Double groups

Josep Planelles

March 12, 2015

1 Some rotational double groups and products of irreps

Two-fold rotational group

$\bar{C}_2$	E	C_2^1	C_2^2	C_2^3	$e^{iM\phi}$ basis
A	1	1	1	1	$M = 0, \pm 2, \pm 4$
B	1	-1	1	-1	$M = \pm 1, \pm 3$
$E_{-3/2}$	1	i	-1	$-i$	$M = 1/2, -3/2$
$E_{3/2}$	1	$-i$	-1	i	$M = -1/2, 3/2$

(1)

Product of irreps for the two-fold rotational group

	A	B	$E_{-3/2}$	$E_{3/2}$
A	A	B	$E_{-3/2}$	$E_{3/2}$
B		A	$E_{3/2}$	$E_{-3/2}$
$E_{-3/2}$			B	A
$E_{3/2}$				B

(2)

Three-fold rotational group

$\bar{C}_3$	E	C_3^1	C_3^2	C_3^3	C_3^4	C_3^5	$e^{iM\phi}$ basis
A	1	1	1	1	1	1	$M = 0, \pm 3$
E_+	1	ϵ	ϵ^*	1	ϵ	ϵ^*	$M = 1, -2$
E_-	1	ϵ^*	ϵ	1	ϵ^*	ϵ	$M = -1, 2$
$E_{1/2}$	1	$-\epsilon^*$	ϵ	-1	ϵ^*	$-\epsilon$	$M = 1/2$
$E_{-1/2}$	1	$-\epsilon$	ϵ^*	-1	ϵ	$-\epsilon^*$	$M = -1/2$
$E_{3/2}$	1	-1	1	-1	1	-1	$M = \pm 3/2$

(3)

with $\epsilon = e^{i\,\frac{2\pi}{3}}$.

Product of irreps for the three-fold rotational group

	A	E_+	E_-	$E_{1/2}$	$E_{-1/2}$	$E_{3/2}$
A	A	E_+	E_-	$E_{1/2}$	$E_{-1/2}$	$E_{3/2}$
E_+		E_-	A	$E_{3/2}$	$E_{1/2}$	$E_{-1/2}$
E_-			E_+	$E_{-1/2}$	$E_{3/2}$	$E_{1/2}$
$E_{1/2}$				E_+	A	E_-
$E_{-1/2}$					E_-	E_+
$E_{3/2}$						A

(4)

Four-fold rotational group

$\bar{C}_4$	E	C_4^1	C_4^2	C_4^3	C_4^4	C_4^5	C_4^6	C_4^7	$e^{iM\phi}$ basis
A	1	1	1	1	1	1	1	1	$M = 0, \pm 4$
B	1	-1	1	-1	1	-1	1	-1	$M = \pm 2$
E_+	1	i	-1	$-i$	1	i	-1	$-i$	$M = 1, -3$
E_-	1	$-i$	-1	i	1	$-i$	-1	i	$M = -1, 3$
$E_{1/2}$	1	ϵ	i	$-\epsilon^*$	-1	$-\epsilon$	$-i$	ϵ^*	$M = 1/2$
$E_{-1/2}$	1	ϵ^*	$-i$	$-\epsilon$	-1	$-\epsilon^*$	i	ϵ	$M = -1/2$
$E_{3/2}$	1	$-\epsilon^*$	$-i$	ϵ	-1	ϵ^*	i	$-\epsilon$	$M = 3/2$
$E_{-3/2}$	1	$-\epsilon$	i	ϵ^*	-1	ϵ	$-i$	$-\epsilon^*$	$M = -3/2$

(5)

with $\epsilon = e^{i\,\frac{\pi}{4}}$.

