Notes on group theory and its application to spettroscopy

(work in progress)

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Contents

1 Recall of matrices definitions and properties

1.1 dimension

The dimension of a square matrix is the number of rows that is equal to the number of columns.

1.2 orthogonal and unitary matrices

It's useful to recall the following definitions:

- inverse of a matrix = $A\ A^{-1} = \mathbb{I}$
- transposed (numerical) matrix A^T = swap each row with the column, in the same order
- orthogonal (numerical) matrix = a real matrix for which the transposed matrix is also inverse: $A\ A^T = \mathbb{I}$. It can be shown that this property is equivalent to the following other: all the rows form an orthonormal set of vectors, and so do all the columns.
- unitary (numerical) matrix = a complex valued matrix A for which the conjugate transposed matrix (also called *hermitian adjoint* and denoted with $A^\dagger$) is also inverse: $A\ A^\dagger = \mathbb{I}$

1.3 trace

The trace of a square matrix as the sum of the elements on the principal diagonal.

Is possible to demonstrate (theorem) that the trace doesn't change if we apply a similarity transformation.

2 Definitions

2.1 Group

Definition 2.1 (definition of a group) *A group G is a set of elements with a binary operation $(G \ X \ G) \rightarrow G$ which assigns to every ordered pair of elements $x, y \in G$ a unique third element of G (usually called the product of x and y) denoted by xy such that the following four properties are satisfied:*

1. *Closure:* $R, S \in G \Rightarrow RS \in G$.
2. *Associative law:* $R, S, K \in G \Rightarrow R(SK) = (RS)K$.
3. *Identity element:* $\exists \ E \in G : ER = RE = R \forall R \in G$.
4. *Inverses:* $\forall R \in G, \exists \ R^{-1} \in G : RR^{-1} = R^{-1}R = E$.

2.1.1 order of a group

Definition 2.2 (order of a group) *the number of elements of a group is called the* order *of the group*

2.1.2 multiplication table

Definition 2.3 (multiplication table) *To describe a finite group, a table that gives the result for all the possible multiplications is used:*

G	E	A_2	A_3
E	A_{11}	A_{12}	A_{13}
A_2	A_{21}	A_{22}	A_{23}
A_2	A_{31}	A_{32}	A_{33}

(cfr appendix G.0.2)

2.1.3 subgroup

Definition 2.4 (subgroup) *A subset of elements of the group that still fulfils the definitions of a group. (note: in a subgroup the identity has to be present)*

2.1.4 similarity transformations

If we choose an element X of the group, we can "transform" it using another element of the group Z and it's inverse Z^{-1} in the following way:

$$Z^{-1}XZ = Y \tag{1}$$

it is easy to show that

$$X = ZYZ^{-1} \tag{2}$$

the two elements of the group, X and Y are said to be *conjugate*, or *similar*, and the transformation is called a similarity transformation.

2.2 Class

A *class* is a complete set of elements which are conjugate to one another. In other words, if I choose an element of the group, and I find *all* the other elements of the group that are *similar* to it, I build the class to which the element belongs to.
In general (but not always) operations of a point group that produce similar effects (i.e. rotations, reflections) are in the same class.
Example, classes of the C_{3v} group (cfr [HB80] page 48)

3 Representations

3.1 definition of representation

In general a group is an "abstract mathematical entity", defined by it's multiplication table (i.e. the relationship between it's elements, i.e. its "internal structure"). So, any group of mathematical objects that is homomorphic to the abstract group is a *representation* of the group. However it is usual to use the term *representation* of a group for any group of square numerical matrices homomorphic to the abstract group, where the "row by column" multiplication between matrices is used as the internal operation of the group.

If each matrix of the representation is different, the matrices group is *isomorphic* to the abstract group, and not only homeomorphic.
To set the notation, if we associate the matrix $D(R)$ to the abstract group element R, we have:

$$\forall R, S \in G, D(R)D(S) = D(RS) \tag{3}$$

This relation provides that the multiplication table of the two groups (abstract and matrices) is the same.

3.2 dimension (or dimensionality) of a representation

Definition 3.1 (dimensionality of a representation) *The dimension of the matrices of a representation is said to be the* dimensionality *(or just* dimension*) of the representation.*

3.3 equivalent representations

Definition 3.2 *two representations are equivalent if exists a single matrix (of any form) that transforms the elements of one representation into the elements of the other*

(cfr [WG59] pag 73)

3.4 irreducible representation

In general the matrices of a representation are *reducible*, i.e. it is possible do partially diagonalise them (with a *similarity transformation*) so that they get the form of a *block* *diagonal matrix*. Since the matrix multiplication will not mix the blocks, *each block will have the same multiplication table*, i.e. each block will be a good representation of the group.

