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3 Exercise - Introduction to Group Theory

3.1 (proof)

An Abelian-group is a group where the elements commute. While the irreducible representation normally are presented in matrices and matrices normally won't commute, it seems highly likely, that only one-dimensonal irreducible representation will form Abelian-groups, since those are only numbers and will commute for sure, since we turn the operation from matrix to "normal" multiplication.

To prove this, we first have to use that each symmetry operation in an Abelian group is in a class itself. Now the sum of the dimensions of the irreducible representations equals the order of the group ($\sum_i l_i^2 = h$), while the number of different classes is equal to the number of different irreducible representations. With the help of this knowledge taken from the theorems, we can contradict:

Each symmetry operation is in a class by itself → The number of symmetry operations (order h of the group) equals the number of classes which equal the number of the irreducible representations. While the order is also defined by $\sum_i l_i^2 = h$, with l_i the dimension of the i-th irreducible representation, the dimension of all irreducible representations has to be one. □

3.2 (D_3 character table)

The list of the matrices for all irreducible representations of the group:

$$E = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad {C_3}^1 = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad {C_3}^2 = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$C_2' = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad C_2'' = \begin{pmatrix} ? & ? & ? \\ ? & ? & ? \\ ? & ? & ? \end{pmatrix} \quad C_2''' = \begin{pmatrix} ? & ? & ? \\ ? & ? & ? \\ ? & ? & ? \end{pmatrix}$$

We therefore get (with the trivial one-dimensional representation and $f\left(E, {C_3}^1, {C_3}^2\right) = 1$ and $f\left(C_2', C_2'', C_2'''\right) = -1$):

	E	${C_3}^1$	${C_3}^2$	C_2'	C_2''	C_2'''
1st irr. rep	1	1	1	1	1	1
2nd irr. rep	1	1	1	-1	-1	-1
3rd irr. rep	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} ? & ? \\ ? & ? \end{pmatrix}$	$\begin{pmatrix} ? & ? \\ ? & ? \end{pmatrix}$

Taking the Traces now of the 3rd irr. reps, we get:

$$\begin{aligned} Tr(E) &= 2 \\ Tr(C_3) &= -1 \\ Tr(C_2) &= 0 \end{aligned}$$

Now using the foregoing and the upper table, we can get the character table of D_3:

D_3	E	$2C_3\,(z)$	$3C_2'$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

(We here used the knowledge of the charactertable, while we were not able to derive the other two C_2-matrices, we only were able to prove it for C_2', but if we would have been able to get the other matrix representations, one could be quite sure, that it would turn out this way.)

3.3 (direct products)

We first give the character table of the point group D_{3h} which we will use to calculate some direct products:

D_{3h}	E	$2C_3\,(z)$	$3C_2'$	$\sigma_h\,(xy)$	$2S_3$	$3\sigma_v$
A_1'	1	1	1	1	1	1
A_2'	1	1	-1	1	1	-1
E'	2	-1	0	2	-1	0
A_1''	1	1	1	-1	-1	-1
A_2''	1	1	-1	-1	-1	1
E''	2	-1	0	-2	1	0

We start calculating:

$$A_1' \otimes A_2' = A_2'$$

$$A_2' \otimes E' = E'$$

which can be seen immediately, since the elements of A_1' all equal 1 and the elements of A_2', for which the E' elements aren't zero, are also 1. Now it get's harder:

$$E' \otimes E'' = ?$$

With

	E	$2C_3\,(z)$	$3C_2'$	$\sigma_h\,(xy)$	$2S_3$	$3\sigma_v$
E'	2	-1	0	2	-1	0
E''	2	-1	0	-2	1	0
$E' \otimes E''$	4	1	0	-4	-1	0

and

$$E'' \otimes E'' = ?$$

	E	$2C_3\,(z)$	$3C_2'$	$\sigma_h\,(xy)$	$2S_3$	$3\sigma_v$
E''	2	-1	0	-2	1	0
E''	2	-1	0	-2	1	0
$E'' \otimes E''$	4	1	0	4	1	0

We now have to reduce this representations. Therefore we first have to check if the representations are reducible, therefore we check the condition for irreducible representations:

$$\sum_R \chi\left[\Gamma_i(R)\right]^* \chi\left[\Gamma_j(R)\right] = h\delta_{ij}$$

with $i = j$ this leads to the condition:

$$\sum_i l_i^2 = h$$

with l_i being the dimension of the i-th irreducible representation of a group of order h. Using the character table of D_3 we find the order of h:

$$\sum_i l_i^2 = 1^2 + 1^2 + 2^2 + 1^2 + 1^2 + 2^2 = 12 = h$$

Therefore the representation will be reducible if $\sum_i l_i^2 = 12$.

$$\begin{aligned} E' \otimes E'' : &\quad 1 \cdot |4|^2 + 2 \cdot |1|^2 + 3 \cdot |0|^2 + 1 \cdot |-4|^2 + 2 \cdot |-1|^2 + 3 \cdot |0|^2 = 36 > 12, \quad \text{reducible} \\ E'' \otimes E'' : &\quad 1 \cdot |4|^2 + 2 \cdot |1|^2 + 3 \cdot |0|^2 + 1 \cdot |4|^2 + 2 \cdot |1|^2 + 3 \cdot |0|^2 = 36 > 12, \quad \text{reducible} \end{aligned}$$

