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1990 J. Phys. A: Math. Gen. 23 2775

(http://iopscience.iop.org/0305-4470/23/13/016)

J. Phys. A: Math. Gen. **23** (1990) 2775–2786. Printed in the UK

Selection rules for vibronic coupling in quasi-one-dimensional solids: II. Helical chains

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Received 1 August 1989, in final form 27 February 1990

Abstract. To identify the Peierls-active modes in conducting polymers and quasi-one-dimensional metals, selection rules for linear vibronic-coupling matrix elements are derived. The symmetrised Kronecker squares of irreducible corepresentations are decomposed into their irreducible constituents, for all the line groups containing a screw axis.

1. Introduction

Study of topological effects of reduced dimensionality has been one of the focal topics in solid state physics in the last decade (Miller 1982, Monceau 1985, Kamimura 1985, Kuzmany *et al* 1985, Skotheim 1986). Vibronic instabilities in quasi-one-dimensional (Q1D) systems are a paramount example of such an effect. As a part of our systematic study of interplay of topology and symmetry in such systems, in the earlier paper (Božović and Božović 1989, hereafter referred to as I) we have determined the selection rules for vibronic coupling for all Q1D solids that can be viewed as eclipsed molecular stacks. In more technical terms (Cracknell 1975), that amounts to decomposing into irreducible components the symmetrised Kronecker square of each corepresentation of each symmorphic line groups; these are $Ln (n = 1, 2, \ldots)$; Lnm, Ln/m, $L\bar{n}$, $Ln2$, $L\bar{n}m$ and $L(\overline{2n})2m$ $(n = 1, 3, \ldots)$ and $Lnmm$, $L(\overline{2n})$, $Ln22$, $L(\overline{2n})2m$ and Ln/mmm $(n = 2, 4, \ldots)$. Here we proceed by dealing with all the line groups that contain a screw axis, i.e. the groups Ln_p $(n = 1, 2, \ldots;\ p = 1, \ldots, n-1)$, isogonal to the point group C_n; Ln_p2 $(n = 1, 3, \ldots;\ p = 1, \ldots, n-1)$ and Ln_p22 $(n = 2, 4, \ldots;\ p = 1, \ldots, n-1)$ isogonal to D_n, $L(2q)_qmc$ $(q = 1, 2, \ldots)$ isogonal to C_{nv}, $L(2q)_q/m$ $(q = 1, 2, \ldots)$ isogonal to C_{nh} and $L(2q)_q/mcm$ $(q = 1, 2, \ldots)$ isogonal to D_{nh}. This class of solids is broad and it includes many materials that have attracted substantial attention recently, e.g. platinum tetracyanates such as $K_2Pt(CN)_4$ and transition metal tetrachalcogenides such as $TaTe_4$, both of which have $L8_4/mcm$ line group symmetry; beryllium hydride $(BeH_2)_x$ which has $L4_2/mcm$; tetrathiatetracene and tetraselenatracene stacks which have $L2_1/mcm$; polysulphurnitride $(SN)_x$ which has $L2_1mc$, and indeed a host of natural and synthetic stereoregular polymers, which in most cases assume one or more helical conformations. Indeed, of particular interest here are those among them which are metallic, or which can be doped to become metallic; in that case vibronic instabilities are indeed expected to occur (Peierls 1955). The tables presented in section 2 enable one to determine all the vibronically active modes of such a system, i.e. all the normal modes Q for which the linear electron–phonon coupling matrix element $\langle e|Q\cdot(\partial V/\partial Q)_0|e'\rangle$ (where $|e\rangle$, $|e'\rangle$ are the degenerate one-electron states at the Fermi level and V is the effective one-electron potential) does not vanish identically. In section 3 we give a couple of examples illustrating this procedure in detail. For the reader's convenience, we also briefly review the line group notation below, and give the character tables of all inequivalent irreducible corepresentations of the line groups under study in the appendix.

A(B): one-dimensional irreducible representation, irrep, of a line group L, even (odd) with respect to the vertical mirror plane;

E: a two-dimensional irrep of L;

G: a four-dimensional irrep of L;

(D, D*): a pair of complex-conjugate irreps, a corepresentation of L;

$\hbar k$: quasi-momentum; we choose $\hbar=1$ and the translation period $a=1$ so that $0<k<\pi$;

$\hbar m$: quasi-angular momentum; $m=1,2,\ldots,(n-2)/2$ for n even and $m=1,2,\ldots,(n-1)/2$ for n odd, where n is the order of the screw axis.

