Modified group projector technique: induced representations

1995 J. Phys. A: Math. Gen. 28 1669

(http://iopscience.iop.org/0305-4470/28/6/020)

J. Phys. A: Math. Gen. 28 (1995) 1669–1679. Printed in the UK

Modified group projector technique: induced representations

M Damnjanović†§ and I Milošević‡

† Faculty of Physics, The University, PO Box 368, 11001 Beograd, Serbia, Yugoslavia

‡ Faculty of Forestry, The University, Kneza Višeslava 1, 11000, Beograd, Serbia, Yugoslavia

Received 11 July 1994, in final form 5 December 1994

Abstract. The group projector technique is developed for the representations of the direct product form, $D = D' \otimes d$, in which one of them has been induced from a representation of a subgroup. It is shown that the group projectors and symmetry-adapted bases are essentially determined in terms of the subgroup representations. To illustrate both the technical and conceptual advantages of the method, it is shown how the calculation of the normal modes of polymers (polyacetylene as an example) can be obtained using the symmetry of the monomer only, and several results of the induction theory are reconsidered within the new framework.

1. Introduction

The induction of the representations from subgroup to group is one of the most powerful methods in the theory of the group representations (Mackey 1952, Altmann 1977). Another group theoretical concept, indispensable in the physical applications, the symmetry-adapted bases, involves the group projector technique (Cornwell 1984, Chen *et al* 1985). This paper is an attempt to develop this technique for the case of the induced representations. To this end the modified version of the group projector method, involving the projectors of the identity representation only, is applied (Damnjanović and Milošević 1984). This allows the more general case, the direct product of the induced representation with any other representation of the group, to be considered. The method is suitable for computer implementation (Davies 1982, Ping *et al* 1989), since it gives a prescription for solving the physically relevant eigenproblems within the space of the initial (subgroup) representation.

To begin with, the group projector technique will briefly be reviewed in order to introduce notation and to clarify the aim of the article. Let $D(G)$ be the representation of the group G in the space $\mathcal{H}_D$. If $D(G)$ decomposes into the irreducible components as $D(G) = \oplus_{\mu=1}^{r} a_\mu D^{(\mu)}(G)$ ($a_\mu = 1, 2, \ldots$), then there exists a symmetry-adapted or standard basis $\{|\mu t_\mu m\rangle \mu = 1, \ldots, r;\, t_\mu = 1, \ldots, a_\mu;\, m = 1, \ldots, \mu\}$ (where $|\mu|$ denotes the dimension of $D^{(\mu)}(G)$) in $\mathcal{H}_D$ satisfying the following conditions:

$$D(g)|\mu t_\mu m\rangle = \sum_{m'=1}^{\mu} D^{(\mu)}_{m'm}(g)|\mu t_\mu m'\rangle. \tag{1}$$

To determine such a basis the group operator technique prescribes the following steps: given the matrices of an irreducible component $D^{(\mu)}(G)$, the operators

$$P^{(\mu)}_{ij}(D, G) \stackrel{\text{def}}{=} \frac{|\mu|}{|G|} \sum_{g\in G} D^{(\mu)*}_{ij}(g) D(g)$$

§ E-mail: EPMFF04@YUBGSS21.BG.AC.YU

are calculated; the operator $P_{11}^{(\mu)}(D, G)$ is the projector, and any basis in its range can take the role of the vectors $|\mu t_\mu 1)$ $(t_\mu = 1, \dots, a_\mu)$, determining the rest of the standard basis as $|\mu t_\mu m\rangle = P_{m1}^{(\mu)}(D, G)|\mu t_\mu 1\rangle$.

A slightly modified procedure, based on the group projectors of the identity representation, $I(G)$, has recently been proposed (Damnjanović and milošević 1984). Given the matrices of each irreducible component, $D^{(\mu)}(G)$ acting in the space $\mathbb{C}^\mu$, the projector $G(D\otimes D^{(\mu)*}) \stackrel{\text{def}}{=} P^{(I)}(D\otimes D^{(\mu)*}, G)$ (in the space $\mathcal{H}_\mu = \mathcal{H}_D \otimes \mathbb{C}^\mu$) should be found (in the cited paper the order of the representations is different, but it is obvious that the choice is unimportant). Its range is a_μ-dimensional; denoting by $\{|\mu t_\mu\rangle_\mu \mid t_\mu = 1, \dots, a_\mu\}$ the basis in the range of this projector, and by $\{|\mu^* m\rangle \mid m = 1, \dots, |\mu|\}$ the basis in the representative space $\mathbb{C}^\mu$ of $D^{(\mu)*}(G)$, the vectors of the symmetry-adapted basis are obtained as the partial scalar products $|\mu t_\mu m\rangle = \langle \mu^* m|\mu t_\mu\rangle_\mu$.

In this paper the modified procedure is applied to the case when $D(G)$ is the direct product of two representations, one of them being induced from a subgroup H. It turns out (section 2) that the group projector $G(D)$ has the significant property: it is determined by the corresponding subgroup projector. When the geometry of the problem is examined (section 3), the class of operators with the same property is singled out. Among them are the relevant physical observables. Therefore, the symmetry-adapted eigenbases, which are important in various physical problems, can easily be found (section 4). The method is simplified when the group G is the weak-direct product, $G = HZ$, of its subgroups (section 5). As an example, calculation of the normal vibrational modes of polyacetylene (section 6) is performed. Together with other concluding remarks, Frobenius' theorem and some related concepts from induction theory are reconsidered to point out the naturalness of the approach.