We could take only one block as representation, and try to (block) diagonalise them. If no more diagonalisation is possible, the representation is said to be an *irreducible representation* (cfr [WG59] pag 73)

4 Theorems on representations

4.1 Important theorems about the orthogonality of the matrix elements of irreducible representations

Theorem 4.1 (Orthogonality relation for the coefficients of an unitary irred. repr.) *(unitary representations) If*

$$D^{(1)}(E), D^{(1)}(A_2), \cdots, D^{(1)}(A_h)$$

and

$$D^{(2)}(E), D^{(2)}(A_2), \cdots, D^{(2)}(A_h)$$

are two inequivalent*, irreducible, unitary representations of the same group, then*

$$\sum_R D^{(1)}(R)^*_{\mu\nu}\; D^{(2)}(R)_{\alpha\beta} = 0 \tag{4}$$

holds for all elements $\mu\nu$ and $\alpha\beta$. For the elements of a single unitary, irreducible representation, we have

$$\sum_R D^{(1)}(R)^*_{\mu\nu}\; D^{(1)}(R)_{\mu'\nu'} = \frac{h}{l_1}\delta_{\mu\mu'}\delta_{\nu\nu'} \tag{5}$$

where h is the order of the group, l_1 is the dimension of the representation, and the symbol $\sum_R$ means sum over all the group elements $E, A_2, A_3, \cdots, A_h$ of the group.
([WG59] theor. 4, pag. 79)

Theorem 4.2 (Orthogonality relation for the coefficients of an irred. repr.) *(general case)*
If

$$D^{(1)}(E), D^{(1)}(A_2), \cdots, D^{(1)}(A_h)$$

and

$$D^{(2)}(E), D^{(2)}(A_2), \cdots, D^{(2)}(A_h)$$

are two inequivalent, *irreducible, representations of the same group (*not necessarily unitary*), then*

$$\sum_R D^{(2)}(R)_{\alpha\beta}\ D^{(1)}(R)^{-1}_{\mu\nu} = 0 \tag{6}$$

holds for all elements $\mu\nu$ and $\alpha\beta$.
For the elements of a single irreducible representation, we have

$$\sum_R D^{(1)}(R)_{\mu\nu}\ D^{(1)}(R^{-1})_{\mu'\nu'} = \frac{h}{l_1}\delta_{\mu\mu'}\delta_{\nu\nu'} \tag{7}$$

([WG59] formula (9.31a) pag. 81)

(remember that for unitary matrices $D^{(1)}(R^{-1}) = [D^{(1)}(R)]^{-1} = D^{(1)}(R)^{\dagger}$, so the case of unitary representations is consistent with this general case)

4.2 irreducible representations and classes

Theorem 4.3 *the number of the irreducible representations of a group is equal to the number of classes of the group.*

(this was not taken from [WG59])

5 Character of a representation

(cfr [WG59], pag 81-83)

5.1 definition of characters

Definition 5.1 (Character of a representation) *Given a representation of a group, for each matrix we can consider its* trace*, which we denote as*

$$\chi^{(j)}(R) \equiv \sum_{\mu=1}^{l_j} D^{(j)}(R)_{\mu\mu}. \tag{8}$$

In this way, for each representation we have a set of h numbers $\chi^{(j)}(E), \chi^{(j)}(A_2), \cdots, \chi^{(j)}(A_h)$. This set of numbers will be called the character *of the representation.*

The specification of a representation by means of the character (set of $\{\chi^{(j)}(R)\}$ values) has the advantage to be invariant under similarity transformations.

