

Modified group-projector technique: subgroups and generators

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Abstract. Instead of the usual procedure involving the family of group operators, only the projector of the identity representation is used to obtain the symmetry-adapted basis. For the product groups, this projector is factorized to the subgroups. So, the whole procedure is reduced to the eigenvalue problem for the operators representing the generators. Avoiding summation over the group, the method is suitable for computer implementations even for infinite groups. Some applications are discussed.

1. Introduction

One of the most important group-theoretical concepts in physics is the standard (or symmetry-adapted) basis (Elliot and Dawber 1979 section 5.3, Jansen and Boon 1967 ch III) which enables us to simplify and sometimes completely solve the eigenproblem of operators commuting with a unitary representation of the symmetry group. Furthermore, such bases are unavoidable when selection rules are sought (Wigner 1959 section 6.3, Messiah 1970 appendix D) and, more generally, they provide the setup for the Wigner–Eckart theorem. To find these bases, group operators are essential.

Let $D(G)$ be a reducible unitary representation in the space \mathcal{H} . The notion of reducibility refers to complex spaces until otherwise specified (Wigner 1959 section 3, Jansen and Boon 1967 ch 2). The frequencies a_μ of the irreducible components $D^{(\mu)}(G)$ can be found by using the characters: $a_\mu = (1/|G|) \sum_g \chi^{(\mu)*}(g) \chi(g)$. Then, $D(G)$ is decomposed into irreducible components in the form $D(G) = \bigoplus_{\mu=1}^s a_\mu D^{(\mu)}(G)$ revealing the decomposition of \mathcal{H} into the irreducible invariant subspaces: $\mathcal{H} = \bigoplus_{\mu=1}^s \bigoplus_{t_\mu=1}^{a_\mu} \mathcal{H}^{\mu t_\mu}$. By choosing an orthonormal sub-basis $\{|\mu t_\mu m\rangle | m = 1, \dots, d_\mu\}$ (d_μ is the dimension of $D^{(\mu)}(G)$) in each of these subspaces, the standard basis in \mathcal{H} is obtained. The action of the operators $D(G)$ in this basis is represented by

$$D(g)|\mu t_\mu m\rangle = \sum_{m'=1}^{d_\mu} D_{m'm}^{(\mu)}(g)|\mu t_\mu m'\rangle$$

i.e. by block-diagonal matrices with irreducible representations within the blocks.

To obtain the standard basis when the matrices $D_{ij}^{(\mu)}(g)$ of the irreducible representations are given, the family of group operators (Jansen and Boon 1967 section III.2.6.)

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$P_{ij}^{(\mu)}(D, G) \stackrel{\text{def}}{=} (d_\mu/|G|) \sum_g D_{ij}^{(\mu)*}(g)D(g)$ has to be calculated. The orthogonality relations imply that $P_{ij}^{(\mu)}(D, G)P_{st}^{(\nu)}(D, G) = P_{it}^{(\mu)}(D, G)\delta_{\mu\nu}\delta_{js}$ and $P_{ij}^{(\mu)\dagger}(D, G) = P_{ji}^{(\mu)}(D, G)$; thus, $P_{ii}^{(\mu)}(D, G)$ are the projectors. The algorithm to obtain the standard basis becomes: for each μ the projector $P_{11}^{(\mu)}(D, G)$ is found, with a basis in the (a_μ -dimensional) range of this projector, say $\{|\mu t_\mu 1\rangle | t_\mu = 1, \dots, a_\mu\}$; finally, the vectors $\{|\mu t_\mu m\rangle \stackrel{\text{def}}{=} P_{m1}^{(\mu)}(D, G)|\mu t_\mu 1\rangle | m = 1, \dots, d_\mu\}$ form the standard sub-basis. In what follows, the group projector $P_{11}^{(I)}(D, G)$ for the identity representation $I(G)$ ($I(g) = 1$) will be denoted by $G(D)$.

This general procedure may appear inconvenient to apply to some specific situations. Since group operators do not involve the whole irreducible representation but only a single matrix element, algebraic operations with them are only related to the structure of the group through the orthogonality relations. Furthermore, for groups with many elements, the summation can be complicated while for infinite groups the direct computer implementation of this technique seems impossible; e.g. the line (Milošević and Damnjanović 1993) and space groups (Altmann 1977) in polymer and crystal physics are infinite.