2. Basic algebraic considerations

Let H be a subgroup of the group G, with the left transversal $Z = \{z_0, \dots, z_{|Z|-1}\}$ $(|Z| = \frac{|G|}{|H|})$; it is assumed that $z_0 = e$, the identity element. It is well known that the inverses of the left transversal form the right transversal, $\{z_0^{-1}, \dots, z_{|Z|-1}^{-1}\}$ and that, if Hg is a right coset of H, then the sets $z_t Hg$ $(t = 0, \dots, |Z| - 1)$ are disjoint. To summarize, G can be partitioned into the forms $G = \cup_t z_t H = \cup_t H z_t^{-1} = \cup_t z_t Hg$. For fixed t, each element g of G uniquely determines $t(g)$ and $h(g, t) \in H$ such that

$$g = z_t h(g, t) z_{t(g)}^{-1}. \tag{2}$$

Given the $|\Delta'|$-dimensional matrix representation $\Delta'(H)$ in the space $\mathcal{H}_{\Delta'}$, the induced $|D'|$-dimensional $(|D'| = |Z||\Delta'|)$ representation $D'(G) = \Delta'(H) \uparrow G$, is constructed as follows. The matrix corresponding to the element $g \in G$ is made of the $|\Delta'|$-dimensional submatrices $D'_{ts}(g)$, which is 0 if the element $z_t^{-1} g z_s$ is not from H, while $D'_{ts}(g) = \Delta'(h)$ if $z_t^{-1} g z_s = h \in H$. Using $|Z|$-dimensional matrices E^{ts}, with elements equal to 0 except that $(E^{ts})_{ts} = 1$, the induced representation takes the form (for convenience, matrices E^{ts} are enumerated by $t, s = 0, \dots, |Z| - 1$, as well as their rows and columns)

$$D'(g) = \sum_{s,t=0}^{|Z|-1} \sum_{h\in H} \delta(z_t^{-1} g z_s, h) E^{ts} \otimes \Delta'(h).$$

Here, the Kronecker function on G (equal to 1 if its arguments coincide and zero otherwise) vanishes whenever the first argument is not from H, while in the opposite case it singles out the element h of H equal to the first argument. Given another representation $d(G)$ in $\mathcal{H}_d$, the matrices of the direct product $D(G) = D'(G) \otimes d(G)$ are $D(g) = \sum_{t,s} \sum_{h \in H} \delta(z_t^{-1} g z_s, h) E^{ts} \otimes \Delta'(h) \otimes d(g)$. Taking into account the factorization (2), this becomes

$$D(g) = \sum_{t=0}^{|Z|-1} E^{tt(g)} \otimes \Delta'(h(g,t)) \otimes d(z_t h(g,t) z_{t(g)}^{-1}). \tag{3}$$

The group projector of the identity representation can be found as the sum of the representative matrices:

$$G(D) = \frac{1}{|G|} \sum_{g \in G} D(g) = \frac{1}{|G|} \sum_t \left\{ \sum_{g \in G} E^{tt(g)} \otimes \Delta'(h(g,t)) \otimes d(z_t h(g,t) z_{t(g)}^{-1}) \right\}.$$

As for the sum in the brackets, the index t is fixed; in view of (2), the sum over g splits into the sums over $h = h(g,t)$ and $s = t(g)$, enumerating for each t all the elements from H and the transversal, respectively. Only the order of terms depends on t, making the sum over h and s independent:

$$G(D) = \frac{1}{|G|} \sum_{ts} \sum_{h \in H} E^{ts} \otimes \Delta'(h) \otimes d(z_t h z_s^{-1}). \tag{4}$$

To clarify the structure of (3) and (4), the direct product of $\Delta'(H)$ with the subduced representation $d(G) \downarrow H$, will be denoted by $\Delta(H)$: $\Delta(h) = \Delta'(h) \otimes d(h)$; also, the *transfer* operators $b_{ts} \stackrel{\mathrm{def}}{=} E^{ts} \otimes I_{\Delta'} \otimes d(z_t)$ ($I_{\Delta'}$ is the identity matrix in $\mathcal{H}_{\Delta'}$), and $B_s \stackrel{\mathrm{def}}{=} \frac{1}{\sqrt{|Z|}} \sum_t b_{ts}$ are introduced. With the abbreviations $b_t = b_{t0}$ and $B = B_0$, (3) and (4) are

$$D(g) = \sum_{t=0}^{|Z|-1} b_t \{E^{00} \otimes \Delta(h(g,t))\} b_{t(g)}^{\dagger} \qquad G(D) = B\{E^{00} \otimes H(\Delta)\} B^{\dagger}. \tag{5}$$

The equalities would hold for any b_{ts} and B_t, if E^{00} was changed to E^{tt}; in the rest of the paper a more general form for some expressions can be obtained analogously. The last relations reveal a similar structure for the operators $D(g)$ and $G(D)$ in $\mathcal{H}_D$: the transfer operators couple them to the subgroup operators in $\mathcal{H}_\Delta(H) = \mathcal{H}_{\Delta'} \otimes \mathcal{H}_d$. This inspires an attempt to study the transfer operators separately, reducing the work to the subgroup only. The following analysis of the geometry of the problem is the cornerstone for the subsequent applications.

3. Geometry and transfer operators

The representative space $\mathcal{H}_{D'}$ of the induced representation decomposes onto the orthogonal sum $\oplus_t \mathcal{H}_{t\Delta'}$, with $\mathcal{H}_{t\Delta'} = (E^{t0} \otimes I_{\Delta'}) \mathcal{H}_{0\Delta'}$. The total space of $D(G)$ is the direct product $\mathcal{H}_{D'} \otimes \mathcal{H}_d$, and trails this decomposition: $\mathcal{H}_D = \oplus_t \mathcal{H}_{t\Delta}$, with $\mathcal{H}_{t\Delta} = \mathcal{H}_{t\Delta'} \otimes \mathcal{H}_d = b_t \mathcal{H}_{0\Delta}$. The spaces $\mathcal{H}_{\Delta'}$ and $\mathcal{H}_\Delta$ are naturally identified with $\mathcal{H}_{0\Delta'}$ and $\mathcal{H}_{0\Delta}$, respectively.

The easily verifiable properties of the transfer operators

$$b_{ts}^{\dagger} b_{pq} = \delta_{tp} E^{sq} \otimes I_\Delta \qquad b_{ts} b_{pq}^{\dagger} = \delta_{sq} E^{tp} \otimes I_{\Delta'} \otimes d(z_t z_p^{-1}) \qquad \operatorname{Tr} b_{ts}^{\dagger} b_{pq} = \delta_{tp} \delta_{sq} |\Delta|$$

immediately yield

$$B_t^{\dagger} B_s = E^{ts} \otimes I_\Delta \qquad B_t B_s^{\dagger} = \frac{1}{|Z|} \delta_{ts} \sum_{pq} E^{pq} \otimes I_{\Delta'} \otimes d(z_p z_q^{-1}) \qquad \operatorname{Tr}(B_t^{\dagger} B_s) = \delta_{ts} |\Delta|. \tag{6}$$

These relations show that $b_t^\dagger b_t$ and $B^\dagger B$ are projectors, with the ranges $R(b_t^\dagger b_t) = R(B^\dagger B) = \mathcal{H}_{0\Delta}$ (thus $b_t^\dagger b_t = B^\dagger B$). Therefore, the transfer operators are partial isometries, satisfying $BB^\dagger B = B$ and $B^\dagger BB^\dagger = B^\dagger$ (and analogously for b_t). The ranges of the transfer operators are $R(B^\dagger) = R(b_t^\dagger) = \mathcal{H}_{0\Delta}$ and $R(b_t) = \mathcal{H}_{t\Delta}$, while $R(B) = R(BB^\dagger)$ mixes all the subspaces $\mathcal{H}_{t\Delta}$. Their null-spaces are $N(B^\dagger) = R^\perp(B)$, $N(b_t^\dagger) = \mathcal{H}_{t\Delta}^\perp$ and $N(B) = N(b_t) = \mathcal{H}_{0\Delta}^\perp$. It should be recalled that the partial isometry bijectively maps the orthocomplement of the null-space onto the range, preserving the scalar products.

