

1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

according to the orthogonality relations. This means that the N functions indeed form an orthogonal basis in the space of all functions on the group. In particular, consider a function $f(K)$ that is constant on conjugacy classes. This function can be expanded in the basis functions.

$$\begin{aligned} f(R) &= \sum_{\alpha ij} f_{\alpha ij} \Gamma_{\alpha}(R)_{ij} \\ &= \sum_{\alpha ij} f_{\alpha ij} (1/N) \sum_{T \in K} \Gamma_{\alpha}(TRT^{-1})_{ij} \\ &= (1/N) \sum_{\alpha ijkl} f_{\alpha ij} \Gamma_{\alpha}(T)_{ik} \Gamma_{\alpha}(R)_{kl} \Gamma_{\alpha}(T^{-1})_{lj} \\ &= (1/N) \sum_{\alpha ijkl} f_{\alpha ij} \Gamma_{\alpha}(R)_{kl} (N/d_{\alpha}) \delta_{ij} \delta_{kl} \\ &= \sum_{\alpha} \sum_{i=1}^{d_{\alpha}} (f_{\alpha ii} / d_{\alpha}) \chi_{\alpha}(R). \end{aligned}$$

This implies that every class function can be written as a linear combination of the character functions. Therefore, the number of such character functions must be equal to or larger than the number of conjugacy classes. On the other hand, the number of dimensions of the space of class functions is k , the number of conjugacy classes. For the scalar product in this space given by

$$f_1 \cdot f_2 \equiv \sum_{i=1}^k (n_i/N) f_1^*(C_i) f_2(C_i)$$

the character functions are orthogonal:

$$\sum_{i=1}^k (n_i/N) \chi_{\alpha}^*(C_i) \chi_{\beta}(C_i) = (1/N) \sum_{R \in K} \chi_{\alpha}^*(R) \chi_{\beta}(R) = \delta_{\alpha\beta}. \quad (1.2.2.34)$$

There are at most k mutually orthogonal functions, and consequently the number of nonequivalent irreducible characters $\chi_{\alpha}(K)$ is exactly equal to the number of conjugacy classes.

As additional result one has the following proposition.

Proposition. The functions $\Gamma_{\alpha}(R)_{ij}$ with $\alpha = 1, 2, \dots, k$ and $i, j = 1, 2, \dots, d_{\alpha}$ form an orthogonal basis in the space of complex functions on the group K . The characters χ_{α} form an orthogonal basis for the space of all class functions.

The characters of a group K can be combined into a square matrix, the *character table*, with entries $\chi_{\alpha}(C_i)$. Besides the orthogonality relations mentioned above, there are also relations connected with *class multiplication constants*. Consider the conjugacy classes C_i of the group K . Formally one can introduce the sum of all elements of a class:

$$M_i = \sum_{R \in C_i} R.$$

It can be proven that the multiplication of two such class sums is the sum of class sums, where such a class sum may occur more than once:

$$M_i M_j = \sum_k c_{ijk} M_k, \quad c_{ijk} \in \mathbb{Z}.$$

The coefficients c_{ijk} are called the *class multiplication constants*. The elements of the character table then have the following properties.

$$(1/N) \sum_{i=1}^k n_i \chi_{\alpha}(C_i) \chi_{\beta}^*(C_i) = \delta_{\alpha\beta}; \quad (1.2.2.35)$$

$$(1/N) \sum_{\alpha=1}^k \chi_{\alpha}(C_i) \chi_{\alpha}^*(C_j) = (1/n_i) \delta_{ij}; \quad (1.2.2.36)$$

$$n_i \chi_{\alpha}(C_i) n_j \chi_{\alpha}(C_j) = d_{\alpha} \sum_{l=1}^k c_{ijl} n_l \chi_{\alpha}(C_l). \quad (1.2.2.37)$$

As an example, consider the permutation group on three letters S_3 . It consists of six permutations. It is a group that is isomorphic with the point group 32. The character table is a 3×3 array, because there are three conjugacy classes (C_i , $i = 1, 2, 3$), and consequently three irreducible representations (Γ_i , $i = 1, 2, 3$) (see Table 1.2.2.1).

