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Irreducible representations of the symmetry groups of polymer molecules: III. Consequences of time-reversal symmetry

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Abstract. Systematic degeneracies of electron and phonon energy spectra of stereoregular polymers are determined by the dimensions of unitary irreducible representations (reps) of line groups (L), as far as the spatial symmetries are concerned. However, time reversal (θ) invariance of the Hamiltonian can bring in some extra degeneracies. These are determined for the reps of all the line groups. A physical interpretation of the results is given in terms of the action of θ onto the quantum numbers arising from line-group symmetry. Finally, corepresentations of the groups $L^A = L + \theta L$ and the corresponding symmetry-adapted bases are also obtained.

1. Introduction

1.1. Representations of line groups and time reversal

Chain-like or quasi one-dimensional physical systems, such as stereoregular polymer molecules but also some well defined, weakly interacting subsystems of certain highly anisotropic materials, are of considerable current research interest (André *et al* 1980, Barišić *et al* 1979). The most important physical means for studying such systems include infrared absorption, Raman scattering, x-photoelectron spectroscopy, etc. The success of these studies depends, however, on our knowledge of the corresponding phonon and electron energy spectra, obtained generally as the solutions of the eigenvalue problems, $H\Psi = \varepsilon\Psi$, of the respective Hamiltonians H. Line groups L (Vujičić *et al* 1977, to be referred to as LG) describe the spatial symmetries of such systems and hence the dimensions of irreducible representations of these groups (Božović *et al* 1978, to be referred to as I, Božović and Vujičić 1980, to be referred to as II) determine the corresponding systematic degeneracies of the mentioned spectra. However, in the case of phonons one finds also that $H\Psi^* = \varepsilon\Psi^*$; since the band structures of polymers are in most cases obtained in the single spinless electron approximation (André *et al* 1980), the same statement is also then valid for electrons. (A comment on the influence of spin will be given later, in § 3.3.) This simple fact can in some cases bring in extra degeneracies and in this paper we find all such cases for the line groups.

More precisely, the problem we solve here is 'what happens to the unitary irreducible representations (reps) of a line group L when it is extended into $L^A = L + \theta L$', where θ is the anti-unitary, antilinear operator of time reversal, for every rep of each L. Notice that in our case θ acts as the complex conjugation (denoted by the asterisk) and commutes with the elements of L: $\theta\Psi = \Psi^*$ and $\theta(R \mid \tau) = (R \mid \tau)\theta$ for every $(R \mid \tau) \in L$. This definition is sufficient for our present purpose; more general situations are dealt with in a recent essay (Domingos 1979) where a clear exposition of physical ideas underlying time-reversal symmetry can be found.

1.2. General methods of determining extra degeneracies

A method to solve the above problem was given long ago (Wigner 1932)†.

Let $d(L)$ be a rep of the group L; one calls it: *type* a *if* $d(L) \sim d^*(L)$ (where $\sim$ denotes the equivalence of two reps) *and both are equivalent to a real representation*; *type* b *if* $d(L) \nsim d^*(L)$; *type* c *if* $d(L) \sim d^*(L)$, *but they are not equivalent to a real representation.*

When L is enlarged into L^A, then: *the degeneracy is doubled if* $d(L)$ *is of type* b *or* c, while *there is no extra degeneracy if* $d(L)$ *is of type* a.

More practical ways to perform the above classification arise from the following two theorems, specialised here to line groups.

Theorem 1. (Herring 1937). *Let*

$$d^*(L) = S^{-1} d(L) S \tag{1}$$

where S is a unitary matrix; *then* $d(L)$ *is of*

type a *iff* $SS^* = I$

type c *iff* $SS^* = -I$.

Theorem 2. (Frobenius and Schur 1906). *Let* $\chi(L)$ *denote the character of* $d(L)$. *Then*

$$\frac{1}{|L|} \sum_{(R|\tau)\in L} \chi[(R \mid \tau)^2] = \begin{cases} 1 & \textit{iff } d(L) \textit{ is of type a} \\ 0 & \textit{iff } d(L) \textit{ is of type b} \\ -1 & \textit{iff } d(L) \textit{ is of type c.} \end{cases}$$

Here $|L|$ is the order of the line group L which is assumed to be made finite via the cyclic boundary conditions (cf I).