In view of this, the first equation (5) clearly manifests the process of the induction. The operator $b_t^\dagger$ maps $\mathcal{H}_{t\Delta}$ bijectively, at first 'rotating' the vectors by $d^\dagger(z_t)$ and then naturally sending them to $\mathcal{H}_{0\Delta}$. The action of $D(g)$ is disassembled to the unitary mappings of $\mathcal{H}_{t(g)\Delta}$ onto $\mathcal{H}_{t\Delta}$ for each t; all of these mappings are essentially given by $\Delta(H)$ in $\mathcal{H}_\Delta$.

Similarly, the second expression (5) describes how the action of the subgroup projector, originally defined in $\mathcal{H}_{0\Delta}$, is extended to the whole space: the first operator $B^\dagger$ transfers the vectors into $\mathcal{H}_{0\Delta}$, preparing them for the projector $E^{00}\otimes H(\Delta)$, while the last B transfers the projections back to $\mathcal{H}_D$. The range of $H(\Delta)$ (more precisely, the range of $E^{00}\otimes H(\Delta)$), being a subspace in $\mathcal{H}_{0\Delta}$, is bijectively mapped by B into $R(B)$, implying that the range of $G(D)$ is a subspace in $R(B)$. The equation (5) is an example of how the action of an operator in $\mathcal{H}_D$ is reduced to the action of the corresponding operator in the subspace $\mathcal{H}_{0\Delta}$. Clearly such a reduction cannot be carried out for all the operators in $\mathcal{H}_D$, and the class of the operators allowing this will be found.

The decomposition of the space $\mathcal{H}_D$ provides the possibility of disassembling any matrix A to the $|\Delta|$-dimensional submatrices: $A = \sum_{pq} E^{pq}\otimes A^{pq}$. Then the transferred operator in $\mathcal{H}_{0\Delta}$ is

$$A^\downarrow \stackrel{\text{def}}{=} B^\dagger AB = E^{00}\otimes\frac{1}{|Z|}\sum_{pq}\beta_p^\dagger A^{pq}\beta_q$$

with $\beta_t = I_{\Delta'}\otimes d(z_t)$; effectively this is the operator $A^{\downarrow 0} = \frac{1}{|Z|}\sum_{pq}\beta_p^\dagger A^{pq}\beta_q$ in $\mathcal{H}_\Delta$. Similarly, given the operator A^0 in $\mathcal{H}_\Delta$, the transferred operator in $\mathcal{H}_D$ is defined by

$$A^{0\uparrow} \stackrel{\text{def}}{=} B(E^{00}\otimes A^0)B = \frac{1}{|Z|}\sum_{pq}E^{pq}\otimes(\beta_p A^0\beta_q^\dagger).$$

These operator mappings are opposite in a sense, but only the last one is injective, and their compositions are:

$$A^{0\uparrow\downarrow 0} = A^0 \qquad A^{\downarrow\uparrow} = \frac{1}{|Z|^2}\sum_{ts}E^{ts}\otimes\sum_{pq}\left(\beta_t\beta_p^\dagger A^{pq}\beta_q\beta_s^\dagger\right).$$

While the first composition is the identical mapping on the operators in $\mathcal{H}_\Delta$, the second one gives the cutoff of A in the subspace $R(B)$. This is equal to the original if and only if both $R(A)$ and $N^\perp(A)$ are subspaces in $R(B)$, i.e. when $A^{\downarrow\uparrow} = BB^\dagger A = ABB^\dagger = A$. The operator A with this property will be called the $R(B)$-*localized* operator. Obviously, the transfer operator B uniquely couples the $R(B)$-localized operators in $\mathcal{H}_D$ to the operators in $\mathcal{H}_\Delta$.

The arguments on the significance of such operators in the physical considerations will be postponed, in order to state immediately a simple but important theorem.

Theorem 1. Let A be an $R(B)$-localized operator in $\mathcal{H}_D$. Then

(i) $(AC)^{\downarrow 0} = A^{\downarrow 0}C^{\downarrow 0}$ and $(CA)^{\downarrow 0} = C^{\downarrow 0}A^{\downarrow 0}$, for any operator C in $\mathcal{H}_D$;

(ii) the eigenvectors of A belonging to $R(B)$ are bijectively mapped by $B^\dagger$ to the eigenvectors of $A^\downarrow$ with the same eigenvalues, i.e. $|x\rangle\in R(B)$ satisfies $A|x\rangle = \alpha|x\rangle$ if and only if $|x\rangle^0 = B^\dagger|x\rangle\in\mathcal{H}_{0\Delta}$ satisfies $A^\downarrow|x\rangle^0 = \alpha|x\rangle^0$.

The first part is obvious, since under the conditions of the theorem $AC = ABB^\dagger C$. Then from $B^\dagger A(BB^\dagger|x\rangle) = \alpha B^\dagger|x\rangle$ follows the second statement.

