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Construction of the symmetry groups of polymer molecules

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Abstract. A derivation of the line groups, which are the symmetry groups of the stereo-regular polymer molecules, is presented.

Every line group is an extension of a one-dimensional translation group by a point group. The point group is either cyclic or a semi-direct product of cyclic groups. The expounded method of derivation of the line groups consists of first extending by the cyclic point groups and then obtaining the rest of the line groups by unification within the Euclidean group. To this purpose, a simple test is given to decide whether two line groups multiply into a third one. The method displays the subgroup structure of the line groups, relevant to the construction of their irreducible representations. All the line groups are derived and tabulated.

1. Introduction: symmetry elements of stereo-regular polymer molecules

The molecules of polymer substances consist of a large number of atoms (up to 10^5 or even more). The shape of these macromolecules is frequently a very long chain. They consist of a great number of identical constituent units, monomers, of the size of ordinary molecules. Those macromolecules which are translationally periodic along a line are called stereo-regular. The translational period, denoted by a (whose length ranges from two to several dozen ångstroms) is a one-dimensional analogue of the primitive cell in crystallography.

A stereo-regular macromolecule is usually characterised by an additional symmetry element—a screw axis, which can be denoted by n_k, where n is a positive integer and k can take the values $0, 1, \ldots, n-1$. This means that the macromolecule coincides with itself if rotated by $2\pi/n$ around the axis of the molecule and subsequently translated by ka/n along the same axis.

To give a few examples, we mention cellulose, having the screw axis 2_1, isotactic polypropylene with 3_1 and polyisobutene with 8_5 etc (Vainshtein 1959, 1966, Miller and Nielsen 1963).

The other possible symmetry elements are mirror and glide planes, denoted by m and c respectively, two-fold rotations perpendicular to the chain, denoted by U (from the German word umklapp) and, of course, combinations of these.

As examples, one can take polymethylene difluoride having m, α-form of gutta-percha which has c, polyvinyl chloride and polyglycine possessing both of them, and

§ Present address: Department of Mathematical Physics, The University, Adelaide, Australia polyisobutene and polytetrafluoroethylene with U (Vainshtein 1959, 1966, Miller and Nielsen 1963).

A macromolecule may, of course, possess a number of symmetry elements simultaneously. To be able to predict as much as possible physically, it is desirable to know all its symmetry elements and their mutual relations. For this it is useful to have a complete classification of all the possible symmetry groups of stereo-regular polymer molecules. These groups belong to the line groups which are the symmetry groups of three-dimensional objects translationally periodic along a line.

It is the aim of this paper to derive and classify all (discrete) line groups, at the same time clarifying their subgroup structure, which we found of great use in our construction of their irreducible representations (required for quantum-mechanical applications).

Of course, the molecules in a real polymer are of finite length; they can be bent, cross-linked and may contain various impurities and defects. Nevertheless, the model of a single isolated infinite linear ideal chain plays a central role in most of the theoretical investigations of polymer molecules. We have here an analogy with the case of the role of the ideal infinite monocrystal in theoretical solid state physics. As a matter of fact, many important physical properties of both of these systems are not very sensitive to deviations of the mentioned kind from the ideal model. The importance of the single chain model for calculation of vibrational spectra of polymers is evident from the book of Zbinden (1964), or the review article of Oleinik and Kompaneyets (1968), etc, and for electronic spectra (band structure) from Duke and O'Leary (1973), Suhai and Ladik (1973), Philpott (1975), Hendeković (1975), etc. The purpose of our work is to enable one to make full use of the symmetries of the single chain models.

2. Definition and general properties of line groups

Having analysed the symmetry elements of the physical objects which are translationally periodic in only one direction, we turn now to a systematic investigation of all the ways in which they can be combined into line groups. By definition the *line groups* are those subgroups of the Euclidean group whose pure translations are integral multiples of one of them. Every transformation of a line group **L** leaves invariant the straight line (known as the invariant line throughout this paper) connecting the centres of masses of the elementary cells (i.e., the structure units of the polymer molecule which are repeated by the pure translations). Such a transformation can be denoted by:

$$(R|v+t), \qquad v \in [0, 1), t \text{ integer}, \tag{1}$$

where R is a proper or improper rotation around a fixed point chosen to lie on the invariant line, whereas v and t determine a fractional and a pure translation respectively along the same line.

