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Symmetrized Kronecker Squares of Irreducible Representations of Line Groups Isogonal to C_n and C_{nv}

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1. Introduction

Line groups are the spatial symmetry groups of three-dimensional objects periodic along a line. They belong to crystallographic groups, and they were first derived by two celebrated crystallographers. C. Hermann and E. Alexander, over sixty years ago [1]. However, they did not arose much interest until late seventies when quasi-one-dimensional metals and conducting polymers became the subject of intense research by physicists and chemists worldwide. For these physical systems, line groups play the role analogous to that of the point groups, for molecules, and space groups, for crystals. Hence, they were rederived [2] rigorously utilising theory of group extensions [3], as was done earlier for the space groups [4]. The normal-subgroup-chain structure was elucidated, and it was utilized to derive [5] all the irreducible representations (ireps) of all the line groups, by the Mackey induction method [6]. Certain selection rules have also been derived [7] by decomposing the Kronecker products of these ireps. Finally, line groups and their ireps found many applications in the Quantum Theory of Polymers, including construction of symmetry adapted bases, symmetrized dynamics equations that provide great numerical savings, labelling the electron and phonon energy bands and identifying their topological character, analysis of vibronic instabilities and identification of the Jahn-Teller active normal modes, phase transitions, etc. [8].

The problem we address here is reduction of the symmetrized Kronecker products of the ireps of line groups. Analogous results have been published already for all the point groups and for some of the space groups and they found applications in the Quantum Chemistry and Solid State Physics [9]. We have used three independent methods to derive and check the entries (the standard character formulae, construction of symmetry-adapted bases, and the direct summation). For brevity, we will omit the details, and refer the reader to standard monographs [6,9]. Instead, we will give a brief summary of the line group notation, and then present the results for all the line groups isogonal to the point groups C_n and C_{nv} in form of tables, to facilitate applications by users whose interest is restricted to testing the selection rules for a particular scattering process.

2. Notations

1D, 2D, 4D : one, two, four-dimensional
L : line group
σ_v : reflection in a vertical mirror plane
A : 1D irep, even with respect to σ_v (if σ_v belongs to L)
B : 1D irep, odd with respect to σ_v
E : 2D irep
G : 4D irep
hk : quasi-momentum
hm : quasi-angular momentum.
For simplicity we choose the units so that $h=1$ and the translation period $a=1$; then

$$-\pi<k<\pi \text{ and } m=\begin{cases} 1,\ 2,\dots,(n-2)/2 & \text{for } n \text{ even} \\ 1,\ 2,\dots,(n-1)/2 & \text{for } n \text{ odd.} \end{cases}$$

SKS : symmetrized Kronecker square
$[D^2]$: *SKS* of the irep **D**.

3. Tables of the symmetrized Kronecker squares of all the irreducible representations of the line groups isogonal to C_n and C_{nv}

Table 1. *SKS* of the ireps of the line groups $Ln\,(n=1, 2,\dots)$

D	k	m	$[D^2]$	k'	m'
kAm	$(-\pi, -\pi/2]$	$(-n/2, -n/4]$**	$k'Am'$	$2k+2\pi$	$2m+n$
		$(-n/4, n/4]$			$2m$
		$(n/4, n/2]$*			$2m-n$
	$(-\pi/2, \pi/2]$	$(-n/2, -n/4]$**		$2k$	$2m+n$
		$(-n/4, n/4]$			$2m$
		$(n/4, n/2]$*			$2m-n$
	$(\pi/2, \pi]$	$(-n/2, -n/4]$**		$2k-2\pi$	$2m+n$
		$(-n/4, n/4]$			$2m$
		$(n/4, n/2]$*			$2m-n$

*for $n>1$ only; **for $n>2$ only.