Product of irreps for the Four-fold rotational group

	A	B	E_+	E_-	$E_{1/2}$	$E_{-1/2}$	$E_{3/2}$	$E_{-3/2}$
A	A	B	E_+	E_-	$E_{1/2}$	$E_{-1/2}$	$E_{3/2}$	$E_{-3/2}$
B		A	E_-	E_+	$E_{-3/2}$	$E_{3/2}$	$E_{-1/2}$	$E_{1/2}$
E_+			B	A	$E_{3/2}$	$E_{1/2}$	$E_{-3/2}$	$E_{-1/2}$
E_-				E_+	$E_{-1/2}$	$E_{-3/2}$	$E_{1/2}$	$E_{3/2}$
$E_{1/2}$					E_+	A	B	E_-
$E_{-1/2}$						E_-	E_+	B
$E_{3/2}$							E_+	A
$E_{-3/2}$								E_+

(6)

The C_{3h} double group.

In this case, the calculation of the character of the horizontal mirror plane σ_h is not trivial for the spin functions. At a first glance, since σ_h does not affect the angle ϕ it may seem that $e^{iM\phi}$ is invariant under σ_h both, for integer and half-integer M. However, since $\mathcal{O}_R f(\mathbf{r}) = f(R^{-1}\mathbf{r})$, one may claim that σ_h change the sign of the z-axis and then that it may affect the functions. This is the case for $z, J_x \pm iJ_y$ that change their sign, while $J_z, x \pm iy$ keep invariant (character unity). What about the spin functions? Let's see first whether or not the character of σ_h for the spin irreps should be different from unit and, then, we will proceed to calculate its value.

We know that in C_{3h} the identity E and the rotation C_3^3 are the same transformation, as it is the two-fold application of σ_h, i.e., $E = C_3^3 = \sigma_h^2$. However, in the C_{3h} double group $C_3^3 = \bar{E}$ which character for the spin function irreducible representations is -1. Then, the character for σ_h^2 should be also -1, i.e., if the function F is double-evaluated in C_{3h} then, $\sigma_h^2 F = -F$. On the other hand, both C_{3h} and double-C_{3h} are abelian or commutative groups and, as a consequence, all their irreps are one-dimensional. Therefore, if $\sigma_h F = \lambda F$, it follows that $\sigma_h^2 F = \lambda^2 F$. And since we have just seen that $\sigma_h^2 F = -F$ we conclude that $\lambda^2 = -1$ and then $\lambda = \pm i$. The sign of the character depends on F, we show next that it is $+i$ for $F = |1/2, -1/2\rangle$ and $-i$ for $F = |1/2, 1/2\rangle$. Now we proceed to calculate them.

Let us consider the spin vector $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z,)$ with $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ and $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$. The action of the mirror symmetry σ_h transforms this vector into $\vec{\sigma}' = (\sigma_{x'}, \sigma_{y'}, \sigma_{z'}) = (-\sigma_x, -\sigma_y, \sigma_z,),$[1] where $\sigma_{x'} = M^\dagger \sigma_x M$, $\sigma_{y'} = M^\dagger \sigma_y M$ and $\sigma_{z'} = M^\dagger \sigma_z M$, $M^\dagger M = \mathbb{I}$, being M the transformation matrix, corresponding to the the σ_h mirror symmetry plane, transforming the spin components. We are looking for a matrix M so that:

$$
\begin{aligned}
\sigma_{x'} = M^\dagger \sigma_x M &= -\sigma_x \\
\sigma_{y'} = M^\dagger \sigma_y M &= -\sigma_y \\
\sigma_{z'} = M^\dagger \sigma_z M &= \sigma_z
\end{aligned}
\tag{7}
$$

