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Subgroups of weak–direct products and magnetic axial point groups

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Abstract. It is shown that all halving subgroups of a group G which is a weak–direct product of two of its subgroups H and K, can be constructed using halving subgroups of H and K. Similarly, if K is of order two, one can find all subgroups of G via the subgroups of H. Using the former method, all of the 31 families of magnetic axial point groups of arbitrary order are determined. These groups are of interest when ferromagnetic and ferroelectric phases of quasi-one-dimensional systems are considered. Also, it is demonstrated that those among the non-crystallographic magnetic axial point groups which are compatible with ferromagnetism (ferroelectricity), admit magnetisation (polarisation) only along the principle axis of rotation.

1. Introduction

Two tasks which are important when properties of the systems whose symmetry is described by line groups (polymers, quasi-one-dimensional systems; Vujičić *et al* 1977) are considered. These can be performed with the aid of a specific structure of the line groups and their isogonal axial point groups.

The first is the determination of the magnetic line and magnetic axial point groups, and arises in the treatment of the ferromagnetic and ferroelectric phases of these systems (Zheludev 1971, Cracknell 1969). The second task is the prediction of changes in structure in phase transitions. In view of some recent approaches to this problem in solid state physics (Ascher 1977, Janovec *et al* 1975, Kopsky 1979) it emerges that this problem reduces to finding subgroups of the isogonal axial point groups (and particularly the epikernels of their irreducible representations).

The specificity of the structure of the line groups and axial point groups is that each of them is either cyclic or a weak–direct product (Jansen and Boon 1967) of two of its subgroups. In the latter case, one of the subgroups is always cyclic (infinite cyclic for the line groups and of order two for the axial point groups), and the second is an axial point group in both cases.

The family of the magnetic groups of a group consists of the group itself, its grey group (which is a direct product of the group with $\Theta = \{e, \theta\}$, the group containing the identity e and θ which is time reversal in the theory of ferromagnetism, or the operation of changing the sign of the polarisation vector in the case of ferroelectricity), and the set of black and white groups (Opechowski and Guccione 1965). To construct all black and white magnetic groups one takes all subgroups of index two of the group and then supplements each of them with its coset multiplied by θ. Hence the decisive part of the construction consists in finding all index-two subgroups of the group.

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In this paper we develop a method which enables one to solve the above problems for the groups that are weak–direct products. In § 2 a theorem concerning the general case of the group G being a weak–direct product of its subgroups H and K is proved. The consequences of this theorem are exploited to find all halving subgroups of G (in § 3), and all subgroups of G when K is of order two (in § 4). In § 5 the magnetic axial point groups are found. Finally (§ 6) the magnetic axial point groups admitting ferromagnetism and ferroelectricity are selected.

2. The main theorem

Let the group G be a *weak–direct product* of two of its subgroups H and K, that is $G = HK$. This means that each element of G is a product of one element of H and one element of K, and that the intersection of H and K contains only the identity element of the group G. Each $g \in G$ determines uniquely a pair $h \in H$ and $k \in K$ such that $g = hk$, and a pair $h' \in H$ and $k' \in K$ such that $g = k'h'$. Semi-direct and direct products are special cases of the weak–direct product.

Now, suppose G′ is a subgroup of $G = HK$. Let us define the sets H′, K′, H_e and K_e as follows:

$$H' \overset{d}{=} \{h' \in H| \quad \exists k \in K \quad h'k \in G'\}, \qquad K' \overset{d}{=} \{k' \in K| \exists h \in H \quad hk' \in G'\},$$

$$H_e \overset{d}{=} H \cap G' \quad \text{and} \quad K_e \overset{d}{=} K \cap G'.$$

H_e and K_e are subgroups of H and K and subsets of H′ and K′ respectively. Thus the subgroup G′ consists only of elements $g' = h'k'$, $h' \in H'$, $k' \in K'$.

Theorem 1. The set of all $k' \in K'$ such that $h'k' \in G'$ for any fixed $h' \in H'$ is a left coset of K_e in K. Analogously, the set of all $h' \in H'$ such that $h'k' \in G'$ for a fixed $k' \in K'$, forms a right coset of H_e in H.