In the tables we also utilise the following abbreviations:

$$r=2k \qquad t=2\pi-2k \qquad w=2m \qquad v=2m-n.$$

2. Tables of irreducible components of the symmetrised Kronecker squares of corepresentations of all the line groups that contain a screw axis

Table 1. Symmetrised Kronecker squares (SKS) of corepresentations of the line groups Ln_p $(n=1,2,\ldots;\ p=1,2,\ldots,n-1)$.

D			$[D^2]-(0A0)$
$(0Am, 0A-m)$		$m<n/4$	$(0Aw, 0A-w)$
		$m=n/4$†	$2(0Aq)$
		$m>n/4$	$(0Av, 0A-v)$
$(kA0, -kA0)$	$k<\pi/2$		$(rA0, -rA0)$
	$k=\pi/2$		$(\pi A0, \pi A-p)$
	$k>\pi/2$		$(tA-p, -tA-p)$
$(kAm, -kA-m)$	$k<\pi/2$	$m<n/4$	$(rAw, -rA-w)$
		$m=n/4$†	$(rAq, -rAq)$
		$m>n/4$	$(rA-v, -rAv)$
	$k=\pi/2$	$m<n/4$	$(\pi Aw, \pi A\bar{w})$‡
		$m=n/4$†	$(\pi Aq, \pi Aq-p)$
		$m>n/4$	$(\pi Av, \pi A\bar{v})$§
	$k>\pi/2$	$m<n/4$	$(tA-w, -tAw)$
		$m=n/4$†	$(tAq, -tAq)$
		$m>n/4$	$(tAv, -tA-v)$
$(kA-m, -kAm)$	$k<\pi/2$	$m<n/4$	$(rA-w, -rAw)$
		$m=n/4$†	$(rAq, -rAq)$
		$m>n/4$	$(rAv, -rA-v)$
	$k=\pi/2$	$m<n/4$	$(\pi Aw, \pi A\bar{w})$‡
		$m=n/4$†	$(\pi Aq, \pi Aq-p)$
		$m>n/4$	$(\pi Av, \pi A\bar{v})$§
	$k>\pi/2$	$m<n/4$	$(tAw, -tA-w)$
		$m=n/4$†	$(tAq, -tAq)$
		$m>n/4$	$(tA-v, -tAv)$

Table 1. (continued)

D			$[D^2]-(0A0)$
$(kAq, -kAq)$‖	$k<\pi/2$		$(rA0, -rA0)$
	$k=\pi/2$		$(\pi A0, \pi A-p)$
	$k>\pi/2$		$(tA0, -tA0)$
$(\pi Am, \pi A\bar{m})$		$m>n/4$	$(0Aw, 0A-w)$
		$m=n/4$†	$2(0Aq)$
		$m>n/4$	$(0Av, 0A-v)$

† Only for $n=2q=4, 8, \ldots$.
‡ $2(\pi Aw)$, for $w=-p/2$ or $w=(n-p)/2$; $\bar{w}=w-q$.
§ $2(\pi Av)$, for $v=-p/2$ or $v=(n-p)/2$; $\bar{v}=v-q$.
‖ Only for $n=2q=2, 4, \ldots$.

Table 2. SKS of corepresentations of the line groups Ln_p2 $(n=1, 3, \ldots)$ and Ln_p22 $(n=2, 4, \ldots)$.

D			$[D^2]-(0A0)$
$(0Em)$		$m<n/4$	$(0Ew)$
		$m=n/4$†	$(0Aq+)+(0Aq-)$
		$m>n/4$	$(0Ev)$
$(kE0)$	$k<\pi/2$		$(rE0)$
	$k=\pi/2$		$(\pi E0)$
	$k>\pi/2$		$(tE0)$
(kEm)	$k<\pi/2$	$m\leqslant n/4$	(rEw)
		$m>n/4$	(rEv)
	$k=\pi/2$	$m\leqslant n/4$	(πEw)‡
		$m>n/4$	(πEv)§
	$k>\pi/2$	$m\leqslant n/4$	(tEw)
		$m>n/4$	(tEv)
(kEq)‖	$k<\pi/2$		$(rE0)$
	$k=\pi/2$		$(\pi E0)$
	$k>\pi/2$		$(tE0)$
(πEm)		$m<n/4$	$(0Ew)$
		$m=n/4$†	$(0Aq+)+(0Aq-)$
		$m>n/4$	$(0Ev)$

† Only for $n=2q=4, 8, \ldots$.
‡ $(\pi Aw+)+(\pi Aw-)$ if $w=-p/2$ or $w=(n-p)/2$.
§ $(\pi Av+)+(\pi Av-)$ if $v=-p/2$ or $v=(n-p)/2$.
‖ Only for $n=2q=2, 4, \ldots$.

