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Zeros of covariant vector fields for the point groups : invariant formulation

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Résumé. — Pour tous les groupes ponctuels (sous-groupes fermés) finis ou continus des groupes orthogonaux O(2) et O(3) nous donnons une base d'intégrité $\theta_i(x)$, $\varphi_\beta(x)$ $\mathbf{e}_\sigma(x)$ pour les polynômes invariants et pour les champs de vecteurs polynomiaux, nous donnons les équations et inégalités définissant les strates (union des orbites de même type). Finalement, nous écrivons des équations donnant les zéros d'un champ de vecteurs covariants sur une strate donnée ; ces équations sont linéaires dans les composantes (invariantes) du champ de vecteurs sur les $\mathbf{e}_\sigma(x)$, les coefficients de ces termes étant eux-mêmes des invariants. Tous ces résultats sont résumés dans des tables et illustrés par un exemple d'application physique de symétrie cubique. La méthode mathématique pour obtenir ces résultats est expliquée de façon à permettre au lecteur de l'appliquer à d'autres groupes.

Abstract. — All finite as well as infinite (matrix) point subgroups of full orthogonal groups in two and three dimensions are considered. For each point group a polynomial integrity basis for invariants and the basic polynomial vector fields are first given. Then, the strata are defined *via* equations and inequalities involving the integrity basis. Finally, equations for zeros of a covariant vector field are given on each stratum in terms of the integrity basis, which appears *via* coefficients in the expansion of the vector field on the vector-field basis. All the results are tabulated and an illustration using the cubic group is presented. Mathematical background sufficient for extensions of the results is also given.

1. Introduction

When a physical system has a symmetry group $\mathcal{G}$, its properties can be studied in terms of $\mathcal{G}$-invariant functions defined on the configuration space on which $\mathcal{G}$ acts. When the action of $\mathcal{G}$ corresponds to a linear representation Γ, we consider instead of $\mathcal{G}$ the matrix group G which represents $\mathcal{G}$. (G is the image of $\mathcal{G}$ under Γ.) The matrix groups with which we deal correspond to the actions of closed subgroups of full orthogonal groups O(l), $l = 1, 2, 3$, on one, two and three dimensional Euclidian (carrier) spaces described by cartesian coordinates. These groups are the ones most frequently met in applications to molecules, solids (macroscopic tensors, electronic structure, Landau theory of phase transitions, etc.), problems concerning spherical bodies (earth, stars), and similar problems. We formulate our methods with sufficient generality that they may be used for other finite or compact groups.

Since Bethe's famous paper [1] on cubic harmonics many papers have been written on the problem of finding independent sets of crystal harmonics. Hopfield [2] recognized that all crystal harmonics of a given symmetry can be written as linear combinations of a few basic ones, with invariant functions as coefficients ; this was well known to the mathematicians (see, e.g. [3], [4] for references). Papers by Meyer [5] and, later, by Killingbeck [6], Kopský [7] and Michel [4] deal with invariants of crystallographic point groups. Other crystal harmonics (covariants, or tensors) were treated by McLellan [8], Patera *et al.* [9] and Kop-

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ský [10, 11]. Since the mid-fifties new mathematical results have appeared (see Stanley [12] for an excellent review) which are directly applicable to these problems; these results have been used and reviewed by Michel *et al.* [4, 13-15].

This paper has several motivations. Not the least, we hope to acquaint solid state physicists with the mathematical methods mentioned above; they provide a powerful tool in problems involving invariants and covariants of space and point groups. References 4 and 13 written with a similar perspective, deal only with polynomial invariants. Here we focus on polynomial covariant vector fields. We develop a new method for finding their zeros associated with a given symmetry. The method involves only invariants of the relevant matrix group G. Such a problem must be solved in many physical applications, such as finding minima of the Landau free energy in phase transitions, minima of a Higgs potential in gauge theories, fixed points of renormalization-group equations, bifurcation points of a nonlinear problem, etc. For each group G, we give canonical equations, in terms of invariants, for zeros of covariant vector fields at each type of symmetry point by G. We also collect results, some known, some given for the first time, concerning subgroups of O(l), $l = 1, 2, 3$. In particular, we list little groups of G and give invariant descriptions for associated strata. We tabulate explicitly the basic polynomial invariants and covariant vector fields.

In the next section, we summarize the mathematical background which would be useful in extending our results to subgroups of O(l), $l \geqslant 4$, or to other representations of relevant physical groups. Physicists interested only in subgroups of O(3) (and not in 4- and 5-dimensional irreductible representations of the icosahedral groups) need only to familiarize themselves with the definitions and notations before proceeding to section 3 where the relevant results are presented.

2. Mathematical background.

2.1 Group actions. — We consider actions of a unitary matrix group G on an n-dimensional vector space E_n. Later on, we shall restrict ourselves to the particular case of real, therefore, orthogonal, representations on real vector spaces. G is given as the representation Γ of a physical symmetry group $\mathcal{G}$; that is, G is the image of $\mathcal{G}$ under Γ (or G = Im $\mathcal{G}$). We emphasize that invariants and covariants on E_n depend only on the image. Since different representations of different groups, or inequivalent representations of the same group, may have the same or equivalent [in $U(n)$!] images, it is advantageous, as pointed out in references 4, 16, to classify and study group representations according to their images.

We denote an arbitrary element (a matrix) of G by g and a vector from E_n by $\mathbf{r}$. The transform of $\mathbf{r}$ by g is written $g.\mathbf{r}$ which in a given basis reads $x_i \to g_{ij}\, x_j$ with a summation over repeated indices; $\mathbf{r}$ may be a configuration space vector and g may be, for example, a rotation matrix.

It is well-known that G defines in E_n certain geometric structures, such as rotation axes and reflection planes, whose points are left invariant by certain elements of G. This leads to the study of little (isotropy) subgroups L of G. By definition the little group L($\mathbf{r}$) of a vector $\mathbf{r}$ of E_n contains all elements of G which leave $\mathbf{r}$ invariant.

By the definition of L($\mathbf{r}$) an element g of G not in L($\mathbf{r}$) transforms $\mathbf{r}$ into $g.\mathbf{r} \neq \mathbf{r}$. The set of all distinct $g.\mathbf{r}$, as g runs through G, is called a G-orbit. Since $\mathrm{L}(g.\mathbf{r}) = g\mathrm{L}(\mathbf{r})\, g^{-1}$ it follows that the little groups of vectors on the same orbit are conjugated; therefore we may label an orbit by $\Omega([\mathrm{L}], \mathbf{r})$ where [L] is the conjugacy class of its little groups and $\mathbf{r}$ is one of its vectors. Furthermore, two different orbits may share little groups; an obvious example is the pair $\Omega([\mathrm{L}], \mathbf{r})$ and $\Omega([\mathrm{L}], \lambda\mathbf{r})$ where λ is a non-zero real number. The union of orbits with the same [L] is called a stratum, denoted by Σ[L].

Strata may be viewed in the following way. Given a little group L we may construct the linear subspace of E_n, denoted E_n^{L} (the notation Fix L is sometimes used), spanned by all vectors invariant under L. For finite groups the dimension i(L) of E_n^{L} is given in terms of characters χ of Γ:

$$i(\mathrm{L}) = \frac{1}{|\mathrm{L}|} \sum_{g \in \mathrm{L}} \chi(g) = \frac{1}{|\mathrm{L}|} \sum_{g \in \mathrm{L}} \operatorname{tr} g\,. \qquad (1)$$

Symmetry subspaces E_n^{L} are a natural generalization of symmetry axes and reflection planes. It can be seen that $\mathrm{L}' > \mathrm{L}$ if $E_n^{\mathrm{L}'} \subset E_n^{\mathrm{L}}$ (incidentally, this relation can be incorporated into an efficient algorithm for determination of all little groups of a discrete group [17, 18]). Therefore, a stratum is given by

$$\Sigma[\mathrm{L}] = \bigcup_{\mathrm{L} \in [\mathrm{L}]} \left(E_n^{\mathrm{L}} - \bigcup_{\mathrm{L}' > \mathrm{L}} E_n^{\mathrm{L}'} \right). \qquad (2)$$

We remark that the topological closure of the stratum is the union of the subspaces E_n^{L} for $\mathrm{L} \in [\mathrm{L}]$.

As an example consider the group SO(3) of three-dimensional rotations around the origin. A vector $\mathbf{r}_0 \neq 0$ is invariant under all rotations around the axis $\{ \lambda \mathbf{r}_0 \}$ and its little group is SO(2). The other rotations of SO(3) acting on $\mathbf{r}_0$ generate the sphere $\| \mathbf{r} \|^2 = \| \mathbf{r}_0 \|^2$, the orbit of $\mathbf{r}_0$. The little group of the origin is the whole group SO(3). Thus, there are two strata, the origin and the rest of space, associated with the classes [SO(3)] and [SO(2)] respectively.

For a compact or finite group there is a natural ordering among classes of little groups. $[\mathrm{L}] < [\mathrm{L}']$ if, by definition, there are $\mathrm{L} \in [\mathrm{L}]$ and $\mathrm{L}' \in [\mathrm{L}']$ such that $\mathrm{L} < \mathrm{L}'$. There is a theorem, not trivial to prove [33], that there is a minimal class $[\mathrm{L}_0]$ whose stratum, the generic stratum, is open dense. In the case of a finite matrix group G, L_0 contains only the identity element.

2.2 INVARIANTS AND COVARIANT VECTOR FIELDS. — Let $D(g)$ be a linear n'-dimensional representation of G carried by the vector space $E_{n'}$. A function $f(\mathbf{r})$ defined on E_n and valued in $E_{n'}$, is called a G-covariant or tensor if for every $g \in G$

$$f(g.\mathbf{r}) = D(g) f(\mathbf{r}) . \tag{3}$$

In this paper, we are mainly interested in two special cases :

1) $E_{n'}$ carries the trivial one-dimensional representation of G, and $D(g) \equiv 1$; then $f(\mathbf{r})$ is called an invariant function;

2) $E_{n'}$ carries the same representation as E_n, so $D(g) = g$; then $f(\mathbf{r})$ is called a covariant vector field, which we write as $\mathbf{f}(\mathbf{r})$.

In the case of SO(3) discussed above, $f(\mathbf{r}) = \| \mathbf{r} \|^2$ is an invariant and $\mathbf{f}(\mathbf{r}) = \| \mathbf{r} \|^2 \mathbf{r}$ is a covariant vector field.

2.3 POLYNOMIALS ON THE REPRESENTATION (CARRIER) SPACE E_n. — To describe the properties of a physical system, we may have to use distributions or functions which are not smooth (infinitely differentiable), but usually smooth functions (which include in particular analytic functions) are sufficient. For a compact (or finite) group Schwarz [19] has shown that G-invariant smooth functions are smooth functions of invariant polynomials. More generally, as we shall see, smooth invariant and covariant vector fields can be expanded on the polynomial basis (which we will introduce for polynomial fields) with smooth functions of polynomial invariants as coefficients. This is our justification for restricting this paper to the study of polynomial invariants and vector fields. In this section, we consider only finite groups and shall say later how the results generalize to the case of infinite compact groups.

