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Symmetrized Kronecker Squares of Irreducible Representations of Line Groups Isogonal to C_{nh}, S_{2n} and D_n

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The reduction coefficients for the symmetrized Kroneker products of the unitary irreducible representations (ireps) are derived for all the line groups isogonal to the point groups $\mathbf{C}_{nh}$, $\mathbf{S}_{2n}$ and $\mathbf{D}_n$ $(n = 1, 2, \ldots)$, respectively.

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1. Introduction

Line groups are the spatial symmetry groups of three-dimensional objects periodic along a line ([1]). They are also subgroups of the full Euclidean group that leave one line invariant. Other than pure mathematical interest, these groups have been studied in the context of Quantuum Physics of quasi-one-dimensional metals and conducting polymers. For these physical systems, line groups play the role analogous to that of the point groups in Quantuum Chemistry, and crystallographic space groups in Solid State Physics.

Line groups can be derived ([2]) by utilizing theory of group extensions ([3]), in analogous way as it was done for the space groups ([4–7]). Using the normal-subgroup-chain structure, it is also possible to derive their unitary irreducible representations (ireps) ([8–10]) by the Mackey induction method ([11]).

In this paper, we report the reduction coefficients of the symmetrized Kronecker products of the ireps of line groups isogonal to the point groups $\mathbf{C}_{nh}$, $\mathbf{S}_{2n}$, and $\mathbf{D}_n$, where $n = 1, 2, \ldots$. These ceofficients play the key role in determining the selection rules for various physical processess in polymer molecules and quasi-one-dimensional solids. Analogous results have been published already for all the point groups and for some of the crystallographic space groups, and they have been utilized extensively by the quantuum chemicists and solid state physicists, [12–14]. More details can be found in [1].

As in [1], we have utilized three independent methods to derive and check the entries: the standard character formulae, construction of symmetry-adapted bases, and the direct summation *a posteriory*.

For the sake of the readers whose interest is restricted to utilizing the selection rules, in Section 2 we have enclosed a brief summary of the line-group-theoretical notation, and then have presented the results in form of tables, one for each family of the line groups under study, in Section 3. The duscussion of the physical interpretation of the results is given separately, in Section 4.

2. Notations

L : line group
SKS : symmetrized Kronecker square
$[D^2]$: SKS of the irep D
$1D$: one-dimensional
$2D$: two-dimensional
σ_H : reflection in a horizontal mirror plane
U : rotation by π around a horizontal axis
$A+$: $1D$ irep, even with respect to σ_H (if σ_H belongs to L) or U (if U belongs to L)
$A-$: $1D$ irep, odd with respect to σ_H or U
E : $2D$ irep
k : quasi-momentum
m : quasi-angular momentum

We choose the units so that $h/2\pi = 1$ and the translation period $a = 1$; then $-\pi < k < \pi$ and $m = 1, 2, \ldots, (n-2)/2$ for n even, and $m = 1, 2, \ldots, (n-1)/2$ for n odd.

3. Tables of SKS of the ireps of line groups isogonal to C_{hn}, S_{2n} and D_n

Table 1. SKS of the ireps of the line groups Ln/m, n = 1, 2, ...

D	k	m	[D²]	k'	m'
(oAm±)	0	(-n/2, -n/4]	(oAm'+)	0	2m+n
	0	(-n/4, n/4]	“	0	2m
	0	(n/4, n/2]	“	0	2m-n
(kEm)	(0,π/2)	(-n/2, -n/4]	(oAm'+)+(k'Em')	2k	2m+n
	(0,π/2)	(-n/4, n/4]	“	2k	2m
	(0,π/2)	(n/4, n/2]	“	2k	2m-n
	(π/2,π)	(-n/2, -n/4]	“	2π-2k	2m+n
	(π/2,π)	(-n/4, n/4]	“	2π-2k	2m
	(π/2,π)	(n/4, n/2]	“	2π-2k	2m-n
	π/2	(-n/2, -n/4]	(oAm'+)+(πAm'+)+(πAm'-)	2π-2k	2m+n
	π/2	(-n/4, n/4]	“	2π-2k	2m
	π/2	(n/4, n/2]	“	2π-2k	2m-n
(πAm±)	π	(-n/2, -n/4]	(oAm'+)	0	2m+n
	π	(-n/4, n/4]	“	0	2m
	π	(n/4, n/2]	“	0	2m-n

Table 2. SKS of the ireps of the line groups $L(2q)_q/m$, q= 1, 2, ...

