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Selection rules for polymers and quasi one-dimensional crystals: II. Kronecker products for the line groups isogonal to D_n

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Abstract. The reduction coefficients for the Kronecker products of irreducible representations of line groups are needed to derive selection rules for various physical processes in polymers and quasi-one-dimensional solids, and in this paper they are tabulated explicitly for all the line groups isogonal to dihedral point groups $D_n = C_n + UC_n$.

The selection rules obtained imply that the quasi-momentum, the quasi-angular momentum, and the parity with respect to the dihedral axis U are all conserved quantities, except that the quasi-angular momentum is increased by $p\hbar$ in Umklapp processes, in the case of a polymer with an n_p screw axis.

1. Introduction

Electronic properties of polymers and quasi one-dimensional conductors are now the focus of intensive theoretical and experimental investigation and thus interest has arisen in studying their symmetry properties and in particular in deriving the selection rules for various physical processes in these systems (Damnjanović *et al* 1983, to be referred to as I). The task essentially consists of determining the reduction (or frequency) coefficients for the Kronecker products of the irreducible representations, reps (Božović *et al* 1978) of the line groups involved. These coefficients have been tabulated for the line groups isogonal to the C_n, C_{nv}, C_{nh} and S_{2n} point groups in I, where the method has also been described. Continuing this programme, in this paper we consider the next class of line groups—those isogonal to the point groups $D_n = C_n + UC_n$, $n = 1, 2, \ldots$, where C_n is a rotation through $2\pi/n$ around the z axis, and U is a rotation through π around the x axis. The same method has been utilised as in I, but the present task is somewhat more difficult in view of the variety of special cases to be discussed.

2. Results

The line groups isogonal to D_n are $Ln2$, $n = 1, 3, \ldots$ and $Ln22$, $n = 2, 4, \ldots$; Ln_p2, $n = 3, 5, \ldots$ and Ln_p22, $n = 2, 4, \ldots$, where $p = 1, 2, \ldots, n-1$. For each of these line

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groups we give (i) the character table, to introduce the rep symbols and to define the ranges of their quantum numbers, and (ii) the table of decompositions of the Kronecker products $D\otimes D'$, for all pairs D, D' of reps of the group considered. Tables (ii) are triangular, in view of the fact that $D\otimes D' \sim D'\otimes D$. The length unit is chosen to coincide with the translational period, to simplify the notation; hence the first Brillouin zone is defined by $k \in (-\pi, \pi]$.

2.1. The symmorphic line groups Ln2, $n=1,3,\ldots$ and Ln22, $n=2,4,\ldots$

Table 1. The characters of the reps of the line groups Ln2, $n=1,3,\ldots$ and Ln22, $n=2,4,\ldots$. Here $s=0,1,\ldots,n-1$; $t=0,\pm1,\ldots$; $\alpha=2\pi/n$; $k\in(0,\pi)$ and m and w take on all the integral values from the intervals $[\frac{1}{2}(1-n),\frac{1}{2}n]$ and $[1,\frac{1}{2}(n-1)]$ respectively. The two-dimensional reps appear only for $n\geq 3$.

rep	$(C_n^s\|t)$	$(UC_n^s\|-t)$
${}_0A_0^{\pm}$	1	±1
${}_0E_w^{-w}$	$2\cos(ws\alpha)$	0
${}_k^{-k}E_m^{-m}$	$2\cos(kt+ms\alpha)$	0
${}_\pi A_0^{\pm}$	$(-1)^t$	$\pm(-1)^t$
${}_\pi E_w^{-w}$	$2(-1)^t\cos(ws\alpha)$	0
and only for $n=2q=2,4,\ldots$		
${}_0A_q^{\pm}$	$(-1)^s$	$\pm(-1)^s$
${}_\pi A_q^{\pm}$	$(-1)^{s+t}$	$\pm(-1)^{s+t}$

As seen from table 2, the product $D\otimes D'$ of two reps of Ln2 or Ln22 is in most cases again a rep of the group considered. However, the result may also be a sum of several reps, and furthermore it may vary with the quantum numbers of D and D' in a non-uniform way. Hence these entries, (1)–(5), are separately discussed below.

(1) One has to distinguish here whether $w+w'=q=\frac{1}{2}n$ or not, and whether $w-w'=0$ or not. Let

$$\theta=\begin{cases} w+w', & \text{if } w+w'\in[2,\frac{1}{2}(n-1)] \\ n-w-w', & \text{if } w+w'\in[\frac{1}{2}(n+1),n-1], \end{cases}$$

(notice that the largest value of $(2+w')$ is $(n-2)$ if n is even), and let

$$\tau=\begin{cases} w'-w, & \text{if } w-w'\in[\frac{1}{2}(3-n),-1] \\ w-w', & \text{if } w-w'\in[1,\frac{1}{2}(n-3)]. \end{cases}$$

Then

$$ {}_0E_w^{-w}\otimes{}_0E_{w'}^{-w'}={}_0E_{w'}^{-w'}\otimes{}_0E_w^{-w}$$

$$=\begin{cases} {}_0E_\theta^{-\theta}+{}_0E_\tau^{-\tau}, & \text{if } w+w'\neq q \text{ and } w\neq w' \\ {}_0E_\theta^{-\theta}+{}_0A_0^{+}+{}_0A_0^{-}, & \text{if } w+w'\neq q \text{ and } w=w' \\ {}_0A_q^{+}+{}_0A_q^{-}+{}_0E_\tau^{-\tau}, & \text{if } w+w'=q \text{ and } w\neq w \\ & \text{(only for } n=4,6,8,\ldots) \\ {}_0A_q^{+}+{}_0A_q^{-}+{}_0A_0^{+}+{}_0A_0^{-}, & \text{if } w+w'=q \text{ and } w=w' \\ & \text{(only for } n=4,8,12,\ldots). \end{cases}$$

Table 2. Decompositions of the Kronecker products of reps of Ln2 and Ln22. The reps $_0A_q^{\pm}$ and $_\pi A_q^{\pm}$ appear only in the Ln22 line groups and the heavily framed part of the tables corresponds only to these groups. The entries (1)–(4) are described in the text, and entry (5) is specified in table 2(a).

