Group Theory

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Introduction

The theory of groups can be developed as an entity independent of its applications as it avoids confusion concerning what is proper to group theory itself and what is special to its applications. The mixture of theory and applications tends, in many cases, to obscure the boundary between them. From this viewpoint, perhaps the most important aspect of group-theoretical applications to physics or chemistry is to consistently disentangle the various concepts. The three major issues are the algebraic structure of the group in question, its corresponding representation theory usually referring to the field of complex numbers $\mathbb{C}$ (as commonly accepted in the quantum theory) and finally, what is essential to the actual physical application.

Properties of Groups

Although some basic knowledge of the group theory is assumed, basic properties are repeated here, thereby also establishing notation and conventions. Let $G = \{e, g, g', g'', \ldots\}$ be a group which is assumed to be finite (e.g., point groups), countable infinite (e.g., crystallographic space groups), or compact continuous (e.g., the three-dimensional proper rotation group $SO(3, \mathbb{R})$ whose corresponding universal covering group $SU(2)$ plays a fundamental role for the spin degree of freedom). Recall that a group G is defined by a set of elements endowed with a certain algebraic structure. Its composition law

$$gg' = g'' \qquad [1]$$

must satisfy the associative law for ordered triplet $g, g', g'' \in G$ of group elements. Likewise, the existence of the unit element and uniquely defined inverses for each $g \in G$ must be guaranteed. Group–subgroup relations of the type $H \subset G$ imply that the group H forms a subset of G, which itself satisfies the group properties and hence is called a subgroup of the group G. A subgroup $N \subset G$ is called a normal subgroup if the conjugation

$$gNg^{-1} = N \qquad [2]$$

maps the subgroup N onto itself for all $g \in G$. Normal subgroups play a fundamental role not only when dealing with images of groups but also when studying features, such as faithfulness, of group representations.

The order of a group, which, loosely speaking, is equal to the number of its elements, is usually denoted by the symbol $|G|$. This symbol implies, for finite groups, the number of its elements, in the case of countable abelian groups, the group volume of their dual groups, and in the case of compact continuous groups, their group volume where the latter are endowed with appropriate Haar measures.

Specific relationships between different groups can be established by means of mappings of the type $\varphi : G \to H$, where G and H are two groups and $\varphi(G) = H$ defines the mapping in detail. Once the mappings satisfy the composition law of the image group H,

$$\varphi(g)\varphi(g') = \varphi(g'') \qquad [3]$$

then such mappings are called homomorphisms, and the associated kernel, denoted by $\ker_{\varphi(G)}$, defines a nontrivial normal subgroup of the pre-image group G. In mathematical terms,

$$\ker_{\varphi(G)} = \{g \in G \mid \varphi(g) = e \in H\} \lhd G \qquad [4]$$

$$G/\ker_{\varphi(G)} \sim H \qquad [5]$$

where the entry $G/\ker_{\varphi(G)}$ denotes the factor group and the special symbol $\lhd$ emphasizes that the subgroup $\ker_{\varphi(G)}$ must form a normal subgroup of the group G. A homomorphism is said to be an isomorphism if and only if the $\ker_{\varphi(G)}$ is trivial, that is, it consists of the identity element of G only. The mapping $\varphi : G \to H$ is called automorphism if and only if the group G is mapped onto itself. For more details on algebraic properties of groups and more advanced concepts, such as extensions of groups, the reader is referred to the "Further reading" section.

Properties of Representations

Every homomorphism $\varphi : G \to T(G)$ of a given group G into a group of nonsingular transformations $T(G) = \{T(g) \mid g \in G\}$ that map an underlying linear n-dimensional vector space $V_{\mathbb{K}}^{n}$ over the field $\mathbb{K}$ onto itself is called a representation of the group G if and only if the corresponding homomorphism property

$$T(g)T(g') = T(gg') = T(g'') \qquad [6]$$

is satisified for all group elements $g, g' \in G$. Such a general representation is called a linear representation of the group G if and only if the linearity condition is satisfied. To be strict, one assumes that

$$T(g)(av + bw) = aT(g)v + bT(g)w \qquad [7]$$

for all vectors $v, w \in V_{\mathbb{K}}^n$ and all $a, b \in \mathbb{K}$. In many applications, especially in quantum mechanics, one assumes $\mathbb{K} = \mathbb{C}$, sometimes one restricts $\mathbb{K} = \mathbb{R}$, whereas for some applications in crystallography, one even restricts $\mathbb{K} = \mathbb{Z}$, where the symbol $\mathbb{Z}$ denotes the ring of integers. For instance, one is inevitably led to the ring of integers when discussing the automorphisms of Bravais lattices. The restriction to the elements of the full rotation group $O(3, \mathbb{R}) = SO(3, \mathbb{R}) \times \mathscr{C}_2$, where the symbol $\mathscr{C}_2 = \{E, J\}$ denotes that the inversion group does not influence the statement. It merely restricts the elements of $GL(3, \mathbb{Z})$ to the elements of point groups $\mathscr{P}(T_{\text{Bravais}})$, which are finite subgroups of $O(3, \mathbb{R})$.