Proof. Note that the identity element e (regarded as an element of H′) occurs in G′ multiplied by $K_e = \{k_1 = e, k_2, \ldots, k_m\}$. If h' is an arbitrary element of H′, then there is at least one element $k' \in K'$ such that $h'k' \in G'$. Furthermore, all the elements $h'k'k_i$ $(i = 2, \ldots, m)$ also belong to G′ since $K_e \subset G'$. Therefore h' is multiplied at least by the left coset of K_e whose representative is k'. The assumption that there exists a $k'' \notin k'K_e$, such that $h'k'' \in G'$ implies the contradiction that K_e contains more than the mentioned m elements.

The following relation is an immediate consequence of the theorem:

$$|G'| = |H'||K_e| = |H_e||K'| \tag{1}$$

($|S|$ denotes the number of elements of a set S).

3. Subgroups of index two in a weak–direct product

In this section the results of theorem 1 will be investigated in detail for the case when G′ is a subgroup of G of index two. Then one has

$$|G'| = |G|/2 = |H||K|/2. \tag{2}$$

Using equations (1) and (2) one can conclude that $|H_e|$ cannot be less than $|H|/2$, and similarly $|K_e|$ cannot be less than $|K|/2$. Because of these constraints $|H_e|$ can take only two values: $|H|$ and $|H|/2$, and analogously $|K_e|=|K|$ or $|K_e|=|K|/2$.

Now we combine these possibilities to count all different index-two subgroups of $G=HK$.

Case (i). If $|H_e|=|H|$, $|K_e|$ must be equal to $|K|/2$, since $|H_e|=|H'|=|H|$ implies $|K'|=|K|/2$, by relation (2). Then G' can be written in the form

$$G'=HK_e. \tag{3}$$

Case (ii). If $|H_e|=|H|/2$, one possibility is $|K_e|=|K|$, and the situation is analogous to the one in case (*i*), that is

$$G'=H_eK. \tag{4}$$

Case (iii) If $|H_e|=|H|/2$, the remaining possibility for $|K_e|$ is $|K_e|=|K|/2$ (with $|K'|=|K|$ and $|H'|=|H|$). By theorem 1, each element of $H^0 \overset{d}{=} H\backslash H_e$ is in G' multiplied by the whole coset of K_e that is with $K^0 \overset{d}{=} K\backslash K_e$, and *mutatis mutandis* for K^0 and H^0. Therefore one has

$$G'=H_eK_e+H^0K^0. \tag{5}$$

Our aim is to find all halving subgroups G' of a given $G=HK$, by making use of halving subgroups of H and K. To this end we construct all the sets: (i) HK_i, (ii) H_jK and (iii) $H_jK_i+H_j^0K_i^0$, where H_j and K_i run over the sets of halving subgroups of H and K respectively (H_j^0 and K_i^0 are the corresponding cosets), and we check which of them are subgroups. As has already been shown, all G' are obtained in this way.

In the first two cases, (i) and (ii), the checking can be done with the aid of the theorem that a necessary and sufficient condition for the product of two subgroups to be a group is their commutation. As for the case (iii), the situation is a little more complicated. A criterion can be formulated as the following theorem:

Theorem 2. Let H_j and K_i be halving subgroups of H and K respectively, with cosets H_j^0 and K_i^0, and $G'=H_jK_i+H_j^0K_i^0$. Further, let H_jK_i be a subgroup of $G=HK$ (that is $H_jK_i=K_iH_j$). Then G' is a subgroup of G iff H_j^0 and K_i^0 commute.

Proof. Suppose the cosets commute. Since $H_jK_i=K_iH_j$ and $H_j^0K_i^0=K_i^0H_j^0$, $K_i^0H_i$ has empty intersections with H_jK_i, $H_j^0K_i^0$ and $H_j^0K_i$. This implies $K_i^0H_j=H_jK_i^0$. Similarly $H_j^0K_i=K_iH_j^0$. Now, by checking that $g'g^{-1}\in G'$ for each $g, g'\in G'$, it can be proved that G' is a group. Suppose now that G' is a group. The elements of $K_i^0H_j^0$, being the inverses of elements of $H_j^0K_i^0$, belong to G'. They cannot be in H_jK_i, since by assumption $H_jK_i=K_iH_j$. Hence $K_i^0H_j^0$ must be equal to $H_j^0K_i^0$.