The symmetry transformation (1) acts as follows:

$$(R|v+t)\boldsymbol{r} = R\boldsymbol{r} + (v+t)\boldsymbol{a}, \tag{2}$$

where $\boldsymbol{a}$ generates all the pure translations in **L**. The composition law, as follows from (2), reads:

$$(R|v+t)(Q|w+q) = (RQ|v+t+Rw+Rq). \tag{3}$$

The unit element is $(E|0)$, and the inverse of $(R|v+t)$ is $(R^{-1}|-R^{-1}v-R^{-1}t)$.

All the elements of $\mathbf{L}$ of the form $(E|t)$, i.e. the pure translations, constitute *the translational subgroup* $\mathbf{T}$, which is invariant in $\mathbf{L}$, i.e. $\mathbf{T} \lhd \mathbf{L}$, because

$$(R|v+t)(E|t')(R|v+t)^{-1} = (E|Rt').$$

The elements of a coset of $\mathbf{T}$ in $\mathbf{L}$ have a common rotational part R:

$$(E|t')(R|v+t) = (R|v+t+t').$$

Each of these rotations R by itself leaves the line invariant, as one can see by applying R to $\boldsymbol{r}$ belonging to the line. As immediately seen from (3), the set of all R for a given $\mathbf{L}$ is a group, which we call *the isogonal point group* of $\mathbf{L}$ and denote by $\mathbf{P}$. Hence every line group $\mathbf{L}$ can be expressed as the sum of $|\mathbf{P}|$ (the order of the group $\mathbf{P}$) cosets of $\mathbf{T}$:

$$\mathbf{L} = \sum_{i=1}^{|\mathbf{P}|} (R_i|v_i)\mathbf{T}, \tag{4}$$

where all $v_i \in [0, 1)$.

Since, as we have concluded, $\mathbf{T} \lhd \mathbf{L}$ and $\mathbf{L}/\mathbf{T} \cong \mathbf{P}$, every line group $\mathbf{L}$ can also be defined as a subgroup of the Euclidean group which is an *extension* (Kurosh 1955) of $\mathbf{T}$ by $\mathbf{P}$, where $\mathbf{P}$ is a point group leaving a line invariant, and $\mathbf{T}$ is a discrete group of translations along the same line.

Involved extension-theoretical methods exist which make use of cohomology theory by which one could construct all the line groups in much the same fashion as was done for the space groups (Ascher and Janner 1965, 1968, Mozrzymas 1974). However, a considerably simpler extension-theoretical method of construction could be developed in the case of line groups (making use of the generalised semi-direct product; see Šijački *et al* 1972).

3. Physically distinct line groups

Before we expound our method of construction of the line groups in detail, we first have to clarify which of them are physically distinct, i.e. to describe the equivalence relation dictated by the problem.

Two line groups are equivalent if a conjugation by a translation and/or a proper rotation takes one into the other, because these transformations do not change the physical properties of the system.

An important characteristic property of the physical systems considered is the existence of the mentioned invariant line for each of them. For simplicity we always choose the z axis to coincide with this line.

In fact, it is then sufficient to consider only conjugations by the transformations which leave the z axis invariant, i.e. by translations along the z axis, by rotations around the same axis through an arbitrary angle, and by rotations around any axis in the x, y plane through 180°. This is so because, as is easily seen, if two line groups are conjugate to each other by any proper Euclidean transformation, they are conjugate also by a transformation of the above restricted kind.

As far as the rotational parts of the symmetry transformations are concerned, any of the mentioned conjugations gives:

$$(Q|w+q)(R|v+t)(Q|w+q)^{-1} = (QRQ^{-1}|\ldots).$$

It follows that the isogonal point groups of equaivalent line groups are necessarily conjugated by proper rotations which leave the z axis invariant; hence only such point groups are equivalent in the framework of line group theory.