Matrix Representations

Every homomorphism $\vartheta : G \to D(G)$ of a given group G into a group of nonsingular matrices represented by $D(G) = \{D(g) \mid g \in G\}$, which are assumed to be finite-dimensional, is called a matrix representation of the group G if and only if the corresponding homomorphism property

$$D(g)D(g') = D(gg') = D(g'') \qquad [8]$$

is satisfied for all group elements $g, g' \in G$. Every matrix representation $\vartheta(G) = D(G)$ of the group G is called faithful if $\ker_{\varphi(G)}$ of the homomorphism is trivial. Every matrix representation of any group G is called unitary if and only if

$$D(g)^{-1} = D(g)^{\dagger} \qquad [9]$$

for all group elements $g \in G$. In the case of finite, countable, or compact continuous groups, it is assumed that every nonsingular matrix representation can be transformed by means of suitable intertwining matrices into unitary ones, if $\mathbb{K} = \mathbb{C}$ is assumed. However, this statement does not make sense if, for instance, $\mathbb{K} = \mathbb{Z}$, the ring of integers, is chosen. In this context, it should be noted that matrix groups are entities in their own right, which need not have any carrier space in order to be able to define them.

Unitary Operator Representations

A homomorphism $\varepsilon : G \to U(G)$ of a given group G into a group of unitary operators, represented by $U(G) = \{U(g) \mid g \in G\}$, that maps an underlying Hilbert space $\mathscr{H}$ over the field $\mathbb{C}$ onto itself is called a unitary operator representation of the group G if and only if the corresponding homomorphism property

$$U(g)U(g') = U(gg') = U(g'') \qquad [10]$$

$$\langle \phi, \psi \rangle_{\mathscr{H}} = \langle U(g)\phi, U(g)\psi \rangle_{\mathscr{H}} \qquad [11]$$

is satisfied for all group elements $g, g' \in G$, together with $U(g^{-1}) = U(g)^{\dagger}$ for all $g \in G$. Here the symbol $\langle ., . \rangle_{\mathscr{H}}$ denotes the scalar product of the $\mathscr{H}$. The most prominent application of this concept concerns the quantum mechanical problems, where the symmetry operations of any Hamiltonian H have to be realized as unitary operators in order to conform to the fundamental rules of quantum mechanics, such as the invariance of the expectation values of operators with respect to unitary conjugation operations.

Unitary Irreducible Matrix Representations

The so-called unitary irreducible matrix representations play the most important role in the vast majority of group-theoretical applications. Hereafter, these representations are called unirreps. Their basic properties are

$$D^{\xi}(g)D^{\xi}(g') = D^{\xi}(gg') \qquad [12]$$

$$D^{\xi}(g^{-1}) = D^{\xi}(g)^{\dagger} \qquad [13]$$

$$\frac{1}{|G|} \sum_{g \in G} D^{\xi}_{ab}(g) D^{\lambda}_{rs}(g)^* = \frac{1}{n(\xi)} \delta_{\xi\lambda}\delta_{ar}\delta_{bs} \qquad [14]$$

$$\sum_{\xi \in \mathscr{A}(G)} \sum_{m,n=1}^{n(\xi)} D^{\xi}_{mn}(g) D^{\xi}_{mn}(g')^* = |G|\delta_{gg} \qquad [15]$$

where the following notations have been introduced and further conventions have been adopted. Let $D^{\xi}(G) = \{D^{\xi}(g) \mid g \in G\}$ denote an $n(\xi)$-dimensional G unirrep. Moreover, [12] represents the composition law, [13] represents the unitarity condition, [14] illustrates the orthogonality relations, and [15] the completeness relations of G unirreps. Finally, the symbol $\mathscr{A}(G) = \{\xi, \lambda, \ldots\}$ denotes the set of G irrep labels, whilst the subscripts a, b, and likewise r, s, or eventually m, n label the rows and columns of the corresponding G unirreps.

Schur's lemma *Let G be a group and $D^{\alpha}(G)$ with $D^{\beta}(G)$ two given G unirreps. Moreover, let S be a matrix such that*

$$D^{\alpha}(g)S = SD^{\beta}(g) \qquad [16]$$

holds true for all group elements $g \in G$. Now, by applying the orthogonality relations [14] of the G unirreps and assuming that equivalent G unirreps are chosen to be, by definition, always identical, one arrives at the following well-known result:

$$S = \begin{cases} O_{\alpha,\beta} & \text{for } \alpha \nsim \beta \\ \delta 1_{\alpha,\alpha} & \text{for } \alpha = \beta \end{cases} \qquad [17]$$

where, in particular, the notation $\alpha \sim \beta$ signifies inequivalent G unirreps and alternatively $\alpha = \beta$ equivalent G unirreps, respectively.

Here the entry $O_{\alpha,\beta}$ denotes the rectangular $n(\alpha) \times n(\beta)$ null matrix, and the entity $1_{\alpha,\alpha}$ the square $n(\alpha) \times n(\alpha)$ unit matrix. Here, only the factor $\delta \in \mathbb{C}$ can be chosen arbitrarily. Schur's lemma, as a special case of the so-called Wigner–Eckart theorem, is one of the most frequently used group-theoretical tools in quantum mechanical applications.

