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(*c*) point groups that have elements in common with $O(3)\backslash SO(3)$ but do not contain $-E$; such groups are isomorphic to a group of the first class, as one can see if one multiplies all elements with determinant equal to -1 by $-E$.

The list of three-dimensional finite point groups is given in Table 1.2.6.1. All isomorphism classes of two-dimensional point groups occur in three dimensions as well. The isomorphism classes occurring here for the first time are:

$C_n \times C_2$: A, B, with $A^n = B^2 = ABA^{-1}B^{-1} = E$;

$D_n \times C_2$: A, B, C with $A^n = B^2 = (AB)^2 = C^2 = ACA^{-1}C^{-1} = BCB^{-1}C^{-1} = E$;

T: A, B, with $A^3 = B^2 = (AB)^3 = E$;

O: A, B, with $A^4 = B^3 = (AB)^2 = E$;

$T \times C_2$: A, B, C, with $A^3 = B^2 = (AB)^3 = C^2 = ACA^{-1}C^{-1} = BCB^{-1}C^{-1} = E$;

$O \times C_2$: A, B, C, with $A^4 = B^3 = (AB)^2 = C^2 = ACA^{-1}C^{-1} = BCB^{-1}C^{-1} = E$;

I: A, B, with $A^5 = B^3 = (AB)^2 = E$;

$I \times C_2$: A, B, C, with $A^5 = B^3 = (AB)^2 = C^2 = ACA^{-1}C^{-1} = BCB^{-1}C^{-1} = E$.

The crystallographic groups among them are given in Table 1.2.6.2.

1.2.2.2. *Representations of finite groups*

As stated in Section 1.2.1, elements of point groups act on physical properties (like tensorial properties) and on wave functions as linear operators. These linear operators therefore generally act in a different space than the three-dimensional configuration space. We denote this new space by V and consider a mapping D from the point group K to the group of nonsingular linear operators in V that satisfies

$$D(R)D(R') = D(RR') \quad \forall\ R, R' \in K. \tag{1.2.2.3}$$

In other words D is a *homomorphism* from K to the group of nonsingular linear transformations $GL(V)$ on the vector space V. Such a homomorphism is called a *representation* of K in V. Here we only consider finite-dimensional representations.

With respect to a basis $\mathbf{e}_i$ $(i = 1, 2, \ldots n)$ the linear transformations are given by matrices $\Gamma(R)$. The mapping Γ from K to the group of nonsingular $n \times n$ matrices $GL(n, R)$ (for a real vector space V) or $GL(n, C)$ (if V is complex) is called an n-dimensional *matrix representation* of K.

If one chooses another basis for V connected to the former one by a nonsingular matrix S, the same group of operators $D(K)$ is represented by another matrix group $\Gamma'(K)$, which is related to $\Gamma(K)$ by S according to $\Gamma'(R) = S^{-1}\Gamma(R)S$ $(\forall\ R \in K)$. Two such matrix representations are called *equivalent*. On the other hand, two such equivalent matrix representations can be considered to describe two different groups of linear operators [$D(K)$ and $D'(K)$] on the same basis. Then there is a nonsingular linear operator T such that $D(R)T = TD'(R)$ $(\forall\ R \in K)$. In this case, the representations $D(K)$ and $D'(K)$ are also called equivalent.

It may happen that a representation $D(K)$ in V leaves a subspace W of V invariant. This means that for every vector $v \in W$ and every element $R \in K$ one has $D(R)v \in W$. Suppose that this subspace is of dimension $m < n$. Then one can choose m basis vectors for V inside the invariant subspace. With respect to this basis, the corresponding matrix representation has elements

$$\Gamma(R) = \begin{pmatrix} \Gamma_1(R) & \Gamma_3(R) \\ 0 & \Gamma_2(R) \end{pmatrix}, \tag{1.2.2.4}$$

where the matrices $\Gamma_1(R)$ form an m-dimensional matrix representation of K. In this situation, the representations $D(K)$ and $\Gamma(K)$ are called *reducible*. If there is no proper invariant subspace the representation is *irreducible*. If the representation is a direct sum of subspaces, each carrying an irreducible representation, the representation is called *fully reducible* or *decomposable*. In the latter case, a basis in V can be chosen such that the matrices $\Gamma(R)$ are direct sums of matrices $\Gamma_i(R)$ such that the $\Gamma_i(R)$ form an irreducible matrix representation. If $\Gamma_3(R)$ in (1.2.2.4) is zero and Γ_1 and Γ_2 form irreducible matrix representations, Γ is fully reducible. For finite groups, each reducible representation is fully reducible. That means that if $\Gamma(K)$ is reducible, there is a matrix S such that

$$\Gamma(R) = S\big[\Gamma_1(R) \oplus \ldots \oplus \Gamma_n(R)\big]S^{-1} = S\begin{pmatrix} \Gamma_1(R) & 0 & \ldots & 0 \\ 0 & \Gamma_2(R) & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & \Gamma_n(R) \end{pmatrix} S^{-1}. \tag{1.2.2.5}$$

In this way one may proceed until all matrix representations $\Gamma_i(K)$ are *irreducible*, *i.e.* do not have invariant subspaces. Then each representation $\Gamma(K)$ can be written as a direct sum

$$\Gamma(R) = S\big[m_1\Gamma_1(R) \oplus \ldots \oplus m_s\Gamma_s(R)\big]S^{-1}, \tag{1.2.2.6}$$

where the representations $\Gamma_1 \ldots \Gamma_s$ are all nonequivalent and the *multiplicities* m_i are the numbers of times each irreducible representation occurs. The nonequivalent irreducible representations Γ_i for which the multiplicity is not zero are the *irreducible components* of $\Gamma(K)$.