It should be noted that this equivalence relation for point groups differs from the one used in crystallography and in molecular physics, where conjugation by *any* proper rotation generates an equivalent point group. All the difference resulting from the mentioned restriction (to conjugation by the rotations leaving the z axis invariant) consists in a possible breaking up of the usual equivalence classes of point groups into smaller ones. Let us now examine in detail this splitting.

To begin with, any point group $\mathbf{P}$ containing an element of at least third order leaves only one line invariant, which, in our case, must be the z axis. If another point group $\mathbf{P}'$ is equivalent to this $\mathbf{P}$ in the usual sense, then they are conjugated by a rotation leaving the z axis invariant, hence, no breaking up of equivalence classes occurs in this case. Here belong the following standard point groups: $\mathbf{C}_n$, $\mathbf{C}_{nv}$, $\mathbf{C}_{nh}$, $\mathbf{D}_n$, and $\mathbf{D}_{nh}$, $n = 3, 4, \ldots$; $\mathbf{S}_{2n}$ and $\mathbf{D}_{nd}$, $n = 2, 3, 4, \ldots$.

On the other hand, two point groups leaving the z axis invariant and containing only involutions (i.e. elements of order two) may be conjugate by the rotation through $\pi/2$ around a horizontal axis. Such groups are equivalent in the standard crystallographic sense, but not with respect to the equivalence we are dealing with. If a standard class contains such a pair of point groups, then it splits into two smaller classes.

The involutions at issue are: I (the inversion through the origin), C_2 and U (the rotations through π around the z axis and a horizontal axis respectively), σ_v and σ_h (the reflections in a vertical and the horizontal planes respectively). In the classes of the groups $\mathbf{S}_2 = \mathbf{C}_i$, $\mathbf{D}_2$ and $\mathbf{D}_{2h}$ no splitting occurs. Finally, the following classes of groups are the result of the mentioned splitting: $\mathbf{C}_2 = \{E, C_2\}$ and $\mathbf{D}_1 = \{E, U\}$; $\mathbf{C}_{1v} = \{E, \sigma_v\}$ and $\mathbf{C}_{1h} = \{E, \sigma_h\}$; $\mathbf{C}_{2h} = \mathbf{C}_2 \times \mathbf{C}_{1h}$ and $\mathbf{D}_{1d} = \mathbf{C}_{1v} \times \mathbf{D}_1$†; $\mathbf{C}_{2v} = \mathbf{C}_2 \times \mathbf{C}_{1v}$ and $\mathbf{D}_{1h} = \mathbf{C}_{1v} \times \mathbf{C}_{1h}$ (they are obviously pairwise conjugate by the rotation through $\pi/2$ around a horizontal axis).

4. Two types of point and line groups

Any (proper or improper) rotation leaving the z axis invariant we call R^+ type if $R\boldsymbol{a} = \boldsymbol{a}$, and R^- type if $R\boldsymbol{a} = -\boldsymbol{a}$. The transformations of the R^+ type are: C_n, $n = 1, 2, \ldots$ (rotations through $2\pi/n$ around the z axis), σ_v, and their products. An R^- transformation can always be written in the form $\sigma_h R^+$.

Therefore, any point group we are dealing with is either of $\mathbf{P}^+$ type, containing only R^+ transformations, or of $\mathbf{P}^-$ type, when it contains also R^- ones. The set of all R^+ transformations in a given $\mathbf{P}^-$ group is obviously an index-two subgroup, $\mathbf{P}^+$. Hence, $\mathbf{P}^-$ can be decomposed into

$$\mathbf{P}^- = \mathbf{P}^+ + R^-\mathbf{P}^+. \tag{5}$$

In particular, the point groups of the $\mathbf{P}^+$ type are $\mathbf{C}_n$ and

$$\mathbf{C}_{nv} = \mathbf{C}_n \wedge \mathbf{C}_{1v}, \qquad n = 1, 2, \ldots \tag{6}$$

($\wedge$ denotes the semi-direct product, SP). The $\mathbf{P}^-$ point groups for $n = 1, 2, \ldots$ can be