Reducible Representations

Let $D(G) = \{D(g) \mid g \in G\}$ be an n-dimensional matrix representation of the group G. This implies that the composition law [8] is satisfied. Every unitary similarity transformation of the G matrix representation, $D(G)$, defined by some n-dimensional unitary matrix $W \in U(n)$ leads to an equivalent matrix representation of the group G:

$$F(g) = WD(g)W^{\dagger} \qquad [18]$$

$$F(g)F(g') = F(gg') \qquad [19]$$

What is common to these equivalent matrix representations $D(G) \sim F(G) \sim \cdots$ are the so-called characters of the corresponding equivalent matrix representations, which by construction are identical:

$$\chi(g) = \operatorname{tr} D(g) = \operatorname{tr} F(g) = \cdots \qquad [20]$$

Accordingly, every set of characters $\{\chi(g) \mid g \in G\}$ is an invariant and loosely speaking, the unique fingerprint of the G matrix representations. Sets of characters, say $\{\chi(g) \mid g \in G\}$ and $\{\tilde{\chi}(g) \mid g \in G\}$ of any given group G are either identical (and, hence, the corresponding matrix representations are equivalent), or different (and the corresponding matrix representations are inequivalent). Thus, this provides an important and simple tool to distinguish matrix representations of any given group G uniquely. Apart from this, one may write

$$\operatorname{tr} D^{\xi}(g) = \chi^{\xi}(g) \qquad [21]$$

$$\frac{1}{|G|} \sum_{g \in G} \chi^{\xi}(g)\chi^{\lambda}(g)^{*} = \delta_{\xi\lambda} \qquad [22]$$

which represent the orthogonality relations of the so-called simple characters that are uniquely assigned to the corresponding G unirreps. These follow immediately from the orthogonality relations [14] by simply carrying out the trace operation for the G unirreps.

A G matrix representation $D(G)$ is called reducible if and only if this matrix representation can be decomposed by means of suitable unitary similarity matrices into a direct sum of small dimensional G matrix representations. Conversely, a G matrix representation $D(G)$ is called irreducible if this matrix representation cannot be decomposed into a direct sum of smaller-dimensional G matrix representations. Note, in passing, that due to the restriction to consider merely finite, countable, and compact continuous Lie groups, one need not distinguish between reducible and completely reducible G matrix representations, since reducibility implies complete reducibility provided that the field $\mathbb{K} = \mathbb{C}$ coincides with the field of complex numbers.

Irreducibility criterion Let $D(G)$ be an m-dimensional G matrix representation. Its corresponding set of characters $\{\chi(g) \mid g \in G\}$, where $\operatorname{tr} D(g) = \chi(g)$ is assumed, has to satisfy

$$\frac{1}{|G|} \sum_{g \in G} |\chi(g)|^2 = \begin{cases} 1, & D(G) \text{ is irreducible} \\ M > 1, & D(G) \text{ is reducible} \end{cases} \qquad [23]$$

where the integer $M > 1$ is uniquely defined by the G matrix representation in question. This criterion is simply applicable and widely used in many practical applications of group-theoretical methods.

Decomposition of reducible matrix representations The decomposition of a reducible m-dimensional G matrix representation $D^{\text{red}}(G)$ into a direct sum of its irreducible constituents is a significant problem. The consistent sequence of the corresponding decomposition formulas may be summarized as follows:

$$D^{\text{red}}(g) = \sum_{\xi \in \mathscr{A}(G)} \oplus m(\text{red}|\xi) D^{\xi}(g) \qquad [24]$$

$$m(\text{red} \mid \xi) = \frac{1}{|G|} \sum_{g \in G} \chi^{\text{red}}(g)\chi^{\xi}(g)^{*} \qquad [25]$$

$$\frac{1}{|G|} \sum_{g \in G} |\chi(g)|^2 = \sum_{\xi \in \mathscr{A}(G)} m(\text{red}|\xi) n(\xi) = M \in \mathbb{Z}^{+} \qquad [26]$$

$$W^{\dagger} D^{\text{red}}(g) W = \sum_{\xi \in \mathscr{A}(G)} \oplus m(\text{red}|\xi) D^{\xi}(g) \qquad [27]$$

$$\{W\}_{j;\xi wa} = W_{j;\xi wa} = \{W_a^{\xi w}\}_j \qquad [28]$$

$$D^{\text{red}}(g) W_a^{\xi w} = \sum_{b=1}^{n(\xi)} D_{ba}^{\xi}(g) W_b^{\xi w} \qquad [29]$$

Several remarks should be made on this set of formulas. First, it should be noted that the unitary m-dimensional similarity matrix W is nonsymmetrically indexed. The row index of W is given by $j = 1, 2, \ldots, m$, whereas its column index is fixed by the ordered triplets (ξ, w, a), where the G irrep label $\xi \in \mathscr{A}(G)$ together with the so-called multiplicity index $w = 1, 2, \ldots, m(\text{red}|\xi)$, and finally the row index $a = 1, 2, \ldots, n(\xi)$, of the G unirrep $D^{\xi}(G)$ have to be taken into account. This nonsymmetrical indexing is common to all types of similarity matrices, for instance, subduction matrices, or Clebsch–Gordan matrices as a special case of subduction matrices. Second, it should be realized that the columns $\{W_a^{\xi w}\}$ of any similarity matrix may be regarded as symmetry adapted vectors, since the transformation formulas [29] represent the prototype of symmetrized states. The basic features of symmetrized states are that they are mutually orthonormal and they transform according to G unirreps. The computation of similarity matrices can be done by applying the so-called projection method, which is briefly discussed later, since the transformation formulas [29] suggest this method. Finally, it should be noted that due to Schur's lemma the similarity matrices W cannot be unique and, hence, have to be fixed by adopting appropriate conventions. The structure of unitary similarity matrices describing this ambiguity can be simply deduced by the following statement.