The aim of this paper is to develop a method to avoid some of the mentioned difficulties. This method should be applicable whenever the described standard one is, i.e. for unitary representations of finite and discrete groups. In the next section, the theorems enabling us to reduce the construction of any group operator to the group projector of the identity representation are proved. Since it does not single out any matrix element, this projector manifestly reflects the group structure (section 3), being expressible through the projectors related to the subgroups. Using this, it is easy to substitute the summation over the group with an eigenproblem (section 4). Finally, besides some remarks on the applicability of the method, an example is given.

2. Projections in the product space

To begin with, the necessary group-theoretical results will be briefly developed. Let $D_1(G)$ and $D_2(G)$ denote two unitary representations of G in the spaces \mathcal{H}_1 and \mathcal{H}_2 (d_1 and d_2 being their dimensions). The corresponding decompositions into irreducible components are $D_i(G) = \oplus_\mu a_\mu^i D^{(\mu)}(G)$ ($i = 1, 2$). In the direct product of these representations $D_1(G) \otimes D_2(G)$, defined in the space $\mathcal{H}_1 \otimes \mathcal{H}_2$, the identity representation $I(G)$ appears $a_I = (1/|G|) \sum_g \chi_1(g)\chi_2(g)$ times (in fact, this is the intertwining number for $D_1(G)$ and $D_2^*(G)$). Since $\chi_i(g) = \sum_\mu a_\mu^i \chi^{(\mu)}(g)$, the orthogonality of the irreducible characters gives $a_I = \sum_\mu a_\mu^1 a_\mu^2$. (here, $D^{(\mu)*}(G)$ denotes the complex conjugated representation of $D^{(\mu)}(G)$). Note that a_I is the dimension of the subspace of the identity representation, i.e. of the range R of the group projector $G(D_1 \otimes D_2) = (1/|G|) \sum_g D_1(g) \otimes D_2(g)$. Obviously, $G(D^{(\mu)*} \otimes D) = P^{(\mu)}(D, G)$ if $D_1(G) = D^{(\mu)}(G)$ is a one-dimensional (irreducible) representation.

Let $\{|i; 1\rangle | i = 1, \dots, d_1\}$ and $\{|b_j\rangle | j = 1, \dots, d_2\}$ be the orthonormal bases in \mathcal{H}_1 and \mathcal{H}_2 , respectively. Any vector $|x\rangle$ from $\mathcal{H}_1 \otimes \mathcal{H}_2$, written as $|x\rangle = \sum_{i,j} \alpha_{ij} |i; 1\rangle \otimes |b_j\rangle$, uniquely defines d_1 vectors in \mathcal{H}_2 through the partial scalar products: $|i; 2\rangle \stackrel{\text{def}}{=} \langle i; 1|x\rangle = \sum_j \alpha_{ij} |b_j\rangle$, $i = 1, \dots, d_1$. The obtained couples $|i; 1\rangle$ and $|i; 2\rangle$ determine $|x\rangle$ in the form $|x\rangle = \sum_{i=1}^{d_1} |i; 1\rangle \otimes |i; 2\rangle$. Note that the vectors $|i; 2\rangle$ may be zero or linearly dependent. The main theorem can now be proposed.

Theorem 1. Let the vectors of the orthonormal basis $\{|i; 1| | i = 1, \dots, d_1\}$ in \mathcal{H}_1 transform according to $D_1(g)|i; 1\rangle = \sum_j D_{1ji}(g)|j; 1\rangle$ and let $|x\rangle = \sum_{i=1}^{d_1} |i; 1\rangle \otimes |i; 2\rangle$ be from R . Then the action of the operators $D_2(g)$ on the vectors $|i; 2\rangle$ is $D_2(g)|i; 2\rangle = \sum_{j=1}^{d_1} D_{1ji}^*(g)|j; 2\rangle$.

Since $D_1(g) \otimes D_2(g)|x\rangle = |x\rangle$, the proof consists of the following sequence of equalities: $D_2(g)|i; 2\rangle = D_2(g)\langle i; 1|x\rangle = D_2(g)\langle i; 1|(D_1(g^{-1}) \otimes D_2(g^{-1}) \sum_{k=1}^{d_1} |k; 1\rangle \otimes |k; 2\rangle) = D_2(g)\langle i; 1|\sum_{k,j=1}^{d_1} D_{1jk}(g^{-1})|j; 1\rangle \otimes (D_2(g^{-1})|k; 2\rangle) = \sum_{k=1}^{d_1} D_{1ki}^*(g)|k; 2\rangle$.