Denote by P the (infinite dimensional) vector space of all polynomials in $\mathbf{r} \in E_n$. It is also a ring. There are two natural compatible decompositions of P as a direct sum. One is

$$P = \bigoplus_{m=0}^{\infty} P^{(m)}, \quad \dim P^{(m)} = \binom{m+n-1}{m} \tag{4}$$

where $P^{(m)}$ is the vector space of all homogeneous polynomials of degree m. Since the action of G on P

$$g.p(\mathbf{r}) \equiv p(g.\mathbf{r}), \quad p(\mathbf{r}) \in P \tag{5}$$

preserves the degree, each $P^{(m)}$ carries a linear representation of G. The character $\chi^{(m)}(g)$ of the G-representation on $P^{(m)}$ is given by the generating function

$$\sum_{m=0}^{\infty} \chi^{(m)}(g)\, t^m = [\det(1 - tg)]^{-1} \tag{6}$$

where t is a dummy variable.

Let α label the different equivalence classes of irreducible representations Γ_α of the group G. We recall that an isotypical (also called factorial) representation of G is a direct sum of equivalent irreducible representations. The second natural decomposition of P is into the direct sum of spaces spanning isotypical representations

$$P = \bigoplus_{\alpha} P_\alpha . \tag{7}$$

P_α is the vector space of α-covariant polynomials. We use $\alpha = 0$ to label the trivial representation, so P_0 is the ring of G-invariant polynomials. A polynomial $p \in P$ may be projected on P_α by an orthogonal projector $\mathcal{P}_\alpha$ given by

$$\mathcal{P}_\alpha\, p(\mathbf{r}) \equiv \frac{\dim \Gamma_\alpha}{|\mathrm{G}|} \sum_{g \in G} \chi_\alpha^*(g)\, p(g^{-1}\,\mathbf{r}) . \tag{8}$$

The multiplicity c_α^m of the irreducible representation Γ_α on the space

$$P_\alpha^{(m)} \equiv P^{(m)} \cap P_\alpha \tag{9}$$

is given by the generating function $M_\alpha(t)$ obtained by forming the Hermitian scalar product of the characters $\chi_\alpha(g)$ and $\chi^{(m)}(g)$

$$M_\alpha(t) \equiv \sum_{m=0}^{\infty} c_\alpha^m\, t^m = \frac{1}{|\mathrm{G}|} \sum_{g \in G} \frac{\chi_\alpha^*(g)}{\det(1 - tg)} . \tag{10}$$

Note that [11]

$$\dim P_\alpha^{(m)} = c_\alpha^m \dim \Gamma_\alpha . \tag{11}$$

For invariant polynomials, the function $M_0(t)$ was first computed by Molien [20]. In the mathematical literature $M_\alpha(t)$ is often called the Poincaré series.

2.4 CASE OF (PSEUDO-) REFLECTION GROUPS. — A pseudo-reflection on E_n is a unitary operator u, of whose n eigenvalues $n - 1$ are equal to one while the n^{th} eigenvalue is a root of unity different from one. The space left invariant by u is called a reflection plane. When the n^{th} eigenvalue is equal to minus one u is equivalent to an orthogonal operator and is simply called a reflection. A group R generated by (pseudo-) reflections is called a (pseudo-) reflection group. Any such matrix group can be decomposed into irreducible groups and the list of irreducible pseudo-reflection groups was determined by Coxeter [21] and Shephard and Todd [22]. They also showed that the Molien function $M_0(t)$ for an irreducible (pseudo-) reflection group can be written in a unique way as

$$M_0(t) = 1/D(t) = \prod_{i=1}^{n} (1 - t^{d_i})^{-1} . \tag{12}$$

They computed the corresponding exponents d_i and showed that they satisfy the relation

$$\prod_{i=1}^{n} d_i = |\mathrm{R}| . \tag{13}$$

As suggested by equations 12 and 13, one can find n algebraically independent homogeneous polynomials $\theta_i(\mathbf{r})$ of respective degrees d_i such that every R-invariant polynomial is a polynomial $\in C[\theta_1, ..., \theta_n]$, the ring of polynomials in $\theta_1, ..., \theta_n$ with complex coefficients. One also says that P_0 is a polynomial ring.

Let us recall a well known example. Let R be the group π_n of $n \times n$ permutations matrices whose all entries are zero except one in each row and each column which is equal to one. The matrix group π_n is a reducible orthogonal representation of the symmetric group S_n, the group of all permutations of n objects. Indeed the one dimensional space of vectors with all coordinates equal is invariant. The orthogonal space of vectors the sum of whose coordinates vanishes carries an $(n-1)$ dimensional irreducible representation of S_n. The reflections in π_n are matrices permuting just two coordinates axes. Since these permutations generate it, π_n is a reflection group. It is well known that any symmetric polynomial in the coordinates $x_1, ..., x_n$ is a polynomial in the θ_i's with $\theta_i = \sum_{j=1}^{n} x_j^i$, $i = 1, ..., n$.

Chevalley [23] for orthogonal groups and Shephard and Todd [22] for unitary groups proved :

Theorem 2.4.1 The ring P_0 of G-invariant polynomials is a polynomial ring if and only if G is a pseudo-reflection group.

Chevalley also proved :

Theorem 2.4.2 For any reflection group R, P is a $|\mathrm{R}|$ dimensional free module over P_0 which transforms under R as the regular representation.

The last theorem extends to pseudo-reflection groups. It is a generalization of an easy-to-prove property : every polynomial in one (real) variable has a unique decomposition

$$p(x) = q_0(x^2) + q_1(x^2)\, x, \tag{14}$$

where q_0 and q_1 are polynomials in x^2, $q_0(x^2) = \frac{1}{2}(p(x) + p(-x))$ and $q_1(x^2) = \frac{1}{2x}(p(x) - p(-x))$. Here, $n = 1$ and R is the two element group O(1).

One can also specify the degrees of the basic polynomials of the module P over the polynomial ring P_0 : the number of basic polynomials of degree s is the coefficient of t^s in the polynomial

$$Q(t) \equiv D(t)\,(1-t)^{-n} = \prod_{i=1}^{n} \sum_{j=0}^{d_i - 1} t^j . \tag{15}$$

The expression *free module* means that the expansion of any $p(\mathbf{r}) \in P$ as a linear combination of the basic polynomials $b_r(\mathbf{r})$, $r = 1, ..., |\mathbf{R}|$, with coefficients in $P_0 = C[\theta_1, ..., \theta_n]$ is unique

$$p(\mathbf{r}) = \sum_{r=1}^{|\mathbf{R}|} q_r(\theta_1, ..., \theta_n)\, b_r(\mathbf{r}) . \tag{16}$$

We give another simple example. The four element group of 2×2 matrices I, $-I$, $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, $\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$ is a reflection group. It is Abelian, so it has four inequivalent irreducible representations of dimension one. Its Molien function is $(1-t^2)^{-2}$, one can take for θ_1 and θ_2, x^2 and y^2, respectively. So P_0 is the ring of all two variable polynomials $q(x^2, y^2)$ and the other three P_α's are xP_0, yP_0 and xyP_0. Thus, for this group equation 16 is explicitly

$$p(x, y) = q_1(x^2, y^2) + q_2(x^2, y^2)\, x + q_3(x^2, y^2)\, y + q_4(x^2, y^2)\, xy . \tag{17}$$

In the tables, section 4, more interesting examples are given.

It is a simple corollary of theorem 2.4.2 that different subspaces P_α are free modules over P_0 each of dimension $(\dim \Gamma_\alpha)^2$. In particular for the vector fields ($\alpha = v$, may be reducible) there are n^2 components of n basic vector fields of degrees $(d_i - 1)$. One can take for the basic vector fields the gradients $\nabla\theta_i$ of the invariants θ_i, $i = 1, ..., n$. So every R-covariant vector field $\mathbf{v}(\mathbf{r})$ has a unique expansion

$$\mathbf{v}(\mathbf{r}) = \sum_{i=1}^{n} q_i(\theta_1, ..., \theta_n)\, \nabla\theta_i . \tag{18}$$

Note that

$$M_v(t) = N_v(t)/D(t) = \left(\sum_{i=1}^{n} t^{d_i - 1}\right)\Big/ D(t) . \tag{19}$$

2.5 FINITE GROUPS NOT GENERATED BY REFLECTIONS. — In this case it can be shown that there exists a polynomial ring $C[\theta_1, ..., \theta_n]$ of n algebraically independent homogeneous G-invariant polynomials $\theta_i(\mathbf{r})$ such that the ring P of polynomials on E_n is a finite free module over $C[\theta_1, ..., \theta_n]$: see for instance Stanley [12]. This author shows that one can always choose the degrees of each $\theta_i(\mathbf{r})$ smaller than or equal to $|\mathrm{G}|$. Moreover, these degrees satisfy a generalization of equation 13

$$\prod_{i=1}^{n} d_i = k\,|\mathrm{G}| \tag{20}$$

where k is an integer greater than one. The module P over $C[\theta_1, ..., \theta_n]$ transforms as a direct sum of k regular representations of G. Similarly, the P_α's are free modules over $C[\theta_1, ..., \theta_n]$ of dimension $k(\dim \Gamma_\alpha)^2$. For instance, the ring P_0 is generated by $(n + k - 1)$ basic polynomials $\theta_i(\mathbf{r})$, $i = 1, ..., n$, and $\varphi_\beta(\mathbf{r})$, $\beta = 1, ..., k-1$ and P_0 is a free $C[\theta_1, ..., \theta_n]$

module of dimension k. That is, every G-invariant polynomial $p_0(\mathbf{r})$ has a unique decomposition

$$p_0(\mathbf{r}) = \sum_{\beta=0}^{k-1} q_\beta(\theta_1, \ldots, \theta_n)\, \varphi_\beta(\mathbf{r}) \qquad (21)$$

where $\varphi_0(\mathbf{r}) \equiv 1$. The basic invariant polynomials θ_i and φ_β form an *integrity basis* for P_0.

For each φ_β, $\beta > 0$, there is an integer power $\nu_\beta > 1$ such that $\varphi_\beta^{\nu_\beta} \in C[\theta_1, \ldots, \theta_n]$. If δ_β = degree $\varphi_\beta(\mathbf{r})$, the corresponding Molien function is

$$M_0(t) = \frac{1 + \sum_{\beta=1}^{k-1} t^{\delta_\beta}}{D(t)} \equiv \frac{N(t)}{D(t)} = \frac{N(t)}{(1-t)^n\, Q(t)} \qquad (22)$$

where $D(t)$ and $Q(t)$ are defined by the equation 15, same as in the case of (pseudo-) reflection groups, with $C[\theta_1, \ldots, \theta_n]$ in place of P_0. Using (10) :

$$k = N(1) = \prod_{i=1} d_i / |\,\mathrm{G}\,| = Q(1)/|\,\mathrm{G}\,| . \qquad (23)$$

We shall call the basic invariants $\theta_i(\mathbf{r})$ and $\varphi_\beta(\mathbf{r})$ the *denominator* and *numerator invariants*, respectively.

Unfortunately, there is no efficient algorithm to determine the *minimal integrity basis*, i.e. the one with the smallest k or, cf. equation 23, with the smallest degrees d_i. It does not correspond necessarily to the case $N(t)$ and $D(t)$ relatively prime (see Stanley [12] for examples).

