Group Theory

Solutions to Problems in Homework Assignment 04

Spring, 2020

1. The multiplication table for the group $D_3 = \{E, D, F, A, B, C\}$ is given by

$$\begin{array}{c|cccccc} & E & D & F & A & B & C \\ \hline E & E & D & F & A & B & C \\ D & D & F & E & B & C & A \\ F & F & E & D & C & A & B \\ A & A & C & B & E & F & D \\ B & B & A & C & D & E & F \\ C & C & B & A & F & D & E \end{array}$$

(a) Determine the dimensions of all the inequivalent irreducible representation of D_3.

(b) Find the character table for D_3.

(a) We found in Homework Assignment 02 that the classes of D_3 are given by

$$C_1 = \{E\},\ C_2 = \{D, F\},\ C_3 = \{A, B, C\}.$$

Because D_3 has three classes, it has three inequivalent irreducible representations. We use d_1, d_2, and d_3 to denote respectively the dimensions of these three inequivalent irreducible representations. We then have

$$d_1^2 + d_2^2 + d_3^2 = 6.$$

The solutions to the above equation are given by

$$d_1 = d_2 = 1,\ d_3 = 2,$$

where we have arranged the three inequivalent irreducible representations in the order of increasing dimensionality. We use Γ^1, Γ^2, and Γ^3 to denote the three inequivalent irreducible representations of D_3 with Γ^1 the identity representation.

(b) We know that, for the two one-dimensional representations, $\chi^{1,2}(C_k) = \pm 1$ with $k = 1, 2, 3$.

i. $\chi^{1,2}(C_1)$. Because $\chi^{1,2}(E) = 1$, we have $\chi^{1,2}(C_1) = 1$.

ii. $\chi^{1,2}(C_2)$. From $D^2 = F$, we have $\chi^{1,2}(D)^2 = \chi^{1,2}(F)$, which implies that $\chi^{1,2}(F) = 1$. We thus have $\chi^{1,2}(C_2) = 1$.

iii. $\chi^{1,2}(C_3)$. Making use of $A^2 = E$, we have $\chi^{1,2}(C_3) = \pm 1$. We choose $\chi^1(C_3) = 1$ so that the characters of all the classes in the identity representation are all equal to one. We then have $\chi^2(C_3) = -1$.

iv. $\chi^3(C_1)$, $\chi^3(C_2)$, and $\chi^3(C_3)$. We use

$$\frac{1}{g}\sum_{T\in G} \chi^p(T)^* \chi^q(T) = \delta_{pq} \text{ and } \frac{1}{g}\sum_{T\in G} |\chi(T)|^2 = 1$$

to determine the characters in the representation Γ^3. We have

$$\begin{aligned} &\chi^3(C_1) + 2\chi^3(C_2) + 3\chi^3(C_3) = 0, \\ &\chi^3(C_1) + 2\chi^3(C_2) - 3\chi^3(C_3) = 0, \\ &\chi^3(C_1)^2 + 2\chi^3(C_2)^2 + 3\chi^3(C_3)^2 = 6. \end{aligned}$$

Subtracting the first two equations, we have $\chi^3(C_3) = 0$. Thus, $\chi^3(C_1) + 2\chi^3(C_2) = 0$, which leads to $\chi^3(C_1) = -2\chi^3(C_2)$. Inserting $\chi^3(C_1) = -2\chi^3(C_2) = 0$ and $\chi^3(C_3) = 0$ into the third equation yields $6\chi^3(C_2)^2 = 6$. Thus, $\chi^3(C_2) = \pm 1$. Choosing the character of the identity element in Γ^3 to be a positive number, we have $\chi^3(C_1) = 2$ and $\chi^3(C_2) = -1$.
Alternatively, we can make use of the fact that $\chi^p(E) = d_p$ to infer that $\chi^3(C_1) = 2$. Then we can obtain $\chi^3(C_2) = -1$ from $\chi^3(C_1) = -2\chi^3(C_2)$. In this approach, the third equation $\chi^3(C_1)^2 + 2\chi^3(C_2)^2 + 3\chi^3(C_3)^2 = 6$ is not used. Note that it is satisfied by the characters determined in this approach.