Theorem 1 offers an algorithm for the derivation of the standard basis. It will be described with the help of the following theorem.

Theorem 2. Let $\{|\mu t_\mu^1 m; 1\rangle\}$ and $\{|\mu t_\mu^2 m; 2\rangle\}$ be the standard bases for the representations $D_1(G)$ and $D_2(G)$ in \mathcal{H}_1 and \mathcal{H}_2 . Then an orthonormal basis in R is

$$\left\{ |\mu t_\mu^1 t_\mu^2\rangle \stackrel{\text{def}}{=} \frac{1}{\sqrt{d_\mu}} \sum_{m=1}^{d_\mu} |\mu^* t_\mu^1 m\rangle \otimes |\mu t_\mu^2 m\rangle | \mu \quad t_\mu^1 = 1, \dots, a_\mu^1 \quad t_\mu^2 = 1, \dots, a_\mu^2 \right\}$$

To prove this, it is sufficient to note that there are exactly $\sum_\mu a_\mu^1 a_\mu^2$ of these vectors, which is also the dimension of R , and that all of them are invariant under $D_1(g) \otimes D_2(g)$. They are orthonormal since so are components in \mathcal{H}_1 and \mathcal{H}_2 .

The standard basis for the reducible representation $D_2(G) = D(G)$ can be found as follows. Let $D^{(\mu)}(G)$ be one of its irreducible components and $\{|\mu^* m\rangle | m = 1, \dots, d_\mu\}$ be the standard basis for the irreducible matrix representation $D_1(G) = D^{(\mu)*}(G)$. First, the projector $G(D^{(\mu)*} \otimes D)$ is to be found. In its a_μ -dimensional range, any orthonormal basis $\{|\mu t_\mu\rangle | t_\mu = 1, \dots, a_\mu\}$ ($t_\mu^1 = 1$ is superfluous, while $t_\mu = t_\mu^2$) can be chosen as the basis of theorem 2. According to theorem 1, the partial scalar products $|\mu t_\mu m\rangle = \langle \mu^* m | \mu t_\mu\rangle$ are the standard vectors. To find the whole standard basis, the procedure has to be worked out for each irreducible component of $D(G)$. Thus, the procedure is reduced to the projectors $G(D^{(\mu)*} \otimes D)$ only. In fact, since $P_{ij}^{(\mu)}(D, G) = \langle \mu^* i | G(D^{(\mu)*} \otimes D) | \mu^* j\rangle$ (partial scalar product), $G(D^{(\mu)*} \otimes D)$ contains the same information as the whole set of the group operators $P_{ij}^{(\mu)}(D, G)$. In this sense, the proposed procedure appears as a modification to the usual one; its advantages will stem from the fact that the projector $G(D)$ reflects the structure of G as will be discussed in the following.

3. Subgroups and their products

The definition of the group projector $G(D)$ can be easily generalized to any subset Y of G : $Y(D) = (1/|Y|) \sum_{g \in Y} D(g)$. Although these operators are not generally projectors, their properties enable us to reduce the calculation of $G(D)$ to some relevant subsets. For further analysis it should be recalled that the group G is the product of its subgroups H and K , $G = HK$, if each element g of G is a product $g = hk$ of the elements h from H and k from K (Jansen and Boon 1967 section I.6). The factors are not unique unless G is the weak direct product of H and K , i.e. unless the intersection subgroup $L = H \cap K$ contains the identity element only: for any $l \in L$ the elements $h' = hl^{-1} \in H$ and $k' = lk$ also give $g = h'k'$. More generally, for any subgroup H of the group G , the left transversal $Z = \{z_0, \dots, z_{|Z|-1}\}$ ($|Z| = |G|/|H|$) can be found; $G = \cup_i z_i H$. If \bar{Z} is the closure of Z , i.e. the minimal subgroup of G containing Z then G is the product $G = \bar{Z}H = H\bar{Z}$. This is the weak direct product if, and only if, $\bar{Z} = Z$, i.e. when Z itself is a subgroup.