Note that this criterion is applicable only when H_jK_i is a subgroup of G itself, but for our purposes this condition will always be fulfilled.

A remark must be made concerning the special case of the direct product ($G=H\otimes K$). All subsets (i), (ii) and (iii) are subgroups, because in that case all required commutations are satisfied.

Thus an algorithm for the derivation of all index-two subgroups of $G=HK$ is obtained.

4. All subgroups of G = HK when K is of order two

When K is of order two ($K = \{e, k\}$) equation (1) yields the following three possibilities: *Case (a).* $|K'| = 1$ (with $|K_e| = 1$). This implies $|H_e| = |H'| = |G'|$ and consequently

$$G' = H_e. \tag{6}$$

Case (b). $|K'| = 2$ and $|K_e| = 2$ (with $|H_e| = |H'| = |G'|/2$). This yields

$$G' = H_e K. \tag{7}$$

Case (c). $|K'| = 2$ and $|K_e| = 1$ (with $|H_e| = |G'|/2$ and $|H'| = |G'|$). Now one has

$$G' = H_e + H_e hk \quad (h \in H \backslash H_e). \tag{8}$$

The situation is similar to the one when index-two subgroups of G are searched for. It has been proved that all subgroups of G = HK are of the forms (a), (b) or (c), but when one tries to obtain all subgroups of G starting with all subgroups H_i of H, then one constructs the sets (6), (7) and (8) and one tests which of them are subgroups.

Subsets (a), i.e. $G' = H_i$ are always subgroups. In the case (b) the commutation of H_i and K is a sufficient and necessary condition for G′ to be a group. In case (c) the following theorem is applied:

Theorem 3. A subset $G' = H_i + H_i hk$ (H_i being a subgroup of H and $h \in H \backslash H_i$) is a subgroup of G = HK ($K = \{e, k\}$) iff the following two conditions are simultaneously satisfied: (1) $hkH_i = H_i hk$ and (2) $(hk)^2 \in H_i$.

Proof. Let G′ be a subgroup of G. Obviously, H_i is a halving subgroup of G′. This implies condition (2) as well as its being invariant (this is sufficient for the validity of (1)). Suppose now that conditions (1) and (2) are fulfilled. Then the fact that G′ is a group follows because $g'g^{-1} \in G'$ for each pair $g, g' \in G'$.

Note that cases (b) and (c) can be treated together, if in equation (8) the condition $h \in H \backslash H_e$ is changed to $h \in H$. Equation (7) is obtained from (8) for $h \in H_e$.

5. The magnetic axial point groups

Axial point groups are point groups consisting of the elements that leave an axis invariant (by definition the z axis). There are seven families of such groups, namely C_n, S_{2n}, C_{nh}, D_n, C_{nv}, D_{nd} and D_{nh} ($n = 1, 2, \ldots$). The groups C_n and S_{2n} are cyclic, with the generators C_n and $\sigma_h C_{2n}$ respectively (C_n is a rotation through $2\pi/n$ around the z axis and σ_h is the reflection in the plane perpendicular to the z axis). The groups of all the other families are semi-direct ($\wedge$) or direct products:

$$\begin{aligned} &C_{nh} = C_n \otimes C_{1h}, \qquad D_n = C_n \wedge D_1, \qquad C_{nv} = C_n \wedge C_{1v}, \\ &D_{nd} = C_{nv} \wedge D_1', \qquad D_{nh} = C_{nv} \otimes C_{1h}, \end{aligned} \tag{9}$$

where $C_{1h} = \{e, \sigma_h\}$, $C_{1v} = \{e, \sigma_v\}$, $D_1 = \{e, U\}$ and $D_1' = \{e, U'\}$ (σ_v is the reflection in a plane containing the z axis, U rotation through π around an axis orthogonal to the z axis, and the prime on U denotes that the angle between the axis of U' and the plane of

σ_v is $\pi/2n$). The following groups are physically equivalent:

$$\begin{aligned} &C_{1h} = C_{1v}, \qquad D_1 = C_2, \\ &D_{1d} = C_{2h}, \qquad D_{1h} = C_{2v}. \end{aligned} \tag{10}$$

Note that in the theory of line groups, these groups are distinct (Vujičić *et al* 1977). Among the axial point groups there are 27 crystallographic groups: C_n, C_{nh} ($n = 1, 2, 3, 4, 6$), C_{nv}, D_n, D_{nh} ($n = 2, 3, 4, 6$), S_{2n} ($n = 1, 2, 3$) and D_{nd} ($n = 2, 3$).