2. Classification of reps of line groups according to the complex conjugation

Making use of theorems 1 and 2, and the tables of reps given in I and II, we have classified the reps of all the line groups according to whether they belong to type a, b or c with respect to the complex conjugation. The results are given in tables 1–15 (for each family of line groups separately). In addition, we give explicitly for every rep d of type b

† The types a, b and c of Frobenius and Schur were denoted in Wigner's article by I, III and II respectively; the first convention was also used by Herring and seems to be prevailing, at least in solid-state physics.

the symbol (i.e. the quantum numbers) of its complex-conjugate rep d^*. The range of the quantum numbers defining such reps is always appropriately restricted so that each pair of mutually conjugate reps appears only once in the tables. For the reps of types a and c, a unitary matrix S satisfying (1) is also given; note that the general solution is $S' = \exp(\mathrm{i}\phi)S$, $0 \leq \phi < 2\pi$ but in the tables we omit this phase factor for the sake of brevity.

Several (more or less obvious) facts have been made use of to further check the entries:

(i) a rep is of type b iff its character is not real;

(ii) one-dimensional reps are of type a if they are real, and of type b otherwise;

(iii) if the character of a rep is real, but the determinants of matrices of that rep are not all real, the rep is of type c;

(iv) two reps differing by real scalar factors are of the same type. (This is the case e.g. for $k = 0$ and $k = \pi/a$ reps of each symmorphic line group, cf I and II.)

The number of non-equivalent reps was controlled via the Burnside theorem (cf Jansen and Boon 1967, Streitwolf 1971).

Remark. The notation for line groups and their reps in these tables is the same as in LG, I and II (with which we assume familiarity). The only exception is that throughout this paper we have chosen the translational period, a, to equal unit length (i.e. $a = 1$); thus here we have ${}_{\pi}A_m$ and $-\pi < k \leq \pi$ as compared with ${}_{\pi/a}A_m$ and $-\pi/a < k \leq \pi/a$ in I, etc.

2.1. *Classification of the reps of the line groups isogonal to C_n*

Table 1. The line groups Ln ($n = 1, 2, 3, \ldots$); their reps are given in table 1 of I. Here $0 < k < \pi$ (note that we have chosen $a = 1$, in contrast to I); $m = 1, 2, \ldots, (n-1)/2$ for n odd and $m = 1, 2, \ldots, (n-2)/2$ for n even.

	For $n = 1, 2, 3, \ldots$						only $n = 2q = 2, 4, 6, \ldots$		
d	${}_0A_0$	${}_0A_m$	${}_kA_0$	${}_kA_m$ †	${}_{\pi}A_0$	${}_{\pi}A_m$	${}_0A_q$	${}_kA_q$	${}_{\pi}A_q$
d^*	${}_0A_0$	${}_0A_{-m}$	${}_{-k}A_0$	${}_{-k}A_{-m}$ †	${}_{\pi}A_0$	${}_{\pi}A_{-m}$	${}_0A_q$	${}_{-k}A_q$	${}_{\pi}A_q$
Type	a	b	b	b	a	b	a	b	a
S	1	/	/	/	1	/	1	/	1

† Here $m = \pm1, \pm2, \ldots, \pm(n-1)/2$ for n odd and $m = \pm1, \pm2, \ldots, \pm(n-2)/2$ for n even.

Table 2. The line groups Ln_p ($n = 2, 3, 4, \ldots; p = 1, 2, \ldots, n-1$); cf table 2 of I. For k and m see the caption of table 1.

	For $n = 1, 2, \ldots; p = 1, 2, \ldots, n-1$					only for n even		only for p even	only for $n-p$ even
d	${}_0A_0$	${}_0A_m$	${}_kA_0$	${}_kA_m$ †	${}_{\pi}A_m$ ‡	${}_0A_{n/2}$	${}_kA_{n/2}$	${}_{\pi}A_{-p/2}$	${}_{\pi}A_{(n-p)/2}$
d^*	${}_0A_0$	${}_0A_{-m}$	${}_{-k}A_0$	${}_{-k}A_{-m}$ †	${}_{\pi}A_{\bar{m}}$ ‡	${}_0A_{n/2}$	${}_{-k}A_{n/2}$	${}_{\pi}A_{-p/2}$	${}_{\pi}A_{(n-p)/2}$
Type	a	b	b	b	b	a	b	a	a
S	1	/	/	/	/	1	/	1	1

† Here $m = \pm1, \pm2, \ldots, \pm(n-1)/2$ for n odd and $m = \pm1, \pm2, \ldots, \pm(n-2)/2$ for n even.
‡ In this case $-p/2 < m < (n-p)/2$ with $\bar{m} = -m-p$ for $-p/2 < m < n/2-p$ and $\bar{m} = n-m-p$ for $n/2-p \leq m < (n-p)/2$.

