International Tables for Crystallography (2006). Vol. D, Section 1.2.5, pp. 53–56.

$$|JM\rangle = \sum_{mm'} \begin{pmatrix} \ell & \ell' & J \\ m & m' & M \end{pmatrix} |\ell m\rangle \otimes |\ell' m'\rangle,$$
$$(J = |\ell - \ell'|, \ldots, \ell + \ell'). \qquad (1.2.4.10)$$

The multiplicity here is always zero or unity, which is the reason why one leaves out the number ℓ in the notation.

If the multiplicity m_γ is unity, the coefficients for given α, β, γ are unique up to a common factor for all i, j, k. This is no longer the case if the multiplicity is larger, because then one can make linear combinations of the basis vectors belonging to Γ_γ. Anyway, one has to follow certain conventions. In the case of $O(3)$, for example, there are the Condon–Shortley phase conventions. The degree of freedom of the Clebsch–Gordan coefficients for given matrix representations Γ_α can be seen as follows. Suppose that there are two basis transformations, S and S', in the tensor product space which give the same reduced form:

$$S(D_\alpha \otimes D_\beta)S^{-1} = S'(D_\alpha \otimes D_\beta)S'^{-1} = D = \bigoplus m_\gamma D_\gamma. \qquad (1.2.4.11)$$

Then the matrix $S'S^{-1}$ commutes with every matrix $D(R)$ ($R \in K$). If all multiplicities are zero or unity, it follows from Schur's lemma that $S'S^{-1}$ is the direct sum of unit matrices of dimension d_γ. If the multiplicities are larger, the matrix $S'S^{-1}$ is a direct sum of blocks which are of the form

$$\begin{pmatrix} \lambda_{11}E & \lambda_{12}E & \ldots & \lambda_{1m_\gamma}E \\ \lambda_{21}E & \lambda_{22}E & \ldots & \lambda_{2m_\gamma}E \\ \vdots & \vdots & \ddots & \vdots \\ \lambda_{m_\gamma 1}E & \ldots & \ldots & \lambda_{m_\gamma m_\gamma}E \end{pmatrix},$$

such that $\mathrm{Det}(\lambda_{ij}) = 1$, and the E's are d_γ-dimensional unit matrices. This means that for multiplicity-free ($m_\gamma \leq 1$) cases, the Clebsch–Gordan coefficients are unique up to a common factor for all coefficients involving one value of γ.

The Clebsch–Gordan coefficients satisfy the following rules:

$$\begin{pmatrix} \alpha & \beta & \gamma \\ i & j & k \quad \ell \end{pmatrix} = \begin{pmatrix} \beta & \alpha & \gamma \\ j & i & k \quad \ell \end{pmatrix}$$

$$\begin{pmatrix} \alpha & \beta & \gamma \\ i & j & k \quad \ell \end{pmatrix} = 0, \text{ if } D_\alpha \otimes D_\beta \text{ does not contain } D_\gamma$$

$$\sum_{k\ell} \begin{pmatrix} \alpha & \beta & \gamma \\ i & j & k \quad \ell \end{pmatrix}^* \begin{pmatrix} \alpha & \beta & \gamma \\ i' & j' & k \quad \ell \end{pmatrix} = \delta_{ii'}\delta_{jj'}$$

$$\sum_{ij} \begin{pmatrix} \alpha & \beta & \gamma \\ i & j & k \quad \ell \end{pmatrix}^* \begin{pmatrix} \alpha & \beta & \gamma \\ i & j & k' \quad \ell' \end{pmatrix} = \delta_{kk'}\delta_{\ell\ell'}.$$

For the basis vectors of the invariant space belonging to the identity representation Γ_1, one has $\gamma = d_\gamma = 1$. Consequently,

$$\psi_\ell = \sum_{ij} \begin{pmatrix} \alpha & \beta & 1 \\ i & j & 1 \quad \ell \end{pmatrix} \mathbf{a}_i \otimes \mathbf{b}_j.$$

1.2.5. Magnetic symmetry

1.2.5.1. *Magnetic point groups*

Until now, the symmetry transformations we have considered affect only spatial variables. In physics, however, time coordinates are also often essential, and time reversal is a very important transformation as well.

