match no. 11 pp. 45-51 1981

THE CONCEPT OF EXTENDED INTEGRITY BASES

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(Received March 1981)

1. Introduction.

In my talk on lattices of stability spaces I had to mention the recently introduced concept of the extended integrity bases[1-6], which is a generalization of the well known concept of integrity bases of invariants[7]. In view of subsequent discussion and critical remarks I would like to review here briefly the present state of the theory with special accent on the practical calculation of these bases.

The subject of the theory is the algebra $\mathcal{P}(L_n)$ of polynomials $p(x)$ on a linear space L_n, $x = x_1e_1+x_2e_2+ \ldots +x_ne_n \in L_n$, on which a finite group G acts as a group of linear operators. In a chosen basis $\{e_i\}$ of L_n, the action of the group G is given by its matrix representation $\Gamma(G)$: $g \longmapsto D(g)$, and $ge_i = D_{ji}(g)e_j$. We say briefly that L_n is a G-module or, more specifically, a $\chi(G)$-module, where $\chi(G)$: $g \longmapsto \chi(g) = \mathrm{Tr}\, D(g)$ is the character of the action of G on L_n. The algebra $\mathcal{P}(L_n)$ is also a G-module, where the action of $g \in G$ on $p(x)$ is defined in the usual way by $gp(x) = p(g^{-1}x)$. The algebra is also a linear space and as such it splits into subspaces $\mathcal{P}(L_n, k)$ of homogeneous polynomials of degree k.

The degrees k provide a natural grading: $\mathcal{P}(L_n) = \bigoplus_{k=0}^{\infty} \mathcal{P}(L_n, k)$, and $\mathcal{P}(L_n, k)\mathcal{P}(L_n, k') = \mathcal{P}(L_n, k+k')$. We shall work here only in the field of complex numbers C, whence $\mathcal{P}(L_n, 0) = C$. It is further $\mathcal{P}(L_n, 1) = \tilde{L}_n$ – the space of linear functions on L_n (an adjoint space to L_n) which is a $\chi^*(G)$-module, because the action of $g \in G$ on $\tilde{L}_n$, in a basis $\{x_i\}$ adjoint to the basis $\{e_i\}$ of L_n, is expressed by matrices $\tilde{D}(g) = D^t(g^{-1})$ adjoint (reciprocal and transposed) to matrices $D(g)$: $gx_i = \tilde{D}_{ji}(g)x_j$. Accordingly, the spaces $\mathcal{P}(L_n, k) = [\tilde{L}_n^k]$ are the symmetrized powers of L_n and hence $[\chi^{k*}(G)]$-modules. For further discussion we fix a full set of matrix ireps (irreducible representations) $\Gamma_\alpha(G)$: $g \longmapsto D^{(\alpha)}(g)$ of the group G and, following Weyl[8], we say that a set $p^{(\alpha)} = (p_{\alpha 1}, p_{\alpha 2}, \ldots, p_{\alpha d_\alpha})$, $d_\alpha = \dim \chi_\alpha(G) = \chi_\alpha(e)$, of polynomials $p_{\alpha i}$ in x, which transform under the action of the group G in the same way as the basis $x_{\alpha i}$ for the adjoint irep $\tilde{\Gamma}_\alpha(G)$: $g \longmapsto \tilde{D}^{(\alpha)}(g)$, i.e. $gp_{\alpha i} = \tilde{D}^{(\alpha)}_{ji}(g)\, p_{\alpha j}$, is a polynomial $\Gamma_\alpha(G)$-covariant (relative invariant in case of one-dimensional ireps, invariant in case of the identity irep). Each $\Gamma_\alpha(G)$-covariant defines a $\chi^*_\alpha(G)$-module – the linear envelope of its components. Covariants themselves form linear spaces $\mathcal{P}^{(\alpha)}(L_n)$ which are composed of spaces $\mathcal{P}^{(\alpha)}(L_n, k)$ of homogeneous polynomial $\Gamma_\alpha(G)$-covariants of degree k. Invariants form a space $\mathcal{P}_1(L_n)$ which is also a subalgebra of the algebra $\mathcal{P}(L_n)$.

As a first step towards the theory of extended integrity bases we shall consider the linear homogeneous bases of spaces of covariants (including the algebra of invariants considered as a linear space). The linear envelope of components of all these covariants is the whole algebra $\mathcal{P}(L_n)$.