We first discuss two special representations. The simplest representation in one-dimensional space is obtained by assigning the number 1 to all elements of K. Obviously this is a representation, called the *identity* or *trivial representation*. Another is the *regular representation*. To obtain this, one numbers the elements of K from 1 to the order N of the group ($|K| = N$). For a given $R \in K$ there is a one-to-one mapping from K to itself defined by $R_i \rightarrow R_j \equiv RR_i$. Consider the $N \times N$ matrix $\Gamma(R)$, which has in the ith column zeros except on line j, where the entry is unity. The matrix $\Gamma(R)$ then has as only entries 0 or 1 and satisfies

$$RR_i = \Gamma(R)_{ji}R_j, \quad (i = 1, 2, \ldots, N). \tag{1.2.2.7}$$

These matrices $\Gamma(R)$ form a representation, the *regular representation* of K of dimension N, as one sees from

$$(R_iR_j)R_k = R_i\sum_{l=1}^{N}\Gamma(R_j)_{lk}R_l = \sum_{l=1}^{N}\sum_{m=1}^{N}\Gamma(R_j)_{lk}\Gamma(R_i)_{ml}R_m = \sum_{m=1}^{N}\big[\Gamma(R_i)\Gamma(R_j)\big]_{mk}R_m = \sum_{m=1}^{N}\Gamma(R_iR_j)_{mk}R_m.$$

A representation in a real vector space that leaves a positive definite metric invariant can be considered on an orthonormal basis for that metric. Then the matrices satisfy

$$\Gamma(R)\Gamma(R)^T = E$$

(^{T} denotes transposition of the matrix) and the representation is *orthogonal*. If V is a complex vector space with positive definite metric invariant under the representation, the latter gives on an orthonormal basis matrices satisfying

$$\Gamma(R)\Gamma(R)^\dagger = E$$

(† denotes Hermitian conjugation) and the representation is *unitary*. A real representation of a finite group is always equivalent with an orthogonal one, a complex representation of a finite group is always equivalent with a unitary one. As a proof of the latter statement, consider the standard Hermitian metric on V: $f(x, y) = \sum_i x_i^* y_i$. Then the positive definite form

$$F(x, y) = (1/N) \sum_{R \in K} f(D(R)x, D(R)y) \qquad (1.2.2.8)$$

is invariant under the representation. To show this, take an arbitrary element R'. Then

$$\begin{aligned} F(D(R')x, D(R')y) &= (1/N) \sum_{R \in K} f(D(R'R)x, D(R'R)y) \\ &= F(x, y). \end{aligned} \qquad (1.2.2.9)$$

With respect to an orthonormal basis for this metric $F(x, y)$, the matrices corresponding to $D(R)$ are unitary. The complex representation can be put into this unitary form by a basis transformation. For a real representation, the argument is fully analogous, and one obtains an orthogonal transformation.

From two representations, $D_1(K)$ in V_1 and $D_2(K)$ in V_2, one can construct the sum and product representations. The *sum representation* acts in the direct sum space $V_1 \oplus V_2$, which has elements $(\mathbf{a}, \mathbf{b})$ with $\mathbf{a} \in V_1$ and $\mathbf{b} \in V_2$. The representation $D_1 \oplus D_2$ is defined by

$$\big[(D_1 \oplus D_2)(R)\big](\mathbf{a}, \mathbf{b}) = (D_1(R)\mathbf{a}, D_2(R)\mathbf{b}). \qquad (1.2.2.10)$$

The matrices $\Gamma_1 \oplus \Gamma_2(R)$ are of dimension $n_1 + n_2$.

The *product representation* acts in the tensor space, which is the space spanned by the vectors $\mathbf{e}_i \otimes \mathbf{e}_j$ $(i = 1, 2, \ldots, \dim V_1;$ $j = 1, 2 \ldots, \dim V_2)$. The dimension of the tensor space is the product of the dimensions of both spaces. The action is given by

$$\big[(D_1 \otimes D_2)(R)\big]\mathbf{a} \otimes \mathbf{b} = D_1(R)\mathbf{a} \otimes D_2(R)\mathbf{b}. \qquad (1.2.2.11)$$

