

# LECTURE NOTES

AS AN AUDIT

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GROUP THEORY APPLIED TO CONDENSED MATTER PHYSICS

PHY889

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# 1 Abstract Groups

By denoting the elements of a group by certain symbols which obey a given rule of multiplication, we obtain the so-called abstract group. In this chapter, we will review some of its properties.

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## 1.1 Translation group

Suppose that the group  $G$  consists of elements  $g_1, g_2, \dots, g_m$ . Let us multiply its elements on the right by some element  $g_\ell$ , i.e., let's carry a right translation along the group.

$$g_1 g_\ell, g_2 g_\ell, \dots, g_m g_\ell \quad (1)$$

We see that each group element is encountered once and only once in this sequence. Suppose that an element could be encountered more than once such that  $g_i g_\ell = g_j g_\ell$ , then this would imply that  $g_i = g_j$  by the existence of the inverse. Since there are as many elements as elements in the group, and they are all unique, then because a group is closed this implies that all elements are represented. Let  $g_\ell$  be an arbitrary element of the group, it is clear that  $(g_\ell g_\ell^{-1}) g_\ell = g_\ell$ , and, consequently, the element  $g_\ell$  also appears in the sequence. Since the number of elements in our sequence is the order of the group, each element can be found in the sequence only once. The sequence of elements  $g_\ell g_1, g_\ell g_2, \dots, g_\ell g_m$  has the same properties.

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## 1.2 Subgroups

A set of elements belonging to a group  $G$ , to which itself forms a group with the same multiplication rule, is a subgroup of  $G$ . The remainder of the group  $G$  cannot form a group since it will not contain the unit element.

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## 1.3 The order of an element

Let us take an arbitrary element  $g_i$  of a group  $G$  and consider the powers of  $g_i, g_i^2, g_i^3, \dots$ . Since we are considering a finite group, the members of this sequence must appear repeatedly. Suppose for example that

$$g_i^{k_1} = g_i^{k_2} = g_i \quad k_2 > k_1 \quad (2)$$

$$\rightarrow g_i^{k_2} = g_i^{k_1} g_i^{k_2 - k_1} = g_i g_i^{k_2 - k_1} = g_i \implies g_i^{k_2 - k_1} = E. \quad (3)$$

The smallest exponent  $h$  for which  $g_i^h = E$  is the order of the element  $g_i$ . The set of elements  $g_i, g_i^2, \dots, g_i^h = E$  is the period of the element  $g_i$ . It is clear that the period of an element of the group is a subgroup of  $G$ . All the elements of this subgroup commute and consequently, the subgroup is Abelian.

If  $h$  is the order of the element  $g_j$ , then  $g_j^{h-1} = g_j^{-1}$ , therefore for finite groups, the existence of the inverse is a consequence of the group order properties.

*Proof.* Recall the definition of a group.

- Composition law.  $\forall a, b \in G, a \cdot b \in G$ .
- Associativity.  $\forall a, b, c \in G, (a \cdot b) \cdot c = a \cdot (b \cdot c)$ .
- Neutral element.  $\exists E \in G \ni \forall a \in G, E \cdot a = a \cdot E = a$ .
- Symmetry.  $\forall a \in G \exists a^{-1} \in G \ni a \cdot a^{-1} = a^{-1} \cdot a = E$ .

The goal of this proof is to show that for finite groups, we can relax the symmetry axiom as it is a consequence of the group order properties. This section already proved most of this proof. ■

### 1.4 Cosets

Let  $H$  be a subgroup of a group  $G$ ,  $h_1, h_2, \dots, h_m$ , where  $m$  is the order of  $H$ . Let us now construct the following sequences of sets of elements of  $G$ .

- Let us take  $g_1$  contained in  $G$ , which is not contained in  $H$ , and construct the set  $g_1 h_1, g_1 h_2, \dots, g_1 h_m$ , which we denote by  $g_1 H$ .
- Now we take another element of  $G$ ,  $g_2 \notin H$ , and set up  $g_2 H$ .

⋮

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As a result, we obtain the sequence  $H, g_1 H, g_2 H, \dots, g_{k-1} H$ . The sets  $g_i H$  are the *left cosets* of the subgroup  $H$ . We shall show that the cosets defined above have no common elements. Let us suppose that the sets  $g_1 H$  and  $g_2 H$  have one common element.

$$g_1 h_1 = g_2 h_2 \rightarrow g_2 = g_1 h_1 h_2^{-1} = g_1 h_3 \quad (4)$$

so that  $g_2$  belongs to the  $g_1 H$  set. But this conflicts with the original assumption that each element of a group  $G$  enters only one of the cosets. Since  $G$  contains  $n$  elements, and each of the cosets contains  $m$  elements, it follows that  $m = \frac{n}{k}$ . The number  $k$  is the index of the subgroup  $H$ . We see that the order of the subgroup is a divisor of the order of the group.