2. Molien series and consecutive Clebsch-Gordan multiplication.

Let $c^{(\alpha)}(L_n, k)$ be the numbers of linearly independent $\Gamma_\alpha(G)$-covariants, homogenous of degree k. This number is the multiplicity with which the irep of the class $\chi_\alpha(G)$ is contained in the symmetrized power $[\chi^k(G)]$. A compact way for calculation of these numbers has its origin in Molien relation[9]:

$$\frac{1}{\mathrm{Det}\,(I - \lambda D(g))} = \sum_{k=0}^{\infty} [\chi^k(g)]\, \lambda^k, \tag{1}$$

where λ is an indeterminate. From the orthogonality of characters one obtains the numbers $c^{(\alpha)}(L_n, k)$ at once as coefficients at k-th degree of the indeterminate λ in the function:

$$F_\alpha(L_n, \lambda) = \frac{1}{N} \sum_{g \in G} \frac{\chi_\alpha(g)}{\mathrm{Det}\,(I - \lambda D(g))} = \sum_{k=0}^{\infty} c^{(\alpha)}(L_n, k)\, \lambda^k. \tag{2}$$

These functions are called Molien functions and the right hand side is the Molien series. The actual calculation of homogeneous bases of covariants can be most suitably performed by consecutive use of Clebsch-Gordan multiplication according to tables of Clebsch-Gordan products[10]. Such approach is useful in tensor calculus where our interest is limited by a finite rank tensor. The Clebsch-Gordan multiplication has been used to calculate and systemize tensorial covariants up to fourth rank for the magnetic point groups[11].

3. The minimal extended integrity bases.

Further we suppose that the order N of G and the dimension n of L_n are finite. It is well known that the algebra $\mathcal{P}_1(L_n)$ of invariants is then finitely generated[7]. The finite set $J_1, J_2, \ldots, J_m$ of invariants in x which generate the algebra $\mathcal{P}_1(L_n)$ in the sense that any other invariant J is expressible as a polynomial $P(J_i)$ in this set is called the integrity basis of invariants. It appears that spaces of covariants which, as linear spaces, are of infinite dimensions (if not void), are also finitely generated in the following sense: There exist finite sets $p_1^{(\alpha)}, p_2^{(\alpha)}, \ldots, p_m^{(\alpha)}$ of $\Gamma_\alpha(G)$-covariants, such that any other $\Gamma_\alpha(G)$-covariant $p^{(\alpha)}$ is expressible in a form of 'linear combination' $\sum_a P_a(J_i)p_a^{(\alpha)}$ with coefficients $P_a(J_i)$ from the algebra of invariants.

We shall use here the terms linear integrity bases of covariants for the sets of generating covariants and extended integrity basis (of algebra $\mathcal{P}(L_n)$ with respect to a chosen set of ireps of G) for the integrity basis of invariants together with linear integrity bases of covariants. As far as I know, the finiteness of linear integrity bases has been first proved by McLellan for subgroups of Coxeter groups[1]. I have proved it first for the case of abelian finite groups[2] and later for the general case of finite groups[4]. My proof grounds on the use of a constructive algorithm which consists of consecutive Clebsch-Gordan multiplication of covariants with elimination of those invariants and covariants which are already expressible through invariants and covariants of lower degrees. This algorithm is also suitable for actual calculation of extended integrity bases. The bases obtained in this way are the minimal extended integrity bases. Construction of the minimal bases does not solve the problem of polynomial invariants and covariants completely – the minimal bases do not, in general case, generate the invariants and covariants in a unique way. To explain the problem of uniqueness, let us briefly consult the literature.

4. Cohen-Macaulay algebras and modules.

The first basic result states, that the number of algebraically independent invariants in the algebra $\mathcal{P}_1(L_n)$ equals just n – the dimension of the space L_n[12]. Let the set of these, so called free invariants, be $I_1, I_2, \ldots, I_n$. These invariants generate the free algebra $\mathcal{P}_f = \mathcal{P}(I_1, I_2, \ldots, I_n)$ which is a subalgebra of $\mathcal{P}_1(L_n)$. It has been further shown that the free algebra $\mathcal{P}_f$ coincides with the whole algebra $\mathcal{P}_1(L_n)$ if the group G, as a group of linear operators on L_n, is a Coxeter group, i.e. a group generated by reflections[13]. More precisely, the algebras coincide, if and only if the group G is generated by pseudoreflections[14]. Generally, the algebra of invariants contains also a set of so called transient invariants $E_1, E_2, \ldots, E_k$ such, that any polynomial invariant is uniquelly expressible in the following way [15]:

$$(3a)\qquad P_o(I_j) + \sum_{a=1}^{k} P_a(I_j)E_a ,$$

where I_j are invariants of that reflection or pseudoreflection group into which the group G can be embedded. For a reason which will becomeapparent in next section, the invariants I_j are also called denominator invariants while the invariants E_i are also called numerator invariants.

An analogous result for covariants has been first obtained for the subgroups of Coxeter groups[1], then for the subgroups of groups generated by pseudoreflections[16], and finally for the general case of finite groups [17]. The result states that there exist such basic sets of $\Gamma_\alpha(G)$-covariants $p_1^{(\alpha)}$, $p_2^{(\alpha)}$, ..., $p_{k_\alpha}^{(\alpha)}$ that any other $\Gamma_\alpha(G)$-covariant can be uniquelly expressed as:

$$(3b) \qquad \sum_{a=1}^{k_\alpha} P_a(I_j)p_a^{(\alpha)} ,$$

where in coefficients $P_a(I_j)$ only the free invariants appear, so that the coefficients belong to the free algebra $\mathcal{P}_f$. Both cases (3a) and (3b) can be united in a statement that the algebra of invariants and the spaces of covariants are expressible as:

$$(4a) \qquad \mathcal{P}_1(L_n) = \mathcal{P}_f.(1 \oplus E_1 \oplus E_2 \oplus \ldots\ldots \oplus E_k),$$

$$(4b) \qquad \mathcal{P}^{(\alpha)}(L_n) = \mathcal{P}_f.(p_1^{(\alpha)} \oplus p_2^{(\alpha)} \oplus \ldots\ldots \oplus p_k^{(\alpha)}).$$

Algebras and spaces of this property are called Cohen-Macaulay algebras and modules or free generated modules over the free algebra $\mathcal{P}_f$.

To distinguish the extended integrity bases which lead to unique expressions (3a) and (3b) we shall call them the canonical extended integrity bases. It is clear that the canonical bases contain the minimal ones and can be derived from them. This, however, requires an additional analysis of algebraic relations between invariants and covariants.

5. The canonical form of Molien functions - denominator and numerator invariants.

It follows directly from (3a), (3b) or (4a), (4b) that Molien functions can be expressed in the following form which will be called canonical form:

$$(5) \qquad F_1(\lambda) = N_1(\lambda)/D(\lambda), \qquad F_\alpha(\lambda) = N_\alpha(\lambda)/D(\lambda),$$

where

$$D(\lambda) = (1 - \lambda^{q_1})(1 - \lambda^{q_2}) \ldots\ldots (1 - \lambda^{q_n}) ,$$

$$(6) \qquad N_1(\lambda) = 1 + \lambda^{p_1} + \lambda^{p_2} + \ldots\ldots + \lambda^{p_k} ,$$

$$N_\alpha(\lambda) = \lambda^{p_{\alpha 1}} + \lambda^{p_{\alpha 2}} + \ldots\ldots + \lambda^{p_{\alpha k_\alpha}} ,$$

and the powers q_1, q_2, ... q_n indicate the degrees of free invariants, p_1, p_2, ... p_k the degrees of transient invariants and $p_{\alpha 1}$, $p_{\alpha 2}$, ... $p_{\alpha k_\alpha}$ the degrees of basic $\Gamma_\alpha(G)$-covariants. Herefrom also the alternative names denominator and numerator invariants.

Molien functions can be calculated from characters and eigenvalues of matrices corresponding to group elements and then brought to the canonical form which indicates the 'possible' structure of canonical extended integrity basis. The problem is that there may exist more than one canonical form and even such canonical formsmay exist which do not correspond to some canonical extended integrity basis. A 'conjecture' that Molien functions determine the integrity basis of invariants has already been made [18] and subsequently rejected in view of a counterexample [19].

6. Fundamental algebras and extended integrity bases of irreducible matrix groups.

So far we have followed the usual approach, in which the group G is considered as the group of linear operators on a certain space L_n. It is of great advantage to consider G as an abstract group and to investigate the problem of extended integrity bases simultaneously for all possible G-modules.