$_0A_0^+$	$_0A_0^+$										
$_0A_0^-$	$_0A_0^-$	$_0A_0^+$									
$_0E_w^{-w}$	$_0E_w^{-w}$	$_0E_w^{-w}$	(1)								
$^{-k}_{k}E_m^{-m}$	$^{-k}_{k}E_m^{-m}$	$^{-k}_{k}E_m^{-m}$	(2)	(5)							
$_\pi A_0^+$	$_\pi A_0^+$	$_\pi A_0^-$	$_\pi E_{w'}^{-w'}$	$^{-\lambda}_{\lambda}E_{-m'}^{m'}$	$_0A_0^+$						
$_\pi A_0^-$	$_\pi A_0^-$	$_\pi A_0^+$	$_\pi E_{w'}^{-w'}$	$^{-\lambda}_{\lambda}E_{-m'}^{m'}$	$_0A_0^-$	$_0A_0^+$					
$_\pi E_w^{-w}$	$_\pi E_w^{-w}$	$_\pi E_w^{-w}$	(3)	(4)	$_0E_w^{-w}$	$_0E_w^{-w}$	(1)				
$_0A_q^+$	$_0A_q^+$	$_0A_q^-$	$_0E_\delta^{-\delta}$	$^{-k'}_{k'}E_\gamma^{-\gamma}$	$_\pi A_q^+$	$_\pi A_q^-$	$_\pi E_\delta^{-\delta}$	$_0A_0^+$			
$_0A_q^-$	$_0A_q^-$	$_0A_q^+$	$_0E_\delta^{-\delta}$	$^{-k'}_{k'}E_\gamma^{-\gamma}$	$_\pi A_q^-$	$_\pi A_q^+$	$_\pi E_\delta^{-\delta}$	$_0A_0^-$	$_0A_0^+$		
$_\pi A_q^+$	$_\pi A_q^+$	$_\pi A_q^-$	$_\pi E_\delta^{-\delta}$	$^{-\lambda}_{\lambda}E_{-\gamma}^{\gamma}$	$_0A_q^+$	$_0A_q^-$	$_0E_\delta^{-\delta}$	$_\pi A_0^+$	$_\pi A_0^-$	$_0A_0^+$	
$_\pi A_q^-$	$_\pi A_q^-$	$_\pi A_q^+$	$_\pi E_\delta^{-\delta}$	$^{-\lambda}_{\lambda}E_{-\gamma}^{\gamma}$	$_0A_q^-$	$_0A_q^+$	$_0E_\delta^{-\delta}$	$_\pi A_0^-$	$_\pi A_0^+$	$_0A_0^-$	$_0A_0^+$
D / D'	$_0A_0^+$	$_0A_0^-$	$_0E_{w'}^{-w'}$	$^{-k'}_{k'}E_{m'}^{-m'}$	$_\pi A_0^+$	$_\pi A_0^-$	$_\pi E_{w'}^{-w'}$	$_0A_q^+$	$_0A_q^-$	$_\pi A_q^+$	$_\pi A_q^-$

where

$$\lambda = \pi - k'$$

$$\delta = q - w'$$

$$\gamma = \begin{cases} q + m' & \text{if } m' \in [-\tfrac{1}{2}(n-1), 0] \\ m' - q & \text{if } m' \in [1, \tfrac{1}{2}n] \end{cases}$$

Table 2 (a). The entry (5) of table 2—decompositions of $^{-k}_{k}E_m^{-m} \otimes {}^{-k'}_{k'}E_{m'}^{-m'}$, with $k \in (0, \pi)$, $k' \in (0, k]$ and $m, m' \in [1, \tfrac{1}{2}n]$.

$k+k'$	$k-k'$	$m+m'$	$m-m'$	$^{-k}_{k}E_m^{-m} \otimes {}^{-k'}_{k'}E_{m'}^{-m'}$
$(0, \pi)$	$(0, \pi)$	M	M_1	$^{-\psi}_{\psi}E_\mu^{-\mu} + {}^{-\kappa}_{\kappa}E_\nu^{-\nu}$
$(\pi, 2\pi)$	$(0, \pi)$	M	M_1	$^{-\zeta}_{\zeta}E_{-\mu}^{\mu} + {}^{-\kappa}_{\kappa}E_\nu^{-\nu}$
π	$(0, \pi)$	M_2	M_1	$_\pi E_\theta^{-\theta} + {}^{-\kappa}_{\kappa}E_\nu^{-\nu}$
		0	M_1	$_\pi A_0^+ + {}_\pi A_0^- + {}^{-\kappa}_{\kappa}E_\nu^{-\nu}$
		$2q$	0	$_\pi A_0^+ + {}_\pi A_0^- + {}^{-\kappa}_{\kappa}E_0^0$ †
		$\pm q$	0	$_\pi A_q^+ + {}_\pi A_q^- + {}^{-\kappa}_{\kappa}E_\nu$ †
$(0, \pi)$	0	M	M_2	$^{-\psi}_{\psi}E_\mu^{-\mu} + {}_0E_\tau^{-\tau}$
		M	0	$^{-\psi}_{\psi}E_\mu^{-\mu} + {}_0A_0^+ + {}_0A_0^-$
		M	$\pm q$	$^{-\psi}_{\psi}E_\mu^{-\mu} + {}_0A_q^+ + {}_0A_q^-$ †
$(\pi, 2\pi)$	0	M	M_2	$^{-\zeta}_{\zeta}E_{-\mu}^{\mu} + {}_0E_\tau^{-\tau}$
		M	0	$^{-\zeta}_{\zeta}E_{-\mu}^{\mu} + {}_0A_0^+ + {}_0A_0^-$
		M	$\pm q$	$^{-\zeta}_{\zeta}E_{-\mu}^{\mu} + {}_0A_q^+ + {}_0A_q^-$ †