Similarly, we can do the same with the right cosets, in constructing the cosets, we have a choice in selecting the element  $g_i$ . It can be shown that for an acceptable choice of the elements  $g_i$ , we can obtain the same set of cosets and the same decomposition. This follows directly from the following theorem.

#### Theorem 1.1

Two cosets  $g_i H$  and  $g_k H$  (being  $g_i, g_k$  any two elements of  $G$ ) either coincide or have no common elements. If these sets have at least one common element  $g_i h_\alpha = g_k h_\beta \rightarrow g_k = g_i h_\alpha h_\beta^{-1} \implies g_k \in g_i H$ . However, any element of the set  $g_k H$  can be represented in the form  $g_k h_j = g_i h_\alpha h_\beta h_\beta^{-1} h_j = g_i h_\gamma$  and will also belong to  $g_i H$ . The group  $G$  can therefore uniquely decompose into (left or right) cosets of subgroup  $H$ .

## 1.5 Conjugate elements and Class

Let  $g$  be an element of the group  $G$  and let us construct the element  $g' = g_i g g_i^{-1}$ ,  $g_i \in G$ . The elements  $g$  and  $g'$  are said to be conjugate. Let us suppose that  $g_i$  runs over all elements of the group  $G$ . We then obtain  $n$  elements, some of which might be equal. Let the number of distinct elements be  $k$ , let us denote them by  $g_1, g_2, \dots, g_k$ . It is clear that this set includes all the elements of the group  $G$ , which are conjugate to the element  $g$ . All the elements of this set are mutually conjugate.

Let

$$g_1 = g_\alpha g g_\alpha^{-1} \quad (5)$$

$$g_2 = g_\beta g g_\beta^{-1}. \quad (6)$$

Then we have

$$g = g_\alpha^{-1} g_1 g_\alpha \quad (7)$$

$$g_2 = g_\beta g_\alpha^{-1} g_1 g_\alpha g_\beta^{-1} = g_\beta g_\alpha^{-1} g_1 (g_\beta g_\alpha^{-1})^{-1}. \quad (8)$$

The set of all the mutually conjugate elements form a *class*. Thus, the elements  $g_1, g_2, \dots, g_k$  form a class of conjugate elements. The number of elements in a class is its order. Any finite group can be denoted into a number of classes of conjugate elements. The unit element of a group is a class by itself. All the elements of a given class have the same order. The product of the elements of two classes consists of whole classes.

$$C_i C_j = \sum_k h_{ijk} C_k \quad (9)$$

where  $k$  is the multiplicity of the class. If  $g_p \in C_i C_j$ , then the entire class  $C_p$  to which  $g_p$  belongs itself belongs to the set  $C_i C_j$ . Let

$$g_p = g_i g_j \cdot \begin{cases} g_i \in C_i \\ g_j \in C_j \end{cases} \quad (10)$$

We then have that for any  $g \in G$ ,

$$g^{-1} g_p g = g^{-1} g_i g g^{-1} g_j g \in C_i C_j \quad (11)$$

it remains to show that each element of the class  $C_p$  enters the set  $C_i C_j$  the same number of times. Suppose that the element  $g_p$  enters twice,  $g_i g_j = g_p$  and  $g'_i g'_j = g_p$ , where  $g_i \neq g'_i$  and  $g_j \neq g'_j$ . Each element  $g'^{-1} g_p g'$  ( $g' \in G$ ) will  $C_p$  then be contained in  $C_i C_j$  at least twice.

$$g'^{-1} g_p g' = g'^{-1} (g_i g_j) g' = (g'^{-1} g_i g') (g'^{-1} g_j g') \quad (12)$$

$$g'^{-1} g_p g' = g'^{-1} (g'_i g'_j) g' = (g'^{-1} g'_i g') (g'^{-1} g'_j g') \quad (13)$$

if we consider the result, it follows that  $g'^{-1} g_i g' \neq g'^{-1} g'_i g'$ . The element  $g'^{-1} g_p g'$  will not be encountered more than twice, since otherwise  $g_p$  would be encountered more than twice, which contradicts the original argument. ■

## 1.6 Invariant subgroup

Let  $H$  be a subgroup of the group  $G$ , and suppose that  $g_i \in G$ . Consider the set of elements  $g_i H g_i^{-1}$ , where  $g_i$  is fixed. That set is also a group, since all the group axioms are satisfied for it. If  $g_i \in H$ , then the similar subgroup will coincide with  $H$ . If  $g_i \notin H$ , then in general we obtain a subgroup of which is different from  $H$ . When the subgroup  $H$  coincide with all its similar subgroups, it is called an invariant subgroup or a normal divisor. An invariant subgroup is represented by the letter  $N$ . It follows from this definition that if an invariant subgroup contains an element  $g \in G$ , then it will also contain the entire class to which  $g$  belongs. The invariant subgroup consists of the whole class of the group.

For an invariant subgroup of  $G$ , the left and right cosets coincide.

$$g_i N = g_i N g_i^{-1} g_i = N g_i \quad \text{since } g_i N g_i^{-1} = N. \quad (14)$$

Any group has two trivial invariant subgroups: the group itself and the unit element. Groups which do not have invariant subgroups other than the trivial ones are called simple. It would be useful to prove that  $NN = N$ .