In order to illustrate a difference between a free and a non-free module we consider a simple example, the two-element group $\{1, -1\}$ in $n = 2$ dimensions. Since it leaves no vector $\mathbf{r} \neq 0$ invariant, and since $|\,\mathrm{G}\,| = 2$, the possible θ's are x^2, y^2 and xy. The Molien function is $(1 + t^2)/(1 - t^2)^2$. In this case the minimal integrity basis corresponds to $k = 2$ and $\theta_1 = x^2$, $\theta_2 = y^2$ and $\varphi_1 = xy$. Hence, every invariant polynomial $p_0(x, y) \in P_0$ can be written as

$$p_0(x, y) = q_1(x^2, y^2) + q_2(x^2, y^2)\, xy . \qquad (24)$$

In that case P is a free $C[x^2, y^2]$ module of dimension $k\,|\,\mathrm{G}\,| = 4$ and the basic polynomials are 1, xy, x and y. Thus, a polynomial $p(x, y) \in P$ can be uniquely written as

$$p(x, y) = p_0(x, y) + p_v(x, y) \qquad (25)$$

with

$$p_v(x, y) = q_3(x^2, y^2)\, x + q_4(x^2, y^2)\, y . \qquad (26)$$

P is also a P_0 module, but it is not a *free* P_0 module. Indeed, to generate all polynomials with coefficients $q \in P_0$ it is sufficient to take as a basis 1, x and y. So, P is a P_0 module. It is not free because the decomposition is not unique; e.g. for $p(x, y) = x^2 y$ one has

$$x^2 y = qx = q' y \qquad (27)$$

with either $q = xy \in P_0$ or $q' = x^2 \in P_0$. Since the group is Abelian the vector representation is reducible and the four ($k.\dim \Gamma_v = nk = 4$) basic vector fields can be chosen as : $\begin{pmatrix} x \\ y \end{pmatrix}, \begin{pmatrix} x \\ -y \end{pmatrix}, \begin{pmatrix} y \\ x \end{pmatrix}, \begin{pmatrix} y \\ -x \end{pmatrix}$.

In the following section, we will treat the cases $\mathrm{G} < \mathrm{R}$. In a more general case, in constructing the basic fields, one must use a brute force method. Namely, one chooses monomials of systematically higher and higher degree, not exceeding $|\,\mathrm{G}\,|$, and applies an appropriate projection operator

$$\mathcal{P}_{\alpha(ij)}\, p(\mathbf{r}) \equiv \frac{\dim \Gamma_\alpha}{|\,\mathrm{G}\,|} \sum_{g \in \mathrm{G}} \Gamma_\alpha^*(g)_{ij}\, p(g^{-1}.\mathbf{r}) \qquad (28)$$

to find the i^{th} component (j is kept fixed) of an α-covariant field. Checking for independence with previously found fields and using the functions $M_\alpha(t)$ one eventually constructs an α-covariant basis.

2.6 SUBGROUPS OF FINITE REFLECTION GROUPS. — If G is not a reflection group but is a subgroup of a reflection group R, $\mathrm{G} < \mathrm{R}$, we can choose for the denominator invariants $\theta_i(\mathbf{r})$ those of R. Then, cf. equation 23, $k = |\,\mathrm{R}\,|/|\,\mathrm{G}\,|$. As we have seen, P is an $|\,\mathrm{R}\,|$-dimensional free module over $C[\theta_1, \ldots, \theta_n]$ which transforms like the regular representation of R. When restricted to G this representation yields k-times the regular representation of G. The basic polynomials $b_r(\mathbf{x})$, equation 16, are exactly the same for both R and G but their covariance properties differ between R and G.

However, it is not guaranteed that this method yields the minimal k, except when $|\,\mathrm{R}\,|/|\,\mathrm{G}\,| = 2$. As shown also by Stanley [3], [12] (the preprint was used and explained in [4]) there is an efficient method when

$$\mathrm{R}' < \mathrm{G} < \mathrm{R} \qquad (29)$$

where R′ is the group generated by the commutators of R (i.e. by the elements of the form $aba^{-1}b^{-1}$). R′ is the smallest invariant subgroup of R such that the quotient R/R′ is an Abelian group. Consequently, irreducible representations of R/R′ yield all inequivalent one dimensional representations of R. Polynomials which transform according to such representations are usually called *quasi-invariants* of R. All quasi invariant polynomials, which transform by a one-dimensional representation χ_α of R, form a one-dimensional P_0 module $P_\alpha = \psi_\alpha(\mathbf{r})\, P_0$. Stanley [3], [12] gave an explicit construction for basic polynomials $\psi_\alpha(\mathbf{r})$. Since we will need this construction only for reflection groups, we explain this slightly simpler case. For any reflection $u \in \mathrm{R}$, $u^2 = 1$ we have $\chi_\alpha(u) = \pm 1$. Stanley's rule is

$$\psi_\alpha(\mathbf{r}) = \prod_{\substack{u = \text{reflection in R} \\ \chi_\alpha(u) = -1}} l_u(\mathbf{r}) \qquad (30)$$

where $l_u(\mathbf{r})$ is the linear form of the hyperplane of the reflection u. As a particular case we can consider the representation $\chi(g) = \det g$. For any reflection $u \in R$, $\det u = -1$, and in that case

$$\psi(\mathbf{r}) = \prod_{u=\text{reflection in R}} l_u(\mathbf{r}) . \tag{31}$$

It was already known that

$$\psi(\mathbf{r}) \sim J(\mathbf{r}) = \det \frac{\partial \theta_i}{\partial x_j} . \tag{32}$$

Indeed, since $J(\mathbf{r})$ is the determinant of the n components of n vectors $\nabla\theta_i$ it is a pseudoscalar which changes sign when one crosses a reflection plane (and only then, as can be seen from theorem 3.1 of the next section). Incidentally, equations 31 and 32 yield for the number of reflections in R :

$$\sum_{i=1}^{n} d_i - n . \tag{33}$$

All quasi invariants of R are quasi invariants of every subgroup of R. When G satisfies (29) then all invariants of G are obtained from the quasi invariants $\psi_\alpha(\mathbf{r})\, P_0$ of R such that $G \leqslant \operatorname{Ker} \chi_\alpha$ (kernel of χ_α), i.e. $\chi_\alpha(g) = 1$ for every $g \in G$. Hence Stanley's theorem : P_0^G, the space of G-invariant polynomials, is a free $P_0 = C[\theta_1, ..., \theta_n]$ module with basis $\psi_\alpha(\mathbf{r})$, $G \leqslant \operatorname{Ker} \chi_\alpha$ (here we used a superscript G in order to distinguish between P_0^G and P_0, the rings of G- and R-invariant polynomials, respectively). That is, for every $p(\mathbf{r}) \in P_0^G$

$$p(\mathbf{r}) = \sum_{\alpha, G \leqslant \operatorname{Ker} \chi_\alpha} q_\alpha \, \psi_\alpha(\mathbf{r}) , \tag{34}$$

where $\psi_0(\mathbf{r}) \equiv 1$ and $q_\alpha \in P_0$. The dimension k of the module P_0^G, is the number of ψ_α in equation 34 and the numerator invariants for G are $\varphi_\alpha(\mathbf{r}) = \psi_\alpha(\mathbf{r})$.

Such explicit algorithms for finding nk basic G-covariant polynomial vector fields are not known. First, one takes $(n + k - 1)$ gradients of the integrity basis but one should also look among quasi-vector fields of R (their components are polynomials which transform like the product of an R-quasi-invariant and an R-covariant vector field), which are G-covariant vector fields. Note that although the number of basic R-quasi-vector fields is precisely kn they are not, in general, basic G-covariant vector fields.

We recall a general method for obtaining from a given covariant, the same type of covariant but of smaller degree : if $p_0(\mathbf{r}) \in P_0^G$, operate on the covariant with the *operator* $p_0(\nabla)$. In three-dimensions a quasi vector field may be obtained by taking a curl $(\nabla \times)$ of a vector field or by forming the cross product of two (quasi) vector fields. Finally, when G is irreducible on the real, but becomes reducible on the complex there is a real orthogonal matrix J which commutes with G and which satisfies

$$-J^2 = J^+ J = 1 . \tag{35}$$

Therefore, if $\mathbf{v}(\mathbf{r})$ is a G-covariant vector field, $J\mathbf{v}$ is another one orthogonal to $\mathbf{v}$, i.e. $(\mathbf{v}, J\mathbf{v}) = 0$, where we use (,) to denote the orthogonal scalar product.

2.7 Orbit space. — The integrity basis for a group G defines a map (function), which we will denote by ω or $\omega(\mathbf{r})$, from E_n into E_{n+k-1}

$$\omega : \mathbf{r} \to \omega(\mathbf{r}) = (\theta_1(\mathbf{r}), ..., \theta_n(\mathbf{r}), \varphi_1(\mathbf{r}), ..., \varphi_{k-1}(\mathbf{r})) . \tag{36}$$

The whole space E_n is mapped onto an n-dimensional (semi-algebraic) surface in E_{n+k-1}. We will call this surface the *orbit space* and we will denote it by $\omega(E_n)$. The usefulness of this concept arises from the fact that ω is constant on any given orbit $\Omega([L], \mathbf{r}_0)$,

$$\omega(\mathbf{r}) = \omega(\mathbf{r}_0) , \quad \mathbf{r} \in \Omega([L], \mathbf{r}_0) , \tag{37}$$

and that it separates orbits [24, 25]. Consequently, all G-invariant structures in E_n, such as orbits and strata, appear also in the orbit space $\omega(E_n)$. Several papers were recently devoted to the relations determining both the surface $\omega(E_n)$ in E_{n+k-1} and the image of the strata in the same space [26-28].

A physical problem which possesses a symmetry G always has « degenerate » solutions which fall on an orbit. Therefore, it is sometimes advantageous to formulate the problem in terms of invariants so that a solution $(\bar{\theta}_1, ..., \bar{\theta}_n, \bar{\varphi}_1, ..., \bar{\varphi}_{k-1})$ in E_{n+k-1} is found first. Only the solutions which fall on the surface $\omega(E_n)$, i.e., ones from the orbit space, are physical ones. Corresponding orbits $\Omega([L], \mathbf{r})$ of solutions in E_n can then be found by employing the inverse map ω^{-1},

$$\Omega([L], \bar{\mathbf{r}}) = \omega^{-1}(\bar{\theta}_1, ..., \bar{\theta}_n, \bar{\varphi}_1, ..., \bar{\varphi}_{k-1}) . \tag{38}$$

The inverse map ω^{-1} depends only on G and is independent of the physical problem in question. Therefore, for a given G, ω^{-1} can be determined once for all. As an illustration, ω^{-1} will be given in section 4 for the cubic group O_h.

2.8 Extension to compact groups. — For (continuous) compact reflection groups we can compute the Poincaré function for invariants : it is of the form $M_0(t) = 1/D(t)$ and the ring of invariant polynomials is a polynomial ring. However, the Chevalley theorem 2.4.2 does not apply. Also, compact groups other than reflection groups can have $M_0(t) = 1/D(t)$. So the problems we wish to solve are more difficult for compact groups in general. These problems happen to be very simple for O(3) and for one-parameter groups, the only compact groups we study here.

Let us again quote the Schwarz theorem [19] which is applicable to compact as well as finite groups : for a compact group G, the G-invariant smooth functions are smooth functions of G-invariant polynomials. With the use of the Malgrange division theorem [29] one can justify expansion of any G-invariant smooth function $s(\mathbf{r})$ into

$$s(\mathbf{r}) = \sum_{\beta=0}^{k-1} s_\beta(\theta_1, ..., \theta_n)\, \varphi_\beta(\mathbf{r}) \quad (39)$$

where s_β's are smooth functions of the denominator invariants (however, not anymore unique) while φ_β's are the numerator invariants. From an identification of the spaces of smooth maps SM(E, E') and SM($E^* \otimes E'$, $\mathbb{R}$), equation 39 can be extended to any type of smooth G-covariant field.