Theorem 5.1 *the characters of the elements in the same class are the same*

(cfr [WG59], end of page 83)

5.2 definition of normalised characters

Let be G a group, and let it consist of k classes $C_1, C_2, \cdots, C_k$, and let $g_1, g_2, \cdots, g_k$ be the number of elements for each class $(g_1 + g_2 + \cdots + g_k = h)$.
Since the characters of the matrices that represent group's elements in the same class are equal, we can introduce the k characters that will be called *characters of the classes*, and will be denoted with

$$\chi^{(j)}(C_\rho)$$

with this notation, the orthogonality relation 7 becomes:

$$\sum_{\rho=1}^{k} \chi^{(j)}(C_\rho)\ \chi^{(j')}(C_\rho)^*\ g_\rho = h\ \delta_{jj'} \tag{9}$$

Definition 5.2 (normalised characters of a representation) *The scalars $\chi^{(j)}(C_\rho) \cdot \sqrt{\frac{g_\rho}{h}}$ are called* normalised characters

6 Theorems on characters

6.1 orthogonality of characters sets

(cfr [WG59] pag 83)

Theorem 6.1 *The set of characters of the irreducible representations of a group form an orthogonal vector system in the space of the group elements. In other words, two characters of two irreducible representations (two vectors of dimension h) are orthogonal:*

$$\sum_R \chi^{(j)}(R)\ \chi^{(j')}(R)^* = h\delta_{jj'} \tag{10}$$

6.2 orthonormality of normalised characters sets

Theorem 6.2 *The normalised characters $\chi^{(j)}(C_\rho)\sqrt{\frac{g_\rho}{h}}$ form an orthonormal vector system in the k-dimensional space of the classes of a group.*

7 Application to quantum mechanics

(cfr. [WG59] cap 11, pag. 102)

7.1 two particles systems

(cfr. [WG59] section 2, pag. 102) Let's consider a system of two indistinguishable particles. Let's assume that the particles have one degree of freedom each. Let's also consider a *non degenerate* eigenvalue of the energy E, and its eigenfunction $\psi(x_1, x_2)$:

$$H\psi(x_1,x_2) = E\psi(x_1,x_2)$$
$$-\frac{\hbar^2}{2m}\left(\frac{\mathrm{d}^2}{\mathrm{d}x_1^2} + \mathrm{d}^2\mathrm{d}x_2^2\right)\ \psi(x_1,x_2) + V(x_1,x_2)\psi(x_1,x_2) = E\psi(x_1,x_2)$$

If the particles are identical, by definition the physics of the system have to be the same if we swap the two particles. To mathematically represent the swapping we introduce an operator P that acts on the wave functions of the system, defined in the following way:

$$P\psi(x_1, x_2) \equiv \psi(x_2, x_1) \tag{11}$$

where with $\psi(x_2, x_1)$ we mean a function where the role of the x_1 and x_2 coordinates is swapped. To the operator P is associated an operator R that acts on the *space of configurations*, and that swaps the coordinates:

$$\begin{aligned} \begin{pmatrix} x_2 \\ x_1 \end{pmatrix} &= R \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \\ \begin{pmatrix} x_2 \\ x_1 \end{pmatrix} &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \end{aligned}$$

The physical significance of P_R is to produce from the wavefunction ψ of a state, the wavefunction $P_R\psi$ in which the role of the particles is interchanged: new coordinates x_1', x_2' play the role of coordinates x_1, x_2.

7.2 more general case: multiple particles

(cfr. [WG59], section 2 pag 104)
(here more insight is needed, to understand why degenerate eigenvalues are mentioned. cfr the book)

We can generalise the concept to a system of more than two particles, each of which have more that one degree of freedom (here x_i run over all the configurations space coordinates):

$$-\frac{\hbar^2}{2m}\left(\frac{\mathrm{d}^2}{\mathrm{d}x_1^2} + \frac{\mathrm{d}^2}{\mathrm{d}x_2^2} + \cdots\right)\ \psi(x_1, x_2, \cdots) + V(x_1, x_2, \cdots)\psi(x_1, x_2, \cdots) = E\ \psi(x_1, x_2, \cdots)$$

and to any possible transformation on the space of configurations (here R must be an orthogonal transformation):

$$\begin{pmatrix} x'_1 \\ x'_2 \\ \vdots \\ x'_n \end{pmatrix} = R \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}. \tag{12}$$

As before, we can define an operator P_R that acts on the wave functions of the system and is associated to R, in the following way:

$$P_R\psi(x'_1, x'_2, \cdots, x'_n) \equiv \psi(x_2, x_1, \cdots, x_n). \tag{13}$$

Two points of the configurations space $\vec{x}$ and $\vec{x'}$ that are transformed into one other by R and it's inverse R^{-1} have to represent the same physical state for the system (by definition of identical particles.

this implies $\Rightarrow$

ψ and $P_R\psi$ also also represent two identical quantum states.