The character table of D_3 is then given by

	$C_1 = \{E\}$	$C_2 = \{D, F\}$	$C_3 = \{A, B, C\}$
Γ^1	1	1	1
Γ^2	1	1	-1
Γ^3	2	-1	0

2. The transformation matrices in two-dimensional real space for the elements of the group $D_3 = \{E, D, F, A, B, C\}$ are given by

$$R(E) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, R(D) = \frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix}, R(F) = \frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix},$$
$$R(A) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, R(B) = \frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ \sqrt{3} & 1 \end{pmatrix}, R(C) = \frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & 1 \end{pmatrix}.$$

The basis functions of a carrier space for D_3 are given by $\psi_1(\vec{\rho}) = x^2F(\rho)$, $\psi_2(\vec{\rho}) = xyF(\rho)$, and $\psi_3(\vec{\rho}) = y^2F(\rho)$, where $F(\rho)$, a function of $\rho = \sqrt{x^2 + y^2}$, ensures that the basis functions are normalizable. Using

$$Q(T)\psi_n(\vec{\rho}) = \psi_n(R(T)^{-1}\vec{\rho}) = \sum_{m=1}^{3} \Gamma(T)_{mn}\psi_m(\vec{\rho}),\ n = 1,\ 2,\ 3,$$

find the representation matrix $\Gamma(F)$ of the element F of D_3. Here $Q(T)$ is the scalar transformation operator and $\vec{\rho}$ is the position vector of a point in two-dimensional real space.

For $T = F$, we have

$$R(F)^{-1} = R(F)^t = \frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix},$$
$$R(F)^{-1}\vec{\rho} = \frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} = \frac{1}{2}\begin{pmatrix} -x - \sqrt{3}\,y \\ \sqrt{3}\,x - y \end{pmatrix}.$$

$Q(F)\psi_n(\vec{\rho})$ for $n = 1,\ 2,\ 3$ are then given by

$$Q(F)\psi_1(\vec{\rho}) = \frac{1}{4}(x + \sqrt{3}y)^2F(\rho) = \frac{1}{4}(x^2 + 2\sqrt{3}\,xy + 3y^2)F(\rho) = \frac{1}{4}\psi_1(\vec{\rho}) + \frac{\sqrt{3}}{2}\psi_2(\vec{\rho}) + \frac{3}{4}\psi_3(\vec{\rho}),$$
$$Q(F)\psi_2(\vec{\rho}) = -\frac{1}{4}(x + \sqrt{3}\,y)(\sqrt{3}\,x - y)F(\rho) = -\frac{1}{4}(\sqrt{3}\,x^2 + 2xy - \sqrt{3}\,y^2)F(\rho)$$
$$= -\frac{\sqrt{3}}{4}\psi_1(\vec{\rho}) - \frac{1}{2}\psi_2(\vec{\rho}) + \frac{\sqrt{3}}{4}\psi_3(\vec{\rho}),$$
$$Q(F)\psi_3(\vec{\rho}) = \frac{1}{4}(\sqrt{3}\,x - y)^2F(\rho) = \frac{1}{4}(3x^2 - 2\sqrt{3}\,xy + y^2)F(\rho) = \frac{3}{4}\psi_1(\vec{\rho}) - \frac{\sqrt{3}}{2}\psi_2(\vec{\rho}) + \frac{1}{4}\psi_3(\vec{\rho}).$$