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## 1.7 The factor group

Let  $N$  be an invariant subgroup of the group  $G$ . Let us decompose  $G$  into the cosets  $N$ ,

$$N, g_1 N, g_2 N, \dots, g_{k-1} N \quad (15)$$

and let's form a set  $g_1 N g_2 N$ , which consists of different elements  $g_1 h_\alpha g_2 h_\beta$ , where  $h_\alpha$  and  $h_\beta$  run independently over the entire subgroup  $N$ . We can see that

$$g_1 N g_2 N = g_1 g_2 g_2^{-1} N g_2 N = g_1 g_2 N N = g_1 g_2 N = g_3 N \quad (16)$$

if the set  $g_1 N g_2 N$  is called the product of sets  $g_1 N$  and  $g_2 N$ , then the product of two cosets of  $N$  will again give a coset  $N$ , since the multiplication of a coset of  $N$  by  $N$  on the right and left does not change these cosets.

$$N g_1 N = g_1 g_1^{-1} N g_1 N = g_1 N N = g_1 N \quad (17)$$

For each coset  $g_i N$ , there is a coset  $g_i^{-1} N$  such that the product is equal to  $N$ .

$$g_i^{-1} N g_i N = N N = N \quad (18)$$

The cosets of an invariant subgroup can be regarded as the elements of a new group in which  $N$  plays the role of the unit element. This group is what we call *the factor group* or *the quotient group* of the invariant subgroup. Its order is equal to the order of  $N$ .

## 1.8 Isomorphism and Homomorphism of groups

If between the elements of two groups there is a one-to-one correspondence which preserves group multiplication, then the groups are *isomorphic*. Let  $G$  and  $\tilde{G}$  be two isomorphic groups, then if elements  $g_i$  and  $g_k$  of  $G$  correspond to the elements  $\tilde{g}_i$  and  $\tilde{g}_k$  of  $\tilde{G}$ , i.e.,  $g_i \leftarrow \tilde{g}_i$ ,  $g_k \leftarrow \tilde{g}_k$ , then  $g_i g_k \rightarrow \tilde{g}_i \tilde{g}_k$ . We can reduce the investigation of a given group to that of another group isomorphic to it.

If to each element of  $G$  there corresponds only one definite element of  $\tilde{G}$ , and to each element of  $\tilde{G}$  a number of elements of  $G$ , and this correspondence is preserved under group multiplication,  $\tilde{G}$  is *homomorphic* to  $G$ . Homomorphism has the following properties:

- If  $\tilde{G}$  is homomorphic to  $G$ , then the element of  $G$  corresponds to the unit element of  $\tilde{G}$ .
- The mutually reciprocal elements of  $G$  correspond to the mutually reciprocal elements of  $\tilde{G}$ .

$$g_i g_k = E \quad \tilde{g}_i \tilde{g}_k = \tilde{E}. \quad (19)$$

- All elements of  $G$ , to which corresponds to the unit element of  $\tilde{G}$  form an invariant subgroup  $N$  of the group  $G$ . Elements  $g'_1, g'_2, \dots, g'_j$  of  $G$  correspond to  $\tilde{E}$  of  $\tilde{G}$ . The product  $g'_i g'_k$  correspond to  $\tilde{E} \tilde{E} = \tilde{E}$ .  $g'_i g'_k = g'_\ell$  and the set  $g'_1, g'_2, \dots, g'_j$  is closed with respect to group multiplication.

From (a), it contains a unit element, but since  $\tilde{E}$  is the inverse of itself and because of (b) for each element  $g'_\ell$  we can find the inverse. From  $\tilde{g} \tilde{E} \tilde{g}^{-1} = \tilde{E}$ , where  $\tilde{g}$  is an arbitrary element of  $\tilde{G}$ , it follows that  $g g_i g^{-1} = g'_f$  for an arbitrary element of  $G$ .

$$g'_1, g'_2, \dots, g'_s \quad (20)$$

forms an *invariant* subgroup of  $G$ .

## 1.9 Exercises

### Exercise 1.1

Consider the group  $S_6$ , symmetric group of order 6, with the elements  $\{E, A, B, C, D, F\}$ .

	E	A	B	C	D	F
E	E	A	B	C	D	F
A	A	E	D	F	B	C
B	B	F	E	D	C	A
C	C	D	F	E	A	B
D	D	C	A	B	F	E
F	F	B	C	E	E	D

1. Find the order of all the elements.

2. Find the possible subgroups.
3. Divide the group into cosets, and verify that this can be done uniquely.
4. Divide the group into classes of conjugate elements.
5. Find the invariant subgroups and verify that the left and right cosets are the same.
6. Write down the multiplication table for the corresponding factor groups.
7. Show that the abstract groups has the following realizations
  - (a) Permutation group of 3 elements.
  - (b) Matrix group of order 2:  $S_6$  can also be 2x2 matrices corresponding to rotations and reflections.

