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Abstract. An extended integrity basis (EIB) of a polynomial algebra in a set of variables on which a finite group operates includes the ordinary integrity basis of invariants and linear integrity bases of covariants. The latter are defined as sets of covariants of a given type such that any other covariant of this type is expressible as a linear combination of basic ones with invariants as coefficients of this combination. A constructive method of derivation, based on successive Clebsch–Gordan reduction and elimination of redundant covariants, is described, and the 'extended Noether's theorem', which states that the EIB of a finite group in a finite set of variables is finite, is proved with its use. It is shown that EIBs in irreducible sets of variables are fundamental for a given group because overall homogeneous EIBs in any set of variables can be constructed with their use for this group. A relationship between this method and theory based on a consideration of Molien series is established. It is shown that the division of invariants into denominator and numerator invariants enables one to construct general invariant functions as well as functional covariants.

1. Introduction

An algebra $\mathscr{P}$ of polynomials $p(\boldsymbol{x})$ in variables $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)$ on which there acts a group G of linear transformations contains a sub-algebra $\mathscr{P}_1$ of invariant polynomials. If the group G and the number n of variables x_i are finite, then the algebra $\mathscr{P}_1$ is generated by a finite set of polynomials called the 'integrity basis' of $\mathscr{P}_1$. This statement is usually referred to as Noether's theorem (Noether 1916, Weyl 1946), though systems of fundamental polynomials had previously been introduced by Hilbert (1890, 1893).

Polynomials which transform by one-dimensional ireps (irreducible representations) of G and sets of polynomials which transform as bases for many-dimensional ireps of G form linear spaces over the field of complex numbers. Such sets will be called here 'covariants' (Weyl 1946); in the one-dimensional case we shall also use the term 'relative invariants' (Burnside 1955). It turns out that these spaces can be generated by finite sets of covariants, called here 'linear integrity bases', in such a way that any covariant of a given type can be expressed as a linear combination of basic ones with invariants as coefficients of the linear combination. The integrity basis of invariants and the linear integrity bases of covariants will together be called the 'extended integrity basis' (EIB) of $\mathscr{P}$ (with respect to a given G), and the statement that the EIB is finite will be referred to as the 'extended Noether's theorem'. The finiteness of linear integrity bases for subgroups of Coxeter groups has been proved by McLellan (1974), who has also shown the structure of covariants using generalised Molien series.

The aim of this paper is: (i) to modify an algorithm for deriving the EIB of abelian groups (Kopský 1975) so that it can be used in the general case; (ii) to prove the 'extended Noether's theorem' with the use of this algorithm; and (iii) to show that, for a given group G, the EIBs in sets of variables belonging to a single irep are fundamental as all other EIBs can be derived from them. These EIBs for ordinary and double crystal point groups will be given explicitly in two further papers (Kopský 1979a,b).

Patera *et al* (1978) and Desmier and Sharp (1978) have recently approached the same problem for ordinary and double point groups with the use of generalised Molien series, following the pattern of McLellan (1974). As this introductory paper seems most convenient for confronting both methods, we include the part concerning Molien series and the structure of $\mathscr{P}_1$ and of spaces of covariants.

Section 2 presents the Clebsch–Gordan (CG) reduction in the form of CG products which give a unified prescription for the construction of covariants on which the construction of EIBs is based. In § 3 we consider the algebras $\mathscr{P}$, $\mathscr{P}_1$ and spaces of covariants as graded algebras and spaces and their characterisation by Molien series. Section 4 contains basic theorems on the structure of EIBs and a discussion of the use of Molien series in comparison with the constructive approach which is given in § 5, where the algorithm is described and the extended Noether's theorem proved with its use.

Throughout we use a shorter-term G-module (Hall 1959) instead of carrier space for a representation of G; if this representation is specified by characters $\chi(g)$, we specify the G-module also more closely as the $\chi(G)$-module. G-modules are considered as linear spaces over the field of complex numbers so that reducibility means complete reducibility. And, to compare our terminology with that of Patera *et al* (1978), let us say that their (Γ_α, Γ)-tensor is our $\Gamma_{0\alpha}$-covariant on the space L_n, which transforms under G by representation Γ.

2. *G*-modules and Clebsch–Gordan reduction

2.1. G-module and its adjoint, functional G-module and covariants

Throughout the paper we consider G as a finite group with κ classes of ireps $\chi_\alpha(G)$, and L_n as a $\chi(G)$-module. In each class $\chi_\alpha(G)$ we also fix one certain matrix irep $\Gamma_{0\alpha}(G)$: $g \to D^{(\alpha)}(g)$ for all further considerations. If n_α is the multiplicity of $\chi_\alpha(G)$ in $\chi(G)$, then L_n splits into a direct sum of minimal (irreducibile) $\chi_\alpha(G)$-modules $L_{\alpha a}$:

$$L_n = \bigoplus_{\alpha=1}^{\kappa} \bigoplus_{a=1}^{n_\alpha} L_{\alpha a}.$$

In a certain basis $\{e_i\}$, $i = 1, 2, \ldots, n = \dim L_n$, we obtain the matrix representation $\Gamma(G)$: $g \to D(g)$; some similarity transformation leads to a basis $\{e_{\alpha a,i}\}$, $i = 1, 2, \ldots, d_\alpha = \chi_\alpha(e) = \dim L_{\alpha a}$, where a set of vectors with fixed α, a spans $L_{\alpha a}$ and defines irep $\Gamma_{0\alpha}(G)$. We write, using summation convention,

$$ge_i = D_{ji}(g)e_j, \qquad ge_{\alpha a,i} = D_{ji}^{(\alpha)}(g)e_{\alpha a,j}. \tag{1}$$

The action of $g \in G$ on a function $f(\boldsymbol{x}, \boldsymbol{y}, \ldots)$ of $\boldsymbol{x}, \boldsymbol{y} \in L_n$ is defined by

$$gf(\boldsymbol{x}, \boldsymbol{y}, \ldots) = f(g^{-1}\boldsymbol{x}, g^{-1}\boldsymbol{y}, \ldots). \tag{2}$$

The space $\tilde{L}_n$ of linear functions on L_n is called adjoint to L_n; its bases $\{\phi_i(\boldsymbol{x}) = x_i\}$ and $\{\phi_{\alpha a,i}(\boldsymbol{x}) = x_{\alpha a,i}\}$, where $\boldsymbol{x} = x_i e_i = x_{\alpha a,i} e_{\alpha a,i}$, are adjoint to bases $\{e_i\}$ and $\{e_{\alpha a,i}\}$ of L_n respectively. From (2) it follows that

$$gx_i = \tilde{D}_{ji}(g)x_j, \qquad gx_{\alpha a,i} = \tilde{D}_{ji}^{(\alpha)}(g)x_{\alpha a,j} \tag{3}$$

where $\tilde{D} = (D^t)^{-1} = (D^{-1})^t$ denotes an adjoint (transposed and reciprocal) matrix to D. Since $\operatorname{tr} \tilde{D} = (\operatorname{tr} D)^*$, $\tilde{L}_n$ is a $\chi^*(G)$-module and splits into

$$\tilde{L}_n = \bigoplus_{\alpha=1}^{\kappa} \bigoplus_{a=1}^{n_\alpha} \tilde{L}_{\alpha a}$$

where $\tilde{L}_{\alpha a}$ are adjoint to $L_{\alpha a}$ $\chi^*_\alpha(G)$-modules spanned by $\{x_{\alpha a,i}\}$.