† Only for $n = 2q$ even.

Table 2(a) (continued) and especially for $k=k'=\frac{1}{2}\pi$.

$m+m'$	$m-m'$	${}^{-k}_{k}E^{-m}_{m}\otimes{}^{-k'}_{k'}E^{-m'}_{m'}$
M_2	M_2	${}_{\pi}E^{-\theta}_{\theta}+{}_{0}E^{-\tau}_{\tau}$
	0	${}_{\pi}E^{-\theta}_{\theta}+{}_{0}A^{+}_{0}+{}_{0}A^{-}_{0}$
	$\pm q$	${}_{\pi}E^{-\theta}_{\theta}+{}_{0}A^{+}_{q}+{}_{0}A^{-}_{q}$ †
0	M_2	${}_{\pi}A^{+}_{0}+{}_{\pi}A^{-}_{0}+{}_{0}E^{-\tau}_{\tau}$
	0	${}_{\pi}A^{+}_{0}+{}_{\pi}A^{-}_{0}+{}_{0}A^{+}_{0}+{}_{0}A^{-}_{0}$
	$\pm q$	${}_{\pi}A^{+}_{0}+{}_{\pi}A^{-}_{0}+{}_{0}A^{+}_{q}+{}_{0}A^{-}_{q}$ ‡
$\pm q$	M_2	${}_{\pi}A^{+}_{q}+{}_{\pi}A^{-}_{q}+{}_{0}E^{-\tau}_{\tau}$ †
	0	${}_{\pi}A^{+}_{q}+{}_{\pi}A^{-}_{q}+{}_{0}A^{+}_{0}+{}_{0}A^{-}_{0}$ ‡
q	$\pm q$	${}_{\pi}A^{+}_{q}+{}_{\pi}A^{-}_{q}+{}_{0}A^{+}_{q}+{}_{0}A^{-}_{q}$ ‡
$2q$	0	${}_{\pi}A^{+}_{0}+{}_{\pi}A^{-}_{0}+{}_{0}A^{+}_{0}+{}_{0}A^{-}_{0}$

† Only for $n=2q$ even.
‡ Only for $n=2q=4,8,\ldots$.

Here $q=n/2$, $M=[-n+1,n]$, $M_1=[-n+1,n-1]$, $M_2=[-n+1,-1]U[1,(n-1)/2]U[(n+1)/2,n-1]$.

$\psi=k+k'$ $\quad\zeta=2\pi-k-k'$ $\quad\kappa=k-k'$

$$\mu=\begin{cases} m+m'+n, & \text{if } m+m'\in[-n+1,-\frac{1}{2}n]\\ m+m', & \text{if } m+m'\in[-\frac{1}{2}(n-1),\frac{1}{2}n]\\ m+m'-n, & \text{if } m+m'\in[\frac{1}{2}(n+1),n]\end{cases}$$

$$\theta=\begin{cases} m+m'+n, & \text{if } m+m'\in[-n+1,-\frac{1}{2}(n+1)]\\ -m-m', & \text{if } m+m'\in[-\frac{1}{2}(n-1),-1]\\ m+m', & \text{if } m+m'\in[1,\frac{1}{2}(n-1)]\\ n-m-m', & \text{if } m+m'\in[\frac{1}{2}(n+1),n-1]\end{cases}$$

$$\nu=\begin{cases} m-m'+n, & \text{if } m-m'\in[-n+1,-\frac{1}{2}n]\\ m-m', & \text{if } m-m'\in[-\frac{1}{2}(n-1),\frac{1}{2}n]\\ m-m'-n, & \text{if } m-m'\in[\frac{1}{2}(n+1),n-1]\end{cases}$$

$$\tau=\begin{cases} m-m'+n, & \text{if } m-m'\in[-n+1,-\frac{1}{2}(n+1)]\\ m'-m, & \text{if } m-m'\in[-\frac{1}{2}(n-1),-1]\\ m-m', & \text{if } m-m'\in[1,\frac{1}{2}(n-1)]\\ m'-m+n, & \text{if } m-m'\in[\frac{1}{2}(n+1),n-1]\end{cases}$$

(2) ${}^{-k}_{k}E^{-m}_{m}\otimes{}_{0}E^{-w'}_{w}={}^{-k}_{k}E^{-\mu}_{\mu}+{}^{-k}_{k}E^{-\nu}_{\nu}$, where

$$\mu=\begin{cases} m+w', & \text{if } m+w'\in[\frac{1}{2}(3-n),\frac{1}{2}n]\\ m+w'-n, & \text{if } m+w'\in[\frac{1}{2}(n+1),n-1]\end{cases}$$

and

$$\nu=\begin{cases} m-w'+n, & \text{if } m-w'\in[1-n,-\frac{1}{2}n]\\ m-w', & \text{if } m-w'\in[\frac{1}{2}(1-n),\frac{1}{2}(n-2)].\end{cases}$$

(3) Special cases appear here when $w+w'=q\equiv\frac{1}{2}n$ and when $w-w'=0$, like in (1).