† We assume here that the axis is perpendicular to the plane because otherwise, i.e. if the axis lies in the plane, $\mathbf{C}_{1v} \times \mathbf{D}_1$ equals $\mathbf{D}_{1h}$.

decomposed as follows (for further convenience we give also their SP forms):

$$\mathbf{S}_{2n} = \mathbf{C}_n + S_{2n}\mathbf{C}_n, \tag{7}$$

where $S_{2n} = \sigma_h C_{2n}$ and it generates $\mathbf{S}_{2n}$;

$$\mathbf{C}_{nh} = \mathbf{C}_n + \sigma_h \mathbf{C}_n = \mathbf{C}_n \wedge \mathbf{C}_{1h}; \tag{8}$$

$$\mathbf{D}_n = \mathbf{C}_n + U\mathbf{C}_n = \mathbf{C}_n \wedge \mathbf{D}_1; \tag{9}$$

$$\mathbf{D}_{nd} = \mathbf{C}_{nv} + U_d \mathbf{C}_{nv} = \mathbf{C}_{nv} \wedge \mathbf{D}'_1 = (\mathbf{C}_n \wedge \mathbf{C}_{1v}) \wedge \mathbf{D}'_1, \tag{10}$$

where the index on U_d denotes that the angle between the axis of this rotation and the plane of σ_v equals $\pi/2_n$, $\mathbf{D}'_1 = \{E, U_d\}$;

$$\mathbf{D}_{nh} = \mathbf{C}_{nv} + \sigma_h \mathbf{C}_{nv} = \mathbf{C}_{nv} \wedge \mathbf{C}_{1h} = (\mathbf{C}_n \wedge \mathbf{C}_{1v}) \wedge \mathbf{C}_{1h}. \tag{11}$$

Analogously, all the line groups are of $\mathbf{L}^+$ or of $\mathbf{L}^-$ type, depending whether the isogonal point groups are of the $\mathbf{P}^+$ or of the $\mathbf{P}^-$ type. Furthermore, it follows from (5) that every line group of $\mathbf{L}^-$ type can be decomposed:

$$\mathbf{L}^- = \mathbf{L}^+ + (R^-|v)\mathbf{L}^+, \tag{12}$$

where $\mathbf{L}^+$ is that index-two subgroup of $\mathbf{L}^-$ whose isogonal point group is precisely $\mathbf{P}^+$ from (5).

The line groups of the $\mathbf{L}^-$ type have the following important property.

For every line group $\mathbf{L}^-$ there exists an equivalent line group for which $v = 0$ in the decomposition (12), i.e.

$$\mathbf{L}^+ + (R^-|v)\mathbf{L}^+ \sim \mathbf{L}^+ + (R^-|0)\mathbf{L}^+. \tag{13}$$

To prove this statement it suffices to note that conjugation by $(E|-v/2)$ does not change any element of $\mathbf{L}^+$, whereas $(E|-v/2)(R^-|v)(E|-v/2)^{-1} = (R^-|0)$.

Thus, the construction of all the line groups is herewith practically reduced to the derivation of all the distinct $\mathbf{L}^+$ groups; all the $\mathbf{L}^-$ groups are then obtained by adding the coset $(R^-|0)\mathbf{L}^+$ to each $\mathbf{L}^+$ group, where R^- is one of the transformations displayed in equations (7)–(11) (if one obtains a group in this way).

5. A method of contruction of the line groups with cyclic isogonal point groups

Let $\mathbf{L}$ be a line group with a cyclic isogonal point group, $\mathbf{P} = \{R_1, R_1^2, \ldots, R_1^n = E\}$. Then the representative $(R_1|v_1)$ of the first coset in the decomposition $\mathbf{L} = \Sigma_{i=1}^n (R_i|v_i)\mathbf{T}$ determines all the others, i.e. $(R_1|v_1)^s\mathbf{T} = (R_1^s|\mathrm{Fr}(v_1 + R_1v_1 + \ldots + R_1^{s-1}v_1))\mathbf{T} = (R_s|v_s)\mathbf{T}$, $s = 2, 3, \ldots, n$ and $\mathrm{Fr}(x)$ denotes the fractional part of the real number x.