D	k	m	$[D^2]$	k'	m'
(oAm±)	0	[-q+1, -q/2]	(oAm'+)	0	2m+2q
	0	[(-q+1)/2, q/2]	"	0	2m
	0	[(q+1)/2, q]	"	0	2m-2q
(kEm)	(0, π/2)	[-q+1, -q/2]	(oAm'+) + (k'Em')	2k	2m+2q
	(0, π/2)	[(-q+1)/2, q/2]	"	2k	2m
	(0, π/2)	[(q+1)/2, q]	"	2k	2m-2q
	(π/2, π)	[-q+1, 0]	"	2π-2k	2m+q
	(π/2, π)	[1, q]	"	2π-2k	2m-q
	π/2	[-q+1, -q/2]	(oAm'+)+(πEm')	2π-2k	2m+2q
	π/2	[(-q+1)/2, q/2]	"	2π-2k	2m
	π/2	[(q+1)/2, q]	"	2π-2k	2m-2q
(πEm)	π	[-q+1, -q/2]	(oA[2m+2q]+)+(oAm'+)+(oAm'-)	0	2m+q
	π	[(-q+1)/2, 0]	(oA2m+)+(oAm'+)+(oAm'-)	0	2m+q
	π	[1, q/2]	(oA2m+)+(oAm'+)+(oAm'-)	0	2m-q
	π	[(q+1)/2, q]	(oA[2m-2q]-)+(oAm'+)+(oAm'-)	0	2m-q

Table 3. SKS of the ireps of the line groups Lν, n= 1, 3, …and L(2ν), n= 2, 4, …

D	k	m	$[D^2]$	k'	m'
(oAm±)	0	(-n/2, -n/4]	(oAm'-)	0	2m+n
	0	(-n/4, n/4]	(oAm'+)	0	2m
	0	(n/4, n/2]	(oAm'-)	0	2m-n
(kEm)	(0,π/2)	(-n/4, n/4]	(oAm'+)+(k'Em')	2k	2m
	(π/2,π)	(-n/2, -n/4]	(oAm'-)+(k'Em')	2π-2k	2m+n
	(π/2,π)	(n/4, n/2]	"	2π-2k	2m-n
	π/2	(-n/2, -n/4]	(oAm'-)+(πAm'+)+(πAm'-)	2π-2k	2m+n
	π/2	(-n/4, n/4]	(oAm'+)+(πAm'+)+(πAm'-)	2π-2k	2m
	π/2	(n/4, n/2]	(oAm'-)+(πAm'+)+(πAm'-)	2π-2k	2m-n
(πAm±)	0	(-n/2, -n/4]	(oAm'-)	0	2m+n
	0	(-n/4, n/4]	(oAm'+)	0	2m
	0	(n/4, n/2]	(oAm'-)	0	2m-n

Table 4. SKS of the ireps of the line groups Ln2, n = 1, 3, ...