this implies $\Rightarrow$

if ψ_χ is a non-degenerate eigenfunction with eigenvalue E_χ the same stationary Schrödinger equation must hold for ψ_χ and $P_R\psi_\chi$:

$$\mathcal{H}\psi_\chi = E\psi_\chi \tag{14}$$

$$\mathcal{H}P_R\psi_\chi = E_\chi P_R\psi_\chi \tag{15}$$

this implies $\Rightarrow$

the hamiltonian of the system $\mathcal{H}$ is *invariant under the action of the operator* P_R

this implies $\Rightarrow$

all the possible transformations $\{R\}$ and $\{P_R\}$ form two isomorphic groups. The "row by column" multiplication for the matrices is the multiplication for the group $\{R\}$, while for the operators $\{P_R\}$ [...] (caution, here the definition of the multiplication for the operators is delicate, cfr [WG59] page 105 - 106)
(cfr. [WG59] section 1, 2, pag 102, 104)

7.3 linearity

(cfr. [WG59] section 3, pag 107)

Theorem 7.1 *Operators* P_R *are linear:*

$$P_R(a\ \psi_1 + b\ \psi_2) = aP_R\psi_1 + bP_R\psi_2 \tag{16}$$

7.4 physical meaning of the invariance group of $\mathcal{H}$

(cfr. [WG59] section 4, pag 107)
For the most part, the group $\{P_R\}$ of the hamiltonian of a quantum system can be determined from *general physical considerations.*

In general, there are physical quantities (observables) from which point of view the state ψ and the state $P_R\psi$ are equivalent: the measurement of the observable gives the same results with the same probabilities.
We say that the observable is *symmetric under the transformation* P_R, and the group of operators $\{P_R\}$ is called the *the symmetry group of the observable* .

Definition 7.1 *The group of the operators that interchange identical particles and plus those that perform rotations of the coordinates reference that leave the system unchanged is called* the symmetry group (or invariance group) of the hamiltonian *of a quantum system.*

7.5 general case of degenerate eigenvalues

Let be E_χ is a degenerate eigenvalue of l degeneracy. This means that there are l linearly independent eigenfunctions

$$\varphi_i \in \{\varphi_1, \varphi_2, \cdots, \varphi_l\} \tag{17}$$

that form a basis for the *eigenspace of degeneracy* of E_χ, for which holds:

$$\mathcal{H}\varphi_i = E_i\varphi_i. \tag{18}$$

If we apply an operator of symmetry P_R to one of these eigenfunctions, this time the fact that $P_R\varphi_i$ has to describe "the same physical state" doesn't mean that $P_R\varphi_i$ is proportional to φ_i (i.e. that $P_R\varphi_i = \kappa\varphi_i$). In this case $P_R\varphi_i$ can be a linear combination of the (17). If we call $D(R)_{\chi\nu}$ the coefficients of this linear combination, we have:

$$P_R\ \varphi_\nu = \sum_{\chi=1}^{l} \underbrace{D(R)_{\chi\nu}}_{coefficient}\ \varphi_\chi. \tag{19}$$

With these definitions, the following theorem holds

Theorem 7.2 *The coefficients defined in (19) form a representation* $\{D(R)\}_{R\in G}$ *of the invariance group of the hamiltonian* G *of the system with dimension* l*.*

Then if we apply a change of base in the eigenspace and move to another eigenbase with a transformation, using a matrix α so that

$$\varphi'_\mu = \sum_{\nu=1}^{l} \alpha_{\nu\mu}\varphi_{nu} \tag{20}$$

it is possible to show that the new representation of the group G obtained from

$$\forall R \in G, P_R \varphi'_\chi = \sum_{\lambda=1}^{l} D'(R)_{\chi\lambda} \varphi'_\lambda \tag{21}$$

is another representation that is *equivalent to the previous* $\{D(R)\}_{R\in G}$*, where the similarity transformation is the matrix* α*.*

In other words, the following theorem holds:

Theorem 7.3 *The representation of the group of invariance for the hamiltonian of a system which belongs to a particular eigenvalue is uniquely determined up to a similarity transformation*

(cfr [WG59] section 6, pag110)

Moreover

Theorem 7.4 *If we start from an orthogonal eigenbase, the particular representation* $\{D(R)\}_{R\in G}$ *(obtained via (19)) is* unitary*.*

(cfr [WG59] section 7, pag111)

wrap-up comment To each eigenvalue of the energy E it is associated a representation of the group of invariance of the system (group of symmetry for the hamiltonain of the group). The dimension of the representation is equal to the degeneracy of the eigenvalue.