Since the theorem applies to the operators transferred to $\mathcal{H}_\Delta$, the analogous statements, $(A^0C^0)^\uparrow = A^{0\uparrow}C^{0\uparrow}$ and $A^0|x\rangle^0 = \alpha|x\rangle^0$ implies $A^{0\uparrow}B|x\rangle^0 = \alpha B|x\rangle^0$, starting from the operators in $\mathcal{H}_\Delta$, are automatically verified. Under the conditions of the theorem, statement (i) states that the transferred operators commute if and only if their originals do; hence, the maps of the normal (Hermitian) operators are normal (Hermitian) again. Consequently, the orthonormal eigenbasis of a normal operator A^0 in $\mathcal{H}_\Delta$ is mapped by B bijectively into the part of the orthonormal eigenbasis of the transferred operator $A^{0\uparrow}$; these vectors span the subspace $R(B)$. In particular, each eigensubspace of $A^{0\uparrow}$ corresponding to a non-vanishing eigenvalue is spanned by some of these vectors. Instead of solving the eigenproblem for A, it suffices to solve it for $A^{\downarrow 0}$. For each eigenvector $|x\rangle^0$ of $A^{\downarrow 0}$, the vector $B|x\rangle^0$ is the eigenvector of A for the same eigenvalue. The definition of B points to the specific simple structure of the obtained eigenvector $B|x\rangle^0$: its component (projection) in the subspace $\mathcal{H}_{t\Delta}$ is

$$|x\rangle^t = \frac{1}{\sqrt{|Z|}} b_t|x\rangle^0. \tag{7}$$

The preservation of the eigenvalues implies that the projectors in $\mathcal{H}_\Delta$ and the $R(B)$-localized projectors in $\mathcal{H}_D$ bijectively correspond, relation (5) being an example of this. This coupling for $BB^\dagger$ and $B^\dagger B = I_\Delta$, in the view of the theorem, means that any operator A in $\mathcal{H}_D$ satisfies $(BB^\dagger A)^{\downarrow 0} = (ABB^\dagger)^{\downarrow 0} = A^{\downarrow 0}$; moreover, if A commutes with $BB^\dagger$ (implying that $R(B)$ is invariant subspace for A), then $A^{\downarrow\uparrow} = BB^\dagger A$.

4. Symmetry-adapted bases

The procedure for finding the symmetry-adapted bases can be adjusted to the considered form of the representation $D(G)$. According to the remark in the introduction, it remains to find the group projectors $G_\mu = G(D \otimes D^{(\mu)^*})$, for each irreducible component of $D(G)$. But, the structure of the representation $D(G) \otimes D^{(\mu)^*}(G)$ is the same as that of $D(G)$: it is the direct product of the induced representation $D'(H) \uparrow G$ with the representation $d(G) \otimes D^{(\mu)^*}(G)$. Thus, the relevant group projector is of the form (5) with $B_\mu = \frac{1}{\sqrt{|Z|}} \sum_t E^{t0} \otimes I_{\Delta'} \otimes d(z_t) \otimes D^{(\mu)^*}(z_t)$ and $\Delta(H) \otimes D^{(\mu)^*}(H)$ instead of Δ:

$$G_\mu = B_\mu\{E^{00} \otimes G_\mu^{\downarrow 0}, H)\}B_\mu^\dagger \qquad G_\mu^{\downarrow 0} = H(\Delta \otimes D^{(\mu)^*}) = H_\mu.$$

Then, according to the theorem, only the basis $|\mu t_\mu\rangle_\mu^0$ in the range of the subgroup projector is to be found. Mapped by B_μ, it produces the basis $|\mu t_\mu\rangle_\mu$ in the range of G_μ, and the wanted symmetry-adapted vectors from $\mathcal{H}_D$ are the partial scalar products $|\mu t_\mu m\rangle = \langle \mu^* m|(B_\mu|\mu t_\mu\rangle_\mu^0)$. Since the vectors $|\mu t_\mu m\rangle^0 \stackrel{\text{def}}{=} \langle\mu^* m|\mu t_\mu\rangle_\mu^0$ obey the relations $\langle\mu^* m|D^{(\mu)^*}(z_s)|\mu t_\mu\rangle_\mu^0 = \sum_{m'}^{\mu} D_{mm'}^{(\mu)^*}(z_s)|\mu t_\mu m'\rangle^0$, the structure of B_μ enables us to solve the whole problem in $\mathcal{H}_\Delta$. That is, in accordance with (7), the component from $\mathcal{H}_{s\Delta}$ of the symmetry-adapted vector $|\mu t_\mu m\rangle$ is determined by the vectors $|\mu t_\mu m\rangle^0$: $|\mu t_\mu m\rangle^s = \frac{1}{\sqrt{|Z|}} E^{s0} \otimes I_{\Delta'} \otimes d(z_s) \otimes D_{mm'}^{(\mu)^*}(z_s)|\mu t_\mu\rangle_\mu^0$; the partial trace gives finally

$$|\mu t_\mu m\rangle^s = \frac{1}{\sqrt{|Z|}} b_s \sum_{m'} D_{mm'}^{(\mu)^*}(z_s)|\mu t_\mu m'\rangle^0. \tag{8}$$

Note that the sum in the last equation defines for each s the vector in $\mathcal{H}_{0\Delta}$, which is mapped to $|\mu t_\mu m\rangle$ by B.

Let $\mathcal{H}_D$, the representative space of $D(G)$, be the state space of a quantum system with the group of symmetry G. Furthermore, let A be an observable describing some property of the system, thus commuting with the representation $D(G)$. There exists the symmetry-adapted eigenbasis of A, i.e. the vectors of the standard basis (1) can be chosen to satisfy $A|\mu t_\mu m\rangle = \alpha_{\mu t_\mu}|\mu t_\mu m\rangle$. If I_{μ^*} denotes the identity operator in the space of the irreducible representation $D^{(\mu)^*}(G)$, then the Hermitian operator $A \otimes I_{\mu^*}$ commutes with $D(G)\otimes D^{(\mu)^*}(G)$, and with the projector G_μ. Therefore, the observable $A_\mu = (A\otimes I_\mu)G_\mu$ is considered, and its eigenbasis in the range of G_μ should be found. Finally, the partial scalar products of the obtained vectors with the vectors $|\mu^* m\rangle$ form the required symmetry-adapted eigenbasis of A.

Within this algorithm theorem 1 offers a shortcut. Since G_μ and A_μ satisfy the conditions of the theorem, it is sufficient to solve the whole problem for the operator $A_\mu^{\downarrow 0} = (A\otimes I_{\mu^*})^{\downarrow 0} G_\mu^{\downarrow 0}$. The obtained eigenvectors of $A_\mu^{\downarrow 0}$ from $R(G_\mu^{\downarrow 0})$ should be transferred by B_μ and the partial scalar products give the eigenbasis. Again, as has been described above, the whole problem can be solved in $\mathcal{H}_\Delta$. Note that within the solving of the eigenproblem of $A_\mu^{\downarrow 0}$, the quantum numbers imposed by symmetry of the subgroup are pointed out and incorporated in the final symmetry-adapted basis.