We shall now derive all index-two subgroups of the axial point groups, in order to find all the magnetic axial point groups.

The cyclic group C_n has no halving subgroups if n is odd, and if $n = 2k$ there is only a cyclic one C_k generated by $C_k = C_n^2$. Analogously, the group S_{2n} has exactly one index-two subgroup, C_n, with the generator $C_n = (\sigma_h C_{2n})^2$. In the rest of the families of axial point groups, the second factors in (9) are of order two (having the identity element as the only element of the halving subgroup).

The groups C_{nh} are the direct products $C_n \otimes C_{1h}$ and therefore all the sets (3), (4) and (5) are subgroups. In the case (i) a subgroup C_n is found. Cases (ii) and (iii) exist only for $n = 2k$, when the only halving subgroup of C_n is C_k. The corresponding subgroups are $G' = C_k \otimes C_{1h} = C_{kh}$ and $G' = C_k + C_k C_{2k}\sigma_h = S_{2k}$.

For the groups of the family $D_n = C_n \wedge D_1$, case (i) yields $G' = C_n$. Again, both cases (ii) and (iii) exist iff $n = 2k$. Equality (4) gives $G' = C_k \wedge D_1 = D_k$. Using (5) one finds $G' = C_k + C_k C_{2k} U$, and since $C_k C_{2k}$ commutes with U, G' is a group by theorem 2. One should note that $C_{2k}U$ is a rotation through π about an axis obtained from that of U by a rotation through $\pi/2n$ about the z axis, and consequently the last G' is again D_k. Hence if n is odd the only halving subgroup of D_n is C_n; for $n = 2k$, there is an additional halving subgroup D_k.

A quite analogous procedure in the case of the family C_{nv} gives C_n as a halving subgroup for each n, and especially for $n = 2k$ there is an additional index two subgroup C_{kv}.

As for the family $D_{nd} = C_{nv} \wedge D_1'$, (3) yields $G' = C_{nv}$. Since C_{nv} has two subgroups of index two, C_n and C_{kv} (the last one for $n = 2k$), two sets of type (ii) can be formed. The first of these is $G' = C_n \wedge D_1' = D_n$ (the axis of the rotation U in D_n is just the same as in D_{nd}) and the second one is $G' = C_{kv}D_1'$. Since the element $U'\sigma_v \in D_1'C_{kv}$ is equal to $C_n\sigma_v U'$, which is not in $C_{kv}D_1'$, one concludes that C_{kv} and D_1' do not commute. Therefore G' is not a subgroup in the latter case. Similarly, there are two possibilities (iii). The first is $G' = C_n + C_n\sigma_v U'$ (commutativity of $C_n\sigma_v$ with U' follows from the relation $U'\sigma_v = C_n\sigma_v U'$), and because of $\sigma_v U' = C_{2n\sigma_h}^{-1}$, one has $G' = S_{2n}$. The second one is $G' = C_{kv} + C_{kv}C_{2k}U'$, and it is not a subgroup since the relation $U'\sigma_v C_{2k} = C_k\sigma_v U'$ with $C_k\sigma_v \notin C_{kv}C_{2k}$ implies noncommutativity of the cosets.

The groups of the remaining family D_{nh} are direct products of C_{nv} with C_{1h}. Case (i) gives $G' = C_{nv}$. Again, there are two sets of type (ii): $G' = C_n \otimes C_{1h} = C_{nh}$ and for $n = 2k$, $G' = C_{kv} \otimes C_{1h} = D_{kh}$. Similarly, the subgroups belonging to case (iii) are $G' = C_n + C_n\sigma_v\sigma_h = D_n$ (note that $\sigma_v\sigma_h = U$), and for $n = 2k$, $G' = C_{kv} + C_{kv}C_{2k}\sigma_h = C_{kv} + C_{kv}U' = D_{kd}$.