If the line group under consideration is of $\mathbf{L}^+$ type, then $R_1v_1 = v_1$ (omitting $\boldsymbol{a}$ for simplicity), so that $(R_s|v_s) = (R_1^s|\mathrm{Fr}(sv_1))$. Therefore, the problem of constructing $\mathbf{L}$ reduces in this case to finding all values of v_1 for which the set $\Sigma_{s=1}^n (R_1^s|\mathrm{Fr}(sv_1))\mathbf{T}$ is a group. It is easily shown that this is the case if and only if $(R_1^n|nv_1) \in \mathbf{T}$. Hence the solutions are

$$v_1 = p/n, \qquad p = 0, 1, \ldots, n-1. \tag{14}$$

In this way one obtains all the solutions; they are all distinct as will be shown later for every particular case separately.

If we consider an $\mathbf{L}^-$-type line group, then the generator R_1 of its isogonal point group must be of R^- type, otherwise it would generate a $\mathbf{P}^+$-type point group. Therefore, $(R_1|v_1)^2 = (R_1^2|0)$, $(R_1|v_1)^3 = (R_1^3|v_1), \ldots$. As $\mathbf{P}^-$ is of an even order, say $2n$, for every $v_1 \in [0, 1)$ the condition $(R_1|v_1)^{2n} \in \mathbf{T}$ is satisfied, and $\Sigma_{s=1}^{2n} (R_1|v_1)^s\mathbf{T}$ is a group. Making use of (13) one can see that each of these line groups is equivalent to one of them, namely to

$$\sum_{s=1}^{2n} (R_1|0)^s\mathbf{T}.$$

In conclusion, for every cyclic point group of $\mathbf{P}^+$ type there exist n distinct line groups, while for any of $\mathbf{P}^-$ type there exists exactly one. In this way for every cyclic point group $\mathbf{P}$ which leaves a line invariant one can construct all the extensions of $\mathbf{T}$ by $\mathbf{P}$ which are subgroups of the Euclidean group.

6. A method of construction of the line groups with non-cyclic isogonal point groups

It is an important fact that every non-cyclic point group we are dealing with is a semi-direct product of two or at most three cyclic ones (cf equations (6) and (8)–(11)).

Let $\mathbf{L}$ be a given line group which is an extension of $\mathbf{T}$ by $\mathbf{P} = \mathbf{P}_1 \wedge \mathbf{P}_2$.

Then $\mathbf{L}_1$ and $\mathbf{L}_2$ are those subgroups of $\mathbf{L}$ which contain $\mathbf{T}$ and whose isogonal point groups are $\mathbf{P}_1$ and $\mathbf{P}_2$ respectively. The subgroup $\mathbf{L}_1$ is invariant in $\mathbf{L}$, the intersection of $\mathbf{L}_1$ and $\mathbf{L}_2$ is $\mathbf{T}$, and the product $\mathbf{L}_1\mathbf{L}_2$ equals $\mathbf{L}$. In other words, $\mathbf{L}$ is a generalised semi-direct product, GSP (Šijački *et al* 1972), of $\mathbf{L}_1$ and $\mathbf{L}_2$.

The above statements give necessary conditions (see theorem 1 in the appendix), so that multiplying every line group $\mathbf{L}_1$ corresponding to $\mathbf{P}_1$ with every line group $\mathbf{L}_2$ corresponding to $\mathbf{P}_2$ one cannot fail to obtain all the line groups $\mathbf{L}$ corresponding to $\mathbf{P} = \mathbf{P}_1 \wedge \mathbf{P}_2$. However, these conditions are not sufficient, i.e. not every product $\mathbf{L}_1\mathbf{L}_2$ is a group.

It is shown in the appendix that the product of $\mathbf{L}_1$ and $\mathbf{L}_2$ defined above is a group if

$$v_2 + R_2 v_1 - R' v_2 = v' + t, \qquad t = 0, \pm 1, \pm 2, \ldots, \tag{15}$$

where $(R_1|v_1)$ and $(R_2|v_2)$ are any coset representatives in $\mathbf{L}_1$ and $\mathbf{L}_2$ respectively, $R' = R_2 R_1 R_2^{-1}$ and v' is the fractional translation corresponding to R'(see from theorem 2 to the end of the appendix).