Recall the definition of the order of an element ([subsection 1.3](#)). Then we can compute for all elements the smallest exponent  $h$  such that  $g^h = E$ . From the table of multiplication, we can see that the order of all the elements except for the unit element and  $F$  and  $D$  is 2. The order of the unit element is 1. The order of  $D$  and  $F$  is 3.

Recall the definition of the subgroup ([subsection 1.2](#)). Then the subgroups are

$$\begin{aligned} &\{E\} \\ &\{A, E\}, \{B, E\}, \{C, E\} \\ &\{D, F, E\} \\ &\{A, B, C, D, E, F\} \end{aligned}$$

Recall the definition of the cosets ([subsection 1.4](#)). Let's start with  $H = \{E\}$ . The left and right cosets are then equal and form  $G$ . Let's continue with  $H = \{A, E\}$ , we then have the left cosets  $\{D, B\}, \{F, C\}$ .



## 2 Representations of point groups

Consider a finite group  $G$  with elements  $g_1, g_2, \dots, g_m$ . If a group  $\hat{T}$  of linear generators  $\hat{T}g_i$  in space  $R$  is homomorphic to  $G$ , then the group  $\hat{T}$  is said to form a representation of  $G$ . Homomorphism leads to  $\hat{T}g_i \cdot \hat{T}g_k = \hat{T}g_i g_k$ . If  $R$  is the  $n$ -dimensional vector space  $R_n$ , then any of its elements  $x$  can be expanded in terms of  $n$  unit vector  $\mathbf{e}_k$  forming the basis of this space.

$$x = x_1 \mathbf{e}_1 + x_2 \mathbf{e}_2 + \dots + x_n \mathbf{e}_n \quad (21)$$

The operator  $\hat{T}g_i$  will be defined if we specify its effect on each of the unit vectors  $\mathbf{e}_k$ . Suppose that

$$\hat{T}g_i \mathbf{e}_k = \sum_{r=1}^n D_{r,k}(g_i) \mathbf{e}_r. \quad (22)$$

To each element  $g_i$  of our group, we can assign a matrix  $\|D_{r,k}(g_i)\|$ . It is also clear that the unit element of the group can be associated with a unit matrix, and the inverse elements can be associated with inverse matrices.

Let us show now that for the matrices  $D$  we have

$$D(g_i)D(g_j) = D(g_i g_j) \quad (23)$$

If we apply  $\hat{T}g_i$  and  $\hat{T}g_j$  successively to the unit vector  $\mathbf{e}_k$ , we obtain

$$\hat{T}g_i \hat{T}g_j \mathbf{e}_k = \hat{T}g_i \sum_r D_{r,k}(g_j) \mathbf{e}_r \quad (24)$$

$$= \sum_{f,r} D_{r,k}(g_j) D_{f,r}(g_i) \mathbf{e}_f. \quad (25)$$

On the other hand

$$\hat{T}g_i \hat{T}g_j \mathbf{e}_k = \hat{T}_{g_i g_j} \mathbf{e}_k \quad (26)$$

$$= \sum_f D_{f,k}(g_i g_j) \mathbf{e}_f. \quad (27)$$

So  $D(g_i)D(g_j) = D(g_i g_j)$  is valid. We will show now that the matrices  $D(g_i)$  form a representation of order  $n$  of the group  $G$ . The space  $R_n$  is the representation space, and the basis of this space is the basis of the representation. By operating with  $\hat{T}g_i$  on an arbitrary vector  $\mathbf{x}$  of space  $R_n$ , we obtain

$$\hat{T}g_i \mathbf{x} = \sum_k x_k \hat{T}g_i \mathbf{e}_k \quad (28)$$

$$= \sum_{k,r} x_k D_{r,k}(g_i) \mathbf{e}_r \quad (29)$$

$$= \sum_r x'_r \mathbf{e}_r \quad (30)$$

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where  $x'_r = \sum_k D_{r,k}(g_i)x_k$ . Let us consider now the change in the representation matrix which occurs when a new basis  $\mathbf{e}'_i$  is taken in the space  $R_n$ , where the new basis is related to  $\mathbf{e}_k$  by the linear transformation

$$\mathbf{e}'_i = \sum_k V_{ki} \mathbf{e}_k \quad (31)$$

$$\mathbf{e}_i = \sum_k \{V^{-1}\}_{k,i} \mathbf{e}'_k. \quad (32)$$

Let us now apply  $\hat{T} g_i$  to  $\mathbf{e}'_i$  by using (Equation 31)

$$\hat{T} g_i \mathbf{e}'_i = \sum_k V_{ki} \hat{T} g_i \mathbf{e}_k \quad (33)$$

$$= \sum_{k,s} V_{k,i} D_{s,k}(g_i) \mathbf{e}_s \quad (34)$$

$$= \sum_{k,s,r} V_{k,i} D_{s,k} \{V^{-1}\}_{r,s} \mathbf{e}'_r \quad (35)$$

$$= \sum_r \{V^{-1}DV\}_{r,i} \mathbf{e}'_r \quad (36)$$

Thus the representation matrices undergo a similar transformation when we transform to the new basis. The representation by the matrices  $V^{-1}DV$  is equivalent to the representation by matrices  $D$ . If the representation matrices are all unitary, the representation is said to be unitary.

