15 Proof of sum relation

We want to demonstrate

$$\sum_{g\in C_k} D^{(i)}(g) = \frac{N_k}{l_i}\chi^{(i)}(C_k)I.$$

In Section 3.7 of the class notes and Section 3.6 of Wu-Ki Tung this is derived up to a constant using Schur's Lemma. This gives

$$\sum_{g\in C_k} D^{(i)}(g) = c\,\chi^{(i)}(C_k)I$$

for some constant c. To find c take the trace of both sides. On the left:

$$\mathrm{Tr}\left[\sum_{g\in C_k} D^{(i)}(g)\right] = \sum_{g\in C_k}\mathrm{Tr}\left[D^{(i)}(g)\right] = \sum_{g\in C_k}\chi^{(i)}(g) = N_k\chi^{(i)}(C_k).$$

On the right:

$$\mathrm{Tr}\left[c\chi^{(i)}(C_k)I\right] = c\chi^{(i)}(C_k)\mathrm{Tr}\,[I] = c\chi^{(i)}(C_k)l_i$$

Comparing the two sides gives $c = N_k/l_i$.

16 Character table of C_{4v}

(a)

The group C_{4v} has as members $\{e, r, r^2, r^3, m_x, m_y, m_p, m_q\}$, where r is a rotation by $\pi/2$ and the m's are mirror reflections: m_x is reflection across the x-axis, m_y across the y-axis, m_p across the line $y = x$, and m_q across the line $y = -x$. We want to find all the irreps of this group. We know that the number of irreps is equal to the number of classes, but let's assume that we don't even know what the classes are. From the orthogonality relations, we know

$$\sum_{i=1}^{n_r} {l_i}^2 = h = 8\ . \tag{1}$$

This means that we must have either 8 1×1 irreps, 2 2×2 irreps, or 4 1×1 and 1 2×2 irreps. There are no other choices. We know that we have a trivial representation, so we need at least 1 1×1 irrep. Also, we know that we could probably find at least one 2×2 irrep by finding how C_{4v} acts on basis vectors $(\hat{e}_x, \hat{e}_y)$ similar to problem 13. So we must have 4 1×1 and 1 2×2 irreps. This means that there are 5 irreps and thus 5 classes. The 1×1 irreps are:

$$D^{(1)}(g) = 1, \forall g \tag{2}$$
$$D^{(2)}(\{e, r, r^2, r^3\}) = 1,\ D^{(2)}(\{m_x, m_y, m_p, m_q\}) = -1 \tag{3}$$
$$D^{(3)}(\{e, r^2, m_x, m_y\}) = 1,\ D^{(3)}(\{r, r^3, m_p, m_q\}) = -1 \tag{4}$$
$$D^{(4)}(\{e, r^2, m_p, m_q\}) = 1,\ D^{(4)}(\{r, r^3, m_x, m_y\}) = -1\ . \tag{5}$$

We can find the 2×2 irrep $D^{(5)}$ by using the same procedure as in problem 13. For example, reflection by m_p sends $(x, y) \to (y, x)$, so $D^{(5)}(m_p)$ is just the matrix which accomplishes this. The answer is:

$$D^{(5)}(e) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad D^{(5)}(r) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{6}$$
$$D^{(5)}(r^2) = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \qquad D^{(5)}(r^3) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{7}$$
$$D^{(5)}(m_x) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \qquad D^{(5)}(m_y) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{8}$$

$$D^{(5)}(m_p) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad D^{(5)}(m_q) = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}. \tag{9}$$

(b)

So far, we still don't know the character classes, but they are easy to figure out once we know all the irreps. First, we can make a character table of every irrep of every group member:

$g \in C_{4v}$	$\chi^{(1)}$	$\chi^{(2)}$	$\chi^{(3)}$	$\chi^{(4)}$	$\chi^{(5)}$
e	1	1	1	1	2
r	1	1	-1	-1	0
r^2	1	1	1	1	-2
r^3	1	1	-1	-1	0
m_x	1	-1	1	-1	0
m_y	1	-1	1	-1	0
m_p	1	-1	-1	1	0
m_q	1	-1	-1	1	0