8 Eigenfunctions and representations

(cfr [WG59] cap. 12 pag. 112)

8.1 Functions belonging to rows of a representation

(cfr [WG59] cap.12, section 1 pag. 112)

Definition 8.1 *Let $D^{(j)}(R)$ be an irreducible unitary representation of dimension l_j of the group of unitary operators P_R, and let $f_1^{(j)}, f_2^{(j)}, \cdots, f_{l_j}^{(j)}$ be l_j wave functions for which*

$$P_R \ f_\mu^{(j)} = \sum_{\lambda=1}^{l_j} D^{(j)}(R)_{\lambda\mu} \ f_\lambda^{(j)} \qquad (\mu \in \{1, 2, \cdots l_j\}) \tag{22}$$

holds for all P_R. A function $f_\chi^{(j)}$ is said to belong to the χ-th row of the irreducible representation $D^{(j)}(R)$ if there exist $l_j - 1$ other "partner" functions $\{f_1^{(j)}, f_2^{(j)}, \cdots, f_{\chi-1}^{(j)}, f_{\chi+1}^{(j)}, \cdots, f_{l_j}^{(j)}\}$ such that all the $f_\lambda(j)$ satisfy (22).

Theorem 8.1 *The relation:*

$$\sum_R D^{(j)}(R)^*_{\chi\chi} P_R \ f_\chi^{(j)} = \frac{h}{l_j} \ f_\chi^{(j)} \tag{23}$$

is necessary and sufficient condition for a function $f_\chi^{(j)}$ to belong to the χ-th row of the irreducible representation $D^{(j)}(R)$.

Theorem 8.2 *a linear combination of functions that belong to the χ-th row of a representation $D^{(j)}$ also belong to the same row of the same representation*

(cfr [WG59] cap.12, section 2 pag. 113)

8.2 linear combinations functions belonging to rows of representations

(cfr [WG59] cap.12, section 3 pag. 113)

Theorem 8.3 *A generic function F of the hilbert space of the wavefunctions of the system can be written as linear combination of functions belonging to rows of the same representation, summing over the group's elements and for each element, on the rows of the representation*

8.3 Orthogonality of functions belonging to rows of irreducible representations

(cfr [WG59] cap.12, section 4 pag. 115)

8.4 Operator that commutes with the operators of a symmetry group

(cfr [WG59] cap.12, section 5 pag. 115)

8.5 Expansion of functions over characters of a symmetry group

(cfr [WG59] cap.12, section 6 pag. 117)
"The general theorems on functions stated here can be summarised by the following statement:"

Theorem 8.4 *Functions belonging to different irreducible representations or to different rows of the same irreducible representation belong to different eigenvalues of some hermitian operator. This operator commutes with all the operators of the symmetry group*

Theorem 8.5 *one irreducible representation correspond to each eigenvalue, and one row of an irreducible representation corresponds to each eigenfunction; the partners of an eigenfunctions (different rows of the same irreducible representation) are the other eigenfunctions belonging to the same degenerate eigenvalue*

(cfr [WG59] cap.12, pag. 119)

Note - Very many eigenvalues will correspond to any given representation

9 Symmetry, representations and perturbation theory

(cfr [WG59] cap.12, section 8-12 pag. 120-123)

1 We can imagine the unperturbed hamiltonian having a certain symmetry group, and the perturbation term to have a different (smaller) one. The lifting of symmetries leads to removal of degeneracy: eigenfunctions that belong to the same irreducible representation of the unperturbed symmetry group, belong to *different* irreducible representations of the perturbed one.

2 the perturbation theory is about diagonalising the perturbation operator, i.e. solving the eigenvalue problem for the perturbation operator.