### 2.1 Examples of representation

- The trivial representation, which is associated with the unit matrix.
- If the group elements are linear transformations, the matrices of these transformations themselves form a representation which is isomorphic to the group.

These are the trivial invariant subgroups.

#### 2.1.1 Quadratic Form

Let's consider the derivation of one of the representations of the group  $C$  of matrices of linear transformations of invariables  $x_1, x_2, \dots, x_n$ ,  $x'_i = \sum_k C_{i,k} x_k$ . But now we are also going to consider the quadratic form

$$\sum_{i,k} a_{i,k} x_i x_k \quad a_{i,k} = a_{k,i} \quad (37)$$

Transformations of the variables  $x_i$  induces a transformation of the coefficients of this form. If we substitute  $x'_j = \sum_s \{C^{-1}\}_{j,s} x'_s$ , we obtain the following quadratic form

$$\sum_{i,k,j,\ell} a_{i,k} \{C^{-1}\}_{i,j} x'_j \{C^{-1}\}_{k,\ell} x'_\ell = \sum_{j,\ell} a'_{j,\ell} x'_j x'_\ell, \quad (38)$$

where

$$a'_{j,\ell} = \sum_{i,k} a_{i,k} \{C^{-1}\}_{i,j} \{C^{-1}\}_{k,\ell} \quad (39)$$

If we use the notation  $A = \|a_{i,k}\|$ , we can write down the transformation rule for the coefficients  $a_{i,k}$  in the matrix form  $A' = C^{-1}AC$ , where  $C^{-1}$  is the transpose of  $C$ . Let's now apply the transformations  $C_1$  and  $C_2$  to  $x_1, x_2, \dots, x_n$ .

$$A'' = C_2^{-1}A'C_2 = C_2^{-1}C_1^{-1}AC_1C_2 \quad (40)$$

$$A'' = (C_2C_1)^{-1}A(C_2C_1) \quad (41)$$

Applications of  $C_1$  and  $C_2$  is equivalent to  $C_2C_1$ . The transformation of the coefficients of the *quadratic form* form themselves a representation.

### 2.1.2 Schrödinger equation and its eigenfunctions

Let's consider a quantum mechanical system described by the Schrödinger equation

$$\left( \frac{-\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right) \psi(\mathbf{r}) = E\psi(\mathbf{r}) \quad (42)$$

We shall assume that the symmetry group for this system consists of orthogonal transformation  $u_s$ , defined by

$$\mathbf{r}' = u_s \mathbf{r} \quad (43)$$

$$\mathbf{r} = u_s^{-1} \mathbf{r}' \quad (44)$$

Since the laplace operator is invariant under any orthogonal transformation of coordinates, this yields to

$$\left( -\frac{\hbar^2}{2m} \nabla^2 + V(u_s^{-1} \mathbf{r}) \right) \psi(u_s^{-1} \mathbf{r}) = E\psi(u_s^{-1} \mathbf{r}) \quad (45)$$

Moreover since the Schrödinger equation is invariant under the  $u_s$  transformation we must have

$$V(u_s^{-1} \mathbf{r}) = V(\mathbf{r}) \quad (46)$$

and therefore, the transformed wave-function

$$\psi'(\mathbf{r}) = \hat{T}_{u_s} \psi(\mathbf{r}) = \psi(u_s^{-1} \mathbf{r}) \quad (47)$$

is also an eigenfunction of the Schrödinger equation with the same eigenvalue. Let's now consider  $\psi_1(\mathbf{r}), \dots, \psi_k(\mathbf{r})$ , a complete set of orthonormal eigenfunctions of this equation, corresponding to eigenvalue  $E$ . We will see that these functions form a basis of a group representation. Each of the transformed functions can be written in the form

$$\hat{T}_{u_s} \psi_i(\mathbf{r}) = \psi_i(u_s^{-1} \mathbf{r}) = \sum_{j=1}^k D_{j,i}(u_s) \psi_j(\mathbf{r}) \quad (48)$$

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$\hat{T}_{u_s} \psi_i(\mathbf{r})$  must also be orthonormal, since a change of the variables through an orthonormal transformation conserves the orthonormalisation condition.

$$\int \psi_i(u_s \mathbf{r}') \psi_j(u_s \mathbf{r}') d\mathbf{r} = \int \psi_i(\mathbf{r}) \psi_j(\mathbf{r}) d\mathbf{r} \quad (49)$$