The time-reversal operation generates a group of order 2 with as elements the unit operator E and the time-reversal operator T. This transformation commutes with transformations of spatial variables. One can consider the combined operation of T and a Euclidean transformation. In other words, we consider the direct product of the Euclidean group $E(d)$ and the time-reversal group of order 2. Elements of this direct product that belong to $E(d)$ are called *orthochronous*, whereas the elements of the coset which are combinations of a Euclidean transformation with T are called *antichronous*. We shall start by considering combinations of T and orthogonal transformations in the physical d-dimensional space. Such combinations generate a subgroup of the direct product of $O(d)$ and the time-reversal group.

There are three types of such groups. First, one can have a group that is already a subgroup of $O(d)$. This group does not have time-reversing elements. A second type of group contains the operator T and is, therefore, the direct product of a subgroup of $O(d)$ with the time-reversal group. The third type of group contains antichronous elements but not T itself. This means that the group contains a subgroup of index 2 that belongs to $O(d)$ and one coset of this subgroup, all elements of which can be obtained from those of the subgroup by multiplication with one fixed time-reversing element which is not T. If one then multiplies all elements of the coset by T, one obtains a group that belongs to $O(d)$ and is isomorphic to the original group. This is the same situation as for subgroups of $O(3)$, which is the direct product of $SO(3)$ with space inversion I. Here also all subgroups of $O(d) \times \mathbb{Z}_2$ are isomorphic to point groups or to the direct product of a point group and $\mathbb{Z}_2$. Magnetic groups can be used to characterize spin arrangements. Because spin inverses sign under time reversal, a spin arrangement is never invariant under T. Therefore, the point groups of the second type are also called *nonmagnetic point groups*. Because time reversal does not play a role in groups of the first type, these are called *trivial magnetic point groups*, whereas the groups of the third type are called *nontrivial magnetic point groups*.

Magnetic point groups are discussed in Chapter 1.5. Orthochronous magnetic point groups (trivial magnetic groups) are denoted by their symbol as a normal point group. Magnetic point groups containing T are denoted by the symbol for the orthochronous subgroup, which is a trivial magnetic group, to which the symbol $1'$ is added. Magnetic point groups that are neither trivial nor contain T are isomorphic to a trivial magnetic point group. They are denoted by the symbol of the latter in which all symbols for antichronous elements are marked with a prime ($'$). For example, $\bar{1}$ is the trivial magnetic group generated by I, $\bar{1}1'$ is the group of four elements generated by I and T, and $\bar{1}'$ is the magnetic group of order 2 generated by the product IT.

Two magnetic point groups are called equivalent if they are conjugated in $O(d) \times \mathbb{Z}_2$ by an element in $O(d)$. This means that under the conjugation antichronous elements go to antichronous elements. The equivalence classes of magnetic point groups are the magnetic crystal classes. There are 32 classes of trivial crystallographic magnetic point groups, 32 classes of direct products with the time-reversal group and 58 classes of nontrivial magnetic crystallographic point groups. They are given in Table 1.2.6.12.

1.2.5.2. *Magnetic space groups*

Magnetic space groups are subgroups of the direct product of the Euclidean group $E(d)$ with the time-reversal group (this direct product is sometimes called the *Shubnikov group*) such that the orthochronous elements together with the products of the antichronous elements and T form a space group in d dimensions. As in the case of magnetic point groups, one can distinguish trivial magnetic groups, which are subgroups of $E(d)$, direct products of a trivial group with the time-reversal group (nonmagnetic) and nontrivial magnetic space groups with antichronous elements but without T. The groups of the third type can be transformed into groups of the first type by multiplication of all antichronous elements by T.