Schur's lemma applied to reducible representations Let G be a group and $\Phi \in \mathrm{GL}(m, \mathbb{C})$ an m-dimensional nonsingular but otherwise arbitrary matrix. Moreover, let $D^{\text{red}\oplus}(G)$, which symbolizes the RHS of [27], be an m-dimensional reducible unitary G matrix representation that is already decomposed into a direct sum of its irreducible constituents. Assume that

$$[\Phi, D^{\text{red}\oplus}(g)] = O \qquad [30]$$

for all group elements $g \in G$. By applying Schur's Lemma to this general situation, one immediately arrives at the following result:

$$\Phi = \sum_{\xi \in \mathscr{A}(G)} \oplus (1_{\alpha,\alpha} \otimes \Phi^{\xi}(m(\text{red}|\xi))) \qquad [31]$$

where the submatrices $\Phi^{\xi}(m(\text{red}|\xi)) \in \mathrm{GL}(m\,(\text{red}|\xi), \mathbb{C})$ are otherwise arbitrary. Of course, if $\Phi \in U(m)$, then $\Phi^{\xi}(m(\text{red}|\xi)) \in U(m(\text{red}|\xi), \mathbb{C})$ must be satisfied. The latter condition reflects the ambiguity of similarity matrices, since W and its counterpart $W\Phi$ are equally well suited to describe identically the decomposition [27], where the phase matrices of the type [31] can be chosen arbitrarily.

The second type of ambiguities emerges from the nonuniqueness of each G unirrep whose dimension is greater than 1. Since every similarity transformation of the type

$$F^{\xi}(g) = W^{\xi\dagger} D^{\xi}(g) W^{\xi} \qquad [32]$$

by means of an arbitray unitary matrix $W^{\xi} \in U(n(\xi))$, yields equivalent G unirreps, they are equally well suited to be used in any application. One then arrives at the following formulas:

$$\bar{W}^{\dagger} D^{\text{red}}(g) \bar{W} = \sum_{\xi \in \mathscr{A}(G)} \oplus m(\text{red} \mid \xi) F^{\xi}(g) \qquad [33]$$

$$\bar{W} = W\Psi \qquad [34]$$

$$\Psi = \sum_{\xi \in \mathscr{A}(G)} \oplus (1_{\alpha,\alpha} \otimes \Phi^{\xi}(m(\text{red}|\xi))) \qquad [35]$$

where, for the sake of brevity, $m(\text{red} \mid \xi) = m(\alpha)$ has been employed; for $m(\alpha) = 0$, the corresponding terms vanish. The combination of both types of ambiguities, namely the occurrence of phase matrices due to Schur's lemma and the transfer to equivalent G unirreps, have led to many unnecessary controversies in the literature. Accordingly, it is generally advised that when comparing results emerging from different sources, one should check whether the intertwining matrices W can be identified by means of phase matrices of the type [31]. If this fails, then the results of at least one source are wrong.

Subduced Representations

Let $H \subset G$ be a given group–subgroup relation, where, for the sake of simplicity, the index $s \in \mathbb{Z}^+$ of the subgroup G in the supergroup G is assumed to be finite. Note that in the case of group–subgroup relations between space groups and sectional layer or penetration rod groups, which are briefly discussed later, this simplifying constraint would be violated. To unify the discussion, let formally

$$G = \sum_{j=1}^{s} \underline{a_j} H \qquad [36]$$

be the left coset decomposition of the group G with respect to the subgroup H, where, for the sake of distinction, coset representatives $\underline{a_j} \in G$ are underlined. Cosets $\underline{a_j} H$ are unique, whereas coset representatives $\underline{a_j} \in G$ are never unique unless the subgroup is trivial.

By definition, the restriction of any given G matrix representation, say $D(G) = \{D(g) \mid g \in G\}$, to the elements of the subgroup H is called subduced matrix representation. Symbolically,

$$D(G) \downarrow H = \{D(h) \mid h \in H\} \qquad [37]$$

which means that only the elements of the subgroup $h \in H$ have to be taken into account. Of course, if $D(G) = D^{\xi}(G)$ forms a G unirrep, then the subduced matrix representation $D^{\xi}(G)\downarrow H$ will in general be reducible. Hence, if a complete set of H unirreps, say $\{L^{\lambda}(H) \mid \lambda \in \mathscr{A}(H)\}$, are known, the corresponding decomposition of the H matrix representations $D^{\xi}(G)\downarrow H$ can be carried out along the lines discussed previously:

$$D^{\xi}(g)\downarrow H \sim \sum_{\lambda \in \mathscr{A}(H)} \oplus m(\xi|\lambda) L^{\lambda}(h) \qquad [38]$$

$$m(\xi|\lambda) = \frac{1}{|H|} \sum_{h \in H} \chi^{\xi}(h)\chi^{\lambda}(h)^{*} \qquad [39]$$

$$W^{\xi\dagger} D^{\xi}(h) W^{\xi} = \sum_{\lambda \in \mathscr{A}(H)} \oplus m(\xi|\lambda) L^{\lambda}(h) \qquad [40]$$

The generalization of these decomposition formulas to the more general situation of reducible G matrix representations subduced to H matrix representations, say $D(G)\downarrow H$, can be readily deduced from formulas [38], [39], and [40].

Clebsch–Gordan Coefficients

The problem of computing for any group G with a fixed complete set of G unirreps, say $\{D^{\xi}(G) \mid \xi \in \mathscr{A}(G)\}$, corresponding Clebsch–Gordan matrices may be viewed as a special case of constructing, for subduced matrix representations, suitable similarity matrices that transform the subduced representation into a direct sum of its subgroup constituents.

