An Introduction to Group Theory

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I have heard many comments from students and colleagues that group theory is so abstract and boring. Is it so? I don't think so. I never feel that group theory is more abstract than quantum mechanics. People get confused because the textbook does not provides concrete examples. In the following notes, I will try to introduce all important and useful concepts in discrete group theory. To make every statement concrete, I choose the dihedral group as the example through out the whole notes.

• Definition of group

A group $\boldsymbol{G}$ is a collection of elements (could be objects or operations) which satisfy the following conditions.

1. For any two elements a and b in the group, the product $a \times b$ is also an element of the group.
2. The multiplication is associative, $(a \times b) \times c = a \times (b \times c)$.
3. There exists an unit element $\mathbf{1}$ in the group such that $\mathbf{1} \times a = a \times \mathbf{1} = a$ for every element a.
4. There must be an inverse (or reciprocal) element a^{-1} of each element a such that $a \times a^{-1} = a^{-1} \times a = \mathbf{1}$.

The above is the definition that you can find in a mathematical textbook. The key point is you need to find the "correct" rule for multiplication and then prove the closure relation (the first criterion) is true. The following three criterions can then be verified straightforwardly.

• Dihedral group

The symmetry of a square is the 4-fold dihedral $\boldsymbol{D}_4$ symmetry. (In general, a dihedral group $\boldsymbol{D}_n$ consists of n-fold rotations and inversion.) To understand a discrete group, we first identify how many elements are in the group, which is called the **order** of the group h. It is obvious that any integer multiples of $\pi/2$ rotations would leave the square invariant. There are four inequivalent rotations of this kind. A mirror inversion of the square is also an invariant transformation. Applying inversion to the previous rotations, we get another four (improper) rotations. Thus, the elements of $\boldsymbol{D}_4$ group are

$$\boldsymbol{D}_4 = \left\{\mathbf{1}, R, R^2, R^3, P, PR, PR^2, PR^3\right\}. \tag{1}$$

That is to say, the order of the group $h = 8$.

• A reducible representation

A more transparent way to realize the $\boldsymbol{D}_4$ group is the modified square dance. Suppose two couples of male and female dancers standing on four vertices of a square. They hold hands with their neighbors during the dance. How many different configurations can you see during the whole dance? The answer is eight! Each configuration is related to the original one by one of the elements in the $\boldsymbol{D}_4$ group. The configuration can be described by a four-dimensional column vector

$$|\text{configuration}\rangle = \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}, \tag{2}$$

where a, b, c, d are four dancers arranged counterclockwise.

A counterclockwise $\pi/2$ rotation R is then represented by a 4×4 matrix. Since R maps (a, b, c, d) to (d, a, b, c), it is

$$R = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}. \tag{3}$$

A π rotation is R^2 which is obtained by multiplying R with itself. You can verify that the rule of multiplication in this representation is just the ordinary matrix multiplication. The matrix of inversion P can be obtained in a similar way,

$$P = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}. \tag{4}$$

From theses two matrices, all eight elements can be constructed as listed in Table 1.

elements	rotations	elements	inverse rotations
$\mathbf{1}$	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	P	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$
R	$\begin{pmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	PR	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$
R^2	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$	PR^2	$\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$
R^3	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}$	PR^3	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$

Table 1: A four dimensional representation of the $\boldsymbol{D}_4$ group

How can we know whether this representation is reducible or not? Here I would like to play a black magic to show how many irreducible representations it contains. First, we take traces of all elements in Table 1, square them and sum them up

$$4^2 + 0^2 + 0^2 + 0^2 + 0^2 + 2^2 + 0^2 + 2^2 = 24. \tag{5}$$

Divided by the order of the group $h = 8$, the number can be decomposed into an unique integer-square sum

$$\frac{24}{8} = 3 = 1^2 + 1^2 + 1^2. \tag{6}$$

This tells us that the four-dimensional representation is reducible and can be decoupled into *three* inequivalent irreducible representations. Since the dimensions add up to four, we conclude that the representation can be decomposed into two distinct one-dimensional representations and a single two-dimensional one.