Making use of

$$Q(T)\psi_n(\vec{\rho}) = \psi_n(R(T)^{-1}\vec{\rho}) = \sum_{m=1}^{3} \Gamma(T)_{mn}\psi_m(\vec{\rho}),\ n = 1,\ 2,\ 3$$

for $T = F$, we obtain

$$\Gamma(F)_{11}\psi_1 + \Gamma(F)_{21}\psi_2 + \Gamma(F)_{31}\psi_3 = \frac{1}{4}\psi_1(\vec{\rho}) + \frac{\sqrt{3}}{2}\psi_2(\vec{\rho}) + \frac{3}{4}\psi_3(\vec{\rho}),$$
$$\Gamma(F)_{12}\psi_1 + \Gamma(F)_{22}\psi_2 + \Gamma(F)_{32}\psi_3 = -\frac{\sqrt{3}}{4}\psi_1(\vec{\rho}) - \frac{1}{2}\psi_2(\vec{\rho}) + \frac{\sqrt{3}}{4}\psi_3(\vec{\rho}),$$
$$\Gamma(F)_{13}\psi_1 + \Gamma(F)_{23}\psi_2 + \Gamma(F)_{33}\psi_3 = \frac{3}{4}\psi_1(\vec{\rho}) - \frac{\sqrt{3}}{2}\psi_2(\vec{\rho}) + \frac{1}{4}\psi_3(\vec{\rho}).$$

Making use of the fact that ψ_1, ψ_2, and ψ_3 are linearly independent, we obtain from the above results

$$\begin{aligned}
\Gamma(F)_{11} &= \frac{1}{4}, \quad \Gamma(F)_{12} = -\frac{\sqrt{3}}{4}, \ \Gamma(F)_{13} = \frac{3}{4}, \\
\Gamma(F)_{21} &= \frac{\sqrt{3}}{2}, \ \Gamma(F)_{22} = -\frac{1}{2}, \quad \Gamma(F)_{23} = -\frac{\sqrt{3}}{2}, \\
\Gamma(F)_{31} &= \frac{3}{4}, \quad \Gamma(F)_{32} = \frac{\sqrt{3}}{4}, \quad \Gamma(F)_{33} = \frac{1}{4}.
\end{aligned}$$

Thus, the representation matrix of the element F is given by

$$\Gamma(F) = \begin{pmatrix} \frac{1}{4} & -\frac{\sqrt{3}}{4} & \frac{3}{4} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{3}{4} & \frac{\sqrt{3}}{4} & \frac{1}{4} \end{pmatrix}.$$

3. Using the information given in the previous problem, find the representation matrix $\Gamma(B)$ of the element B of D_3.

For $T = B$, we have

$$\begin{aligned}
R(B)^{-1} &= R(B)^t = \frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ \sqrt{3} & 1 \end{pmatrix}, \\
R(B)^{-1}\vec{\rho} &= \frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ \sqrt{3} & 1 \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} = \frac{1}{2}\begin{pmatrix} -x + \sqrt{3}\,y \\ \sqrt{3}\,x + y \end{pmatrix}.
\end{aligned}$$

$Q(B)\psi_n(\vec{\rho})$ for $n = 1, 2, 3$ are then given by

$$\begin{aligned}
Q(B)\psi_1(\vec{\rho}) &= \frac{1}{4}(-x + \sqrt{3}y)^2 F(\rho) = \frac{1}{4}(x^2 - 2\sqrt{3}\,xy + 3y^2)F(\rho) = \frac{1}{4}\psi_1(\vec{\rho}) - \frac{\sqrt{3}}{2}\psi_2(\vec{\rho}) + \frac{3}{4}\psi_3(\vec{\rho}), \\
Q(B)\psi_2(\vec{\rho}) &= \frac{1}{4}(-x + \sqrt{3}\,y)(\sqrt{3}\,x + y)F(\rho) = \frac{1}{4}(-\sqrt{3}\,x^2 + 2xy + \sqrt{3}\,y^2)F(\rho) \\
&= -\frac{\sqrt{3}}{4}\psi_1(\vec{\rho}) + \frac{1}{2}\psi_2(\vec{\rho}) + \frac{\sqrt{3}}{4}\psi_3(\vec{\rho}), \\
Q(B)\psi_3(\vec{\rho}) &= \frac{1}{4}(\sqrt{3}\,x + y)^2 F(\rho) = \frac{1}{4}(3x^2 + 2\sqrt{3}\,xy + y^2)F(\rho) = \frac{3}{4}\psi_1(\vec{\rho}) + \frac{\sqrt{3}}{2}\psi_2(\vec{\rho}) + \frac{1}{4}\psi_3(\vec{\rho}).
\end{aligned}$$