The translation subgroup U of a magnetic space group G is the intersection of G and $T(d) \times \{E, T\}$. The factor group G/U is (isomorphic to) a subgroup of $O(d) \times \{E, T\}$. For trivial magnetic space groups, the point group is a subgroup of $O(d)$. For direct products with $\{E, T\}$, the translation group is the direct product of an orthochronous lattice with $\{E, T\}$ and the point group is a subgroup of $O(d)$. Magnetic space groups with antichronous elements but without T have either a translation subgroup consisting of orthochronous elements or one with antichronous elements as well. In the first case, the point group is a subgroup of $O(d) \times \{E, T\}$ and contains antichronous elements; in the second case, one may always choose orthochronous elements for the coset representatives with respect to the translation group, and the point group is a subgroup of $O(d)$. Therefore, nontrivial magnetic space groups without T have either the same lattice or the same point group as the space group of orthochronous elements.

Two magnetic space groups are equivalent if they are affine conjugated *via* a transformation with positive determinant that maps antichronous elements on antichronous elements. Then there are 1656 equivalence classes: 230 classes of trivial groups with only orthochronous elements, 230 classes of direct products with $\{E, T\}$ and 1191 classes with nontrivial magnetic groups.

1.2.5.3. *Transformation of tensors*

Vectors and tensors transforming in the same way under Euclidean transformations may behave differently when time reversal is taken into account. As an example, both the electric field **E** and magnetic field **B** transform under a rotation as a position vector. Under time reversal, the former is invariant, but the latter changes sign. Therefore, the magnetic field is called a pseudovector field under time reversal. Under spatial inversion, the field **E** changes sign, as does a position vector, but the field **B** does not. Therefore, the magnetic field is also a pseudovector under central inversion. The electric polarization induced by an electric field is given by the electric susceptibility, a magnetic moment induced by a magnetic field is given by the magnetic susceptibility and in some crystals a magnetic moment is induced by an electric field *via* the magneto-electric susceptibility. Under the four elements of the group generated by $T = 1'$ and $I = \bar{1}$, the fields and susceptibility tensors transform according to

	E	$\bar{1}$	$1'$	$\bar{1}'$
E	1	−1	1	−1
B	1	1	−1	−1
χ_{ee}	1	1	1	1
χ_{mm}	1	1	1	1
χ_{me}	1	−1	−1	1

Here $\bar{1}' = \bar{1}1'$.

In general, a vector transforms as the position vector **r** under rotations and changes sign under $\bar{1}$, but not under $1'$. A pseudovector under $\bar{1}$ or (respectively and) $1'$ gets an additional minus sign. The generalization to tensors is straightforward.

$$gT_{i_1\ldots i_n} = \varepsilon_P \varepsilon_T \sum_{j_1\ldots j_n} \left(\prod_{k=1}^{n} R_{i_k j_k} \right) T_{j_1\ldots j_n}, \qquad (1.2.5.1)$$

where ε_P and ε_T are ± 1, depending on the pseudotensor character with respect to space and time reversal, respectively.

Under a rotation $[R \in SO(d)]$, a vector transforms according to a representation characterized by the character $\chi(R)$ of the representation. In two dimensions $\chi = 2\cos\varphi$ and in three dimensions $\chi = 1 + 2\cos\varphi$, if φ is the rotation angle. Under IR the character gets an additional minus sign, under RT it is the same, and under RIT there is again an additional minus sign. For pseudovectors, either under I or T or both, there are the extra factors ε_P, ε_T and $\varepsilon_P \varepsilon_T$, respectively. As an example, the character

Table 1.2.5.1. *Character of the representations corresponding to the electric and magnetic fields in point groups 222, 2′2′2 and 2′mm′*

n_i is the number of invariants.

Point group	**E**				n_i	**B**				n_i
222	3	−1	−1	−1	0	3	−1	−1	−1	0
$2'2'2$	3	−1	−1	−1	0	3	1	1	−1	1
$2'mm'$	3	−1	1	1	1	3	1	−1	1	1

of the representations corresponding to the electric and magnetic fields in two orthorhombic point groups (222, $2'2'2$ and $2'mm'$) are given in Table 1.2.5.1.