A set $f^{(\alpha)} = (f_{\alpha 1}, f_{\alpha 2}, \ldots, f_{\alpha d_\alpha})$ of functions on L_n is called a (functional) $\Gamma_{0\alpha}$-covariant if

$$g f_{\alpha i} = \tilde{D}^{(\alpha)}_{ji}(g) f_{\alpha j}. \tag{4}$$

In the case of the identity irep ($\alpha = 1$) we say that f_1 is an invariant; in the case of one-dimensional ireps we also use the term relative invariant. The sets $x^{(\alpha)}_a = (x_{\alpha a,1}, x_{\alpha a,2}, \ldots, x_{\alpha a,d_\alpha})$ are linear $\Gamma_{0\alpha}$-covariants. The properties of covariants are discussed in Weyl (1946), who introduced this term.

2.2. *Clebsch–Gordan products of covariants*

Instead of tabulating the CG coefficients like, for example, Koster *et al* (1963) did, we prefer to present the CG reduction by means of CG products. To do it in a standardised way, we introduce a set of typical covariants $x^{(\alpha)} = (x_{\alpha 1}, x_{\alpha 2}, \ldots, x_{\alpha d_\alpha})$, $\alpha = 1, 2, \ldots, \kappa$. We then take the complete set of typical variables $x_{\alpha i}$, looking for transformation properties of their bilinear combinations. Let $\Gamma_\alpha \otimes \Gamma_\beta = \Gamma_\beta \otimes \Gamma_\alpha = \ldots \oplus (\alpha\beta\mu)\Gamma_\mu \oplus \ldots$, $[\Gamma^2_\alpha] = \ldots \oplus [\alpha\alpha\mu]\Gamma_\mu \oplus \ldots$, and $\{\Gamma^2_\alpha\} = \ldots \oplus \{\alpha\alpha\mu\}\Gamma_\mu \oplus \ldots$. Then there exist $(\alpha\beta\mu)$ linearly independent $\Gamma_{0\mu}$-covariants, called CG products of $x^{(\alpha)}$, $x^{(\beta)}$,

$$(x^{(\alpha)}, x^{(\beta)})^{(\mu)}_m \quad \text{and also } (x^{(\beta)}, x^{(\alpha)})^{(\mu)}_m, \qquad m = 1, 2, \ldots, (\alpha\beta\mu) \tag{5}$$

with components

$$(x^{(\alpha)}, x^{(\beta)})^{(\mu)}_{m,k} = \sum_{i,j} (\alpha i \beta j \,|\, \mu k)_m x_{\alpha i} x_{\beta j}. \tag{6}$$

The CG coefficients can be chosen to satisfy $(\alpha i \beta j \,|\, \mu k)_m = (\beta j \alpha i \,|\, \mu k)_m$ and to form symmetric and antisymmetric CG products for $\alpha \neq \beta$:

$$(x^{(\alpha)}, x^{(\beta)})^{(\mu)}_m \pm (x^{(\beta)}, x^{(\alpha)})^{(\mu)}_m. \tag{7}$$

If $\alpha = \beta$, then the total number of $\Gamma_{0\mu}$-covariants, which are linearly independent CG products of $x^{(\alpha)}$ with itself, is $(\alpha\alpha\mu) = [\alpha\alpha\mu] + \{\alpha\alpha\mu\}$, and it is possible to make a choice of $[\alpha\alpha\mu]$ symmetric and of $\{\alpha\alpha\mu\}$ antisymmetric CG products. The symmetry and antisymmetry is more clearly seen if we distinguish one of the covariants by a prime.

Neglecting normalisation we can write a complete set of bilinear covariants into a convenient table which gives a prescription for the multiplication of covariants in the general case. Such tables for crystal point groups have already been given (Kopský 1976a,b); for crystallographic double point groups we shall give them in the second of the subsequent papers (Kopský 1979b) together with the EIBs.

The CG product $(f^{(\alpha)}, f^{(\beta)})^{(\mu)}_m$ of covariants $f^{(\alpha)}$, $f^{(\beta)}$ is defined by (6), where we replace x by f. If $f^{(\alpha)}$, $f^{(\beta)}$ are defined on different spaces (on different variables), then all their CG products are linearly independent for all $d_\alpha d_\beta$ binoms $f_{\alpha i} f_{\beta j}$ are linearly independent. This, however, need not be true if the spaces of variables for the two covariants have non-vanishing intersection. In this case we can formally construct the CG products as well, but some of them may vanish or be connected by linear relations.

The simplest example is provided by the antisymmetric product of the covariant with itself. An important property of CG products is their distributivity:

$$\left(\sum_a z_a f_a^{(\alpha)}, \sum_b z'_b f_b^{(\beta)}\right)_m^{(\mu)} = \sum_{a,b} z_a z'_b (f_a^{(\alpha)}, f_b^{(\beta)})_m^{(\mu)} \tag{8}$$

where z_a, z'_b are complex numbers.

2.3. Invariant Clebsch–Gordan products

Two typical covariants $\boldsymbol{x}^{(\alpha)}$ and $\boldsymbol{x}^{(\beta)}$ produce an invariant CG product $(\boldsymbol{x}^{(\alpha)}, \boldsymbol{x}^{(\beta)})_1$ as many times as given by the reduction coefficient

$$(\alpha\beta 1) = \frac{1}{N} \sum_{g\in G} \chi_\alpha(g)\chi_\beta(g).$$

This number is 1 if $\chi_\alpha(G) = \chi_\beta^*(G)$, and zero otherwise. Let us recall the Frobenius–Schur (1906) test by which we distinguish three kinds of ireps:

$$\frac{1}{N}\sum_{g\in G} \chi_\alpha(g^2) = \begin{cases} 1 \text{ real} & \text{(integer, 1st kind)} \\ -1 \text{ complex} & \text{(half-integer, 2nd kind)} \\ 0 \text{ half-real} & \text{(3rd kind).} \end{cases} \tag{9}$$

The irep is half-real only if $\chi_\alpha(G)$ is complex; then there exists a class $\chi_\beta(G) = \chi_\alpha^*(G)$ not equivalent to $\chi_\alpha(G)$, and $(\alpha\beta 1) = 1$. The character $\chi_\alpha(G)$ is real if the irep is real or complex, and hence in both these cases $(\alpha\alpha 1) = 1$. However,

$$[\alpha\alpha 1] = \frac{1}{2N}\sum_{g\in G} (\chi_\alpha^2(g) + \chi_\alpha(g^2))$$

and

$$\{\alpha\alpha 1\} = \frac{1}{2N}\sum_{g\in G} (\chi_\alpha^2(g) - \chi_\alpha(g^2)).$$

Substituting (9) into these two relations, we obtain $[\alpha\alpha 1] = 1$, $\{\alpha\alpha 1\} = 0$ for a real irep, and $[\alpha\alpha 1] = 0$, $\{\alpha\alpha 1\} = 1$ for a complex irep. Thus we have:

Theorem 1. Each typical covariant $\boldsymbol{x}^{(\alpha)}$ couples into an invariant CG product $(\boldsymbol{x}^{(\alpha)}, \boldsymbol{x}^{(\beta)})_1$ with just one type of covariant $\boldsymbol{x}^{(\beta)}$. If the irep $\Gamma_{0\alpha}(G)$ is half-real, then the covariant $\boldsymbol{x}^{(\beta)}$ belongs to a complex conjugate irep $\Gamma_{0\beta}(G)$ which is not equivalent to $\Gamma_{0\alpha}(G)$. If $\Gamma_{0\alpha}(G)$ is real or complex, then $\boldsymbol{x}^{(\alpha)}$ couples into an invariant CG product only with itself; this product is symmetric in the first case and antisymmetric in the second case. There exist, therefore, only the following types of invariants:

$$\sum_{i,j} (\alpha i\beta j|1) x_{\alpha i} x_{\beta j}, \qquad \Gamma_\alpha = \Gamma_\beta^*, \text{ half-real ireps,}$$

$$\sum_{i,j} (\alpha i\alpha j|1) x_{\alpha i} x_{\alpha j}, \begin{cases} (\alpha i\alpha j|1) = (\alpha j\alpha i|1), & \Gamma_\alpha \text{ real;} \\ (\alpha i\alpha j|1) = -(\alpha j\alpha i|1), & \Gamma_\alpha \text{ complex.} \end{cases}$$

3. Polynomial algebra on a G-module

3.1. Homogeneous and overall homogeneous grading

The set $\mathscr{P}(L_n)$ of polynomials on L_n is a graded G-module and an algebra. The natural grading is given by the degrees $k = 0, 1, 2, \ldots$ of homogeneous polynomials, and $\mathscr{P}(L_n)$ can be written as a direct sum

$$\mathscr{P}(L_n) = \bigoplus_{k=0}^{\infty} \mathscr{P}(L_n, k). \tag{10}$$

Here $\mathscr{P}(L_n, 0) = \mathbb{C}$, the field of complex numbers, $\mathscr{P}(L_n, 1) = \tilde{L}_n$, and $\mathscr{P}(L_n, k) = [\tilde{L}_n^k]$, the space of kth-degree homogeneous polynomials. A finer grading is obtained if we split L_n into the direct sum of its minimal submodules $L_{\alpha a}$ and express $\mathscr{P}(L_n)$ as a direct product

$$\mathscr{P}(L_n) = \bigotimes_{\alpha=1}^{\kappa} \bigotimes_{a=1}^{n_\alpha} \mathscr{P}(L_{\alpha a}) \tag{11}$$

of its subalgebras $\mathscr{P}(L_{\alpha a})$, each of which has its own grading

$$\mathscr{P}(L_{\alpha a}) = \bigoplus_{k_{\alpha a}=0}^{\infty} \mathscr{P}(L_{\alpha a}, k_{\alpha a}). \tag{12}$$

We denote by $\boldsymbol{k} = (\ldots k_{\alpha a} \ldots) = \Sigma_{\alpha,a} k_{\alpha a} \mathbf{1}_{\alpha a}$ the degrees of overall homogeneous polynomials, i.e. of polynomials homogeneous of degree $k_{\alpha a}$ separately on each of $L_{\alpha a}$. The set of degrees $\boldsymbol{k}$ is a lattice $\mathscr{K}$ (Hall 1959, chap. 8) in which: (i) inclusion relation $\boldsymbol{k} \leq \boldsymbol{k}'$ means $k_{\alpha a} \leq k'_{\alpha a}$ for each α, a, the sharp inclusion holding if $k_{\alpha a} < k'_{\alpha a}$ at least for one α, a; (ii) the least upper bound $\boldsymbol{k}' \cup \boldsymbol{k}''$ and the greatest lower bound $\boldsymbol{k}' \cap \boldsymbol{k}''$ is that $\boldsymbol{k} = \Sigma_{\alpha,a} k_{\alpha a} \mathbf{1}_{\alpha a}$ for which each $k_{\alpha a}$ is the greater and lower of the $k'_{\alpha a}$ and $k''_{\alpha a}$, respectively. The lattice $\mathscr{K}$ contains the least element $\boldsymbol{k} = 0$, but not the greatest element, and satisfies the Jordan–Dedekind condition: the lengths of all ascending chains from $\boldsymbol{k} = 0$ to any given $\boldsymbol{k}$ is the same and equals $k = |\boldsymbol{k}| = \Sigma_{\alpha,a} k_{\alpha a}$, the total degree. The lengths of all chains between two given $\boldsymbol{k}_1$, $\boldsymbol{k}_2$ are also the same and equal $k_1 - k_2$ (chains ascending or descending for positive or negative values of $k_1 - k_2$ respectively).

In this notation we have:

$$\mathscr{P}(L_n, k) = \bigoplus_{|\boldsymbol{k}|=k} \mathscr{P}(L_n, \boldsymbol{k}), \qquad \mathscr{P}(L_n, \boldsymbol{k}) = \bigotimes_{\alpha=1}^{\kappa} \bigotimes_{a=1}^{n_\alpha} \mathscr{P}(L_{\alpha a}, k_{\alpha a}) \tag{13}$$

and, using either (11) or (13),

$$\mathscr{P}(L_n) = \bigoplus_{\boldsymbol{k} \in \mathscr{K}} \mathscr{P}(L_n, \boldsymbol{k}) = \bigoplus_{k=0}^{\infty} \bigoplus_{|\boldsymbol{k}|=k} \left(\bigotimes_{\alpha=1}^{\kappa} \bigotimes_{a=1}^{n_\alpha} \mathscr{P}(L_{\alpha a}, k_{\alpha a}) \right)$$

$$= \bigotimes_{\alpha=1}^{\kappa} \bigotimes_{a=1}^{n_\alpha} \left(\bigoplus_{k_{\alpha a}=0}^{\infty} \mathscr{P}(L_{\alpha a}, k_{\alpha a}) \right). \tag{14}$$

The fine grading performed here can be used with respect to any division of L_n into its subspaces. However, the grading used here is preserved by the group G, and the fine grading is the finest one which is preserved by G. This is important, as it is only in this case that the spaces $\mathscr{P}(L_n, \boldsymbol{k})$ are G-modules.

3.2. Algebra of invariants and spaces of covariants

The set $\mathscr{P}_1(L_n)$ of invariant polynomials on L_n is a subalgebra of $\mathscr{P}(L_n)$. Relative invariants and components of $\Gamma_{0\alpha}$-covariants form linear spaces $\mathscr{P}_i^{(\alpha)}(L_n)$ which are subspaces of $\mathscr{P}(L_n)$. The covariants themselves also form linear spaces which we shall write formally as

$$\boldsymbol{\mathscr{P}}^{(\alpha)}(L_n) = (\mathscr{P}_1^{(\alpha)}(L_n), \mathscr{P}_2^{(\alpha)}(L_n), \ldots, \mathscr{P}_{d_\alpha}^{(\alpha)}(L_n)).$$

The linear basis of $\mathscr{P}_1(L_n)$ together with components of covariants which form bases of $\boldsymbol{\mathscr{P}}^{(\alpha)}(L_n)$'s form a complete basis of $\mathscr{P}(L_n)$. The grading of the $\mathscr{P}(L_n)$ is transferred to the algebra $\mathscr{P}_1(L_n)$ and to spaces $\boldsymbol{\mathscr{P}}^{(\alpha)}(L_n)$, so that

$$\mathscr{P}_1(L_n) = \bigoplus_{k=0}^{\infty} \mathscr{P}_1(L_n, k) = \bigoplus_{\boldsymbol{k}\in\mathscr{K}} \mathscr{P}_1(L_n, \boldsymbol{k}) \tag{15a}$$

$$\boldsymbol{\mathscr{P}}^{(\alpha)}(L_n) = \bigoplus_{k=0}^{\infty} \boldsymbol{\mathscr{P}}^{(\alpha)}(L_n, k) = \bigoplus_{\boldsymbol{k}\in\mathscr{K}} \boldsymbol{\mathscr{P}}^{(\alpha)}(L_n, \boldsymbol{k}) \tag{15b}$$