We have now found all the halving subgroups of the axial point groups. To derive the black and white axial point groups one has to add to these subgroups their cosets multiplied by θ (in the Schönflies notation this is denoted by giving the group and its halving subgroups in brackets). The results are summarised in table 1, in which the grey groups are given, as well as the ordinary axial point groups. In the table, the

Table 1. The magnetic axial point groups: The groups are given in both Schönflies and international notations. Each family of the magnetic groups begins with an ordinary axial group, the black and white groups follow, and the grey group is given last.

	Schönflies		International	
	n even $(2k)$	n arbitrary	n even	n odd
1		C_n	n	n
2	$C_n(C_k)$		n'	
3		$C_n \otimes \Theta$	$n1'$	$n1'$
4		S_{2n}	$(\overline{2n})$	$\bar{n}$
5		$S_{2n}(C_n)$	$(\overline{2n})'$	$\bar{n}'$
6		$S_{2n} \otimes \Theta$	$(\overline{2n})1'$	$\bar{n}1'$
7		C_{nh}	n/m	$(\overline{2n})$
8		$C_{nh}(C_n)$	n/m'	$(\overline{2n})'$
9	$C_{nh}(S_{2k})$		n'/m'	
10	$C_{nh}(C_{kh})$		n'/m	
11		$C_{nh} \otimes \Theta$	$n/m1'$	$(\overline{2n})1'$
12		D_n	$n22$	$n2$
13		$D_n(C_n)$	$n2'2'$	$n2'$
14	$D_n(D_k)$		$n'22'$	
15		$D_n \otimes \Theta$	$n221'$	$n21'$
16		C_{nv}	nmm	nm
17		$C_{nv}(C_n)$	$nm'm'$	nm'
18	$C_{nv}(C_{kv})$		$n'mm'$	
19		$C_{nv} \otimes \Theta$	$nmm1'$	$nm1'$
20		D_{nd}	$(\overline{2n})2m$	$\bar{n}m$
21		$D_{nd}(S_{2n})$	$(\overline{2n})2'm'$	$\bar{n}m'$
22		$D_{nd}(D_n)$	$(\overline{2n})'2m'$	$\bar{n}'m'$
23		$D_{nd}(C_{nv})$	$(\overline{2n})'2'm$	$\bar{n}'m$
24		$D_{nd} \otimes \Theta$	$(\overline{2n})2m1'$	$\bar{n}m1'$
25		D_{nh}	n/mmm	$(\overline{2n})2m$
26		$D_{nh}(C_{nh})$	$n/mm'm'$	$(\overline{2n})2'm'$
27		$D_{nh}(D_n)$	$n/m'm'm'$	$(\overline{2n})'2m'$
28		$D_{nh}(C_{nv})$	$n/m'mm$	$(\overline{2n})'2'm$
29	$D_{nh}(D_{kd})$		$n'/m'm'm$	
30	$D_{nh}(D_{kh})$		n'/mmm'	
31		$D_{nh} \otimes \Theta$	$n/mmm1'$	$(\overline{2n})2m1'$

international notation is used together with that of Schönflies (Bradley and Cracknell 1972).

Besides the 7 families of axial point groups, 7 families of grey and 17 of black and white axial point groups have been obtained. Among them there are 27 crystallographic axial point groups which have already been listed, their 27 grey and 52 associated black and white groups (note that by (10) one has $D_2(D_1) = D_2(C_2)$, $D_{2h}(D_{1h}) = D_{2h}(C_{2v})$ and $D_{2h}(D_{1d}) = D_{2h}(C_{2h})$), and these results are known (e.g. Bradley and Cracknell 1972).

6. Magnetic axial point groups admitting ferromagnetism and ferroelectricity

To determine whether a system with a symmetry of a given magnetic axial point group M can be ferromagnetic or ferroelectric, we use the following procedure. If a system is ferromagnetic (ferroelectric) there must be at least one component of the magnetisation (polarisation) vector which is invariant under all transformations of M, that is, transforms according to the identical representation of M.

The magnetisation (polarisation) vector transforms according to the vector representation $D^{(1)}$ of the rotational group SO(3) and, being an axial (polar) vector, according to the representation $D^{(1)+}$ $[D^{(1)-}]$ of the full rotation–reflection group $O(3) = SO(3) \otimes \{e, I\}$ (I is the spatial inversion). Furthermore, it changes sign under the operation θ, and thus belongs to the representation $D^{(1)+-}$ $[D^{(1)--}]$ of $O(3) \otimes \Theta$.