The two one-dimensional representations are equal to their character. A representative representation for the third character is generated by matrices

$$\Gamma_3(A) = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}, \quad \Gamma_3(B) = \begin{pmatrix} 1 & -1 \\ 0 & -1 \end{pmatrix}$$

and the group of matrices is equivalent to an orthogonal group with generators

$$\Gamma_3(A)' = \begin{pmatrix} -\frac{1}{2} & \frac{1}{2}\sqrt{3} \\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{pmatrix}, \quad \Gamma_3(B)' = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The character table is in agreement with the class multiplication table

$$\begin{array}{lll} C_1 C_1 = C_1 & C_2 C_1 = C_2 & C_3 C_1 = C_3 \\ C_1 C_2 = C_2 & C_2 C_2 = 2C_1 + C_2 & C_3 C_2 = 2C_3 \\ C_1 C_3 = C_3 & C_2 C_3 = 2C_3 & C_3 C_3 = 3C_1 + 3C_2. \end{array}$$

1.2.2.6. The representations for point groups in one, two and three dimensions

For the irreducible representations of the point groups, it is necessary to know something about the structure of these groups. Since the representations of isomorphic groups are the same, one can restrict oneself to representatives of the isomorphism classes. In the following, we give a brief description of the structure of the point groups in spaces up to three dimensions. The character tables are given in Section 1.2.6. For the infinite series of groups (C_n and D_n), the crystallographic members are given explicitly separately.

(i) C_n . Cyclic groups are Abelian. Therefore, each element is a conjugacy class on itself. Irreducible representations are one-dimensional. The representation is determined by its value on a generator. Since $A^n = E$, the character $\chi(A)$ of an irreducible representation is an n th root of unity. There are n one-dimensional representations. For the p th irreducible representation, one has $\chi^{(p)}(A) = \exp(2\pi ip/n)$.

(ii) D_n . From the defining relations, it follows that A^p and A^{-p} ($p = 1, 2, \dots, n$) form a conjugacy class and that $A^p B$ and $A^{p+2} B$ belong to the same class. Therefore, one has to distinguish the

 Table 1.2.2.1. Character table for $S_3 \sim D_3$

Elements Symbols	(1) E	(123) A	(132) A^2	(23) B	(13) $A^2 B$	(12) AB
Class Order	C_1 1	C_2 3		C_3 2		
Γ_1	1	1	1	1	1	1
Γ_2	1	1	1	-1	-1	-1
Γ_3	2	-1	-1	0	0	0

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cases of even n from those of odd n . For odd n , one has a class consisting of E (order 1), $(n-1)/2$ classes with elements $A^{\pm p}$, and one class with all elements $A^p B$ (order 2). For even n , there is a class consisting of E (order 1), one with $A^{n/2}$, and $(n-2)/2$ classes with $A^{\pm p}$. The other elements form two classes of order 2 elements, one with the elements $A^p B$ for p odd, the other with $A^p B$ for p even.

The number of one-dimensional irreducible representations is the order of the group (N) divided by the order of the *commutator group*, which is the group generated by all elements $aba^{-1}b^{-1}$ ($a, b \in K$). For n odd this number is 2, for n even it is 4. In addition there are two-dimensional irreducible representations: $(n-1)/2$ for odd n , $n/2 - 1$ for even n .

(iii) T, O, I . The conjugacy classes of the tetrahedral, the octahedral and the icosahedral groups T, O and I , respectively, are given in the tables in Section 1.2.6.

(iv) $K \times C_2$. Because the generator of C_2 commutes with all elements of the group, the number of conjugacy classes of the direct product $K \times C_2$ is twice that for K . If A is the generator of C_2 and C_i are the classes of K , then the classes of the direct product are C_i and $C_i A$. The element A , which commutes with all elements of the direct product, is in an irreducible representation represented by a multiple of the identity. Because A is of order 2, the factor is ± 1 . Therefore, the character table looks like

$$\chi(K \times C_2) = \begin{pmatrix} \chi(K) & \chi(K) \\ \chi(K) & -\chi(K) \end{pmatrix}.$$

The n irreducible representations where A is represented by $+E$ are called *gerade* representations, the other, where A is represented by $-E$, are called *ungerade*.