The requirement $[A, D(g)] = 0$ for each g in G imposes some conditions on the matrix elements of A. If coset representatives are taken for g, a straightforward calculation yields:

$$\beta_p^\dagger A^{pq}\beta_q = \Delta(h(z_q, p))\beta_{p(z_q)}^\dagger A^{p(z_q)0} \qquad A^{\downarrow 0} = \frac{1}{|Z|}\sum_{qp}\Delta^\dagger(h(z_p^{-1}, q))\beta_q^\dagger A^{q0}. \tag{9}$$

Note that the sufficient condition for validity of (9) is that A commutes with the operators representing the transversal.

5. Special case: the transversal is a subgroup

In the previous sections no restriction on the structure of the group has been imposed, and the conclusions are quite general. Some additional results can be derived when the group G is the weak-direct product (Jansen and Booth 1967) of its subgroups H and Z, i.e. when the transversal itself is a subgroup of G. This immediately simplifies calculations, since $h(z_s, t) = e$ and $z_{t(z_s)} = z_s^{-1}z_t$. For example, the expression (9) becomes

$$A^{pq} = \beta_q A^{p(z_q)0}\beta_q^\dagger \qquad A^{\downarrow 0} = \sum_p \beta_p^\dagger A^{p0}. \tag{10}$$

It has been shown (Damnjanović and Milošević 1984) that the group projectors reflect the group structure: $G(D) = H(D)Z(D)$. Using $\Delta(e) = I_\Delta$ in the matrices $D(z_s)$ from (5), the second factor-projector is: $Z(D) = \frac{1}{|Z|}\sum_t D(z_t) = \frac{1}{|Z|}\sum_t b_t \sum_s b_{t(s)}^\dagger = BB^\dagger$. The last equality holds due to the group property of Z: for fixed t, $z_{t(z_s)}$ runs over the Z, i.e. the second sum is independent on t. Thus the subspace $R(B)$ is more clearly described as the range of $Z(D)$. Looking backward to the general case, it becomes clear that $BB^\dagger$ is $\overline{Z}(D)$, the projector for the subgroup generated by the transversal.

Leaving aside other theoretical aspects, the case when Z is a cyclic subgroup will be considered. If $z_1 = z$ is the generator of Z, the elements of the transversal are $z_t = z^t$. Then, it is easily seen that $t(z_s) = t - s$, and with $\beta \stackrel{\text{def}}{=} \beta_1$ the equations (10) read:

$$A^{pq} = \beta^q A^{p-q,0}\beta^{q^\dagger} \qquad A^{\downarrow 0} = \sum_p \beta^{p^\dagger} A^{p0}. \tag{11}$$

Since $d(G) \downarrow Z$ is a representation of the cyclic group Z, it can be decomposed onto the irreducible ones, which are all of the form $d^{(k)}(z^s) = e^{iks}$. Therefore, there exists a unitary matrix S, such that $\beta^{s^\dagger} = S\,\mathrm{diag}(e^{ik_1 s}, \ldots, e^{ik_\Delta s})S^\dagger$ (each k_t least $|\Delta'|$ times). Then (11) becomes a Fourier-type relation of the operators A and $A^{\downarrow 0}$:

$$S^\dagger A^{\downarrow 0} S = \sum_s \mathrm{diag}(e^{ik_1 s}, \ldots, e^{ik_\Delta s})(S^\dagger A^{s0} S) \qquad \text{or} \qquad A^{\downarrow 0}_{ij} = \sum_{tp} S_{it} S^\dagger_{tp} \sum_s e^{ik_t s} A^{s0}_{pj}. \tag{12}$$

Let it be noted here that groups with such a structure frequently appear in the physics of discrete systems. All the point groups are of this type. The symmorphic space groups essentially have the same structure, since the translational group is the direct product of three cyclic groups; taking it for Z, the last expression is obtained again, with p and q being three-dimensional integer vectors. In particular, each line group (Milošević and Damnjanović 1992) is the weak-direct products of one point group and one infinite cyclic group.

6. Example: normal modes of polyacetylene

Trans-polyacetylene is the simplest planar polymer. The equilibrium coordinates of the carbon and hydrogen atom of the sth monomer are (Chien 1984): $\boldsymbol{R}_{\mathrm{C}}(s) = ((-1)^s X_{\mathrm{C}}, 0, sa)$ and $\boldsymbol{R}_{\mathrm{H}}(s) = ((-1)^s X_{\mathrm{H}}, 0, sa)$, where $a = 1.24$ Å is half of the translational unit of the polymer, while $X_{\mathrm{C}} = 0.33$ Å and $X_{\mathrm{H}} = 1.41$ Å. The symmetry group of this polymer is (Milošević and Damnjanović 1993) the line group $G = \boldsymbol{L}2_1/mcm = \boldsymbol{D}_{1h}\boldsymbol{2}_1$, i.e. the weak-direct product of the point group $H = \boldsymbol{D}_{1h} = \{e, \sigma_x, \sigma_h, U_x\}$ (σ_x and σ_h are the reflections in the xz and xy planes, U_x is the rotation for π around x axis) and the infinite cyclic group $Z = \boldsymbol{2}_1$ generated by $z = (C_2 a)$ (the rotation for π around the z axis followed by the translation for a along the z axis). Obviously, the monomer with $s = 0$ is invariant under the subgroup H, and the rest of the polymer is obtained by the action of Z on this monomer.