In conclusion, if one has all the line groups $\mathbf{L}_1$ which are the extensions of $\mathbf{T}$ by the point group $\mathbf{P}_1$ and analogously for $\mathbf{L}_2$ and $\mathbf{P}_2$, then all the line groups $\mathbf{L}$ of $\mathbf{P} = \mathbf{P}_1 \wedge \mathbf{P}_2$ are obtained by multiplying those $\mathbf{L}_1$ and $\mathbf{L}_2$ for which the practical compatibility test (15) is satisfied. It is sufficent to take for R_1 and R_2 the generators of $\mathbf{P}_1$ and $\mathbf{P}_2$ respectively, so that in practice one has to solve at most two simple equations.

7. Results and discussion

The line groups were first derived by Hermann (1928); for subsequent treatments see Alexander (1929), Shubnikov (1940), Belov (1956). The relevance of line groups for polymers was discussed by Vainshtein (1959, 1966) and also by Tobin (1955, 1960), Elliott (1969), Zbinden (1964), Oleinik and Kompaneyets (1968).

By the method expounded we have constructed all the line groups. The results are presented in table 1.

Table 1. Classification of the line groups. Every element of a line group can be obtained from the listed general form by choosing $s=0,1,\ldots,n-1$, $r=0,1,\ldots,q-1$ where $q=n/2$ and $t=0,\pm1,\ldots$. For every point group, the first line group listed is symmorphic (i.e. $\mathbf{L}=\mathbf{T}\wedge\mathbf{P}$), while the rest of them are non-symmorphic. Further, $p=1,2,\ldots,n-1$.

Point group ($n=1,2,\ldots$)	Corresponding line groups: n odd	n even	General form of elements
$\mathbf{C}_n$	$\mathbf{L}n$		$(C_n^s\|t)$
	$\mathbf{L}n_p$		$(C_n^s\|\mathrm{Fr}(sp/n)+t)$
$\mathbf{C}_{nv}$	$\mathbf{L}nm$	$\mathbf{L}nmm$	$(C_n^s\|t)$, $(\sigma_v C_n^s\|t)$
	$\mathbf{L}nc$	$\mathbf{L}ncc$	$(C_n^s\|t)$, $(\sigma_v C_n^s\|1/2+t)$
		$\mathbf{L}(2q)_q mc$	$(C_{2q}^{2r}\|t)$, $(C_{2q}^{2r+1}\|1/2+t)$, $(\sigma_v C_{2q}^{2r}\|t)$, $(\sigma_v C_{2q}^{2r+1}\|1/2+t)$
$\mathbf{C}_{nh}$	$\mathbf{L}n/m$		$(C_n^s\|t)$, $(\sigma_h C_n^s\|t)$
		$\mathbf{L}(2q)_q/m$	$(C_{2q}^{2r}\|t)$, $(C_{2q}^{2r+1}\|1/2+t)$, $(\sigma_h C_{2q}^{2r}\|t)$, $(\sigma_h C_{2q}^{2r+1}\|1/2+t)$
$\mathbf{S}_{2n}$	$\mathbf{L}\bar{n}$	$\mathbf{L}(\overline{2n})$	$(C_{2n}^{2s}\|t)$, $(\sigma_h C_{2n}^{2s+1}\|t)$
$\mathbf{D}_n$	$\mathbf{L}n2$	$\mathbf{L}n22$	$(C_n^s\|t)$, $(UC_n^s\|t)$
	$\mathbf{L}n_p2$	$\mathbf{L}n_p22$	$(C_n^s\|\mathrm{Fr}(sp/n)+t)$, $(UC_n^s\|\mathrm{Fr}(sp/n)+t)$
$\mathbf{D}_{nd}$	$\mathbf{L}\bar{n}m$	$\mathbf{L}(\overline{2n})2m$	$(C_n^s\|t)$, $(\sigma_v C_n^s\|t)$, $(U_d C_n^s\|t)$, $(U_d\sigma_v C_n^s\|t)$
	$\mathbf{L}\bar{n}c$	$\mathbf{L}(\overline{2n})2c$	$(C_n^s\|t)$, $(\sigma_v C_n^s\|1/2+t)$, $(U_d C_n^s\|t)$, $(U_d\sigma_v C_n^s\|1/2+t)$
$\mathbf{D}_{nh}$	$\mathbf{L}(\overline{2n})2m$	$\mathbf{L}n/mmm$	$(C_n^s\|t)$, $(\sigma_v C_n^s\|t)$, $(\sigma_h C_n^s\|t)$, $(\sigma_h\sigma_v C_n^s\|t)$
	$\mathbf{L}(\overline{2n})2c$	$\mathbf{L}n/mcm$	$(C_n^s\|t)$, $(\sigma_v C_n^s\|1/2+t)$, $(\sigma_h C_n^s\|t)$, $(\sigma_h\sigma_v C_n^s\|1/2+t)$
		$\mathbf{L}(2q)_q/mcm$	$(C_{2q}^{2r}\|t)$, $(C_{2q}^{2r+1}\|1/2+t)$, $(\sigma_v C_{2q}^{2r}\|t)$, $(\sigma_v C_{2q}^{2r+1}\|1/2+t)$, $(\sigma_h C_{2q}^{2r}\|t)$, $(\sigma_h C_{2q}^{2r+1}\|1/2+t)$, $(\sigma_h\sigma_v C_{2q}^{2r}\|t)$, $(\sigma_h\sigma_v C_{2q}^{2r+1}\|1/2+t)$