Table 2. *SKS* of ireps of the line groups $Ln_p (p=1, 2, \dots, n\text{-}1)$

D	p	k	m	$[D^2]$	k'	m'
kAm	$[1, n/2)$	$(-\pi, -\pi/2]$	$(-n/2, (2p-n)/4]$	$k'Am'$	$2k+2\pi$	$2m-p+n$
			$((2p-n)/4, (2p+n)/4]$			$2m-p$
			$((2p+n)/4, n/2]$			$2m-p-n$
		$(-\pi/2, \pi/2]$	$(-n/2, -n/4]$		$2k$	$2m+n$
			$(-n/4, n/4]$		$2m$	
			$(n/4, n/2]$		$2m-n$	
		$(\pi/2, \pi]$	$(-n/2, (-2p-n)/4]$		$2k-2\pi$	$2m+p+n$
			$((-2p-n)/4, (n-2p)/4]$		$2m+p$	
			$((n-2p)/4, n/2]$		$2m+p-n$	
	$(n/2, n-1]$	$(-\pi, -\pi/2]$	$(-n/2, (2p-3n)/4]$		$2k+2\pi$	$2m-p+2n$
			$((2p-3n)/4, (2p-n)/4]$		$2m-p+n$	
			$((2p-n)/4, n/2]$		$2m-p$	
		$(-\pi/2, \pi/2]$	$(-n/2, -n/4]$		$2k$	$2m+n$
			$(-n/4, n/4]$		$2m$	
			$(n/4, n/2]$		$2m-n$	
		$(\pi/2, \pi)$	$(-n/2, (n-2p)/4]$		$2k-2\pi$	$2m+p$
			$((n-2p)/4, (3n-2p)/4]$		$2m+p-n$	
			$((3n-2p)/4, n/2]$		$2m+p-2n$	
	$n/2$	$(-\pi, -\pi/2]$	$(-n/2, 0]$	$2k+2\pi$	$2m-p+n$	
			$(0, n/2]$		$2m-p$	
		$(-\pi/2, \pi/2]$	$(-n/2, -n/4]$	$2k$	$2m+n$	
			$(-n/4, n/4]$			$2m$
			$(n/4, n/2]$		$2m=n$	
		$(\pi/2, \pi)$	$(-n/2, 0]$	$2k=2\pi$	$2m+p$	
			$(0, n/2]$		$2m+p-n$	

Table 3. *SKS* of the ireps of the line groups $Lnm (n=1, 2, \dots)$

D	k	m	$[D^2]$	k'	m'
kAo; kBo	$(-\pi, -\pi/2]$	0	$k'Ao$	$2k+2\pi$	0
	$(-\pi/2, \pi/2]$	0		$2k$	0
	$(\pi/2, \pi]$	0		$2k-2\pi$	0
kEm	$(-\pi, -\pi/2]$	$[1, (n-1)/4]$	$k'Ao+k'Em'$	$2k+2\pi$	$2m$
		$[(n+1)/4, (n-1)/2]$			$n-2m$
	$(-\pi/2, \pi/2]$	$[1, (n-1)/4]$		$2k$	$2m$
		$[(n+1)/4, (n-1)/2]$			$n-2m$
	$(\pi/2, \pi]$	$[1, (n-1)/4]$		$2k-2\pi$	$2m$
		$[(n+1)/4, (n-1)/4]$			$n-2m$

Table 4. *SKS* of the ireps of the line groups *Lnmm* ($n=2, 4, \ldots$)

D	k	m	$[D^2]$	k'	m'
kAo; kBo	$(-\pi, -\pi/2]$		$k'Ao$	$2k+2\pi$	
kAq; kBq	$(-\pi/2, \pi/2]$			$2k$	
	$(\pi/2, \pi]$			$2k-2\pi$	
kEm	$(-\pi, -\pi/2]$	$[1, (n-2)/4]$	$k'Ao+k'Em'$	$2k+2\pi$	$2m$
		$[(n+2)/4, (n-2)/2]$			$n-2m$
	$(-\pi/2, \pi/2]$	$[1, (n-2)/4]$		$2k$	$2m$
		$[(n+2)/4, (n-2)/2]$			$n-2m$
	$(\pi/2, \pi]$	$[1, (n-2)/4]$		$2k-2\pi$	$2m$
		$[(n+2)/4, (n-2)/2]$			$n-2m$
	$(-\pi, -\pi/2]$	$n/4$	$k'Ao+k'Aq+k'Bq$	$2k+2\pi$	
	$(-\pi/2, \pi/2]$			$2k$	
	$(\pi/2, \pi]$			$2k-2\pi$	