Table 3. SKS of corepresentations of the line groups $L(2q)_q mc$ ($q = 1, 2, \ldots$).

D			$[D^2] - (0A0)$
$(0Em)$		$m < q/2$	$(0Ew)$
		$m = q/2$†	$(0Aq) + (0Bq)$
		$m > q/2$	$(0Ev)$
$(kA0, -kA0)$	$k < \pi/2$		$(rA0, -rA0)$
	$k = \pi/2$		$(\pi A0, \pi Aq)$
	$k > \pi/2$		$(tAq, -tAq)$
$(kB0, -kB0)$	$k < \pi/2$		$(rA0, -rA0)$
	$k = \pi/2$		$(\pi A0, \pi Aq)$
	$k > \pi/2$		$(tA0, -tAq)$
$(kEm, -kEm)$	$k < \pi/2$	$m < q/2$	$(rEw, -rEw) + (rA0, -rA0) + (0Ew) + (0B0)$
		$m = q/2$†	$(rAq, -rAq) + (rBq, -rBq) + (rA0, -rA0)$ $+ (0Aq) + (0Bq) + (0B0)$
		$m > q/2$	$(rEv, -rEv) + (rA0, -rA0) + (0Ev) + (0B0)$
	$k = \pi/2$	$m < q/2$	$(\pi Ew, \pi E\bar{w})$‡ $+ (\pi A0, \pi Aq) + (0Ew) + (0B0)$
		$m = q/2$†	$2(\pi A0, \pi Aq) + (\pi B0, \pi Bq) + (0Aq) + (0Bq) + (0B0)$
		$m > q/2$	$(\pi Ev, \pi E\bar{v})$§ $+ (\pi A0, \pi Aq) + (0Ev) + (0B0)$
	$k > \pi/2$	$m < q/2$	$(tEw, -tEw) + (tAq, -tAq) + (0Ew) + (0B0)$
		$m = q/2$†	$(tAq, -tAq) + (tA0, -tA0) + (tB0, -tB0) + (0Aq) + (0B0)$
		$m > q/2$	$(tEv, -tEv) + (tAq, -tAq) + (0Ev) + (0B0)$
$(kAq, -kAq)$	$k < \pi/2$		$(rA0, -rA0)$
	$k = \pi/2$		$(\pi A0, \pi Aq)$
	$k > \pi/2$		$(tAq, -tAq)$
$(kBq, -kBq)$	$k < \pi/2$		$(rA0, -rA0)$
	$k = \pi/2$		$(\pi A0, \pi Aq)$
	$k > \pi/2$		$(tAq, -tAq)$
$(\pi A0, \pi Aq)$			$2(0Aq)$
$(\pi B0, \pi Bq)$			$2(0Aq)$
$(\pi Em, \pi E\bar{m})$		$m < q/2$	$2(0Ew) + (0E\bar{w}) + 2(0Aq) + (0B0)$
$(\pi Eq/2)$			$(0Aq) + (0B0)$

† Only for $q = 2, 4, \ldots$.

‡ $2(\pi Ew)$ for $w = q/2$.

§ $2(\pi Ev)$ for $v = q/2$; $\bar{w} = w - q$; $\bar{v} = v - q$.

Table 4. SKS of corepresentations of the line groups $L(2q)_q/m$ $(q = 1, 2, \ldots)$.

