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Little groups of irreps of $O(3)$, $SO(3)$, and the infinite axial subgroups

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Abstract

A new chain criterion, for the determination of little groups, is presented. This result distinguishes massive (rotationally inequivalent) irrep basis functions and allows for multiple branching paths; consequently, it is suitable for application to Lie groups. Applied to the groups $O(3)$, $SO(3)$, $D_{\infty h}$, D_{∞}, $C_{\infty v}$, $C_{\infty h}$, and C_{∞}, the result enables the enumeration of all possible little groups, together with their associated basis functions. These results are relevant to the determination of the symmetry of a material from its linear and nonlinear optical properties and to the choices of order parameters for symmetry breaking in liquid crystals.

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1. Introduction

Little groups, or isotropy groups, have proved extremely valuable in many disciplines. Essentially, the little group is the exact symmetry, or the largest possible group of transformations, under which a mathematical object, specifically an irreducible representation (irrep), is invariant. Formally, if $|\lambda l\rangle$ is a component (basis function) of an irrep λ of a group G, then the little group $H_{\lambda l}$ may be defined as $H_{\lambda l} = \{g \in G | g|\lambda l\rangle = |\lambda l\rangle\}$. If two irrep vectors λ_a and λ_b exist such that $\lambda_a = g\lambda_b$, then it is clear that λ_a and λ_b must have the same intrinsic symmetry, only re-oriented by the operation g. The corresponding little groups are conjugate and, as such, are equivalent, $H_{\lambda_a} \sim H_{\lambda_b}$. Consequently, the set of all possible different little groups of λ will be discrete, even when G is a Lie group. A three-dimensional irrep of $O(3)$, such as an electric field vector, exemplifies this; it is well known that this irrep only has one possible little group ($C_{\infty v}$) although the three components of the irrep may be combined in uncountably many different ways, such that the C_{∞} symmetry axis may be rotated to point in any direction. This infinite freedom makes the enumeration of all possible little groups of the irreps of Lie groups non-trivial; for discrete groups one may in principle test the behaviour of some $|\lambda l\rangle$ under the application of all the elements of G in turn, but when G is a Lie group the number of elements is uncountably infinite and so the direct approach becomes impossible.

The aim of this paper is to provide a method for enumerating the little groups of Lie groups, and then to apply it to the group $O(3)$ and all of its Lie sub-groups. The value of such results is significant, as applications of the little group concept cover the gamut of theoretical physics and applied mathematics. The utility of the group theoretical approach to symmetry breaking problems arises because, often, the symmetries of solutions do not depend on the details of the governing equations, only their symmetry. Complete solutions still require analysis of the governing equations, but group theoretical selection rules may reduce the manifold of possibilities to a manageable number.

In bifurcation theory (e.g. Keller and Antman 1969), when a bifurcation occurs the symmetry of the solution is often a subgroup of that of the ground state. Examples include the spherical Bénard problem, which involves finding the steady states in the buckling of an elastic spherical shell (like a red blood cell) or in the convection of a viscous fluid confined between two concentric spherical shells (like the magma between the crust and the core of the Earth). It has been successfully approached via the Liapunov–Schmidt reduction (Sattinger 1978), which is contingent upon knowledge of the little groups of $O(3)$ (Ihrig and Golubitsky 1984). A similar problem is that of finding the equilibrium of a rotating self-gravitating fluid. The relevant equations depend on the square of the angular momentum. Consequently, they and their unbifurcated solutions (known as Maclaurin ellipsoids) are invariant under the group $D_{\infty h}$. The first symmetry breaking solutions were found by Jacobi (1834) and are known as the Jacobi ellipsoids (symmetry group D_{2h}). Poincaré (1885) made further contributions. It was not until relatively recently (Constantinescu 1979) that a complete (infinite) set of solutions were found for bifurcations from both the Maclaurin and Jacobi ellipsoids using the little groups of $D_{\infty h}$ and D_{2h}, respectively.

Little groups are frequently used in physics when spontaneous symmetry breaking occurs; solution of the Higgs potential minimum problem often relies on knowledge of the little groups of the relevant representation of the gauge group (Girardi *et al* 1982, p 381). Similar tactics may be adopted to find the symmetry of a system described by the Landau theory of second order phase transitions (Jarić 1986). Since a transition occurs from a more symmetrical group (say G) to a less symmetrical group (say H) one may describe the system in terms of the irreps of G. The order parameter belongs to the identity representation of H but not to the identity representation of G. Thus, a reduction of symmetry $G \to H \subsetneq G$ is most appropriately quantified by an order parameter that has H for its little group. Little group techniques successfully predict all known superfluid phases of He^3 (Vollhardt and Wölfle 1990) and provide the starting point for all phenomenological theories of them. One similar area where little groups have, perhaps, been under-exploited is in the phase transitions of liquid crystals. The nematic and cholesteric phases involve symmetry breaking from $O(3)$, whilst smectic and hexatic phases often break $D_{\infty h}$ symmetry.

Another application that we have in mind is the determination of the symmetry of a system by (for example) experimental measurement of its optical properties, both linear and nonlinear. It is well known that the symmetry of a system may be ascertained to some degree from its spectra, but that the extent to which the symmetry can be pinned down varies with the technique used. For example, the dielectric tensor ε of a crystal usually has a higher symmetry than the crystal point group G: ε is biaxial (diagonal) if $G \subseteq D_{2h}$, uniaxial (diagonal and with $\varepsilon_{xx} = \varepsilon_{yy}$) if $G \nsubseteq D_{2h}$ but $G \subseteq D_{\infty h}$, and isotropic otherwise. The reason is conspicuous from section 5; such a symmetric even-parity second-rank tensor must transform under $O(3)$ as $l^\pi = 0^+ \oplus 2^+$, and the relevant little groups—$O(3)$, $D_{\infty h}$ and D_{2h}—dictate the appropriate form of the tensor. The same mathematics may be applied to justify the manner in which the moment of inertia tensor of undergraduate physics can be represented by an ellipsoid, even for objects with far less or even no symmetry. Another problem that may be similarly elucidated arises in ligand-field theory where experimentalists often use tabulations by point group of the symmetry conditions on ligand-field parameters (Newman 1971). In establishing the non-zero and related elements of such objects, it is normal to assume a particular axis system. However, many spectroscopic fitting techniques (such as the fitting of the parameters in a crystal-field Hamiltonian to an observed energy level spectrum) are ignorant of the coordinate system used in the theory, and are vulnerable to the associated introduction of unphysically high numbers of parameters. Such results, familiar in the folklore of crystal-field theory, can be put on a firmer foundation by recognizing them as consequences of the identification of little groups for the relevant $O(3)$ tensors. For example, in the ligand-field theory of a system with symmetry C_{4h} inclusion of the parameter A^4_{4-} (the coefficient of the corresponding tesseral harmonic Z^l_m with $l = 4$, $m = 4-$) in a level fitting program leads to indeterminancy in the fitting procedure, because its value is arbitrary in the sense that one may rotate the coordinates about the z axis by any angle ϕ, changing the relative size of this parameter and A^4_{4+}; hence a least squares fit becomes indefinite through the ambiguity in the choice of ϕ. Instead, one should define A^4_{4-} to be zero, as if the symmetry were D_{4h}. Section 5 gives a group-theoretic reason for this observation: D_{4h}, but not C_{4h}, is a little group for $l = 4^+$ (the parity of a crystal-field Hamiltonian is positive since it acts within the d-electron manifold), and the tensorial structure appropriate to D_{4h} should therefore be used.

The results presented here are therefore of immediate interest in the theory of liquid crystal phase transitions and in the identification of molecular symmetries from their spectra. They are, however, of far more general application, as indicated above.

2. Chain criteria for little group identification

Several authors have investigated the little groups of the rotation group $SO(3)$. No fully reliable algorithm for determining the little groups of $O(3)$ or $SO(3)$ has previously been reported.

Listings have been made of the little groups of the irreps (l^π where $l = 0, 1, 2, \ldots$, and $\pi = \pm 1$) of $O(3)$. In many works, a chain criterion has been the central consideration. Such criteria have been discussed extensively (Birman 1966, Goldrich and Birman 1968, Boccara 1973, Cracknell *et al* 1976, Lorenc *et al* 1980, Birman 1982, Jarić 1982, Przystawa 1982, Gaeta 1984). The chain criterion has passed through several modifications in the literature, and the little group listing alters with each modification. Problems in the analysis of Boccara (1973), for example, are mentioned in appendix A. The remainder of this section begins with a critical examination of the two most important works on the little groups of $O(3)$, those of Michel (1980) and of Ihrig and Golubitsky (1984). Then, in section 2.3, our main result, the massive chain criterion, which allows correct enumeration of the little groups of $O(3)$, is presented.

2.1. Michel criterion

A systematic determination of the little groups of $SO(3)$ was made by Michel (1980). He used a form of the chain criterion (his lemma 2) except in the case of all cyclic groups, where little groups were determined by inspection. The present work gives two small corrections to Michel's list. First, $SO(3)$ is only trivially a little group for a non-identity irrep. Second, Michel's identification of D_2 as a little group for $l = 3$ is incorrect (see appendix A). This indicates an inadequacy in his chain criterion. The aim of this paper is to find an approach that generates the correct little groups and to extend the analysis to find the most general vector in the group representation space for a given little group, generalizing these results to cover irreps of the full rotation group $O(3)$. Michel notes that this is trivial in the case of positive parity representations if one knows the results for $SO(3)$. This is because the full rotation group is an outer direct product group: $O(3) = SO(3) \times Z_2 = Z_2 \times SO(3)$, where Z_2 denotes the parity (inversion) group. Thus, if a representation belongs to the identity irrep of Z_2, its little groups will simply be the direct product of Z_2 with the relevant $SO(3)$ little groups. In the case of negative parity no such simple prescription exists as improper operations may still be present (as in the intrinsic symmetry of a true vector such as the electric field, the symmetry of which is $C_{\infty v}$).

In his lemma 2 and table A.2, Michel (1980) used a group subduction criterion which may be rephrased in the following form. If H is to be a little group of an orthogonal irrep $\lambda\,(G)$, for a strictly larger intermediate subgroup H' such that $H \subset H' \subset G$, and in particular for a group H' adjacent to H in this group coupling chain, then

$$c_\lambda(H') < c_\lambda\,(H)\,. \tag{1}$$

In this equation $c_\lambda\,(H)$ is the subduction frequency for H in $\lambda(G)$, namely the number of occurrences of the identity irrep $0\,(H)$ in $\lambda\,(G)$; it is readily determined from the Weyl trace formula $c_\lambda(H) = \sum_{h\in H} \chi^{\lambda(G)}\,(h)\,/\,|H|$.

From the above chain criterion the largest group H that has a particular $c_\lambda(H)$ is the little group of that particular linear combination of basis functions. If one moves from a little group to the next group up the group chain then the value of $c_\lambda(H)$ decreases because that increase in symmetry removes one or more of the basis functions that were allowed at the lower symmetry. The little group is then the maximal symmetry of some linear combination of basis functions. A simple illustration of the application of this chain criterion is given in appendix A, where the tables give the group–subgroup branching relations needed for the use of the chain criterion for the 32 crystallographic point groups and also for other groups of interest in our applications. The entries are the subduction frequencies, or number of times the invariant $0(H)$ occurs in $\lambda(G)$. Equation (1) is a useful necessity condition for H to be a little group.

Jarić (1982) noted the failure of the chain criterion to be sufficient for a Lie group. There are two reasons for the lack of sufficiency. Even for finite groups equation (1) can fail to be a sufficiency condition, because multiple group–subgroup coupling chains connecting H' and H need special consideration. In addition, the little group is the *maximal* symmetry group as its symmetry elements do not have to share the axes of the same elements in the parent group. Every function in the basis set can have its own orientation relative to the supergroup axes. For example, C_s is not a little group of $1^-(O(3))$ in spite of its conformity to this chain criterion. The conformity is shown because the vector irrep $1^-\,(O(3))$ branches twice to $0\,(C_s)$, once more than in any of its supergroups C_{5h}, C_{5v}, C_{2h}, C_{2v}, C_{3v} which are maximally connected (i.e. which have no intervening group in the chain). However, these numbers reflect the fact that all the components are tied to the same choice of rotation axes and mirror plane. When the axis choice can be tailored individually to the basis functions their symmetry is seen to be much higher than this, and in fact the little group of the functions in $1^-\,(O_3)$ is uniquely $C_{\infty v}$, the intrinsic symmetry group of any polar vector. As another example, $2(SO\,(3))$ reduces to more invariants in the maximal subgroup C_2 of D_2 than it does in D_2 itself; again, more invariants appear at the C_1 level. However, C_1 and C_2 are not little groups of $2(SO\,(3))$. The (real and orthogonal) basis functions $Z^2_{1+} = xz$, $Z^2_{2+} = x^2 - y^2$ in $2\,(SO\,(3))$ both have D_2 symmetry, but about different axes. In addition, their linear combination has no two-fold symmetry about an axis in the same plane; yet it has D_2 symmetry about oblique axes.