Making use of

$$Q(T)\psi_n(\vec{\rho}) = \psi_n(R(T)^{-1}\vec{\rho}) = \sum_{m=1}^{3}\Gamma(T)_{mn}\psi_m(\vec{\rho}), \ n = 1, 2, 3$$

for $T = B$, we obtain

$$\begin{aligned}
\Gamma(B)_{11}\psi_1 + \Gamma(B)_{21}\psi_2 + \Gamma(B)_{31}\psi_3 &= \frac{1}{4}\psi_1(\vec{\rho}) - \frac{\sqrt{3}}{2}\psi_2(\vec{\rho}) + \frac{3}{4}\psi_3(\vec{\rho}), \\
\Gamma(B)_{12}\psi_1 + \Gamma(B)_{22}\psi_2 + \Gamma(B)_{32}\psi_3 &= -\frac{\sqrt{3}}{4}\psi_1(\vec{\rho}) + \frac{1}{2}\psi_2(\vec{\rho}) + \frac{\sqrt{3}}{4}\psi_3(\vec{\rho}), \\
\Gamma(B)_{13}\psi_1 + \Gamma(B)_{23}\psi_2 + \Gamma(B)_{33}\psi_3 &= \frac{3}{4}\psi_1(\vec{\rho}) + \frac{\sqrt{3}}{2}\psi_2(\vec{\rho}) + \frac{1}{4}\psi_3(\vec{\rho}).
\end{aligned}$$

Making use of the fact that ψ_1, ψ_2, and ψ_3 are linearly independent, we obtain from the above results

$$\begin{aligned}
&\Gamma(F)_{11} = \frac{1}{4}, && \Gamma(F)_{12} = -\frac{\sqrt{3}}{4}, && \Gamma(F)_{13} = \frac{3}{4}, \\
&\Gamma(F)_{21} = -\frac{\sqrt{3}}{2}, && \Gamma(F)_{22} = \frac{1}{2}, && \Gamma(F)_{23} = \frac{\sqrt{3}}{2}, \\
&\Gamma(F)_{31} = \frac{3}{4}, && \Gamma(F)_{32} = \frac{\sqrt{3}}{4}, && \Gamma(F)_{33} = \frac{1}{4}.
\end{aligned}$$

Thus, the representation matrix of the element B is given by

$$\Gamma(B) = \begin{pmatrix} \frac{1}{4} & -\frac{\sqrt{3}}{4} & \frac{3}{4} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{3}{4} & \frac{\sqrt{3}}{4} & \frac{1}{4} \end{pmatrix}.$$

4. Show that, if the projection operators P^p_{mn} and P^q_{jk} belong to two unitary irreducible representations Γ^p and Γ^q of G that are not equivalent if $p \neq q$ (but are identical if $p = q$), then $P^p_{mn} P^q_{jk} = \delta_{pq}\delta_{nj} P^q_{mk}$.

Making use of

$$P^p_{mn} = \frac{d_p}{g} \sum_{T \in G} \Gamma^p(T)^*_{mn} Q(T),$$

we have

$$\begin{aligned}
P^p_{mn} P^q_{jk} &= \frac{d_p d_q}{g^2} \sum_{T_1, T_2 \in G} \Gamma^p(T_1)^*_{mn} \Gamma^q(T_2)^*_{jk} Q(T_1) Q(T_2) \\
&= \frac{d_p d_q}{g^2} \sum_{T_1, T_2 \in G} \Gamma^p(T_1)^*_{mn} \Gamma^q(T_2)^*_{jk} Q(T_1 T_2).
\end{aligned}$$