In general, if K and H are finite groups with irreducible representations $D_{1\alpha}(K)$ and $D_{2\beta}(H)$, the *outer tensor product* acts on the tensor product $V_1 \otimes V_2$ of representation spaces as

$$(D_{1\alpha}(R) \otimes D_{2\beta}(R')) \mathbf{a} \otimes \mathbf{b} = (D_{1\alpha}(R) \mathbf{a}) \otimes (D_{2\beta}(R') \mathbf{b}),$$

$$\mathbf{a} \in V_1, \mathbf{b} \in V_2. \quad (1.2.2.38)$$

With the irreducibility criterion, one checks that this is an irreducible representation of $K \times H$. Moreover, $D_{1\alpha} \otimes D_{2\beta}$ is equivalent with $D_{1\alpha'} \otimes D_{2\beta'}$ if and only if $\alpha = \alpha'$ and $\beta = \beta'$. This means that one obtains all nonequivalent irreducible representations of $K \times H$ from the outer tensor products of the irreducible representations of K and H . If the group H is C_2 , there are two irreducible representations of C_2 , both one-dimensional. That means that the tensor product simplifies to a normal product. If $H = C_2$ and $D_{2\beta}(H)$ is the trivial representation, one has from (1.2.2.38)

$$D_{\alpha g}(R) = D_{\alpha}(R), \quad D_{\alpha g}(RA) = D_{\alpha}(R), \quad R \in K$$

$$D_{\alpha u}(R) = D_{\alpha}(R), \quad D_{\alpha u}(RA) = -D_{\alpha}(R).$$

The letters g and u come from the German *gerade* (even) and *ungerade* (odd). They indicate the sign of the operator associated with the generator A of C_2 : $+1$ for g representations, -1 for u representations. The number of nonequivalent irreducible representations of $K \otimes C_2$ is twice that of K .

Schur's lemma and the orthogonality relations and theorems derived above are formulated for complex representations and are, generally, not valid for integer or real representations. Nevertheless, many physical properties can be described using representation theory, but being real quantities they sometimes require a slightly different treatment. Here we shall discuss the relation between the complex representations and *physical or real representations*. Consider a real matrix representation $\Gamma(K)$. If it is reducible over complex numbers, it can be fully reduced. When is an irreducible component itself real? A first condition is clearly that its character is real. This is, however, not sufficient. A real representation can by a complex basis transformation be put

into a complex form and such a transformation does not change the character. Therefore, a better question is: which complex irreducible representations can be brought into real form? Consider a complex irreducible representation with a real character. Then it is equivalent with its complex conjugate *via* a matrix S :

$$\Gamma(R) = S\Gamma^*(R)S^{-1}, \quad R \in K.$$

Here one has to distinguish two different cases. To make the distinction between the two cases one has the following:

Proposition. Suppose that $\Gamma(K)$ is a complex irreducible representation with real character, and S a matrix intertwining $\Gamma(K)$ and its complex conjugate. Then S satisfies either $SS^* = E$ or $SS^* = -E$. In the former case, there exists a basis transformation that brings $\Gamma(K)$ into real form, in the latter case there is no such basis transformation.

Proposition. If $\Gamma(K)$ is a complex irreducible representation with real character $\chi(K)$, the latter satisfies

$$(1/N) \sum_{R \in K} \chi(R^2) = \pm 1.$$

If the right-hand side is $+1$, the representation can be put into real form, if it is -1 it cannot. (Proofs are given in Section 1.2.5.5.)

Consequently, a complex irreducible representation $\Gamma(K)$ is equivalent with a real one if $\chi(R) = \chi^*(R)$ and $\sum_R \chi(R^2) = N$. If that is not the case, a real representation containing $\Gamma(K)$ as irreducible component is the matrix representation

$$\frac{1}{2} \begin{pmatrix} \Gamma(R) + \Gamma^*(R) & i(\Gamma(R) - \Gamma^*(R)) \\ -i(\Gamma(R) - \Gamma^*(R)) & \Gamma(R) + \Gamma^*(R) \end{pmatrix} \sim \begin{pmatrix} \Gamma(R) & 0 \\ 0 & \Gamma^*(R) \end{pmatrix}. \quad (1.2.2.39)$$

The basis transformation is given by

$$S = \begin{pmatrix} E & E \\ -iE & iE \end{pmatrix}.$$

The dimension of the physically irreducible representation is $2d$, if d is the dimension of the complex irreducible representation $\Gamma(K)$. In summary, there are three types of irreducible representation:

- (1) First kind: $\chi(K) = \chi^*(K)$, $\sum_{R \in K} \chi(R^2) = +N$, dimension of real representation d ;
- (2) Second kind: $\chi(K) = \chi^*(K)$, $\sum_{R \in K} \chi(R^2) = -N$, dimension of real representation $2d$;
- (3) Third kind: $\chi(R) \neq \chi(R)^*$, $\sum_{R \in K} \chi(R^2) = 0$, dimension of real representation $2d$.