These examples show that the symmetries of all these functions cannot be tested at once within a global choice of axes by counting the increases in the number c_λ of invariants as the symmetry is lowered simply by removing group elements relative to those axes. An approach is needed in which bases are allowed to be fully flexible so as to investigate the maximal symmetry of any function.

2.2. *Ihrig and Golubitsky criterion*

Michel (1980) left the Parthian challenge: 'we leave to the reader the study of the representations 1−'. The challenge was taken up by Ihrig and Golubitsky (1984). Their work is the most sophisticated to date and has been accepted by subsequent workers as the definitive result.

Ihrig and Golubitsky (1984) observe: 'unfortunately, Michel's criterion for determining when a subgroup is actually an isotropy subgroup (lemma 2) is incorrect as stated', and 'in section 5 we give a correct version of this lemma (see lemma 5.3). Its proof is involved. It seems likely that the condition we give is both necessary and sufficient though we have not been able to prove this'. Our results show that their lemma 5.3 is necessary but not sufficient for the group $O(3)$, and not all their identifications are correct.

Initially, Ihrig and Golubitsky (1984) undertake to find the maximal little groups of $O(3)$, stating: 'it is harder for a system to break more symmetries than less'. This, the so-called maximality conjecture, has been part of the folklore of phase transition and gauge field theory for 20 years. Its general applicability was disproved by Jarić (1983). Ihrig and Golubitsky (1984) then embark on the task of finding all of the little groups of $O(3)$, a task described as 'a much more difficult calculation'.

Ihrig and Golubitsky's (1984) central result, proposition 5.3, is another refinement of the chain criterion. Rather than depending on an increase in the total subduction frequency, Ihrig and Golubitsky propose that the following inequality must be satisfied in a $H' \supset H$ if H is to be a little group of $\lambda\,(G)$:

$$c_\lambda(H') - \dim N_{\mathrm{G}}\left(H'\right) < c_\lambda(H) - \dim N_{\mathrm{G}}\left(H, H'\right). \qquad (2)$$

In this the following definitions are used. As above, $c_V(G)$ (which Ihrig and Golubitsky write as $\dim V^G$) is the subduction frequency for the group G in the vector V, namely the number of occurrences of the identity irrep $0(G)$ in the set V. In the case of c_λ $V = V_\lambda$, the set of basis functions of the irrep $\lambda\,(G)$.

The normalizer $N_{\mathrm{G}}\,(H)$ of any $H \subset G$ is the largest subgroup of G that contains H as an invariant subgroup: $N_{\mathrm{G}}\,(H) \equiv \{g \in G \mid gHg^{-1} = H\}$ (see Fraleigh 1994). For $K \subset H$, $N_{\mathrm{G}}\,(K, H) \equiv \{g \in G \mid gHg^{-1} \supset K\}$. For a group, $\dim G$ is the Lie group dimension of the manifold of G, namely the number of infinitesimal generators in G. As we deal only with subgroups of $O(3)$, $\dim G = 3$ if $G = O(3)$ or $SO(3)$, $\dim G = 1$ if G is one of the infinite axial groups, and $\dim G = 0$ if G is a finite group. The normalizer of a finite subgroup of $O(3)$ is usually also a finite group and so of dimension zero. The exceptions are the normalizers of any of the Abelian subgroups of $O(3)$. Any subgroup of an Abelian group is an invariant subgroup, so that the normalizer of any Abelian subgroup of $O(3)$ will always contain C_∞ and will thus always be one-dimensional.

This refinement of the chain criterion by Ihrig and Golubitsky (1984), introducing the dimensions of the normalizers, shows cognisance of the basic problems with the Michel criterion, and is closer to a sufficiency condition. The differences are discussed in sections 2.3, 5.2 and appendix A. We note here that the little groups of $SO(3)$ generated by their method mostly agree with Michel (1980), including the erroneous assignment of D_2 in $l = 3$; they disagree with Michel (1980) by assigning O and not T as a little group of $l = 3$;

these changes are retrograde as erroneous. For positive parity irreps of $O(3)$, their results are completely incorrect; none of the groups they list are little groups. For negative parity irreps in $O(3)$ their results are not consistently presented. On the most favourable rationalization of this problem, they are incorrect in assigning T as a little group in $l = 3^-, 4^-$. It follows that equation (2) is not sufficient.

2.3. Massive chain criterion

We introduce now a modified criterion which we call the massive chain criterion; we find it to be fully reliable as a sufficiency as well as necessity condition within subgroups of $G = O(3)$. This criterion states that $H \subset G$ is a little group of an orthogonal irrep $\lambda\,(G)$ if and only if for each strictly larger and adjacent group H' (so that $H \subset H' \subset \cdots \subset G$),

$$c_\lambda(H') - f_\lambda^0\left(H'\right) < c_\lambda(H) - f_\lambda^0\,(H)\,. \tag{3}$$

Here we call $f_\lambda^0\,(H)$ the massless subduction frequency; it will be defined below. $f_\lambda^0\,(H)$ redeems the failure of earlier chain criteria to recognize adequately that the shape of a basis function is independent of any $O(3)$ rotation, and that the attendant freedom of its axis choice has to be taken into account in determining whether it is an invariant with respect to any potential little group H. Comparing equations (1)–(3), we note that the massless subduction frequency $f_\lambda^0\,(H)$ plays the role of Ihrig and Golubitsky's correction term $\dim N_{\rm G}(H, H')$ in refining the Michel criterion. We shall illustrate that $f_\lambda^0(H)$ can differ from $\dim N_{\rm G}(H, H')$ by more than a constant even in subgroups of $O(3)$.

Another practical difference with both Michel (1980) and with Ihrig and Golubitsky (1984) is the emphasis on checking the criterion in each possible coupling chain $H' \supset H$. This is an important check when there are multiple chains, to avoid H being credited with little group character when that application should really be to some higher group. This explains at least some of the explicit errors in earlier work.

Let $V_\lambda\,(H)$ be the subset of functions in V_λ (a set of orthogonal functions forming a basis of $\lambda\,(G)$) that are invariant under H. The basis is chosen to maximize the number of functions in the subset $V_\lambda\,(H)$. The dimension of V_λ is therefore c_λ, the number of occurrences of $0\,(H)$ in λ. At this stage no transformations of G may be applied to demonstrate such an H-invariance; the basis functions, once chosen, are fixed and elements of G that are retained in its subgroup H have unchanged orientations.

We now define the massless subduction frequency by determining the extent to which the members of $V_\lambda(H)$ are in fact equivalent under transformations of G. We partition $V_\lambda\,(H)$ into two sets, a 'massless' subset $V_\lambda^0\,(H)$ and a 'massive' subset $V_\lambda^m\,(H)$, so that each member of $V_\lambda^0\,(H)$ when transformed by a suitable element of G is identical to some member of $V_\lambda^m\,(H)$. The partition is made so as to maximize the dimension $f_\lambda^0\,(H)$ of $V_\lambda^0\,(H)$ within the irrep λ. In other words, G-equivalent functions in V_λ are separated, one being partitioned off to $V_\lambda^0\,(H)$ until no two members of $V_\lambda^m\,(H)$ are identical under a transformation of G. $V_\lambda^m\,(H)$ contains one and only one of each of the shapes represented by the members of V_λ; $V_\lambda^0\,(H)$ contains any duplicate shapes (functions which are equivalent under G-transformation). This defines the 'massless subduction frequency' $f_\lambda^0\,(H)$. The massive subduction frequency is the dimension $f_\lambda^m\,(H)$ of $V_\lambda^m\,(H)$, and is therefore given by

$$f_\lambda^m\,(H) = c_\lambda - f_\lambda^0\,(H)\,. \tag{4}$$

The terms 'massless' and 'massive' are chosen in analogy with Higgs theory (see, for example, Weinberg 1996) where a unitarity transformation (the analogue of the G operations above, and in particular to rotations for $SO(3)$) removes the basis functions of the gauge group that correspond to massless particles. The analogy is particularly close when little groups are applied to spontaneous symmetry breaking. Only massive components contribute to the homogeneous Hamiltonian. The massless components become important in the inhomogeneous part of the Hamiltonian because they give rise to Goldstone modes, and the number of Goldstone modes must equal the number of massless components.

With these definitions, equation (3) then gives

$$f_\lambda^m(H') < f_\lambda^m(H) . \tag{5}$$

When this inequality holds, a new shape (characterized independently of its orientation) has appeared, and because it is invariant under H and not under any supergroup H' its symmetry is H. This is the condition for H to be a little group of $\lambda(H)$. By construction, then, equation (3) takes fully into account the complications in the subduction formula caused by the freedom of axis choice.

We now search for an algorithm to calculate the massless subduction frequency $f_\lambda^0(H)$ in subgroups of $G = O(3)$ and $SO(3)$. First, the value of $f_\lambda^0(H)$ is limited by the need to have at least one massive function, $f_\lambda^m(H) \geqslant 1$ within a finite subspace V_λ of dimension dim V_λ (or $|\lambda|$). Hence $f_\lambda^0(H) \leqslant \dim V_\lambda - 1$, which is $2l$ in the irrep $l^\pi(O(3))$. The next aspect is the extent to which linearly independent functions can be generated from any basis function while respecting H symmetries. The general rule for this pays particular attention to the degrees of freedom of the group; linear independence is then possible because of the continuous value of the possible rotation (Ihrig and Golubitsky 1984). There are three cases to consider. We summarize the results here; illustrations of such points are discussed in the next section.

First, if there are no symmetry axes in H (i.e. for $H = C_i$ or C_1), all basis functions are H-invariant; $V_\lambda(H) = V_\lambda$; any rotation of $O(3)$ will carry any basis function into another H-invariant function. Using the three generators of $SO(3)$, three linearly independent functions can be generated from any member of $V_\lambda^m(H)$ by rotation if the space is sufficiently big (dim $V_\lambda > 2$), so that in these cases $f_\lambda^0(H) = 3$.

Second, for the groups $H = O(3)$, $SO(3)$, $D_{\infty h}$, D_∞, $C_{\infty v}$, Y_h, Y, O_h, O, T_h, T_d, T, D_{nh}, D_{nd}, D_n, C_{nv} there are at least two non-collinear symmetry axes. Hence any member of $V_\lambda(H)$, being invariant under H, must also have a fixed orientation, and must be uniquely aligned with these two axes. No continuous rotational degrees of freedom exist to preserve the H-invariance and yet secure linear independence of any basis function, and so no massless basis functions are possible: $f_\lambda^0(H) = 0$.

Third, if all the symmetry axes of H are the same, as for $H = C_{\infty h}$, C_∞, C_{nh}, C_{ni}, C_n, S_n, C_s at most one generator of $O(3)$ can act to change the orientation of any function nontrivially. In the case of the Abelian groups $H = C_{\infty h}$, C_∞ dim $V_\lambda = 1$, there is no possibility of a massless function and even this rotation is powerless to make the original basis function $\exp \mathrm{i}m\phi$ linearly independent of its rotated form; $f_\lambda^0(H) = 0$ in these groups. In the remaining groups (C_{nh}, C_{ni}, C_n, S_n, C_s) no such simplification arises and, corresponding to the number of generators, $f_\lambda^0(H) = 1$ if dim $V_\lambda > 1$.

We now enshrine this argument and its conclusions in a formula. The number of degrees of freedom of the group H, the Lie dimension of the normalizer group of H, is defined as dim $N_{\mathrm{G}}(H)$; it gives information on the number of independent H-invariant basis functions which might be obtained from a member of the massive subset by an equal number of types of rotations (Ihrig and Golubitsky 1984). Because of the above-mentioned problem with C_∞ and $C_{\infty h}$ (and this is one point of departure from Ihrig and Golubitsky (1984) in this paper), we should subtract from dim $N_{\mathrm{G}}(H)$ the Lie dimension of H, dim H; this denotes the one situation in which one degree of freedom fails to generate an independent basis function (the third case above). That this is the only category of exceptional cases is confirmed by inspection, and that confirmation (together with the provision of a number of illustrations) is the function of sections 3–5 in the argument of this paper. Taking into account the dimensional restriction discussed above, we may then define

$$\bar{f}_\lambda(H) = \dim N_G(H) - \dim H \qquad f_\lambda^0(H) = \min\left[(\dim V_\lambda - 1), \bar{f}_\lambda(H)\right]. \tag{6}$$

This completes the definition of the massive chain criterion. The results of its application are tabulated in appendix B.