9.1 Symmetric perturbation

(cfr [WG59] section 8 pag. 120)

Theorem 9.1 *Under a symmetric perturbation, an eigenvalue with an irreducible representation retains its representation, and there is no splitting*

Theorem 9.2 *Under a symmetric perturbation, an eigenvalue with a reducible representation will be in general split in different eigenvalues. If the representation is reduced into an irreducible representation with* a_1 *occurrences of the* $D^{(1)}(R)$ *irreducible representation,* a_2 *occurrences of* $D^{(2)}(R)$ *and so forth, in the perturbed system there will be* a_1 *eigenvalues with irreducible representation* $D^{(1)}(R)$*,* a_2 *with* $D^{(2)}(R)$ *and so forth. These values will be in general different.*

A Appendix - Other theorems on representations

A.1 theor. on the dimensions of irreducible representations

Theorem A.1 *The sum of the squares of the dimensions of all the inequivalent irreducible representations of a group is equal to the order of the group.*

(for the proof cfr appendix H)

A.2 theor. on equivalent representations

Theorem A.2 *If the same similarity transformation is applied to all the matrices of a representation, we obtain another representation, that is said to be* equivalent*.*

Proof: If $\Gamma'(A) = S^{-1}\Gamma(A)S$ is the similarity transformation, then let's show that the transformed matrices have the same "group structure" (i.e. the product):

$$\begin{aligned}\Gamma'(A)\Gamma'(B) &= \left[S^{-1}\Gamma(A)S\right]\left[S^{-1}\Gamma(B)S\right] \\ &= S^{-1}\Gamma(A)SS^{-1}\Gamma(B)S \\ &= S^{-1}\Gamma(A)\,\mathbb{I}\,\Gamma(B)S \\ &= S^{-1}\Gamma(A)\Gamma(B)S \\ &= S^{-1}\Gamma(AB)S \\ &= \Gamma'(AB)\end{aligned}$$

A.3 theor. on unitary repr.

Theorem A.3 *Any representation by matrices with nonvanishing determinants can be transformed into a representation by unitary matrices through a similarity transformation ([WG59] theor. 1, pag. 74)*

(this is a preparation for theorem 4.1)

A.4 theor. on equivalent representations

Theorem A.4 *If two repr. are unitary and equivalent (equivalent means that exist "a matrix" of any form that transforms the one into the other) then the two repr. can be transformed into one another by a unitary transf. ([WG59] theor. 1a, pag. 78)*

(this is a preparation for theorem 4.1)

B Appendix - other theorems on characters

B.1 unicity of characters

Corollary B.1 *Two inequivalent irreducible representations cannot have the same character. Irreducible representations with equal characters are equivalent.*

B.2 characters and classes

Corollary B.2 *In a given representation, elements of the same class have the same character*

Thus, in stating the set of characters for a representation it suffices to give the character for one element of each class of the group. This can be considered the character of the class.

B.3 reduction of a representation

Theorem B.3 *The irreducible components of an irreducible representation are uniquely determined (except for order). In other words, a reducible representation has an unique set of irreducible representations that forms it.*

B.4 characters of reducible representations

Theorem B.4 *The number of times an irreducible representation appears in the reduced form of a reducible representation is completely determined by the character of the representation*

Corollary B.5 *Equality of the characters is necessary and sufficient condition for the equivalence of two representations*

C characters of the C_{3V} group [Web10]

D Mulliken symbols

(cfr. [HB80] page 49 and 50)

E Direct product of groups [Wik10a]

In group theory one can define the direct product of two groups $(G, *)$ and (H, o), denoted by $G \times H$. For *abelian groups* which are written additively, it may also be called the direct sum of two groups, denoted by $G \oplus H$.
It is defined as follows:

- as set of the elements of the new group, take the "cartesian product" of the sets of elements of G and H, that is$\{(g, h) : g \in G, h \in H\}$;
- on these elements put an operation, defined elementwise:

$$(g, h) \times (g', h') = (g * g', h \circ h') \tag{24}$$

(Note the operation * may be the same as $\circ$.)

This construction gives a new group. It has a normal subgroup isomorphic to G (given by the elements of the form $(g, 1)$), and one isomorphic to H (comprising the elements (1, h)).

The reverse also holds, there is the following recognition theorem: If a group K contains two normal subgroups G and H, such that $K = GH$ and the intersection of G and H contains only the identity, then $K = G \times H$. A relaxation of these conditions gives the [[semidirect product]].

As an example, take as G and H two copies of the unique (up to isomorphisms) group of order 2, C_2: say $\{1, a\}$ and$\{1, b\}$. Then $C_2 \times C_2 = \{(1, 1), (1, b), (a, 1), (a, b)\}$, with the operation element by element. For instance, $(1, b)*(a, 1) = (1*a, b*1) = (a, b), and (1, b)* (1, b) = (1, b_2) = (1, 1)$.