where $\mathscr{P}_1(L_n, k) = \mathscr{P}_1(L_n) \cap \mathscr{P}(L_n, k)$ and $\mathscr{P}_1(L_n, \boldsymbol{k}) = \mathscr{P}_1(L_n) \cap \mathscr{P}(L_n, \boldsymbol{k})$ are spaces of homogeneous and overall homogeneous invariants of degrees k and $\boldsymbol{k}$ respectively. Analogously $\mathscr{P}_i^{(\alpha)}(L_n, k) = \mathscr{P}_i^{(\alpha)}(L_n) \cap \mathscr{P}(L_n, k)$ and $\mathscr{P}_i^{(\alpha)}(L_n, \boldsymbol{k}) = \mathscr{P}_i^{(\alpha)}(L_n) \cap \mathscr{P}(L_n, \boldsymbol{k})$ are spaces of the ith components of homogeneous and overall homogeneous $\Gamma_{0\alpha}$-covariants of degrees k and $\boldsymbol{k}$ respectively, from which we compose the spaces $\boldsymbol{\mathscr{P}}^{(\alpha)}(L_n, k)$, $\boldsymbol{\mathscr{P}}^{(\alpha)}(L_n, \boldsymbol{k})$ of these covariants.

Let us finally note that

$$\mathscr{P}(L_n, k) = \bigoplus_{\alpha=1}^{\kappa} \bigoplus_{i=1}^{d_\alpha} \mathscr{P}_i^{(\alpha)}(L_n, k) \tag{16}$$

and analogously for $\mathscr{P}(L_n, \boldsymbol{k})$. Further, we denote polynomial $\Gamma_{0\alpha}$-covariants by $\boldsymbol{p}^{(\alpha)}(\boldsymbol{k})$, the degree being indicated in parentheses.

3.3. Construction of linear bases of covariants by successive Clebsch–Gordan reduction

First we shall discuss the construction of overall homogeneous bases of $\Gamma_{0\alpha}$-covariants. Tables of CG products allow the construction of higher-degree covariants from lower-degree ones. Let $\mathscr{P}(L_n, \boldsymbol{k}) = \oplus_{\alpha,i}\mathscr{P}_i^{(\alpha)}(L_n, \boldsymbol{k})$ and $\mathscr{P}(L_n, \boldsymbol{k}') = \oplus_{\beta,j}\mathscr{P}_j^{(\beta)}(L_n, \boldsymbol{k}')$ be the spaces of overall homogeneous polynomials of degrees $\boldsymbol{k}$ and $\boldsymbol{k}'$ respectively, and let the sets of covariants $\boldsymbol{p}_a^{(\alpha)}(\boldsymbol{k})$, $\boldsymbol{p}_b^{(\beta)}(\boldsymbol{k}')$, complete and linearly independent, be known. Then we can construct the space $\mathscr{P}(L_n, \boldsymbol{k}+\boldsymbol{k}') = \oplus_{\mu,k}\boldsymbol{\mathscr{P}}_k^{(\mu)}(L_n, \boldsymbol{k}+\boldsymbol{k}')$ as a linear envelope of components of CG products $(\boldsymbol{p}^{(\alpha)}(\boldsymbol{k}), \boldsymbol{p}^{(\beta)}(\boldsymbol{k}'))_m^{(\mu)}$.

Generally not all of these covariants are linearly independent. The case when they are is covered by the following:

Theorem 2. It is possible to write $\mathscr{P}(L_n, \boldsymbol{k}+\boldsymbol{k}')$ as a direct product

$$\mathscr{P}(L_n, \boldsymbol{k}+\boldsymbol{k}') = \mathscr{P}(L_n, \boldsymbol{k}) \otimes \mathscr{P}(L_n, \boldsymbol{k}') \tag{17}$$

if and only if $\boldsymbol{k} \cap \boldsymbol{k}' = \boldsymbol{K} \in \mathscr{K}_0$, where $\mathscr{K}_0$ is the sublattice of $\mathscr{K}$ corresponding to degrees of variables belonging to one-dimensional ireps only.

Proof. The number

$$N(d,k)=\binom{d+k-1}{d-1}$$

of linearly independent polynomials of degree k in d variables satisfies the inequality $N(d,k)N(d,k')\geq N(d,k+k')$, where equality holds if and only if $d=1$ or if one of $k, k'=0$. Taking into account that $\dim \mathscr{P}(L_n,\boldsymbol{k})=\Pi_{\alpha,a}N(d_{\alpha a},k_{\alpha a})$ we see that the dimensions of both sides of (17) coincide if and only if $\boldsymbol{k}\cap\boldsymbol{k}'\in\mathscr{K}_0$.

It is easy to conclude that in this case the covariants constructed are linearly independent. Overall homogeneous covariants can be constructed by successive application of this procedure, starting with linear covariants $\boldsymbol{x}_a^{(\alpha)}$ and following ascending chains in $\mathscr{K}$. In view of theorem 2 it is, however, of advantage to construct first the covariants in sets $\{x_{\alpha a,i}\}$ for fixed α, a, i.e. the covariants relevant to subalgebras $\mathscr{P}(L_{\alpha a})$, and then to construct the whole algebra as direct product (11). Another advantage of this approach is that all algebras $\mathscr{P}(L_{\alpha a})$ are alike and may be considered as copies of one algebra $\mathscr{P}(L_\alpha)$, described in a set of typical variables. This is just another version of the 'symbolic method' in the theory of invariants (Weitzenböck 1923). These algebras for ordinary and double crystal point groups will be considered in two further papers (Kopský 1979a,b).

3.4. *Molien series and their generalisation*

A powerful analytic characteristic of graded algebras and spaces is given by Molien series. The grading of $\mathscr{P}_1(L_n)$ and of $\boldsymbol{\mathscr{P}}^{(\alpha)}(L_n)$ is described by functions

$$F_1(L_n,\lambda)=\sum_{k=0} n_1(L_n,k)\lambda^k, \qquad F_\alpha(L_n,\lambda)=\sum_{k=0} n_\alpha(L_n,k)\lambda^k \tag{18}$$

where λ is an indeterminate; $n_1(L_n,k)=\dim\mathscr{P}_1(L_n,k)$ and $n_\alpha(L_n,k)=\dim\boldsymbol{\mathscr{P}}^{(\alpha)}(L_n,k)$ are the numbers of linearly independent invariants and Γ_{0a}-covariants of degree k respectively.

Theorem 3 (*generalised Molien theorem*). The above defined functions equal

$$F_1(L_n,\lambda)=\frac{1}{N}\sum_{g\in G}\frac{1}{\det(I-\lambda D(g))} \tag{19a}$$

$$F_\alpha(L_n,\lambda)=\frac{1}{N}\sum_{g\in G}\frac{\chi_\alpha^*(g)}{\det(I-\lambda D(g))}. \tag{19b}$$

Both relations follow from the known fact that the coefficient at λ^k in the expansion of

$$\det(I-\lambda D(g))^{-1}=\sum_{k=0}^{\infty}[\chi^k(g)]\lambda^k$$

is the symmetrised kth power of the representation $\chi(G)$: $g\to D(g)$ acting on L_n (Molien 1897, Burnside 1955). The functions $F_1(L_n,\lambda)$ are regularly used in the theory of invariants, while the generalised $F_\alpha(L_n,\lambda)$'s were introduced relatively recently by McLellan (1974). The whole algebra $\mathscr{P}(L_n)$ is a free algebra generated by $\{x_i\}$, and its Molien function is

$$F(L_n,\lambda)=\frac{1}{(1-\lambda)^n}=\sum_{k=0}^{\infty}\binom{n+k-1}{n-1}\lambda^k. \tag{20}$$