Note that $N_G(H) \supseteq H$, so that $\dim N_G(H) - \dim H \geqslant 0$. The number of massless components of an irrep that subduces some group is not just the number of degrees of freedom in orienting the basis functions, but this quantity minus the number of generators in the group. The term $(\dim V_\lambda - 1)$ is important only for small irreps, with $|\lambda| \leqslant 3$, which are easily dealt with by inspection.

For $|\lambda| > 3$, the Ihrig and Golubitsky (1984) criterion, equation (2), and the massive chain criterion of equation (3) agree if

$$\dim N_G(H, H') = \dim N_G(H) + \dim H' - \dim H. \tag{7}$$

In many cases this holds true. Ihrig and Golubitsky consider the case of $H = C_n$ and $H' = C_\infty$ in some detail and find that $\dim N_G(H, H') = \dim N_G(H)$. Our above-mentioned point of departure reflects the fact that $\dim C_\infty = 1$ although $\dim C_n = 0$, violating equation (7) and making the increase in the number of massless components in going from C_∞ to C_n equal to one, not zero. This illustrates the insufficiency of the criterion of equation (2). The difference between $f_\lambda^0(C_\infty)$ and $f_\lambda^0(C_n)$ explains why we use a stronger criterion than do Ihrig and Golubitsky (1984). The above analysis certainly confirms that Ihrig and Golubitsky's proposition 5.3 is a necessity condition within the group $O(3)$, and as such is a stronger condition than that of Michel (1980).

Although the massive chain criterion only provides a slightly stronger inequality than that of Ihrig and Golubitsky's work for some cases in respect of $O(3)$, it is unwise to conclude that these two different inequalities will provide much the same results when applied to more complicated Lie groups. Indeed, that these two different inequalities provide similar results for $O(3)$ can be understood through consideration of the concept of the normalizer group. Since the normalizer of any group with respect to $O(3)$ is, by definition, a subgroup of $O(3)$, it follows that its dimension can only be three (if it is $O(3)$ or $SO(3)$), one (if it is one of the infinite axial groups) or zero (if it is any finite group). The dimension of a Lie group is identified in all of this work with the dimension of its group manifold. If one considered a group with a larger manifold (for example the group $SU(5)$, which is 24-dimensional) then it seems likely that discrepancies could become much more significant.

This analysis explains why, when inequality 5.3 of Ihrig and Golubitsky (1984) is so similar to equation (5), these authors identify some little groups incorrectly. The case of the group D_2 for $l = 3(SO(3))$ is instructive; this case is also incorrectly identified as a little group by Michel (1980). Previous authors would not have found this to be a little group if they had deployed the correct form of the chain criterion for dealing with multiple inequivalent group chains, namely, if they had required the criterion to hold for each possible H' such that $H' \supset H$.

Finally, we note that Ihrig and Golubitsky's (1984) results (corollaries 6.7 and 6.9) and our results (section 6) for little groups of $O(3)$ for $l \geqslant 30$ are in complete agreement.

3. The infinite axial groups

We now determine the little groups of all irreps of C_∞, $C_{\infty h}$, $C_{\infty v}$, D_∞ and $D_{\infty h}$. While some of these are well known, this is a complete list and the results give a useful illustration of the concept of massless functions, a vital step in the recognition of a more general chain criterion. One example of the physical interest of these groups is that in nematic liquid crystals we start not from $O(3)$ but from D_∞ or $D_{\infty h}$, since it is the reduction of this symmetry which may be the decisive step.

The group C_∞, isomorphic to the group $U(1)$, has one-dimensional irreps; for the irrep labelled m the basis function is the complex number of unit modulus: $m \to \mathrm{e}^{\mathrm{i}m\phi}$. Inspection or Michel's chain criterion (equation 1) show that the little groups are C_∞ for $m = 0$ and $C_{|m|}$ for all other m.

In $C_{\infty h}$ also the irreps are one-dimensional. To apply the chain criterion we need the branchings $C_{\infty h} \supset C_{nh}$, C_{ni} (n odd), C_∞; C_{nh} (n even) $\supset C_n$, C_i, C_s; C_{nh} (n odd) $\supset C_n$, C_s; $C_{ni} \supset C_n$, C_i; $C_n \supset C_1$, the lower-order cases of which are tabulated in appendix B. The little groups (with the relevant irreps in brackets) are as follows: $C_{\infty h}(0^+)$, $C_\infty(0^-)$, $C_i(1^+)$, $C_s(1^-)$; $C_{nh}(n^+)$ and $C_n(n^-)$ for n even, $n \geqslant 2$; $C_{ni}(n^+)$ and $C_{nh}(n^-)$ for n odd, $n \geqslant 3$.

The one-dimensional irreps of the groups $C_{\infty v}$, D_∞ and $D_{\infty h}$ may be dealt with similarly, generalizing the tabulated branchings to $C_{\infty v} \supset C_{nv}$, C_∞; $C_{nv} \supset C_n$, C_s. These groups all have two-dimensional representations, and the Michel chain criterion is not sufficient. Consider the first two-dimensional irrep 1 of $C_{\infty v}$. The only non-zero subduction frequencies are $c_1(C_s) = 1$ and $c_1(C_1) = 2$.

C_s is clearly a little group for the irrep 1, because C_s is the first group for which the massive subduction frequency is non-zero. If the dimension of the representation vector is one, it cannot have any massless components. Since there exists only a single axis of symmetry (the direction perpendicular to the plane) and no infinitesimal generators, any representation vector that subduces the identity of C_s and that has C_s as its little group must have exactly one massless component. Now consider the irrep spanned by $\{Z_m^{1^-}\}$, where $Z_{m\pm}^l$ is a tesseral harmonic. This subduces the group $C_{\infty v}$ once (which as we have seen is its only little group). The subduction frequency of the group C_{nv} remains unity for all $n > 1$. The group C_{1v} is the group C_s and its identity representation is subduced twice by the irrep $Z_m^{1^-}$. However, according to the new rules, this is not a new little group because the massive subduction frequency must be the ordinary subduction frequency minus one (for the one massless component). Since the massive subduction frequency remains equal to one, the shape of the representation function and hence its little group cannot have changed.

However, C_1 is not so clear. The basis functions of $\lambda = 1$, the tesseral harmonics Z_{1+}^l and Z_{1-}^l, transform into each other under rotations, and a linear combination of them has the same symmetry as either of the functions individually. It follows that there is only one little group for the irrep 1 and that its most general representation vector is two-dimensional. The same argument applies to all irreps of this group for $m > 0$; a linear combination of the basis functions $\sin m\phi$ and $\cos m\phi$ is another sinusoidal function with the same period. The little groups for each irrep, stated in brackets with the dimension of the basis functions, are: $C_{\infty v}$ (0, 1); C_s (1, 2); C_{nv} (n, 2).

A similar approach suffices in the cases of the two-dimensional irreps of D_∞ and $D_{\infty h}$, and inspection of either basis function gives each little group. For D_∞ the little groups are $D_\infty\,(A_1, 1)$, $C_\infty\,(A_2, 2)$, $C_2\,(E_1, 2)$, $D_n\,(E_n, 2)$. For $D_{\infty h}$, we have $D_{\infty h}(A_1^+, 1)$, $D_\infty(A_1^-, 1)$, $C_{\infty h}(A_2^+, 1)$, $C_{\infty v}(A_2^-, 1)$; $C_{2h}(E_1^\pm, 2)$, $D_{nh}(E_n^+, 2)$ and $D_{nd}(E_n^-, 2)$ for n even; $D_{nd}(E_n^+, 2)$ and $D_{nh}(E_n^-, 2)$ for n odd.

4. Inspection of the $O(3)$ little group analysis

We claim the massive chain criterion to give the full solution of the problem. However, we aim in this and the next section to illustrate and confirm its conclusions by inspection of the results.

Ultimately establishing the sufficiency of a chain condition involves the explicit demonstration of a function within the irrep space with the symmetry of the candidate little group. This is a safeguard against producing yet another abstract argument in favour of yet another inadequate criterion. We might first inspect the symmetry elements of any function with respect to a global axis choice, then convert the results of this inspection into a sufficiency condition by showing that no rotation of axes will reveal new symmetry elements.

In the following, we use an inspection-based approach to examine the individual functions $\{|\lambda l\rangle \mid l \in \lambda\}$ of the chosen basis for the irrep space λ. Their maximal symmetries will be called the *basis* little groups. For $G = O(3)$, $\lambda = l^{\pi}$, and we choose as basis the tesseral harmonics $|\lambda l\rangle \rightarrow \eta Z^{l}_{m\pm}(\theta, \phi)$ (suppressing the arguments for simplicity), $m = 0, 1, 2, \ldots, l$ with a scalar or pseudoscalar factor η to adjust the parity from polar to axial respectively (scalar if $\pi = (-1)^{l}$, pseudoscalar otherwise). Inspection of the symmetries and identification of the little group of each such function is particularly straightforward, the best choice of axes being conspicuous for such fundamental functions. This nomenclature cannot avoid the arbitrariness of the basis choice. However, an optimal or even near-optimal choice of basis (in our case the tesseral harmonics) enables the identification of a maximal number of little groups at the basis level, leaving fewer to be found in the later steps.

We must consider other little groups corresponding to the symmetries of all possible linear combinations $\sum_l a_l|\lambda l\rangle$ of the basis vectors $\{|\lambda l\rangle \mid l \in \lambda\}$. The literature is ambivalent about the necessity of this, but we believe that any linear combination is of as much interest in our applications as are the basis functions. General linear combinations are those for which the same little group applies to functions for a continuous range of the coefficients $\{a_l\}$ of the basis functions $\{|\lambda l\rangle\}$. The consideration of general linear combinations is a trivial problem for vectors; all linear combinations give another vector of the same parity and so the same little group. Determining the symmetry of a general linear combination is nontrivial, interesting and analytically solvable for second rank tensors $2(SO(3))$, i.e. the $l = 2$ irrep of $SO(3)$ (and similarly for $O(3)$). Here the existence of higher symmetries for oblique axes is very important. For higher irreps l of $O(3)$, we proceed by a combination of inspection with guidance from the chain criterion and the group-chain pedigree of any invariant function.

Suppose that two basis functions $|\lambda l_1\rangle$, $|\lambda l_2\rangle$ with little groups H_1, H_2 are linearly combined. The linear combination obviously includes all joint symmetries, and possibly no others. Hence their common symmetry elements will make $H_{12} = H_1 \cap H_2$ a candidate little group. (The intersection $\cap$ needs to be performed recognizing that the axes of H_1 and H_2 may not be parallel, this being already ascertained in the step of discovering the basis little groups.) Hence the invariant count in H_{12}, a subgroup of H_1 and of H_2, satisfies $c_\lambda(H_{12}) \geqslant c_\lambda(H_1) + c_\lambda(H_2)$. This relation follows from the linear independence of the basis functions $|\lambda l_1\rangle$, $|\lambda l_2\rangle$ which demonstrate the basis little group status of H_1 and H_2, because each of these increments the invariant count. As little groups, H_1, H_2 have at least one invariant each, so that each term in this inequality is nonzero. If, for at least one of the group–subgroup paths $H_1 \supset H_{12}$, $H_2 \supset H_{12}$ any intermediate group H', if it exists, has no invariants extra to those of the higher group H_1 or H_2, the invariant count $c_\lambda(H_{12})$ is greater than that of an adjacent higher group and the Michel chain criterion is obeyed. However, before one can conclude that H_{12} is a little group, it needs to be verified that a linear combination of basis functions has no further symmetries which are generated by the linear combination, and that its symmetries are exhibited only by a suitable axis rotation.