Using these preliminary considerations, one can prove the following theorem.

Theorem 3. Let $D(G)$ be a unitary representation of the group G .

- (i) If $Y^{-1} \stackrel{\text{def}}{=} \{y^{-1} | y \in Y\}$ then $(Y^{-1})(D) = Y^\dagger(D)$.
- (ii) For a closed subset Y (i.e. $YY = Y$) in G , $Y(D)$ is idempotent, $Y^2(D) = Y(D)$.
- (iii) If H and K are subgroups of G , then $(HK)(D) = H(D)K(D)$ and this is the projector if $HK = KH$ is also a subgroup; in particular, when G is the product of its subgroups H and K , then $G(D)$ is factorized into subgroup projectors: $G(D) = H(D)K(D)$.
- (iv) If H is a subgroup of G with the left transversal Z then $G(D) = Z(D)H(D) = \overline{Z}(D)H(D)$.

The first two statements follow directly from the unitarity of $D(G)$ and the definition of $Y(D)$. To prove the third part—note that if h_i and k_j are the left and right coset representatives of L in H and K , respectively, i.e. $H = \cup_i h_i L$ and $K = \cup_j L k_j$ —all the pairs h, k such that $g = hk$ (for given $g \in HK$) belong to the same cosets of L in H and K , respectively. Indeed, if $g = hk = h'k'$ with $h = h_i l_h$, $h' = h_{i'} l_{h'}$, $k = l_k k_j$ and $k' = l_{k'} k_{j'}$, it follows from $hk = h'k'$ that $h_i^{-1} h_i (l_h l_k) = (l_{h'} l_{k'}) k'_j k_j^{-1}$ and $i' = i$, $j = j'$ and $l_h l_k = l_{h'} l_{k'} = l$. Once the transversals $\{h_i\}$ and $\{k_j\}$ are chosen, the elements of HK are uniquely factorized in the form $g = h_i l k_j$, $l \in L = H \cap K$. So, the orders of the mentioned subsets are related by $|G| = |H||K|/|L|$. The product of the subgroup projectors, when $h = h_i l$ and $k = l' k_j$ are substituted, becomes

$$H(D)K(D) = \frac{1}{|H||K|} \sum_{h,k} D(hk) = \frac{1}{|H||K|} \sum_i D(h_i) \sum_{l,l'} D(l') \sum_j D(k_j) = (HK)(D).$$

HK is a subgroup if, and only if, $HK = KH$ which implies that $H(D)$ and $K(D)$ commute and ensures that $(HK)(D)$ is again a projector. The last part is obtained when in $G(D) = 1/(|Z||H|) \sum_{z,h} D(z)D(h)$ the summation over H is performed giving the sum of the transversal representatives multiplied by $H(D)$.

Applied to the results of the preceding sections, this theorem enables us to reduce the group-projector technique to some subgroup and its transversal: for any irreducible component $D^{(\mu)}(G)$ of $D(G)$ the representation $D^{(\mu)*}(G) \otimes D(G)$ is constructed and the relevant group projector factorized: $G(D^{(\mu)*} \otimes D) = Z(D^{(\mu)*} \otimes D)H(D^{(\mu)*} \otimes D)$. Both factors are projectors, particularly for the product groups. Afterwards, the determination of the standard basis is prescribed by theorem 2.

4. Projectors of the cyclic groups

All the operators of the representation $D(G)$ of a cyclic group G with generator g are powers of $D(g)$. Hence, there exists a unitary operator U such that $UD(g)U^{-1}$ is the diagonal matrix with eigenvalues e^{ik_s} ($s = 1, \dots, d$; d is the dimension of $D(G)$) on the diagonal. The corresponding eigenspaces are the irreducible invariant subspaces for $D(G)$ and the irreducible subrepresentations (always one dimensional) are generated by the eigenvalues. g^t is represented by a phase factor $D^{(\mu)}(g^t) = e^{ik_\mu t}$ particularly within an irreducible representation.