General outer direct-product groups General outer direct-product groups are groups of the type $G_1 \otimes G_2$ where the given groups G_1 and G_2 are assumed not to be isomorphic. Its group elements are, by definition, the ordered pairs (g_1, g_2), where $g_1 \in G_1$ and $g_2 \in G_2$ are chosen independently. In mathematical terms,

$$G_1 \otimes G_2 = \{(g_1, g_2) \mid g_1 \in G_1;\ g_2 \in G_2\} \qquad [41]$$

$$(g_1, g_2) * (g_1', g_2') = (g_1 g_1', g_2 g_2') \qquad [42]$$

where its composition law, given by [42], is an immediate consequence of the definition of the outer direct-product set. Moreover, the order $|G_1 \otimes G_2|$ of the outer direct-product group $G_1 \otimes G_2$ is given by the product of the orders $|G_1|$ and $|G_2|$ of the respective groups G_1 and G_2.

Special outer direct-product groups Let G be a group and the specific construction

$$G \otimes G = \{(g, g') \mid g, g' \in G)\} = G^2 \qquad [43]$$

its corresponding outer direct-product group, whose group elements are again the ordered pairs (g, g'), where, analogously to the general situation, the group elements $g, g' \in G$ are to be chosen independently. Its composition law is again given by the rule

$$(g, g') * (\tilde{g}, \tilde{g}') = (g\tilde{g}, g'\tilde{g}') \qquad [44]$$

and shows, amongst others, that for the order of the outer direct-product group, $|G \otimes G| = |G|^2$ must be valid. Obviously, the subset

$$G \boxtimes G = \{(g, g) \mid g \in G\} = G^{[2]} \sim G \qquad [45]$$

must form a subgroup of the outer direct-product group $G \otimes G$ which is isomorphic to the original group G. It is common to denote the special group $G \boxtimes G$ as a twofold Kronecker product group. The generalization to n-fold outer direct-product groups G^n and n-fold Kronecker product groups $G^{[n]}$ is immediate.

Unirreps of special outer direct-product groups The G^2 unirreps of the special outer direct-product group $G \otimes G = G^2$ are simply obtained by the construction of ordered pairs of direct matrix products of G unirreps, say $D^{\xi}(G)$ and $D^{\eta}(G)$, where $\xi, \eta \in \mathscr{A}(G)$. Accordingly, one can summarize that

$$D^{\xi\otimes\eta}(g, g') = D^{\xi}(g) \otimes D^{\eta}(g') \qquad [46]$$

$$(\xi \otimes \eta) \in \mathscr{A}(G^2) \qquad [47]$$

$$\dim D^{\xi\otimes\eta}(g, g') = n(\xi)n(\eta) \qquad [48]$$

for all $(g, g') \in G^2$, where especially the elements $(\xi, \eta) = (\xi \otimes \eta)$ of the index set $\mathscr{A}(G^2)$ of the outer direct-product group G^2 are denoted by the symbols $(\xi \otimes \eta)$ to emphasize the outer direct-product group structure. Now, if one restricts G^2 to its Kronecker product subgroup $G^{[2]}$,

$$\begin{aligned} D^{\xi\otimes\eta}(G^2)\downarrow G^{[2]} &= D^{\xi,\eta}(G) \\ &= \{D^{\xi,\eta}(g) = D^{\xi}(g) \otimes D^{\eta}(g) \mid g \in G\} \end{aligned} \qquad [49]$$

then one arrives at $n(\xi)n(\eta)$-dimensional G matrix representations, which in general are reducible.

Clebsch–Gordan matrices By definition, the corresponding similarity matrices are nothing but the unitary Clebsch–Gordan matrices whose matrix elements are the Clebsch–Gordan coefficients. In mathematical terms

$$D^{\xi,\eta}(g) \sim \sum_{\zeta\in\mathscr{A}(G)} \oplus m(\xi,\eta|\zeta) D^{\zeta}(g) \qquad [50]$$

$$m(\xi,\eta\mid\zeta) = \frac{1}{|G|}\sum_{g\in G} \chi^{\xi}(g)\chi^{\eta}(g)\chi^{\zeta}(g)^{*} \qquad [51]$$

$$C^{\xi,\eta\dagger} D^{\xi,\eta}(g) C^{\xi,\eta} = \sum_{\zeta\in\mathscr{A}(G)} \oplus m(\xi,\eta|\zeta) D^{\zeta}(g) \qquad [52]$$

$$\{C^{\xi,\eta}\}_{jk;\zeta wa} = C^{\xi,\eta}_{jk;\zeta wa} = \left(\begin{array}{cc|c} \xi & \eta & \zeta w \\ j & k & a \end{array}\right) \qquad [53]$$

where, as already pointed out, the corresponding Clebsch–Gordan coefficients $C^{\xi,\eta}_{jk;\zeta wa}$ are nonsymmetrically indexed. The row index of Clebsch–Gordan matrices $C^{\xi,\eta}$ are given by the ordered pairs (j,k), where $j = 1,2,\ldots,n(\xi)$ and $k = 1,2,\ldots,n(\eta)$, whereas their column indices are fixed by the ordered triplets (ζ,w,a), where the G irrep label $\zeta\in\mathscr{A}(G)$ together with the so-called multiplicity index $w = 1,2,\ldots,m(\xi,\eta|\zeta)$, and finally the row index $a = 1,2,\ldots,n(\zeta)$ of the relevant G unirreps $D^{\zeta}(G)$ have to be taken into account. The round bracket symbol occurring on the RHS of [53] is frequently used to symbolize Clebsch–Gordan coefficients but many other types of symbols may appear in applications.