As an example, consider linear combinations in $l = 2$. $Z^2_{2-} \propto xy$ is a D_2 invariant in the chain $O(3) - O_h - O - T - D_2$ (forcing the C_2' axis through the cube edge) while $Z^2_{2+} \propto x^2 - y^2$ is a D_2 invariant in the chain $O(3) - O_h - D_{4h} - D_4 - D_2$ (forcing the C_2' axis to a face centre). In this way the possibilities for extra little groups become denumerable, as in the chain criterion analysis, and can be given geometric character. Some of the subtler points in implementing this are exemplified by Reid and Butler (1982). The program RACAH was used to confirm the symmetry of some more complicated basis functions. While this approach was restricted as above to a subset of axis choices and so still has a 'basis function' flavour, the axis choices are very much more numerous and apposite, and the results are adequate in their variety to cover all the possible little groups revealed by the chain criterion. For example, neither inspection of common symmetry elements nor the program RACAH captures the retention of D_2 symmetry in a general linear combination of Z^2_{2+} and Z^2_{2-}, which is easily revealed by a suitable rotation about the z axis; however, either of these functions suffices to illustrate the little group character of D_2 in a way which is conveniently covered by its symmetry elements under the standard axis choice.

Special linear combinations may exist in which only a unique set of coefficients will give the symmetry in question. The chain criterion of equation (1) is a reliable indicator since the requisite linear combination will be unique to the group in question and the invariant count will not be reflected in a supergroup. In the tesseral harmonic basis we use, such special combinations may be expected at rank 4 (for a cubic function necessarily involving the special linear combination of equation (10)).

C_i and C_1 might be expected to be little groups in all irreps of $O(3)$, for positive and negative parity respectively, as the probable symmetries (i.e. no rotational symmetry) of a fully general linear combination of the basis functions. As noted below, this argument does not work in the cases $l = 1, 2$. We now give a general approach to understanding this, and the allied results for $l \geqslant 3$; and not only this, but a general attack on the problem of dealing with the variation and uncertainty of the axis choice that best reveals the symmetry of each linear combination.

If any linear combination $\sum_{m\pm} a_{m\pm} Z^l_{m\pm}$ is invariant under a general rotation operator $O_\phi(\boldsymbol{n})$ with representation matrix $O^l_{mm'}(\phi, \boldsymbol{n})$, where ϕ has an arbitrary axis $\boldsymbol{n}$,

$$O^l_{mm'}(\phi, \boldsymbol{n})\, a_{m'} = a_m. \tag{8}$$

Hence $|\boldsymbol{O}^l(\phi, \boldsymbol{n}) - \boldsymbol{I}| = 0$, and because under a rotation of $\boldsymbol{n}$ to the z axis, $\boldsymbol{O}^l(\phi, \boldsymbol{n}) - \boldsymbol{I} = \boldsymbol{R}(\boldsymbol{O}^l(\phi, \boldsymbol{z}) - \boldsymbol{I})\boldsymbol{R}^\dagger$, the determinant of a matrix product is the product of the determinants, $|\boldsymbol{O}^l(\phi, \boldsymbol{z}) - \boldsymbol{I}| = 0$. Conversely, any rotation operator $O_\phi(\boldsymbol{z})$ (and therefore any $O_\phi(\boldsymbol{n})$) satisfies $|\boldsymbol{O}_\phi(\boldsymbol{n}) - \boldsymbol{I}| = 0$ in the basis Z^l_m, since it leaves Z^l_0 unchanged. We ask now that the condition for a particular linear combination be invariant under any such rotation. A minimum condition is that both ϕ and $\boldsymbol{n}$ have to be chosen appropriately to the choice of $\{a_m\}$. To explore this, for convenience we switch temporarily to a spherical harmonic basis, in which $O^l_{mm'}(\phi, \boldsymbol{z}) = \delta_{mm'} \exp(\mathrm{i}m\phi)$ and we use the corresponding component labels $\pm m$. With this substitution equation (8), while making no demand of a_0, requires the following conditions on the possible linear combinations which are invariant under O_ϕ. First $a_1 = a_{-1} = 0$; it is not possible for the factor $\exp(\pm\mathrm{i}\phi) - 1$ to vanish for nontrivial ϕ. This vanishing of $a_{\pm 1}$ can always be achieved by a judicious choice of the two Euler angles (rotating the function $a_m Z^l_m$) and so defining the direction of the axis $\boldsymbol{n}$. Since for $l = 1$ this concludes the requirements, and is always possible for any ϕ given an appropriate axis $\boldsymbol{n}$, a general linear combination of $l = 1$ functions always has at least C_∞ symmetry. This line of argument may be extended to $l \geqslant 2$ (see appendix C), but the reliability of the massive chain criterion (section 2.3) reduces the importance of this to a check.

5. Lower-order little groups of $O(3)$ and $SO(3)$

We distinguish polar (true) and axial tensors: polar tensors of rank l reflect 'naturally', having parity $\pi = \pi_l \equiv (-1)^l$, whereas axial tensors of that rank have parity $-\pi_l$. The basis functions

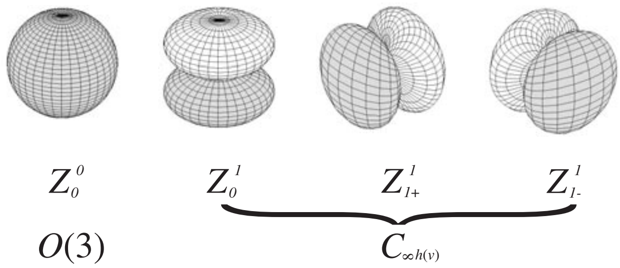

Figure 1. Basis functions of $l = 0, 1$ ($O(3)$). Some of the relevant little groups are indicated below, the bracketed indices indicating the changes between positive and negative parity in $O(3)$ and between $O(3)$ and $SO(3)$.

under consideration, with the relevant basis little groups as established by inspection, are depicted in the various figures; little groups for positive parity are on the left, and for negative parity on the right, in each figure.

5.1. $l = 0, 1$

For $l = 0$ we have trivially the basis function η and the following little groups.

Positive parity: 0^+ *(polar: invariant).* η is a scalar, and the little group is the full group $O(3)$.

Negative parity; 0^- *(axial, pseudoscalar).* η is a pseudoscalar, and the little group is the full group $SO(3)$.

For $l = 1$, figure 1 shows the angular dependence of the basis functions $\eta\{Z^1_{m\pm}\}$ (the labels $m\pm$ denote the full set $0, 1\pm, \ldots, l\pm$ in general).

Positive parity 1^+ *(pseudovector, axial).* η is a pseudoscalar. By inspection the basis little group is $C_{\infty h}$. (This preserves an axial vector. Under $\sigma_h = \sigma_{xy}$, a reflection in the xy plane normal to the C_∞ axis, a plain 1^- spherical harmonic reverses; the pseudoscalar factor also reverses and restores the sign; a magnetic field is unchanged by a reflection in a plane to which it is perpendicular.)

Negative parity 1^- *(natural, polar).* η is a scalar. The basis little group is $C_{\infty v}$ which preserves a polar vector in the reflection plane.

For either parity, any linear combination can only give another such vector, with the same symmetry. Note that C_i is not a little group of 1^+, or C_1 of 1^-; the symmetry of a general linear combination of $l = 1$ functions is always at least C_∞. This illustrates that the chain criterion fails as a necessity condition, even for finite groups, since (in the case of positive parity for example) the value (3) of c_1 (C_i) is greater than for any supergroup (appendix B). A proof that C_∞ is the minimum rotational symmetry is given in section 4.

We note that equations (5) and (6) yield these results; the dim $V_\lambda - 1$ restriction requires $f^0 < 3$. According to the above $f^0 = 0$ for $D_{\infty h}$, $C_{\infty h}$, $C_{\infty v}$, and according to appendix 2 the nonzero subduction frequencies are $c_{1+}(C_{\infty h}) = 1 = c_{1-}$ $(C_{\infty v})$.

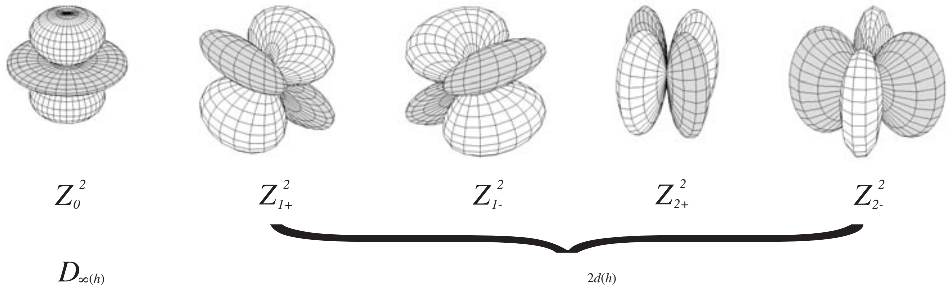

Figure 2. Basis functions of $l = 2$ ($O(3)$) as for figure 1.

5.2. $l = 2$

The case of $l = 2$ is nontrivial. However, it is familiar in the form of the representations found in the inertia tensor of rigid bodies in classical mechanics. Such tensors contain both the 0 and 2 irreps of $SO(3)$, and are isomorphic to a real symmetric traceless 3×3 matrix. Figure 2 shows the basis functions $\eta\{Z^2_{m\pm}\}$. The functions $\eta\{Z^2_{m\pm}|m > 0\}$ are equal modulo a rotation.

Positive parity 2^+ *(natural, polar).* η is a scalar. The maximal symmetries of ηZ^2_0 and $\eta\{Z^2_{m\pm}|m > 0\}$ give $D_{\infty h}$ and D_{2h}, respectively. The axes of the former are standard (z for C_∞, x say for C_2 in D_∞); the axes of the latter are oblique and m-dependent. This is a dramatic example as to why merely working out intersections of groups is not reliable in analysing linear combinations; the D_2 axes of the functions $\{Z^2_{m\pm}|m > 0\}$ are all different. This also illustrates why C_i is not necessarily a little group of l^+.

Negative parity 2^- *(pseudotensor, axial).* η is a pseudoscalar. The maximal symmetries of ηZ^2_0 and $\{\eta Z^2_{m\pm}|m > 0\}$ are D_∞ and D_{2d}, respectively. As for the case of positive parity, the axes of the former are standard (z for C_∞, x say for C_2 in D_∞); the axes of the latter are oblique and m-dependent.

The general linear combination of $\{Z^2_{m\pm}\}$, $a(2z^2-x^2-y^2)+2bxy+2cyz+2dzx+e(x^2-y^2)$ can be written $(x, y, z)M(x, y, z)^{\mathrm{T}}$ where the matrix M and its eigenvector matrix R are

$$M = \begin{pmatrix} e-a & b & d \\ b & -e-a & c \\ d & c & 2a \end{pmatrix} \qquad R = \begin{pmatrix} w_{11} & w_{21} & w_{31} \\ w_{12} & w_{22} & w_{32} \\ w_{13} & w_{23} & w_{33} \end{pmatrix}. \tag{9}$$

Since M is symmetric and real (Hermitian), its eigenvalues λ_a are real and its eigenvectors $\boldsymbol{w}_a$ are orthogonal in the sense $\boldsymbol{w}^*_a \cdot \boldsymbol{w}_b = 0$. Hence the eigenvector matrix R where w_{ab} is the bth component of w_a is unitary and also diagonalizes $M : RMR^\dagger = \mathrm{diag}\,(\{\lambda_a\})$. Since the matrix elements (as well as the eigenvalues) are real, the basis vectors can be chosen to be real, and R is orthogonal and so a rotation matrix. This defines a basis change under which such a linear combination can be reduced to a linear combination of the diagonal terms x^2, y^2 and z^2, i.e. the functions Z^2_0, Z^2_{2+}, whose combined rotational symmetry is D_2. Hence D_2 is the minimal symmetry of a general linear combination at $l = 2$, and no new little groups arise.

Another way of understanding this result is to note that symmetric functions of second rank must be linear combinations of x^2, xy, y^2, xz, yz, z^2. Of these the invariant $x^2 + y^2 + z^2 \sim 0$ can be removed, leaving 5 rank two functions, according to the symmetric square of the vector irrep in $SO(3)$: $1^{\otimes\{2\}} = 2 \oplus 0$. Three coefficients (of xy, yz, zx say) can be chosen to be zero by appropriate choice of a rotation (the three Euler angles). This leaves two functions, $x^2 - y^2 \sim Z^2_{2+}$ and $3z^2 - r^2 \sim Z^2_0$.

Once again this illustrates the failure of the Michel chain criterion as a necessity condition, since (in the case of positive parity for example) the value (5) of c_2 (C_i) is greater than for any supergroup (see appendix B). Another proof that D_{2h} (for positive parity) and D_2 (for negative parity) is the minimum symmetry is given in section 4.

5.3. $l = 3$

It was proved in section 4 that, for $l \geqslant 3$, a truly general linear combination cannot have any rotational symmetry element. Hence C_i and C_1 are little groups for positive and negative parity, respectively.