The potential of this system is $U = \frac{1}{2}\sum_{s,t}\sum_{\alpha,\beta} U^{s\alpha}_{t\beta}$, with $s, t = 0, \pm 1, \ldots$ and $\alpha, \beta = C, H$. The two-particle interactions depend on the types of particle and their distances only: $U^{s\alpha}_{t\beta}(|\boldsymbol{r}_{s\alpha} - \boldsymbol{r}_{t\beta}|) = U_{\alpha\beta}(s - t)$. Its second derivative at the equilibrium configuration is denoted by $U''_{\alpha\beta}(s - t)$. Being cyclic, all the y coordinates are ignored. In the view of this, the infinite-dimensional polymer configurational space $\mathcal{H}_D$ is decomposed onto the orthogonal sum $\mathcal{H}_D = \oplus_s \mathcal{H}_s$ of the four-dimensional monomeric spaces $\mathcal{H}_s$ (two dimensions for each atom). To find the normal modes, the eigenproblem of the (infinite-dimensional) dynamical matrix

$$W^{s\alpha i}_{t\beta j} = \frac{1}{\sqrt{m_\alpha m_\beta}} \frac{\partial^2 U(\boldsymbol{R})}{\partial r_{s\alpha i}\partial r_{t\beta j}} \qquad (i, j = x, z)$$

should be solved. This matrix can be written in the form $W = \sum_{st} E^{st} \otimes W^{st}$, where W^{st} is the four-dimensional matrix with the elements $W^{s\alpha i}_{t\beta j}$. In agreement with (11), only the blocks W^{s0} will be studied carefully. For

$$R^\alpha_\beta(s) = \frac{\begin{pmatrix} (X_\alpha - (-1)^s X_\beta)^2 & sa((-1)^s X_\alpha - X_\beta) \\ sa((-1)^s X_\alpha - X_\beta) & s^2a^2 \end{pmatrix}}{(X_\alpha - (-1)^s X_\beta)^2 + s^2a^2}$$

these matrices for $s \neq 0$ or $\alpha \neq \beta$ are $W^{s\alpha i}_{0\beta j} = -\frac{1}{\sqrt{m_\alpha m_\beta}} U''_{\alpha\beta}(s)(R^\alpha_\beta(s))^i_j$. As is well known, the translational invariance of the whole system, i.e. the conservation of the momenta, manifests as $\sum_{s\alpha}\sqrt{m_\alpha m_\beta}W^{s\alpha i}_{0\beta j}=0$, implying $W^{0\alpha i}_{0\alpha j}=-\sum'_{s\beta}\sqrt{\frac{m_\beta}{m_\alpha}}W^{s\beta i}_{0\alpha j}$ (the primed sum is performed over pairs s,β different from $0,\alpha$).

The form of $R^\alpha_\beta(s)$ and the fact that the potential is a real even function of s (i.e. of the distance), lead to some special properties of the matrix elements $w^{\alpha i}_{\beta j}(k)=\sum_s W^{s\alpha i}_{0\beta j}e^{-iks}$ from (12). For $i=j$ they are real and even in k, satisfying

$$w^{\alpha i}_{\beta i}(k)=w^{\beta i}_{\alpha i}(k)=\sum_s W^{s\alpha i}_{0\beta i}\cos(ks).$$

On the contrary, for $i\neq j$, they are pure imaginary and odd in k, with

$$w^{\alpha x}_{\beta z}(k)=w^{\alpha z}_{\beta x}(k)=-w^{\beta x}_{\alpha z}(\pi+k)=\mathrm{i}\sum_s W^{s\alpha i}_{0\beta j}\sin(ks)$$

(vanishing for $k=0,\pi$). For convenience, $w^{Ci}_{Cj}(k)$, $w^{Hi}_{Hj}(k)$ and $w^{Ci}_{Hj}(k)$ will be denoted by $C^i_j(k)$, $H^i_j(k)$ and $w^i_j(k)$, respectively.

The matrix W commutes with the dynamical representation $S^V(G)=D(G)$ of G, which is the direct product of the permutational $D'(G)=S(G)$ and the vector representation $d(G)=V(G)$. It is easy to calculate:

$$V(\sigma_x)=V(e)=I_2 \qquad V(\sigma_h)=V(U_x)=-V(z)=\begin{pmatrix}1&0\\0&-1\end{pmatrix}$$

(I_2 is the two-dimensional identity matrix). Each type of atom forms one e_1 orbit of G, with H as the stabilizer group (Milošević and Damnajanović 1993). This means that in the monomer permutational representation $\Delta'(H)=Y(H)$ the elements of H are represented by $Y(h)=I_2$, and that the monomer dynamical representation is diagonal $\Delta(H)=Y(H)\otimes V(H)=\mathrm{diag}(V(H),V(H))$. Since the representation $S(G)$ is induced from the $Y(H)$, i.e. $S(G)=Y(H)\uparrow G$, the eigenproblem of W can be solved at the level of the monomer using the developed theory.

The irreducible components of the dynamical representation of the polyacetylene are (Milošević and Damnjanović 1993, table 14):

$$\begin{aligned}S^V(G)=2{}_0A_0^+ + 2{}_0A_0^- + 2{}_0A_1^+ + 2{}_0A_1^- + 4{}_\pi E_A + \sum_{k\in(0,\pi)}(4_k^{-k}E_{A_0}+4_k^{-k}E_{A_1})\\ +2{}_0B_1^+ + 2{}_0B_0^+ + 2{}_\pi E_B + \sum_{k\in(0,\pi)}(2_k^{-k}E_{B_0}+2_k^{-k}E_{B_1}).\end{aligned}$$

The representations in the second line, containing the label B, are related to the displacements along the y axis (in Milošević I and Damnjanović M (1993) the full vector representation is considered), implying $W^{\downarrow 0}_\mu=0$ in these cases. As for remaining irreducible components of $S^V(G)$, the operator $W^{\downarrow 0}_\mu$ should be found, and its eigenproblem solved. The relevant matrices for the irreducible representations are given in the table 1.

The projectors $H_\mu=H(\Delta\otimes D^{(\mu)^*})$ are $P_+=\mathrm{diag}(1,0,1,0)$ for $D^{(\mu)}={}_0A_0^+,{}_0A_1^+$, $P_-=\mathrm{diag}(0,1,0,1)$ for $D^{(\mu)}={}_0A_0^-,{}_0A_1^-$,

$$P_E=\tfrac{1}{2}\mathrm{diag}\left(\begin{pmatrix}1&1\\1&1\end{pmatrix},\begin{pmatrix}1&-1\\-1&1\end{pmatrix},\begin{pmatrix}1&1\\1&1\end{pmatrix},\begin{pmatrix}1&-1\\-1&1\end{pmatrix}\right)$$

for $D^{(\mu)}={}_k^{-k}E_{A_0},{}_k^{-k}E_{A_1},{}_\pi E_A$.