D			$[D^2] - (0A0+)$
$(0Am\pm, 0A-m\pm)$		$m < q/2$	$(0Aw+, 0A-w+)$
		$m = q/2$†	$2(0Aq+)$
		$m > q/2$	$(0Av+, 0A-v+)$
$(kE0)$	$k < \pi/2$		$(rE0)$
	$k = \pi/2$		$(\pi E0)$
	$k > \pi/2$		$(tE0)$
$(kEm, kE-m)$	$k < \pi/2$	$m < q/2$	$(rEw, rE-w) + (rE0) + (0Aw+, 0A-w+) + (0A0-)$
		$m = q/2$†	$2(rEq) + (rE0) + 2(0Aq+) + (0A0-)$
		$m > q/2$	$(rEv, rE-v) + (rE0) + (0Av+, 0A-v+) + (0A0-)$
	$k = \pi/2$	$m < q/2$	$(\pi Ew, \pi E\bar{w})$‡ $+ (\pi E0) + (0Aw+, 0A-w+) + (0A0-)$
		$m = q/2$†	$3(\pi E0) + 2(0Aq+) + (0A0-)$
		$m > q/2$	$(\pi Ev, \pi E\bar{v})$§ $+ (\pi E0) + (0Av+, 0A-v+) + (0A0-)$
	$k > \pi/2$	$m < q/2$	$(tEw, tE-w) + (tE0) + (0Aw+, 0A-w+) + (0A0-)$
		$m = q/2$†	$2(tEq) + (tE0) + 2(0Aq+) + (0A0-)$
		$m > q/2$	$(tEv, tE-v) + (tE0) + (0Av+, 0A-v+) + (0A0-)$
(kEq)	$k < \pi/2$		$(rE0)$
	$k = \pi/2$		$(\pi E0)$
	$k > \pi/2$		$(tE0)$
$(\pi E0)$			$(0Aq+) + (0Aq-)$
$(\pi Em, \pi E\bar{m})$		$m < q/2$	$2(0Aw+, 0A-w+) + (0Aw-, 0A-w-) + (0Aq+)$ $+ (0Aq-) + (0A0-)$
$(\pi Eq/2)$			$(0Aq+) + (0A0-)$

† Only for $q = 2, 4, \ldots$.
‡ $2(\pi Ew)$ for $w = q/2$.
§ $2(\pi Ev)$ for $v = q/2$; $\bar{w} = w - q$; $\bar{v} = v - q$.

Table 5. SKS of corepresentations of the line groups $L(2q)_q/mcm$ ($q = 1, 2, \ldots$).

D			$[D^2] - (0A0+)$
$(0Em\pm)$		$m < q/2$	$(0Ew+)$
		$m = q/2$†	$(0Aq+) + (0Bq+)$
		$m > q/2$	$(0Ev+)$
$(kEA0)$	$k < \pi/2$		$(rEA0)$
	$k = \pi/2$		$(\pi EA0)$
	$k > \pi/2$		$(tEAq)$
$(kEB0)$	$k < \pi/2$		$(rEA0)$
	$k = \pi/2$		$(\pi EA0)$
	$k > \pi/2$		$(tEAq)$
(kGm)	$k < \pi/2$	$m < q/2$	$(rGw) + (rEA0) + (0Ew+) + (0B0-)$
		$m = q/2$†	$(rEAq) + (rEBq) + (rEA0) + (0Aq+) + (0Bq+) + (0B0-)$
		$m > q/2$	$(rGv) + (rEA0) + (0Ev+) + (0B0-)$
	$k = \pi/2$	$m < q/2$	$(\pi Gw) + (\pi EA0) + (0Ew+) + (0B0-)$
		$m = q/2$†	$2(\pi Eq/2+) + (\pi EA0) + (0Aq+) + (0Bq+) + (0B0-)$
		$m > q/2$	$(\pi Gv) + (\pi EA0) + (0Ev+) + (0B0-)$
	$k > \pi/2$	$m < q/2$	$(tGw) + (tEAq) + (0Ew+) + (0B0-)$
		$m = q/2$†	$(tEA0) + (tEB0) + (tEAq) + (0Aq+) + (0Bq+) + (0B0-)$
		$m > q/2$	$(tGv) + (tEAq) + (0Ev+) + (0B0-)$
$(kEAq)$	$k < \pi/2$		$(rEA0)$
	$k = \pi/2$		$(\pi EA0)$
	$k > \pi/2$		$(tEAq)$
$(kEBq)$	$k < \pi/2$		$(rEA0)$
	$k = \pi/2$		$(\pi EA0)$
	$k > \pi/2$		$(tEAq)$
$(\pi EA0)$			$(0Aq+) + (0Aq-)$
$(\pi EB0)$			$(0Aq+) + (0Aq-)$
(πGm)		$m < q/2$	$2(0Ew+) + (0Ew-) + (0Aq+) + (0Bq+) + (0B0+)$
$(\pi Eq/2\pm)$			$(0Aq+) + (0B0-)$

† Only for $q = 2, 4, \ldots$.