Needless to repeat that Clebsch–Gordan matrices are not unique, which is not only due to Schur's lemma but also to their representation dependence. Apart from this, it is worth stressing the possible appearance of the so-called multiplicity index w in the case of twofold Kronecker product decompositions. In fact, the appearance of the multiplicity index w depends on the structure of the group G in question. A group G is called simple reducible if and only if the multiplicities $m(\xi,\eta|\zeta)$ occurring in the so-called Clebsch–Gordan series [52] are at most 1. Accordingly, a group G is called simple reducible if and only if

$$0 \leqslant m(\xi,\eta|\zeta) \leqslant 1 \qquad [54]$$

is satisfied for all G irrep labels $\xi,\eta,\zeta\in\mathscr{A}(G)$. Groups of this type are, for instance, SU(2) or its homomorphic image SO(3,$\mathbb{R}$), and certainly abelian groups, whereas in particular three-dimensional crystallographic space groups $\mathscr{G}$ are nonsimple reducible. This has as an important consequence that an additional ambiguity arises in the computation of Clebsch–Gordan coefficients and their potential applications.

Induced Representations

By definition, induced matrix representations are obtained by assuming a given group–subgroup relation, say $H\subset G$ with [36] as its left coset decomposition, and extending by means of the so-called induction procedure a given H matrix representation $D(H)$ to an induced G matrix representation $D^{\uparrow G}(G)$. To be more strict, induced G matrix representations are defined by the following expressions:

$$D^{\uparrow G}_{\underset{\sim}{a},\underset{\sim}{b}}(g) = \delta_{\underset{\sim}{a}H,g\underset{\sim}{b}H} D(\underset{\sim}{a}^{-1}g\underset{\sim}{b}) \qquad [55]$$

$$\delta_{\underset{\sim}{a}H,g\underset{\sim}{b}H} = \left\{\begin{array}{ll} 1, & \underset{\sim}{a}^{-1}g\underset{\sim}{b}\in H \\ 0, & \text{otherwise} \end{array}\right\} \qquad [56]$$

$$\dim D^{\uparrow G}(G) = |G:H| \dim D(H) \qquad [57]$$

where, in part, a matrix representation has been employed and the notation $|G:H| = s$ has been introduced to stress the fact that the dimensions of the induced G matrix representations increase by the index of H in G. Moreover, if $D(H)$ defines a reducible H matrix representation, then the corresponding induced G matrix representation $D^{\uparrow G}(G)$ must be reducible in any case. Conversely, if $D(H) = D^{\lambda}(H)$ defines an H unirrep, then the corresponding induced G matrix representation $D^{\lambda\uparrow G}(G)$ still need not necessarily be a G unirrep. On the contrary, induced G matrix representations of the type $D^{\lambda\uparrow G}(G)$ are in general reducible and may be decomposed into direct sums of G unirreps in the same manner as before. The corresponding decomposition formulas read

$$D^{\lambda\uparrow G}(g) \sim \sum_{\zeta\in\mathscr{A}(G)} m(\lambda\uparrow G|\zeta) D^{\zeta}(g) \qquad [58]$$

$$m(\lambda\uparrow G|\zeta) = \frac{1}{|G|}\sum_{g\in G} \chi^{\lambda\uparrow G}(g)\chi^{\zeta}(g)^{*} \qquad [59]$$

$$m(\lambda\uparrow G|\zeta) = m(\zeta\downarrow H|\lambda) \qquad [60]$$

$$S^{\lambda\uparrow G\dagger} D^{\lambda\uparrow G}(g) S^{\lambda\uparrow G} = \sum_{\zeta\in\mathscr{A}(G)} m(\lambda\uparrow G|\zeta) D^{\zeta}(g) \qquad [61]$$

$$\{S^{\lambda\uparrow G}\}_{\underset{\sim}{a}k;\zeta wa} = S^{\lambda\uparrow G}_{\underset{\sim}{a}k;\zeta wa} \qquad [62]$$

where the matrix elements $S^{\lambda\uparrow G}_{\underset{\sim}{a}k;\zeta wa}$ of the subduction matrices $S^{\lambda\uparrow G}$ are nonsymmetrically indexed. The row indices of $S^{\lambda\uparrow G}$ are given by the ordered pairs $(\underset{\sim}{a},k)$ where $\underset{\sim}{a}\in G:H$ and $k = 1,2,\ldots,n(\lambda)$, whereas their column indices are fixed by the ordered triplets (ζ,w,a), where the G irrep label $\zeta\in\mathscr{A}(G)$ together with the so-called multiplicity index

$w = 1, 2, \ldots, m(\lambda \uparrow G|\zeta)$, and finally the row index $a = 1, 2, \ldots, n(\zeta)$ of the relevant G unirreps $D^{\zeta}(G)$ have to be taken into account. Finally, the relations [60] describe the Frobenius reciprocity law, which, for instance, is extensively discussed in several textbooks.

Group-Theoretical Methods in Physics

Up to now, exclusively group-theoretical aspects, such as their algebraic structure and associated properties, and representation-theoretic aspects with special emphasis on the decomposition of reducible representations into direct sums of their irreducible constituents have been dealt with. This section discusses how group-theoretical methods can be applied in physical applications. The physical applications cover a wide range of, not only quantum mechanics but also classical applications (e.g., classical mechanics or hydrodynamics are possible candidates for these methods). Here the discussions are confined to standard applications in quantum mechanics.

Symmetry Groups of Hamiltonians

The first task is to construct a unitary operator representation of a given group, say G, with respect to the Hilbert space $\mathscr{H}$, which is the carrier space for the considered Hamiltonian H in question. Accordingly, it is assumed that there exits a homomorphism $\varepsilon : G \rightarrow U(G)$ of the given group G into a group of unitary operators which are represented by $U(G) = \{U(g) \mid g \in G\}$ that map the underlying Hilbert space $\mathscr{H}$ over the field $\mathbb{C}$ onto itself.