Let θ and τ be defined as in (1), then

$$
{}_{\pi}E_{w}^{-w} \otimes {}_{0}E_{w'}^{-w'} = \begin{cases} {}_{\pi}E_{\theta}^{-\theta} + {}_{\pi}E_{\tau}^{-\tau}, & \text{if } w+w' \neq q \text{ and } w \neq w' \\ {}_{\pi}E_{\theta}^{-\theta} + {}_{\pi}A_{0}^{+} + {}_{\pi}A_{0}^{-}, & \text{if } w+w' \neq q \text{ and } w = w' \\ {}_{\pi}A_{q}^{+} + {}_{\pi}A_{q}^{-} + {}_{\pi}E_{\tau}^{-\tau}, & \text{if } w+w' = q \text{ and } w \neq w' \\ & \text{(only for } n = 4, 6, 8, \ldots) \\ {}_{\pi}A_{q}^{+} + {}_{\pi}A_{q}^{-} + {}_{\pi}A_{0}^{+} + {}_{\pi}A_{0}^{-}, & \text{if } w+w' = q \text{ and } w = w' \\ & \text{(only for } n = 4, 8, 12, \ldots). \end{cases}
$$

(4) ${}_{\pi}E_{w}^{-w} \otimes {}^{-k'}_{k'}E_{m'}^{-m'} = {}^{-\lambda}_{\lambda}E_{-\mu}^{\mu} + {}^{-\lambda}_{\lambda}E_{\nu}^{-\nu}$, where $\lambda = \pi - k'$, μ is defined as in (2), and

$$
\nu = \begin{cases} w - m', & \text{if } w - m' \in [\tfrac{1}{2}(2-n), \tfrac{1}{2}n] \\ w - m' - n, & \text{if } w - m' \in [\tfrac{1}{2}(n+1), n-1]. \end{cases}
$$

(5) Depending on the values of $k+k'$, $k-k'$, $m+m'$ and $m-m'$, many special cases have to be distinguished of the decomposition of ${}^{-k}_{k}E_{m}^{-m} \otimes {}^{-k'}_{k'}E_{m'}^{-m'}$; to facilitate reference they are all tabulated separately, in table 2(*a*). We assume that $k \geqslant k'$; in the opposite case just interchange ${}^{-k}_{k}E_{m}^{-m}$ and ${}^{-k}_{k'}E_{m'}^{-m'}$.

2.2. The non-symmorphic line groups Ln_p2, $n = 3, 5, \ldots$, and Ln_p2 $n = 2, 4, \ldots$, with $p = 1, \ldots, n-1$

(6) Special cases appear here if $v' - w = g \equiv -\tfrac{1}{2}p$ and/or $w + v' = h \equiv \tfrac{1}{2}(n-p)$. Let

$$
\beta = \begin{cases} w' + v, & \text{if } w' + v \in [\tfrac{1}{2}(1-p), \tfrac{1}{2}(n-p-1)] \\ n - p - w' - v, & \text{if } w' + v \in [\tfrac{1}{2}(n-p+1), \tfrac{1}{2}(2n-p-1)], \end{cases}
$$

Table 3. The characters of the reps of the line groups Ln_p2, $n = 3, 5, \ldots, p = 1, 2, \ldots, n-1$ and Ln_p22, $n = 2, 4, \ldots$, $p = 1, 2, \ldots, n-1$. For s, t, k, α, m and w see the caption of table 1; v takes on all the integral values from the interval $[\tfrac{1}{2}(1-p), \tfrac{1}{2}(n-p-1)]$; $\bar{v} = -p - v$ if $v \in [\tfrac{1}{2}(1-p), \tfrac{1}{2}(n-2p-1]$ and $\bar{v} = n - p - v$ if $v \in [\tfrac{1}{2}(n-2p+1), \tfrac{1}{2}(n-p-1)]$. In the case of $L2_122$ there are no two-dimensional reps.

rep	$(C_n^s \mid t + sp/n)$	$(UC_n^s \mid -t - sp/n)$
${}_{0}A_{0}^{\pm}$	1	± 1
${}_{0}E_{w}^{-w}$	$2\cos(ws\alpha)$	0
${}^{-k}_{k}E_{m}^{-m}$	$2\cos(kt + ksp/n + ms\alpha)$	0
${}_{\pi}E_{v}^{\bar{v}}$	$2(-1)^t \cos[(v + \tfrac{1}{2}p)s\alpha]$	0
and only for $n = 2q = 2, 4, \ldots$		
${}_{0}A_{q}^{\pm}$	$(-1)^s$	$\pm(-1)^s$
and only for $p = -2g = 2, 4, \ldots$		
${}_{\pi}A_{g}^{\pm}$	$(-1)^t$	$\pm(-1)^t$
and only for $n - p = 2h = 2, 4, \ldots$		
${}_{\pi}A_{h}^{\pm}$	$(-1)^{s+t}$	$\pm(-1)^{s+t}$

Table 4. Decomposition of Kronecker products of reps of Ln_p2 and Ln_p22. The reps ${}_0A_q^{\pm}$ appear only when $n=2q$ is even, the reps ${}_0A_g^{\pm}$ only when $p=-2g$ is even, and the reps ${}_0A_h^{\pm}$ only when $n-p=2h$ is even. For entries (1) and (2) see §2.1; the entries (6)–(8) are described in the text below, and the entry (9) in table 4(a).