Let $T_1 T_2 = T$. Then, we can express T_2 as $T_2 = T_1^{-1} T$. Changing the dummy summation group element variables from T_1 and T_2 to T and T_1, we have

$$\begin{aligned}
P^p_{mn} P^q_{jk} &= \frac{d_p d_q}{g^2} \sum_{T, T_1 \in G} \Gamma^p(T_1)^*_{mn} \Gamma^q(T_1^{-1} T)^*_{jk} Q(T) \\
&= \frac{d_p d_q}{g^2} \sum_{T, T_1 \in G} \Gamma^p(T_1)^*_{mn} \sum_{\ell} \Gamma^q(T_1^{-1})^*_{j\ell} \Gamma^q(T)^*_{\ell k} Q(T).
\end{aligned}$$

Making use of the fact that $\Gamma^q(T_1)$ is a unitary matrix, we have $\Gamma^q(T_1^{-1})^*_{j\ell} = \Gamma^q(T_1)_{\ell j}$. The above result then becomes

$$P^p_{mn} P^q_{jk} = \frac{d_p d_q}{g^2} \sum_{\ell} \sum_{T, T_1 \in G} \Gamma^p(T_1)^*_{mn} \Gamma^q(T_1)_{\ell j} \Gamma^q(T)^*_{\ell k} Q(T).$$

Making use of the orthogonal relation

$$\frac{1}{g} \sum_{T_1 \in G} \Gamma^p(T_1)^*_{mn} \Gamma^q(T_1)_{\ell j} = \frac{1}{d_q} \delta_{pq} \delta_{m\ell} \delta_{nj},$$

we have

$$\begin{aligned}
P^p_{mn} P^q_{jk} &= \frac{d_p}{g} \delta_{pq} \delta_{nj} \sum_{T \in G} \sum_{\ell} \delta_{m\ell} \Gamma^q(T)^*_{\ell k} Q(T) \\
&= \frac{d_p}{g} \delta_{pq} \delta_{nj} \sum_{T \in G} \Gamma^p(T)^*_{mk} Q(T).
\end{aligned}$$

Making use of the definition of the projector operators, we have

$$P^p_{mn} P^q_{jk} = \delta_{pq} \delta_{nj} P^p_{mk}.$$

5. Choosing $\phi(\vec{r}) = (xy + yz)e^{-r}$, construct the basis functions for the two-dimensional irreducible representation Γ^5 of the crystallographic point group D_4.

We first write down the projection operators P^5_{11} and P^5_{22}. We have

$$\begin{aligned}
P^5_{11} &= \frac{1}{4} \sum_{T \in D_4} \Gamma^5(T)^*_{11} Q(T) = \frac{1}{4}\big[Q(E) + Q(C_{2x}) - Q(C_{2y}) - Q(C_{2z})\big], \\
P^5_{22} &= \frac{1}{4} \sum_{T \in D_4} \Gamma^5(T)^*_{22} Q(T) = \frac{1}{4}\big[Q(E) - Q(C_{2x}) - Q(C_{2y}) + Q(C_{2z})\big].
\end{aligned}$$

From the above expressions, we see that, to evaluate $P^5_{11}\phi(\vec{r})$ and $P^5_{22}\phi(\vec{r})$, we need first to evaluate $Q(E)\phi(\vec{r})$, $Q(C_{2x})\phi(\vec{r})$, $Q(C_{2y})\phi(\vec{r})$, and $Q(C_{2z})\phi(\vec{r})$. We know that $Q(E)\phi(\vec{r}) = \phi(\vec{r})$. From $Q(T)\phi(\vec{r}) = \phi(R(T)^{-1}\vec{r})$ and

$$R(C_{2x})^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix},\ R(C_{2y})^{-1} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix},\ R(C_{2z})^{-1} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

we have

$$Q(C_{2x})\phi(\vec{r}) = (-xy + yz)e^{-r},\ Q(C_{2y})\phi(\vec{r}) = -(xy + yz)e^{-r},\ Q(C_{2z})\phi(\vec{r}) = (xy - yz)e^{-r}.$$