If two elements are in the same class, their characters must match in every representation. From this table, it is clear that the 5 character classes are: $C_1 = \{e\}, C_2 = \{r^2\}, C_3 = \{r, r^3\}, C_4 = \{m_x, m_y\}$, and $C_5 = \{m_p, m_q\}$. Thus the character table is

N_k	C_k	$\chi^{(1)}$	$\chi^{(2)}$	$\chi^{(3)}$	$\chi^{(4)}$	$\chi^{(5)}$
1	C_1	1	1	1	1	2
1	C_2	1	1	1	1	-2
2	C_3	1	1	-1	-1	0
2	C_4	1	-1	1	-1	0
2	C_5	1	-1	-1	1	0

17 Proof: abelian representation is similar to a diagonal rep

Let A and B be elements of the abelian representation and $\vec{x_i}$ be an eigenvector of A with eigenvalue a_i. $BA\vec{x_i} = Ba_i\vec{x_i} = a_i(B\vec{x_i})$. Because A and B commute, this must be equal to $AB\vec{x_i}$, which implies $B\vec{x_i}$ is also and eigenvector of A corresponding to eigenvalue a_i. This can only be true in general if $B\vec{x_i}$ is a constant times $\vec{x_i}$, *i.e.* if $\vec{x_i}$ is also an eigenvector of B. In other words, A and B must share the same eigenvectors if they commute. The matrix composed of these eigenvectors is a similarity transform diagonalizing both A and B, hence the representation is similar to a diagonal representation.

18 Invariant subspaces on D_3

This is by far the hardest problem in this set. There are several ways to arrive at the answer, with varying degrees of rigor. First, I'll give the answer then discuss a couple of possible solutions.

The invariant subspaces of the function

$$f(x, y) = ax^2 + bxy + cy^2 + dx + ey + h$$

on the point group D_3 are given by the basis functions $\{x^2 + y^2\}$, $\{xy, x^2 - y^2\}$, $\{x, y\}$, and $\{1\}$. Both one-dimensional subspaces transform like the trivial irreducible representation. The two-dimensional subspaces transform like the two-dimensional irrep.

Some people chose to write the answer in terms of the coefficients rather than the basis functions. This is also ok: $\{a + c\}$, $\{b, a - c\}$, $\{d, e\}$, and $\{h\}$.

18.1 Solution by algebraic arguments

First, because all of the elements of D_3 are linear with respect to x and y, they cannot change the polynomial order of the terms. This immediately splits the function space into subspaces by polynomial order: $\{x^2, xy, y^2\}$, $\{x, y\}$, and $\{1\}$.

Also, the operators are unitary. One consequence of unitarity is that the operators preserve lengths. This means $x^2 + y^2$ must be invariant. This leaves the quadratic subspaces as $\{x^2 + y^2\}$ and $\{xy, g(x, y)\}$, where $g(x, y)$ is some function orthogonal to the other basis functions. A good choice is $g(x, y) = x^2 - y^2$.

The last check is to see if either of the two-dimensional subspaces can be further decomposed. Testing the effects of the group operators on these subspaces should convince you that these subspaces are not further reduceable.

To summarize, the subspaces are $\{x^2 + y^2\}$, $\{xy, x^2 - y^2\}$, $\{x, y\}$, and $\{1\}$.

18.2 Solution by algebraic arguments in polar coordinates

Change to polar coordinates: $x = r\cos\phi$; $y = r\sin\phi$. Then the function becomes:

$$f(r, \phi) = ar^2\cos^2\phi + br^2\cos\phi\sin\phi + cr^2\sin^2\phi + dr\cos\phi + er\sin\phi + h$$

Making use of the double-angle trigonometry relations reveals

$$f(r, \phi) = r^2[\tfrac{1}{2}(a + c) + \tfrac{1}{2}(a - c)\cos(2\phi) + \tfrac{1}{2}b\sin(2\phi)] + r[d\cos\phi + e\sin\phi] + h$$

In this new notation the group elements are

$$\begin{array}{ccc} e : \phi \to \phi & C_3 : \phi \to \phi + 2\pi/3 & C_3^{-1} : \phi \to \phi - 2\pi/3 \\ C_2 : \phi \to -\phi & C_2' : \phi \to -\phi - 2\pi/3 & C_2'' : \phi \to -\phi + 2\pi/3 \end{array}$$