For bases $\mathbf{e}_i$ $(i = 1, 2, \ldots, d_1)$ for V_1 and $\mathbf{e}'_j$ $(j = 1, 2, \ldots, d_2)$ for V_2, a basis for the tensor product of spaces is given by

$$\mathbf{e}_i \otimes \mathbf{e}'_j, \quad i = 1, \ldots, d_1;\ j = 1, 2, \ldots, d_2, \qquad (1.2.2.12)$$

and with respect to this basis the representation of K is given by matrices

$$(\Gamma_1 \otimes \Gamma_2)(R)_{ik,jl} = \Gamma_1(R)_{ij}\Gamma_2(R)_{kl}. \qquad (1.2.2.13)$$

As an example of these operations, consider

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \oplus \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix};$$

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix}.$$

If two representations $D_1(K)$ and $D_2(K)$ are equivalent, there is an operator S such that

$$SD_1(R) = D_2(R)S \quad \forall\, R \in K.$$

This relation may also hold between sets of operators that are not necessarily representations. Such an operator S is called an *intertwining operator*. With this concept we can formulate a theorem that strictly speaking does not deal with representations but with intertwining operators: *Schur's lemma*.

Proposition. Let M and N be two sets of nonsingular linear transformations in spaces V (dimension n) and W (dimension m), respectively. Suppose that both sets are irreducible (the only invariant subspaces are the full space and the origin). Let S be a linear transformation from V to W such that $SM = NS$. Then either S is the null operator or S is nonsingular and $SMS^{-1} = N$.

Proof: Consider the image of V under S: $\mathrm{Im}_S V \subseteq W$. That means that $S\mathbf{r} \in \mathrm{Im}_S V$ for all $\mathbf{r} \in V$. This implies that $NS\mathbf{r} = SM\mathbf{r} \in \mathrm{Im}_S V$. Therefore, $\mathrm{Im}_S V$ is an invariant subspace of W under N. Because N is irreducible, either $\mathrm{Im}_S V = 0$ or $\mathrm{Im}_S V = W$. In the first case, S is the null operator. In the second case, notice that the kernel of S, the subspace of V mapped on the null vector of W, is an invariant subspace of V under M: if $S\mathbf{r} = 0$ then $NS\mathbf{r} = 0$. Again, because of the irreducibility, either Ker_S is the whole of V, and then S is again the null operator, or $\mathrm{Ker}_S = 0$. In the latter case, S is a one-to-one mapping and therefore nonsingular. Therefore, either S is the null operator or it is an isomorphism between the vector spaces V and W, which are then both of dimension n. With respect to bases in the two spaces, the operator S corresponds to a nonsingular matrix and $M = S^{-1}NS$.

This is a very fundamental theorem. Consequences of the theorem are:

(1) If N and M are nonequivalent irreducible representations and $SM = NS$, then $S = 0$.

(2) If a matrix S is singular and links two irreducible representations of the same dimension, then $S = 0$.

(3) A matrix S that commutes with all matrices of an irreducible complex representation is a multiple of the identity. Suppose that an $n \times n$ matrix S commutes with all matrices of a complex irreducible representation. S can be singular and is then the null matrix, or it is nonsingular. In the latter case it has an eigenvalue $\lambda \neq 0$ and $S - \lambda E$ commutes with all the matrices. However, $S - \lambda E$ is singular and therefore the null matrix: $S = \lambda E$. This reasoning is only valid in a complex space, because, generally, the eigenvalues λ are complex.

1.2.2.3. *General tensors*

Suppose a group K acts linearly on a d-dimensional space V: for any $v \in V$ one has

$$Rv \in V \quad \forall\, R \in K, v \in V.$$

For a basis $\mathbf{a}_i$ in V this gives a matrix group $\Gamma(K)$ *via*

$$R\mathbf{a}_i = \sum_{j=1}^{d} \Gamma(R)_{ji}\mathbf{a}_j, \quad R \in K. \qquad (1.2.2.14)$$

The matrix group $\Gamma(K)$ is a matrix representation of the group K.

Consider now a linear function f on V. Because

$$f\left(\sum_{i=1}^{d} \xi_i \mathbf{a}_i\right) = \sum_{i=1}^{d} \xi_i f(\mathbf{a}_i),$$

the function is completely determined by its value on the basis vectors $\mathbf{a}_i$. A second point is that these linear functions form a vector space because for two functions f_1 and f_2 the function $\alpha_1 f_1 + \alpha_2 f_2$ is a well defined linear function. The vector space is called the *dual space* and is denoted by V^*. A basis for this space is given by functions $f_1, \ldots, f_d$ such that

$$f_i(\mathbf{a}_j) = \delta_{ij},$$

because any linear function f can be written as a linear combination of these vectors with as coefficients the value of f on the basis vectors $\mathbf{a}_i$:

$$f = \sum_{i=1}^{d} f(\mathbf{a}_i) f_i \Leftrightarrow f\Big(\sum_{k=1}^{d} \xi_k \mathbf{a}_k\Big) = \sum_{k=1}^{d} \xi_k \sum_{i=1}^{d} f(\mathbf{a}_i) f_i(\mathbf{a}_k) = \sum_{k=1}^{d} \xi_k f(\mathbf{a}_k).$$