Positive parity 3^+ *(pseudotensor, axial).* When we apply the massive chain criterion (using the group branchings and subduction frequencies of appendix B) for $l = 3^+$, the only groups for which the subduction frequency increases also exhibit an increase in the massive subduction frequency. These groups are $C_{\infty h}$, T_h, D_{3d}, C_{3i}, C_{2h} and C_i.

These results are the same as those of Michel (1980, table A.2) except that they do not include the group D_{2h}. Ihrig and Golubitsky (1984) also find the group D_{2h} in this case. The reason that D_{2h} is not included here is that it is a subgroup of T_h, and the subduction frequency is the same (1) for both these groups. This error probably arose because the subduction frequency does increase in the chain $D_{\infty h} \supset D_{nh} \supset D_{2h}$ because the subduction frequency for all such supergroups of D_{2h} is zero. This illustrates the need to test the chain criterion for all possible supergroups.

Negative parity 3^- *(natural, polar).* Application of the massive chain criterion to the case of the seven-dimensional irrep of $O(3)$ with negative parity yields the little groups: $C_{\infty v}$, T_d, D_{3h}, C_{3v}, C_{2v}, C_s and C_1. There are other groups for which the subduction frequency increases. However, in all of these cases the massive subduction frequency is the same as that of a supergroup. For example, the group S_4 has a subduction frequency of 2, but a massive subduction frequency of 1 in common with its supergroup T_d. Detailed inspection generates the same results as those above. The detailed inspection method in 3^- needs care over whether the group C_2 should be included in the set of little groups. Any linear combination of Z^3_0, $Z^3_{2\pm}$ has C_{2v} symmetry, because this group is the intersection of their symmetry elements. But Z^3_{3+} and Z^3_{2-} have only C_2 for a common symmetry group, suggesting that C_2 is a new little group for 3^-. In fact, an arbitrary linear combination of these functions has the full C_{2v} symmetry. Such a linear combination can be generated from another that obviously has C_{2v} symmetry, $a\left(Z^3_0 + Z^3_2\right) + bZ^3_{-2}$, when rotated by the transformation: $x \to -z$, $y \to y$, $z \to x$. This also shows that the choice of the two vectors with C_{2h} symmetry for 3^+ simply amounts to a choice of coordinate system.

The basis functions connected with these little groups in 3^+, 3^- are listed in appendix C, because of their interest in calculation of property tensors. Figure 3 gives the form of the full basis for $l = 3$, and the tables of section 6 indicate the symmetries of these functions.

5.4. $l = 4$

As for $l = 3$, C_i and C_1 are general little groups for positive and negative parity, respectively. We inspect the symmetries of the basis functions $\eta\{Z^4_{m\pm}\}$ (figure 5, table B.3) for the basis little groups.

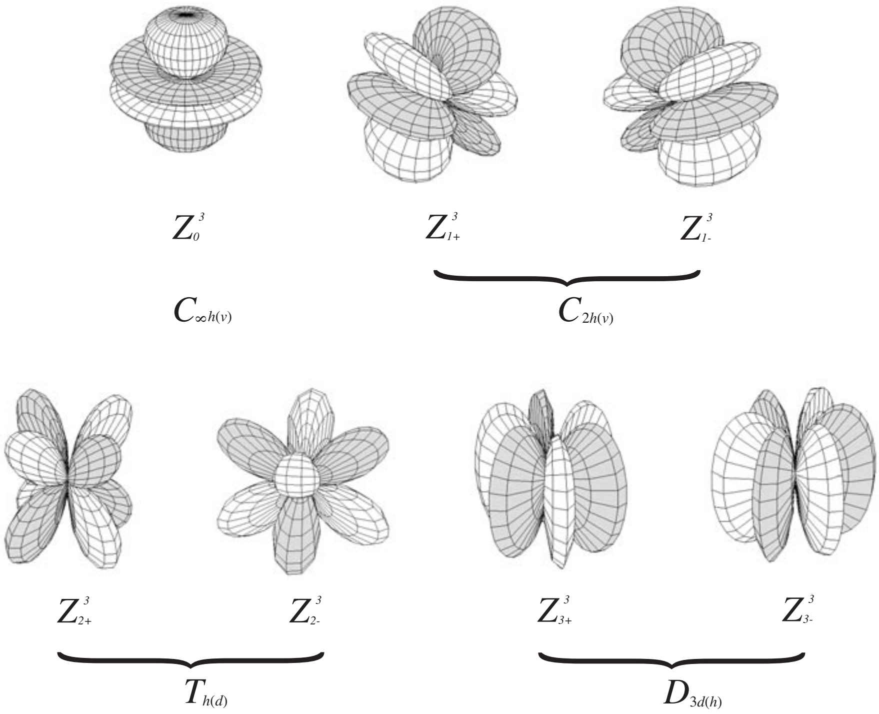

Figure 3. Basis functions of $l = 3$ ($O(3)$) as for figure 1.

Positive parity 4^+. The basis little groups are $D_{\infty h}$, C_{2h}, D_{2h}, D_{3d}, D_{4h} (for $|m| = 0, 1, 2, 3, 4$, respectively).

Negative parity 4^-. The basis little groups are D_∞, C_{2v}, D_{2d}, D_{3h}, D_{4d} (for $|m| = 0, 1, 2, 3, 4$, respectively).

We form a histogram from the relevant column ($4\pm$) of table B.1 of the numbers of invariants, and inspect the points of increase as the symmetry is lowered. For *positive* parity ($l^\pi = 3^+$), $D_{\infty h}$, O_h have 1 invariant. D_{4h}, D_{3d} have 2 invariants. D_{2h}, C_{3i}, C_{4h} have 3 invariants. C_{2h} has 5 invariants. C_i has 7 invariants. This accounts for the basis and general little groups, and also gives the candidates O_h, C_{3i} and C_{4h}.

O_h is a little group, an example of such an invariant being the special combination

$$\zeta = \left(\sqrt{7}Z^4_0 + \sqrt{5}Z^4_{4+}\right)/2\sqrt{3}. \tag{10}$$

Such results (see appendix C for others) are most easily obtained from RACAH.

C_{3i} possesses 3 invariants; it is a subgroup of 2 basis little groups, $D_{\infty h}$ and D_{3d}, giving two invariants from Z^4_0 and Z^4_{3+}. The third invariant therefore has to be sought elsewhere. Table B.3 shows that the only possible additional function is Z^4_{3-}. However, its inclusion with Z^4_0 and Z^4_{3+} can be frustrated by a rotation about z, and the combination of Z^4_0 with either Z^4_{3+} or Z^4_{3-} has a higher symmetry. Hence C_{3i} is not a little group. (If we seek it from ζ of equation (10), on the grounds that C_{3i} is also a subgroup of O_h, we then have to rotate ζ so that the C_3 axis is common, and the basis reduces to the set Z^4_0, Z^4_{3+}, Z^4_{3-}.)

This leaves C_{4h}. This is a subgroup of $D_{\infty h}$ and O_h (whose invariants, involving as they do different linear combinations of Z_0^4 and Z_{4+}^4, are linearly independent), and has a third invariant. The four-fold axis shows (from table B.3) that this can only arise from another linear combination of Z_0^4 and $Z_{4\pm}^4$, but this can be frustrated by a rotation about z. Hence C_{4h} is not a little group.

Hence O_h is the only general little group for 4^+.

For *negative parity* 4^-(axial), D_∞, O, D_{2d} and D_{3h} have 1 invariant; D_4, D_3, S_4, C_{3h} and C_{2v} have 2 invariants; D_2, C_3 and C_4 have 3 invariants; C_s has 4 invariants; C_2 has 5 invariants, and C_1 has 7 invariants. This confirms the little group status of D_∞, C_{2v}, D_{2d}, D_{3h}, D_{4d} and C_1; this leaves O, D_4, D_3, D_2, S_4, C_{3h}, C_4, C_3, C_2, C_s to be discussed. We seek invariant functions for each of these groups from the set $\{Z_0^4, Z_{2\pm}^4, Z_{3\pm}^4, Z_{4\pm}^4\}$ as before.

O is a little group from equation (10).

D_4 and C_4 both require a four-fold axis, and so must be found in the subset $\{Z_0^4, Z_{4\pm}^4\}$. A z rotation eliminates, say, Z_{4-}^4, and from table B.3 the remaining joint symmetry includes a two-fold operation and so is indeed D_4, which becomes a little group. Since this symmetry is higher than C_4, the latter is not a little group; its candidacy assumed the necessity of admixing Z_{4-}^4. A similar argument is true for S_4, the claim for whose candidacy also requires both of $Z_{4\pm}^4$.

D_3, C_{3h} and C_3 all require a three-fold axis, and so must be found in the subset $\{Z_0^4, Z_{3\pm}^4\}$. A z rotation eliminates, say, Z_{3-}^4, and from table B.3 the remaining joint symmetry elements, C_{3z}, C_{2y} and C_{2e} give D_3 as the only little group. In particular, no reflection is possible. The appearance of C_{3h} from the chain criterion is understandable on the basis of the combination $Z_{3\pm}^4$, itself neutralized by a z rotation, and similarly C_3 on the basis of combining Z_0^4, $Z_{3\pm}^4$.

The subset $\{Z_0^4, Z_{2+}^4\}$ similarly reveals D_2 as a little group, and the elimination of Z_{2-}^4 by rotation also eliminates C_2.

This leaves C_s, whose candidacy is explained by noting that the linear combination of $\{Z_{2-}^4, Z_{3-}^4, Z_{4-}^4\}$ has from table B.3 only the reflection symmetry σ_{xz}. One of these three functions can be eliminated by z rotation. If we choose this to be Z_{3-}^4, not only is σ_{xz} common to both the remaining functions, but C_{2z} is also present. Hence C_s is not a little group.

Hence O, D_4, D_3 and D_2 are general little groups for 4^-.

6. Little groups for any l

The subgroups of $O(3)$ and their group–subgroup relations are well known; in seeking a general solution we require analytical formulae for the subduction frequencies of these various groups. First, consider the tetrahedral group T. From the Weyl trace formula from section 2.2 and noting from its character table that T contains the following elements (with multiplicities in brackets): $C_1(1)$, $C_3(4)$, $C_3^2(4)$, $C_2(3)$ the subduction frequency is given by

$$\begin{aligned} c_\lambda(T) &= \frac{1}{12}\left(\frac{\sin\left(\left(l+\frac{1}{2}\right)2\pi\right)}{\sin(\pi)} + 8\frac{\sin\left(\left(l+\frac{1}{2}\right)\frac{2\pi}{3}\right)}{\sin\left(\frac{\pi}{3}\right)} + 3\frac{\sin\left(\left(l+\frac{1}{2}\right)\pi\right)}{\sin\left(\frac{\pi}{2}\right)}\right) \\ &= \frac{1}{12}(2l+1) + \frac{4}{9}\sqrt{3}\left(\sin\frac{\pi}{3}(2l+1)\right) + \frac{1}{4}\left(\sin\frac{\pi}{2}(2l+1)\right) \\ &\equiv 2\left[\frac{l}{3}\right] + \left[\frac{l}{2}\right] - l + 1 \end{aligned}$$

where the last equivalence follows for l being an integer. The square bracket denotes the floor function, namely the largest integer less than or equal to the argument. This result also applies to the group T_h for positive parity irreps. The same procedure allows us to determine formulae for other subduction frequencies such as Y and O (also in $SO(3)$; these hold also for $O(3)$ for either parity) and Y_h and O_h (for positive parity), also a formula can be obtained for T_d (for negative parity) as given in tables B.1 and B.2. For the moment we concentrate on $SO(3)$ and table B.1.

Ihrig and Golubitsky (1984) augment the trace formula and correctly generate subduction frequencies for groups such as C_n for arbitrary values of n. For this presentation we proceed partly via inspection as deployed initially by Ihrig and Golubitsky in the groups C_∞ and C_n and then apply the massive chain criterion. The dimension of the fixed point set must be unity for C_∞ because there is just one tesseral harmonic basis function, Z_0^l, that is invariant under infinitesimal rotations about an axis. From our earlier discussion the subduction frequency for C_∞ must be equal to the massive subduction frequency (i.e. unity). Furthermore, as Ihrig and Golubitsky also observe, the fixed point set for the group C_n will include all basis functions where n divides $|m|$. It follows that the fixed point set will always include the basis function $m = 0$ and twice (one for $+m$ and one for $-m$) the floor of l divided by n. The case of C_1 has already been dealt with, the conclusion being that it is a little group for all $l \geqslant 3$ with a subduction frequency of $2l + 1$.