Clearly these operations do not effect the first or last terms of $f(r, \phi)$, which are therefore each invariant subspaces. The $\cos(2\phi)$ and $\sin(2\phi)$ terms mix and form a 2-dimensional subspace. Similarly, the $\cos\phi$ and $\sin\phi$ terms form a 2-d invariant subspace. To summarize, the invariant subspaces are $\{r^2\}$, $\{r^2\cos(2\phi), r^2\sin(2\phi)\}$, $\{r\cos\phi, r\sin\phi\}$, and $\{1\}$. Changing back to rectangular coordinates gives the answer above.

(This trick works because D_3 is isomorphic to C_{3v} which is a subgroup of the full 2-dimensional rotation group $C_{\infty v}$. Many problems involving point groups can be simplified this way or by using spherical coordinates.)

18.3 Solution by transforming matrices into block-diagonal form

This solution is more involved than the others but is general and can be applied to more complex problems. It is also the method most students attempted, so I'll explain it in some detail. The basic idea is

1. Express the group elements as matrices in the basis of original function as explained above.
2. Use characters to determine the decomposition of this representation into irreps.
3. Construct a block-diagonal form consisting of direct sums of the irreps found above.
4. Find a similarity transform which takes the original matrices into the new block-diagonal form.
5. Perform the same similarity transform on the original basis vectors to get the basis vectors of the invariant subspaces (one subspace per irrep instance).

To begin, the original definition of the function $f(x, y)$ suggests using a basis $\{x^2, xy, y^2, x, y, 1\}$. In this basis, the function $f(x, y)$ can be expressed as a vector: $\vec{f} = [a, b, c, d, e, h]$. The elements of the group D_3 can then be expressed as 6 by 6 matrices which multiply into the vector $\vec{(f)}$. Calling the new representation D_V, for example:

$$ef(x, y) \leftrightarrow D_V(e)\vec{f} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \\ d \\ e \\ h \end{pmatrix}$$

The matrices representing other elements can be found by applying the rule

$$gf(x, y) = f(g^{-1}x, g^{-1}y)$$

(where g is some element in the group) and then comparing coefficients of the original basis set. (The use of the inverse element above is a choice of convention. Some books use the original element instead of the inverse.)

For example, if the element C_3 is the mapping $x \to -\frac{1}{2}x - \frac{\sqrt{3}}{2}y, y \to \frac{\sqrt{3}}{2}x - \frac{1}{2}y$, then

$$\begin{aligned} C_3 f(x,y) &= f(C_3^{-1}x, C_3^{-1}y) = f(-\tfrac{1}{2}x + \tfrac{\sqrt{3}}{2}y, -\tfrac{\sqrt{3}}{2}x - \tfrac{1}{2}y) \\ &= (\tfrac{1}{4}a + \tfrac{\sqrt{3}}{4}b + \tfrac{3}{4}c)x^2 + (-\tfrac{\sqrt{3}}{2}a - \tfrac{1}{2}b + \tfrac{\sqrt{3}}{2}c)xy + (\tfrac{3}{4}a - \tfrac{\sqrt{3}}{4}b + \tfrac{1}{4}c)y^2 \\ &\quad +(-\tfrac{1}{2}d - \tfrac{\sqrt{3}}{2}e)x + (\tfrac{\sqrt{3}}{2}d - \tfrac{1}{2}e)y + h \\ D_V(C_3) &= \begin{pmatrix} \frac{1}{4} & \frac{\sqrt{3}}{4} & \frac{3}{4} & 0 & 0 & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 & 0 & 0 \\ \frac{3}{4} & -\frac{\sqrt{3}}{4} & \frac{1}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \end{aligned}$$

To find the decomposition of the 6 by 6 representation into irreducible representations, calculate the trace of the matrices for at least one element per class (*i.e.* find the characters of the 6 by 6 rep). For example the trace of $D_V(C_3)$ is zero. It's helpful to write these characters on the character table:

$\mathbf{D_3}$	E	$2C_3$	$3C_2$	
A_1	1	1	1	
A_2	1	1	-1	
E	2	-1	0	
D_V	6	0	2	$\leftarrow$ our 6 by 6 rep.