The group G being represented by the corresponding unitary operator group $U(G) = \{U(g) \mid g \in G\}$ is called a symmetry group of the Hamiltonian H if and only if the Hamiltonian commutes with all unitary operators:

$$[H, U(g)] = O \quad \forall g \in G \tag{63}$$

Moreover, assume that the eigenvalue problem for the Hamiltonian H has been solved, which implies that not only the corresponding eigenvalues, denoted by $\lambda \in \mathbb{R}$, but also suitably orthonormalized eigenstates $\{\Phi_j^{\lambda} \mid j = 1, 2, \ldots, \deg \lambda\}$ for each eigenvalue are known. The existence of a symmetry group G of the Hamiltonian H implies

$$H\Phi_j^{\lambda} = \lambda \Phi_j^{\lambda}$$
$$\Leftrightarrow H(U(g)\Phi_j^{\lambda}) = \lambda (U(g)\Phi_j^{\lambda}) \tag{64}$$

that the corresponding eigenspaces $\mathscr{H}^{\lambda} \subset \mathscr{H}$, which are uniquely associated with the eigenvalues $\lambda \in \mathbb{R}$ the Hamiltonian H, have to be G-invariant subspaces of the original Hilbert space $\mathscr{H}$. Clearly, the "bigger" and the "more noncommutative" the symmetry group G, the more useful the symmetry group G. Once the so-called symmetry adapted states, which are discussed below, are known, the application of Schur's lemma leads at least to a partial solution of the eigenvalue problem. Obviously, if every G-invariant subspace $\mathscr{H}^{\lambda}$ turns out to be irreducible, then the eigenvalue problem for H is completely solved, and the degeneracy of the eigenvalues is sometimes said to be generic with respect to the group G. Conversely, if some of the subspaces $\mathscr{H}^{\lambda}$ are reducible, then the degeneracy of the corresponding eigenvalues is sometimes said to be nongeneric with respect to the group G.

Symmetrization of States

One of the most popular group-theoretical applications in quantum mechanics consists of symmetry, adapting given sets of states, say $\{\Phi\} = \{\Phi_1, \Phi_2, \ldots, \Phi_n\}$. In mathematical terms, it implies that, out of the given set of states $\{\Phi\}$, some new sets of states be constructed systematically whose elements transform according to given G unirreps and are mutually orthonormal. Such bases are usually called G-symmetrized states or simply symmetry-adapted states. The standard method to achieve the symmetry adaptation of states is the so-called projection method. The set of operators

$$\{E_{jk}^{\xi}\} = \{E_{jk}^{\xi} \mid \xi \in \mathscr{A}(G);\ j, k = 1, 2, \ldots, n(\xi)\} \tag{65}$$

$$E_{jk}^{\xi} = \frac{n(\xi)}{|G|} \sum_{g \in G} D_{jk}^{\xi}(g)^{*} U(g) \tag{66}$$

are the so-called units of the corresponding group algebra $\mathscr{A}(G)$ whose general elements are arbitrary linear combinations of the group elements. Clearly, if and only if G is finite, then $|\{E_{jk}^{\xi}\}| = |G|$, which, loosely speaking, remains valid if the group G is countable or even compact continuous but has to be refined correspondingly, since the group volumes of their dual groups have to be taken into account. In fact, this represents a topological subtlety. Apart from this, one has

$$\{E_{jk}^{\xi}\}^{\dagger} = E_{kj}^{\xi} \tag{67}$$

$$E_{jk}^{\xi} E_{mn}^{\eta} = \delta_{\xi\eta} \delta_{km} E_{jn}^{\xi} \tag{68}$$

$$U(g) E_{jk}^{\xi} = \sum_{\ell=1}^{n(\xi)} D_{\ell j}^{\xi}(g) E_{\ell k}^{\xi} \tag{69}$$

$$\sum_{\xi \in \mathscr{A}(G)} \sum_{k=1}^{n(\xi)} E_{kk}^{\xi} = 1_{\mathscr{H}} \tag{70}$$

where the extra symbol $1_{\mathscr{H}}$ denotes the unit operator of the underlying Hilbert space $\mathscr{H}$. It follows from [67] and [68] that the operators $\{E^{\xi}_{kk} \mid \xi \in \mathscr{A}(G);\ k = 1, 2, \ldots, n(\xi)\}$ are projection operators, whereas the remaining operators are shift operators that intertwine mutually orthogonal subspaces that belong to any given $\xi \in \mathscr{A}(G)$ but different $k = 1, 2, \ldots, n(\xi)$.

Step 1 First, one proves that the n-dimensional subspace which is the linear hull of the set of functions $\{\Phi_1, \Phi_2, \ldots, \Phi_n\}$ denoted by $\mathscr{H}_n$ is in fact a G-invariant subspace. For simplicity, assume that the set of functions $\{\Phi\}$ forms an orthonormal basis. Accordingly, $\langle \Phi_j, \Phi_k \rangle_{\mathscr{H}} = \delta_{jk}$ for all pairs Φ_j, Φ_k of basis functions. By virtue of the transformation law given by the expressions

$$U(g)\Phi_j = \sum_{k=1}^{n} D^{\Phi}_{kj}(g)\Phi_k \qquad [71]$$

$$D^{\Phi}(g) \sim \sum_{\xi \in \mathscr{A}(G)} m(D^{\Phi}(G)|\xi) D^{\xi}(g) \qquad [72]$$

$$\dim D^{\Phi}(G) = n = \sum_{\xi \in \mathscr{A}(G)} m(D^{\Phi}(G)|\xi) n(\xi) \qquad [73]$$

one defines an n-dimensional G matrix representation, which in general forms a reducible representation. Relation [73] presents the obvious dimension check to be carried out from the outset.