Examples of the three cases:

- (1) The matrices

$$D(A) = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} \quad \text{and} \quad D(B) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

generate a group that forms a faithful representation of the dihedral group $D_4 = 422$, for which the character table is given in Table 1.2.6.5. If one uses the same numbering of conjugacy classes, its character is $\chi(C_i) = 2, 0, -2, 0, 0$. It is an irreducible representation ($2^2 + 2^2 = N = 8$) with real character. The sum of the characters of the squares of the elements is $2 + 2 \times (-2) + 2 + 2 \times 2 + 2 \times 2 = 8 = N$. Therefore, it is equivalent to a real matrix representation, e.g. with

$$D'(A) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \quad \text{and} \quad D'(B) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

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(2) The matrices

$$D(A) = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} \text{ and } D(B) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

generate a group that is a faithful representation of the quaternion group of order 8. This group has five classes: E , $\{A, A^3\}$, $\{B, B^3\}$, $\{BA, AB\}$ and A^2 . The character of the elements is $\chi(R) = 2, 0, 0, 0, -2$ for the five classes. Then

$$(1/8) \sum_R \chi(R^2) = -1,$$

which means that the representation is essentially complex. A real physically irreducible representation of the group is generated by

$$\begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \text{ and } \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$

and the generated group is a crystallographic group in four dimensions.

(3) The complex number $\exp(2\pi i/n)$ generates a representation of the cyclic group C_n . For $n > 2$ the representation is not equivalent with its complex conjugate. Therefore, it is not a physical representation. The physically irreducible representation that contains this complex irreducible component is generated by

$$\begin{pmatrix} \cos(2\pi/n) & -\sin(2\pi/n) \\ \sin(2\pi/n) & \cos(2\pi/n) \end{pmatrix} \simeq \begin{pmatrix} \exp(2\pi i/n) & 0 \\ 0 & \exp(-2\pi i/n) \end{pmatrix}.$$

All complex irreducible representations of the finite point groups in up to three dimensions with real character can be put into a real form. This is not true for higher dimensions, as we have seen in the example of the quaternion group.

1.2.2.7. Tensor representations

When V_1, \dots, V_n are linear vector spaces, one may construct tensor products of these spaces. There are many examples in physics where this notion plays a role. Take the example of a particle with spin. The wave function of the particle has two components, one in the usual three-dimensional space and one in spin space. The proper way to describe this situation is *via* the tensor product. In normal space, a basis is formed by spherical harmonics Y_{lm} , in spin space by the states $|ss_z\rangle$. Spin-orbit interaction then plays in the $(2l+1)(2s+1)$ -dimensional space with basis $|lm\rangle \otimes |ss_z\rangle$. Another example is a physical tensor, e.g. the dielectric tensor ϵ_{ij} of rank 2. It is a symmetric tensor that transforms under orthogonal transformations exactly like a symmetric bi-vector with components $v_i w_j + v_j w_i$, where v_i and w_i ($i = 1, 2, 3$) are the components of vectors \mathbf{v} and \mathbf{w} . A basis for the space of symmetric bi-vectors is given by the six vectors $(\mathbf{e}_i \otimes \mathbf{e}_j + \mathbf{e}_j \otimes \mathbf{e}_i)$ ($i \leq j$). The space of symmetric rank 2 tensors has the same transformation properties.

A basis for the tensor space $V_1 \otimes V_2 \otimes \dots \otimes V_n$ is given by $\mathbf{e}_{1i} \otimes \mathbf{e}_{2j} \otimes \dots \otimes \mathbf{e}_{nk}$, where $i = 1, 2, \dots, d_1; j = 1, 2, \dots, d_2; \dots; k = 1, 2, \dots, d_n$. Therefore the dimension of the tensor product is the product of the dimensions of the spaces V_i (see also Section 1.1.3.1.2). The tensor space consists of all linear combinations with real or complex coefficients of the basis vectors. In the summation one has the multilinear property

$$\left(\sum_{i=1}^{d_1} c_{1i} \mathbf{e}_{1i} \right) \otimes \left(\sum_{j=1}^{d_2} c_{2j} \mathbf{e}_{2j} \right) \otimes \dots = \sum_{ij\dots} c_{1i} c_{2j} \dots \mathbf{e}_{1i} \otimes \mathbf{e}_{2j} \otimes \dots \quad (1.2.2.40)$$

In many cases in practice, the spaces V_i are all identical and then the dimension of the tensor product $V^{\otimes n}$ is simply d^n .