Table 5. *SKS* of the ireps of the line groups *Lnc* ($n=1, 3, \ldots$)

D	k	m	$[D^2]$	k'	m'
kAo; kBo	$(-\pi, -\pi/2]$	0	$k'Bo$	$2k+2\pi$	0
	$(-\pi/2, \pi/2]$	0	$k'Ao$	$2k$	0
	$(\pi/2, \pi]$	0	$k'Bo$	$2k-2\pi$	0
kEm	$(-\pi, -\pi/2]$	$[1, (n-1)/4]$	$k'Bo+k'Em'$	$2k+2\pi$	$2m$
		$[(n+1)/4, (n-1)/2]$		$n-2m$	
	$(-\pi, -\pi/2]$	$[1, (n-1)/4]$	$k'Ao+k'Em'$	$2k$	$2m$
		$[(n+1)/4, (n-1)/2]$		$n-2m$	
	$(\pi/2, \pi]$	$[1, (n-1)/4]$	$k'Bo+k'Em'$	$2k-2\pi$	$2m$
		$[(n+1)/4, (n-1)/2]$		$n-2m$	

Table 6. *SKS* of the ireps of the line groups $Lncc\,(n=2, 4,\ldots)$

D	k	m	$[D^2]$	k'	m'
kAo; kBo;	$(-\pi, -\pi/2]$		$k'Ao$	$2k+2\pi$	
kAq; kBq	$(-\pi/2, \pi/2]$		$k'Ao$	$2k$	
	$(\pi/2, \pi]$		$k'Bo$	$2k-2\pi$	
kEm	$(-\pi, -\pi/2]$	$[1, (n-1)/4]$	$k'Bo+k'Em'$	$2k+2\pi$	$2m$
		$[(n+1)/4, (n-1)/2]$			$n-2m$
	$(-\pi/2, \pi/2]$	$[1, (n-1)/4]$	$k'Ao+k'Em'$	$2k$	$2m$
		$[(n+1)/4, (n-1)/2]$			$n-2m$
	$(\pi/2, \pi]$	$[1, (n-1)/4]$	$k'Bo+k'Em'$	$2k-2\pi$	$2m$
		$[(n+1)/4, (n-1)/2]$			$n-2m$
	$(-\pi, -\pi/2]$	$n/4$	$k'Bo+k'Aq+k'Bq$	$2k+2\pi$	
	$(-\pi/2, \pi/2]$	$n/4$	$k'Ao+k'Aq+k'Bq$	$2k$	
	$(\pi/2, \pi]$	$n/4$	$k'Bo+k'Aq+k'Bq$	$2k-2\pi$	

Table 7. *SKS* of the ireps of the line groups $L(2q)_q mc\,(q=1, 2,\ldots)$

D	k	m	$[D^2]$	k'	m'
kAo; kBo;	$(-\pi, -\pi/2]$		$k'Aq$	$2k+2\pi$	
kAq; kBq	$(-\pi/2, \pi/2]$		$k'Ao$	$2k$	
	$(\pi/2, \pi]$		$k'Aq$	$2k-2\pi$	
kEm	$(-\pi, -\pi/2]$	$[1, (q-1)/2]$	$k'Aq+k'Em'$	$2k+2\pi$	$q-2m$
		$[(q+1)/2, q-1]$			$2m-q$
	$(-\pi/2, \pi/2]$	$[1, (q-1)/2]$	$k'Ao+k'Em'$	$2k$	$2m$
		$[(q+1)/2, q-1]$			$2q-2m$
	$(\pi/2, \pi]$	$[1, [q-1)/2]$	$k'Aq+k'Em'$	$2k-2\pi$	$q-2m$
		$[(q+1)/2, q-1]$			$2m-q$
	$(-\pi, -\pi/2]$	$q/2$	$k'Ao+k'Bo+k'Aq$	$2k+2\pi$	
	$(-\pi/2, \pi/2]$	$q/2$	$k'Ao+k'Aq+k'Bq$	$2k$	
	$(\pi/2, \pi]$	$q/2$	$k'Ao+k'Bo+k'Aq$	$2k-2\pi$	