Matrices  $\|D_{i,j}(u_s)\|$  should be unitary, and hence, to each transformation  $u_s$  form the symmetry group of the Schrödinger equation, we can assign a unitary matrix of order  $k$ . Let us consider  $u_s$  and  $u_t$  to be transformations in the group. Their successive applications

$$\hat{T}_{u_s} \hat{T}_{u_t} \psi_i(\mathbf{r}) = \hat{T}_{u_s} \psi_i(u_t^{-1} \mathbf{r}) \quad (50)$$

$$= \psi_i(u_t^{-1} u_s^{-1} \mathbf{r}) \quad (51)$$

$$= \psi_i((u_s u_t)^{-1} \mathbf{r}) \quad (52)$$

$$\sum_{\ell=1}^k D_{\ell,\ell}(u_s u_t) \psi_{\ell}(\mathbf{r}). \quad (53)$$

On the other hand

$$\hat{T}_{u_s} \hat{T}_{u_t} \psi_i(\mathbf{r}) = \hat{T}_{u_s} \sum_{j=1}^k D_{j,i}(u_t) \psi_j(\mathbf{r}) \quad (54)$$

$$\sum_{j=1}^k D_{j,i}(u_t) \sum_{\ell=1}^k D_{\ell,j}(u_s) \psi_{\ell}(\mathbf{r}) \quad (55)$$

$$= \sum_{\ell=1}^k \{D(u_s) D(u_t)\}_{\ell,i} \psi_{\ell}(\mathbf{r}). \quad (56)$$

$\Rightarrow$  With each energy eigenvalue, we can associate a representation and establish the possible types of symmetry of the wave functions without explicitly solving the Schrödinger equation.

### 2.2 Existence of an equivalent unitary representation

We shall show that any representation of a finite group is equivalent to a unitary representation. Suppose that we have a representation  $D$  of the group  $G$  consisting of the elements  $g_1, g_2, \dots, g_m$ . We regard the representation matrices  $D(g_i)$  as the transformation matrices in a  $n$ -dimensional space  $R_n$   $\mathbf{x}(x_1, x_2, \dots, x_n)$  and  $\mathbf{y}(y_1, y_2, \dots, y_n)$  are vectors in this space. The scalar product will be defined

$$(\mathbf{x}, \mathbf{y}) = x_1 y_1 + x_2 y_2 + \dots + x_n y_n \quad (57)$$

and  $D(g_i)$  transforms the vector  $\mathbf{x}$  into the vector  $\mathbf{x}^{(i)}$

$$\mathbf{x}^{(i)} = D(g_i) \mathbf{x} \quad (58)$$

$$x_{\alpha}^{(i)} = \sum_{\beta} D_{\alpha,\beta}(g_i) x_{\beta}. \quad (59)$$

## 2.2 Existence of an equivalent unitary representation

Let's suppose that  $D(g_i)$  is not unitary, and it does not conserve the scalar product. We shall show that it is possible to choose a new basis in  $R_n$  such that the transformation matrices for vector components will be unitary. We take the average of the scalar product over the group and construct the expression

$$\sum_{i=1}^m (D(g_i)\mathbf{x}, D(g_i)\mathbf{y}) = \sum_{i=1}^m (\mathbf{x}^{(i)}, \mathbf{y}^{(i)}). \quad (60)$$

This can be written as

$$\sum_{i=1}^m (\mathbf{x}^{(i)}, \mathbf{y}^{(i)}) = (L\mathbf{x}, L\mathbf{y}) \quad (61)$$

where  $L$  is a linear transformation.

$$\sum_{i=1}^m (D(g_i)\mathbf{x}, D(g_i)\mathbf{y}) = \left( \sum_{i=1}^m D^\dagger(g_i)D(g_i)\mathbf{x}, \mathbf{y} \right) \quad (62)$$

The matrix  $D^\dagger(g_i)D(g_i)$  is Hermitian, and it can be reduced to a diagonal form through a unitary transformation  $V$

$$d = V^{-1} \sum_{i=1}^m D^\dagger(g_i)D(g_i)V. \quad (63)$$

If we substitute  $D(g_i) = V^{-1}D(g_i)V$ , we can write

$$d = \sum_{i=1}^m V^{-1}D^\dagger(g_i)VV^{-1}D(g_i)V \quad (64)$$

$$= \sum_{i=1}^m \tilde{D}^\dagger(g_i)\tilde{D}(g_i) \quad (65)$$

and the diagonal elements of the matrices  $d$  are given by

$$d_{\alpha,\alpha} = \sum_{i=1}^m \sum_{\beta=1}^n \tilde{D}_{\alpha,\beta}^\dagger(g_i)\tilde{D}_{\alpha,\beta}(g_i) \quad (66)$$

$$= \sum_{i=1}^m \sum_{\beta=1}^n |\tilde{D}_{\alpha,\beta}(g_i)|^2. \quad (67)$$