It's easy to see that 2 times the first row plus 2 times the third row equals the last row. So our representation contains two instances of A_1 and two instances of E: $D_V = 2A_1 \oplus 2E$.

The third step is to construct the block-diagonal forms, which I'll call the $\widetilde{D}_V$ representation. For example

$$\widetilde{D}_V(C_3) = \left(\begin{array}{c|cc|cc|c} 1 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 & 0 & 0 \\ 0 & \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ 0 & 0 & 0 & \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & 1 \end{array}\right).$$

The lines show the separation between subspaces.

The next step is find a matrix S such that $SD_VS^{-1} = \widetilde{D}_V$. Note that this is not the same as diagonalizing $D_V(g)$ for some particular element g (except in the case where the representation is composed entirely of 1-d irreps *a la* Problem 16, which doesn't apply here). The transform must hold for all elements of the group. Some students diagonalized a particular element (often in Mathematica which gave weird complex-number answers) and incorrectly asserted that this transformation applies to the entire group.

For our problem the diagonalization can almost be found by inspection.

$$S = \begin{pmatrix} 1/\sqrt{2} & 0 & 1/\sqrt{2} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 1/\sqrt{2} & 0 & -1/\sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

In this particular case $S^{-1} = S$ and it is easy to verify $SD_VS^{-1} = \widetilde{D}_V$.

The final step is to apply the transformation onto the "function" $\vec{f}$.

$$S\vec{f} = \begin{pmatrix} 1/\sqrt{2} & 0 & 1/\sqrt{2} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 1/\sqrt{2} & 0 & -1/\sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \\ d \\ e \\ h \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}}(a+c) \\ b \\ \frac{1}{\sqrt{2}}(a-c) \\ d \\ e \\ h \end{pmatrix}$$

This new vector is divided into subspaces in the same way as the block-diagonal form $\widetilde{D}_V$. Comparing the coefficients to the original polynomial function given the breakdown into invariant subspaces $\{\frac{\sqrt{2}}{2}(x^2+y^2)\}\})$, $\{xy, \frac{\sqrt{2}}{2}(x^2-y^2)\}$, $\{x, y\}$, and $\{1\}$. (These differ from the originally given answer by some constants because the original answer wasn't normalized.)

18.4 Solution by projection operators

Although it wasn't covered in class and no student attempted it, another solution is to use projection operators to pick out the components belonging to the various irreps. This is discussed in Section 4.2 of Wu-Ki Tung.

18.5 Solution by comparison to published character tables

This solution is the most likely "real-world" solution, but borders on cheating for purposes of this assignment. Many published character tables list example basis functions for each irrep. These basis functions can be used to decompose the function $f(x, y)$.

For example, from the website
`http://newton.ex.ac.uk/research/qsystems/people/goss/symmetry/CharacterTables.html`
the character table for D_3 is given as

$\mathbf{D_3}$	E	$2C_3$	$3C_2$		
A_1	1	1	1		x^2+y^2, z^2
A_2	1	1	-1	z, I_z	
E	2	-1	0	(x, y), (I_x, I_y)	(x^2-y^2, xy), (xz, yz)

(Note that this table is transposed compared to those in the class notes.) The classes are listed along the top, with the numbers preceding the class names indicating the number of elements in that class. The irreducible representations are listed on the left side, using a common naming convention. The functions listed on the right are examples of possible basis functions which transform like the given representation. Note that other basis functions are possible – these are only simple examples. (The notations like I_x represent axial vectors pointing in the appropriate direction. Axial vectors are quantities like angular momentum that do not change direction upon inversion of the coordinates.)

Fortunately for the purposes of solving this problem we only need terms up to second order, which happen to be included in this table. The answer can be read directly from the table. (Constant terms always transform like the trivial rep.) In our function $f(x, y)$ there are two instances on the irrep A_1 corresponding to basis functions $\{x^2+y^2\}$ and $\{1\}$ and two instances of the two-dimensional irrep E corresponding to basis functions $\{x, y\}$ and $\{x^2-y^2, xy\}$.