Let's check whether our conclusion is correct or not. Applying an unitary transformation U

$$U = \frac{1}{2}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & -i & -1 & i \\ 1 & i & -1 & -i \end{pmatrix}, \qquad \text{and} \qquad UU^\dagger = \mathbf{1}, \tag{7}$$

to all elements of the group, the representation of the group becomes

$$R' = URU^\dagger = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \end{pmatrix}, \qquad P' = UPU^\dagger = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix}. \tag{8}$$

You should convince yourself that the matrices after the transformation still form a representation of the same group. All elements in the group now are block diagonal with two one-dimensional blocks and a single two-dimensional one. So, what we said previously is correct. The most fascinating thing about group theory is you can never imagine many beautiful consequences come out from the seemingly trivial criterions! Hopefully you would pick up the tricks to play the black magic and show it to other people who haven't learned group theory yet.

• Rules of multiplication

Once you identify all elements in a group, the next thing is to build up the multiplication table, i.e. rules to multiply two elements together. Since there are eight elements in the $\boldsymbol{D}_4$ group, we need to build up a 8×8 table. However, the actual work is much less than this. Three rules of multiplication are enough to complete the task. The first two are straightforward,

$$R^4 = \mathbf{1}, \qquad P^2 = \mathbf{1}. \tag{9}$$

The third one is related to the fact that the order of multiplication is important for the $\boldsymbol{D}_4$ group because it might lead to different results. For example, the two elements P and R do not commute

$$[P, R] = PR - RP \neq 0. \tag{10}$$

When elements of the group do not commute, it is called a non-Abelian group. The third rule is

$$PR = (PR)^{-1} = R^{-1}P^{-1} = R^3P, \tag{11}$$

which tells us how to change the order of multiplications. All other rules can be derived from the above ones. For instance,

$$PR^3 = RP, \qquad PR^2 = R^2 P \tag{12}$$

• Subgroup and coset

If a collection of elements of the group also satisfies all criterions of a group, it is called a **subgroup**. The following are the subgroups of the $\boldsymbol{D}_4$ group,

$$\begin{aligned}
N = 1, &\quad \boldsymbol{S}_1 = \{\mathbf{1}\}; \\
N = 2, &\quad \boldsymbol{S}_2 = \{\mathbf{1}, R^2\}, \\
&\quad \boldsymbol{S}_3 = \{\mathbf{1}, P\}, \boldsymbol{S}_4 = \{\mathbf{1}, PR\}, \boldsymbol{S}_5 = \{\mathbf{1}, PR^2\}, \boldsymbol{S}_6 = \{\mathbf{1}, PR^3\}; \\
N = 4, &\quad \boldsymbol{S}_7 = \{\mathbf{1}, R, R^2, R^3\}, \\
&\quad \boldsymbol{S}_8 = \{\mathbf{1}, R^2, P, PR^2\}; \\
N = 8, &\quad \boldsymbol{S}_9 = \{\mathbf{1}, R, R^2, R^3, P, PR, PR^2, PR^3\}.
\end{aligned} \tag{13}$$

We notice that the unit element itself $\boldsymbol{S}_1$ and the whole group $\boldsymbol{S}_9$ are *always* subgroups of the original group.

The concept of subgroup is rather useful because it provides us a way to divide the original group into smaller sets with equal number of elements. Before explaining what I mean, we need to introduce another important terminology, **cosets**. (Trust me. I have tried to reduce all terminologies to a minimum.) Take an element of the group x and multiply it to all elements in the subgroup $\boldsymbol{S}$, another collection of elements are constructed, i.e.

$$\boldsymbol{C}_r(x) = \boldsymbol{S} \times x, \qquad \boldsymbol{C}_l(x) = x \times \boldsymbol{S}. \tag{14}$$

Depending on whether you multiply the element x on the right or left sides, the corresponding sets are called right and left cosets. Let us work out all cosets for the subgroup $\boldsymbol{S}_3$. The right cosets are

$$\{\mathbf{1}, P\}, \{R, PR\}, \{R^2, PR^2\}, \{R^3, PR^3\}, \tag{15}$$

while the left cosets are

$$\{\mathbf{1}, P\}, \{R, PR^3\}, \{R^2, PR^2\}, \{R^3, PR\}. \tag{16}$$

You probably notice that the number of inequivalent elements in each cosets are the same as the order of the subgroup. (It can be shown but I didn't show it here. Show it yourself!) Thus the original group can be viewed as sum of all cosets

$$\begin{aligned} G &= \boldsymbol{S}_3 \oplus R \times \boldsymbol{S}_3 \oplus R^2 \times \boldsymbol{S}_3 \oplus R^3 \times \boldsymbol{S}_3, \\ &= \boldsymbol{S}_3 \oplus \boldsymbol{S}_3 \times R \oplus \boldsymbol{S}_3 \times R^2 \oplus \boldsymbol{S}_3 \times R^3, \end{aligned} \tag{17}$$