2.2. Classification of the reps of the line groups isogonal to C_{nv}

Table 3. The line groups Lnm ($n = 1, 3, 5, \ldots$) and Lnmm ($n = 2, 4, 6, \ldots$); cf table 4 in I. Here $0 < k < \pi$; $m = 1, 2, \ldots, (n-1)/2$ for n odd, while $m = 1, 2, \ldots, (n-2)/2$ for n even; $p = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$.

For $n = 1, 2, 3, \ldots$									
d	${}_0A_0$	${}_0B_0$	${}_0E_{m,-m}$	${}_kA_0$	${}_kB_0$	${}_kE_{m,-m}$	${}_\pi A_0$	${}_\pi B_0$	${}_\pi E_{m,-m}$
d^*	${}_0A_0$	${}_0B_0$	${}_0E_{m,-m}$	${}_{-k}A_0$	${}_{-k}B_0$	${}_{-k}E_{m,-m}$	${}_\pi A_0$	${}_\pi B_0$	${}_\pi E_{m,-m}$
Type	a	a	a	b	b	b	a	a	a
S	1	1	P	/	/	/	1	1	P

and only for $n = 2q = 2, 4, 6, \ldots$						
d	${}_0A_q$	${}_0B_q$	${}_kA_q$	${}_kB_q$	${}_\pi A_q$	${}_\pi B_q$
d^*	${}_0A_q$	${}_0B_q$	${}_{-k}A_q$	${}_{-k}B_q$	${}_\pi A_q$	${}_\pi B_q$
Type	a	a	b	b	a	a
S	1	1	/	/	1	1

Table 4. The line groups Lnc ($n = 1, 3, 5, \ldots$) and Lncc ($n = 2, 4, 6, \ldots$); cf table 5 in I. For k, m and P see the caption of table 3; $F = \begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}$. (i) The data for the reps ${}_0A_0$, ${}_0B_0$, ${}_0E_{m,-m}$, ${}_0A_q$, ${}_0B_q$, ${}_kA_0$, ${}_kB_0$, ${}_kE_{m,-m}$, ${}_kA_q$ and ${}_kB_q$ coincide with those given in table 3 for the respective reps of Lnm and Lnmm.

(ii)	For $n = 1, 2, 3, \ldots$		only $n = 2q = 2, 4, 6, \ldots$
d	${}_\pi A_0$	${}_\pi E_{m,-m}$	${}_\pi A_q$
d^*	${}_\pi B_0$	${}_\pi E_{m,-m}$	${}_\pi B_q$
Type	b	c	b
S	/	F	/

Table 5. The line groups L$(2q)_q mc$ ($n = 2q = 2, 4, 6, \ldots$); cf table 6 in I. Here $0 < k < \pi$ and $I = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$. (i) For ${}_0A_0$, ${}_0B_0$, ${}_0E_{m,-m}$, ${}_0A_q$, ${}_0B_q$, ${}_kA_0$, ${}_kB_0$, ${}_kE_{m,-m}$, ${}_kA_q$ and ${}_kB_q$ cf table 3.

(ii)	For $q = 1, 2, 3, \ldots$			only $q = 2v = 2, 4, 6, \ldots$
d	${}_\pi A_0$	${}_\pi B_0$	${}_\pi E_{m,-m}$ †	${}_\pi E_{v,-v}$
d^*	${}_\pi A_q$	${}_\pi B_q$	${}_\pi E_{\bar{m},-\bar{m}}$	${}_\pi E_{v,-v}$
Type	b	b	b	a
S	/	/	/	I

† Here $m = 1, 2, \ldots, (q-1)/2$ for q odd and $m = 1, 2, \ldots, (q-2)/2$ for q even; $\bar{m} = q - m$.