3. Examples

To illustrate how these tables can be utilised, let us consider a staggered stack of identical diatomic molecules shown in figure 1. The spatial symmetry of this model polymer is described by the line group $L4_2/mcm$. Let us assume that each atom contributes one relevant atomic orbital of the $l = 0$ type (i.e. s, p, d_z, etc), and let t_1 and t_2 denote the intra- and inter-molecular transfer integrals as indicated in figure 1. Within the tight-binding scheme, the electronic energy bands are given as

$$E(kA_0) = 2t_1 + 2t_2 \cos ka$$

$$E(kE_1) = 2t_2 \cos ka$$

$$E(kA_2) = -2t_2 + 2t_2 \cos ka.$$

If we assume that $t_1 < 0$, $t_2 < 0$ and $|t_2| > |t_1|$, to avoid band overlapping, the two outer bands A0 and A2 are non-degenerate; the middle E_1 band is twofold degenerate throughout the Brillouin zone. Notice that this *band degeneracy* is frequent in Q1D crystals, thus making line-group-theoretical considerations more generally useful than,

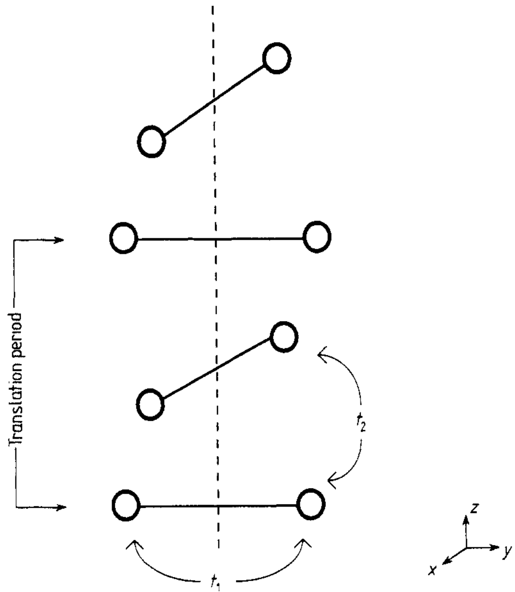

Figure 1.

for example, the analogous space group ones; in the latter case, the limiting factor is the relative scarcity of the special (high-symmetry) k vectors as compared to the overwhelming abundance of the general (low-symmetry) ones.

Let us consider the two simplest non-trivial cases: when each molecule contributes one electron so that the lowest A0 band is half-filled, and when each molecule contributes two electrons so that the middle E_1 band is half-filled.

Case 1. Here, the Fermi level states correspond to

$$D = (\pi/2A0) + (-\pi/2A0) = (\pi/2EA0).$$

From table 5, entry (kEA0), case $k = \pi/2$, we find that

$$[\pi/2EA_0^2] = (\pi EA0) + (0A0+).$$

(Notice that we have added the identity corepresentation, which indeed appears in every $[D^2]$, but which was omitted from tables 1-5 for brevity.)

Now, one has to construct the vibration modes that transform according to the corepresentation (πEA0). That can be done utilising the standard methods for constructing symmetry adapted bases; for application of those techniques to the line groups see Božović and Delhalle (1984). The resulting displacement modes are shown in figures 2 and 3; notice that these modes are pairwise-degenerate. The implication is an existence of a vibronic (or charge-density wave) instability with a complex order parameter. This *is* unusual since we were dealing with a single (i.e. non-degenerate) half-filled band; in the simple Peierls model with commensurability $n = 2$, one would have had a real order parameter. Notice also that in addition to the longitudinal, displacive Peierls mode (figure 2), we have a possible transverse distortive instability (figure 3), which differs from both the Peierls case and the examples considered in I.

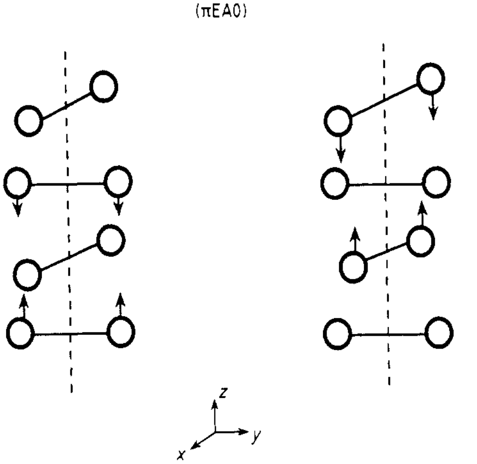

Figure 2.