We can now decompose the reducible representations using the formula:

$$m_i = \frac{1}{h}\sum_i c_i \chi\left[\Gamma_i(R)\right]^* \chi\left[\Gamma_i(R)\right]$$

where m_i stands for the irreducible representations ($m_1 = A_1'$, $m_2 = A_2'$, $m_3 = E'$, $m_4 = A_1''$, $m_5 = A_2''$, $m_6 = E''$). We now decompose, starting from $E' \otimes E''$:

$$\begin{aligned}
A_1' &= \frac{1}{12}\left[1 \cdot 1 \cdot 4 + 2 \cdot 1 \cdot 1 + 3 \cdot 1 \cdot 0 + 1 \cdot 1 \cdot (-4) + 2 \cdot 1 \cdot (-1) + 3 \cdot 1 \cdot 0\right] = \frac{1}{12}(4 + 2 - 4 - 2) = 0 \\
A_2' &= \frac{1}{12}\left[1 \cdot 1 \cdot 4 + 2 \cdot 1 \cdot 1 + 3 \cdot (-1) \cdot 0 + 1 \cdot 1 \cdot (-4) + 2 \cdot 1 \cdot (-1) + 3 \cdot (-1) \cdot 0\right] = \frac{1}{12}(4 + 2 - 4 - 2) = 0 \\
E' &= \frac{1}{12}\left[1 \cdot 2 \cdot 4 + 2 \cdot (-1) \cdot 1 + 3 \cdot 0 \cdot 0 + 1 \cdot 2 \cdot (-4) + 2 \cdot (-1) \cdot (-1) + 3 \cdot 0 \cdot 0\right] = \frac{1}{12}(8 - 2 - 8 + 2) = 0 \\
A_1'' &= \frac{1}{12}\left[1 \cdot 1 \cdot 4 + 2 \cdot 1 \cdot 1 + 3 \cdot 1 \cdot 0 + 1 \cdot (-1) \cdot (-4) + 2 \cdot (-1) \cdot (-1) + 3 \cdot (-1) \cdot 0\right] = \frac{1}{12}(4 + 2 + 4 + 2) = 1 \\
A_2'' &= \frac{1}{12}\left[1 \cdot 1 \cdot 4 + 2 \cdot 1 \cdot 1 + 3 \cdot (-1) \cdot 0 + 1 \cdot (-1) \cdot (-4) + 2 \cdot (-1) \cdot (-1) + 3 \cdot 1 \cdot 0\right] = \frac{1}{12}(4 + 2 + 4 + 2) = 1 \\
E'' &= \frac{1}{12}\left[1 \cdot 2 \cdot 4 + 2 \cdot (-1) \cdot 1 + 3 \cdot 0 \cdot 0 + 1 \cdot (-2) \cdot (-4) + 2 \cdot 1 \cdot (-1) + 3 \cdot 0 \cdot 0\right] = \frac{1}{12}(8 - 2 + 8 - 2) = 1
\end{aligned}$$

now for $E'' \otimes E''$:

$$\begin{aligned}
A_1' &= \frac{1}{12}\left[1 \cdot 1 \cdot 4 + 2 \cdot 1 \cdot 1 + 3 \cdot 1 \cdot 0 + 1 \cdot 1 \cdot 4 + 2 \cdot 1 \cdot 1 + 3 \cdot 1 \cdot 0\right] = \frac{1}{12}(4 + 2 + 4 + 2) = 1 \\
A_2' &= \frac{1}{12}\left[1 \cdot 1 \cdot 4 + 2 \cdot 1 \cdot 1 + 3 \cdot (-1) \cdot 0 + 1 \cdot 1 \cdot 4 + 2 \cdot 1 \cdot 1 + 3 \cdot (-1) \cdot 0\right] = \frac{1}{12}(4 + 2 + 4 + 2) = 1
\end{aligned}$$

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\begin{aligned}
E' &= \frac{1}{12}\left[1\cdot 2\cdot 4+2\cdot(-1)\cdot 1+3\cdot 0\cdot 0+1\cdot 2\cdot 4+2\cdot(-1)\cdot 1+3\cdot 0\cdot 0\right]=\frac{1}{12}\left(8-2+8-2\right)=1\\
A_1'' &= \frac{1}{12}\left[1\cdot 1\cdot 4+2\cdot 1\cdot 1+3\cdot 1\cdot 0+1\cdot(-1)\cdot 4+2\cdot(-1)\cdot 1+3\cdot(-1)\cdot 0\right]=\frac{1}{12}\left(4+2-4-2\right)=0\\
A_2'' &= \frac{1}{12}\left[1\cdot 1\cdot 4+2\cdot 1\cdot 1+3\cdot(-1)\cdot 0+1\cdot(-1)\cdot 4+2\cdot(-1)\cdot 1+3\cdot 1\cdot 0\right]=\frac{1}{12}\left(4+2-4-2\right)=0\\
E'' &= \frac{1}{12}\left[1\cdot 2\cdot 4+2\cdot(-1)\cdot 1+3\cdot 0\cdot 0+1\cdot(-2)\cdot 4+2\cdot 1\cdot 1+3\cdot 0\cdot 0\right]=\frac{1}{12}\left(8-2-8+2\right)=0
\end{aligned}
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This leads to

$$
\begin{aligned}
E'\otimes E'' &= A_1''+A_2''+E''\\
E''\otimes E'' &= A_1'+A_2'+E'
\end{aligned}
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