The number of invariant components is the multiplicity of the trivial representation in the representation to which the tensor belongs. The nonzero invariant field components are B_z for $2'2'2$, E_x and B_y for $2'mm'$. These components can be constructed by means of projection-operator techniques, or more simply by solving the linear equations representing the invariance of the tensor under the generators of the point group. For example, the magnetic field vector B transforms to $(-B_x, B_y, -B_z)$ under m_y and to $(B_x, B_y, -B_z)$ under m_z, and this gives the result that all components are zero except B_y.

1.2.5.4. *Time-reversal operators*

In quantum mechanics, symmetry transformations act on state vectors as unitary or anti-unitary operators. For the Schrödinger equation for one particle without spin,

$$\hbar i \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = H\Psi(\mathbf{r}, t), \qquad (1.2.5.2)$$

the operator that reverses time is the complex conjugation operator θ with

$$\theta\Psi(\mathbf{r}, t) = \Psi^*(\mathbf{r}, t) \qquad (1.2.5.3)$$

satisfying

$$\hbar i \frac{\partial}{\partial t} \Psi^*(\mathbf{r}, -t) = H\Psi^*(\mathbf{r}, -t),$$

which is the time-reversed equation.

This operator is *anti-linear* $[\theta(\alpha\Psi + \beta\Phi) = \alpha^*\theta\Psi + \beta^*\Phi]$ and has the following commutation relations with the operators **r** and **p** for position and momentum:

$$\theta\mathbf{r}\theta^{-1} = \mathbf{r}, \quad \theta\mathbf{p}\theta^{-1}. \qquad (1.2.5.4)$$

For a Euclidean transformation $g = \{R|\mathbf{a}\}$, the operation on the state vector is given by the unitary operator

$$T_g\Psi(\mathbf{r}) = \Psi(g^{-1}\mathbf{r}) = \Psi(R^{-1}(\mathbf{r} - \mathbf{a})). \qquad (1.2.5.5)$$

The two operators θ and T_g commute. Therefore, if g is an orthochronous element of the symmetry group, the corresponding operator is T_g, and if gT is an antichronous element the operator is θT_g. The operator θT_g is also *anti-unitary*: it is anti-linear and conserves the absolute value of the Hermitian scalar product: $|\langle \theta T_g \Psi | \theta T_g \Phi \rangle| = |\langle \Psi | \Phi \rangle|$.

If the particle has a spin, the time-reversal operator has to have the commutation relation

$$\theta\mathbf{S}\theta^{-1} = -\mathbf{S} \qquad (1.2.5.6)$$

with the spin operator **S**. For a spin-$\frac{1}{2}$ particle, the spin operators are $S_i = \hbar\sigma_i/2$ in terms of the Pauli matrices. Then the time-reversal operator is

$$T_T = \sigma_2\theta. \qquad (1.2.5.7)$$

The operators corresponding to the elements of a magnetic symmetry group are generally (anti-)unitary operators on the state vectors. These operators form a representation of the magnetic symmetry group.

$$T_g T_{g'} = T_{gg'}. \tag{1.2.5.8}$$

In principle, they even form a projective representation, but as discussed before for particles without spin the factor system is trivial, and for particles with spin one can take as the symmetry group the double group of the symmetry group.

1.2.5.5. *Co-representations*

Suppose the magnetic point group G has an orthochronous subgroup H and an antichronous coset $H' = aH$ for some antichronous element a. The elements of H are represented by unitary operators, those of H' by anti-unitary operators. These operators correspond to matrices in the following way. Suppose Φ_j are the elements of a basis of the state vector space. Then

$$T_g\Phi_j = \sum_k M(g)_{kj}\Phi_k, \quad g \in G. \tag{1.2.5.9}$$

The matrices M do not form a matrix representation in the usual sense. They satisfy the relations

$$\begin{aligned} M(g_1g_2) &= M(g_1)M(g_2) \quad g_1 \in H \\ &= M(g_1)M^*(g_2) \quad g_1 \in H', \end{aligned} \tag{1.2.5.10}$$

as one verifies easily. Matrices satisfying these relations are called *co-representations* of the group G.