In general, for each subgroup, you can construct two distinct cosets (right and left). Sometimes, you find the right and left cosets of some subgroups are identical. These subgroups are called *invariant subgroups*. We will elaborate on this point later on.

Since the whole group can be decomposed into sum of cosets which have the same number of elements as the order of the corresponding subgroup, *the order of a subgroup is a divisor of the order of the group.* In this case, the order of the subgroup can only be $1, 2, 4, 8$, as can be seen easily in Eq. 13.

• Classes and characters

Another way to divide the original group into smaller pieces is by classes. At first, you might not appreciate the power of it. But, you would be completely surprised how much information is embedded and eventually realize that this is right spot to search black magics in group theory! Two elements A and B are in the same **class** if they are related as

$$x^{-1}Ax = B, \tag{18}$$

where x is an element of the group. Notice that we just need one element to do the job. It is not necessary that the relation holds for all elements in the group.

Apparently the unit element always forms a class. To search for other classes, you need to sit down and try it out. Five classes can be found for the $\boldsymbol{D}_4$ group,

$$\boldsymbol{C}_1 = \{\mathbf{1}\}, \boldsymbol{C}_2 = \{R^2\}, \boldsymbol{C}_3 = \{R, R^3\}, \boldsymbol{C}_4 = \{P, PR^2\}, \boldsymbol{C}_5 = \{PR, PR^3\}. \tag{19}$$

What is the use of it? The number of classes $k = 5$ looks like an "ugly" number here since it is not even a divisor of the order $h = 8$. Looking into the classes, they don't even have the same number of elements. If you then think it is just boring mathematics, well, think again.

After long and tedious proof, a great theorem tells us that the number of class k equals the number of inequivalent irreducible representations of the group. The first time I learned this, I was totally impressed. This mean that the $\boldsymbol{D}_4$ group has five irreducible representations.

Now let's turn to another important concept, **character**, or just the simple trace. For all elements in the same class, they are related by a similar transformation. As a consequence, the traces of elements in the same class are identical. Another important theorem quoted here without proof is

$$\sum_G |\chi(G)|^2 = h \sum_\nu a_\nu^2, \tag{20}$$

where a_i is the times that the i-th irreducible representation appears. This provides us a way to check whether the representation is reducible. At the beginning of the notes, we calculated the square of characters of each elements and sum them up to 24. Divided by the order of the group, we find

$$\sum_\nu a_\nu^2 = 3. \tag{21}$$

It then lead to our conclusion before.

• Invariant subgroup

Combining the concepts of subgroups and classes become even more powerful. Suppose all elements of the subgroup satisfy the relation

$$g^{-1}\boldsymbol{S}g = \boldsymbol{S}, \tag{22}$$

where g denotes all elements in the whole group, this subgroup is called an **invariant subgroup**. Two straightforward consequences are (1) an invariant subgroup must be a direct sum of classes, (2) there are no distinction between right and left cosets. The invariant subgroups of the $\boldsymbol{D}_4$ group are

$$\boldsymbol{S}_2 = \{\mathbf{1}, R^2\}, \tag{23}$$

$$\boldsymbol{S}_7 = \{\mathbf{1}, R, R^2, R^3\}. \tag{24}$$

You should verify the two results I just raised above.