3. Zeros of covariant vector fields.

We consider a finite orthogonal group G acting on a real E_n. Given a polynomial vector field $\mathbf{v}(\mathbf{r})$,

$$\mathbf{v}(g.\mathbf{r}) = g.\mathbf{v}(\mathbf{r})\,, \quad g \in \mathrm{G}\,, \quad (40)$$

we want to find its zeros. That is, we want to solve for $\mathbf{r}$ the system of equations

$$\mathbf{v}(\mathbf{r}) = 0\,. \quad (41)$$

We recall that a covariant polynomial vector field can be expanded

$$\mathbf{v}(\mathbf{r}) = \sum_{\sigma=1}^{nk} q_\sigma(\theta_1, ..., \theta_n)\, \mathbf{e}_\sigma(\mathbf{r}) \quad (42)$$

where $\mathbf{e}_\sigma(\mathbf{r})$ are basic (for $C[\theta_1, ..., \theta_n]$ module) covariant polynomial fields.

At a point $\mathbf{r}_0$, by using (40) for $g \in \mathrm{L}(\mathbf{r}_0)$ and the definition of $E_n^{\mathrm{L}(\mathbf{r}_0)}$, we have

$$g.\mathbf{v}(\mathbf{r}_0) = \mathbf{v}(\mathbf{r}_0) \quad (43)$$

implying $\mathbf{v}(\mathbf{r}_0)$ is in $E_n^{\mathrm{L}(\mathbf{r}_0)}$ and thus in the closure of $\Sigma[\mathrm{L}(\mathbf{r}_0)]$. Hence, at a given particular point $\mathbf{r}_0$ of an m-dimensional stratum there cannot be more than m linearly independent basic fields $\mathbf{e}_\sigma(\mathbf{r}_0)$ (since G is finite, the topological dimension m of the stratum is equal to the dimension of the subspace $E_n^{\mathrm{L}(\mathbf{r}_0)}$). Also there cannot be fewer than m. For a proof, let $\hat{n}$ be an arbitrary unit vector in $E_n^{\mathrm{L}(\mathbf{r}_0)}$. Then we can construct a covariant polynomial vector field which is along $\hat{n}$ at $\mathbf{r}_0$. Such a field is the gradient of $F(\mathbf{r})$, $\nabla F(\mathbf{r})$, with

$$F(\mathbf{r}) = \prod_{g \in \mathrm{G}} \left[a \,\| \mathbf{r} - g.\mathbf{r}_0 \|^2 + (\mathbf{r} - g.\mathbf{r}_0, g.\hat{n})\right], \quad (44)$$

where a is any real number

$$a > \operatorname*{Max}_{g \notin \mathrm{L}(\mathbf{r}_0)} \frac{(g.\mathbf{r}_0 - \mathbf{r}_0, g.\hat{n})}{\| g.\mathbf{r}_0 - \mathbf{r}_0 \|^2} \quad (45)$$

and $\| \mathbf{r} \|^2 \equiv (\mathbf{r}, \mathbf{r})$. Since $\hat{n}$ may be in any one of the m linearly independent directions and since each corresponding field $\nabla F(\mathbf{r})$ can be expanded like equation 42 the proof is complete. Thus,

Theorem 3.1 Values of basic G-covariant vector fields (and also of gradients of the integrity basis) at $\mathbf{r}$ span $E_n^{\mathrm{L}(\mathbf{r})}$, the tangent plane at $\mathbf{r}$ to the stratum $\Sigma[\mathrm{L}(\mathbf{r})]$. The theorem extends to compact groups if one replaces $E_n^{\mathrm{L}(\mathbf{r})}$ by the « invariant slice » (see e.g. Ref. 26).

Let us denote the m basic vector fields whose values are linearly independent at $\mathbf{r} \in E_n^{\mathrm{L}(\mathbf{r})}$ by $\mathbf{e}'_1(\mathbf{r}), ..., \mathbf{e}'_m(\mathbf{r})$, $m = \dim E_n^{\mathrm{L}(\mathbf{r})}$. In general, $\mathbf{e}'_\sigma(\mathbf{r})$ cannot be chosen so that they form a *global basis* on $\Sigma[\mathrm{L}(\mathbf{r})]$, i.e. a linearly independent set of vectors not only at $\mathbf{r}$ but everywhere on $\Sigma[\mathrm{L}(\mathbf{r})]$. For example, in the tables of section 4, a *global basis* does not exist for some strata of the groups S_{2n}, $n \geqslant 1$. Additional discussion of the global basis is given in appendix A.

As explained in section 2.7 our goal is to replace (41) by conditions in terms of the integrity basis only. The rational is that by going to the orbit space not only do we remove unnecessary degeneracy but we sometimes obtain equations of lower degree than those found directly in E_n using e.g. a recent method by Jarić [30]. In order to achieve our goal we first need equations and inequalities describing each stratum Σ[L] in orbit space. They can be found using a method by Jarić [28]. Second, on each stratum the basic fields $\mathbf{e}'_\sigma(\mathbf{r})$ need to be determined (we always choose a basis of the lowest possible degree). Equation 41 is then replaced, on a given stratum Σ[L], by $m = \dim E_n^{\mathrm{L}}$ equations

$$(\mathbf{v}(\mathbf{r}), \mathbf{e}'_\sigma(\mathbf{r})) = 0, \quad \sigma = 1, ..., m\,. \quad (46)$$

These equations can be written explicitly in terms of the integrity basis by using (42) and by calculating explicitly the $nk \times nk$ matrix $M(\theta_1, ..., \theta_n, \varphi_1, ..., \varphi_{k-1})$

$$M_{\alpha\beta}(\theta_1, ..., \theta_n, \varphi_1, ..., \varphi_{k-1}) = (\mathbf{e}_\alpha(\mathbf{r}), \mathbf{e}_\beta(\mathbf{r}))\,. \quad (47)$$

For closed subgroups of O(2) and O(3) calculations of the matrix M are illustrated in appendices B, C and D. The system of equations 46 can often be simplified and we give in the tables its lowest degree equivalent.

4. Tables for closed subgroups of O(2) and O(3).

The closed subgroups of O(2) are the Lie group SO(2) and the two families of finite groups, C_n and C_{nv}, which are isomorphic to cyclic and dihedral groups Z_n and D_n. We use here the usual notation of the physical and chemical literature (see e.g. [31]). For instance, C_∞ and $\mathrm{C}_{\infty v}$ stand for SO(2) and O(2), respectively.

Lie subgroups of SO(3) are C_∞ and D_∞, whereas the finite subgroups are C_n, D_n, T, O and Y. The last three are irreducible and leave invariant some regular polyhedra : tetrahedron for T, cube and octahedron for O, icosahedron and dodecahedron for Y. It is well known that subgroups of O(3) can be obtained from those of SO(3) by adding the spatial inversion (− I) in one of two ways :

Table I*a*. — *Two-dimensional point groups* (G) : *Denominator* (θ_i) *and numerator* (φ_β) *invariants and basic vector fields* ($\mathbf{e}_\sigma$). *Cartesian coordinates x and y are chosen so that the origin is a fixed point and the x-axis is a reflection axis.* $\hat{i}$ *and* $\hat{j}$ *denote the unit vectors in the x and y directions respectively. The radius vector is* $\boldsymbol{\rho} = x\hat{i} + y\hat{j}$, $\rho^2 = x^2 + y^2$. *Other quantities entering the table are defined as follows :* $\gamma_n = \operatorname{Re}(x + iy)^n$; $\sigma_n = \operatorname{Im}(x + iy)^n$; $J\boldsymbol{\rho} = -y\hat{i} + x\hat{j}$.

G $\leqslant$ O(2)	θ_i	φ_β	$\mathbf{e}_\sigma$
$C_{\infty v}$ = O(2)	$\theta_1 = \rho^2$	$\varphi_0 = 1$	$\mathbf{e}_1 = \boldsymbol{\rho}$
C_∞ = SO(2)	$\theta_1 = \rho^2$	$\varphi_0 = 1$	$\mathbf{e}_1 = \boldsymbol{\rho}$ $\mathbf{e}_2 = J\boldsymbol{\rho}$
C_{nv} $n \geqslant 2$	$\theta_1 = \rho^2$ $\theta_2 = \gamma_n$	$\varphi_0 = 1$	$\mathbf{e}_1 = \boldsymbol{\rho}$ $\mathbf{e}_2 = \frac{1}{n}\nabla\gamma_n$
C_n $n \geqslant 2$	$\theta_1 = \rho^2$ $\theta_2 = \gamma_n$	$\varphi_0 = 1$ $\varphi_1 = \sigma_n$	$\mathbf{e}_1 = \boldsymbol{\rho}$ $\mathbf{e}_2 = J\boldsymbol{\rho}$ $\mathbf{e}_3 = \frac{1}{n}\nabla\gamma_n$ $\mathbf{e}_4 = \frac{1}{n}\nabla\sigma_n$
C_s	$\theta_1 = x$ $\theta_2 = y^2$	$\varphi_0 = 1$	$\mathbf{e}_1 = \hat{i}$ $\mathbf{e}_2 = y\hat{j}$
C_1	$\theta_1 = x$ $\theta_2 = y$	$\varphi_0 = 1$	$\mathbf{e}_1 = \hat{i}$ $\mathbf{e}_2 = \hat{j}$

G	Σ[L]	zeros of $\mathbf{v} = \Sigma_\sigma\, q_\sigma(\theta)\, \mathbf{e}_\sigma$
$C_{\infty v}$	$\Sigma[C_{\infty v}]$ $\Sigma[C_s]$	——— $q_1 = 0$
C_∞	$\Sigma[C_\infty]$ $\Sigma[C_1]$	——— $q_1 = q_2 = 0$
C_{nv}	$\Sigma[C_{nv}]$ $\Sigma[C_s^{(\pm)}]$ $\Sigma[C_1]$	——— $q_1\theta_1 + q_2\theta_2 = 0$ $q_1 = q_2 = 0$
C_n	$\Sigma[C_n]$ $\Sigma[C_1]$	——— $q_1\theta_1 + q_3\theta_2 + q_4\varphi_1 = 0$ $q_2\theta_1 - q_3\varphi_1 + q_4\theta_2 = 0$
C_s	$\Sigma[C_s]$ $\Sigma[C_1]$	$q_1 = 0$ $q_1 = q_2 = 0$
C_1	$\Sigma[C_1]$	$q_1 = q_2 = 0$

Table I*b*. — *Two-dimensional point groups* (G) : *Classes of little groups* ([*L*]), *relations determining corresponding stratum* ($\Sigma[L]$) *and the global basis on* E_2^L ($\mathbf{e}_\sigma$). *The relations are given in terms of invariants; the relations necessary in orbit space, but redundant in the carrier space, are enclosed in curly brackets. For the group* C_n, *the last row gives an algebraic relation satisfied on each stratum by the non-trivial numerator invariant. See table* I*a for definitions of the invariants and the vector fields.*

G $\leqslant$ O(2)	[L]	Σ[L]	$\mathbf{e}'_\sigma$ ([b])
$C_{\infty v}$	$[C_{\infty v}]$ $[C_s]$	$\theta_1 = 0$ $\theta_1 > 0$	0 $\mathbf{e}_1$(2)
C_∞	$[C_\infty]$ $[C_1]$	$\theta_1 = 0$ $\theta_1 > 0$	0 $\mathbf{e}_1, \mathbf{e}_2$
C_{nv}	$[C_{nv}]$ $[C_s^{(\pm)}]$ ([a]) $[C_1]$	$\theta_1 = 0$, $\{\theta_2 = 0\}$ $\theta_1 > 0$, $\theta_2^2 = \theta_1^n$ $\theta_1 > 0$, $\theta_1^n > \theta_2^2$	0 $\mathbf{e}_1$ $\mathbf{e}_1, \mathbf{e}_2$
C_n	$[C_n]$ $[C_1]$	$\theta_1 = 0$, $\{\theta_2 = 0\}$ $\theta_1 > 0$, $\theta_1^n > \theta_2^2$	0 $\mathbf{e}_1, \mathbf{e}_2$
	$\varphi_1^2 = \theta_1^n - \theta_2^2$		
C_s	$[C_s]$ $[C_1]$	$\theta_2 = 0$ $\theta_2 > 0$	$\mathbf{e}_1$ $\mathbf{e}_1, \mathbf{e}_2$
C_1	$[C_1]$	The whole space	$\mathbf{e}_1, \mathbf{e}_2$

([a]) For n odd the two classes, $[C_s^{(+)}]$ and $[C_s^{(-)}]$, coincide; for n even they are disjoint and correspond to $\theta_2 = \pm\,\theta_1^{n/2}$.