A co-representation is irreducible if there is no proper invariant subspace. If a co-representation is reducible, there is a basis transformation S that brings the matrices into a block form. For co-representations, a basis transformation S with

$$S\Phi_i = \sum_{j=1}^{m} S_{ji}\Phi_j \tag{1.2.5.11}$$

transforms the matrices according to

$$M(h) \to S^{-1}M(h)S, \quad M(ah) \to S^{-1}M(ah)S^*, \quad (h \in H). \tag{1.2.5.12}$$

Here a is the coset representative of the antichronous elements. The co-representation restricted to the orthochronous subgroup H gives an ordinary representation of H which is not necessarily irreducible even if the co-representation is irreducible. Suppose that $\Phi_1 \ldots \Phi_m$ form a basis for the irreducible co-representation of G and that the restriction to H is also irreducible. The elements $T_a\Phi_1, \ldots, T_a\Phi_m$ form another basis for the space, and on this basis the representation matrices of H follow from

$$T_hT_a\Phi_i = T_aT_{a^{-1}ha}\Phi_i = \sum_{j=1}^{m} M(a^{-1}ha)^*_{ji}T_a\Phi_j. \tag{1.2.5.13}$$

Because both bases are bases for the same irreducible space, it means that the (ordinary) representations $M(H)$ and $M(a^{-1}Ha)^*$ are equivalent.

If the representation $M(H)$ is reducible, there is a basis $\varphi_1, \ldots, \varphi_d$ for the irreducible representation $D(H)$. A basis for the whole space then is given by

$$\varphi_1, \ldots, \varphi_d, T_a\varphi_1, \ldots, T_a\varphi_d,$$

because the co-representation of G would be reducible if the last d vectors were dependent on the first d. On this basis, the matrices for the co-representation become

$$\begin{aligned} M(h) &= \begin{pmatrix} D(h) & 0 \\ 0 & D(a^{-1}ha)^* \end{pmatrix}, \\ M(ah) &= \begin{pmatrix} 0 & D(aha) \\ D(h)^* & 0 \end{pmatrix}, \quad h \in H, a \in H' \end{aligned} \tag{1.2.5.14}$$

because

$$\begin{aligned} T_ah\varphi_i &= T_a\sum_j D(h)_{ji}\varphi_j = \sum_j D(h)^*_{ji}T_a\varphi_j \\ T_ahT_a\varphi_i &= T_aha\varphi_i = \sum_j D(aha)_{ji}\varphi_j. \end{aligned}$$

The two irreducible components for $M(H)$ can be either equivalent or non-equivalent. If they are not equivalent the co-representation is indeed irreducible, because a basis transformation S that leaves the matrices $M(h)$ the same is necessarily of the form $\lambda E \oplus \mu E$ because of Schur's lemma, and such a matrix cannot bring the matrices $D(ah)$ into a reduced form. In this case, the co-representation $M(G)$ is irreducible, in agreement with the starting assumption, and the dimension m is twice the dimension of the representation $D(H)$: $m = 2d$.

If the two irreducible components $D(H)$ and $D(a^{-1}Ha)^*$ are equivalent, there is a basis transformation U such that

$$D(a^{-1}ha)^* = U^{-1}D(h)U \quad \forall\, h \in H.$$

The basis transformation

$$T = \begin{pmatrix} 1 & 0 \\ 0 & U^{-1} \end{pmatrix}$$

then gives a new matrix co-representation for G:

$$\begin{aligned} M(h) &\to T^{-1}M(h)T = \begin{pmatrix} D(h) & 0 \\ 0 & D(h) \end{pmatrix}, \\ M(ah) &\to T^{-1}M(ah)T^* = \begin{pmatrix} 0 & D(aha)U^{*-1} \\ UD(h)^* & 0 \end{pmatrix}. \end{aligned}$$

The most general basis transformation S that leaves $M(h)$ in the same form is then

$$S = \begin{pmatrix} \lambda E & \mu E \\ \rho E & \sigma E \end{pmatrix}. \tag{1.2.5.15}$$