D	k	m	$[D^2]$	k'	m'
(oAo±)	0	0	(oAo+)	0	0
(oEm)	0	[1, (n-1)/4]	(oAo+)+(oEm')	0	2m
	0	[(n+1)/4, (n-1)/2]	"	0	n-2m
(kEm)	(0,π/2)	[-(n-1)/2, (-n-1)/4]	(oAo+)+(k'Em')	2k	2m+n
	(0,π/2)	[(-n+1)/4, (n-1)/4]	"	2k	2m
	(0,π/2)	[(n+1)/4, (n-1)/2]	"	2k	2m-n
	(π/2,π)	[-(n-1)/2, (-n-1)/4]	"	2π-2k	-2m-n
	(π/2,π)	[(-n+1)/4, (n-1)/4]	"	2π-2k	-2m
	(π/2,π)	[(n+1)/4, (n-1)/2]	"	2π-2k	-2m+n
	π/2	0	(oAo+)+(πAo+)+(πAo-)	0	0
	π/2	[-(n-1)/2, (-n-1)/4]	(oAo+)+(πEm')	0	2m+n
	π/2	[(-n+1)/4, -1]	"	0	-2m
	π/2	[1, (n-1)/4]	"	0	2m
	π/2	[(n+1)/4, (n-1)/2]	"	0	-2m+n
(πAo±)	0	0	(oAo+)	0	0
(πEm)	0	[1, (n-1)/4]	(oAo+)+(oEm')	0	2m
	0	[(n+1)/4, (n-1)/2]	"	0	n-2m

Table 5. SKS of the ireps of the line groups Ln22, n = 2q = 2, 4, ...

D	k	m	$[D^2]$	k'	m'
(oAo±)	0	0	(oAo+)	0	0
(oEm)	0	[1, (n-2)/4]	(oAo+)+(oEm')	0	2m
		[(n+2)/4, (n-2)/2]	"	0	n-2m
	0	n/4	(oAo+)+(oAq+)+(oAq-)	0	0
(oAq±)	0	0	(oAo+)	0	0
(kEm)	(0,π/2)	[(-n+2)/2, -n/4]	(oAo+)+(k'Em')	2k	2m+n
	(0,π/2)	[(-n+2)/4, n/4]	"	2k	2m
	(0,π/2)	[(n+2)/4, n/2]	"	2k	2m-n
	(π/2,π)	[(-n+2)/2, (-n-2)/4]	"	2π-2k	-2m-n
	(π/2,π)	[-n/4, (n-2)/4]	"	2π-2k	-2m
	(π/2,π)	[n/4, n/2]	"	2π-2k	-2m+n
	π/2	[(-n+2)/2, (-n-2)/4]	(oAo+)+(πEm')	0	2m+n
	π/2	[(-n+2)/4, -1]	"	0	-2m
	π/2	[1, (n-2)/4]	"	0	2m
	π/2	[(n+2)/4, (n-1)/2]	"	0	-2m+n
	π/2	0	(oAo+)+(πAo+)+(πAo-)	0	0
	π/2	n/2	"	0	0
	π/2	±n/4	(oAo+)+(πAq+)+(πAq-)	0	0
(πAo±)	0	0	(oAo+)	0	0
(πAq±)	0	0	(oAo+)	0	0
(πEm)	0	[1, (n-2)/4]	(oAo+)+(oEm')	0	2m
	0	[(n+2)/4, (n-2)/2]	"	0	n-2m
	0	n/4	(oAo+)+(oAq+)+(oAq-)	0	0

Table 6. SKS of the ireps of the line groups Ln_p2, n = 1, 3, ..., p = 1, 2, ..., n-1.

D	k	m	$[D^2]$	k'	m'
(oAo±)	0	0	(oAo+)	0	0
(oEm)	0	[1, (n-1)/4]	(oAo+)+(oEm')	0	2m
	0	[(n+1)/4, (n-1)/2]	"	0	n-2m
(kEm)	*	*see Table 6.a	(oAo+)+(k'Em') *see Table 6.a	*	*
	π/2	-p/4, for p even	(oAo+)+(πA-p/2+)+(πA-p/2-)	0	-p/2
	π/2	(2n-p)/4, for p even	"		-p/2
	π/2	(-n-p)/4	(oAo+)+(πA[n-p]/2+)+(πA[n-p]/2-)	0	0
	π/2	(n-p)/4	"	0	0
	π/2	[(-n+1)/2, (-n-p)/4)	(oAo+)+(πEm')	0	2m+n
	π/2	((-n-p)/4, -p/4)	"	0	-2m-p
	π/2	(-p/4, (n-p)/4)	"	0	2m
	π/2	((n-p)/4, (2n-p)/4)	"	0	n-2m-p
	π/2	((2n-p)/4, (n-1)/2]	"	0	2m-n
(πA-p/2±)	0	0	(oAo+)	0	0
(πA[n-p]/2±)	0	0	(oAo+)	0	0
(πEm)	0	[(-p+1)/2, (n-2p-1)/4]	(oAo+)+(oEm')	0	2m+p
	0	[(n-2p+1)/4, (n-p-1)/2]	"	0	n-2m-p