([b]) dim Σ[L], when different from dim E_2^L, is given in parentheses.

←

Table I*c*. — *Two-dimensional point groups* (G) : *Zeros of a general vector field* $\mathbf{v} = \Sigma_\sigma\, q_\sigma(\theta)\, \mathbf{e}_\sigma$ *at each stratum* $\Sigma[L]$. *The basic fields and relations determining the strata are given in tables* I*a and* I*b respectively. A dash in the last column indicates that* $\mathbf{v} = 0$ *reduces to an identity.*

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i) From a group H < SO(3), generate G = H ∪ (− I) H < O(3) which is isomorphic to H × Z_2. In this fashion one finds $C_{\infty h}$, $D_{\infty h}$, S_{2n} and D_{nd} (n odd), C_{nh} and D_{nh} (n even), T_h, O_h and Y_h.

ii) From a group H < SO(3) which has a subgroup K of index two generate a group G < O(3) isomorphic to H by multiplying elements of H not in K by (− I).

In this way one finds $C_{\infty v} = O(2)$, C_{nh} and D_{nh} (n odd), S_{2n} and D_{nd} (n even), C_{nv} and T_d.

The explicit forms of the invariant and covariant basic fields depend on the choice of coordinates. The choice we make is indicated in the table captions. Traditionally, the z-axis is the rotation axis of order n; moreover, when the group has in addition axes of order two, one of them is the x-axis. Similarly by convention, one of the reflection planes of C_{nv}, if not fixed by previous choice for two-fold rotation axes, is the xOz plane.

The tables are organized in the following way. A division is made according to the type of the groups. For example, tables I contain all closed subgroups of O(2); tables II contain all Lie subgroups of O(3); tables III to VIII contain all finite subgroups of O(3). For each type the tables are broken into three : in (*a*) the basic fields are defined; in (*b*) the isotropy groups and equations of corresponding strata are given; in (*c*) the lowest degree equivalents of equation 46 are written for each stratum and in orbit space.

In choosing basic fields there is definite arbitrarines. For example, one could wish to choose harmonic polynomials whenever possible. However, an arbitrary linear combination of harmonic polynomials with coefficients in $C[\theta_1, ..., \theta_n]$ is not necessarily a harmonic polynomial. In order to extract the harmonic component of a polynomial, a procedure due to Lohe [32] is useful :

$$p(\mathbf{r}) \to p(\mathbf{r} - r^2(2N+3)^{-1}\,\nabla)\,1\,, \qquad (48)$$

Table II*a*. — *Three-dimensional point groups* (G). *Lie subgroups of* O(3) : *Denominator* (θ_i) *and numerator* (φ_β) *invariants and basic vector fields* ($\mathbf{e}_\sigma$). *Cartesian coordinates x, y and z are chosen so that the origin is a fixed point and the z axis is the preferred one.* $\hat{i}$, $\hat{j}$ *and* $\hat{k}$ *denote unit vectors in the x, y and z directions respectively. The radius vector is* $\mathbf{r} = x\hat{i} + y\hat{j} + z\hat{k}$, $r^2 = x^2 + y^2 + z^2$, *the radius vector in the xy plane is* $\boldsymbol{\rho} = x\hat{i} + y\hat{j}$, $\rho^2 = x^2 + y^2$ *and* $J\boldsymbol{\rho} = -y\hat{i} + x\hat{j}$.

G ⩽ O(3)	θ_i	φ_β	$\mathbf{e}_\sigma$
O(3)	$\theta_1 = r^2$	$\varphi_0 = 1$	$\mathbf{e}_1 = \mathbf{r}$
SO(3)	$\theta_1 = r^2$	$\varphi_0 = 1$	$\mathbf{e}_1 = \mathbf{r}$
$D_{\infty h}$	$\theta_1 = \rho^2$ $\theta_2 = z^2$	$\varphi_0 = 1$	$\mathbf{e}_1 = \boldsymbol{\rho}$ $\mathbf{e}_2 = z\hat{k}$
D_∞	$\theta_1 = \rho^2$ $\theta_2 = z^2$	$\varphi_0 = 1$	$\mathbf{e}_1 = \boldsymbol{\rho}$ $\mathbf{e}_2 = z\hat{k}$ $\mathbf{e}_3 = zJ\boldsymbol{\rho}$
$C_{\infty h}$	$\theta_1 = \rho^2$ $\theta_2 = z^2$	$\varphi_0 = 1$	$\mathbf{e}_1 = \boldsymbol{\rho}$ $\mathbf{e}_2 = z\hat{k}$ $\mathbf{e}_3 = J\boldsymbol{\rho}$
$C_{\infty v}$	$\theta_1 = \rho^2$ $\theta_2 = z$	$\varphi_0 = 1$	$\mathbf{e}_1 = \boldsymbol{\rho}$ $\mathbf{e}_2 = \hat{k}$
C_∞	$\theta_1 = \rho^2$ $\theta_2 = z$	$\varphi_0 = 1$	$\mathbf{e}_1 = \boldsymbol{\rho}$ $\mathbf{e}_2 = \hat{k}$ $\mathbf{e}_3 = J\boldsymbol{\rho}$

Table II*b*. — *Three-dimensional point groups* (G). *Lie subgroups of* O(3) : *Classes of little groups* ([L]), *relations determining corresponding stratum* (Σ[L]) *and the global basis on* E_3^L ($\mathbf{e}'_\sigma$). *The relations are given in terms of invariants* (*orbit space*). *See table* II*a for definitions of the invariants and the vector fields.*

G ⩽ O(3)	[L]	Σ[L]	$\mathbf{e}'_\sigma$ ([a])
O(3)	[O(3)]	$\theta_1 = 0$	0
	$[C_{\infty v}]$	$\theta_1 > 0$	$\mathbf{e}_1(3)$
SO(3)	[SO(3)]	$\theta_1 = 0$	0
	$[C_\infty]$	$\theta_1 > 0$	$\mathbf{e}_1(3)$
$D_{\infty h}$	$[D_{\infty h}]$	$\theta_1 = \theta_2 = 0$	0
	$[C_{\infty v}]$	$\theta_2 > 0;\ \theta_1 = 0$	$\mathbf{e}_2$
	$[C_{2v}]$	$\theta_2 = 0;\ \theta_1 > 0$	$\mathbf{e}_1(2)$
	$[C_s]$	$\theta_2 > 0;\ \theta_1 > 0$	$\mathbf{e}_1, \mathbf{e}_2(3)$
D_∞	$[D_\infty]$	$\theta_1 = \theta_2 = 0$	0
	$[C_\infty]$	$\theta_2 > 0;\ \theta_1 = 0$	$\mathbf{e}_2$
	$[C_2]$	$\theta_2 = 0;\ \theta_1 > 0$	$\mathbf{e}_1(2)$
	$[C_1]$	$\theta_1 > 0;\ \theta_2 > 0$	$\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$
$C_{\infty h}$	$[C_{\infty h}]$	$\theta_1 = \theta_2 = 0$	0
	$[C_\infty]$	$\theta_2 > 0;\ \theta_1 = 0$	$\mathbf{e}_2$
	$[C_s]$	$\theta_2 = 0;\ \theta_1 > 0$	$\mathbf{e}_1, \mathbf{e}_3$
	$[C_1]$	$\theta_1 > 0;\ \theta_2 > 0$	$\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$
$C_{\infty v}$	$[C_{\infty v}]$	$\theta_1 = 0$	$\mathbf{e}_2$
	$[C_s]$	$\theta_1 > 0$	$\mathbf{e}_1, \mathbf{e}_2(3)$
C_∞	$[C_\infty]$	$\theta_1 = 0$	$\mathbf{e}_2$
	$[C_1]$	$\theta_1 > 0$	$\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$

([a]) dim Σ[L], when different from dim E_3^L, is given in parenthesis.

Table II*c*. — *Three-dimensional point groups* (G). *Lie subgroups of* O(3) : *Zeros of a general vector field* $\mathbf{v} = \Sigma_\sigma q_\sigma(\sigma)\,\mathbf{e}_\sigma$ *at each stratum* Σ[L]. *The basic fields and relations determining the strata are given in tables* II*a and* II*b respectively. A dash in the last column indicates that* $\mathbf{v} = 0$ *reduces to an identity.*

$G \leqslant O(3)$	Σ[L]	Zeros of $\mathbf{v} = \Sigma_\sigma q_\sigma(\theta)\,\mathbf{e}_\sigma$
O(3)	Σ[O(3)] $\Sigma[C_{\infty v}]$	—— $q_1 = 0$
SO(3)	Σ[SO(3)] $\Sigma[C_\infty]$	—— $q_1 = 0$
$D_{\infty h}$	$\Sigma[D_{\infty h}]$ $\Sigma[C_{\infty v}]$ $\Sigma[C_{2v}]$ $\Sigma[C_s]$	—— $q_2 = 0$ $q_1 = 0$ $q_1 = q_2 = 0$
D_∞	$\Sigma[D_\infty]$ $\Sigma[C_\infty]$ $\Sigma[C_2]$ $\Sigma[C_1]$	—— $q_2 = 0$ $q_1 = 0$ $q_1 = q_2 = q_3 = 0$
$C_{\infty h}$	$\Sigma[C_{\infty h}]$ $\Sigma[C_\infty]$ $\Sigma[C_s]$ $\Sigma[C_1]$	—— $q_2 = 0$ $q_1 = q_3 = 0$ $q_1 = q_2 = q_3 = 0$
$C_{\infty v}$	$\Sigma[C_{\infty v}]$ $\Sigma[C_s]$	$q_2 = 0$ $q_1 = q_2 = 0$
C_∞	$\Sigma[C_\infty]$ $\Sigma[C_1]$	$q_2 = 0$ $q_1 = q_2 = q_3 = 0$

where $N = \mathbf{r}.\nabla$ is an operator which multiplies a homogeneous polynomial by its degree.

Some of the results listed in our tables have been known previously and they have been double checked here. Several errors which appeared in previous publications have been detected and they are discussed in appendix E.