2.3. Classification of the reps of the line groups isogonal to C_{nh}

Table 6. The line groups Ln/m ($n = 1, 2, 3, \ldots$); cf table 8 in I. For k, m and P see the caption of table 3.

	For $n = 1, 2, 3, \ldots$						only $n = 2q = 2, 4, 6, \ldots$		
d	${}_0A_0^\pm$	${}_0A_{m'}^\pm$	${}_k^{-k}E_0$	${}_k^{-k}E_m$	${}_\pi A_0^\pm$	${}_\pi A_m^\pm$	${}_0A_q^\pm$	${}_k^{-k}E_q$	${}_\pi A_q^\pm$
d^*	${}_0A_0^\pm$	${}_0A_{-m}^\pm$	${}_k^{-k}E_0$	${}_k^{-k}E_{-m}$	${}_\pi A_0^\pm$	${}_\pi A_{-m}^\pm$	${}_0A_q^\pm$	${}_k^{-k}E_q$	${}_\pi A_q^\pm$
Type	a	b	a	b	a	b	a	a	a
S	1	/	P	/	1	/	1	P	1

Table 7. The line groups $L(2q)_q/m$ ($n = 2q = 2, 4, 6, \ldots$); cf table 9 in I. For k, m and P see the caption of table 3. (i) For the reps ${}_0A_0^\pm$, ${}_0A_m^\pm$, ${}_0A_q^\pm$, ${}_k^{-k}E_0$, ${}_k^{-k}E_m$, ${}_k^{-k}E_q$ see the corresponding entries of table 6.

(ii)	For $q = 1, 2, 3, \ldots$		only for $q = 2v = 2, 4, 6, \ldots$
d	${}_\pi E_q^0$	${}_\pi E_m^{-\tilde m}$ †	${}_\pi E_v^{-v}$
d^*	${}_\pi E_q^0$	${}_\pi E_{\tilde m}^{-m}$	${}_\pi E_v^{-v}$
Type	a	a	a
S	P	/	I

† Here $m = 1, 2, \ldots, (q-1)/2$ for q odd and $m = 1, 2, \ldots, (q-2)/2$ for q even; $\tilde m = q - m$.

2.4. Classification of the reps of the line groups isogonal to S_{2n}

Table 8. The line groups $L\bar n$ ($n = 1, 3, 5, \ldots$) and $L(\overline{2n})$ ($n = 2, 4, 6, \ldots$); cf table 11 in I. For k, m and P see the caption of table 3; $F = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$.

	For $n = 1, 2, 3, \ldots$						only $n = 2q = 2, 4, 6, \ldots$		
d	${}_0A_0^\pm$	${}_0A_m^\pm$	${}_k^{-k}E_0$	${}_k^{-k}E_m$	${}_\pi A_0^\pm$	${}_\pi A_m^\pm$	${}_0A_q^+$	${}_k^{-k}E_q$	${}_\pi A_q^+$
d^*	${}_0A_0^\pm$	${}_0A_{-m}^\pm$	${}_k^{-k}E_0$	${}_k^{-k}E_{-m}$	${}_\pi A_0^\pm$	${}_\pi A_{-m}^\pm$	${}_0A_q^-$	${}_k^{-k}E_q$	${}_\pi A_q^-$
Type	a	b	a	b	a	b	b	c	b
S	1	/	P	/	1	/	/	F	/

2.5. Classification of the reps of the line groups isogonal to D_n

Table 9. The line groups $Ln2$ ($n = 1, 3, 5, \ldots$) and $Ln22$ ($n = 2, 4, 6, \ldots$); cf table 13 in I. For k, m and P see the caption of table 3. All these reps are of type a.

	For $n = 1, 2, 3, \ldots$						only $n = 2q = 2, 4, 6, \ldots$		
d	${}_0A_0^\pm$	${}_0E_m^{-m}$	${}_k^{-k}E_0$	${}_k^{-k}E_m^{-m}$ †	${}_\pi A_0^\pm$	${}_\pi E_m^{-m}$	${}_0A_q^\pm$	${}_k^{-k}E_q$	${}_\pi A_q^\pm$
S	1	P	P	P	1	P	1	P	1

† Here $m = \pm 1, \pm 2, \ldots, \pm(n-1)/2$ for n odd and $m = \pm 1, \pm 2, \ldots, \pm(n-2)/2$ for n even.