I remind here some properties of the σ_i Pauli matrices that can be checked by replacing σ_i by its matrix representation: $\sigma_x\sigma_x = \sigma_y\sigma_y = \sigma_z\sigma_z = \mathbb{I}$, $\sigma_y\sigma_z = i\sigma_x$, $\sigma_z\sigma_y = -i\sigma_x$, $\sigma_z\sigma_x = i\sigma_y$, $\sigma_x\sigma_z = -i\sigma_y$. Finally, $\sigma_i^\dagger = \sigma_i$, $i = x, y, z$. These relations prompt the matrix M to be $M = -i\,\sigma_z$ ($M^\dagger = i\,\sigma_z$), as we check now:

$$
M^\dagger \sigma_z M = (i)\,(-i)\,\sigma_z\,\sigma_z\,\sigma_z = \sigma_z
$$

[1] Please realize that spin is not a polar but an axial vector. A mirror symmetry plane containing an axial vector change its direction while a perpendicular mirror leaves the vector invariant. Then, since the σ_h mirror symmetry plane contains σ_x and σ_y and it is perpendicular to σ_z, it changes the sign of the first two components and leaves the last one invariant.

$$
\begin{aligned}
M^\dagger \sigma_x M &= \sigma_z\,\sigma_x\,\sigma_z = \sigma_z\,(-i\,\sigma_y) = -i\,(-i\,\sigma_x) = -\sigma_x \\
M^\dagger \sigma_y M &= \sigma_z\,\sigma_y\,\sigma_z = \sigma_z\,(i\,\sigma_x) = i\,(i\,\sigma_y) = -\sigma_y
\end{aligned} \tag{8}
$$

Next we consider the action of M on the spin functions $|1/2,1/2\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $|1/2,-1/2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$:

$$
\begin{aligned}
M|1/2,1/2\rangle &= -i\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = -i\begin{pmatrix} 1 \\ 0 \end{pmatrix} = -i\,|1/2,1/2\rangle \\
M|1/2,-1/2\rangle &= -i\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = -i\begin{pmatrix} 0 \\ -1 \end{pmatrix} = i\,|1/2,-1/2\rangle
\end{aligned} \tag{9}
$$

Therefore, the mirror σ_h character for the irrep with basis $|1/2,1/2\rangle$ is $\chi(\sigma_h) = -i$, while the character corresponding toe $|1/2,-1/2\rangle$ is $\chi(\sigma_h) = i$.

In order to calculate the remaining characters, we take into account general definitions or properties like: $S_3^+ = \sigma_h\,C_3^+$, then $\chi(S_3^+) = \chi(\sigma_h)\chi(C_3^+)$; $\bar{\sigma}_h = \bar{E}\sigma_h$; $\bar{S}_3^+ = \bar{C}_3^+\sigma_h$, etc.[2] resulting:

	E	C_3^+	C_3^-	σ_h	S_3^+	S_3^-	$\bar{E}$	$\bar{C}_3^+$	$\bar{C}_3^-$	$\bar{\sigma}_h$	$\bar{S}_3^+$	$\bar{S}_3^-$	basis
$E_{1/2}$	1	$-\omega^*$	ω	$-i$	$i\,\omega^*$	$-i\,\omega$	-1	ω^*	$-\omega$	i	$-i\,\omega^*$	$i\,\omega$	$\|1/2,1/2\rangle$
$E_{-1/2}$	1	$-\omega$	ω^*	i	$-i\,\omega$	$i\,\omega^*$	-1	ω	$-\omega^*$	$-i$	$i\,\omega$	$-i\,\omega^*$	$\|1/2,-1/2\rangle$

(10)

Next we consider $|3/2,\pm 3/2\rangle$. In order to calculate the characters we take into account that $|3/2,3/2\rangle = |1,1\rangle|1/2,1/2\rangle$ and $|3/2,-3/2\rangle = |1,-1\rangle|1/2,-1/2\rangle$. Therefore, we just multiply irreps, i.e., $E_{3/2} = E'_+ \otimes E_{1/2}$ and $E_{-3/2} = E'_- \otimes E_{-1/2}$, yielding e.g.,