	D \ D'	${}_0A_0^+$	${}_0A_0^-$	${}_0E_{w'}^{-w'}$	${}_{k'}^{-k'}E_{m'}^{-m'}$	${}_\pi E_{v'}^{\bar v'}$	${}_0A_q^+$	${}_0A_q^-$	${}_\pi A_g^+$	${}_\pi A_g^-$	${}_\pi A_h^+$	${}_\pi A_h^-$
	${}_0A_0^+$	${}_0A_0^+$										
	${}_0A_0^-$	${}_0A_0^-$	${}_0A_0^+$									
	${}_0E_w^{-w}$	${}_0E_w^{-w}$	${}_0E_w^{-w}$	(1)								
	${}_k^{-k}E_m^{-m}$	${}_k^{-k}E_m^{-m}$	${}_k^{-k}E_m^{-m}$	(2)	(9)							
	${}_\pi E_v^{\bar v}$	${}_\pi E_v^{\bar v}$	${}_\pi E_v^{\bar v}$	(6)	(7)	(8)						
n even	${}_0A_q^+$	${}_0A_q^+$	${}_0A_q^-$	${}_0E_\delta^{-\delta}$	${}_{k'}^{-k'}E_\gamma^{-\gamma}$	${}_\pi E_d^{\bar d}$	${}_0A_0^+$					
	${}_0A_q^-$	${}_0A_q^-$	${}_0A_q^+$	${}_0E_\delta^{-\delta}$	${}_{k'}^{-k'}E_\gamma^{-\gamma}$	${}_\pi E_d^{\bar d}$	${}_0A_0^-$	${}_0A_0^+$				
p even	${}_\pi A_g^+$	${}_\pi A_g^+$	${}_\pi A_g^-$	${}_\pi E_b^{\bar b}$	${}_\lambda^{-\lambda}E_\varepsilon^{-\varepsilon}$	${}_0E_e^{-e}$	${}_\pi A_h^+$	${}_\pi A_h^-$	${}_0A_0^+$			
	${}_\pi A_g^-$	${}_\pi A_g^-$	${}_\pi A_g^+$	${}_\pi E_b^{\bar b}$	${}_\lambda^{-\lambda}E_\varepsilon^{-\varepsilon}$	${}_0E_e^{-e}$	${}_\pi A_h^-$	${}_\pi A_h^+$	${}_0A_0^-$	${}_0A_0^+$		
$n-p$ even	${}_\pi A_h^+$	${}_\pi A_h^+$	${}_\pi A_h^-$	${}_\pi E_c^{-\bar c}$	${}_\lambda^{-\lambda}E_\rho^{-\rho}$	${}_0E_f^{-f}$	${}_\pi A_g^+$	${}_\pi A_g^-$	${}_0A_q^+$	${}_0A_q^-$	${}_0A_0^+$	
	${}_\pi A_h^-$	${}_\pi A_h^-$	${}_\pi A_h^+$	${}_\pi E_c^{\bar c}$	${}_\lambda^{-\lambda}E_\rho^{-\rho}$	${}_0E_f^{-f}$	${}_\pi A_g^-$	${}_\pi A_g^+$	${}_0A_q^-$	${}_0A_q^+$	${}_0A_0^-$	${}_0A_0^+$
							n even		p even		$n-p$ even	

$b=\frac{1}{2}(2w'-p)$ $\quad c=\frac{1}{2}(n-p-2w')$

$d=q-p-v'$ $\quad e=\frac{1}{2}(2v'+p)$

$f=\frac{1}{2}(n-p-2v')$ $\quad g=-\frac{1}{2}p$

$h=\frac{1}{2}(n-p)$ $\quad \delta=q-w'$

$\lambda=\pi-k'$

and where

$$\gamma=\begin{cases} q+m', & \text{if } m'\in[1-q,0] \\ m'-q, & \text{if } m'\in[1,q] \end{cases}$$

$$\varepsilon=\begin{cases} -\frac{1}{2}(2m'+p), & \text{if } m'\in[\frac{1}{2}(1-n),\frac{1}{2}(n-p-1)] \\ \frac{1}{2}(2n-2m'-p), & \text{if } m'\in[\frac{1}{2}(n-p+1),\frac{1}{2}n] \end{cases}$$

$$\rho=\begin{cases} -\frac{1}{2}(n+p+2m'), & \text{if } m'\in[\frac{1}{2}(1-n),-\frac{1}{2}(p+1)] \\ \frac{1}{2}(n-p-2m'), & \text{if } m'\in[\frac{1}{2}(1-p),\frac{1}{2}n] \end{cases}$$

and

$$\phi=\begin{cases} w-v'-p, & \text{if } v'-w\in[\frac{1}{2}(1-n-p),-\frac{1}{2}(p+1)] \\ v'-w, & \text{if } v'-w\in[\frac{1}{2}(1-p),\frac{1}{2}(n-p-1)], \end{cases}$$