Let us now determine the diagonal matrix  $d^{1/2}$ , whose elements are  $\{d^{1/2}\}_{\alpha,\alpha} = \sqrt{d_{\alpha,\alpha}}$ . So  $d^{1/2}d^{1/2} = d$  and if we use the self = conjoint property of  $d^{1/2}$ , we have

$$\sum_{i=1}^m (\mathbf{x}^{(i)}, \mathbf{y}^{(i)}) = (VdV^{-1}\mathbf{x}, \mathbf{y}) \quad (68)$$

$$= (d^{1/2}d^{1/2}V^{-1}\mathbf{x}, V^{-1}\mathbf{y}) \quad (69)$$

$$= (d^{1/2}V^{-1}\mathbf{x}, d^{1/2}V^{-1}\mathbf{y}). \quad (70)$$

## 2 Representations of point groups

We can go to

$$(L\mathbf{x}, L\mathbf{y}) \rightarrow L = d^{1/2}V^{-1}. \quad (71)$$

We can also show that the representation of  $G$  given by the matrices  $LDL^{-1}$  is unitary. For an arbitrary element  $g_k$  of  $G$ ,

$$(LD(g_k)\mathbf{x}, LD(g_k)\mathbf{y}) = (L\mathbf{x}, L\mathbf{y}). \quad (72)$$

Prove it for next class.

### 2.3 Reducible and irreducible representations

Suppose that a representation  $D$  of the group  $G$  is given in a space  $R_n$ . If in the space  $R_n$  there is a subspace  $R_k$ , with  $k < n$ , which is invariant under all transformations  $D$ , i.e., if for  $x \in R_k$  we have a  $D_x \in R_k$ , the representation is *reducible*. Let us take the first  $k$  unit vectors in the space  $R_n$  as the unit vectors of the subspace  $R_k$ . The representation matrix must have the following form:

$$\begin{pmatrix} D_{11} & D_{12} & \dots & D_{jk} & D_{1k+1} & \dots & D_{1n} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ D_{k1} & D_{k2} & \dots & D_{kk} & D_{kk+1} & \dots & D_{kn} \\ 0 & \dots & \dots & 0 & D_{k+1k+1} & \dots & D_{k+1n} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & \dots & 0 & D_{nk+1} & \dots & D_{nn} \end{pmatrix} \quad (73)$$

If on the other hand we cannot define an invariant subspace in  $R_n$ , the representation is *irreducible*. We shall show that if a reducible representation  $D$  is unitary, the orthogonal complement of the subspace  $R_k$ , which we denote  $R_{n-k}$ , is also invariant under the transformation of  $D$ .

Let us consider  $x \in R_k, y \in R_{n-k}$  and  $(x, y) = 0$ . Since the subspace  $R_k$  is invariant ( $D_g(x), y = 0$ ), but as we know

$$(D(g)x, y) = (x, D^\dagger(g)y) = (x, D^{-1}(g)y) \quad (74)$$

$$= (x, D(g^{-1})y) = 0, \quad (75)$$

and hence  $D(g^{-1})y \in R_{n-k}$ . When  $g$  runs over the entire group, the inverse element  $g^{-1}$  will also do so. So (Equation 75) is satisfied for all matrices of the representation in question, and the invariance  $R_{n-k}$  is proved.

If we take the unit vectors of the subspace  $R_k$ , as the first  $k$  vectors, and the remaining  $n-k$  unit vectors as the vectors of the subspace  $R_{n-k}$ , the representation matrix will be quasi-diagonal.

$$\begin{pmatrix}
 D_{11} & D_{12} & \dots & D_{jk} & 0 & \dots & 0 \\
 \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
 D_{k1} & D_{k2} & \dots & D_{kk} & 0 & \dots & 0 \\
 0 & \dots & \dots & 0 & D_{k+1k+1} & \dots & D_{k+1n} \\
 \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
 0 & \dots & \dots & 0 & D_{nk+1} & \dots & D_{nn}
 \end{pmatrix} \quad (76)$$

If the space  $R$  can be resolved into invariant subspaces, in each of them an irreducible representation is realised, then the representation  $D$  is *fully reducible*. With a suitable choice of unit vectors, the matrix of this representation is block diagonal. From this discussion, it follows that

- A unitary representation of a group is always irreducible or fully reducible.
- Any representation of a finite group is either again irreducible or fully reducible.

If a representation  $D$  is reducible, its matrices can be reduced to a quasi-diagonal form by going under the new system of unit vectors. We note that in this case, the representation matrices undergo the similarity transformation:  $D \rightarrow V^{-1}DV$ , where  $V$  is the unitary matrix relating the unit vectors of the old and new basis.

A representation  $D$  is reducible if there exists a non-singular matrix  $V$  such that  $V^{-1}DV$  is block-diagonal.