The subduction frequency of D_∞ for all odd l must equal zero as only even l basis functions contain even powers of $\cos\theta$ (θ being the polar variable) and so only they have the two-fold symmetry perpendicular to the infinity-fold axis found in the group D_∞. Thus even l irreps subduce the identity representation of D_∞ once. The only other subgroups of $SO(3)$ are the groups D_n for all $n > 1$. If l is even the fixed point set obviously includes $m = 0$ (little group D_∞). It is clear from the case of C_n that basis functions for which m is an integer multiple of n will contribute to the fixed point set of D_n. However, they will only contribute to the fixed point set in such a way that the two-fold axes perpendicular to the n-fold axis coincide for all basis functions. This means that only one basis function for a given $|m|$ will contribute to the fixed point set. For even l and even n one may choose all appropriate m to be positive. For even l and odd n one may choose odd m negative and even m positive. For odd l one must exclude $m = 0$ (little group C_∞). If n is even one may take all relevant m to be negative. When n is odd one may choose the odd m positive and the even m negative. The preceding results with the massive chain criterion (section 2.3) produce the complete set of results for the little groups of $SO(3)$ in table B.1. The basis functions for the groups T, O and Y are not as simply stated; only particular combinations of the tesseral harmonic basis functions have the requisite symmetry. They may be determined for any particular case by using the program RACAH (appendix C). In this sense group branching arguments fully accommodate the effects of axis freedom.

We now consider little groups of irreps of $O(3)$. The results for positive parity irreps are trivially derived from the little groups of $SO(3)$ (see caption to table B.2); the subduction frequencies and representation vectors are exactly the same for these irreps. The case of negative parity may be attacked in exactly the same way as that of positive parity. The only caution applies to finding the general vectors for cases such as D_n where one must again be sure that the two-fold axes of different basis functions coincide. Also, one must be sure that basis functions that are included in the fixed point set do actually possess the requisite symmetry. For example, the group D_{4d} does not contain D_{2d}; the supergroups of D_{nd} are D_{pnd} where p is any odd positive integer. The cases of D_{nh}, C_{nh} and S_n are similar. The results for $l > 0$ are given in table B.2. In our choice of basis we follow the convention (see section 5.3) in which the massless components that are eliminated are those with $m = 1\pm$ and one of the smallest $|m| > 1$ possible where necessary (often $m = 2-$).

The group O_h is maximally connected to $O(3)$: there are no subgroups of $O(3)$ that are supergroups of O_h. It follows that O_h will be a little group for any irrep that subduces its identity more than zero times (except the identity irrep $l^\pi = 0^+$). The same is true of the group Y_h. In the case of the groups O, Y and T_d one may note that they are only connected to $O(3)$

via inversion supergroups. It follows that, since these non-inversion groups can only be little groups of negative parity irreps and since inversion groups are always subduced zero times by negative parity irreps, then they will be little groups for any negative parity irrep l^π, $l > 0$ for which $c_\lambda > 0$. Since the subduction frequency is partly a periodic function and partly a linear function, the largest value of l for which the subduction frequency could be zero is obtained by comparing the linear part to the largest negative value generated by the periodic part. This gives the little groups in the first 5 rows of table B.2.

The cases of T_h for positive parity and T for negative parity require a further observation. Suppose for some irrep of a group G there exist at least two little groups: A and B. Further, suppose that A and B are not group–subgroup related. It follows that at least one of the massive components of the most general representation vector with little group A must be different from that with little group B. The representation vector that subduces the identity representation of any subgroup of A must contain all of the components of the representation vector that subduces the identity of A. The same is true for any subgroup of B. Now consider a group C that is a subgroup of both A and B. It follows immediately that the massive subduction frequency of C must be strictly greater than that of either A or B (whichever is the larger). Hence C must also be a little group of G for the irrep under consideration. This means that both T_h (supergroups Y_h and O_h) and T (supergroups Y, O and T_d) must be little groups for all l^π (respectively positive and negative parity) greater than or equal to 30. Since the subduction frequencies given above must be the massive subduction frequencies for these groups (which have non-collinear axes) it is a simple matter to apply the massive chain criterion for all l less than 30. This procedure determines that table B.2 gives the only irreps for which T_h and T are little groups.

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Appendix A. Comparisons with earlier work and chain criteria

We give here some details of where previous work differs from this paper, and a simple example of the use of subduction.

Boccara (1973) observes that the representation l^+ (for odd l) subduces the identity of C_∞. This is true, but C_∞ is not the relevant little group as claimed. Boccara states: 'pseudo-tensorial order parameters cannot be used to characterise phases with unproper symmetry elements'. One counterexample is given by the pseudotensorial irrep 1^+ of $O(3)$ (the symmetry of the magnetic field) which contains the little group $C_{\infty h}$ and so an improper element (the mirror reflection σ_h). Indeed, the irreducible Cartesian tensor manifestation of all irreps l^+ will be pseudotensorial for all odd l. If an irrep transforms as the identity (+) representation of the inversion group, its little group must contain the inversion, an improper symmetry element. Many of the pseudotensorial irreps that have negative parity have little groups that contain reflection or rotation–reflection elements. Boccara also neglects all of the octahedral, tetrahedral and icosahedral groups, and we note that, contrary to Boccara, $3^- \downarrow 0\,(D_2)$.

Ihrig and Golubitsky (1984) use a group notation which is translated into the Schönflies notation by: $O(2) \to D_\infty$, $O(2)^- \to C_{\infty v}$, $I \to Y$, $O^- \to T_d$, $D_n^z \to C_{nv}$, $Z_n \to C_n$, $1 \to C_1$; $D_{2n}^d \to D_{nd}$ when n is even and $D_{2n}^d \to D_{nh}$ when n is odd; $D_2^d \to C_{2v}$, $Z_{2n}^- \to S_{2n}$ when n is even and $Z_{2n}^- \to C_{nh}$ when n is odd ($Z_2^- \to C_s$); the inversion group corresponding to the rotation group G is $K \oplus G$. In $SO(3)$, Ihrig and Golubitsky (1984) agree with Michel (1980) except for the seven-dimensional irrep: $l = 3$. Here, Ihrig erroneously finds O where Michel (1980) correctly finds T. In common with Michel (1980) Ihrig and Golubitsky (1984) include (erroneously, as we show) the group D_2 as a little group for $l = 3$. For rotation–reflection groups, a fundamental problem is that Ihrig and Golubitsky do not specify the parity of the $O(3)$ irreps under discussion. In the case of positive parity, none of the little groups are correctly identified. Entries in their table B.2 are inconsistent with their theorem 6.8 (Ihrig and Golubitsky 1984). For example, in their table B.2 the groups listed include D_{3h} (for $l^{\pi} = 3^-$) and D_{5h} (for $l^{\pi} = 5^-$). Their theorem 6.8 (part f) includes the statement: 'D^d_{2n}, for $1 < n < l$ except D^d_4 when $l = 3$'. For D_{3h} (for $l^{\pi} = 3^-$) and D_{5h} (for $l^{\pi} = 5^-$) to enter, this relation should rather contain: $1 < n \leqslant l$; the strict inequality would be an error according to the present work, and is inconsistent with their tabulation of C_2 and T under $l^{\pi} = 3^-$. The present work agrees with the first inequality as strict; however, this is inconsistent with their listing of D^d_2 for $l^{\pi} = 5^-$. We retain the first inequality as strict and interpret the strictness of their second inequality as a typographical error. On this favourable reading, the little groups of $O(3)$ of theorem 6.8 of Ihrig and Golubitsky (1984) give results in agreement with the present results for negative parity (only), except for their inclusion of T as a little group of 3^- and 4^-. From appendix B, we note that T_d supplants T as the proper little group in 3^-, and O similarly supplants T in 4^-; the relevant subduction frequencies do not increase on descending from these groups to T. In each case, just this part of the multiple branching diagram fails to satisfy the chain criterion.

Jarić (1986) quotes this work; his own work does not resolve these problems. Some minor corrections to Jarić (1986) may be noted. Figure 1 of Jarić covers all invariants constructible from powers of a rank L tensor via a sequence of ladder diagrams in which all lines have rank L. Jarić's ladder construction gives an overdetermined set of invariants (in fact an infinite set of relations), of which the first two alone are pure: $l = 0, L$. The remaining ones are arbitrarily written linear combinations of these and the other $2L - 2$ independent invariants. There are linear combinations between these when some or all the rank L terminals are equal, corresponding to the reductions that occur when symmetrization of the product is made. If they are equal in pairs, the tree angular momenta are even, halving the number of invariants from $2L$ to L. When all four terminals are equal, the further linear relations that must exist are unknown; Jarić appeals to the integrity basis analysis result of Bistricky *et al* (1982) to show that the number of invariants is halved again. It is better to have a single tree diagram as in Jarić's $\bar{I}^{4,1}_L$, not a sequence of ladder diagrams, and to allow all values $l = 0, 1, 2, \ldots, 2L$ of the coupled irreps consistent with Kronecker products, not just L. This labels the possible independent invariants uniquely—completely and without repetition—in the case that no symmetrizations are applicable and the terminal tensors are different (though all of rank L). (Jarić's equations (2.1) and (2.2) need a factor $2\sin^2\phi/2$ in the integrand to give the correct measure; this does not affect his conclusions.) Applications of integrity basis theory are discussed by McLellan (1980), and graphical methods have been used for integrity bases in $SO(n)$ by Ichinose and Ikeda (1997). The integrity bases of $O(3)$ have been extended to the case of several tensors and related to angular momentum coupling trees for spin 1 and $\frac{1}{2}$ (Minard *et al* 1983, Riddell and Stedman 1984, Stedman 1990).

Finally, we give a simple but nontrivial application of the chain criteria, namely the little groups of the tetrahedral group T. Consider the group chains $T \supset D_2 \supset C_2 \supset C_1$; $T \supset C_3 \supset C_1$. From character theory we obtain for irrep A the subduction frequencies $c_A(T, D_2, C_3, C_2, C_1) = 1$. Hence the little group of A is T (as is appropriate for the identity representation). For the irrep E the frequencies are: $c_E(T) = 0$, $c_E(D_2) = 1$, $c_E(C_2) = 1$, $c_E(C_3) = 0$, $c_E(C_1) = 1$. Hence D_2 is the little group for E (or E', the complex conjugate irrep). The three-dimensional irrep F has the subduction frequencies: $c_F(T) = 0$, $c_F(D_2) = 0$, $c_F(C_2) = 1$, $c_F(C_3) = 1$, $c_F(C_1) = 3$. Hence one of the basis functions of F has the little group C_2 while another has the little group C_3. Finally the linear combination of these two may be combined with the third basis function, reducing the symmetry to that of the trivial little group C_1. This gives the little groups of the irreps of the tetrahedral group as T [1](A), D_2 [1] (E, E'), C_2 [1], C_3 [1], C_1 [3](F). The numbers in square brackets indicate the dimension of the most general vector in the representation space of T that has this little group.

Appendix B. Tables relevant to little group analysis

Tables B.1 and B.2 give the results of deducing the little groups from the massive chain criterion. Table B.3 gives the subduction frequencies $C_\lambda(H)$ from the Weyl trace formula, as used for the traditional criteria. Tables B.4 and B.5 give the little groups of $SO(3)$ ($l = 0$–4) and $O(3)$ ($l = 0$–9), both parities respectively.

Table B.1. Irreps of $SO(3)$ for which the stated groups are little groups when $l > 0$. The special cases for Y are $l = 6$, 10, 12, 15, 16, 18, 20–22, 24–28. Representation vectors for Y, O, T may be determined from RACAH for each l (see appendix C for examples). $\kappa \equiv (-1)^k$.