Under this basis transformation, the matrices $M(ah)$ become

$$S^{-1}M(ah)S^* = \frac{1}{(\lambda\sigma - \mu\rho)}\mathcal{M}$$

with

$$\begin{aligned} \mathcal{M}_{11} &= -\lambda^*\mu UD(h)^* + \rho^*\sigma D(aha)U^{*-1} \\ \mathcal{M}_{12} &= |\sigma|^2D(aha)U^{*-1} - |\mu|^2UD(h)^* \\ \mathcal{M}_{21} &= |\lambda|^2UD(h)^* - |\rho|^2D(aha)U^{*-1} \\ \mathcal{M}_{22} &= \lambda\mu^*UD(h)^* - \rho\sigma^*D(aha)U^{*-1}. \end{aligned}$$

This is block diagonal if

$$|\mu|^2UU^*D(a^{-1}ha)U^{*-1}U^* = |\sigma|^2D(aha)$$

and analogous expressions for $|\lambda|^2$ and $|\rho|^2$ also hold.

The transformation matrix U satisfies $UU^* = \pm D(a^2)$, as one can show as follows. From the definition

$$D(a^{-1}ha)^* = U^{-1}D(h)U$$

follow the two relations

$$D(a^{-2}ha^2) = U^{*-1}U^{-1}D(h)UU^*$$
$$D(a^{-2}ha^2) = D(a^2)^{-1}D(h)D(a^2).$$

(Notice that $a^2 \in H$.) Because $D(H)$ is irreducible, it follows that $UU^*D(a^{-2})$ is a multiple of the identity: $UU^* = \chi D(a^2)$. The factor χ is real because

$$D(a^2)^* = U^{-1}D(a^2)U = U^{-1}UU^*U/\chi$$

and

$$D(a^2)^* = U^*U/\chi^*.$$

Hence $\chi = \chi^* = \pm 1$.

The conditions for the transformed matrix $M(ah)$ to be block diagonal then read

$$\pm|\mu|^2 D(a^2)D(a^{-1}ha) = |\sigma|^2 D(aha), \quad (1.2.5.16)$$

with the corresponding expressions for λ and ρ. If χ is equal to -1, these equations do not have a solution. However, when $\chi = +1$ there is a solution, which means that the co-representation is reducible, contrary to the assumption. Therefore, this situation can not occur.

One can summarize these considerations in the following theorem.

Theorem 1. If the restriction of an irreducible co-representation to the orthochronous subgroup is reducible, then either the (two) irreducible components are non-equivalent, or they are equivalent and connected by a basis transformation U for which $UU^* = -D(a^2)$. If the restriction $M(H)$ is irreducible, it is equivalent to $M(a^{-1}Ha)^*$.

In the former case, the dimension of the co-representation is twice that of the restriction, in the latter case they are equal. Therefore, one has the following corollary.

Corollary. A d-dimensional irreducible representation of the orthochronous subgroup H can occur as irreducible component of the restriction of an irreducible co-representation of G with dimension m with

$m = 2d$ if $D(H)$ nonequivalent to $D(a^{-1}Ha)^*$

$m = 2d$ if $D(H)$ equivalent to $D(a^{-1}Ha)^*$ and $UU^* = -D(a^2)$

$m = d$ if $D(H)$ equivalent to $D(a^{-1}Ha)^*$ and $UU^* = +D(a^2)$.