Table 7. SKS of the ireps of the line groups Ln_p22, n = 2, 4, ..., p = 1, 2, ..., n-1.

D	k	m	$[D^2]$	k'	m'
(oAo±)	0	0	(oAo+)	0	0
(oAq±)	0	0	(oAo+)	0	0
(oEm)	0	[1, (n-1)/4]	(oAo+)+(oEm')	0	2m
	0	[(n+1)/4, (n-2)/2]	"	0	n-2m
	0	n/4	(oAo+)+(oAq+)+(oAq-)	0	0
(kEm)	**	**see Table 7.a	(oAo+)+(k'Em') **see Table 7.a	**	**
	π/2	-p/4	(oAo+)+(πA-p/2+)+(πA-p/2-)	0	0
	π/2	(2n-p)/4	"	0	0
	π/2	(-n-p)/4	(oAo+)+(πA[n-p]/2+)+(πA[n-p]/2-)	0	0
	π/2	(n-p)/4	"	0	0
	π/2	[(-n+2)/2, (-n-p)/4)	(oAo+)+(πEm')	0	2m+n
	π/2	((-n-p)/4, -p/4)	"	0	-2m-p
	π/2	(-p/4, (n-p)/4)	"	0	2m
	π/2	((n-p)/4, (2n-p)/4)	"	0	n-2m-p
	π/2	((2n-p)/4, n/2]	"	0	2m-n
(πA-p/2±)	0	0	(oAo+)	0	0
(πA[n-p]/2±)	0	0	(oAo+)	0	0
(πEm)	0	[(-p+1)/2, (n-2p-2)/4]	(oAo+)+(oEm')	0	2m+p
	0	[(n-2p+2)/4, (n-p-1)/2]	"	0	n-2m-p
	0	(n-2p)/4	(oAo+)+(oAq+)+(oAq-)	0	0

***Table 6.a**

k	m	p	k'	m'
(0,π/2)	[(-n+1)/2, (-n-1)/4]	[1, n-1]	2k	2m+n
(0,π/2)	[(-n+1)/4, (n-1)/4]	[1, n-1]	2k	2m
(0,π/2)	[(n+1)/4, (n-1)/2]	[1, n-1]	2k	2m-n
(π/2,π)	[(-n+1)/2, (-n-2p-1)/4]	[1, (n-3)/2]	2p-2k	-n-2m-p
(π/2,π)	[-(n-2p+1)/4, (n-2p-1)/4]	[1, (n-1)/2]	2p-2k	-2m-p
(π/2,π)	[(-n+1)/2, (n-2p-1)/4]	[(n-1)/2, n-1]	2p-2k	-2m-p
(π/2,π)	[(n-2p+1)/4, (n-1)/2]	[1, (n+1)/2]	2p-2k	n-2m-p
(π/2,π)	[(n-2p+1)/4, (3n-2p-1)/4]	[(n+1)/2, n-1]	2p-2k	n-2m-p
(π/2,π)	[(3n-2p+1)/4, (n-1)/2]	[(n+3)/2, n-1]	2p-2k	2n-2m-p