	E	C_3^+	C_3^-	σ_h	S_3^+	S_3^-	$\bar{E}$	$\bar{C}_3^+$	$\bar{C}_3^-$	$\bar{\sigma}_h$	$\bar{S}_3^+$	$\bar{S}_3^-$	basis
E'_+	1	ω	ω^*	1	ω	ω^*	1	ω	ω^*	1	ω	ω^*	$\|1,1\rangle$
$E_{1/2}$	1	$-\omega^*$	ω	$-i$	$i\,\omega^*$	$-i\,\omega$	-1	ω^*	$-\omega$	i	$-i\,\omega^*$	$i\,\omega$	$\|1/2,1/2\rangle$
$E_{3/2}$	1	-1	1	$-i$	i	$-i$	-1	1	-1	i	$-i$	i	$\|3/2,3/2\rangle$

(11)

The irrep $E_{-3/2}$ is the dual or complex conjugate of $E_{3/2}$ (in the same way that E'_+, E'_- on the one side and $E_{1/2}$, $E_{-1/2}$ on the other hand, are duals.

One can alternatively build all angular momentum irreps from that of $|1/2,\pm 1/2\rangle$ just by calculating the different powers. For example for positive components we have that

$$
|1,1\rangle = |1/2,1/2\rangle|1/2,1/2\rangle
$$

[2] Also we realize some angular identities like $e^{i\,\frac{2\pi}{6}} = -e^{-i\,\frac{2\pi}{3}} = -\omega^*$, $e^{i\,\frac{4\pi}{6}} = e^{i\,\frac{2\pi}{3}} = \omega$, etc.

$$\begin{aligned} |3/2,3/2\rangle &= |1/2,1/2\rangle|1/2,1/2\rangle|1/2,1/2\rangle \\ |2,2\rangle &= |1/2,1/2\rangle|1/2,1/2\rangle|1/2,1/2\rangle|1/2,1/2\rangle, \quad \text{etc.} \end{aligned} \tag{12}$$

Therefore the characters are:

	E	C_3^+	C_3^-	σ_h	S_3^+	S_3^-	$\bar{E}$	$\bar{C}_3^+$	$\bar{C}_3^-$	$\bar{\sigma}_h$	$\bar{S}_3^+$	$\bar{S}_3^-$	basis
$\|1/2,1/2\rangle$	1	$-\omega^*$	ω	$-i$	$i\,\omega^*$	$-i\,\omega$	-1	ω^*	$-\omega$	i	$-i\,\omega^*$	$i\,\omega$	$\|1/2,1/2\rangle$
$\|1/2,1/2\rangle^2$	1	ω	ω^*	-1	$-\omega$	$-\omega^*$	1	ω	ω^*	-1	$-\omega$	$-\omega^*$	$\|1,1\rangle$
$\|1/2,1/2\rangle^3$	1	-1	1	i	$-i$	i	-1	1	-1	$-i$	i	$-i$	$\|3/2,3/2\rangle$
$\|1/2,1/2\rangle^4$	1	ω^*	ω	1	ω^*	ω	1	ω^*	ω	1	ω^*	ω	$\|2,2\rangle$
$\|1/2,1/2\rangle^5$	1	$-\omega$	ω^*	$-i$	$i\,\omega$	$-i\,\omega^*$	-1	ω	$-\omega^*$	i	$-i\,\omega$	$i\,\omega^*$	$\|5/2,5/2\rangle$
$\|1/2,1/2\rangle^6$	1	1	1	-1	-1	-1	1	1	1	-1	-1	-1	$\|3,3\rangle$

(13)

When we compare the results obtained by one and another method, e.g. referred to $|3/2,3/2\rangle$, we find out two different results (!) In particular, we see that the character of the horizontal mirror symmetry σ_h are different. The reason is that C_{3h} introduces an additional symmetry to the angular momentum symmetry. Now we have two different $|3/2,3/2\rangle$ functions. Those we may call bonding (invariants under σ_h) and those we call anti-bonding, that have a node at σ_h. Since the σ_h character of $|1/2,1/2\rangle$ is $-i$, the one of $|1/2,1/2\rangle^2$ is -1, i.e. anti-bonding, while the function $x+i\,y \equiv e^{i\,\phi}$ is invariant under σ_h (bonding). The bonding $J=1$ angular momentum functions are like the antibonding where X, Y, and Z are replaced by J_x, J_y, and J_z, e.g $|3/2,3/2^a\rangle = -\frac{1}{\sqrt{2}}|(X+i\,Y)\uparrow\rangle$ vs. $|3/2,3/2^b\rangle = -\frac{1}{\sqrt{2}}|(J_x+i\,J_y)\uparrow\rangle$. Next we enclose the complete character table.