then

$$
{}_0E_w^{-w} \otimes {}_\pi E_{v'}^{\bar{v}'} = \begin{cases} {}_\pi E_\beta^{\bar\beta} + {}_\pi E_\phi^{\bar\phi}, & \text{if } v'-w \neq g \text{ and } w+v' \neq h \\ {}_\pi A_h^+ + {}_\pi A_h^- + {}_\pi E_\phi^{\bar\phi}, & \text{if } v'-w \neq g \text{ and } w+v' = h \\ & \text{(only for } n-p=2,4,\ldots) \\ {}_\pi E_\beta^{\bar\beta} + {}_\pi A_g^+ + {}_\pi A_g^-, & \text{if } v'-w = g \text{ and } w+v' \neq h \\ & \text{(only for } p=2,4,\ldots,n-1) \\ {}_\pi A_h^+ + {}_\pi A_h^- + {}_\pi A_g^+ + {}_\pi A_g^-, & \text{if } v'-w = g \text{ and } w+v' = h \\ & \text{(only for } n=4,8,\ldots, \text{and} \\ & p=2,4,\ldots,n-2). \end{cases}
$$

Notice that $v'-w=g$ and $w+v'=h$ implies that $w=\frac{1}{4}n$ and $v'=\frac{1}{4}(n-2p)$.

(7) ${}_\pi E_v^{\bar v} \otimes {}^{-k}_{k}E_{m'}^{-m'} = {}^{-\lambda}_{\lambda}E_\mu^{-\mu} + {}^{-\lambda}_{\lambda}E_\nu^{-\nu}$ where

$$
\mu = \begin{cases} -p-v-m', & \text{if } v+m' \in [\frac{1}{2}(2-n-p), \frac{1}{2}(n-2p-1)] \\ n-p-v-m', & \text{if } v+m' \in [\frac{1}{2}(n-2p+1), \frac{1}{2}(2n-p-1)]. \end{cases}
$$

(Notice that the smallest value of $(v+m')$ is $\frac{1}{2}(4-n-p)$ if both n and p are even, and that the largest value of $(v+m')$ is $\frac{1}{2}(2n-p-3)$ if both n and p are odd),

$$
\nu = \begin{cases} m'-v+n, & \text{if } m'-v \in [\frac{1}{2}(p+2-2n), -\frac{1}{2}(n+1)] \\ m'-v, & \text{if } m'-v \in [\frac{1}{2}(1-n), \frac{1}{2}n] \\ m'-v-n, & \text{if } m'-v \in [\frac{1}{2}(n+1), \frac{1}{2}(n+p-1)]. \end{cases}
$$

(Notice that the smallest value of $(m'-v)$ is $\frac{1}{2}(p+4-2n)$ if both n and p are even, and that the largest value of $(m'-v)$ is $\frac{1}{2}(n+p-3)$ if n is odd and p is even.)

(8) One has to distinguish here whether $v+v'+p=q\equiv\frac{1}{2}n$ and/or $v-v'=0$. Let

$$
\omega = \begin{cases} -v-v'-p, & \text{if } v+v' \in [\frac{1}{2}(1-n), -1], \\ v+v'+p, & \text{if } v+v' \in [1, \frac{1}{2}(n-1)], \\ n-v-v'-p, & \text{if } v+v' \in [\frac{1}{2}(n+1), n-1]; \end{cases}
$$

and

$$
\tau = \begin{cases} v'-v, & \text{if } v-v' \in [\frac{1}{2}(1-n), -1], \\ v-v', & \text{if } v-v' \in [1, \frac{1}{2}(n-1)]; \end{cases}
$$

then

$$
{}_\pi E_v^{\bar v} \otimes {}_\pi E_{v'}^{\bar v'} = \begin{cases} {}_0E_\omega^{-\omega} + {}_0E_\tau^{-\tau}, & \text{if } v+v'+p \neq q \text{ and } v \neq v' \\ {}_0E_\omega^{-\omega} + {}_0A_0^+ + {}_0A_0^-, & \text{if } v+v'+p \neq q \text{ and } v = v' \\ {}_0A_q^+ + {}_0A_q^- + {}_0E_\tau^{-\tau}, & \text{if } v+v'+p = q \text{ and } v \neq v' \\ & \text{(only for } n=4,6,\ldots) \\ {}_0A_q^+ + {}_0A_q^- + {}_0A_0^+ + {}_0A_0^-, & \text{if } v+v'+p = q \text{ and } v = v' \\ & \text{(only for } n=4,6,\ldots, \text{and} \\ & q-p=2,4,\ldots). \end{cases}
$$

(9) The possible special cases of the decomposition of ${}^{-k}_{k}E_m^{-m} \otimes {}^{-\lambda'}_{\lambda'}E_{m'}^{-m'}$ are given in table 4a. We assume that $k \geqslant k'$, as in (5).

3. Discussions

Since $D_n = C_n + UC_n$, all the line groups considered in this paper are of the form $Ln_p + (U|0)Ln_p$, where $p = 0, 1, \ldots, n-1$. The quantum numbers arising from Ln_p symmetry are the quasi-momentum $k\hbar$ and the quasi-angular momentum $m\hbar$ (Božović *et al* 1978). It is easily seen that $(U|0)$ reverts both momenta, so that $\{\varepsilon_\lambda(m, k), \lambda = 1, 2, \ldots\} = \{\varepsilon_\lambda(-m, -k), \lambda = 1, 2, \ldots\}$ and the energy eigenvalues can be labelled by the pairs $\{(k, m), (-k, -m)\}$. Let $\psi = k_v + k_i$, $\mu = m_v + m_i$, $\kappa = k_v - k_i$ and $\nu = m_v - m_i$; then the selection rules derived in § 2 in fact state that a matrix element $\langle f|v|i\rangle$ vanishes unless (k_f, m_f) coincides either with one of the labels (ψ, μ), $(-\psi, -\mu)$ or with one of the labels (κ, ν), $(-\kappa, -\nu)$. For symmorphic line groups $Ln2$ ($n = 1, 3, \ldots$) and $Ln22$ ($n = 2, 4, \ldots$) this implies that $\langle f|v|i\rangle = 0$ unless

$$k_v \pm k_i = k_f (\mathrm{mod}\ 2\pi), \qquad m_v \pm m_i = m_f (\mathrm{mod}\ n).$$