It should be noted that there are five different operators β, giving rise to the five operators $(W\otimes I_{\mu^*})^{\downarrow 0}$ by (12). All of them are essentially of two types. As for the one-dimensional

Table 1. The matrices of the irreducible components of the dynamical representation of polyacetylene. After the label of the irreducible representation in the first column, the corresponding representative matrices follow (columns 2–6). In the last column the matrices $\beta^{t^s} = I_2 \otimes V(z^s) \otimes D^{(\mu)}(z^s)$ are given. $P = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $K(k) = \begin{pmatrix} e^{ik} & 0 \\ 0 & e^{-ik} \end{pmatrix}$ and $F^s(k) = \mathrm{diag}(e^{i(\pi+k)s}, e^{i(\pi-k)s}, e^{iks}, e^{-iks}, e^{i(\pi+k)s}, e^{i(\pi-k)s}, e^{iks}, e^{-iks})$.

Rep.	e	σ_x	σ_h	U_x	z	β^{t^s}
${}_0A_0^{\pm}$	1	1	± 1	± 1	1	$\mathrm{diag}((-1)^s, 1, (-1)^s, 1)$
${}_0A_1^{\pm}$	1	1	± 1	± 1	-1	$\mathrm{diag}(1, (-1)^s, 1, (-1)^s)$
${}_0B_0^{+}$	1	-1	1	-1	1	$\mathrm{diag}((-1)^s, 1, (-1)^s, 1)$
${}_0B_1^{+}$	1	-1	1	-1	-1	$\mathrm{diag}(1, (-1)^s, 1, (-1)^s)$
${}_k^{-k}E_{A_0}$	I_2	I_2	P	P	$K(\frac{k}{2})$	$F^s(\frac{k}{2})$
${}_k^{-k}E_{A_1}$	I_2	I_2	P	P	$K(\pi+\frac{k}{2})$	$F^s(\pi+\frac{k}{2})$
${}_{\frac{\pi}{a}}E_A$	I_2	I_2	P	P	$K(\frac{\pi}{2})$	$F^s(\frac{\pi}{2})$
${}_k^{-k}E_{B_0}$	I_2	$-I_2$	P	$-P$	$K(\frac{k}{2})$	$F^s(\frac{k}{2})$
${}_k^{-k}E_{B_1}$	I_2	$-I_2$	P	$-P$	$K(\pi+\frac{k}{2})$	$F^s(\pi+\frac{k}{2})$
${}_{\frac{\pi}{a}}E_B$	I_2	$-I_2$	P	$-P$	$K(\frac{\pi}{2})$	$F^s(\frac{\pi}{2})$

representations the result is

$$w_q = \begin{pmatrix} C_x^x(\bar{q}) & 0 & w_x^x(\bar{q}) & 0 \\ 0 & C_z^z(q) & 0 & w_z^z(q) \\ w_x^x(\bar{q}) & 0 & H_x^x(\bar{q}) & 0 \\ 0 & w_z^z(q) & 0 & H_z^z(q) \end{pmatrix}.$$

Here, $q = 0$ and $q = \pi$ for the representations ${}_0A_0^{\pm}$ and ${}_0A_1^{\pm}$, respectively, and $\bar{q} = \pi + q$. Similarly, for the two-dimensional representations

$$W_q = \begin{pmatrix} C_x^x(\bar{q}) & 0 & -C_z^x(q) & 0 & w_x^x(\bar{q}) & 0 & w_z^x(\bar{q}) & 0 \\ 0 & C_x^x(\bar{q}) & 0 & C_z^x(q) & 0 & w_x^x(\bar{q}) & 0 & -w_z^x(\bar{q}) \\ C_z^x(q) & 0 & C_z^z(q) & 0 & w_z^x(q) & 0 & w_z^z(q) & 0 \\ 0 & -C_z^x(q) & 0 & C_z^z(q) & 0 & -w_z^x(q) & 0 & w_z^z(q) \\ w_x^x(\bar{q}) & 0 & -w_z^x(q) & 0 & H_x^x(\bar{q}) & 0 & -H_z^x(q) & 0 \\ 0 & w_x^x(\bar{q}) & 0 & w_z^x(q) & 0 & H_x^x(\bar{q}) & 0 & H_z^x(q) \\ -w_z^x(\bar{q}) & 0 & w_z^z(q) & 0 & H_z^x(q) & 0 & H_z^z(q) & 0 \\ 0 & w_z^x(\bar{q}) & 0 & w_z^z(q) & 0 & -H_z^x(q) & 0 & H_z^z(q) \end{pmatrix}$$

where $q = \frac{k}{2}$, $q = \pi + \frac{k}{2}$ and $q = \frac{\pi}{2}$ for the representations ${}_q^{-q}E_{A_0}$, ${}_q^{-q}E_{A_1}$ and ${}_{\pi}E_A$, respectively.

It remains to multiply these matrices by the group projectors, and to solve the eigenproblems of the products. The dimensions of the eigenproblems are essentially equal to the frequencies of the corresponding irreducible components, i.e. two for the one-dimensional and four for two-dimensional components. If

$$a_0^i(q) = \frac{C_i^i(q) + H_i^i(q)}{2} \qquad \kappa_i(q) = \frac{2w_i^i(q)}{C_i^i(q) - H_i^i(q)}$$

$$a_1^i(q) = (1 + \kappa^{-2}(q))^{-\frac{1}{2}} \qquad a_3^i(q) = (1 + \kappa^2(q))^{-\frac{1}{2}}$$

and

$$\omega_{\pm}^i(q) = \frac{C_i^i(q) + H_i^i(q)}{2} \pm \frac{C_i^i(q) - H_i^i(q)}{2}\sqrt{1 + \kappa^2(q)} \qquad \text{for } i = x, z$$

the eigenvalues and the eigenvectors for the one-dimensional representations are:

$$
\begin{aligned}
{}_0A_0^+ :&\quad \omega_\pm^x(\pi),\ \frac{1}{\sqrt{2(1\pm a_3^x(\pi))}}(1\pm a_3^x(\pi),0,\pm a_1^x(\pi),0)\\
{}_0A_1^+ :&\quad \omega_\pm^x(0),\ \frac{1}{\sqrt{2(1\pm a_3^x(0))}}(1\pm a_3^x(0),0,\pm a_1^x(0),0)\\
{}_0A_0^- :&\quad \omega_\pm^z(0),\ \frac{1}{\sqrt{2(1\pm a_3^z(0))}}(0,1\pm a_3^z(0),0,\pm a_1^z(0))\\
{}_0A_1^- :&\quad \omega_\pm^z(\pi),\ \frac{1}{\sqrt{2(1\pm a_3^z(\pi))}}(0,1\pm a_3^z(\pi),0,\pm a_1^z(\pi)).
\end{aligned}
$$

The translational invariance, expressed as $m_{\mathrm{C}}C_i^i(0) = m_{\mathrm{H}}H_i^i(0) = -\sqrt{m_{\mathrm{C}}m_{\mathrm{H}}}w_i^i(0)$, gives $\omega_+^i(0) = 0$, revealing the translational x and z modes ${}_0A_1^+$ and ${}_0A_0^-$. The eigenvectors coordinates should be multiplied by the square roots of the corresponding atomic masses, to get the precise geometrical notion of the vibrations of the monomer with $s = 0$, and the additional action of β^s gives, due to (8) the displacements in the sth monomer. The two-dimensional representations can be treated along the same lines, but the results are omitted, being lengthy enough, with no essentially different point.