Of primary importance in this approach are the fundamental algebras $\mathcal{P}(L_\alpha)$ defined on minimal (irreducible) $\chi_\alpha(G)$-modules L_α and their canonical bases [2-6]. Both the algebra $\mathcal{P}(L_\alpha)$ and its canonical basis are determined by the irreducible matrix group Im $\Gamma_\alpha(G)$. The matrices of this group form a faithful irep of the factor group $\mathcal{H}_\alpha = G/H_\alpha$, where $H_\alpha = \ker \Gamma_\alpha(G)$. According to representation generating theorem there exist polynomial $\Gamma_\gamma(\mathcal{H}_\alpha)$-covariants to each irep $\chi_\gamma(\mathcal{H}_\alpha)$ of the group $\mathcal{H}_\alpha$. With reference to the group G these covariants are the $\Gamma_\gamma(G)$-covariants, where $\Gamma_\gamma(G)$ is the irep of G engendered of the irep $\Gamma_\gamma(\mathcal{H}_\alpha)$ of $\mathcal{H}_\alpha$. The group G can be here a normal extension of any group H_α by the factor group $\mathcal{H}_\alpha$.

To calculate the canonical extended integrity basis of any algebra $\mathcal{P}(L_n)$, where L_n is a $\chi(G)$-module, we need to know only the canonical bases of fundamental algebras $\mathcal{P}(L_\alpha)$ relevant to the group G, and the Clebsch-Gordan multiplication table for this group. Then we proceed as follows: The space L_n splits into a direct sum of n_α (the multiplicity of $\chi_\alpha(G)$ in $\chi(G)$) minimal $\chi_\alpha(G)$-modules $L_{\alpha a}$, each of which forms an algebra $\mathcal{P}(L_{\alpha a})$. The whole algebra $\mathcal{P}(L_n)$ is the direct product of all $\mathcal{P}(L_{\alpha a})$. The algebras $\mathcal{P}(L_{\alpha a})$ are just copies of the algebra $\mathcal{P}(L_\alpha)$. The copies of free invariants are free invariants in $\mathcal{P}(L_n)$, the copies of transient invariants are also transient invariants and, of course, we obtain also the copies of covariants. In addition to all these invariants and covariants which are obtained by copying from fundamental algebras we have to add all invariants and covariants which are obtained by Clebsch-Gordan multiplication of bases of fundamental algebras. The bases thus obtained will be the canonical basis of the algebra $\mathcal{P}(L_n)$.

Polynomial covariants obtained in this procedure are not only homogeneous on L_n, they are homogeneous on each of the spaces $L_{\alpha a}$. It is, accordingly, possible to introduce the Molien functions of fine grading, with indeterminates $\lambda_{\alpha a}$ for each space $L_{\alpha a}$. The calculation of these functions from Molien functions of fundamental algebras can be performed by consecutive use of the formula [3,4]:

$$(7) \qquad F_\gamma(L_n \oplus L_m, \lambda_1, \lambda_2) = \sum_{\alpha,\beta} (\alpha\beta\gamma) F_\alpha(L_n, \lambda_1) . F_\beta(L_m, \lambda_2),$$

which holds if the spaces L_n and L_m are distinct and in which $(\alpha\beta\gamma)$ are the reduction coefficients.

If $F_\alpha(L_n, \lambda_1) = N_\alpha(\lambda_1)/D(\lambda_1)$ and $F_\beta(L_m, \lambda_2) = N_\beta(\lambda_2)/D(\lambda_2)$ are in their canonical form corresponding to an actual canonical basis, then $F_\gamma(L_n \oplus L_m, \lambda_1, \lambda_2) = N_\gamma(\lambda_1, \lambda_2)/D(\lambda_1, \lambda_2)$ are also in the canonical form, where $D(\lambda_1, \lambda_2) = D(\lambda_1).D(\lambda_2)$ and

$$(8) \qquad N_\gamma(\lambda_1, \lambda_2) = \sum_{\alpha,\beta} (\alpha\beta\gamma) N_\alpha(\lambda_1) . N_\beta(\lambda_2).$$

Moreover, this canonical form describes an actual canonical basis of the algebra $\mathcal{P}(L_n \oplus L_m)$.