4. Discussions

Of principal interest here is to look for the selection rules in the form of conservation laws for the quantum numbers k (the quasi-momentum), m (the quasiangular momentum), and A/B (the mirror-reflection parity). By inspecting the Tables 1 – 7 one can verify that all three quantum numbers are conserved, for all the symmorphic line groups (Ln, $n=1, 2,\ldots$; Lnm, $n=1, 3,\ldots$, and $Lnmm$, $n=2, 4,\ldots$). They are conserved also in the remaining, nonsymmorphic line groups (Ln_p, $n=2, 3,\ldots, p=2,\ldots, n\text{-}1$; Lnc, $n=1, 3,\ldots$, $Lncc$, $n=2, 4,\ldots$, and $L(2q)_q mc$, $q=1, 2,\ldots$), provided that $-\pi/2<k<\pi/2$. The latter condition implies restriction to the so-called 'normal' scattering processes. In the opposite case, one has an 'Umklapp' process, for which we find that $A\rightarrow B$, $B\rightarrow A$ and $m\rightarrow 2m\pm p$ (the sign depending on whether the reciprocal-lattice vector is added or subtracted). Indeed, this non-conservation arises from the fact that the point group C_n is isogonal to the line group L_{n_p}, but it is not (isomorphous to) a subgroup of Ln_p. The same is true for C_{nv} and Ln, $Lncc$ and $L(2q)_q mc$; for more details, see Ref. 7.

References

1. C. Hermann. *Z. Kristallogr.*, **69**, 1928, 250; E. Alexander, ibid, **70**, 1929, 367.
2. M. Vujicic, I. Borovic, F. Herbut. *J. Phys. A. Math. Gen.*, **10**, 1971, 1271.
3. A. G. Kurosh. The Theory of Groups, vol. 1. Chelsea, New York, 1955.
4. E. Ascher, A. Janner. *Helv. Phys. Acta*, **38**, 1965, 551; *Commun. Math. Phys.*, **11**, 1968, 138; J. Mozrzymas, *Rep. Math. Phys.*, **6**, 1974, 29; ibid, **6**, 1974, 83.
5. I. Bozovic, M. Vujicic, F. Herbut. *J. Phys. A. Math. Gen.*, **11**, 1978, 2133; I. Bozovic, M. Vujicic, ibid, **14**, 1981, 777; I. Bozovic, N. Bozovic, ibid, **14**, 1981, 1825.
6. S. L. Altmann. Induced Representations in Crystals and Molecules. Academic, London, 1977.
7. M. Damnjanovic, I. Bozovic, N. Bozovic. *J. Phys. A. Math. Gen.*, **16**, 1983, 3937; ibid, **17**, 1984, 747; ibid, **17**, 1984, 2599; ibid, **18**, 1985, 923.
8. I. Bozovic, J. Delhalle. *Phys. Rev., B*, **29**, 1984, 4733; I. Bozovic, ibid, **29**, 1984, 6586; ibid, **32**, 1985, 8136; ibid, **33**, 1986, 5956; M. Koch, F. F. Seelig. *Int. J. Quant. Chem.*, **32**, 1987, 249.
9. A. P. Cracknell. Group Theory in Solid State Physics. Taylor and Francis, London, 1975; H. W. Streitwolf. Group Theory in Solid State Physics. MacDonald, London, 1971; M. Lax. Symmetry Principles in Solid State and Molecular Physics. Wiley, New York, 1974.

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