Table 10. The line groups Ln_p2 ($n = 3, 5, 7, \ldots$) and Ln_p22 ($n = 2, 4, 6, \ldots$); cf table 14 in I. For k, m and P see the caption of table 3. (i) ${}_0A_0^\pm$, ${}_0E_m^{-m}$, ${}_0A_q^\pm$, ${}_k^{-k}E_0$, ${}_k^{-k}E_m^{-m}$, ${}_k^{-k}E_q$ same as in table 9. All these reps are of type a.

(ii)	For $n = 1, 2, 3, \ldots$; $p = 1, \ldots, n-1$	only for p even	only for $n - p$ even
d	${}_\pi E_m^{\tilde m}$ †	${}_\pi A_{-p/2}^\pm$	${}_\pi A_{(n-p)/2}^\pm$
S	P	1	1

† Here $-p/2 < m < (n-p)/2$; $\tilde m = -m - p$ for $-p/2 < m < n/2 - p$ and $\tilde m = n - m - p$ for $n/2 - p \leq m < (n-p)/2$.

2.6. *Classification of the reps of the line groups isogonal to D_{nd}*

Table 11. The line groups L$\bar{n}m$ ($n = 1, 3, 5, \ldots$) and L$(\overline{2n})2m$ ($n = 2, 4, 6, \ldots$); cf tables 5 and 6 in II. Here k, m and P are the same as in table 3;

$$\mathrm{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \text{and} \qquad Q = \begin{pmatrix} 0 & M \\ M & 0 \end{pmatrix}$$

where

$$M = \begin{pmatrix} \exp(\mathrm{i}m\alpha/2) & 0 \\ 0 & \exp(-\mathrm{i}m\alpha/2) \end{pmatrix} \qquad \alpha = 2\pi/n.$$

For $n = 1, 2, 3, \ldots$

d	$_0A_0^\pm$	$_0B_0^\pm$	$_0E^\pm_{m,-m}$	$^{-k}_{k}E_{A0}$	$^{-k}_{k}E_{B0}$	$^{-k}_{k}G_{m,-m}$	$_\pi A_0^\pm$	$_\pi B_0^\pm$	$_\pi E^\pm_{m,-m}$
S	1	1	P	P	P	Q	1	1	P

All these reps are of type a.

and only for $n = 2q = 2, 4, 6, \ldots$

d	$_0E_q$	$^{-k}_{k}E^{B_q}_{A_q}$	$_\pi E_q$
d^*	$_0E_q$	$^{-k}_{k}E^{A_q}_{B_q}$	$_\pi E_q$
Type	a	b	a
S	I	/	I

Table 12. The line groups L$\bar{n}c$ ($n = 1, 3, 5, \ldots$) and L$(\overline{2n})2c$ ($n = 2, 4, 6, \ldots$); cf table 7 in II. For k, m and P see the caption of table 3. (i) The data for the reps $_0A_0^\pm$, $_0B_0^\pm$, $_0E^\pm_{m,-m}$, $_0E_q$, $^{-k}_{k}E_{A0}$, $^{-k}_{k}E_{B0}$, $^{-k}_{k}G_{m,-m}$, $^{-k}_{k}E^{B_q}_{A_q}$ and $^{-k}_{k}E^{A_q}_{B_q}$ coincide with the corresponding ones in table 11.

(ii)	For $n = 1, 2, 3, \ldots$		only $n = 2q = 2, 4, 6, \ldots$
d	$_\pi E_0$	$_\pi E^+_{m,-m\pi}$	$A_q^\pm$
d^*	$_\pi E_0$	$_\pi E^-_{m,-m}$	$_\pi B_q^\pm$
Type	a	b	b
S	P	/	/

2.7. *Classification of the reps of the line groups isogonal to D_{nh}*

Table 13. The line groups L$(\overline{2n})2m$ ($n = 1, 3, 5, \ldots$) and Ln/mmm ($n = 2, 4, 6, \ldots$); cf tables 8 and 9 in II. For k, m and P see the caption of table 3; $I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ and $H = \begin{pmatrix} 0 & P \\ P & 0 \end{pmatrix}$. All these reps are of type a.