****Table 7.a**

k	m	p	k'	m'
(0, π/2)	[(-n+2)/2, -n/4]	[1, n-1]	2k	2m+n
(0, π/2)	[(-n+2)/4, n/4]	[1, n-1]	2k	2m
(0, π/2)	[(n+2)/4, n/2]	[1, n-1]	2k	2m-n
(π/2, π)	[(-n+2)/2, (-n-2p-2)/4]	[1, (n-6)/2]	2π-2k	-n-2m-p
(π/2, π)	[(-n-2p)/4, n-2p-2)/4]	[1, (n-4)/2]	2π-2k	-2m-p
(π/2, π)	[(-n+2)/2, (n-2p-2)/4]	[(n-4)/2, n-1]	2π-2k	-2m-p
(π/2, π)	[(n-2p)/4, n/2]	[1, (n-2)/2]	2π-2k	n-2m-p
(π/2, π)	[(n-2p)/4, (3n-2p-2)/4]	[(n-2)/2, n-1]	2π-2k	n-2m-p
(π/2,π)	[(3n-2p)/4, n/2]	[n/2, n-1]	2π-2k	2n-2m-p

4. Discussions

The main goal here is to deduce the selection rules in the form of conservation laws for the relevent line-group theoretical quantuum numbers: k (the quasi-momentum), m (the quasi-angular momentum) and $\pm$ (the parity with respect to the reflection in σ_H, the horizontal mirror plane, or U, the horizontal rotation by π).

Starting from the quasi-momentum, we can see that it is conserved in all cases. If the initial state has the quasi-momentum k and the final state has $-k$, the perturbation must have $-2k$. In the case that $\pm 2k$ sticks outside the first Brillouin zone, an "Umklapp" happens, the reduced quasi-momentum of the perturbation is $2k \pm 2\pi$.

The quasi-angular momentum m is also conserved in the cases when the generating rotation $(Cn|0)$ belongs to the line group. This is the case in all the symmorphic line groups, viz. the groups $\mathbf{L}n/m$, $n = 1, 2, \ldots$; $\mathbf{L}\bar{n}$, $n = 1, 2, \ldots$; and $\mathbf{L}n22$, $n = 2, 4, \ldots$. Since the order of the rotation subgroups is finite, n, one has that $m \hat{=} m(\text{mod } n)$. In the present case, this allows that $m' = 2m \pm n$.

In the remaining, non-symmorphic line groups, viz. $\mathbf{L}(2q)_q/m$, $q = 1, 2, \ldots$; $\mathbf{L}n_p2$, $n = 1, 3, \ldots$, and $p = 1, 2, \ldots, n-1$; $\mathbf{L}n_p22$, $n = 2, 4, \ldots,$, $p = 1, 2, \ldots, n-1$; the rotations are coupled with fractional translations. The corresponding group generators are $(C_{2q}|1/2)$ and $(C_n|p/n)$, respectively. For this reason, the above equivalence changes into $m \hat{=} m(\text{mod } n - p)$. Therefore, we get $m' = 2m \pm q$, $2m \pm 2q$ and $m' = 2m \pm (n - p)$, respectively.

Finally, the parity with respect to σ_H is preserved without exceptions in all the line groups isogonal to $\mathbf{C}_{nh}$, since each of these contains $(\sigma_H|0)$. The symmetrized Kronecker squares thus must be even with respect to σ_H. This is a very strong restriction: in this case, only even perturbations can cause strong (first-order) scattering.

The situation is analogous in al the line groups isogonal to $\mathbf{D}_n$, since each of these contains $(U|0)$. Here, all the allowed perturbations must be even with respect to U.

The line group isogonal to $\mathbf{S}_{2n}$ depart from this general pattern, because in this case the rotations and reflections are coupled; the group generators include $(S_{2n}|0)$, where $S_{2n} = \sigma_H C_{2n}$. For this reason, whenever the quasi-angular momentum undergroes an "Umklapp", i.e., a jump by n, the parity is reversed. In other words, odd perturbations are allowed for m larger than $n/4$, while even ones are allowed for smaller values of m.

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