Therefore, the group projector $P^{(\mu)}(D, G) = G(D^{(\mu)*} \otimes D)$ takes the form

$$G(D^{(\mu)*} \otimes D) = U^{-1} \text{diag} \left(\frac{1}{|G|} \sum_t e^{i(k_1 - k_\mu)t}, \dots, \frac{1}{|G|} \sum_t e^{i(k_d - k_\mu)t} \right) U.$$

The non-vanishing sums are for $k_x = k_\mu$ being equal to 1. In other words, R is the eigenspace of $D(g)$ for the eigenvalue $D^{(\mu)}(g)$ and instead of the summation over the group, only the eigenprojector of $D^{(\mu)*}(g) \otimes D(g)$ for the eigenvalue 1 is to be calculated. This also remains true for the infinite cyclic groups when direct summation is not possible and this fact can be exploited in the related computational methods.

The generality of the presented considerations becomes clear when it is realized that, besides the finite groups, most of the discrete groups applied in physics can be factorized as the product of the cycles of their generators. For example, all the crystallographic point groups are products of cyclic groups (Altmann 1977, p 268) and the line groups are of the form $L = ZP$ where Z is a cyclic infinite group and P is one of the axial point groups which are themselves products of the cyclic groups (Damjanović 1981). In all these cases the group projectors can be found by solving the eigenproblems for the generators. As for the space groups, the translational subgroup is the direct product of three infinite cyclic groups (the subgroup projector is to be within three eigenvalue problems) while the transversal is finite, making the last part of theorem 3 applicable. In addition, it should be mentioned that when H is the invariant subgroup, since it is the translational subgroup, $Z(D)$ commutes with $H(D)$.

5. Discussion

The group-operator technique is reduced to the group projectors $G(D^{(\mu)*} \otimes D)$ of the identity representation. It appears that the vectors in the range of this projector, i.e. the fixed points of the operators of $D^{(\mu)*}(G) \otimes D(G)$ are those coupling the corresponding vectors of the standard bases for $D^{(\mu)*}(G)$ and $D(G)$. This provides an algorithm for constructing the standard basis of $D(G)$: for each irreducible subrepresentation $D^{(\mu)}(G)$, the projector $G(D^{(\mu)*} \otimes D)$ should be found together with an orthonormal basis in its range. For each vector of this basis, partial scalar products with the known standard basis for $D^{(\mu)*}(G)$ (usually the absolute basis) give the standard basis for $D(G)$. Note that the order in the direct product is unimportant; the whole method can be worked out with the choice $G(D \otimes D^{(\mu*)})$.

In this form, the group-projector technique does not involve any isolated matrix elements but only the whole matrices of the related representations. Essentially, this has been exploited to show that in the most general case of the group factorizing into subgroups $G = H_1 H_2 \dots$ (with no restriction on their intersection) and their factor groups, the projector $G(D^{(\mu)*} \otimes D)$ is the product of the corresponding projectors $H_i(D^{(\mu)*} \otimes D)$ of subduced (or restricted) representations to the subgroups. Moreover, for the groups factorizable in this sense into the cycles of the generators, it turns out that the whole problem is equivalent to the determination of the eigenspaces for the eigenvalue 1 for the operators representing generators of G in $D^{(\mu)*}(G) \otimes D(G)$, even in the case of infinite discrete groups. In this sense the proposed scheme generalizes the subgroup method used in the solid-state physics.

The structural conditions required in the theorems are weak enough such that the results refer to all the discrete groups relevant in physics. This offers the opportunity to apply the technique in the calculations with obvious advantage when infinite groups are involved. Due to the relation $a_\mu = \text{Tr } G(D^{(\mu)*} \otimes D)$, it may be preferable to calculate even the frequencies of the irreducible representations by this technique. It should be mentioned that these results have already been implemented in the computer program POLSym, employing the line groups in polymer physics (Milošević and Damjanović 1992).

The same concept can obviously be extended to compact factorizable Lie groups in which the usual group-projector method is based on the bi-invariant measure. While the

structural considerations remain the same, the appropriate elements of the Lie algebra and the null-spaces of the operators representing them should be used instead of the generators of the discrete groups and the eigenspaces for the eigenvalue 1. The connection of this approach with Cartan's seems to be an interesting question but far beyond the scope of this paper.