Since we feel that the method of construction of the line groups might be applicable also to other group-theoretical problems in physics, a more detailed presentation has been prepared as an internal report†.

An extensive list of polymers, each classified according to the line group which is its symmetry group, has been presented (Božović and Vidaković 1976). All the irreducible representations of the line groups have been derived in a thesis (Božović 1975) and it is hoped to publish the results.

Appendix

A group $\mathbf{E}$ is called an extension of a group $\mathbf{K}$ by a group $\mathbf{G}$, and denoted by $(i, \mathbf{E}, s)$, if it

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contains a normal subgroup $i(\mathbf{K})$ isomorphic to $\mathbf{K}$, such that $\mathbf{E}/i(\mathbf{K})$ is isomorphic to $\mathbf{G}$ (Kurosh 1955, Michel 1964). Diagrammatically, one describes the above situation by a short exact sequence of homomorphisms:

$$1 \to \mathbf{K} \xrightarrow{i} \mathbf{E} \xrightarrow{s} \mathbf{G} \to 1. \tag{A.1}$$

We denote by s^{-1} the multi-valued inverse map of the homomorphism $s: \mathbf{E} \to \mathbf{G}$, $\mathrm{Ker}(s) = i(\mathbf{K})$. The map s^{-1} takes the elements of $\mathbf{G}$ onto the cosets of $i(\mathbf{K})$ in $\mathbf{E}$.

We are interested in the case when $\mathbf{G}$ is a semi-direct product (SP) of its two subgroups:

$$\mathbf{G} = \mathbf{G}_1 \wedge \mathbf{G}_2, \tag{A.2}$$

which actually means

$$\mathbf{G}_1 \lhd \mathbf{G}, \qquad \mathbf{G}_2 < \mathbf{G}, \qquad \mathbf{G}_1 \cap \mathbf{G}_2 = \{e\}, \qquad \mathbf{G} = \mathbf{G}_1\mathbf{G}_2. \tag{A.3a, b, c, d}$$

We propose first to extend each of these factors separately, and then to unify the extensions. This is found to be a substantially simplified procedure.

Let us first give the necessary conditions for the outlined construction.

