1	-1	1	1	-1	1
E_g	2	-1	0	2	-1	0	1
A_{1u}	1	1	1	-1	-1	-1	1
A_{2u}	1	1	-1	-1	-1	1	1
E_u	2	-1	0	-2	1	0	1

(l)

$\bar{6}m^12^1$	62^12^1	$6/m^1$	$6^1/m$	$6m^1m^1$	E	S_3^-	C_3^+	σ_h	C_3^-	S_3^+	$\bar{6}m^12^1$	62^12^1	$6/m^1$	$6^1/m$	$6m^1m^1$
					E	C_6^+	C_3^+	C_2	C_3^-	C_6^-					
A'	A	A	A'	A	1	1	1	1	1	1	1	1	1	1	1
${}^1E''$	${}^1E_1$	${}^1E_1$	${}^1E''$	${}^1E_1$	1	$-\omega^*$	ω	-1	ω^*	$-\omega$	1	1	3	3	1
${}^2E''$	${}^2E_1$	${}^2E_1$	${}^2E''$	${}^2E_1$	1	$-\omega$	ω^*	-1	ω	$-\omega^*$	1	1	3	3	1
A''	B	B	A''	B	1	-1	1	-1	1	-1	1	1	1	1	1
${}^2E'$	${}^2E_2$	${}^2E_2$	${}^2E'$	${}^2E_2$	1	ω	ω^*	1	ω	ω^*	1	1	3	3	1
${}^1E'$	${}^1E_2$	${}^1E_2$	${}^1E'$	${}^1E_2$	1	ω^*	ω	1	ω^*	ω	1	1	3	3	1

(m)

$6/mm^1m$	E	C_6^+	C_3^+	C_2	C_3^-	C_6^-
A_g	1	1	1	1	1	1
${}^1E_{1g}$	1	$-\omega^*$	ω	-1	ω^*	$-\omega$
${}^2E_{1g}$	1	$-\omega$	ω^*	-1	ω	$-\omega^*$
B_g	1	-1	1	-1	1	-1
${}^2E_{2g}$	1	ω	ω^*	1	ω	ω^*
${}^1E_{2g}$	1	ω^*	ω	1	ω^*	ω
A_u	1	1	1	1	1	1
${}^1E_{1u}$	1	$-\omega^*$	ω	-1	ω^*	$-\omega$
${}^2E_{1u}$	1	$-\omega$	ω^*	-1	ω	$-\omega^*$
B_u	1	-1	1	-1	1	-1
${}^2E_{2u}$	1	ω	ω^*	1	ω	ω^*
${}^1E_{2u}$	1	ω^*	ω	1	ω^*	ω

I	S_3^-	S_6^-	σ_h	S_6^+	S_3^-	$6/mm^1m^1$
1	1	1	1	1	1	1
1	$-\omega^*$	ω	-1	ω^*	$-\omega$	1
1	$-\omega$	ω^*	-1	ω	$-\omega^*$	1
1	-1	1	-1	1	-1	1
1	ω	ω^*	1	ω	ω^*	1
1	ω^*	ω	1	ω^*	ω	1
-1	-1	-1	-1	-1	-1	1
-1	ω^*	$-\omega$	1	$-\omega^*$	ω	1
-1	ω	$-\omega^*$	1	$-\omega$	ω^*	1
-1	1	-1	1	-1	1	1
-1	$-\omega$	$-\omega^*$	-1	$-\omega$	$-\omega^*$	1
-1	$-\omega^*$	$-\omega$	-1	$-\omega^*$	$-\omega$	1

(n)

$6^1/mm^1m$	$6/m^1m^1m^1$	$6/m^1mm$	E / E / E	σ_h / C_{2z} / C_{2z}	$C_3^\pm$ / $C_3^\pm$ / $C_3^\pm$	$S_3^\mp$ / $C_6^\pm$ / $C_6^\pm$	C_{2i}' / C_{2i}' / σ_{di}	σ_{vi} / C_{2i}'' / σ_{vi}	$6^1/mm^1m$	$6/m^1m^1m^1$	$6/m^1mm$
A_1'	A_1	A_1	1	1	1	1	1	1	1	1	1
A_2'	A_2	A_2	1	1	1	1	-1	-1	1	1	1
A_1''	B_1	B_2	1	-1	1	-1	1	-1	1	1	1
A_2''	B_2	B_1	1	-1	1	-1	-1	1	1	1	1
E''	E_1	E_1	2	-2	-1	1	0	0	1	1	1
E'	E_2	E_2	2	2	-1	-1	0	0	1	1	1