We will illustrate the use of the tables on an example of an O_h-covariant vector field. Let $\mathbf{v}$ be an O_h-covariant inhomogeneous vector field of seventh degree in x, y, z. Such a field can be written using the basis given in table IV*a* as

$$\mathbf{v} = q_1(\theta)\,\mathbf{e}_1 + q_2(\theta)\,\mathbf{e}_2 + q_3(\theta)\,\mathbf{e}_3\,, \qquad (49)$$

where we used a shorthand $\theta = (\theta_1, \theta_2, \theta_3)$. Since $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$ are of first, third and fifth degree, respectively, in x, y, z the polynomials q_1, q_2 and q_3 are of degree six, four and two, respectively. Thus, in the most general case

$$\begin{aligned} q_1 &= a_{11} + a_{12}\,\theta_1 + a_{13}\,\theta_1^2 + a_{14}\,\theta_2 + a_{15}\,\theta_1^3 + \\ &\quad + a_{16}\,\theta_1\,\theta_2 + a_{17}\,\theta_3 \\ q_2 &= a_{21} + a_{22}\,\theta_1 + a_{23}\,\theta_1^2 + a_{24}\,\theta_2 \qquad (50) \\ q_3 &= a_{31} + a_{32}\,\theta_1\,, \end{aligned}$$

Table III*a*. — *Three dimensional point groups* (G). *Icosahedral groups* (Y_h, Y) : *Denominator* (θ_i) *and numerator* (φ_β) *invariants and basic vector fields* ($\mathbf{e}_\sigma$). *Cartesian coordinates x, y and z are chosen so that the origin is a fixed point and the five-fold axes pass through the* 12 *vertices of an icosahedron at* $(\pm\,\tau, \pm 1, 0)$, $(0, \pm\,\tau, \pm 1)$, $(\pm 1, 0, \pm\,\tau)$, *where* $\tau = \frac{1}{2}(\sqrt{5} + 1)$. $\mathbf{r}$ *denotes the radius vector and* $r^2 = x^2 + y^2 + z^2$. *Other quantities entering the tables are* :

$$\begin{aligned} I_6' &= (\tau x^2 - y^2)(\tau y^2 - z^2)(\tau z^2 - x^2)\,; \\ I_{10} &= (x+y+z)(x-y-z)(y-z-x)(z-y-x)\,\times \\ &\times (\tau^{-2}\,x^2 - \tau^2\,y^2)(\tau^{-2}\,y^2 - \tau^2\,z^2)(\tau^{-2}\,z^2 - \tau^2\,x^2)\,; \\ J_{15} &= 4\,\tau^3\,xyz(\tau x + \tau^{-1}\,y + z)(-\tau x + \tau^{-1}\,y + z) \\ &\times (\tau x - \tau^{-1}\,y + z)(\tau x + \tau^{-1}\,y - z)(x + \tau y + \tau^{-1}\,z) \\ &\times (x - \tau y + \tau^{-1}\,z)(x + \tau y - \tau^{-1}\,z)(-x + \tau y + \tau^{-1}\,z) \\ &\times (\tau^{-1}\,x + y + \tau z)(\tau^{-1}\,x + y - \tau z)(-\tau^{-1}\,x + y + \tau z) \\ &\times (\tau^{-1}\,x - y + \tau z)\,. \end{aligned}$$

G	θ_i	φ_β	$\mathbf{e}_\sigma$
Y_h	$\theta_1 = r^2$ $\theta_2 = I_6'$ $\theta_3 = I_{10}$	$\varphi_0 = 1$	$\mathbf{e}_1 = \mathbf{r}$ $\mathbf{e}_2 = \frac{1}{2}\nabla I_6'$ $\mathbf{e}_3 = \frac{1}{2}\nabla I_{10}$
Y	$\theta_1 = r^2$ $\theta_2 = I_6'$ $\theta_3 = I_{10}$	$\varphi_0 = 1$ $\varphi_1 = J_{15}$	$\mathbf{e}_1 = \mathbf{r}$ $\mathbf{e}_2 = \frac{1}{2}\nabla I_6'$ $\mathbf{e}_3 = \frac{1}{2}\nabla I_{10}$ $\mathbf{e}_4 = \mathbf{e}_1 \times \mathbf{e}_2$ $\mathbf{e}_5 = \mathbf{e}_1 \times \mathbf{e}_3$ $\mathbf{e}_6 = \mathbf{e}_2 \times \mathbf{e}_3$

where a_{ij} are arbitrary constants and the basic invariants are given in table IV*a*.

Zeros of a seventh degree O_h-covariant vector field determine low symmetry phases which occur in Perovskites during a ferroelectric phase transition described by a Landau free energy F of eighth degree

$$\begin{aligned} F = a_{01}\,\theta_1 &+ a_{02}\,\theta_1^2 + a_{03}\,\theta_2 + a_{04}\,\theta_1^3 + \\ &+ a_{05}\,\theta_1\,\theta_2 + a_{06}\,\theta_3 + a_{07}\,\theta_1^4 + a_{08}\,\theta_1^2\,\theta_2 \\ &+ a_{09}\,\theta_1\,\theta_3 + a_{00}\,\theta_2^2\,. \qquad (51) \end{aligned}$$

In this case $\mathbf{v} = \nabla F$ and only ten a_{ij} of equation 50 are independent : ($a_{11} = 2\,a_{01}$, $a_{12} = 4\,a_{02}$, $a_{13} = 6\,a_{04}$, $a_{14} = 2\,a_{05}$, $a_{15} = 8\,a_{07}$, $a_{16} = 4\,a_{08}$, $a_{17} = 2\,a_{09}$, $a_{21} = 4\,a_{03}$, $a_{22} = 4\,a_{05}$, $a_{23} = 4\,a_{08}$, $a_{24} = 8\,a_{00}$, $a_{31} = 6\,a_{06}$, $a_{32} = 6\,a_{09}$)

Table III*b*. — *Three-dimensional point groups* (G). *Icosahedral grops* (Y_h, Y) : *Classes of little groups* ([L]), *relations determining corresponding straum* (Σ[L]) *and the global basis on* E_3^L (e'_σ). *The relations are given in terms of invariants; the relations necessary in orbit space, but redundant in the carrier space, are enclosed in curly brackets. The last row for* Y *gives an algebraic relation satisfied on each stratum by the non-trivial numerator invariant. See table* III*a for definitions of the invariants and the vector fields.* $\tau = \frac{1}{2}(1 + \sqrt{5})$.

G	[L]	Σ[L]	e'_σ
Y_h	[Y_h]	$\theta_1 = 0, \{ \theta_2 = \theta_3 = 0 \}$	0_1
	[C_{5v}]	$\theta_1 > 0, \theta_2 = -\frac{(2\tau+1)}{5}\theta_1^3, \left\{ \theta_3 = \frac{(2\tau-1)}{125}\theta_1^5 \right\}$	e_1
	[C_{3v}]	$\theta_1 > 0, \theta_2 = \frac{(2\tau+1)}{27}\theta_1^3, \left\{ \theta_3 = \frac{5(2\tau-1)}{81}\theta_1^5 \right\}$	e_1
	[C_{2v}]	$\theta_1 > 0, \theta_2 = \theta_3 = 0$	e_1
	[C_s]	$\theta_1 > 0, -\frac{(2\tau+1)}{5}\theta_1^3 < \theta_2 < \frac{(2\tau+1)}{27}\theta_1^3, \theta_3 > (7-4\tau)\theta_2\theta_1^2,$ $4\theta_1^9\theta_2^2 - 8\theta_1^7\theta_2\theta_3(3+4\tau) - 91\theta_1^6\theta_2^3(3-2\tau) + 4\theta_1^5\theta_3^2(5+8\tau) + 159\theta_1^4\theta_2^2\theta_3(1-2\tau) + 688\theta_1^3\theta_2^4(13-8\tau) + 325\theta_1^2\theta_2\theta_3(1+2\tau) - 720\theta_1\theta_2^3\theta_3(7-4\tau) - 1\,728\,\theta_2^5(55-34\tau) - 25\theta_3^3(11+18\tau) = 0$	e_1, e_2
	[C_1]	$\left\{ \theta_1 > 0, -\frac{(2\tau+1)}{5}\theta_1^3 < \theta_2 < \frac{(2\tau+1)}{27}\theta_1^3, \theta_3 > (7-4\tau)\theta_2\theta_1^2 \right\},$ $4\theta_1^9\theta_2^2 - 8\theta_1^7\theta_2\theta_3(3+4\tau) - 91\theta_1^6\theta_2^3(3-2\tau) + 4\theta_1^5\theta_3^2(5+8\tau) + 159\theta_1^4\theta_2^2\theta_3(1-2\tau) + 688\theta_1^3\theta_2^4(13-8\tau) + 325\theta_1^2\theta_2\theta_3^2(1+2\tau) - 720\theta_1\theta_2^3\theta_3(7-4\tau) - 1\,728\,\theta_2^5(55-34\tau) - 25\theta_3^3(11+18\tau) > 0$	e_1, e_2, e_3
Y	[Y]	$\theta_1 = 0, \{ \theta_2 = \theta_3 = 0 \}$	0
	[C_5]	$\theta_1 > 0, \theta_2 = -\frac{(2\tau+1)}{5}\theta_1^3, \left\{ \theta_3 = \frac{(2\tau-1)}{125}\theta_1^5 \right\}$	e_1
	[C_3]	$\theta_1 > 0, \theta_2 = \frac{(2\tau+1)}{27}\theta_1^3, \left\{ \theta_3 = \frac{5(2\tau-1)}{81}\theta_1^5 \right\}$	e_1
	[C_2]	$\theta_1 > 0, \theta_2 = \theta_3 = 0$	e_1
	[C_1]	$\theta_1 > 0, -\frac{(2\tau+1)}{5}\theta_1^3 < \theta_2 < \frac{(2\tau+1)}{27}\theta_1^3, \theta_3 > (7-4\tau)\theta_2\theta_1^2$	e_1, e_2, e_4
	$4\varphi_1^2 = 4\theta_1^9\theta_2^2 - 8\theta_1^7\theta_2\theta_3(3+4\tau) - 91\theta_1^6\theta_2^3(3-2\tau) + 4\theta_1^5\theta_3^2(5+8\tau) + 159\theta_1^4\theta_2^2\theta_3(1-2\tau) + 688\theta_1^3\theta_2^4(13-8\tau) + 325\theta_1^2\theta_2\theta_3^2(1+2\tau) - 720\theta_1\theta_2^3\theta_3(7-4\tau) - 1\,728\,\theta_2^5(55-34\tau) - 25\theta_3^3(11+18\tau) \{ \geqslant 0 \}$		

Table III*c*. — *Three-dimensional point groups* (G). *Icosahedral groups* (Y_h, Y) : *Zeros of a general vector field* $\mathbf{v} = \Sigma_\sigma q_\sigma(\theta)\, \mathbf{e}_\sigma$ *at each stratum* $\Sigma[L]$. *The basic fields and relations determining the strata are given in tables* III*a* *and* III*b*, *respectively*. $\tau \equiv \frac{1}{2}(1 + \sqrt{5})$. *A dash in the last column indicates that* $\mathbf{v} = 0$ *reduces to an identity.*