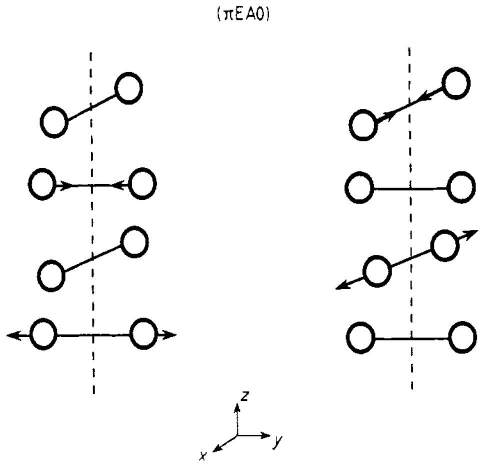

Figure 3.

Case 2. Here, there are four degenerate states at the Fermi level, which belong to

$$D = (\pi/2E_1) + (-\pi/2E_1) = (\pi/2G_1).$$

From table 5, entry (kGm), case $k = \pi/2$ and $m = 1$, we find that

$$[\pi/2G_1^2] = 2(\pi E_1+) + (\pi EA0) + (0A_2+) + (0B_2+) + (0B0-) + (0A0+)$$

where we have added the identical corepresentation, as explained above. The additional vibronically active modes are shown in figures 4 and 5. Of these, the (πE_1+) modes are twofold-degenerate and displacive; ($0A_2+$) mode is non-degenerate and distortive, and ($0B_2+$) is non-degenerate and displacive; all of them are transverse. Notice that, despite the fact that $k_F = \pi/2$, the latter two modes have $k = 0$ rather than $k = \pi$; that is again unusual and it originates from the presence of the screw axis, i.e. of the mixing of rotational and translational symmetries. There are no modes of ($0B0-$) symmetry. The ($0B_2+$) mode is the libration mode; if $|t_2| \ll |t_1|$, as would probably be the case in

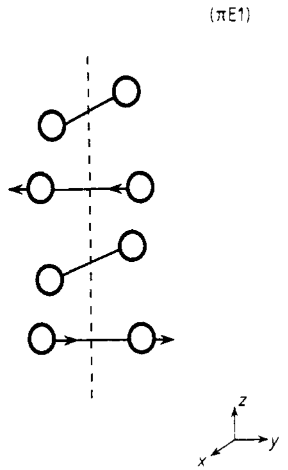

Figure 4.

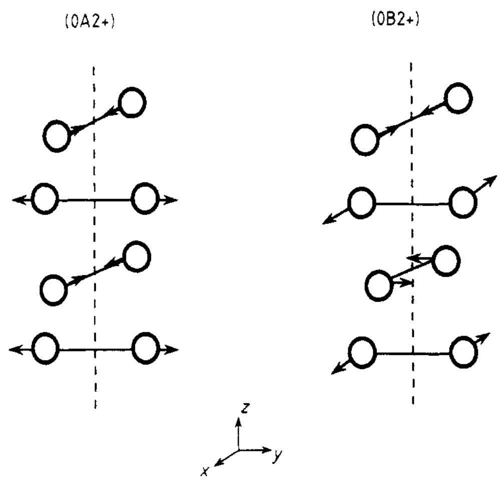

Figure 5.

reality, this mode would likely be lowest-frequency one, and one would expect it to dominate the instability.

4. Conclusions and discussions

Compared to those of I, the selection rules listed here show certain similarities; for instance, notice the appearance of Kronecker multiplicity coefficients larger than one. In those cases, additional restrictions on the allowed matrix elements can be obtained via the Wigner–Eckart theorem. Next, four-dimensional irreducible components of $[D^2]$ are seen to appear in tables 3–5. The importance of this fact stems from possible occurrence of a four-dimensional order parameter in the Peierls-distorted phase. That can generate physics much richer from that of the simple Peierls model (where the order parameter is two or one dimensional); particularly exciting is the possibility of two independent Goldstone modes emerging simultaneously (Božović 1985a, b). The fact that four-dimensional corepresentations do not appear in tables 1 and 2 is not an accident: a screw axis of order larger than two is not compatible with simultaneous occurence of mirror or glide planes, which is needed to couple (k, m) to $(-k, -m)$, and thus make electronic energy bands twofold degenerate throughout the Brillouin zone. It is also interesting to note that four-dimensional vibronically active phonon modes never appear in conjunction with electronic states at the Brillouin zone centre or boundaries, even when those states have the necessary twofold (or even fourfold!) band degeneracy. This precludes occurrence of the double-Goldstone-mode anomaly mentioned above in QID solids with even number of electrons per unit cell (unless there is an accidental band overlap); in general, doping will be required to generate partially occupied bands.