$i=1, 2, 3.$

(o)

m^13	$\bar{4}^13m^1$	4^132^1	E	C_{2m}	C_{3j}^-	C_{3j}^+	m^13	$\bar{4}^13m^1$	4^132^1
A	A	A	1	1	1	1	1	1	1
${}^1E$	${}^1E$	${}^1E$	1	1	ω	ω^*	3	1	1
${}^2E$	${}^2E$	${}^2E$	1	1	ω^*	ω	3	1	1
T	T	T	3	-1	0	0	1	1	1

$m=x, y, z.$ $j=1, 2, 3, 4.$

(p)

$m3m^1$	E	C_{2m}	C_{3j}^-	C_{3j}^+	I	σ_m	S_{6j}^+	S_{6j}^-	$m3m^1$
A_g	1	1	1	1	1	1	1	1	1
${}^1E_g$	1	1	ω	ω^*	1	1	ω	ω^*	1
${}^2E_g$	1	1	ω^*	ω	1	1	ω^*	ω	1
T_g	3	−1	0	0	3	−1	0	0	1
A_u	1	1	1	1	−1	−1	−1	−1	1
${}^1E_u$	1	1	ω	ω^*	−1	−1	$-\omega$	$-\omega^*$	1
${}^2E_u$	1	1	ω^*	ω	−1	−1	$-\omega^*$	$-\omega$	1
T_u	3	−1	0	0	−3	1	0	0	1

$m=x, y, z.\qquad j=1, 2, 3, 4.$

(q)

m^13m^1	m^13m	E / E	$C_{3j}^\pm$ / $C_{3j}^\pm$	C_{2m} / C_{2m}	C_{2p} / σ_{dp}	$C_{4m}^\pm$ / $S_{4m}^\pm$	m^13m^1	m^13m
A_1	A_1	1	1	1	1	1	1	1
A_2	A_2	1	1	1	−1	−1	1	1
E	E	2	−1	2	0	0	1	1
T_1	T_1	3	0	−1	−1	1	1	1
T_2	T_2	3	0	−1	1	−1	1	1

Table VII. Matrices for degenerate reps.

$$\alpha=\begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix};\quad \beta=\begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix};$$

$$\varepsilon=\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix};\quad \kappa=\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix};$$

$$\lambda=\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix};\quad \mu=\begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & 1/2 \end{pmatrix};$$

$$\nu=\begin{pmatrix} -1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & 1/2 \end{pmatrix};\quad \rho=\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

(g)

H of $4/m^1m^1m^1$ $422(D_4)$	H of $4/m^1mm$ $4mm(C_{4v})$	H of $4^1/m^1m^1m$ $\bar{4}2m(D_{2d})$	Matrix
E	E	E	ε
C_{2z}	C_{2z}	C_{2z}	$-\varepsilon$
C_{4z}^+	C_{4z}^+	S_{4z}^+	$-\rho$
C_{4z}^-	C_{4z}^-	S_{4z}^-	ρ
C_{21}''	σ_{d1}	σ_{d1}	κ
C_{22}''	σ_{d2}	σ_{d2}	$-\kappa$
C_{21}'	σ_{v1}	C_{21}'	λ
C_{22}'	σ_{v2}	C_{22}'	$-\lambda$

(j)

	Matrix
E	ε
C_3^+	β
C_3^-	α
C_{21}' or σ_{d1}	λ
C_{22}' or σ_{d2}	μ
C_{23}' or σ_{d3}	ν

(k)

	Matrix for E_g	Matrix for E_u
E	ε	ε
C_3^+	β	β
C_3^-	α	α
C_{21}'	λ	λ
C_{22}'	μ	μ
C_{23}'	ν	ν
I	ε	$-\varepsilon$
S_6^-	β	$-\beta$
S_6^+	α	$-\alpha$
σ_{d1}	λ	$-\lambda$
σ_{d2}	μ	$-\mu$
σ_{d3}	ν	$-\nu$

(n)