The tensor product of n identical spaces carries in an obvious way a representation of the permutation group S_n of n elements. A permutation of n elements is always the product of pair exchanges. The action of the permutation (12), that interchanges spaces 1 and 2, is given by

$$P_{12} \mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \dots = \mathbf{e}_j \otimes \mathbf{e}_i \otimes \mathbf{e}_k \otimes \dots \quad (1.2.2.41)$$

Two subspaces are then of particular interest, that of the tensors that are invariant under all elements of S_n and those that get a minus sign under pair exchanges. These spaces are the spaces of fully *symmetric* and *antisymmetric* tensors, respectively.

If the spaces V_1, \dots, V_n carry a representation of a finite group K , the tensor product space carries the product representation.

$$\begin{aligned} \mathbf{e}_{1j_1} \otimes \mathbf{e}_{2j_2} \otimes \dots \\ = \bigotimes_{i=1}^n \mathbf{e}_{ij_i} \rightarrow \sum_{k_1 k_2 \dots} \Gamma_1(R)_{k_1 j_1} \Gamma_2(R)_{k_2 j_2} \dots \mathbf{e}_{1k_1} \otimes \mathbf{e}_{2k_2} \otimes \dots \end{aligned} \quad (1.2.2.42)$$

The matrix $\Gamma(R)$ of the tensor representation is the tensor product of the matrices $\Gamma_i(R)$. In general, this representation is reducible, even if the representations Γ_i are irreducible. The special case of $n = 2$ has already been discussed in Section 1.2.2.3.

From the definition of the action of $R \in K$ on vectors in the tensor product space, it is easily seen that the character of R in the tensor product representation is the product of the characters of R in the representations Γ_i :

$$\chi(R) = \prod_{i=1}^n \chi_i(R). \quad (1.2.2.43)$$

The reduction in irreducible components then occurs with the multiplicity formula.

$$m_\alpha = (1/N) \sum_{R \in K} \chi_\alpha^*(R) \prod_{i=1}^n \chi_i(R). \quad (1.2.2.44)$$

If the tensor product representation is a real representation, the physically irreducible components can be found by first determining the complex irreducible components, and then combining with their complex conjugates the components that cannot be brought into real form.

The tensor product of the representation space V with itself has a basis $\mathbf{e}_i \otimes \mathbf{e}_j$ ($i, j = 1, 2, \dots, d$). The permutation (12) transforms this into $\mathbf{e}_j \otimes \mathbf{e}_i$. This action of the permutation becomes diagonal if one takes as basis $\mathbf{e}_i \otimes \mathbf{e}_j + \mathbf{e}_j \otimes \mathbf{e}_i$ ($1 \leq i \leq j \leq d$, spanning the space $V_s^{\otimes 2}$) and $\mathbf{e}_i \otimes \mathbf{e}_j - \mathbf{e}_j \otimes \mathbf{e}_i$ ($1 \leq i < j \leq d$, spanning the space $V_a^{\otimes 2}$). If one considers the action of K , one has with respect to the first basis $\chi(R) = \chi_\alpha(R)^2$ if V carries the representation with character $\chi_\alpha(K)$. With respect to the second basis, one sees that the character of the permutation $P = (12)$ is given by $\frac{1}{2}d(d+1) - \frac{1}{2}d(d-1) = d$. The action of the element $R \in K$ on the second basis is

$$R(\mathbf{e}_i \otimes \mathbf{e}_j \pm \mathbf{e}_j \otimes \mathbf{e}_i) = \sum_{kl} (\Gamma_\alpha \otimes \Gamma_\alpha)(R)_{kl,ij} (\mathbf{e}_i \otimes \mathbf{e}_j \pm \mathbf{e}_j \otimes \mathbf{e}_i).$$

This implies that both $V_s^{\otimes 2}$ and $V_a^{\otimes 2}$ are invariant under R . The character in the subspace is

$$\chi^+(R) = \sum_{k \leq l} (\Gamma_\alpha \otimes \Gamma_\alpha)(R)_{kl,kl} \quad (1.2.2.45)$$

for the symmetric subspace and

$$\chi^-(R) = \sum_{k < l} (\Gamma_\alpha \otimes \Gamma_\alpha)(R)_{kl,kl} \quad (1.2.2.46)$$