As for the differences, we have emphasised in I the fact that both quasi-momentum and quasi-angular momentum were strictly conserved there. This is true here only for so-called 'normal' scattering processes in which $2k < \pi$ (the Brillouin zone edge); in umklapp processes where $2k \geqslant \pi$, the quasi-angular momentum also undergoes a jump according to the rule $(k, m) \to (k+2\pi, m-p)$. Indeed, the underlying reason is that the n_p screw axis mixes rotational and translational symmetry operations $(C_n|0)$ and $(E|p/n)$, none of which itself belongs to the line group under study; for more details see Damnjanović *et al* (1983).

Appendix

In what follows, we give the character tables of the irreducible corepresentations of all the line groups that contain screw axes. The characters are listed only for the necessary elements (coset representatives); that is sufficient to identify the corepresentations.

The following notation is utilised throughout tables A1–A5:

$$s = 0, 1, \ldots, n-1 \qquad r = 0, 1, \ldots, q-1$$

$$\alpha = 2\pi/n \qquad t = 0, \pm 1, \pm 2, \ldots.$$

Table A1. The characters of irreducible corepresentations of the line groups Ln_p $(n = 1, 2, \ldots; p = 0, 1, \ldots, n-1)$.

D	$(C_n^s \vert t + sp/n)$
$(0A0)$	1
$(0Am, 0A-m)$	$2\cos(ms\alpha)$
$(0Aq)$†	$(-1)^s$
$(kA0, -kA0)$	$2\cos(kt + ksp/n)$
$(kAm, -kA-m)$	$2\cos(ms\alpha + kt + ksp/n)$
$(kAq, -kAq)$†	$2(-1)^s\cos(kt + ksp/n)$
$(\pi Am, \pi A\bar{m})$‡	$2(-1)^t\cos(ms\alpha + ps\alpha/2)$
$(\pi A-p/2)$§	$(-1)^t$
$(\pi A(n-p)/2)$‖	$(-1)^{s+t}$

† Only for $n = 2q = 2, 4, \ldots$.
‡ $\bar{m} = -m - p$.
§ Only for $p = 2, 4, \ldots$.
‖ Only for $n - p = 2, 4, \ldots$.

Table A2. The characters of irreducible corepresentations of the line groups Ln_p2 ($n = 1, 3, \ldots$) and Ln_p22 ($n = 2, 4, \ldots$).

D	$(C_n^s \vert t + sp/n)$	$(U \vert 0)$
$(0A0\pm)$	1	± 1
$(0Em)$	$2\cos(ms\alpha)$	0
$(0Aq\pm)$†	$(-1)^s$	± 1
$(kE0)$	$2\cos(kt + ksp/n)$	0
(kEm)	$2\cos(ms\alpha + kt + ksp/n)$	0
(kEq)†	$2(-1)^2\cos(kt + ksp/n)$	0
(πEm)	$2(-1)^{t+sp/n}\cos(ms\alpha + sp\alpha/2)$	0
$(\pi A - p/2\pm)$‡	$(-1)^{t+sp/n}$	± 1
$(\pi A(n - p/2)\pm)$§	$(-1)^{t+s+sp/n}$	± 1

† Only for $n = 2q = 2, 4, \ldots$.
‡ Only for $p = 2, 4, \ldots$.
§ Only for $n - p = 2, 4, \ldots$.

Table A3. The characters of irreducible corepresentations of line groups $L(2q)_q mc$ ($q = 1, 2, \ldots$).