The three cases from theorem (1) can be distinguished by the following theorem:

Theorem 2. The irreducible representation $D(H)$ with character $\chi(H)$ belongs to the respective cases of theorem (1) if

$$\sum_{h\in H} \chi(ahah) = \begin{cases} 0 & \text{for the first case} \\ -N & \text{for the second case} \\ N & \text{for the third case.} \end{cases} \quad (1.2.5.17)$$

The proof of theorem (2) goes as follows. We have

$$\sum_{h\in H} \chi(ahah) = \sum_{h\in H}\sum_{i=1}^{d} D(ahah)_{ii} = \sum_{i,k,l} D(a^2)_{ik} \sum_{h\in H} D(a^{-1}ha)_{kl}D(h)_{li}, \quad (1.2.5.18)$$

and this gives zero if $D(H)$ and $D(a^{-1}Ha)^*$ are non-equivalent, because of the orthogonality relations. If the two representations are equivalent, we take for convenience unitary representations. Then there is a unitary matrix U with

$$D(a^{-1}ha)^* = U^{-1}D(h)U.$$

Then we have

$$\begin{aligned}\sum_{h\in H} \chi(ahah) &= \sum_{ik\ell mn} D(a^2)_{ik}(U^{*-1})_{km} \sum_{h\in H} D(h)^*_{mn}U_{n\ell}D(h)_{\ell i} \\ &= (N/d)\sum_{i,k,\ell} D(a^2)_{ik}(U^{*-1})_{k\ell}U^*_{i\ell} \\ &= (N/d)\sum_{i,k} D(a^2)_{ik}(U^*U)_{ik} \\ &= \pm(N/d)\sum_{i,k} D(a^2)_{ik}D(a^{-2})_{ki} = \pm N.\end{aligned}$$

This proves theorem (2).

In the special case of a group G in which the time reversal $1'$ occurs as element, one may choose $a = 1'$. In this case, a^2 is the identity and the expressions simplify. Theorem (1) now states that an irreducible d-dimensional representation $D(H)$ of an orthochronous group can occur as irreducible component in the restriction of an irreducible m-dimensional co-representation of $H \times \{E, 1'\}$, with

$m = 2d$ if $D(H)$ nonequivalent to $D(H)^*$

$m = 2d$ if $D(H) = UD(H)^*U^{-1}$ and $UU^* = -E$

$m = d$ if $D(H) = UD(H)^*U^{-1}$ and $UU^* = +E$,

which correspond to, respectively, [*cf.* theorem (2)]

$$\sum_{h\in H} \chi(h^2) = \begin{cases} 0 \\ -N \\ +N \end{cases}. \quad (1.2.5.19)$$

For a spinless particle, the time-reversal operator is the complex conjugation θ. This generates a co-representation of the group $\mathbb{Z}_2$. The symmetry group is the direct product of the point group H and $\mathbb{Z}_2$. Compared to the degeneracy d of a state characterized by the irreducible representation $D(H)$, the degeneracy is double ($m = 2d$) for the first two cases and the same for the third case. When it is a particle with spin $\frac{1}{2}$, the time-reversal operator is $\sigma_2\theta$, which is of order 4. If one takes for the coset representative a the time reversal, one has $D(a^2) = -E$. Therefore, the degeneracy is now doubled in the first and third case, and the same for the second. This is Kramer's degeneracy.

1.2.6. Tables

In the following, a short description of the tables is given in order to facilitate consultation without reading the introductory theoretical Sections 1.2.2 to 1.2.5.

Table 1.2.6.1. Finite point groups in three dimensions. The point groups are grouped by isomorphism class. There are four infinite families and six other isomorphism classes. (Notation: C_n for the cyclic group of order n, D_n for the dihedral group of order $2n$, T, O and I the tetrahedral, octahedral and icosahedral groups, respectively). Point groups of the first class are subgroups of $SO(3)$, those of the second class contain $-E$, and those of the third class are not subgroups of $SO(3)$, but do not contain $-E$ either. The families C_n and D_n are also isomorphism classes of two-dimensional finite point groups.

Table 1.2.6.2. Among the infinite number of finite three-dimensional point groups, 32 are crystallographic.

Table 1.2.6.3. Character table for the cyclic groups C_n. The generator is denoted by α. The number of elements in the conjugacy classes (n_i) is one for each class. The order is the smallest nonnegative power p for which $A^p = E$. The n irreducible representations are denoted by Γ_i.

Table 1.2.6.4. Character tables for the dihedral groups D_n of order $2n$. n_i is the number of elements in the conjugacy class C_i. The irreducible representations are denoted by Γ_i.

references