We then have

$$\begin{aligned}
P^5_{11}\phi(\vec{r}) &= \frac{1}{4}\big[Q(E)\phi(\vec{r}) + Q(C_{2x})\phi(\vec{r}) - Q(C_{2y})\phi(\vec{r}) - Q(C_{2z})\phi(\vec{r})\big] \\
&= \frac{1}{4}\big[(xy + yz) + (-xy + yz) + (xy + yz) - (xy - yz)\big]e^{-r} \\
&= yze^{-r}, \\
P^5_{22}\phi(\vec{r}) &= \frac{1}{4}\big[Q(E)\phi(\vec{r}) - Q(C_{2x})\phi(\vec{r}) - Q(C_{2y})\phi(\vec{r}) + Q(C_{2z})\phi(\vec{r})\big] \\
&= \frac{1}{4}\big[(xy + yz) - (-xy + yz) + (xy + yz) + (xy - yz)\big]e^{-r} \\
&= xye^{-r}.
\end{aligned}$$

Therefore, the basis functions for the two-dimensional irreducible representation Γ^5 of the crystallographic point group D_4 are

$$\psi_1(\vec{r}) = Ayze^{-r},\ \psi_2(\vec{r}) = -Axye^{-r},$$

where A is the normalization constant and is given by

$$A = (xye^{-r}, xye^{-r})^{-1/2}.$$

In the above expression of $\psi_2(\vec{r})$, we used an overall minus sign to be consistent with the result obtained by using $\psi_2(\vec{r}) = P^5_{21}\psi_1(\vec{r})$. This is permissible because the normalization constant of a basis function can be determined only within a phase factor of magnitude of unity.

We now rederive $\psi_2(\vec{r})$ by making use of $\psi_2(\vec{r}) = P^5_{21}\psi_1(\vec{r})$ with P^5_{21} given by

$$P^5_{21} = \frac{1}{4} \sum_{T \in D_4} \Gamma^5(T)^*_{21} Q(T) = \frac{1}{4}\big[Q(C_{4y}) - Q(C^{-1}_{4y}) + Q(C_{2c}) - Q(C_{2d})\big].$$

From

$$R(C_{4y})^{-1} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix},\ R(C_{4y}^{-1})^{-1} = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix},\ R(C_{2c})^{-1} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix},\ R(C_{2d})^{-1} = \begin{pmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{pmatrix},$$

we have

$$\begin{aligned}
R(C_{4y})^{-1}\vec{r} &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} z \\ y \\ -x \end{pmatrix}, \\
R(C_{4y}^{-1})^{-1}\vec{r} &= \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -z \\ y \\ x \end{pmatrix}, \\
R(C_{2c})^{-1}\vec{r} &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} z \\ -y \\ x \end{pmatrix}, \\
R(C_{2d})^{-1}\vec{r} &= \begin{pmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -z \\ -y \\ -x \end{pmatrix}.
\end{aligned}$$

From $Q(T)\psi_1(\vec{r}) = \psi_1(R(T)^{-1}\vec{r})$, we have

$$Q(C_{4y})\psi_1(\vec{r}) = -xye^{-r},\ Q(C_{4y}^{-1})\psi_1(\vec{r}) = xye^{-r},\ Q(C_{2c})\psi_1(\vec{r}) = -xye^{-r},\ Q(C_{2d})\psi_1(\vec{r}) = xye^{-r}.$$

We then have

$$\begin{aligned}
\psi_2(\vec{r}) &= P_{21}^5\psi_1(\vec{r}) \\
&= \frac{1}{4}\big[Q(C_{4y}) - Q(C_{4y}^{-1}) + Q(C_{2c}) - Q(C_{2d})\big]\psi_1(\vec{r}) \\
&= \frac{1}{4}\big[-Axye^{-r} - Axye^{-r} - Axye^{-r} - Axye^{-r}\big] \\
&= -Axye^{-r}.
\end{aligned}$$