G	Σ[L]	Zeros of $\mathbf{v} = \Sigma_\sigma q_\sigma(\theta)\, \mathbf{e}_\sigma$
Y_h	$\Sigma[Y_h]$	———
	$\Sigma[C_{5v}]$	$25\, q_1 - 15(2\tau + 1)\, \theta_1^2\, q_2 + (2\tau - 1)\, \theta_1^4\, q_3 = 0$
	$\Sigma[C_{3v}]$	$81\, q_1 + 9(2\tau + 1)\, \theta_1^2\, q_2 + 25(2\tau - 1)\, \theta_1^4\, q_3 = 0$
	$\Sigma[C_{2v}]$	$q_1 = 0$
	$\Sigma[C_s]$	$\theta_1 q_1 + 3\, \theta_2 q_2 + 5\, \theta_3 q_3 = 0$ $3\, \theta_2 q_1 + \frac{1}{4}[-7(2\tau + 1)\, \theta_1^2\, \theta_2 + (18\tau + 11)\, \theta_3]\, q_2 +$ $+ \frac{1}{4}[(1 - 2\tau)\, \theta_1^4\, \theta_2 + 3(2\tau + 1)\, \theta_1^2\, \theta_3 + 8(4\tau - 7)\, \theta_1\, \theta_2^2]\, q_3 = 0$
	$\Sigma[C_1]$	$q_1 = q_2 = q_3 = 0$
Y	$\Sigma[Y]$	———
	$\Sigma[C_5]$	$25\, q_1 - 15(2\tau + 1)\, \theta_1^2\, q_2 + (2\tau - 1)\, \theta_1^4\, q_3 = 0$
	$\Sigma[C_3]$	$81\, q_1 + 9(2\tau + 1)\, \theta_1^2\, q_2 + 25(2\tau - 1)\, \theta_1^4\, q_3 = 0$
	$\Sigma[C_2]$	$q_1 = 0$
	$\Sigma[C_1]$	$\theta_1 q_1 + 3\, \theta_2 q_2 + 5\, \theta_3 q_3 + \varphi_1 q_6 = 0$ $3\, \theta_2 q_1 + \frac{1}{4}[-7(2\tau + 1)\, \theta_1^2\, \theta_2 + (18\tau + 11)\, \theta_3]\, q_2 +$ $+ \frac{1}{4}[(1 - 2\tau)\, \theta_1^4\, \theta_2 + 3(2\tau + 1)\, \theta_1^2\, \theta_3 + (4\tau - 7)\, \theta_1\, \theta_2^2]\, q_3 - \varphi_1 q_6 = 0$ $\varphi_1 q_3 + \frac{1}{4}[-7(2\tau + 1)\, \theta_1^3\, \theta_2 + (18\tau + 11)\, \theta_1\, \theta_3 - 36\, \theta_2^2]\, q_4 +$ $+ \frac{1}{4}[(1 - 2\tau)\, \theta_1^5\, \theta_2 + 3(2\tau + 1)\, \theta_1^3\, \theta_3 + 8(4\tau - 7)\, \theta_1^2\, \theta_2^2 - 60\, \theta_2\, \theta_3]\, q_5$ $+ \frac{1}{4}[3(1 - 2\tau)\, \theta_1^4\, \theta_2^2 + 44(2\tau + 1)\, \theta_1^2\, \theta_2\, \theta_3$ $+ 24(4\tau - 7)\, \theta_1\, \theta_2^3 - 5(18\tau + 11)\, \theta_3^2]\, q_6 = 0\,.$

To determine zeros of **v** directly in terms of x, y, z one has to solve system of 3 equations of seventh degree, which in addition depend on thirteen arbitrary parameters. The idea of our method is to solve, instead, for the zeros of **v** in terms of the invariants θ. Corresponding orbits in x, y, z can then be determined from the inverse of $\theta = \omega(\mathbf{r})$ which depends only on G (not on **v**) and can be given once for all. Let us first determine the inverse map for O_h.

Table IV*a*. — *Three-dimensional point groups* (G). *Octahedral groups* (O_h, O) : *Denominator* (θ_i) *and numerator* (φ_β) *invariants and basic vector fields* ($\mathbf{e}_\sigma$). *Cartesian coordinates x, y and z are chosen so that the origin is a fixed point and x-, y- and z-axes are the four-fold axes.* **r** *is the radius vector,* $r^2 = x^2 + y^2 + z^2$. *Other quantities entering the tables are defined as follows :*

$$I_4 = x^4 + y^4 + z^4 ; \quad I_6 = x^6 + y^6 + z^6 ;$$
$$J_9 = xyz(x^2 - y^2)(y^2 - z^2)(z^2 - x^2) .$$

G	θ_i	φ_β	$\mathbf{e}_\sigma$
O_h	$\theta_1 = r^2$ $\theta_2 = I_4$ $\theta_3 = I_6$	$\varphi_0 = 1$	$e_1 = \mathbf{r}$ $e_2 = \frac{1}{4}\nabla I_4$ $e_3 = \frac{1}{6}\nabla I_6$
O	$\theta_1 = r^2$ $\theta_2 = I_4$ $\theta_3 = I_6$	$\varphi_0 = 1$ $\varphi_1 = J_9$	$\mathbf{e}_1 = \mathbf{r}$ $\mathbf{e}_2 = \frac{1}{4}\nabla I_4$ $\mathbf{e}_3 = \frac{1}{6}\nabla I_6$ $\mathbf{e}_4 = \mathbf{e}_1 \times \mathbf{e}_2$ $\mathbf{e}_5 = \mathbf{e}_1 \times \mathbf{e}_3$ $\mathbf{e}_6 = \mathbf{e}_2 \times \mathbf{e}_3$

Table IV*b*. — *Three-dimensional point groups* (G). *Octahedral groups* (O_h, O) : *Classes of little groups* ([L]), *relations determining corresponding stratum* (Σ[L]) *and the global basis on* E_3^{L} ($\mathbf{e}'_\sigma$). *The relations are given in terms of invariants ; the relations necessary in orbit space, but redundant in the carrier space, are enclosed in curly brackets. For the group* O *the last row gives an algebraic relation satisfied on each stratum by the non-trivial numerator invariant. See table* IV *a for definitions of the invariants and the vector fields.*

G	[L]	Σ[L]	$\mathbf{e}'_\sigma$
O_h	[O_h]	$\theta_1 = 0, \{ \theta_2 = \theta_3 = 0 \}$	0
	[C_{4v}]	$\theta_1 > 0, \theta_2 = \theta_1^2, \{ \theta_3 = \theta_1^3 \}$	$\mathbf{e}_1$
	[C_{3v}]	$\theta_1 > 0, 3\theta_2 = \theta_1^2, \{ 9\theta_3 = \theta_1^3 \}$	$\mathbf{e}_1$
	[C_{2v}]	$\theta_1 > 0, 2\theta_2 = \theta_1^2, \{ 4\theta_3 = \theta_1^3 \}$	$\mathbf{e}_1$
	[C_s]	$\theta_1 > 0, 3\theta_2 > \theta_1^2, 2\theta_3 > (3\theta_1\theta_2 - \theta_1^3)$, $-\theta_1^6 + 9\theta_1^4\theta_2 - 8\theta_1^3\theta_3 - 21\theta_1^2\theta_2^2 + 36\theta_1\theta_2\theta_3 + 3\theta_2^3 - 18\theta_3^2 = 0$	$\mathbf{e}_1, \mathbf{e}_2$
	[C'_s]	$\theta_1 > 0, 2\theta_1^2 > 2\theta_2 > \theta_1^2, \theta_1^3 - 3\theta_1\theta_2 + 2\theta_3 = 0$	$\mathbf{e}_1, \mathbf{e}_2$
	[C_1]	$\theta_1 > 0, \theta_1^3 - 3\theta_1\theta_2 + 2\theta_3 > 0$, $-\theta_1^6 + 9\theta_1^4\theta_2 - 8\theta_1^3\theta_3 - 21\theta_1^2\theta_2^2 + 36\theta_1\theta_2\theta_3 + 3\theta_2^3 - 18\theta_3^2 > 0$, $\{ \theta_2 < \theta_1^2 \}$	$\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$
O	[O]	$\theta_1 = 0, \{ \theta_2 = \theta_3 = 0 \}$	0
	[C_4]	$\theta_1 > 0, \theta_2 = \theta_1^2, \{ \theta_3 = \theta_1^3 \}$	$\mathbf{e}_1$
	[C_3]	$\theta_1 > 0, 3\theta_2 = \theta_1^2, \{ 9\theta_3 = \theta_1^3 \}$	$\mathbf{e}_1$
	[C_2]	$\theta_1 > 0, 2\theta_2 = \theta_1^2, 4\theta_3 = \theta_1^3$	$\mathbf{e}_1$
	[C_1]	$\theta_1 > 0, \theta_1^3 - 3\theta_1\theta_2 + 2\theta_3 \geqslant 0$, $-\theta_1^6 + 9\theta_1^4\theta_2 - 8\theta_1^3\theta_3 - 21\theta_1^2\theta_2^2 + 36\theta_1\theta_2\theta_3 + 3\theta_2^3 - 18\theta_3^2 \geqslant 0$, $\{ \theta_2 \leqslant \theta_1^2 \}$	$\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_4$
	$36\varphi_1^2 = (-\theta_1^6 + 9\theta_1^4\theta_2 - 8\theta_1^3\theta_3 - 21\theta_1^2\theta_2^2 + 36\theta_1\theta_2\theta_3 + 3\theta_2^3 - 18\theta_3^2) \times$ $\times (\theta_1^3 - 3\theta_1\theta_2 + 2\theta_3) \{ \geqslant 0 \}$		

Table IV*c*. — *Three-dimensional point groups* (G). *Octahedral groups* (O_h, O) : *Zeros of a general vector field* $\mathbf{v} = \Sigma_\sigma q_\sigma(\theta)\, \mathbf{e}_\sigma$ *at each stratum* Σ[L]. *The basic fields and relations determining the strata are given in tables* IV*a* *and* IV*b*, *respectively. A dash in the last column indicates that* $\mathbf{v} = 0$ *reduces to an identity.*

G	Σ[L]	Zeros of $\mathbf{v} = \Sigma_\sigma q_\sigma(\theta)\, \mathbf{e}_\sigma$
O_h	$\Sigma[O_h]$	————
	$\Sigma[C_{4v}]$	$q_1 + \theta_1 q_2 + \theta_1^2 q_3 = 0$
	$\Sigma[C_{3v}]$	$9 q_1 + 3 \theta_1 q_2 + \theta_1^2 q_3 = 0$
	$\Sigma[C_{2v}]$	$4 q_1 + 2 \theta_1 q_2 + \theta_1^2 q_3 = 0$
	$\Sigma[C_s]$	$\theta_1 q_1 + \theta_2 q_2 + \theta_3 q_3 = 0$
		$6 \theta_2 q_1 + 6 \theta_3 q_2 + (\theta_1^4 - 6 \theta_1^2 \theta_2 + 8 \theta_1 \theta_3 + 3 \theta_2^2) q_3 = 0$
	$\Sigma[C_s']$	$q_2 + \theta_1 q_3 = 0$
		$2 q_1 + (\theta_2 - \theta_1^2) q_3 = 0$
	$\Sigma[C_1]$	$q_1 = q_2 = q_3 = 0$
O	$\Sigma[O]$	————
	$\Sigma[C_4]$	$q_1 + \theta_1 q_2 + \theta_1^2 q_3 = 0$
	$\Sigma[C_3]$	$9 q_1 + 3 \theta_1 q_2 + \theta_1^2 q_3 = 0$
	$\Sigma[C_2]$	$4 q_1 + 2 \theta_1 q_2 + \theta_1^2 q_3 = 0$
	$\Sigma[C_1]$	$\theta_1 q_1 + \theta_2 q_2 + \theta_3 q_3 + \varphi_1 q_6 = 0$
		$6 \theta_2 q_1 + 6 \theta_3 q_2 + (\theta_1^4 - 6 \theta_1^2 \theta_2 + 8 \theta_1 \theta_3 + 3 \theta_2^2) q_3 - \varphi_1 q_5 = 0$
		$6 \varphi_1 q_3 + 6(\theta_1 \theta_3 - \theta_2^2) q_4 + (\theta_1^5 - 6 \theta_1^3 \theta_2 + 8 \theta_1^2 \theta_3 + 3 \theta_1 \theta_2^2 - 6 \theta_2 \theta_3) q_5 +$ $+ (\theta_1^4 \theta_2 - 6 \theta_1^2 \theta_2^2 + 8 \theta_1 \theta_2 \theta_3 + 3 \theta_2^3 - 6 \theta_3^2) q_6 = 0$