It should be emphasized that the modified group projector technique enabled us to reduce all the calculations of the normal modes (i.e. infinite-dimensional problem) to the monomeric level (finite-dimensional); as has been explained in (Damnjanović and Milošević 1984), it remains to solve a few eigenproblems of finite-dimensional matrices for the eigenvalue 1, to derive the normal modes and frequencies. Let us mention here that this procedure has already been implemented in the computer program POLSym to find the normal modes, and some other characteristics of polymers.

7. Concluding remarks

The connection between a representation of the subgroup and the induced representation of the group is analysed. The results enable us to solve the problem of the symmetry-adapted eigenbases at the level of the subgroup solely, pointing out the relevance of the quantum numbers based on the subgroup symmetry.

The proposed group projector technique appears as a natural method to deal with the induced representations. Although it seems that the most of the induction theory can be interpreted within this concept, only several theorems (Altmann 1977, section 11) will be re-derived here in order to illustrate the basic ideas. To begin with, recall that the trace of the projector $G(D\otimes D^{(\mu)*})$ is the frequency of the irreducible representation $D^{(\mu)}(G)$ in the representation $D(G)$. Then a radically shortened proof of the Frobenius reciprocity theorem is offered: with $D(G) = (\Delta^{(\nu)}(H)\uparrow G)\otimes D^{(\mu)*}(G)$, i.e. $\Delta(H) = \Delta^{(\nu)}(H)\otimes(D^{(\mu)*}(G)\downarrow H)$, expression (5) implies that the frequency of $D^{(\mu)}(G)$ in $\Delta^{(\nu)}(H)\uparrow G$ is equal to the frequency of the irreducible representation $\Delta^{(\nu)*}(H)$ in $D^{(\mu)*}(G)\downarrow H$, i.e. to the frequency of $\Delta^{(\nu)}(H)$ in $D^{(\mu)}(G)\downarrow H$. The Burnside theorem appears as the special case for $H = \{e\}$ and $\Delta^{(\nu)}(H) = 1$; the induced representation $D'(G)$ is just the regular one, while the subgroup projector becomes $H(1\otimes D^{(\mu)*}) = I_{\mu^*}$, with the trace equal to μ. The frequency theorem for the induced representations, stating that the frequencies of $I(G)$ in $\Delta(H)\uparrow G$ and $I(H)$ in $\Delta(H)$ are equal, is an immediate consequence of (5), for $d(G) = I(G)$. The theorem on the equivalence of the representations $D_1(G) = (\Delta(H)\uparrow G)\otimes d(G)$ and $D_2(G) = \{\Delta(H)\otimes(d(G)\downarrow H)\}\uparrow G$ is similarly proved: for any irreducible representation $D^{(\mu)}(G)$, both the projectors $G(D_1 \otimes D^{(\mu)^*})$ and $G(D_2 \otimes D^{(\mu)^*})$ are transferred to the subgroup projector $H(\Delta \otimes d \otimes D^{(\mu)^*})$, and thereby their traces are equal. Further, the transitivity of induction, i.e. the equivalence of $D = \Delta(K) \uparrow G$ with $(\Delta(K) \uparrow H) \uparrow G$ for $K < H < G$, is seen as the double transferring: $G(D \otimes D^{(\mu)^*}) = B_H H((\Delta(K) \uparrow H) \otimes D^{(\mu)^*}) B_H^\dagger = B_H B_K K(\Delta \otimes D^{(\mu)^*}) B_K^\dagger B_H^\dagger$ (with the obvious meaning of B_H and B_K), guaranteeing the same irreducible components for both the representations.

The dynamical representation of the discrete system, which is important when the normal modes are sought, is the direct product of the vector representation and the permutational representation. The latter is often obtained as the induced representation, from the permutational representation of the stabilizer group of a subsystem. In such cases the developed theory enables us to work with the subsystem and its symmetry group only. A typical example, treated in this paper, is the polymer, the normal modes of which can be derived through the procedure involving one monomer only. It is important to note that there are other physical situations quite analogous to this (Elliot and Dawker 1979). For example, when the molecular orbitals are calculated as the linear combination of the atomic orbitals, the procedure is the same as that for the normal modes, only the vector representation has to be substituted with another one (some of the irreducible representations of the full rotational group, subduced to the orthogonal subgroup of G) (Wigner 1959). The method suggested has been implemented within the computer program POLSym (Milošević and Damnjanović 1992), designed for calculations in polymer physics.

Acknowledgment

This work is supported by National Science Foundation, grant E-01-01.

References

Altmann S L 1977 *Induced Representations in Crystals and Molecules* (London: Academic)
Chen J Q, Gao M J and Ma G Q 1985 *Rev. Mod. Phys.* 211
Chien J C W 1984 *Polyacetylene* (London: Academic)
Cornwell J F 1984 *Group Theory in Physics* (London: Academic)
Damnjanović M and Milošević I 1984 *J. Phys. A: Math. Gen.* 27 4859–66
Davies B L 1982 *Physica* A **114** 507–17
Elliot J P and Dawber P G 1979 *Symmetry in Physics* (London: Macmillan)
Jansen L and Boon M 1967 *Theory of Finite Groups: Applications in Physics* (Amsterdam: North-Holland)
Mackey G 1952 *Ann. Math.* **55** 101–39
Milošević I and Damnjanović M 1992 *Preprint FPBU* 01/92
——1993 *Phys. Rev.* B **47** 7805–18
Ping J L, Zheng Q R, Chen B Q and Chen J Q 1989 *Comput. Phys. Commun.* **52** 355–73
Wigner E P 1959 *Group Theory and its Applications to the Quantum Mechanics of Atomic Spectra* (New York: Academic)