These conservation laws are valid also for non-symmorphic line groups Ln_p2 ($n = 3, 5, \ldots$) and Ln_p22 ($n = 2, 4, \ldots$), where $p = 1, \ldots, n-1$, as long as one considers normal processes only. However, $\psi = k_v + k_i$ can fall outside the first Brillouin zone, in which case $\langle f|v|i\rangle$ describes an Umklapp process. The above conservation law is then modified: $\langle f|v|i\rangle = 0$ unless

$$k_v + k_i - 2\pi = k_f, \qquad m_v + m_i + p = m_f (\mathrm{mod}\ n)$$

or

$$k_v - k_i = k_f \qquad m_v - m_i = m_f (\mathrm{mod}\ n).$$

Notice that in the Ln_p groups and in their supergroups, (k, m) is equivalent to $(k - 2\pi, m - p)$, and in this sense m is coupled to k, because rotations are coupled to (fractional) translations in these groups.

Table 4(a). The entry (9) of table 4—the decompositions of ${}^{-k}_{k}E^{-m}_{m} \otimes {}^{-k}_{k'}E^{-m'}_{m}$, with $k \in (0, \pi]$, $k' \in (0, k)$ and $m, m' \in [1, \frac{1}{2}n]$.

$k + k'$	$k - k'$	$m + m'$	$m - m'$	${}^{-k}_{k}E^{-m}_{m} \otimes {}^{-k'}_{k'}E^{-m'}_{m'}$
$(0, \pi)$	$(0, \pi)$	M	M_1	${}^{-\psi}_{\psi}E^{-\mu}_{\mu} + {}^{-\kappa}_{\kappa}E^{-\nu}_{\nu}$
$(\pi, 2\pi)$	$(0, \pi)$	M	M_1	${}^{-\zeta}_{\zeta}E^{-\sigma}_{\sigma} + {}^{-\kappa}_{\kappa}E^{-\nu}_{\nu}$
π	$(0, \pi)$	M_3	M_1	${}_{\pi}E^{\bar{\omega}}_{\omega} + {}^{-\kappa}_{\kappa}E^{-\nu}_{\nu}$
		$g, n+g$	M_1	${}_{\pi}A^{+}_{g} + {}_{\pi}A^{-}_{g} + {}^{-\kappa}_{\kappa}E^{-\nu}_{\nu}$ †
		$\pm h$	M_1	${}_{\pi}A^{+}_{h} + {}_{\pi}A^{-}_{h} + {}^{-\kappa}_{\kappa}E^{-\nu}_{\nu}$ ‡
$(0, \pi)$	0	M	M_2	${}^{-\psi}_{\psi}E^{-\mu}_{\mu} + {}_{0}E^{-\tau}_{\tau}$
		M	0	${}^{-\psi}_{\psi}E^{\mu}_{\mu} + {}_{0}A^{+}_{0} + {}_{0}A^{-}_{0}$
		M	$\pm q$	${}^{-\psi}_{\psi}E^{\mu}_{\mu} + {}_{0}A^{+}_{q} + {}_{0}A^{-}_{q}$ §
$(\pi, 2\pi)$	0	M	M_2	${}^{-\zeta}_{\zeta}E^{-\sigma}_{\sigma} + {}_{0}E^{-\tau}_{\tau}$
		M	0	${}_{-\zeta}^{\zeta}E^{-\sigma}_{\sigma} + {}_{0}A^{+}_{0} + {}_{0}A^{-}_{0}$
		M	$\pm q$	${}_{-\zeta}^{\zeta}E^{-\sigma}_{\sigma} + {}_{0}A^{+}_{q} + {}_{0}A^{-}_{q}$ §

† Only for p even, $g = -\frac{1}{2}p$.
‡ Only for $(n-p)$ even, $h = \frac{1}{2}(n-p)$.
§ Only for n even, $q = \frac{1}{2}n$.

Table 4(a). (continued) and especially for $k=k'=\frac{1}{2}\pi$.

$m+m'$	$m-m'$	${}^{-k}_{k}E^{-m}_{m} \otimes {}^{-k'}_{k'}E^{-m'}_{m'}$
M_3	M_3	${}_{\pi}E^{\bar{\omega}}_{\omega} + {}_{0}E^{-\tau}_{\tau}$
M_3	0	${}_{\pi}E^{\bar{\omega}}_{\omega} + {}_{0}A^{+}_{0} + {}_{0}A^{-}_{0}$
M_3	$\pm q$	${}_{\pi}E^{\bar{\omega}}_{\omega} + {}_{0}A^{+}_{q} + {}_{0}A^{-}_{q}$ (only for n even)
$g, n+g$	M_3	${}_{\pi}A^{+}_{g} + {}_{\pi}A^{-}_{g} + {}_{0}E^{-\tau}_{\tau}$ (p even)
$g, n+g$	0	${}_{\pi}A^{+}_{g} + {}_{\pi}A^{-}_{g} + {}_{0}A^{+}_{0} + {}_{0}A^{-}_{0}$ ($\frac{1}{2}p$ even)
$g, n+g$	$\pm q$	${}_{\pi}A^{+}_{g} + {}_{\pi}A^{-}_{g} + {}_{0}A^{+}_{q} + {}_{0}A^{-}_{q}$ (n, p even)
$\pm h$	M_3	${}_{\pi}A^{+}_{h} + {}_{\pi}A^{-}_{h} + {}_{0}E^{-\tau}_{\tau}$ ($n-p$ even)
$\pm h$	0	${}_{\pi}A^{+}_{h} + {}_{\pi}A^{-}_{h} + {}_{0}A^{+}_{0} + {}_{0}A^{-}_{0}$ ($\frac{1}{2}(n-p)$ even)
$\pm h$	$\pm q$	${}_{\pi}A^{+}_{h} + {}_{\pi}A^{-}_{h} + {}_{0}A^{+}_{q} + {}_{0}A^{-}_{q}$ ($\frac{1}{2}n, \frac{1}{2}p$ even)