Comparing numbers of independent polynomials and of covariants of any degree, we find that Molien series satisfy a relation

$$\sum_{\alpha=1}^{\kappa} d_\alpha F_\alpha(L_n, \lambda) = F(L_n, \lambda). \tag{21}$$

To describe the fine grading by $\boldsymbol{k}$, we assign to each subset $\{x_{\alpha a,i}\}$ or, in other words, to each space $L_{\alpha a}$, its own indeterminate $\lambda_{\alpha a}$; we shall write for brevity $\boldsymbol{\lambda}^{\boldsymbol{k}} = \ldots \lambda_{\alpha a}^{k_{\alpha a}} \ldots$. Then we define Molien series by

$$F_1(L_n, \boldsymbol{\lambda}) = \sum_{\boldsymbol{k}\in\mathcal{K}} n_1(L_n, \boldsymbol{k})\boldsymbol{\lambda}^{\boldsymbol{k}}, \qquad F_\alpha(L_n, \boldsymbol{\lambda}) = \sum_{\boldsymbol{k}\in\mathcal{K}} n_\alpha(L_n, \boldsymbol{k})\boldsymbol{\lambda}^{\boldsymbol{k}} \tag{22}$$

where again $n_1(L_n, \boldsymbol{k}) = \dim \mathcal{P}_1(L_n, \boldsymbol{k})$, $n_\alpha(L_n, \boldsymbol{k}) = \dim \mathcal{P}^{(\alpha)}(L_n, \boldsymbol{k})$. The Molien series for the whole algebra $\mathcal{P}(L_n)$ is now

$$F(L_n, \boldsymbol{\lambda}) = \sum_{\boldsymbol{k}\in\mathcal{K}} n(L_n, \boldsymbol{k})\boldsymbol{\lambda}^{\boldsymbol{k}} = \prod_{\alpha=1}^{\kappa} \prod_{a=1}^{n_\alpha} F(L_{\alpha a}, \lambda_{\alpha a}) \tag{23}$$

where $F(L_{\alpha a}, \lambda_{\alpha a}) = 1/(1-\lambda_{\alpha a})^{d_\alpha}$. Again the relation

$$\sum_{\alpha=1}^{\kappa} d_\alpha F_\alpha(L_n, \boldsymbol{\lambda}) = F(L_n, \boldsymbol{\lambda}) \tag{24}$$

must hold.

Molien series with fine grading are used by Solomon (1977), Patera *et al* (1978) and Stanley (1978). Recalling the previous section we conclude that, if $L_n \cap L_m$ is empty, we can write Molien series for $\mathcal{P}^{(\mu)}(L_n \oplus L_m)$ as

$$F_\mu(L_n \oplus L_m; \boldsymbol{\lambda}_1, \boldsymbol{\lambda}_2) = \sum_{\alpha,\beta} (\alpha\beta\mu) F_\alpha(L_n, \boldsymbol{\lambda}_1) F_\beta(L_m, \boldsymbol{\lambda}_2). \tag{25}$$

Molien series for subalgebras $\mathcal{P}(L_{\alpha a})$ become in this connection of great importance as other series can be constructed from them using (25) successively. Since all these subalgebras are copies of $\mathcal{P}(L_\alpha)$ over the typical module L_α, the series will have the same form differing only by indeterminates $\lambda_{\alpha a}$. For $\mathcal{P}(L_\alpha)$ we write

$$F_\beta(L_\alpha, \lambda_\alpha) = \sum_{k_\alpha=0}^{\infty} n_\beta(L_\alpha, \lambda_\alpha)\lambda_\alpha^{k_\alpha} = \frac{1}{N}\sum_{g\in G} \frac{\chi_\beta^*(g)}{\det(I - \lambda_\alpha D^{(\alpha)}(g))} \tag{26}$$

with the dimensionality relation

$$\sum_{\alpha=1}^{\kappa} d_\beta F_\beta(L_\alpha, \lambda_\alpha) = F(L_\alpha, \lambda_\alpha) = \frac{1}{(1-\lambda_\alpha)^{d_\alpha}}. \tag{27}$$

These series and composition formula (25) are considered by Patera *et al* (1978). A link between this description and multiplication (11) of subalgebras $\mathcal{P}(L_{\alpha a})$ is obvious.

4. Extended integrity bases

Unless stated otherwise, invariants and covariants in the following are polynomial invariants and covariants.

4.1. Extended Noether's theorem

Theorem 4 (extended Noether's theorem). (i) There exists a finite set of (homogeneous or overall homogeneous if desired) invariants J_l which generate the algebra $\mathscr{P}_1(L_n)$ in the sense that any invariant J is expressible as a polynomial $J = P(J_l)$.

(ii) To each $\Gamma_{0\alpha}(G)$ there exists a finite set of $\Gamma_{0\alpha}$-covariants $\boldsymbol{p}_a^{(\alpha)}$ (again homogeneous or overall homogeneous if desired) which generate $\boldsymbol{\mathscr{P}}^{(\alpha)}(L_n)$ in the sense that any $\Gamma_{0\alpha}$-covariant $\boldsymbol{p}^{(\alpha)}$ is expressible as

$$\boldsymbol{p}^{(\alpha)} = \sum_a J_a \boldsymbol{p}_a^{(\alpha)} \tag{28}$$

where $J_a \in \mathscr{P}_1(L_n)$ are invariants.

Part (i) of the theorem is the ordinary Noether's theorem. Sets of generating invariants are called integrity bases; for sets of generating covariants we propose the term 'linear integrity bases', and together we shall call these sets the 'extended integrity basis'. A constructive proof of part (ii) will be given in the next section together with the description of an algorithm for the construction of a *minimal* EIB.

A more intricate problem then to find the EIBs is to find a unique expression of an invariant or of a covariant in terms of generating ones. The theory of invariants is well developed in this direction, and here are the most important results:

Theorem 5. The algebra $\mathscr{P}_1(L_n)$ contains just n algebraically independent invariants $I_1, I_2, \ldots, I_n$ (homogeneous or overall homogeneous if desired); see, for example, the book by Burnside (1955).

Hence $\mathscr{P}_1(L_n)$ contains a free subalgebra $\mathscr{P}_{1\mathrm{d}}(L_n)$ generated by $I_1, I_2, \ldots, I_n$.

Theorem 6. $\mathscr{P}_{1\mathrm{d}}(L_n) \equiv \mathscr{P}_1(L_n)$ if and only if the group G (as a group of transformations on L_n) is generated by reflections or by pseudo-reflections.

The 'if' part of this theorem for reflection groups has been proved by Coxeter (1951); see also Coxeter and Moser (1972). The theorem has been completed by Sheppard and Todd (1954) and Chevalley (1955).

Theorem 7. If G and $n = \dim L_n$ are finite, then $\mathscr{P}_1(L_n)$ is Cohen–Macaulay algebra or, in other words, there exists a set of invariants $E_1, E_2, \ldots, E_m$, m finite, such that $\mathscr{P}_1(L_n) = \mathscr{P}_{1\mathrm{d}}(L_n)(1 \oplus E_1 \oplus E_2 \oplus \ldots \oplus E_m)$, so that any invariant is uniquely expressible as

$$J = P_0(I_l) + \sum_k E_k P_k(I_l) \tag{29}$$

(Hochster and Eagon 1971, Stanley 1978).