For $n = 1, 2, 3, \ldots$

d	$_0A_0^\pm$	$_0B_0^\pm$	$_0E^\pm_{m,-m}$	$^{-k}_{k}E_{A0}$	$^{-k}_{k}E_{B0}$	$^{-k}_{k}G_{m,-m}$	$_\pi A_0^\pm$	$_\pi B_0^\pm$	$_\pi E^\pm_{m,-m}$
S	1	1	P	P	P	H	1	1	P

and only for $n = 2q = 2, 4, 6, \ldots$

d	$_0A_q^\pm$	$_0B_q^\pm$	$^{-k}_{k}E_{A_q}$	$^{-k}_{k}E_{B_q}$	$_\pi A_q^\pm$	$_\pi B_q^\pm$
S	1	1	P	P	1	1

Table 14. The line groups $L(\overline{2n})2c$ ($n = 1, 3, 5, \ldots$) and Ln/mcc ($n = 2, 4, 6, \ldots$); cf table 10 in II. For k, m and P see the caption of table 3. (i) For ${}_0A_0^\pm$, ${}_0B_0^\pm$, ${}_0E_{m,-m}^\pm$, ${}_0A_q^\pm$, ${}_0B_q^\pm$, ${}_k^{-k}E_{A0}$, ${}_k^{-k}E_{B0}$, ${}_k^{-k}G_{m,-m}$, ${}_k^{-k}E_{A_q}$ and ${}_k^{-k}E_{B_q}$ see table 13.

(ii)	For $n = 1, 2, 3, \ldots$		only $n = 2q = 2, 4, 6, \ldots$
d	${}_\pi E_0$	${}_\pi E_{m,-m}^+$	${}_\pi E_q$
d^*	${}_\pi E_0$	${}_\pi E_{m,-m}^-$	${}_\pi E_q$
Type	a	b	a
S	P	/	P

Table 15. The line groups $L(2q)_q/mcm$ ($n = 2q = 2, 4, 6, \ldots$); cf table 11 in II. For k, m and P see the caption of table 3; $I = \left(\begin{smallmatrix}1 & 0\\ 0 & 1\end{smallmatrix}\right)$ and $H = \left(\begin{smallmatrix}0 & P\\ P & 0\end{smallmatrix}\right)$. (i) ${}_0A_0^\pm$, ${}_0B_0^\pm$, ${}_0E_{m,-m}^\pm$, ${}_0A_1^\pm$, ${}_0B_q^\pm$, ${}_k^{-k}E_{A0}$, ${}_k^{-k}E_{B0}$, ${}_k^{-k}G_{m,-m}$, ${}_k^{-k}E_{A_q}$ and ${}_k^{-k}E_{B_q}$ as in table 13. All these reps are of type a.

(ii)	For $q = 1, 2, 3, \ldots$			only $q = 2v = 2, 4, 6, \ldots$
d	${}_\pi E_{A0}^{A_q}$	${}_\pi E_{B0}^{B_q}$	${}_\pi G_{m,-m}^{\bar{m},-\bar{m}}$ †	${}_\pi E_{v,-v}^\pm$
S	P	P	H	I

† Here $m = 1, 2, \ldots, (q-1)/2$ for q odd and $m = 1, 2, \ldots, (q-2)/2$ for q even; $\bar{m} = q - m$.

3. Further applications

3.1. *Coreps and* UMAM *reps of* $L^A = L + \theta L$

In accordance with our physical motivation, attention was focused onto extra degeneracies arising from time-reversal invariance of the Hamiltonian; however, tables 1–15 contain more information. The *grey line group* $L^A = L + \theta L = L \otimes \{E, \theta\}$ contains both linear and antilinear operators so that one might use irreducible corepresentations (coreps; cf Jansen and Boon 1967) or unitary matrix–antimatrix representations (UMAM reps; cf Herbut *et al* 1980), to label the bands etc. Now, given a rep $d(L)$, the data presented in the above tables are sufficient to write down the corresponding coreps or UMAM reps immediately; the recipes (Jansen and Boon 1967, Herbut *et al* 1980) are summarised in table 16.