Some other related problems should be mentioned in this context. The first of these is a prescription for calculating the Clebsch–Gordan coefficients. If, in the direct product of two irreducible representations $D^{(\mu)}(G)$ and $D^{(\nu)}(G)$, the irreducible component $D^{(\lambda)}(G)$ occurs once then the Clebsch–Gordan coefficients are the scalar products $\langle \mu m \nu n | \mu \nu \lambda l \rangle$ of the standard basis $|\mu \nu \lambda l\rangle$ (in the product space) with the vectors $|\mu m \nu n\rangle = |\mu m\rangle \otimes |\nu n\rangle$ of the product of the standard bases (in the factor spaces). In view of section 2, the range of the projector $G(D^{(\lambda)*} \otimes D^{(\mu)} \otimes D^{(\nu)})$ is one dimensional and for a chosen normalized vector $|\mu \nu \lambda\rangle$ the standard basis is $|\mu \nu \lambda l\rangle = \langle \lambda^* l | \mu \nu \lambda \rangle$ (partial scalar product). Therefore, the Clebsch–Gordan coefficients can be calculated as $\langle \mu m \nu n | \mu \nu \lambda l \rangle = \langle \mu m \nu n | \langle \lambda^* l | \mu \nu \lambda \rangle$. Assuming that all the bases involved ($|\mu m\rangle$, $|\nu n\rangle$ and $|\lambda^* l\rangle$) are absolute, it turns out that the Clebsch–Gordan coefficients are just the coordinates of $|\mu \nu \lambda\rangle$.

It is well known that there is a standard eigenbasis of the Hermitian operator H commuting with the representation $D(G)$. In fact, the group operators commute with H also and the ranges of the projectors $P_{ii}^{(\mu)}(D, G)$ are invariant for H . This enables us to solve the eigenvalue problems separately in the ranges of $P_{ii}^{(\mu)}(D, G)$ for each μ and to reveal the other symmetry-adapted eigenvectors through the use of the group operators. In the proposed scheme, the role of H is taken by the operator $I \otimes H$ commuting with the representation $D^{(\mu)*}(G) \otimes D(G)$. The subspace R is invariant for this operator and by solving the eigenproblems in these subspaces (for each μ) we obtain the basis in R . This is the basis $|\mu 1 t_{\mu}^2\rangle$ used in theorem 2; it is easy to verify that the standard basis of the original space derived in the theorem is an eigenbasis of H .

At the end of the paper the concepts introduced are illustrated by an example concerning the line groups (Milošević and Damjanović 1993). The group $L = L(2n)_n mc$ is the weak direct product $L = ZP$ of the infinite cyclic group of the screw axis $Z = (2n)_1 = \{(C_{2n}|\frac{1}{2})^t | t = 0, \pm 1, \dots\}$ and the point group $P = C_{nv} = \{C_n^j C_2^s | j = 0, 1; s = 0, \dots, n-1\}$. The Clebsch–Gordan series of the square of the irreducible two-dimensional representation $E = {}_k E_{m, -m}$ for $m \neq \frac{1}{4}$ is $E^2 = E' + A + B$ with $E' = 2{}_k E_{2m, -2m}$, $A = 2{}_k A_0$ and $B = 2{}_k B_0$ (Damjanović *et al* 1983). The scheme presented in the paper will be applied to find the Clebsch–Gordan coefficients. The factorized projector $L(D') = Z(D')P(D')$ is used with D' being $D'_E = E^r \otimes E^2$, $D'_A = A^* \otimes E^2$ and $D'_B = B^* \otimes E^2$. While the subgroup projector of C_{nv} is found by the standard technique, the other factor is constructed as the eigenprojector for the eigenvalue 1 of the operator $D'(C_{2n}|\frac{1}{2})$, thus avoiding the infinite summation.

The representative matrices are ($\alpha = 2\pi/n$)

$$E((C_{2n}|\frac{1}{2})^t \sigma_v^j C_n^s) = e^{ikt/2} \text{diag}(e^{im\alpha/2}, e^{-im\alpha/2}) M_2^j \text{diag}(e^{ims\alpha}, e^{-ims\alpha})$$

$$A((C_{2n}|\frac{1}{2})^t \sigma_v^j C_n^s) = e^{ikt/2} \quad B((C_{2n}|\frac{1}{2})^t \sigma_v^j C_n^s) = (-1)^j e^{ikt/2}$$

and

$$E^2((C_{2n}|\frac{1}{2})^t \sigma_v^j C_n^s) = e^{ikt} \text{diag}(e^{im\alpha}, 1, 1, e^{-im\alpha}) M_4^j \text{diag}(e^{2ims\alpha}, 1, 1, e^{-2ims\alpha})$$

where M_n is the n -dimensional off-diagonal matrix

$$M_n = \begin{pmatrix} 0 & \dots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \dots & 0 \end{pmatrix}.$$