This result is of great importance because it admits a generalisation. Indeed, if an invariant function f_1 on L_n can be developed into a power series, then by rearranging terms of the same degree we can bring it to the form

$$f_1 = f_0(I_l) + \sum_k E_k f_k(I_l) \tag{30}$$

where $f_0(I_l)$, $f_k(I_l)$ are now functions. Functions of three-dimensional vectors, invariant under crystal point groups, were given in this form by Döring (1958).

Of the same importance for covariants is:

Theorem 8. Any $\Gamma_{0\alpha}$-covariant is expressible as

$$\boldsymbol{p}^{(\alpha)} = \sum_a P_a(I_l)\boldsymbol{p}_a^{(\alpha)} \tag{31}$$

where the number of $\boldsymbol{p}_a^{(\alpha)}$'s is finite. This has been proved by McLellan (1974) for subgroups of Coxeter groups. The proof can be carried out in the same way for any finite group which can be embedded in some group generated by pseudo-reflections. The invariants I_l in both cases are invariants of this pseudo-reflection group. The constructive proof of the extended Noether's theorem given in § 5 holds, on the other hand, for any finite group. Again we can generalise (31) to get a functional form

$$f^{(\alpha)} = \sum_a f_a(I_l)\boldsymbol{p}_a^{(\alpha)} \tag{32}$$

of a covariant on L_n. Due to their relationship to Molien series (§ 4.3) the invariants I_l and E_k are called denominator and numerator invariants (McLellan 1974). Other terms—free and transient invariants—are used, for example, by Sloane (1977).

4.2. *Fundamental algebras for a finite group*

All theorems formulated in § 4.1 hold for the typical algebras $\mathscr{P}(L_\alpha)$ as well. The EIBs of these algebras, α-running ireps of the group G, are fundamental for this group. With their use we can determine the EIB for any $\mathscr{P}(L_n)$. Indeed, the subalgebras $\mathscr{P}(L_{\alpha a})$ are copies of $\mathscr{P}(L_\alpha)$, so that adjoining indices a to variables $x_{\alpha,i}$ we get the EIBs of the $\mathscr{P}(L_{\alpha a})$'s at once from the EIB of $\mathscr{P}(L_\alpha)$. All copies of invariants and covariants in typical variables will certainly belong to the EIB of $\mathscr{P}(L_n)$ if the originals belong to the EIB of $\mathscr{P}(L_\alpha)$, and each of them will be a polynomial in a single set of $x_{\alpha a,i}$. Particularly, the copies of denominator invariants will again be denominator invariants, and their total number will be just

$$n = \sum_{\alpha=1}^{\kappa} d_\alpha n_\alpha$$

because there are d_α of them for each $\mathscr{P}(L_{\alpha a})$ and the total number of $\mathscr{P}(L_{\alpha a})$ is n_α. Further, we shall have invariants and covariants in which variables belonging to different $\mathscr{P}(L_{\alpha a})$'s will be coupled. These can be obtained by multiplication of subalgebras according to CG tables with elimination of redundant ones as described by the algorithm below. All invariants obtained in this way will be numerator ones because the denominator ones are already exhausted.

One possible and useful generalisation is at hand. As all $\mathscr{P}(L_{\alpha a})$'s are copies of $\mathscr{P}(L_\alpha)$, so are the products $\mathscr{P}(L_{\alpha a})\otimes\mathscr{P}(L_{\alpha a'})$ copies of $\mathscr{P}(L_\alpha)\otimes\mathscr{P}(L'_\alpha)$, and so on for greater numbers of $\mathscr{P}(L_{\alpha a})$'s in the product. Preliminary investigation leads us to believe that the EIB of a product

$$\mathscr{P}(L_N) = \bigotimes_{\alpha=1}^{\kappa} \bigotimes_{a=1}^{d_\alpha} \mathscr{P}(L_{\alpha a}) \tag{33}$$

plays, in the case of non-abelian groups, the same role as the typical EIB of abelian groups, i.e. it already describes all possible EIBs. Notice that here $N = \dim L_N$ is the order of the group G; L_N can be interpreted as the group ring of G, and the representation of G on L_N is its regular representation.

4.3. *Denominator and numerator of Molien series*

Proposition. If invariants of $\mathscr{P}_1(L_n)$ are expressible by (29), and $\Gamma_{0\alpha}$-covariants of $\mathscr{P}^{(\alpha)}(L_n)$ by (31), then Molien series are of the form

$$F_1(L_n, \lambda) = N_1(\lambda)/D(\lambda), \qquad F_\alpha(L_n, \lambda) = N_\alpha(\lambda)/D(\lambda) \tag{34}$$

where

$$D(\lambda) = \prod_{j=1}^{n} (1-\lambda^{q_j}), \qquad N_1(\lambda) = 1 + \sum_{k=1}^{m} \lambda^{p_k}, \qquad N_\alpha(\lambda) = \sum_a \lambda^{p_{\alpha a}}.$$

Here q_j, p_k and $p_{\alpha a}$ are the degrees of homogeneous basic invariants I_j, E_k and covariants $\boldsymbol{p}_a^{(\alpha)}$. Analogous expressions will be obtained with $\boldsymbol{\lambda}, \boldsymbol{q}_j, \boldsymbol{p}_k$ and $\boldsymbol{p}_{\alpha a}$ if the basic invariants and covariants are overall homogeneous. According to § 4.2 the $\boldsymbol{q}_j$'s will be the degrees in single sets $x_{\alpha a, i}$ i.e. $\boldsymbol{q}_{j_{\alpha a}} \mathbf{1}_{\alpha a}$, and the denominator expressible as

$$D(\boldsymbol{\lambda}) = \prod_{\alpha=1}^{\kappa} \prod_{a=1}^{n_\alpha} D_\alpha(\lambda_{\alpha a})$$

where

$$D_\alpha(\lambda_{\alpha a}) = \prod_{j_{\alpha a}=1}^{d_\alpha} (1-\lambda_{\alpha a}^{q_{j_{\alpha a}}}).$$

The proposition follows at once from definitions (18) and (22).

It is so far not clear whether this proposition can be reversed. If it can, then Molien series can be calculated relatively easily from (19) and brought to the form (34) which gives information about the structure of EIBS: numbers and degrees of denominator and numerator invariants and of basic covariants. The invariants and covariants can then be calculated by brute force. This is exactly what Patera *et al* (1978) did for finite subgroups of SO(3), and Desmier and Sharp (1978) for finite subgroups of SU(2).

Mallows and Sloane (1973) conjectured tentatively (for invariants) that reversal of the proposition is possible. Further, the following counter-example has been discussed from which it follows that the conjecture is generally false (Sloane 1977, Stanley 1978). The algebra of invariants generated by diag$(-1,-1,1)$ and diag$(1,1,\mathrm{i})$ acting on $L_3 = (x_1, x_2, x_3)$ is $\mathscr{P}_1(L_3) = \mathscr{P}_{1\mathrm{d}}[x_1^2, x_2^2, x_3^4](1 \oplus x_1 x_2)$, and its Molien series

$$F_1(L_3, \lambda) = \frac{1+\lambda^2}{(1-\lambda^2)^2(1-\lambda^4)} = \frac{1}{(1-\lambda^2)^3}$$

admits a second form of the type (34) to which there is evidently no corresponding integrity basis (the inner reason for this is that the group is not a subgroup of a pseudo-reflection group with three quadratic invariants). It is, however, easy to resolve this example using fine grading which gives Molien series

$$F_1(L_3; \lambda_1, \lambda_2, \lambda_3) = \frac{1+\lambda_1\lambda_2}{(1-\lambda_1^2)(1-\lambda_2^2)(1-\lambda_3^4)}$$

with no problem of the above type.