Table 16. (i) Construction of coreps $D(L^A)$ out of given reps $d(L)$.

Type of d	$D(R\,|\,\tau)$	$D(\theta)$	$D[\theta(R\,|\,\tau)] = D(\theta)D(R\,|\,\tau)^*$
a	$d(R\,|\,\tau)$	S	$Sd^*(R\,|\,\tau)$
b	$\begin{pmatrix} d(R\,|\,\tau) & 0 \\ 0 & d^*(R\,|\,\tau) \end{pmatrix}$	$\begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & d(R\,|\,\tau) \\ d^*(R\,|\,\tau) & 0 \end{pmatrix}$
c	$\begin{pmatrix} d(R\,|\,\tau) & 0 \\ 0 & d(R\,|\,\tau) \end{pmatrix}$	$\begin{pmatrix} 0 & S \\ -S & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & Sd^*(R\,|\,\tau) \\ -Sd^*(R\,|\,\tau) & 0 \end{pmatrix}$

(ii) Construction of UMAM reps $D^A(L^A)$ out of $d(L)$:

$$D^A(R\,|\,\tau) = D(R\,|\,\tau) \qquad D^A(\theta) = D(\theta)K \tag{2a}$$

$$D^A[\theta(R\,|\,\tau)] = D^A(\theta)D^A(R\,|\,\tau) = D[\theta(R\,|\,\tau)]K \tag{2b}$$

where $D(R\,|\,\tau)$, $D(\theta)$ and $D[\theta(R\,|\,\tau)]$ are defined in (i) and K is the *antimatrix* (cf Herbut *et al* 1980), such that $KM = M^*K$ for every matrix M. Conceptual and mnemotechnical advantages of the UMAM rep concept arise from the homomorphism, which is restored by (2*b*).

Note that two coreps of L^A are equivalent iff they subduce equivalent reps of L (Jansen and Boon 1967, p 174) so that for reps of types a and c the matrices S and $S' = \exp(i\phi)S$ give rise to equivalent coreps. Tables 1–15 were designed to produce a complete set of non-equivalent coreps and hence only one matrix S has been given for each such rep; for the same reason each pair of conjugate reps of type b appears only once in these tables.

3.2. *Symmetry adapted bases*

If a symmetry adapted basis (SAB) $\{\psi_1, \ldots, \psi_n\}$ for a rep $d(L)$ is known, the data quoted in tables 1–15 enable one to write down the corresponding SAB for the corep $D(L^A)$, in which the latter will be in its standard form as given in table 16. Let $\phi_i = \Sigma_{j=1}^{n} S_{ji}^{*}\psi_j^{*}$, $i = 1, \ldots, n$. Then the required SAB for $D(L^A)$ is

$$\{\psi_1+\phi_1, \ldots, \psi_n+\phi_n\} \qquad \text{if } d(L) \text{ is of type a}$$

$$\{\psi_1, \ldots, \psi_n, \psi_1^*, \ldots, \psi_n^*\} \qquad \text{if } d(L) \text{ is of type b}$$

$$\{\psi_1, \ldots, \psi_n, \phi_1, \ldots, \phi_n\} \qquad \text{if } d(L) \text{ is of type c.}$$

Proofs of these statements are given for cases a and b in Jansen and Boon (1967); a proof for the third case can be easily reconstructed along the same lines.

3.3. *Influence of spin*

The classification of reps given here resolves the problem of finding extra degeneracies induced by time-reversal symmetry also when one deals with half-integral spins. In that case (cf Streitwolf 1971): *the degeneracy is doubled for type* a *and* b reps, *while there is no extra degeneracy for type* c reps. This might be of relevance for those approaches to electron spectra of polymers that go beyond the restricted Hartree–Fock method, such as alternant molecular orbitals, AMO (Calais 1980) or different orbitals for different spins, DODS (Kertész *et al* 1976, 1979) schemes etc.

4. Concluding remarks

The tables 1–15 enable a user to determine effortlessly whether time-reversal symmetry brings in some extra degeneracies of electron bands or vibration branches of a polymer or not; the task we set in the introduction is thus solved. However, a brief discussion of some overall aspects of the results obtained might be in order.