The representations D' of the subgroup C_{nv} can be found by substituting $t = 0$

$$D'_E(\sigma_v^j C_n^s) = M_3^j \text{diag}(1, e^{-2ims\alpha}, e^{-2ims\alpha}, e^{-4ims\alpha}, e^{4ims\alpha}, e^{2ims\alpha}, e^{2ims\alpha}, 1)$$

$$D'_A(\sigma_v^j C_n^s) = {}_k E_{m,-m}^2(\sigma_v^j C_n^s) \quad \text{and} \quad D'_B(\sigma_v^j C_n^s) = (-1)^j {}_k E_{m,-m}^2(\sigma_v^j C_n^s).$$

The subgroup projectors $P(D') = (1/2n) \sum_{s=0}^{n-1} \sum_{j=0}^1 D'(\sigma_v^j C_n^s)$ are

$$P(D'_E) = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$P(D'_A) = \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \text{and} \quad P(D'_B) = \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

As for the generator $(C_{2n}|1/2)$, the representative matrices are

$$D'_E(C_{2n}|1/2) = \text{diag}(1, e^{-i\alpha}, e^{-i\alpha}, e^{-2i\alpha}, e^{2i\alpha}, e^{i\alpha}, e^{i\alpha}, 1)$$

$$D'_A(C_{2n}|1/2) = D'_B(C_{2n}|1/2) = \text{diag}(e^{i\alpha}, 1, 1, e^{-i\alpha}).$$

Consequently, the projectors $Z(D')$, being the eigenprojectors of these matrices are $Z(D'_E) = \text{diag}(1, 0, 0, 0, 0, 0, 0, 1)$ and $Z(D'_A) = Z(D'_B) = \text{diag}(0, 1, 1, 0)$.

Finally, the projectors for the whole line group $L(2n)_n mc$ are the products of the corresponding factor-projectors

$$L(D'_E) = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

while $L(D'_A)$ and $L(D'_B)$ are equal to those found for the subgroup C_{nv} . The eigenvectors in the ranges of these projectors are: $|EEE'\rangle = (1, 0, 0, 0, 0, 0, 0, 1)^T$ for D'_E , $|EEA\rangle = (1/\sqrt{2})(0, 1, 1, 0)^T$ for D'_A and $|EEB\rangle = (1/\sqrt{2})(0, 1, -1, 0)^T$ for D'_B .

It remains to find the standard basis and the Clebsch-Gordan coefficients. Denoting the absolute bases in the irreducible representative spaces by $\{|E1\rangle, |E2\rangle\}$, $\{|E'1\rangle, |E'2\rangle\}$, $\{|A1\rangle\}$, $\{|B1\rangle\}$, the coefficients are the coordinates of the found vectors $|EEE'\rangle$, $|EEA\rangle$ and $|EEB\rangle$. The non-vanishing ones are

$$\begin{aligned} \langle E1E1 | EEE'1\rangle &= \langle E2E2 | EEE'2\rangle = 1 \\ \langle E1E2 | EEA1\rangle &= \langle E2E1 | EEA1\rangle = 1/\sqrt{2} \\ \langle E1E2 | EEB1\rangle &= -\langle E2E1 | EEB1\rangle = 1/\sqrt{2}. \end{aligned}$$

References

- Altmann S L 1977 *Induced Representations in Crystals and Molecules* (London: Academic)
- Damnjanović M 1981 *J. Phys. A: Math. Gen.* **14** 1055–63
- Damnjanović M, Božović I and Božović N 1983 *J. Phys. A: Math. Gen.* **16** 3937–47
- 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)
- Messiah A 1970 *Quantum Mechanics* (Amsterdam: North-Holland)
- Milošević I and Damnjanović M 1992 *Preprint FPBU 01/92*
- 1993 *Phys. Rev. B* **47** 7805–18
- Wigner E P 1959 *Group Theory and its Applications to the Quantum Mechanics of Atomic Spectra* (New York: Academic)