H	$c_l(H)$	General	Special l	Representation vectors
Y	$\left[\frac{l}{5}\right]+\left[\frac{l}{3}\right]+\left[\frac{l}{2}\right]-l+1$	$l \geqslant 30$	Caption	—
O	$\left[\frac{l}{4}\right]+\left[\frac{l}{3}\right]+\left[\frac{l}{2}\right]-l+1$	$l \geqslant 12$	4, 6, 8, 9, 10	—
T	$2\left[\frac{l}{3}\right]+\left[\frac{l}{2}\right]-l+1$	$l \geqslant 9$	3, 6, 7	—
D_∞	1	l even	—	Z_0^l
C_∞	1	l odd	—	Z_0^l
D_n	$\left[\frac{l}{n}\right]$	l odd, $2 \leqslant n \leqslant l \geqslant 4$	$l = n = 3$	$Z_{n,-\kappa}^l, Z_{2n,-\kappa}^l, Z_{3n,-\kappa}^l \cdots$
D_n	$\left[\frac{l}{n}\right]+1$	l even, $2 \leqslant n \leqslant l \geqslant 4$	$l = n = 2$	$Z_0^l, Z_{n\kappa}^l, Z_{2n\kappa}^l, Z_{3n\kappa}^l \cdots$
C_n	$2\left[\frac{l}{n}\right]+1$	l even, $2 \leqslant n \leqslant l/2$	—	$Z_0^l, Z_{n+}^l, Z_{2n+}^l, Z_{3n+}^l \cdots$
C_n	$2\left[\frac{l}{n}\right]+1$	l odd, $2 \leqslant n \leqslant l$	—	$Z_0^l, Z_{n+}^l, Z_{2n+}^l, Z_{3n+}^l \cdots$
C_1	$2l+1$	$l \geqslant 3$	—	$Z_0^l, Z_{2+}^l, Z_{3\pm}^l, Z_{4\pm}^l, \ldots$

Table B.2. Irreps l^- ($O(3)$) for which the stated (non-inversion) groups are little groups when $l > 0$. The little groups for irreps $l^+(O(3))$ are the inversion groups, and the results may be obtained from table B.1 with the mappings $D_\infty \to D_{\infty h}$, $C_\infty \to C_{\infty h}$, $Y \to Y_h$, $O \to O_h$, $T \to T_h$, ($D_n \to D_{nh}$, $C_n \to C_{nh}$ if n is even), ($D_n \to D_{nd}$, $C_n \to C_{ni}$ if n is odd). The special cases for Y are $l = 6$, 10, 12, 15, 16, 18, 20–22, 24–28. $\kappa \equiv (-1)^k$, $\mu \equiv (-1)^l$, $\nu \equiv \kappa\mu$.

H	$c_{l^\pi}(H)$	General	Special cases	Representation vectors
Y	$\left[\frac{l}{5}\right]+\left[\frac{l}{3}\right]+\left[\frac{l}{2}\right]-l+1$	$l \geqslant 30$	Caption	—
O	$\left[\frac{l}{4}\right]+\left[\frac{l}{3}\right]+\left[\frac{l}{2}\right]-l+1$	$l \geqslant 12$	4, 6, 8, 9, 10	—

Table B.2. (Continued)

H	$c_{l^\pi}(H)$	General	Special cases	Representation vectors
T_d	$\left[\frac{l+2}{4}\right]+\left[\frac{l}{3}\right]+\left[\frac{l+1}{2}\right]-l$	$l \geqslant 9$	3, 6, 7	—
T	$2\left[\frac{l}{3}\right]+\left[\frac{l}{2}\right]-l+1$	$l \geqslant 12$	6, 9, 10	—
D_∞	1	l even	—	Z^l_0
$C_{\infty v}$	1	l odd	—	Z^l_0
D_{nd}	$[(l+n)/2n]$	n even, $2 \leqslant n \leqslant l \geqslant 4$	$n=l=2$	$Z^l_{n\nu}, Z^l_{3n\nu}, Z^l_{5n\nu}\cdots$
D_{nh}	$[(l+n)/2n]$	n odd, $2 \leqslant n \leqslant l \geqslant 4$	$n=l=3$	$Z^l_{n\nu}, Z^l_{3n\nu}, Z^l_{5n\nu}\cdots$
D_n	$\left[\frac{l}{n}\right]+1$	l even, $2 \leqslant n \leqslant l$	—	$Z^l_0, Z^l_{n\kappa}, Z^l_{2n\kappa}, Z^l_{3n\kappa}\cdots$
D_n	$\left[\frac{l}{n}\right]$	l odd, $2 \leqslant n \leqslant l/2$	—	$Z^l_{n,-\kappa}, Z^l_{2n,-\kappa}, Z^l_{3n,-\kappa}\cdots$
C_{nv}	$\left[\frac{l}{n}\right]$	l even, $2 \leqslant n \leqslant l/2$	—	$Z^l_{n-}, Z^l_{2n-}, Z^l_{3n-}\cdots$
C_{nv}	$\left[\frac{l}{n}\right]+1$	l odd, $2 \leqslant n \leqslant l$	—	$Z^l_0, Z^l_{n+}, Z^l_{2n+}, Z^l_{3n+}\cdots$
C_{nh}	$2\left[\frac{l+n}{2n}\right]$	n odd, $3 \leqslant n \leqslant l/3$	—	$Z^l_{n+}, Z^l_{3n\pm}, Z^l_{5n\pm}\cdots$
C_s	$2\left[\frac{l+n}{2n}\right]$	l even, $l \geqslant 4$	—	$Z^l_0, Z^l_{2+}, Z^l_{3+}, \ldots, Z^l_{l+}$
C_s	$2\left[\frac{l+n}{2n}\right]$	l odd, $l \geqslant 3$	—	$Z^l_{2-}, Z^l_{3-}, \ldots, Z^l_{l-}$
S_{2n}	$2\left[\frac{l+n}{2n}\right]$	n even, $2 \leqslant n \leqslant l/3$	—	$Z^l_{n+}, Z^l_{3n\pm}, Z^l_{5n\pm}\cdots$
C_n	$2\left[\frac{l}{n}\right]+1$	$2 \leqslant n \leqslant l/2$	—	$Z^l_0, Z^l_{n\pm}, Z^l_{2n\pm}, \ldots$
C_1	$2l+1$	$l \geqslant 3$	—	$Z^l_0, Z^l_{2+}, Z^l_{3\pm}, \ldots, Z^l_{l\pm}$

Table B.3. Adjacent group branchings $H \supset K$, $H \subset H'$ (for Lie groups and groups with n-fold symmetry axes where $n \leqslant 6$), and (except for the column headed $\bar{f}_\lambda$) subduction frequencies $c_\lambda(H)$ for the irreps l^π, within $O(3)$ for $l \leqslant 6$. These frequencies were calculated from the computer program RACAH vol 3.1 (Butler 1995). The corresponding massive subduction frequency $f^m_\lambda(H)$ is obtained by subtracting the massless subduction frequency $f^0_\lambda(H)$ from the tabulated entries (equation (4)). From equation (6) $f^0_\lambda(H)$ is the smaller of $2l$ and $\bar{f}_\lambda(H)$, which is also tabulated.

H	Adjacent groups	$\bar{f}_\lambda$	0^-	1^+	1^-	2^+	2^-	3^+	3^-	4^+	4^-	5^+	5^-	6^+	6^-
C_1	$\subset C_5, C_2, C_i, C_s, C_3$	3	1	3	3	5	5	7	7	9	9	11	11	13	13
C_i	$\supset C_1; \subset C_{5i}, C_{2h}, C_{3i}$	3	0	3	0	5	0	7	0	9	0	11	0	13	0
C_s	$\supset C_1; \subset C_{5h}, C_{5v}, C_{2h}, C_{2v}, C_{3v}$	1	0	1	2	3	2	3	4	5	4	5	6	7	6
C_2	$\supset C_1; \subset C_4, C_{2h}, D_3, D_2, C_6$	1	1	1	1	3	3	3	3	5	5	5	5	7	7
C_{2h}	$\supset C_2, C_i, C_s; \subset C_{4h}, D_{2h}, C_{6h}, D_{3d}$	1	0	1	0	3	0	3	0	5	0	5	0	7	0
C_{2v}	$\supset C_2, C_s; \subset C_{4v}, D_{2d}, D_{2h}, C_{6v}$	0	0	0	1	2	1	1	2	3	2	2	3	4	3
C_3	$\supset C_1; \subset T, D_3, C_6, C_{3i}, C_{3v}, C_{3h}$	1	1	1	1	1	1	3	3	3	3	3	3	5	5
C_{3h}	$\supset C_3, C_s; \subset D_{3h}, C_{6h}$	1	0	1	0	1	0	1	2	1	2	1	2	3	2
C_{3i}	$\supset C_3, C_i; \subset T_h, C_{6h}, D_{3d}$	1	0	1	0	1	0	3	0	3	0	3	0	5	0
C_{3v}	$\supset C_3, C_s; \subset T_d, C_{6v}, D_{3h}, D_{3d}$	0	0	0	1	1	0	1	2	2	1	1	2	3	2

Table B.3. (Continued.)

H	Adjacent groups	$\bar{f}_\lambda$	0^-	1^+	1^-	2^+	2^-	3^+	3^-	4^+	4^-	5^+	5^-	6^+	6^-
C_4	$\supset C_2; \subset C_\infty, C_{4h}, C_{4v}, D_4$	1	1	1	1	1	1	1	1	3	3	3	3	3	3
C_{4h}	$\supset C_4, C_{2h}, S_4; \subset C_{\infty h}, D_{4h}$	1	0	1	0	1	0	1	0	3	0	3	0	3	0
C_{4v}	$\supset C_4, C_{2v}; \subset C_{\infty v}, D_{4d}, D_{4h}$	0	0	0	1	1	0	0	1	2	1	1	2	2	1
C_5	$\supset C_1; \subset C_{5i}, C_{5h}, C_{5v}, D_5, C_\infty$	1	1	1	1	1	1	1	1	1	1	3	3	3	3
C_{5h}	$\supset C_5, C_s; \subset D_{5h}$	1	0	0	1	1	0	1	0	1	0	1	2	1	2
C_{5i}	$\supset C_5, C_i; \subset D_{5d}, C_{\infty h}$	1	0	1	0	1	0	1	0	1	0	3	0	3	0
C_{5v}	$\supset C_5, C_s; \subset C_{\infty v}, D_{5d}$	0	0	0	1	1	0	0	1	1	0	1	2	2	1
C_6	$\supset C_3, C_2; \subset C_\infty, D_6, C_{6h}, C_{6v}$	1	1	1	1	1	1	1	1	1	1	1	1	3	3
C_{6h}	$\supset C_6, C_{3h}, C_{3i}, C_{2h}; \subset C_{\infty h}, D_{6h}$	1	0	1	0	1	0	1	0	1	0	1	0	3	0
C_{6v}	$\supset C_6, C_{2v}, C_{3v}; \subset C_{\infty v}, D_{6h}$	0	0	0	1	1	0	0	1	1	0	0	1	2	1
C_∞	$\supset C_6, C_5, C_4; \subset C_{\infty h}, D_\infty$	0	1	1	1	1	1	1	1	1	1	1	1	1	1
$C_{\infty h}$	$\supset C_\infty, C_{6h}, C_{5i}, C_{4h}; \subset D_{\infty h}$	0	0	1	0	1	0	1	0	1	0	1	0	1	0
$C_{\infty v}$	$\supset C_\infty, C_{6v}, C_{5v}, C_{4v}; \subset D_{\infty h}$	0	0	0	1	1	0	0	1	1	0	0	1	1	0
D_2	$\supset C_2; \subset D_{2d}, T, D_4, D_{2h}, D_6$	0	1	0	0	2	2	1	1	3	3	2	2	4	4
D_{2d}	$\supset D_2, C_{2v}, S_4; \subset D_{4h}, D_{6d}, T_d$	0	0	0	0	1	1	0	1	2	1	1	1	2	2
D_{2h}	$\supset D_2, C_{2h}, C_{2v}; \subset D_{4h}, D_{6h}, T_h$	0	0	0	0	2	0	1	0	3	0	2	0	4	0
D_3	$\supset C_3, C_2; \subset O, Y, D_6, D_{3d}, D_{3h}$	0	1	0	0	1	1	1	1	2	2	1	1	3	3
D_{3d}	$\supset D_3, C_{3i}, C_{3v}, C_{2h}; \subset O_h, Y_h, D_{6h}$	0	0	0	0	1	0	1	0	2	0	1	0	3	0
D_{3h}	$\supset D_3, C_{3h}, C_{3v}; \subset D_{6h}, D_{6d}$	0	0	0	0	1	0	0	1	1	1	0	1	2	1
D_4	$\supset D_2, C_4; \subset D_\infty, O, D_{4h}$	0	1	0	0	1	1	0	0	2	2	1	1	2	2
D_{4d}	$\supset D_4, C_{4v}; \subset D_{\infty h}$	0	0	0	0	1	0	0	0	1	1	0	1	1	1
D_{4h}	$\supset D_4, C_{4h}, C_{4v}, D_{2h}, D_{2d}; \subset O_h, D_{\infty h}$	0	0	0	0	1	0	0	0	2	0	1	0	2	0
D_5	$\supset C_5, C_2; \subset D_{5d}, D_{5h}, D_\infty, Y$	0	1	0	0	1	1	0	0	1	1	1	1	2	2
D_{5d}	$\supset D_5, C_{5i}, C_{5v}, C_{2h}; \subset D_{\infty h}$	0	0	0	0	1	0	0	0	1	0	1	0	2	0
D_{5h}	$\supset D_5, C_{5h}; \subset D_{\infty h}$	0	0	0	0	1	0	0	0	1	0	0	1	1	1
D_6	$\supset D_3, D_2, C_6; \subset D_\infty, D_{6h}, D_{6d}$	0	1	0	0	1	1	0	0	1	1	0	0	2	2
D_{6d}	$\supset D_6, D_{2d}; \subset D_{\infty h}$	0	0	0	0	1	0	0	0	1	0	0	0	1	1
D_{6h}	$\supset D_6, D_{2h}, D_{3h}, D_{3d}, C_{6h}, C_{6v}; \subset D_{\infty h}$	0	0	0	0	1	0	0	0	1	0	0	0	2	0
D_∞	$\supset C_\infty, D_6, D_5, D_4; \subset D_{\infty h}, SO(3)$	0	1	0	0	1	1	0	0	1	1	0	0	1	1
$D_{\infty h}$	$\supset D_\infty, C_{\infty v}, D_{6h}, D_{5d}, D_{4h}; \subset O(3)$	0	0	0	0	1	0	0	0	1	0	0	0	1	0
Y	$\supset T, D_5, D_3, C_{5v}; \subset SO(3), Y_h$	0	1	0	0	0	0	0	0	0	0	0	0	1	1
Y_h	$\supset Y, D_{5d}; \subset O(3)$	0	0	0	0	0	0	0	0	0	0	0	0	1	0
O	$\supset T, D_4, D_3; \subset SO(3), O_h$	0	1	0	0	0	0	0	0	1	1	0	0	1	1
$O(3)$	$\supset SO(3), D_{\infty h}, Y_h, O_h$	0	0	0	0	0	0	0	0	0	0	0	0	0	0
O_h	$\supset O, T_d, T_h, D_{3d}, D_{4h}, C_{3i}; \subset O(3)$	0	0	0	0	0	0	0	0	1	0	0	0	1	0
S_4	$\supset C_2; \subset C_{4h}, D_{2d}$	1	0	1	0	1	2	1	2	3	2	3	2	3	4
$SO(3)$	$\supset D_\infty, Y, O; \subset O(3)$	0	1	0	0	0	0	0	0	0	0	0	0	0	0
T	$\supset D_2, C_3; \subset O, Y, T_h, T_d$	0	1	0	0	0	0	1	1	1	1	0	0	2	2
T_d	$\supset T, D_{2d}; \subset O_h$	0	0	0	0	0	0	0	1	1	0	0	0	1	1
T_h	$\supset T, D_{2h}, C_{3i}; \subset O_h, Y_h$	0	0	0	0	0	0	1	0	1	0	0	0	2	0