H of $6^1/mm^1m$ $\bar{6}m2$ (D_{3h})			H of $6/m^1m^1m^1$ 622 (D_6)			H of $6/m^1mm$ $6mm$ (C_{6v})		
	Matrices			Matrices			Matrices	
	E'	E''		E_1	E_2		E_1	E_2
E	ε	ε	E	ε	ε	E	ε	ε
C_3^-	α	α	C_6^-	$-\beta$	α	C_6^-	$-\beta$	α
C_3^+	β	β	C_6^+	$-\alpha$	β	C_6^+	$-\alpha$	β
C_{21}'	λ	$-\lambda$	C_3^-	α	β	C_3^-	α	β
C_{22}'	μ	$-\mu$	C_3^+	β	α	C_3^+	β	α
C_{23}'	ν	$-\nu$	C_2	$-\varepsilon$	ε	C_2	$-\varepsilon$	ε
σ_{v1}	λ	λ	C_{21}'	λ	λ	σ_{v1}	λ	λ
σ_{v2}	μ	μ	C_{22}'	μ	ν	σ_{v2}	μ	ν
σ_{v3}	ν	ν	C_{23}'	ν	μ	σ_{v3}	ν	μ
σ_h	ε	$-\varepsilon$	C_{21}''	$-\lambda$	λ	σ_{d1}	$-\lambda$	λ
S_3^-	α	$-\alpha$	C_{22}''	$-\mu$	ν	σ_{d2}	$-\mu$	ν
S_3^+	β	$-\beta$	C_{23}''	$-\nu$	μ	σ_{d3}	$-\nu$	μ

(q)

			Matrix
$E, C_{2x}, C_{2y}, C_{2z}$			ε
$C_{31}^+, C_{32}^+, C_{33}^+, C_{34}^+$			β
$C_{31}^-, C_{32}^-, C_{33}^-, C_{34}^-$			α
$C_{4z}^+, C_{4z}^-, C_{2a}, C_{2b}$	or	$S_{4z}^-, S_{4z}^+, \sigma_{da}, \sigma_{db}$	λ
$C_{4x}^+, C_{4x}^-, C_{2d}, C_{2f}$		$S_{4x}^-, S_{4x}^+, \sigma_{dd}, \sigma_{df}$	μ
$C_{4y}^+, C_{4y}^-, C_{2c}, C_{2e}$		$S_{4y}^-, S_{4y}^+, \sigma_{dc}, \sigma_{de}$	ν

(o), (p), (q)

For the triply degenerate representations in case (p) the matrices for the elements $I\times R$, where R is an element in column one, are the same as for R in T_g and are minus those for R in T_u. In case (q) the matrix of an element in column two or three is given by postmultiplying the given matrix, which is for the element in column one, by

$$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \text{ for } T_1$$

$$\text{or } \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \text{ for } T_2.$$

(p), (q)	(q)	(q)	Matrix
E	C_{2a}	σ_{da}	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
C_{31}^+	C_{4y}^-	S_{4y}^+	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$
C_{31}^-	C_{4x}^+	S_{4x}^-	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$
C_{32}^+	C_{4y}^+	S_{4y}^-	$\begin{pmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}$
C_{32}^-	C_{4x}^-	S_{4x}^+	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{pmatrix}$
C_{33}^+	C_{2c}	σ_{dc}	$\begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$
C_{33}^-	C_{2f}	σ_{df}	$\begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{pmatrix}$

C_{34}^{+}	C_{2e}	σ_{de}	$\begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}$
C_{34}^{-}	C_{2d}	σ_{dd}	$\begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{pmatrix}$
C_{2x}	C_{4z}^{-}	S_{4z}^{+}	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
C_{2y}	C_{4z}^{+}	S_{4z}^{-}	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
C_{2z}	C_{2b}	σ_{db}	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

§ 6. Example of use of Tables

We now consider as an example in the use of these tables the case of m^13. To use Tables V, VI and VII to find the coreps of this magnetic point group we use columns two and four of Table V; column two refers the reader to the appropriate section of Table VI, and column four states which element from $R(\boldsymbol{G}-\boldsymbol{H})$ was used as $\boldsymbol{a}_0$ in the construction of Table VI. As Wigner[1)] demonstrates, the actual choice of $\boldsymbol{a}_0$ does not affect the coreps when they are finally derived but does involve differences in the algebra of their derivation; however, having made a choice of $\boldsymbol{a}_0$ for a particular group it is important to keep to that choice when writing down all the coreps. A useful check of the derivation of the types of the coreps in Table VI can be made by deriving them using several different choices of $\boldsymbol{a}_0$, and this has in fact been done, in each case at least two different $\boldsymbol{a}_0$ have been used (except in the trivial case where $(\boldsymbol{G}-\boldsymbol{H})$ contains only one element anyway). Thus for m^13 we refer to section (o) of Table VI where we see that reps A and T of $\boldsymbol{H}$ lead to coreps of the first type with $\boldsymbol{\beta}=+\mathbf{1}$ and therefore $\boldsymbol{\beta}^{-1}\boldsymbol{\beta}=+\boldsymbol{\Delta}(\boldsymbol{a}_0^2)$. For reps ${}^1E$ and ${}^2E$ the coreps derived from them are of the third type. Therefore in all these cases, knowing $\boldsymbol{a}_0=RI$ from column four of Table V and, where relevant, $\boldsymbol{\beta}$, it is straightforward to write down the matrices $\boldsymbol{D}(\boldsymbol{u})$ and $\boldsymbol{D}(\boldsymbol{a}_0\boldsymbol{u})$ in each of the coreps of the magnetic group m^13 using Eqs. (4·2)–(4·4) of APC I. This will yield just the matrices which were previously obtained for this group in § 4.