With a direct product, we get some natural group homomorphisms for free: the projection maps $\pi_1 \colon G \times H \to G \quad \text{by} \quad \pi_1(g, h) = g$, $\pi_2 \colon G \times H \to H \quad \text{by} \quad \pi_2(g, h) = h$ called the "'coordinate functions"'.

Also, every homomorphism f on the direct product is totally determined by its component functions $f_i = \pi_i \circ f$.

For any group $(''G'', *)$, and any integer $n \geq 0$, multiple application of the direct product gives the group of all n-tuples G^n (for $n = 0$ the trivial group). Examples: Z^n R^n (with additional vector space structure this is called Euclidean space)

F Notation [Wik10b]

In geometry a point group in three dimensions is an isometry group in three dimensions that leaves the origin fixed (correspondingly, an isometry group of a sphere).

It is a *subgroup* of the orthogonal group $O(3)$, the group of all isometries which leave the origin fixed, or correspondingly, the group of orthogonal matrices. O(3) itself is a subgroup of the Euclidean group E(3) of all isometries.

Symmetry groups of objects are isometry groups. Accordingly, analysis of isometry groups is analysis of possible symmetries. All isometries of a bounded 3D object have one or more common fixed points. We choose the origin as one of them.

Symmetry groups of objects are isometry groups. Accordingly, analysis of isometry groups is analysis of possible symmetries. All isometries of a bounded 3D object have one or more common fixed points. We choose the origin as one of them. The symmetry group of an object is sometimes also called full symmetry group, as opposed to its rotation group or proper symmetry group, the intersection of its full symmetry group and the rotation group SO(3) of the 3D space itself. The rotation group of an object is equal to its full symmetry group if and only if the object is chiral.

F.1 List of symmetry operations

The operations of symmetry allowed for an object form a group, where the multiplication is represented by the action of two operations taken one after the other.

Here we list the possible *punctual* symmetry operations (punctual = leave at least one point non-moved. Non punctual (spatial) symmetry operations are *translations*.

symbol	**name**	**description**
E	identity	leave the object unchanged
σ	reflection	
C_n	rotation	rotate of an angle $2\pi/n$ around an axis
S_n	improper rotation	rotation of $2\pi/n$ followed by a reflection through a plane perpendicular to the axis of rotation
i	inversion	map all points at the same distance but the other side of the "inversion centre", along their connecting line

The following holds:

$S_2 \equiv i$.

F.1.1 number of rotation symmetries

theorem: the smallest angle of rotaional symmetry is 360/6, i.e he rotational series C_n has 6 members, wih $1 \leq n \leq 6$.

proof

see solid state noes

G The point groups

Here is the list of all the possible *point* groups

(to be updated! - cfr [HB80] page 26)

C_n	n-fold rotational symmetry	cyclic symmetry
C_{nh}	n-fold rotational symmetry with an additional reflection symmetry plane perpendicular to the rotation axis (horizontal plane)	cyclic symmetry
C_{nv}	n-fold rotational symmetry with additional reflection symmetry planes containing the rotation axis (vertical planes)	cyclic symmetry
D_n	n-fold rotational symmetry	dihedralsymmetry
D_{nh}	n-fold rotational symmetry with an additional reflection symmetry plane perpendicular to the rotation axis (horizontal plane)	dihedralsymmetry
D_{nd}	n-fold rotational symmetry with additional reflection symmetry planes containing the rotation axis (vertical planes)	dihedralsymmetry
S_{2n}	n-fold rotational symmetry with additional reflection symmetry planes containing the rotation axis (vertical planes)	rotation and inversion about the origin (also called “improper rotation”)

G.0.2 Example of a group

the identity, the rotation of $2\pi/3$ (C_3) and the rotation of $2\pi(2/3)$ ($C_3C_3 = C_3^2$) form a group. To describe the multiplication of this group, a table is used:

C_3	E	C_3	C_3^2
E	E	C_3	C_3^2
C_3	C_3	C_3^2	E
C_3^2	C_3^2	C_3	E

H proof of the theorem on the dimensions of irreducible representations

(cfr A.1)

Statement - The sum of the squares of the dimensions of all the inequivalent irreducible representations of a group is equal to the order of the group.