7. Discussion.

Let us now discuss the existing methods for calculation of the canonical extended integrity bases. **1.** The method of McLellan[1,6] is based on embedding the group G, as a group of linear operators on L_n, in a pseudoreflection group. This method is perharps the most rigorous (there are no problems with correspondence of Molien series and bases in canonical form). It requires, however, a special consideration of each G-module L_n. **2.** Patera et al[3] start from calculation of Molien series for the fundamental algebras. The Molien functions are then brought to the canonical form and the canonical extended integrity bases calculated by brute force with help of the knowledge of numbers and degrees of its elements. Despite the fact that canonical bases of fundamental algebras for all images of ireps of ordinary and double point groups have been calculated in this way, there are two weak points in it: we have no guarrancy that the canonical form of Molien functions corresponds to the basis and even if it does, the corresponding members of the basis cannot be calculated ad hoc. **3.** My method is based on the use of algorithm which employs the Clebsch-Gordan multiplication tables [2,4,5,10]. As already said, this algorithm leads in the first instance to the minimal bases. Let us notice, however, that in cases so far calculated, the minimal bases of fundamental algebras coincide with the canonical ones.

In my opinion, the most promising and effective approach to the calculation of canonical extended integrity bases for fundamental algebras is the combination of Clebsch–Gordan multiplication with Molien functions. Both the canonical bases and Clebsch–Gordan multiplication tables are already known for the ordinary and double crystallographic point groups[2–5,10] so that the canonical extended integrity bases can be calculated for any representation of these groups. The knowledge of the covering groups and projective representations of crystal point groups[20] and the approach to representations of space groups via images of ireps of little groups, presented by Prof. Michel and Prof. Mozrzymas at this meeting, will hopefully enable us to extend the theory to space groups, adding a new powerfull apparatus to the theory of their representations and to the theory of interactions in solid state.

Acknowledgement: I owe my thanks to authors of several references for informing me about their work prior to publication (refs. 3,6,16). Prof. McLellan has first pointed to methe importance of what I call here the canonical bases (ref.6) of which I was not aware at the time of my first contribution(ref.2) in the subject. Critical remarks of Prof. Michel who pointed to mesome errors in my tables (ref.5) are appreciated. I thank also Prof. Neubüser for helpful discussion and Prof. Dress for helping me to collect some new information.

References:

1. A.G.McLellan, J.Phys.C: Solid St. Phys. 7 (1974), 8326.
2. V.Kopský, J.Phys.C: Solid St. Phys. 8 (1975), 3251.
3. J.Patera, R.T.Sharp, and P.Winternitz, J.Math.Phys. 19 (1978), 2362.
P.E.Desmier and R.T.Sharp, J.Math.Phys. 20 (1979), 74.
4. V.Kopský, J.Phys.A: Math.Gen. 12 (1979), 429.
5. V.Kopský, J.Phys.A: Math.Gen. 12 (1979), 943 and 958.
6. A.G.McLellan, J.Phys.C: Solid St. Phys. 12 (1979), 753.
7. E.Noether, Math.Ann. 77 (1916), 89.
8. H.Weyl: Classical Groups. Princeton UP, 1946.
9. T.Molien, Sber.Preuss.Akad.Wiss. (1897), 1152.
10. V.Kopský, J.Phys.C: Solid St. Phys. 9 (1976), 3391 and 3405.
11. V.Kopský, Acta Cryst. A35 (1979), 83 and 95.
12. W.Burnside: Theory of Groups of Finite Order. Dover, New York, 1955.
13. H.S.M.Coxeter, Duke Math.J. 18 (1951), 765.
14. G.S.Sheppard and J.A.Todd, Can.J.Math. 6 (1954), 274.
C.Chevalley, Amer.J.Math. 77 (1955), 778.
15. M.Hochster and J.A.Eagon, Amer.J.Math. 93 (1971), 1020.
16. R.P.Stanley, J.Algebra 49 (1977), 134.
17. R.P.Stanley, Bull.Amer.Math.Soc. 1 (1979), 443.
18. C.L.Mallows and N.J.A.Sloane, Proc.Camb.Phil.Soc. 7 (1973), 435.
19. N.J.A.Sloane, Amer.Math.Monthly 84 (1977), 82.
20: L.L.Boyle and K.F:Green, Phil.Trans.Roy.Soc.(London) 288 (1978), 237.