Each magnetic point group is a subgroup of the group $O(3) \otimes \Theta$. The representation of M according to which the magnetisation (polarisation) is transformed is the subduced representation $D^{(1)+-}(O(3)\otimes\Theta)\downarrow M\,[D^{(1)--}(O(3)\otimes\Theta)\downarrow M]$ of $O(3)\otimes\Theta$ onto M. Therefore, if M admits spontaneous magnetisation (polarisation) then this subduced representation is reducible and at least one of its irreducible components is the identical representation of M. The corresponding vector, carrying the identical representation,

Table 2. The magnetic axial point groups which are compatible with a ferromagnetic phase of the system: For each of these groups (left-hand column) the admissible directions of the magnetisation vector are given (right-hand column).

C_n	$n = 1$	x, y, z
	$n = 2, 3, \ldots$	z
$C_2(C_1)$		x, y
S_{2n}	$n = 1$	x, y, z
	$n = 2, 3, \ldots$	z
C_{nh}	$n = 1, 2, \ldots$	z
$C_{1h}(C_1)$		x, y
$C_{2h}(S_2)$		x, y
D_1		x
$D_n(C_n)$	$n = 1$	y, z
	$n = 2, 3, \ldots$	z
$D_2(D_1)$		x
C_{1v}		y
$C_{nv}(C_n)$	$n = 1$	x, z
	$n = 2, 3, \ldots$	z
$C_{2v}(C_{1v})$		y
D_{1d}		y
$D_{nd}(S_{2n})$	$n = 1$	x, z
	$n = 2, 3, \ldots$	z
$D_{nh}(C_{nh})$	$n = 1, 2, \ldots$	z
$D_{1h}(D_1)$		x
$D_{1h}(C_{1v})$		y
$D_{2h}(D_{1d})$		y

Table 3. The magnetic axial point groups which are compatible with a ferroelectric phase of the system: For each of these groups (left hand column) the admissible directions of the polarisation vector are given (right hand column).

C_n	$n=1$	x, y, z
	$n=2, 3, \ldots$	z
$C_2(C_1)$		x, y
$S_{2n}(C_n)$	$n=1$	x, y, z
	$n=2, 3, \ldots$	z
C_{1h}		x, y
$C_{nh}(C_n)$		z
$C_{2h}(C_{1h})$		x, y
D_1		x
$D_n(C_n)$	$n=1$	z, y
	$n=2, 3, \ldots$	z
$D_2(D_1)$		x
C_{nv}	$n=1$	x, z
	$n=2, 3, \ldots$	z
$C_{1v}(C_1)$		y
$C_{2v}(C_{1v})$		x
$D_{1d}(D_1)$		y
$D_{nd}(C_{nv})$	$n=1$	x, z
	$n=2, 3, \ldots$	z
D_{1h}		x
$D_{1h}(C_{1h})$		y
$D_{nh}(C_{nv})$	$n=1, 2, \ldots$	z
$D_{2h}(D_{1h})$		x

is just the invariant component of magnetisation (polarisation). It can be determined using the group projectors (Lyubarsky 1960) or directly by inspection.

Groups that admit ferromagnetism, together with the possible directions of the magnetisation vector, are given in table 2, and in table 3 the analogous results for ferroelectricity are presented.

7. Conclusions

When the symmetry group of a considered system is a weak–direct product of two of its subgroups, one can use this property to find its halving subgroups and consequently the whole family of the corresponding magnetic groups. It turns out that the axial point groups and line groups are of this structure, and in this paper all the magnetic axial point groups are derived.

Among the 31 families of magnetic axial point groups (17 of them are black and white) those which admit ferromagnetism and ferroelectricity are emphasised. It has been shown that spontaneous magnetisation and polarisation of a system with the symmetry of a non-crystallographic magnetic axial point group has always the direction of the principal axis of rotation.

Subgroups of any index of the axial point groups as well as the magnetic line groups have been already found by the method described in this work, and the results will be reported in a forthcoming paper. Work on the matrix–antimatrix representations of these magnetic groups (Herbut *et al* 1980) is in progress.

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