### 3 Schur's Lemmas

#### 3.1 Schur's First Lemma

*A matrix which commutes with all the matrices of an irreducible representation is a multiple of the unit matrix.*

Let  $D(g)$  represent the matrices of an irreducible representation of order  $n$  of the group  $G$ ,  $g \in G$ . Let's suppose the matrix  $M$  commutes with all the matrices  $D(g)MD(g) = D(g)M$ . Let  $R_n$  represent the space in which  $D(g)$  is realised. In this space, there should at least be one eigenvector of  $M$ , we denote it  $x$ , such that  $Mx = \lambda x$ . If we apply the transformation with the representation matrix  $D(g)$  to the vector  $x$  will have that

$$D(g)\bar{x} = \bar{x}g. \quad (77)$$

This resulting vector is also an eigenvector of  $M$  with the same eigenvalue  $\lambda$ .

$$M\bar{x}_g = MD(g)x = \lambda D(g)\bar{x} \quad (78)$$

$$= \lambda \bar{x}_g. \quad (79)$$

It follows that the space of eigenvectors of the matrix  $M$  corresponding to the same eigenvalue is invariant under the transformation  $D(g)$ . But since  $D(g)$  is irreducible, it follows that this subspace should coincide with the entire  $R_n$ , and the matrix  $M$  multiplying by any vector of the space  $R_n$  by  $\lambda$ , should be of the form

$$M = \begin{pmatrix} \lambda & \dots & 0 \\ 0 & \ddots & 0 \\ 0 & \dots & \lambda \end{pmatrix} \quad (80)$$

If a representation is fully reducible, i.e., its matrices have the quasi-diagonal form, one will always find a matrix which is not a multiple of the unit matrix and which commutes with all the matrices of this representation. Once we verify that this matrix can be taken to be the diagonal matrix in which diagonal element corresponding to the different blocks are not equal to one another.

#### 3.2 Schur's Second Lemma

##### Theorem 3.2

*Let  $D^{(j)}(g)$  and  $D^{(i)}(g)$  be the matrices of two irreducible non-equivalent representations of a group  $G$  of order  $n_1$  and  $n_2$ , respectively. Then, any rectangular matrix  $M$  with  $n_1$  columns and  $n_2$  rows which satisfies this equation*

$$MD^{(i)}(g) = D^{(i)}(g)M, \quad \forall g \in G \quad (81)$$

*is a null matrix.*



*Proof.* Let us take the Hermitian conjugate on both sides

$$D^{(i)\dagger}(g)M^\dagger = M^\dagger D^{(i)\dagger}(g) \quad (82)$$

$D^{(i)}(g)$  and  $D^{(j)}(g)$  are unitary.

$$D^{(1)-1}(g)M^\dagger = M^\dagger D^{(2)-1}(g) \quad (83)$$

$$D^{(1)}(g^{-1})M^\dagger = M^\dagger D^{(2)}(g^{-1}) \quad (84)$$

If  $g$  runs over the entire group, then  $g^{-1}$  also do so. (Equation 31) can also be re-written as

$$D^{(1)}(g)M^\dagger = M^\dagger D^{(2)}(g). \quad (85)$$

Let's multiply both sides on the left by the matrix  $M$ .

$$MD^{(2)}M^\dagger = MM^\dagger D^{(2)}(g) \quad (86)$$

$$D^{(2)}(g)MM^\dagger = MM^\dagger D^{(2)}(g) \quad (87)$$

According to Schur's first lemma, we conclude that  $MM^\dagger$  must be a multiple of the unit matrix.

$$MM^\dagger = \lambda E_{n_2} \quad (88)$$

First case:  $n_1 = n_2$ . In this case,  $M$  must be singular  $\det M = 0$ . If this was not the case, the  $MD^{(2)}(g) = D^{(2)}(g)M$  should yield the condition for the equivalence of the representation

$$D^{(1)} = M^{-1}D^{(2)}M. \quad (89)$$

But this would mean  $D^{(1)}$  and  $D^{(2)}$  are isomorphic, which is not true by hypothesis.  $M$  cannot be invertible  $\implies \det M = 0$ . If we take

$$MM^\dagger = \lambda E_{n_2} \quad (90)$$

$$\lambda = \sum_j M_{ij} \bar{M}_{ij} \quad (91)$$

$$\det M \det M^\dagger = \lambda^{n_2} \quad (92)$$

$$\lambda = 0 = \sum_j |M_{ij}|^2 \implies M_{ij} = 0 \quad (93)$$

In the other case,  $n_2 > n_1$ . We augment the matrix  $M$  so that it becomes a square matrix with  $n_2 n_1$  rows and columns. We do the same to  $M^\dagger$ . If we denote the two matrices  $\tilde{M}$  and  $\tilde{M}^\dagger$ ,

$$\tilde{M} \tilde{M}^\dagger = \lambda E_{n_2} \quad (94)$$

$$\det \tilde{M}^\dagger = \det \tilde{M} = 0 \implies M_{ij} = 0. \quad (95)$$

■

**Exercise 3.2**

Prove that any representation of a simple group (one without a normal divisor) is isomorphic to the group itself.

**Exercise 3.3**

Use Schur's first lemma to show that all irreducible representations of an Abelian group are of order 1.

**Exercise 3.4**

Use Schur's first lemma to show that the sum of irreducible representation matrices corresponding to the elements of a given class is a multiple of the unit matrix.

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## References