G	θ_i	φ_β	$\mathbf{e}_\sigma$
T_h	$\theta_1 = r^2$ $\theta_2 = I_4$ $\theta_3 = I_6$	$\varphi_0 = 1$ $\varphi_1 = J_6$	$\mathbf{e}_1 = \mathbf{r}$ $\mathbf{e}_2 = \frac{1}{4} \nabla I_4$ $\mathbf{e}_3 = \frac{1}{6} \nabla I_6$ $\mathbf{e}_4 = \mathbf{e}_1 \times \nabla I_3$ $\mathbf{e}_5 = \mathbf{e}_2 \times \nabla I_3$ $\mathbf{e}_6 = I_3\, \mathbf{e}_1 \times \mathbf{e}_2$
T_d	$\theta_1 = r^2$ $\theta_2 = I_3$ $\theta_3 = I_4$	$\varphi_0 = 1$	$\mathbf{e}_1 = \mathbf{r}$ $\mathbf{e}_2 = \nabla I_3$ $\mathbf{e}_3 = \frac{1}{4} \nabla I_4$
T	$\theta_1 = r^2$ $\theta_2 = I_3$ $\theta_3 = I_4$	$\varphi_0 = 1$ $\varphi_1 = J_6$	$\mathbf{e}_1 = \mathbf{r}$ $\mathbf{e}_2 = \nabla I_3$ $\mathbf{e}_3 = \frac{1}{4} \nabla I_4$ $\mathbf{e}_4 = \mathbf{e}_1 \times \mathbf{e}_2$ $\mathbf{e}_5 = \mathbf{e}_1 \times \mathbf{e}_3$ $\mathbf{e}_6 = \mathbf{e}_2 \times \mathbf{e}_3$

←

Table V*a*. — *Three-dimensional point groups* (G). *Tetrahedral groups* (T_h, T_d, T) : *Denominator* (θ_i) *and numerator* (φ_β) *invariants and basic vector fields* ($\mathbf{e}_\sigma$). *Cartesian coordinates x, y and z are so chosen that the origin is a fixed point and the three-fold axes pass through vertices of a tetrahedron at* (1, 1, 1), (− 1, − 1, 1), (1, − 1, − 1), (− 1, 1, − 1). $\mathbf{r}$ *is the radius vector,* $r^2 = x^2 + y^2 + z^2$. *Other quantities entering the tables are defined as follows :*

$$I_3 = xyz \; ; \; I_4 = x^4 + y^4 + z^4 \; ;$$
$$I_6 = x^6 + y^6 + z^6 \; ;$$
$$J_6 = (x^2 - y^2)(y^2 - z^2)(z^2 - x^2) .$$

Let $\bar{\theta}_1$, $\bar{\theta}_2$, $\bar{\theta}_3$ be particular values of the invariants θ_1, θ_2, θ_3. The corresponding orbit in x, y, z is found from, cf. table IV*a*,

$$\begin{aligned} x^2 + y^2 + z^2 &= \bar{\theta}_1 \\ x^4 + y^4 + z^4 &= \bar{\theta}_2 \\ x^6 + y^6 + z^6 &= \bar{\theta}_3 . \end{aligned} \qquad (52)$$

Table V*b*. — *Three-dimensional point groups* (G). *Tetrahedral groups* (T_h, T_d, T) : *Classes of little groups* ([L]), *relations determining corresponding stratum* (Σ[L]) *and the global basis on* $E_3^{\perp}$ ($\mathbf{e}'_\sigma$). *The relations are given in terms of invariants ; the relations necessary in orbit space, but redundant in the carrier space, are enclosed in curly brackets. The last rows for groups* T_h *and* T *give albebraic relations satisfied on each stratum by the non-trivial numerator invariants. See table* V*a for definitions of the invariants and the vector fields.*

G	[L]	Σ[L]	$\mathbf{e}'_\sigma$
T_h	[T_h]	$\theta_1 = 0, \{ \theta_2 = \theta_3 = 0 \}$	0
	[C_{2v}]	$\theta_1 > 0, \theta_2 = \theta_1^2, \{ \theta_3 = \theta_1^3 \}$	$\mathbf{e}_1$
	[C_3]	$\theta_1 > 0, 3\,\theta_2 = \theta_1^2, \{ 9\,\theta_3 = \theta_1^3 \}$	$\mathbf{e}_1$
	[C'_s]	$\theta_1 > 0, \theta_2 < \theta_1^2, \theta_1^3 - 3\,\theta_1\,\theta_2 + 2\,\theta_3 = 0,$ $\{ 2\,\theta_2 \geqslant \theta_1^2 \}$	$\mathbf{e}_1, \mathbf{e}_4$
	[C_1]	$\theta_1 > 0, 3\,\theta_2 > \theta_1^2, \theta_1^3 - 3\,\theta_1\,\theta_2 + 2\,\theta_3 > 0, \{ \theta_2 \leqslant \theta_1^2 \}$	$\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_4$
	$6\,\varphi_1^2 = -\,\theta_1^6 + 9\,\theta_1^4\,\theta_2 - 8\,\theta_1^3\,\theta_3 - 21\,\theta_1^2\,\theta_2^2 + 36\,\theta_1\,\theta_2\,\theta_3 + 3\,\theta_2^3 - 18\,\theta_3^2 \{ \geqslant 0 \}$		
T_d	[T_d]	$\theta_1 = 0, \{ \theta_2 = \theta_3 = 0 \}$	0
	[C_{3v}]	$\theta_1 > 0, 3\,\theta_3 = \theta_1^2, \{ 27\,\theta_2^2 = \theta_1^3 \}$	$\mathbf{e}_1$
	[C_{2v}]	$\theta_1 > 0, \theta_3 = \theta_1^2, \{ \theta_2 = 0 \}$	$\mathbf{e}_1$
	[C_s]	$\theta_1 > 0, 3\,\theta_1^2 > 3\,\theta_3 > \theta_1^2,$ $-\,\theta_1^6 + 4\,\theta_1^4\,\theta_3 + 20\,\theta_1^3\,\theta_2^2 - 5\,\theta_1\,\theta_3^2 - 36\,\theta_1\,\theta_2^2\,\theta_3 - 108\,\theta_2^4 + 2\,\theta_3^3 = 0$	$\mathbf{e}_1, \mathbf{e}_2$
	[C_1]	$\theta_1 > 0, 3\,\theta_1^2 > 3\,\theta_3 > \theta_1^2,$ $-\,\theta_1^6 + 4\,\theta_1^4\,\theta_3 + 20\,\theta_1^3\,\theta_2^2 - 5\,\theta_1\,\theta_3^2 - 36\,\theta_1\,\theta_2^2\,\theta_3 - 108\,\theta_3^4 + 2\,\theta_3^3 > 0$	$\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$
T	[T]	$\theta_1 = 0, \{ \theta_2 = \theta_3 = 0 \}$	0
	[C_3]	$\theta_1 > 0, 3\,\theta_3 = \theta_1^2, \{ 27\,\theta_2^2 = \theta_1^3 \}$	$\mathbf{e}_1$
	[C_2]	$\theta_1 > 0, \theta_3 = \theta_1^2, \{ \theta_2 = 0 \}$	$\mathbf{e}_1$
	[C_1]	$-\,\theta_1 > 0, 3\,\theta_1^2 > 3\,\theta_3 > \theta_1^2$	$\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_4$
	$4\,\varphi_1^2 = -\,\theta_1^6 + 4\,\theta_1^4\,\theta_3 + 20\,\theta_1^3\,\theta_2^2 - 5\,\theta_1^2\,\theta_3^2 - 36\,\theta_1\,\theta_2^2\,\theta_3 - 108\,\theta_2^4 + 2\,\theta_3^3 \{ \geqslant 0 \}$		

This system of equations can be solved analytically leading to (at the most) 48 solutions $(\bar{x}, \bar{y}, \bar{z})$

$$(\bar{x}, \bar{y}, \bar{z}) = (\pm\, \lambda_i^{1/2}(\bar{\theta}), \pm\, \lambda_j^{1/2}(\bar{\theta}), \pm\, \lambda_k^{1/2}(\bar{\theta}))\,, \quad (53)$$

where $\pm$ signs are independent, $i, j, k = 1, 2, 3$, $i \neq j \neq k \neq i$, and $\lambda_i(\bar{\theta})$ are the three solutions (possibly degenerate) of the cubic equation in λ

$$\lambda^3 - \bar{\theta}_1\,\lambda^2 + \frac{1}{2}(\bar{\theta}_1^2 - \bar{\theta}_2)\,\lambda - \frac{1}{6}(\bar{\theta}_1^3 - 3\,\bar{\theta}_1\,\bar{\theta}_2 + 2\,\bar{\theta}_3) = 0\,. \quad (54)$$

By construction, $(\bar{x}, \bar{y}, \bar{z})$ will be real at each stratum and, conversely, the reality condition determines the orbit space.

We use tables IV*b* and IV*c* in order to find $\bar{\theta}_1, \bar{\theta}_2, \bar{\theta}_3$ for which $\mathbf{v} = 0$. For example, at $\Sigma[C_1]$ the equations for $\bar{\theta}_1, \bar{\theta}_2, \bar{\theta}_3$ are $q_1 = q_2 = q_3 = 0$, which using (50) have the solution

$$\begin{aligned}
\bar{\theta}_1 &= -\,\frac{a_{31}}{a_{32}} \\
\bar{\theta}_2 &= -\,\frac{a_{21}}{a_{24}} + \frac{a_{22}\,a_{31}}{a_{24}\,a_{32}} - \frac{a_{23}\,a_{31}^2}{a_{24}\,a_{32}^2} \\
\bar{\theta}_3 &= -\,\frac{a_{11}}{a_{17}} + \frac{a_{12}\,a_{31}}{a_{17}\,a_{32}} - \frac{a_{13}\,a_{31}^2}{a_{17}\,a_{32}^2} + \frac{a_{15}\,a_{31}^3}{a_{17}\,a_{32}^3} + \\
&\quad + \left(\frac{a_{14}}{a_{17}} - \frac{a_{16}\,a_{31}}{a_{17}\,a_{32}}\right)\left(\frac{a_{21}}{a_{24}} - \frac{a_{22}\,a_{31}}{a_{24}\,a_{32}} + \frac{a_{23}\,a_{31}^2}{a_{24}\,a_{32}^2}\right).
\end{aligned} \quad (55)$$

In (55) we assumed $a_{17}\,a_{24}\,a_{32} \neq 0$, other cases can be treated similarly.