Table B.4. Little groups H of irreps of $SO(3)$ for $l \leqslant 4$, and for $n \leqslant 4$ in D_n, C_n; a prescription for general l, n is in table B.1. Nonzero entries indicate little groups, the numbers being the appropriate subduction frequencies c_λ.

l	0	1	2	3	4
$SO(3)$	1	—	—	—	—
D_∞	—	—	3	—	3
C_∞	—	3	—	3	—

Table B.4. (Continued)

l	0	1	2	3	4
O	—	—	—	—	4
T	—	—	—	4	—
D_4	—	—	—	—	5
D_3	—	—	—	4	5
D_2	—	—	5	—	6
C_3	—	—	—	5	—
C_2	—	—	—	5	7
C_1	—	—	—	7	9

Table B.5. Little groups H of irreps of $O(3)$ for $l \leqslant 9$, and for $n \leqslant 9$ in D_n, C_n; a prescription for general l, n is in table B.2. Nonzero entries indicate little groups, the numbers being the appropriate subduction frequencies c_λ.

H	l^+	0	1	2	3	4	5	6	7	8	9
$O(3)$		1	—	—	—	—	—	—	—	—	—
$D_{\infty h}$		—	—	3	—	3	—	3	—	3	—
$C_{\infty h}$		—	3	—	3	—	3	—	3	—	3
Y_h		—	—	—	—	—	—	4	—	—	—
O_h		—	—	—	—	4	—	4	—	4	4
T_h		—	—	—	4	—	—	5	4	—	5
D_{9d}		—	—	—	—	—	—	—	—	—	4
D_{8h}		—	—	—	—	—	—	—	—	5	4
D_{7d}		—	—	—	—	—	—	—	4	5	4
D_{6h}		—	—	—	—	—	—	5	4	5	4
D_{5d}		—	—	—	—	—	4	5	4	5	4
D_{4h}		—	—	—	—	5	4	5	4	6	5
D_{3d}		—	—	—	4	5	4	6	5	6	6
D_{2h}		—	—	5	—	6	5	7	6	8	7
C_{9i}		—	—	—	—	—	—	—	—	—	5
C_{8h}		—	—	—	—	—	—	—	—	—	5
C_{7i}		—	—	—	—	—	—	—	5	—	5
C_{6h}		—	—	—	—	—	—	—	5	—	5
C_{5i}		—	—	—	—	—	5	—	5	—	5
C_{4h}		—	—	—	—	—	5	—	5	7	7
C_{3i}		—	—	—	5	—	5	7	7	7	9
C_{2h}		—	—	—	5	7	7	9	9	11	11
C_i		—	—	—	7	9	11	13	15	17	19
H	l^-	0	1	2	3	4	5	6	7	8	9
$SO(3)$		1	—	—	—	—	—	—	—	—	—
D_∞		—	—	3	—	3	—	3	—	3	—
$C_{\infty v}$		—	3	—	3	—	3	—	3	—	3
Y		—	—	—	—	—	—	4	—	—	—
O		—	—	—	—	4	—	4	—	4	4
T_d		—	—	—	4	—	—	4	4	—	4
T		—	—	—	—	—	—	5	—	—	5
D_{9h}		—	—	—	—	—	—	—	—	—	4
D_9		—	—	—	—	—	—	—	—	—	—
D_{8d}		—	—	—	—	—	—	—	—	4	4

Table B.5. (Continued)

H	l^+	0	1	2	3	4	5	6	7	8	9
D_8		—	—	—	—	—	—	—	—	5	—
D_{7h}		—	—	—	—	—	—	—	4	4	4
D_7		—	—	—	—	—	—	—	—	5	—
D_{6d}		—	—	—	—	—	—	4	4	4	4
D_6		—	—	—	—	—	—	5	—	5	—
D_{5h}		—	—	—	—	—	4	4	4	4	4
D_5		—	—	—	—	—	—	5	—	5	—
D_{4d}		—	—	—	—	4	4	4	4	4	4
D_4		—	—	—	—	5	—	5	—	5	5
D_{3h}		—	—	—	4	4	4	4	4	4	5
D_3		—	—	—	—	5	—	5	5	5	6
D_{2d}		—	—	4	—	4	4	5	5	5	5
D_2		—	—	5	—	5	5	6	6	6	7
C_{9v}		—	—	—	—	—	—	—	—	—	5
C_{8v}		—	—	—	—	—	—	—	—	—	5
C_{7v}		—	—	—	—	—	—	—	5	—	5
C_{6v}		—	—	—	—	—	—	—	5	—	5
C_{5v}		—	—	—	—	—	5	—	5	—	5
C_{4v}		—	—	—	—	—	5	—	5	5	6
C_{3v}		—	—	—	5	—	5	5	6	5	7
C_{2v}		—	—	—	5	5	6	6	7	7	8
S_4		—	—	—	—	—	—	6	6	6	6
C_{3h}		—	—	—	—	—	—	—	—	—	6
C_s		—	—	—	6	6	8	8	10	10	12
C_4		—	—	—	—	—	—	—	—	7	7
C_3		—	—	—	—	—	—	7	7	7	9
C_2		—	—	—	—	7	7	9	9	11	11
C_1		—	—	—	7	9	11	13	15	17	19

Appendix C. Inspection in higher irreps of $SO(3)$, and basis functions

If $l > 1$, then in addition, either $a_2 = a_{-2} = 0$ or $\phi = \pm\pi$ (so that $\exp(\pm 2\mathrm{i}\phi) = 1$), i.e. a two-fold rotation only is possible. Also for $l > 1$, the freedom of choosing a rotation by 3 Euler angles leaves one degree of freedom, the third Euler angle, to be exploited as required. In the case $l = 2$ we can choose the third Euler angle to make the coefficient of, say, Z^l_{-2} zero; this leaves the functions Z^2_0, Z^2_{2+} as adequate to describe any linear combination. Since any linear combination of these functions has the D_2 rotational symmetry which they share, this is the minimum rotational symmetry in $l = 2$. In addition these functions (with even m) have compatible reflection symmetries, so that in the case of even parity a general linear combination has D_{2h} symmetry.

If $l > 2$, then in addition, either $a_3 = a_{-3} = 0$ or $\phi = \pm 2\pi/3$, i.e. only a three-fold rotation can evade the necessity of requiring $a_{\pm 3} = 0$. Since a two- and three-fold rotation are not compatible, it is impossible to avoid imposing at least 3 conditions on $a_{\pm 2}$ and $a_{\pm 3}$ (3 rather than 4, because of the possibility of using the third Euler angle to cancel the fourth); and so it is impossible for a general linear combination at $l = 3$ to have a nontrivial rotational symmetry. However, the symmetry of a general linear combination of the full basis set $\{Z^3_{m\pm}\}$ can be simplified by an appropriate axis choice to restrict the number of functions under consideration to $\{Z^3_0, Z^3_{2\pm}, Z^3_{3\pm}\}$ with the free choice of one linear relation between the coefficients $a_{2\pm}$, $a_{3\pm}$ (for example $a_{2-} = 0$). Since the reflection symmetries of $Z^3_{3\pm}$ (where m is odd) are incompatible with those of the other functions (with even m), no reflection plane can survive in general in the case $l > 2$. Hence C_i and C_1 are the maximal symmetries of a general linear form and so little groups for positive and negative parity respectively for $l > 2$.

This proceeds similarly for higher l; for $l = 4$ we can consider a general linear combination as a combination of $\{Z^4_0, Z^4_{2\pm}, Z^4_{3\pm}, Z^4_{4\pm}\}$ with the coefficient of one of the Z^4_{m-} functions being set to zero. Special functions and their little groups at $l = 4$ include equation (10) for O and at $l = 6$ include Y: $(\sqrt{11}Z^6_0 - \sqrt{14}Z^6_5)/5$; O: $(-Z^6_0 + \sqrt{7}Z^6_4)/\sqrt{8}$; T: $(-Z^6_0 + \sqrt{7}Z^6_4)/\sqrt{8}$, $(-\sqrt{11}Z^6_2 + \sqrt{5}Z^6_6)/4$.

Since the little groups of positive parity irreps are determined purely by their rotational symmetry we need only consider pure rotations in using the inspection method. The tesseral harmonic basis functions in 3^+ have the following symmetries (confirmed by the program RACAH): Z^3_0: $C_{\infty h}$, $Z^3_{1\pm}$: C_{2h}, $Z^3_{2\pm}$: T_h, $Z^3_{3\pm}$: D_{3d}. A general linear combination of Z^l_{m+} with Z^l_{m-} will always have the same symmetry as Z^l_{m+} for the reasons discussed in section 4. We may now consider all possible linear combinations of the above. This is essentially a combinatorial exercise although we use the fact that it is always possible to remove $Z^3_{1\pm}$ and one other function with $m > 0$, say Z^3_{m-}, by performing the appropriate rotation. The results are as follows: Z^3_0, Z^3_{2+}: C_{2h}, Z^3_0, Z^3_{3+}: C_{3i}, Z^3_{2-}, Z^3_{3+}: C_{2h}, $Z^3_{2+}, Z^3_{3\pm}$: C_i, $Z^3_0, Z^3_{2+}Z^3_{3\pm}$: C_i. In short, the massive chain criterion finds all possible little groups. The massive subduction frequency also gives the number of massive components of the most general representation vector that has a particular little group. The vectors which are appropriate for different l, H are indicated in tables B.1, B.2. The convention by which the massless components are removed is that of sections 5.3 and 6. According to the above we could have chosen Z^3_{-2}, Z^3_3 as the vector for C_{2h} instead of Z^3_0, Z^3_2. These two vectors actually belong to the same stratum.

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