First, a variety of possibilities is realised. Thus e.g. Ln_p2 line groups have only type a reps, Ln/m have both a and b, and Lnc have a, b and c in spite of similar structure of these groups and their reps. If we focus our attention on the quantum numbers distinguishing the reps we also observe substantial differences. Thus e.g.

(i) θ-symmetry connects $_kE_{1,-1}$ and $_{-k}E_{1,-1}$ reps of $L4_2mc$, thus bringing in extra two-fold *star* degeneracy (i.e. $\varepsilon(k) = \varepsilon(-k)$);

(ii) similarly; θ couples $^{-k}_{k}E_1$ and $^{-k}_{k}E_{-1}$ reps of $L4_2/m$, but here it brings in extra two-fold *band* degeneracy (i.e. $\varepsilon(m=1) = \varepsilon(m=-1)$ throughout the Brillouin zone), while

(iii) in the case of $^{-k}_{k}E_1^{-1}$ rep of $L4_22$ simply nothing happens when θ is added. (The notions we use here are familiar in solid-state physics where analogous situations are encountered; for a good account see e.g. Streitwolf (1971), Cracknell (1975).

To recognise some general trends in this variety of cases we have to resort to somewhat more elaborate group theoretical concepts. First, note that here we are dealing with *solvable* groups possessing normal subgroup chains like e.g.

$$T \lhd \mathrm{L}n \lhd \mathrm{L}nc \lhd \mathrm{L}\bar{n}c \tag{3}$$

or

$$T \lhd \mathrm{L}(2q)_q \lhd \mathrm{L}(2q)_q mc \lhd \mathrm{L}(2q)_q/mcm \tag{4}$$

etc. (Here $H \lhd G$ means that H is a normal subgroup of G.) Utilising this fact we use the ${}_kA_m$ reps (all of which are one-dimensional) of the $\mathrm{L}n_p$ line groups as building blocks to induce all the others (cf LG, I and II).

Next, observe that the quantum numbers of ${}_kA_m$ (namely k and m) have kinematical meaning—they describe quasi-momentum (related to the translational symmetry) and quasi-angular momentum (related to the screw-axis symmetry) of a particle (or a quasi-particle), respectively. As expected from this physical interpretation, the action of θ on these two quantum numbers is given by

$$\theta : k \to -k \qquad \theta : m \to -m. \tag{5}$$

At first sight some exceptions to this rule seem to appear for some special values of k and m, namely $k = 0$ or $k = \pi$ and $m = 0$ or $m = q = n/2$. However, these cases also start fitting into the scheme (5) as soon as one takes into account appropriate 'periodicity relations' for these reps, e.g.

$${}_kA_m(\mathrm{L}n_p) = {}_{k+2\pi}A_{m-p}(\mathrm{L}n_p) \tag{6}$$

etc, enabling conversions like ${}_{-\pi}A_m = {}_{\pi}A_{m-p}$ to be made.

Then, we can proceed upwards along the subgroup chain, similar to (3) or (4), by adding new spatial symmetry transformations (σ_v, σ_h or U) and building the reps of in this way enlarged groups (i.e. *minimal extensions*; cf LG, I and II for the line groups and Herbut *et al* (1973) for a general account). The action on k and m—again in accordance with their physical meaning—can be summarised as:

$$\sigma_\mathrm{v} : \begin{matrix} m \to -m \\ k \to k \end{matrix} \qquad \sigma_\mathrm{h} : \begin{matrix} m \to m \\ k \to -k \end{matrix} \qquad U : \begin{matrix} m \to -m \\ k \to -k \end{matrix} \tag{7}$$

(with the same explanation valid for the above-mentioned special values of k and m).

Now we are in a position to understand why additional time-reversal symmetry produced such different effects in the examples (i)–(iii) given above. The systematic band degeneracy (among ${}_kA_1(\mathrm{L}4_2)$ and ${}_kA_{-1}(\mathrm{L}4_2)$ states for each k point in the Brillouin zone) is produced by σ_v in case (i) and by joint action of σ_h and θ in case (ii), while it is absent in case (iii), as follows from (5) and (7). We further conclude that this band degeneracy will be lifted by e.g. a homogeneous magnetic field parallel to the chain axis in case (ii), while it will be still preserved in case (i). A similar analysis can be readily performed for every line group.

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