D	$(C_{2q}^{2r} \vert t)$	$(C_{2q}^{2r+1} \vert t + 1/2)$	$(\sigma_v \vert 0)$
$(0A0)$	1	1	1
$(0B0)$	1	1	-1
$(0Em)$	$2\cos(2mr\alpha)$	$2\cos[m(2r+1)\alpha]$	0
$(0Aq)$	1	-1	1
$(0Bq)$	1	-1	-1
$(kA0, -kA0)$	$2\cos(kt)$	$2\cos[k(t+\frac{1}{2})]$	2
$(kB0, -kB0)$	$2\cos(kt)$	$2\cos[k(t+\frac{1}{2})]$	-2
$(kEm, -kEm)$	$4\cos(2mr\alpha)\cos(kt)$	$4\cos[m(2r+1)\alpha)\cos[k(t+\frac{1}{2})]$	0
$(kAq, -kAq)$	$2(-1)^s\cos(kt)$	$2(-1)^s\cos[k(t+\frac{1}{2})]$	2
$(kBq, -kBq)$	$2(-1)^s\cos(kt)$	$2(-1)^s\cos[k(t+\frac{1}{2})]$	-2
$(\pi A0, \pi Aq)$	$2(-1)^t$	0	2
$(\pi B0, \pi Bq)$	$2(-1)^t$	0	-2
$(\pi Em, \pi E\bar{m})$†	$4(-1)^t\cos(2mr\alpha)$	0	0
$(\pi Eq/2)$‡	$2(-1)^{t+r}$	0	0

† $\bar{m} = q - m$.
‡ Only for $q = 2, 4, \ldots$.

Table A4. The characters of irreducible corepresentations of the line groups $L(2q)_q/m$ ($q = 1, 2, \ldots$).

D	$(C_{2q}^{2r} \vert t)$	$(C_{2q}^{2r+1} \vert t+\frac{1}{2})$	$(\sigma_h \vert 0)$
$(0A0\pm)$	1	1	± 1
$(0Am\pm, 0A-m\pm)$	$2\cos(2mra)$	$2\cos[m(2r+1)a]$	± 2
$(0Aq\pm)$	$(-1)^s$	$(-1)^s$	± 1
$(kE0)$	$2\cos(kt)$	$2\cos[k(t+\frac{1}{2})]$	0
$(kEm, kE-m)$	$4\cos(2mr\alpha)\cos(kt)$	$4\cos[m(2r+1)\alpha]\cos[k(t+\frac{1}{2})]$	0
(kEq)	$2\cos(kt)$	$-2\cos[k(t+\frac{1}{2})]$	0
$(\pi E0)$	$2(-1)^t$	0	0
$(\pi Em, \pi E\bar{m})$†	$4(-1)^t\cos(2mr\alpha)$	0	0
$(\pi Eq/2)$‡	$2(-1)^{r+t}$	0	0

† $\bar{m} = q - m$.
‡ Only for $q = 2, 4, \ldots$.

Table A5. The characters of irreducible corepresentations of the line groups $L(2q)_q/mcm$ ($q = 1, 2, \ldots$).

D	$(C_{2q}^{2r}\|t)$	$(C_{2q}^{2r+1}\|t+1/2)$	$(\sigma_v\|0)$	$(\sigma_h\|0)$
$(0A0\pm)$	1	1	1	±1
$(0B0\pm)$	1	1	-1	±1
$(0Em\pm)$	$2\cos(2mr\alpha)$	$2\cos[m(2r+1)\alpha]$	0	±2
$(0Aq\pm)$	1	-1	1	±1
$(0Bq\pm)$	1	-1	-1	±1
$(kEA0)$	$2\cos(kt)$	$2\cos[k(t+\frac{1}{2})]$	2	0
$(kEB0)$	$2\cos(kt)$	$2\cos[k(t+\frac{1}{2})]$	-2	0
(kGm)	$4\cos(2mr\alpha)\cos(kt)$	$4\cos[m(2r+1)\alpha]\cos[k(t+\frac{1}{2})]$	0	0
$(kEAq)$	$2\cos(kt)$	$-2\cos[k(t+\frac{1}{2})]$	2	0
$(kEBq)$	$2\cos(kt)$	$-2\cos[k(t+\frac{1}{2})]$	-2	0
$(\pi EA0)$	$2(-1)^t$	0	2	0
$(\pi EB0)$	$2(-1)^t$	0	-2	0
(πGm)	$4(-1)^t\cos(2mr\alpha)$	0	0	0
$(\pi Eq/2\pm)$†	$2(-1)^{t+r}$	0	0	0

† Only for $q = 2, 4, \ldots$.

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