$\bar{C}_{3h}$	E	C_3^+	C_3^-	σ_h	S_3^+	S_3^-	$\bar{E}$	$\bar{C}_3^+$	$\bar{C}_3^-$	$\bar{\sigma}_h$	$\bar{S}_3^+$	$\bar{S}_3^-$	basis
$K1$	1	1	1	1	1	1	1	1	1	1	1	1	J_z
$K2$	1	ω	ω^*	1	ω	ω^*	1	ω	ω^*	1	ω	ω^*	$x+iy$
$K3$	1	ω^*	ω	1	ω^*	ω	1	ω^*	ω	1	ω^*	ω	$x-iy$
$K4$	1	1	1	-1	-1	-1	1	1	1	-1	-1	-1	z
$K5$	1	ω	ω^*	-1	$-\omega$	$-\omega^*$	1	ω	ω^*	-1	$-\omega$	$-\omega^*$	J_x+iJ_y
$K6$	1	ω^*	ω	-1	$-\omega^*$	$-\omega$	1	ω^*	ω	-1	$-\omega^*$	$-\omega$	J_x-iJ_y
$K7$	1	$-\omega$	ω^*	i	$-i\omega$	$i\omega^*$	-1	ω	$-\omega^*$	$-i$	$i\omega$	$-i\omega^*$	$J_{-1/2}$
$K8$	1	$-\omega^*$	ω	$-i$	$i\omega^*$	$-i\omega$	-1	ω^*	$-\omega$	i	$-i\omega^*$	$i\omega$	$J_{1/2}$
$K9$	1	$-\omega$	ω^*	$-i$	$i\omega$	$-i\omega^*$	-1	ω	$-\omega^*$	i	$-i\omega$	$i\omega^*$	
$K10$	1	$-\omega^*$	ω	i	$-i\omega^*$	$i\omega$	-1	ω^*	$-\omega$	$-i$	$i\omega^*$	$-i\omega$	
$K11$	1	-1	1	i	$-i$	i	-1	1	-1	$-i$	i	$-i$	
$K12$	1	-1	1	$-i$	i	$-i$	-1	1	-1	i	$-i$	i	

(14)

and the table of products of irreps.

	K_1	K_2	K_3	K_4	K_5	K_6	K_7	K_8	K_9	K_{10}	K_{11}	K_{12}
K_1	K_1	K_2	K_3	K_4	K_5	K_6	K_7	K_8	K_9	K_{10}	K_{11}	K_{12}
K_2		K_3	K_1	K_5	K_6	K_4	K_{10}	K_{12}	K_8	K_{11}	K_7	K_9
K_3			K_2	K_6	K_4	K_5	K_{11}	K_9	K_{12}	K_7	K_{10}	K_8
K_4				K_1	K_2	K_3	K_9	K_{10}	K_7	K_8	K_{12}	K_{11}
K_5					K_3	K_1	K_8	K_{11}	K_{10}	K_{12}	K_9	K_7
K_6						K_2	K_{12}	K_7	K_{11}	K_9	K_8	K_{10}
K_7							K_6	K_1	K_3	K_4	K_5	K_2
K_8								K_5	K_4	K_2	K_3	K_6
K_9									K_6	K_1	K_2	K_5
K_{10}										K_5	K_6	K_3
K_{11}											K_4	K_1
K_{12}												K_4

(15)