Theorem 1. If $(i, \mathbf{E}, s)$ is an extension of $\mathbf{K}$ by $\mathbf{G} = \mathbf{G}_1 \wedge \mathbf{G}_2$, then $\mathbf{E}_1 = s^{-1}(\mathbf{G}_1)$ and $\mathbf{E}_2 = s^{-1}(\mathbf{G}_2)$ are extensions of $\mathbf{K}$ by $\mathbf{G}_1$ and $\mathbf{G}_2$, respectively, and

$$\mathbf{E}_1 \lhd \mathbf{E}, \qquad \mathbf{E}_2 < \mathbf{E}, \qquad \mathbf{E}_1 \cap \mathbf{E}_2 = i(\mathbf{K}), \qquad \mathbf{E} = \mathbf{E}_1\mathbf{E}_2; \tag{A.4a, b, c, d}$$

$$s^{-1}(g_2)s^{-1}(g_1)[s^{-1}(g_2)]^{-1} = s^{-1}(g_2 g_1 g_2^{-1}), \tag{A.4e}$$

for every $g_1 \in \mathbf{G}_1$, and every $g_2 \in \mathbf{G}_2$.

In theorem 1 we assumed $\mathbf{E}$ to be given in advance. The inverse problem—how to construct $\mathbf{E}$ via $\mathbf{E}_1$ and $\mathbf{E}_2$—is more important. The following theorem establishes a method of solution of this problem for a certain class of cases.

Theorem 2. For given $\mathbf{G} = \mathbf{G}_1 \wedge \mathbf{G}_2$ and $\mathbf{K}$, let $(i, \mathbf{E}_1, s_1)$ and $(i, \mathbf{E}_2, s_2)$ be extensions of $\mathbf{K}$ by $\mathbf{G}_1$ and by $\mathbf{G}_2$ respectively, such that they both are subgroups of a larger group $\mathbf{F}$, and $\mathbf{E}_1 \cap \mathbf{E}_2 = i(\mathbf{K})$. Further let

$$s_2^{-1}(g_2)s_1^{-1}(g_1)[s_2^{-1}(g_2)]^{-1} = s_1^{-1}(g_2 g_1 g_2^{-1}), \tag{A.5}$$

for every $g_1 \in \mathbf{G}_1$, and every $g_2 \in \mathbf{G}_2$. Then: (i) $\mathbf{E} = \mathbf{E}_1\mathbf{E}_2$ is a group; (ii) $i(\mathbf{K}) \lhd \mathbf{E}$; and (iii) $\mathbf{E}/i(\mathbf{K}) \cong \mathbf{G}$, i.e. $\mathbf{E}$ is an extension of $\mathbf{K}$ by $\mathbf{G}$.

Remark. In practice, it is sufficient to test (A.5) for generators of $\mathbf{G}_1$ and $\mathbf{G}_2$ only, since s_1^{-1} and s_2^{-1} give isomorphisms of $\mathbf{G}_1$ onto $\mathbf{E}_1/i(\mathbf{K})$ and $\mathbf{G}_2$ onto $\mathbf{E}_2/i(\mathbf{K})$ respectively, and conjugation is a homomorphism.

In order to apply the test (A.5) to the line groups, we specialise it as follows. Since here $\mathbf{G} = \mathbf{P}$, $\mathbf{K} = \mathbf{T}$, $\mathbf{E} = \mathbf{L}$, $\mathbf{F}$ is the Euclidean group, $g = R$, we have $s^{-1}(R) = (R|v)\mathbf{T}$, and (A.5) takes the form

$$(R_2|v_2)\mathbf{T}(R_1|v_1)\mathbf{T}(R_2|v_2)^{-1}\mathbf{T} = (R'|v')\mathbf{T}, \tag{A.6}$$

where $R' = R_2R_1R_2^{-1}$, and v' is the corresponding fractional translation.

Finally, we arrive at the following very practical test:

$$v_2 + R_2v_1 - R_2R_1R_2^{-1}v_2 = v' + t, \tag{A.7}$$

where v' corresponds to $R' = R_2 R_1 R_2^{-1}$. The test is satisfied, i.e. $\mathbf{L}_1\mathbf{L}_2$ is a group, if equation (A.7) has a solution among $t = 0, \pm 1, \pm 2, \ldots$. It is sufficient to apply (A.7) to the generators of $\mathbf{P}_1$ and $\mathbf{P}_2$ only (cf the above remark).

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