So far we have used $\boldsymbol{\Delta}(\boldsymbol{a}_0^2)=+\mathbf{1}$ where $\boldsymbol{a}_0^2$ contains a factor R^2. This applies to the case of a system with integral rather than half-integral spin magnetic moments. For the case of half-integral spins the only effect is to change over the first and second types of coreps. Therefore for the case of half-integral spins, the coreps listed in Table VI as being of the first type are now of the second type.

§ 7. The consequences of invariance under time inversion

The conventional treatment of systems having time-reversal symmetry, also due to Wigner[10] and neatly summarised by Herring[11] and Elliott,[12] although it was developed long before the derivation of the magnetic point groups and space groups, is exactly equivalent to the consideration of the theory of the corepresentations of the grey magnetic groups.

The effect of the operation of time inversion is to reverse the spin magnetic moment of an atom or ion and therefore a crystal which is invariant under the operation of time inversion belongs to one of the type II Shubnikov groups or "grey" groups. The type II Shubnikov group, $\boldsymbol{M}$, is given by Eq. (2·1),

$$\boldsymbol{M}=\boldsymbol{G}+R\boldsymbol{G} \tag{7·1}$$

so that it is natural to choose as $\boldsymbol{a}_0$ the operation of time inversion itself. For an electron with spin $S=1/2$, $R^2=(-1)^{2S}=-1$ and therefore

$$\boldsymbol{\Delta}(\boldsymbol{a}_0^2)=-\mathbf{1}. \tag{7·2}$$

The reps $\boldsymbol{\Delta}(\boldsymbol{u})$ of the unitary subgroup $\boldsymbol{G}$ are just the ordinary space-group reps, and there are three possibilities to consider:

(i) $\boldsymbol{\Delta}(\boldsymbol{u})$ is real

(ii) $\boldsymbol{\Delta}(\boldsymbol{u})$ is complex and is equivalent to $\boldsymbol{\Delta}(\boldsymbol{u})^*$

and (iii) $\boldsymbol{\Delta}(\boldsymbol{u})$ is complex and is not equivalent to $\boldsymbol{\Delta}(\boldsymbol{u})^*$.

In case (i) then the reps $\boldsymbol{\Delta}(\boldsymbol{u})$ and $\bar{\boldsymbol{\Delta}}(\boldsymbol{u})\,(=\boldsymbol{\Delta}(\boldsymbol{u})^*)$ are obviously not only equivalent but also identical so that $\boldsymbol{\beta}=+\mathbf{1}$ and therefore $\boldsymbol{\beta\beta}^*=+\mathbf{1}$ so that by Eq. (7·2)

$$\boldsymbol{\beta\beta}^*=-\boldsymbol{\Delta}(\boldsymbol{a}_0^2) \tag{7·3}$$

and the corep of $\boldsymbol{M}$ is of the second type and is given by Eq. (4·3) of APC I which shows that there is an extra degeneracy. In case (ii) $\boldsymbol{\Delta}(\boldsymbol{u})$ and $\bar{\boldsymbol{\Delta}}(\boldsymbol{u})$ $(=\boldsymbol{\Delta}(\boldsymbol{u})^*)$ are equivalent but necessarily not identical and $\boldsymbol{\beta\beta}^*=-\mathbf{1}$, therefore

$$\boldsymbol{\beta\beta}^*=-\mathbf{1}=+\boldsymbol{\Delta}(\boldsymbol{a}_0^2). \tag{7·4}$$

The coreps of $\boldsymbol{M}$ are therefore of the first type and are given by Eq. (4·2) of APC I and there is thus no extra degeneracy in this case. Finally in case (iii) the corep of $\boldsymbol{M}$ is obviously of the third type and is given by Eq. (4·4) of APC I. Thus case (iii) leads to an extra degeneracy. Summarising then we find

(i) an extra degeneracy

(ii) no extra degeneracy

and (iii) an extra degeneracy.

For an even number of electrons $R^2=(-1)^{2S}=+1$ so that $\boldsymbol{\Delta}(\boldsymbol{a}_0^2)=+\mathbf{1}$ and the results for cases (i) and (ii) are interchanged, while the result for case (iii) is left unaltered.

The above conclusions are just the same as those of the more conventional view of time reversal originally due to Wigner[10] and neatly summarised in Heine's book[8] § 19.

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