This indicates that the conjecture is perhaps true for Molien series of our typical algebras, but so far we do not know a rigorous answer.

4.4. Reducible and irreducible invariants and covariants

Invariants behave under G like numbers, so that 'linear combinations' $\Sigma_a J_a f_a^{(\alpha)}$ of $\Gamma_{0\alpha}$-covariants with $J_a \in \mathscr{P}_1(L_n)$ are again $\Gamma_{0\alpha}$-covariants, and the distributive rule (8) for CG products

$$\left(\sum_a I_a f_a^{(\alpha)}, \sum_b I'_b f_b^{(\beta)}\right)_m^{(\mu)} = \sum_{a,b} I_a I'_b (f_a^{(\alpha)}, f_b^{(\beta)})_m^{(\mu)} \tag{35}$$

holds also for invariants as coefficients.

However, $\boldsymbol{\mathscr{P}}^{(\alpha)}(L_n)$ cannot be considered as vector space over $\mathscr{P}_1(L_n)$, since the latter is an algebra but not a field. Consequently a linear relation $\Sigma_a J_a \boldsymbol{p}_a^{(\alpha)} = 0$ does not imply that one of $\boldsymbol{p}_a^{(\alpha)}$, say $\boldsymbol{p}_b^{(\beta)}$, is expressible as $\Sigma_{a\neq b} J'_a \boldsymbol{p}_a^{(\alpha)}$, and the linear independence over $\mathscr{P}_1(L_n)$ cannot be introduced.†

Instead we shall introduce a concept of reducibility.

Definition: (i) An invariant J is said to be reducible if it can be expressed as a polynomial $P(I_i)$ without a linear term in some set of invariants I_i.

(ii) A $\Gamma_{0\alpha}$-covariant $\boldsymbol{p}^{(\alpha)}$ is said to be reducible if it can be expressed as a combination $\boldsymbol{p}^{(\alpha)} = \Sigma_a J_a \boldsymbol{p}_a^{(\alpha)}$, where $\boldsymbol{p}_a^{(\alpha)}$ is some set of $\Gamma_{0\alpha}$-covariants and J_a-invariants without a constant term. Otherwise we say that the invariant or covariant is irreducible.

Lemma 1. (i) The set $\mathscr{P}_{1r}(L_n)$ of reducible invariants is a linear subspace and also a subalgebra of $\mathscr{P}_1(L_n)$.

(ii) The set $\boldsymbol{\mathscr{P}}_r^{(\alpha)}(L_n)$ of reducible covariants is a linear subspace of the space $\boldsymbol{\mathscr{P}}^{(\alpha)}(L_n)$.

Proof. It is sufficient to realise that a linear combination or a product of polynomials without linear terms is again a polynomial without a linear term, and that the product of a polynomial without a constant term and any polynomial is again a polynomial without a constant term.

Lemma 2. If at least one covariant in a CG product is reducible, then the CG product is reducible. Consequently, whatever covariants may be constructed by successive CG multiplication from a reducible covariant, all of them will be reducible.

5. Minimal extended integrity basis and its derivation

5.1. Minimal extended integrity basis

Irreducible invariants and covariants do not generally form spaces. Let us define spaces of homogenous or overall homogeneous reducible invariants and covariants by $\mathscr{P}_{1r}(L_n, k) = \mathscr{P}_1(L_n) \cap \mathscr{P}_r(L_n, k)$ and analogously for $\boldsymbol{k}$ and for $\boldsymbol{\mathscr{P}}_r^{(\alpha)}(L_n, k)$ or $\boldsymbol{\mathscr{P}}_r^{(\alpha)}(L_n, \boldsymbol{k})$ with the use of spaces of components. To complete the spaces $\mathscr{P}_1(L_n, \boldsymbol{k})$ and $\boldsymbol{\mathscr{P}}^{(\alpha)}(L_n, \boldsymbol{k})$ we have to choose some complementary subspaces $\mathscr{P}_{1c}(L_n, \boldsymbol{k})$ or $\boldsymbol{\mathscr{P}}_c^{(\alpha)}(L_n, \boldsymbol{k})$, so that $\mathscr{P}_1(L_n, \boldsymbol{k}) = \mathscr{P}_{1c}(L_n, \boldsymbol{k}) \oplus \mathscr{P}_{1r}(L_n, \boldsymbol{k})$, and $\boldsymbol{\mathscr{P}}^{(\alpha)}(L_n, \boldsymbol{k}) = \boldsymbol{\mathscr{P}}_c^{(\alpha)}(L_n, \boldsymbol{k}) \oplus \boldsymbol{\mathscr{P}}_r^{(\alpha)}(L_n, \boldsymbol{k})$.

† See discussion (Kopský 1978) of a theorem formulated by Hopfield (1960) and given in the book by Lax (1974) as theorem 3.8.1.

Theorem 9. Whatever complementary subspaces $\mathscr{P}_{1c}(L_n, \boldsymbol{k})$, $\boldsymbol{\mathscr{P}}_c^{(\alpha)}(L_n, \boldsymbol{k})$ and whatever linear bases $J_i(\boldsymbol{k})$, $\boldsymbol{p}_a^{(\alpha)}(\boldsymbol{k})$ in them we choose, the latter will always be the minimal EIB of $\mathscr{P}(L_n)$ with respect to group G. Instead of $\boldsymbol{k}$ we may use k.

Proof. Any $\boldsymbol{p}^{(\alpha)}$ is expressible as a sum of $\boldsymbol{p}^{(\alpha)}(\boldsymbol{k})$, and any $\boldsymbol{p}^{(\alpha)}(\boldsymbol{k})$ as a linear combination of $\boldsymbol{p}_a^{(\alpha)}(\boldsymbol{k})$ plus reducible covariant $\boldsymbol{p}_r^{(\alpha)}(\boldsymbol{k})$. The latter is, according to definition, a sum of covariants $J(\boldsymbol{k}')\boldsymbol{p}^{(\alpha)}(\boldsymbol{k}-\boldsymbol{k}')$, where $0<\boldsymbol{k}'<\boldsymbol{k}$. Applying this procedure successively to $\boldsymbol{p}^{(\alpha)}(\boldsymbol{k}-\boldsymbol{k}')$ and so on, we clearly arrive at a form $\boldsymbol{p}^{(\alpha)}=\Sigma_a J_a \boldsymbol{p}_a^{(\alpha)}$, and, if the original $\boldsymbol{p}^{(\alpha)}$ was reducible, J_a will not contain a constant term. Quite analogously we carry out the proof for invariants. It follows from definition that such an EIB is minimal.

The minimal integrity basis must contain all denominator invariants but not necessarily all numerator invariants. The only case in which all numerator invariants are in the minimal integrity basis is when every polynomial $Q(E_k)$ without linear term belongs to $\mathscr{P}_{1d}(L_n)$. The relations $Q(E_k)=P(I_i)$ form the so-called syzygies (Hilbert 1890, Weitzenböck 1923).

5.2. Constructive proof of the extended Noether's theorem

Part (i) of the theorem is the well known ordinary Noether's theorem. To prove part (ii) we need a lemma.