Step 2 Let $m(D^{\Phi}(G)|\xi) > 0$, then one knows that the corresponding subspaces constructed by means of the projection operators

$$\mathscr{H}^{\xi,k}_n = E^{\xi}_{kk} \mathscr{H}_n \qquad [74]$$

$$\dim \mathscr{H}^{\xi,k}_n = m(D^{\Phi}(G) \mid \xi) \qquad [75]$$

have the same dimension for each $k = 1, 2, \ldots, n(\xi)$, as otherwise the projection method would contain inconsistencies.

Step 3 Next, one constructs for the fixed G irrep label $\xi \in \mathscr{A}(G)$ (where $m(D^{\Phi}(G)|\xi) > 0$ is assumed) and for a fixed row index, say $k = k_0 = 1$, an orthonormalized basis of the $m(D^{\Phi}(G)|\xi)$-dimensional subspace $\mathscr{H}^{\xi,k_0}_n$ by applying the Gram–Schmidt orthonormalization procedure. Symbolically, as a result of the projection method,

$$E^{\xi}_{k_0k_0}\{\Phi\} \rightarrow \{\Psi^{\xi,w}_{k_0} \mid w = 1, 2, \ldots, m(D^{\Phi}(G)|\xi)\} \qquad [76]$$

$$\langle \Psi^{\xi,w}_{k_0}, \Psi^{\xi,v}_{k_0} \rangle_{\mathscr{H}} = \delta_{wv} \qquad [77]$$

Step 4 In order to obtain for the fixed G irrep label $\xi \in \mathscr{A}(G)$ (where $m(D^{\Phi}(G)|\xi) > 0$ is assumed) the remaining partner functions, one has to employ the corresponding shift operators:

$$\Psi^{\xi,w}_j = E^{\xi}_{jk_0} \Psi^{\xi,w}_{k_0}, \quad j = 1, 2, \ldots, n(\xi) \qquad [78]$$

$$\langle \Psi^{\xi,w}_j, \Psi^{\xi,v}_{\ell} \rangle_{\mathscr{H}} = \delta_{wv}\delta_{j\ell} \qquad [79]$$

$$U(g)\Psi^{\xi,w}_j = \sum_{\ell=1}^{n(\xi)} D^{\xi}_{\ell j}(g) \Psi^{\xi,w}_{\ell} \qquad [80]$$

Step 5 Finally, in order to obtain a complete basis of the n-dimensional G-invariant subspace $\mathscr{H}_n$ that consists of G-symmetrized states which are mutually orthonormal and which satisfy the transformation law [80], one has to repeat the steps described previously for all G irrep labels $\xi \in \mathscr{A}(G)$, where the corresponding multiplicities $m(D^{\Phi}(G)|\xi)$ are different from zero.

Coupling of Product States

Another important application of group-theoretical methods in quantum mechanics concerns the coupling of states, where the constituents are assumed to transform according to G unirreps, and where the coupled product states likewise should possess specific transformation properties. Let $\Psi^{\xi}_j \in \mathscr{H}_1$ and, equivalently, $\Phi^{\eta}_k \in \mathscr{H}_2$ be two sets of G-symmetrized states, where states of the type

$$\Lambda^{\xi \otimes \eta}_{jk} = \Psi^{\xi}_j \otimes \Phi^{\eta}_k \in \mathscr{H}_1 \otimes \mathscr{H}_2 \qquad [81]$$

should be transformed into such linear combinations, so that the new states transform according to G unirreps of the twofold Kronecker product group $G^{[2]}$ which is isomorphic to G. Starting from the transformation law

$$U(g, g')\Lambda^{\xi\otimes\eta}_{jk} = \sum_{j'=1}^{n(\xi)} \sum_{k'=1}^{n(\eta)} \{D^{\xi\otimes\eta}(g)\}_{j'k',jk} \Lambda^{\xi\otimes\eta}_{j'k'} \qquad [82]$$

which refers to the special outer direct-product group $G \otimes G$, one readily infers that the product states [81] transform according to G^2 unirreps. The aim is to find such linear combinations of the states [81] such that they transform according to G unirreps. The desired transformation coefficients are just the all such cases, one need not compute the corresponding reduced matrix elements. Not surprisingly, this is an important statement when investigating selection rules, such as the Stark effect for the spectral properties of the hydrogen atom, or when dealing with electron–phonon interactions in solids. However, if the respective Clebsch–Gordan coefficients are nonzero, then one has to compute the corresponding reduced matrix elements, but which might be much more complicated than to simply compute directly the original matrix elements.

See also: Group Theory in Materials Science, Applications; Magnetic Point Groups and Space Groups.

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Further Reading

Altmann SL (1977) *Induced Representations in Crystals and Molecules: Point, Space, and Non-rigid Molecule Groups*. London: Academic Press.

Bassani F and Pastori PG (1975) *Electronic States and Optical Transitions in Solids*. Oxford: Pergamon.

Bradley CJ and Cracknell AP (1972) *The Mathematical Theory of Symmetry in Solids*. Oxford: Clarendon.

Condon EU and Shortley GH (1935) *The Theory of Atomic Spectra*. Cambridge: Cambridge University Press.

Jansen L and Boon M (1976) *The Theory of Finite Groups. Applications to Physics*. Amsterdam: North-Holland.

Wigner EP (1959) *Group Theory and its Application to the Quantum Mechanics of Atomic Spectra*. New York: Academic.