Proof - Let's consider a representation of a group:

$$D^{(1)}(E), D^{(1)}(A_2), \cdots, D^{(1)}(A_h)$$

If we fix two integers μ and ν smaller than the dimension l_1 of the representation, we can associate to each element of the group the $\mu\nu$ element of the irreducible representation

$$D^{(1)}(A_1)_{\mu\nu} = \mathfrak{v}_{A_1}^{(\mu\nu)} \ ; \ D^{(1)}(A_2)_{\mu\nu} = \mathfrak{v}_{A_2}^{(\mu\nu)} \ ; \cdots ; \ D^{(1)}(A_h)_{\mu\nu} = \mathfrak{v}_{A_h}^{(\mu\nu)}$$

where h is the order of the group.
In this way we can define l_1^2 vectors of length h.
Theorem 4.2 means that every pair of these l_1^2 vectors are orthogonal. Moreover, the same theorem states that if we choose another inequivalent irreducible representation

$$D^{(2)}(E), D^{(2)}(A_2), \cdots, D^{(2)}(A_h)$$

of the same group, and we define

$$D^{(2)}(A_1)_{\alpha\beta} = \mathfrak{w}_{A_1}^{(\alpha\beta)} \ ; \ D^{(2)}(A_2)_{\alpha\beta} = \mathfrak{w}_{A_2}^{(\alpha\beta)} \ ; \cdots ; \ D^{(2)}(A_h)_{\alpha\beta} = \mathfrak{w}_{A_h}^{(\alpha\beta)}$$

we have that all the l_1^2 $\mathfrak{v}$ vectors are orthogonal to all the l_2^2 $\mathfrak{w}$. Note that vectors $\mathfrak{v}$ and $\mathfrak{w}$ have the same length h, which is the order of the group.

Let's now consider all the inequivalent irreducible representations of the same group, each of which has dimensionality l_j. Let their number be c. We can assume that all the representations are unitary.

From theorem 4.1 we can write that:

$$\left.\begin{array}{l} \sum_R \sqrt{\frac{l_j}{h}}\, D^{(j)}(R)_{\mu\nu} \ \ \sqrt{\frac{l_{j'}}{h}}\, D^{(j')}(R)^*_{\mu'\nu'} = \delta_{jj'}\delta_{\mu\mu'}\delta_{\nu\nu'} \\ \forall \mu,\nu \le l_j; \quad \mu'\nu' \le l_{j'}; \quad j,j' \le c \end{array}\right\} \tag{25}$$

that means that the $l_1^2 + l_2^2 + \cdots + l_c^2$ h-dimensional vectors

$$\mathfrak{v}_R^{(j)(\mu\nu)} = [D^{(j)}(R)]_{\mu\nu}$$

are mutually orthogonal. Since the space of h dimension there can exist at most h orthogonal vectors, it follows that $l_1^2 + l_2^2 + \cdots + l_c^2 \le h$.

It can be shown (omitted here) that the equality holds.

I Proof of theorem 7.2 (representation of eigenspace of degeneracy)

Recap - G is the symmetry group of the hamiltonian of a system. E_χ is a degenerate eigenvalue of l degeneracy, and $\varphi_i \in \{\varphi_1, \varphi_2, \cdots, \varphi_l\}$ is the eigenbase of the eigenspace of degeneracy. Given $R \in G$ we have that the transformed eigenfunction is not proportional to the starting eigenfunction, but is still in the eigenspace (i.e. is a linear combination):

$$P_R\, \varphi_\nu = \sum_{\chi=1}^{l} \underbrace{D(R)_{\chi\nu}}_{coefficient}\ \varphi_\chi.$$

The theorem states: *The coefficients of the linear combination form a representation* $\{D(R)\}_{R\in G}$ *of* G *with dimension* l.

Let's consider another operator of the symmetry group P_S with $S \in G$, for which holds

$$P_S\varphi_\chi = \sum_{\lambda=1}^{l} D(S)_{\lambda\chi}\varphi_\lambda \tag{26}$$

If we apply P_S to both sides of (19):

$$\begin{aligned}
P_S P_R \varphi_\nu &= P_S \sum_{\chi=1}^{l} D(R)_{\chi\nu}\varphi_\chi \\
&= \sum_{\chi=1}^{l} D(R)_{\chi\nu} P_S \varphi_\chi \qquad (P_S \text{ is linear}) \\
&= \sum_{\chi=1}^{l} D(R)_{\chi\nu} \sum_{\lambda=1}^{l} D(R)_{\lambda\chi}\varphi_\lambda \qquad (\text{we have expanded } P_S\varphi_\chi)
\end{aligned}$$

[...] to be continued, cfr [WG59] pag 109

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