For each invariant subgroup, a factor group can be constructed by its cosets. Notice that the elements of a factor group are *cosets* but not *elements* of the original group.

$$\boldsymbol{F}_2 = \Big\{\{\mathbf{1}, R^2\}, \{P, PR^2\}, \{R, R^3\}, \{PR, PR^3\}\Big\}, \tag{25}$$

$$\boldsymbol{F}_7 = \Big\{\{\mathbf{1}, R, R^2, R^3\}, \{P, PR, PR^2, PR^3\}\Big\} \tag{26}$$

The beautiful thing about factor groups is the original group is homomorphic to the factor groups. It is not hard too see that $\boldsymbol{F}_2$ and $\boldsymbol{F}_7$ are isomorphic $\boldsymbol{D}_2$ and $\boldsymbol{Z}_2$. Thus the $\boldsymbol{D}_4$ group is homomorphic to both groups.

• Irreducible representations

Finally, we would say something about irreducible representations. As stated (without proof) before, the number of inequivalent irreducible representation is the number of classes k. Another theorem tells us more about irreducible representations,

$$\sum_{\nu=1}^{k} d_\nu^2 = h, \tag{27}$$

where k is the number of classes in the group and d_ν is the dimension of the corresponding irreducible representation. If the order of the group is not too big, the dimensions of all possible irreducible representations can be determined uniquely. In this case, the constraint is

$$\sum_{\nu=1}^{5} d_\nu^2 = 8 = 1^2 + 1^2 + 1^2 + 1^2 + 2^2. \tag{28}$$

Obviously all dimensions must be either one or two. It shouldn't be hard to figure out that the answer must be four one-dimensional and a two-dimensional irreducible representations which can be found in Table 2.

How can we construct these representation from scratch? It is tough and random. You just need to try it out several times and eventually you would have a better feeling about it. Let's get back to our square dance and I will show you a way to construct the most complicated irreducible representation of the $\boldsymbol{D}_4$ group (of course, it is still pretty simple). Imagine now you do not care about the distinction between individual dancers and just want to know the pattern of male and female. The configuration can be described in a more compact way,

$$|\text{configuration}\rangle = \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \begin{pmatrix} F(-1) \\ F \\ M \\ M(1) \end{pmatrix} \doteq \begin{pmatrix} -1 \\ 1 \end{pmatrix}, \tag{29}$$

where I extract components a and d to form a two-dimensional vector.

To relate different configurations described by two-component vectors, each elements of the group is represented by 2×2 matrices,

$$R = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = i\sigma_2, \qquad P = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} = -\sigma_1. \tag{30}$$

All other elements can be calculated by the rules of multiplication. Now, I hope you have some basic familiarity of the group theory and also some excitement of the surprises we go through in the notes. From just four criterions, it is really impressive that some much hidden information is embedded.

ν	P	R
s	1	1
s_p	-1	1
$d_{x^2-y^2}$	1	-1
d_{xy}	-1	-1
$\begin{pmatrix} p_x \\ p_y \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$

Table 2: Irreducible representations for $\boldsymbol{D}_4$ group. All eigenstates can be classified into these five different representations.

• More theorems ...

There are more theorems of the group theory which I didn't mention in previous sections. The first one is the grand orthogonality theorem for irreducible representations. Take a matrix component of all elements, it forms a $h-$dimensional vector. You found all these vectors, constructed in different representation, or at different columns and rows are orthogonal,

$$\sum_G D^{(\nu)*}_{\alpha\beta}(G) D^{(\nu')}_{\alpha'\beta'}(G) = \left(\frac{h}{d_\nu}\right) \delta_{\nu\nu'}\delta_{\alpha\alpha'}\delta_{\beta\beta'}, \tag{31}$$

where d_j is the dimension of the representation. Another orthogonality theorem is about the characters. The characters in each representation can be viewed as a vector. They are also orthogonal,

$$\sum_G \chi^{(\nu)*}(G)\chi^{(\nu')}(G) = h\delta_{\nu\nu'}. \tag{32}$$

A very useful lemma follows. Suppose a reducible representation consists of a_ν times of $\nu-$th irreducible representation. The character in this representation is

$$\chi(G) = \sum_\nu a_\nu \chi^{(\nu)}(G). \tag{33}$$

From this we can deduce

$$a_\nu = \left(\frac{1}{h}\right) \sum_G \chi^{(\nu)*}(G)\chi(G), \tag{34}$$

and also

$$\left(\frac{1}{h}\right) \sum_G |\chi(G)|^2 = \sum_\nu a_\nu^2. \tag{35}$$

These theorems are extremely useful in decompose a reducible representation into irreducible ones.