Here $q=\frac{1}{2}n$, $g=-\frac{1}{2}p$, $h=\frac{1}{2}(n-p)$, $M=[-n+1, n]$, $M_1=M\backslash\{n\}$, $M_2=M\backslash\{-\frac{1}{2}n, \frac{1}{2}n, n\}$, $M_3=M\backslash\{-\frac{1}{2}p, \frac{1}{2}(p-n), \frac{1}{2}(n-p), \frac{1}{2}(2n-p)\}$, $\psi=k+k'$, $\zeta=2\pi-k-k'$, $\kappa=k-k'$.

$$\mu=\begin{cases} m+m'+n, & \text{if } m+m'\in[1-n, -\frac{1}{2}n] \\ m+m', & \text{if } m+m\in[\frac{1}{2}(1-n), \frac{1}{2}n] \\ m+m'-n, & \text{if } m+m'\in[\frac{1}{2}(n+1), n] \end{cases}$$

$$\sigma=\begin{cases} -n-m-m'-p, & \text{if } m+m'\in[1-n, -\frac{1}{2}(n+2p)] \\ & \quad\text{(only for } p\leqslant\frac{1}{2}(n-2)) \\ -m-m'-p, & \text{if } m+m'\in[\frac{1}{2}(1-n-2p), \frac{1}{2}(n-2p)] \\ n-m-m'-p, & \text{if } m+m'\in[\frac{1}{2}(n-2p+1), \frac{1}{2}(3n-2p)] \\ 2n-m-m'-p, & \text{if } m+m'\in[\frac{1}{2}(3n-2p+1), n] \\ & \quad\text{(only for } p\geqslant\frac{1}{2}(n+1)) \end{cases}$$

$$\omega=\begin{cases} m+m'+n, & \text{if } m+m'\in[1-n, -\frac{1}{2}(n+p+1)] \\ -p-m-m', & \text{if } m+m'\in[\frac{1}{2}(1-n-p), -\frac{1}{2}(p+1)] \\ m+m', & \text{if } m+m'\in[\frac{1}{2}(1-p), \frac{1}{2}(n-p-1)] \\ n-p-m-m', & \text{if } m+m'\in[\frac{1}{2}(n-p+1), \frac{1}{2}(2n-p-1)] \\ m+m'-n, & \text{if } m+m'\in[\frac{1}{2}(2n-p+1), n] \end{cases}$$

$$\nu=\begin{cases} m-m'+n, & \text{if } m-m'\in[1-n, -\frac{1}{2}n] \\ m-m', & \text{if } m-m'\in[\frac{1}{2}(1-n), \frac{1}{2}n] \\ m-m'-n, & \text{if } m-m'\in[\frac{1}{2}(n+1), n-1] \end{cases}$$

$$\tau=\begin{cases} m-m'+n, & \text{if } m-m'\in[1-n, -\frac{1}{2}(n+1)] \\ m'-m, & \text{if } m-m'\in[\frac{1}{2}(1-n), -1] \\ m-m', & \text{if } m-m'\in[1, \frac{1}{2}(n-1)] \\ m'-m+n, & \text{if } m-m'\in[\frac{1}{2}(n+1), n-1] \end{cases}$$

Next, in all the line groups considered here, for $k=0$ and $k=\pi$, the eigenstates with non-chiral m (i.e. with $m=0$ or, if n is even, with $m=\frac{1}{2}n$) have well defined parity with respect to $(U|0)$, say $\eta=+1$ for even states and $\eta=-1$ for odd states. Then $\langle f|v|i\rangle\neq 0$ requires that $\eta_f=\eta_v\eta_i$ and in this sense the parity with respect to $(U|0)$ is conserved, also.

Finally, in addition to spatial (i.e. line-group) symmetry, the standard effective one-electron Hamiltonians utilised in quantum theory of polymers (André 1980, Kèrtesz *et al* 1980, Karpfen 1982) are also invariant with respect to the time reversal θ, and hence one has to consider the extended, grey line groups like $\mathrm{L}^{A}n2 = \mathrm{L}n2 + \theta\mathrm{L}n2$, etc. Fortunately, the reps of line groups isogonal to D_n are all (Božović and Božović 1981) of the Frobenius–Schur type (a), and hence such an extension does not affect the above selection rules. However, more complex Hamiltonians have been proposed also (Calais 1980, Kertèsz *et al* 1976, Kertèsz *et al* 1979), which go beyond the restricted Hartree–Fock description of electron band structures of polymers, and which in principle require the double-valued reps of the line groups to be considered.

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