Lemma 3. Let us adjoin a space $L_{\beta b}$ to L_n, or a covariant $\boldsymbol{x}_b^{(\beta)}$ to the original set. Let further $I(\boldsymbol{k}+\boldsymbol{1}_{\beta b}) \in \mathscr{P}_1(L_n \oplus L_{\beta b})$ be an invariant of first degree in $\boldsymbol{x}_b^{(\beta)}$, so that $\boldsymbol{k} \cap \boldsymbol{1}_{\beta b}=0$. Then there exists just one $\Gamma_{0\alpha}$-covariant $\boldsymbol{p}^{(\alpha)}(\boldsymbol{k})$, where $(\alpha\beta 1)=1$, such that $I(\boldsymbol{k}+\boldsymbol{1}_{\beta b})=(\boldsymbol{p}^{(\alpha)}(\boldsymbol{k}), \boldsymbol{x}_b^{(\beta)})_1$, and the invariant is reducible if and only if $\boldsymbol{p}^{(\alpha)}(\boldsymbol{k})$ is reducible.

Proof. According to theorem 1 there is only one type of covariant which couples with $\boldsymbol{x}_b^{(\beta)}$ into invariants, and to get the degree $\boldsymbol{k}+\boldsymbol{1}_{\beta b}$ we must use a covariant from $\boldsymbol{\mathscr{P}}^{(\alpha)}(L_n, \boldsymbol{k})$. Let $\boldsymbol{p}_a^{(\alpha)}(\boldsymbol{k})$ be the linear basis of $\boldsymbol{\mathscr{P}}^{(\alpha)}(L_n, \boldsymbol{k})$. Since $\boldsymbol{k} \cap \boldsymbol{1}_{\beta b}=0$, the set of invariants $I_a(\boldsymbol{k}+\boldsymbol{1}_{\beta b})=(\boldsymbol{p}_a^{(\alpha)}(\boldsymbol{k}),\ \boldsymbol{x}_b^{(\beta)})_1$ is a linear basis of $\mathscr{P}_1(L_n \oplus L_{\beta b}, \boldsymbol{k}+\boldsymbol{1}_{\beta b})$. Therefore $I(\boldsymbol{k}+\boldsymbol{1}_{\beta b})=\Sigma_a c_a I_a(\boldsymbol{k}+\boldsymbol{1}_{\beta b})$ if and only if $I(\boldsymbol{k}+\boldsymbol{1}_{\beta b})=(\boldsymbol{p}^{(\alpha)}(\boldsymbol{k}), \boldsymbol{x}_b^{(\beta)})_1$, where $\boldsymbol{p}^{(\alpha)}(\boldsymbol{k})=\Sigma_a c_a \boldsymbol{p}_a^{(\alpha)}(\boldsymbol{k})$. If $\boldsymbol{p}^{(\alpha)}(\boldsymbol{k})$ is reducible, then $I(\boldsymbol{k}+\boldsymbol{1}_{\beta b})$ is certainly also reducible. If $I(\boldsymbol{k}+\boldsymbol{1}_{\beta b})$ is reducible, then it is expressible as a sum

$$\sum_{a, \boldsymbol{k}_1+\boldsymbol{k}_2=\boldsymbol{k}} I_a(\boldsymbol{k}_1) I_a(\boldsymbol{k}_2+\boldsymbol{1}_{\beta b})$$

and invariants $I_a(\boldsymbol{k}_2+\boldsymbol{1}_{\beta b})$ are expressed as CG products $(\boldsymbol{p}_a^{(\alpha)}(\boldsymbol{k}_2), \boldsymbol{x}_b^{(\beta)})_1$. Hence

$$I(\boldsymbol{k}+\boldsymbol{1}_{\beta b})=\sum_{a, \boldsymbol{k}_1+\boldsymbol{k}_2=\boldsymbol{k}} (I_a(\boldsymbol{k}_1)\boldsymbol{p}_a^{(\alpha)}(\boldsymbol{k}_2), \boldsymbol{x}_b^{(\beta)})_1=(\boldsymbol{p}^{(\alpha)}(\boldsymbol{k}), \boldsymbol{x}_b^{(\beta)})_1$$

where

$$\boldsymbol{p}^{(\alpha)}(\boldsymbol{k})=\sum_{a, \boldsymbol{k}_1+\boldsymbol{k}_2=\boldsymbol{k}} I_a(\boldsymbol{k}_1)\boldsymbol{p}_a^{(\alpha)}(\boldsymbol{k}_2)$$

is reducible.

Let us now suppose that part (ii) of theorem 4 does not hold. Then there exists at least one type of covariant for which the linear integrity basis $\boldsymbol{p}_a^{(\alpha)}(\boldsymbol{k})$ is infinite. If we adjoin a new covariant $x_b^{(\beta)}$ to the system such that it couples into invariants with $p_a^{(\alpha)}(k)$, then, according to lemma 3, all invariant CG products $(p_a^{(\alpha)}(k), x_b^{(\beta)})_1$ are linearly independent and irreducible. Hence the integrity basis of invariants on $L_n \oplus L_{\beta b}$ will be infinite, in contradiction to the ordinary Noether's theorem.

5.3. The algorithm

The algorithm is exceedingly easy for abelian groups. In this case all spaces of overall homogeneous covariants (relative invariants) are one-dimensional, based on single monomials which are either reducible or irreducible. The product of the form (33) then provides the typical EIB of the group in question (Kopský 1975).

In the general case we proceed to determine some bases of complementary subspaces which according to theorem 9 provide the minimal EIB. To do it we construct, for a given degree k, provided we have already the bases for lower degrees, first the space $\mathscr{P}_r^{(\alpha)}(L_n, k)$ by taking all products $I(k-k')p_a^{(\alpha)}(k')$ of basic (irreducible) lower-degree covariants with sets of linear bases of invariants of appropriate degrees $k-k'$. The linear envelope of these covariants is just the space $\mathscr{P}_r^{(\alpha)}(L_n, k)$, and it is a standard problem of linear algebra to find some of its linear bases (check of one, say the first, component of the covariant suffices).

Further we construct 'enough' CG products of the type $(p_b^{(\beta)}(k_1), p_c^{(\gamma)}(k_2))_a^{(\mu)}$ with $k_1+k_2=k$ and $p_b^{(\beta)}(k_1)$, $p_c^{(\gamma)}(k_2)$ irreducible to complete the basis of $\mathscr{P}^{(\alpha)}(L_n, k)$. It is sufficient to consider only one pair of degrees k_1, k_2 because this already grants that all space $\mathscr{P}^{(\alpha)}(L_n, k)$ will be spanned. Some of the covariants obtained this way will belong to $\mathscr{P}_r^{(\alpha)}(L_n, k)$, and it is again standard to determine the complementary ones. At a certain stage we shall find that all the covariants constructed thus are already reducible; then the procedure is cut off for all $K \geq k$. Invariants are constructed analogously; the basis of $\mathscr{P}_{1r}(L_n, k)$ is, however, constructed from polynomials in lower-degree invariants. To construct the complementary basis we again use only irreducible covariants. Dimensionality relations provide a suitable check of whether 'enough' covariants and invariants were constructed. Throughout the calculation we keep a record of irreducible covariants already obtained and of all linearly independent invariants.

This is a description of the algorithm in its general form. In practice, however, we shall proceed to construct first the EIBs of typical algebras. These, for the ordinary and for the double crystal point groups, will be considered in two further papers (Kopský 1979a,b).

6. Discussion

The construction of EIBs with use of CG products is a self-checking procedure which also gives an insight into relations between covariants of different types and degrees. On the other hand, the method based on a consideration of Molien series has the advantage that we know in advance the numbers and degrees of basic covariants and invariants. The problem of calculation of these covariants and of selection of the irreducible ones must, however, still be faced. Our impression from calculating EIBs of double point groups in which we have used both methods (we received the preprint by Patera *et al* (1978) before completing these bases) is that they are complementary rather than competing.

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