



Group Theory

Solutions to the Problems in Homework Assignment 07

Spring, 2020

Consider a particle of mass μ confined to a square in two dimensions whose vertices are located at $(z, x) = (1, 1), (1, -1), (-1, -1),$ and $(-1, 1)$ on the zOx plane. The potential is zero within the square and infinite on the edges of the square. The eigenfunctions $\psi_{mn}(z, x)$ of the Hamiltonian of the particle are of the form

$$\psi_{mn}(z, x) \propto \begin{cases} \cos(k_m z) \cos(k_n x), & \text{if both } m \text{ and } n \text{ are odd,} \\ \cos(k_m z) \sin(k_n x), & \text{if } m \text{ is odd but } n \text{ is even,} \\ \sin(k_m z) \cos(k_n x), & \text{if } m \text{ is even but } n \text{ is odd,} \\ \sin(k_m z) \sin(k_n x), & \text{if both } m \text{ and } n \text{ are even,} \end{cases}$$

where $k_m = m\pi/2$, $k_n = n\pi/2$, and m and n are positive integers. The corresponding eigenvalues are given by

$$E_{mn} = \frac{\pi^2 \hbar^2}{8\mu} (m^2 + n^2).$$

The symmetry group of the Hamiltonian H_0 is D_4 whose character table is given by

	$C_1 = \{E\}$	$C_2 = \{C_{2x}, C_{2z}\}$	$C_3 = \{C_{2y}\}$	$C_4 = \{C_{4y}, C_{4y}^{-1}\}$	$C_5 = \{C_{2c}, C_{2d}\}$
Γ^1	1	1	1	1	1
Γ^2	1	1	1	-1	-1
Γ^3	1	-1	1	1	-1
Γ^4	1	-1	1	-1	1
Γ^5	2	0	-2	0	0

1. For which irreducible representations do the eigenfunctions $\psi_{11}(z, x)$ and $\psi_{22}(z, x)$ form bases respectively?

Through inspection, we find the following transformation matrices for the elements of D_4 in two dimensions with the position vector of a point given by (z, x)

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

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

The transformation generated by the element T of D_4 on a basis function $\phi_i^p(z, x)$ in representation Γ^p is given by

$$Q(T)\phi_i^p(z, x) = \phi_i^p(z', x') = \sum_{j=1}^{d_p} \Gamma^p(T)_{ji} \phi_j^p(z, x),$$

where

$$\begin{pmatrix} z' \\ x' \end{pmatrix} = R(T) \begin{pmatrix} z \\ x \end{pmatrix}.$$

From the above transformation matrices of the elements of D_4 , we have

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

For $\psi_{11}(z, x) \propto \cos(\pi z/2) \cos(\pi x/2)$, we have $Q(T)\psi_{11}(z, x) = \psi_{11}(z, x)$ for all $T \in D_4$. Since $\psi_{11}(z, x)$ is a complete basis set by itself, $\psi_{11}(z, x)$ is the basis of a one-dimensional irreducible representation. Noting that $Q(T)\psi_{11}(z, x) = \psi_{11}(z, x)$ for all $T \in D_4$, we see that the characters of the elements are all equal to one. Thus, $\psi_{11}(z, x)$ forms the basis for the one-dimensional identity representation Γ^1 .

For $\psi_{22}(z, x) \propto \sin(\pi z) \sin(\pi x)$, we have

$$\begin{aligned} Q(E)\psi_{22}(z, x) &= \psi_{22}(z, x), & Q(C_{2x})\psi_{22}(z, x) &= -\psi_{22}(z, x), & Q(C_{2y})\psi_{22}(z, x) &= \psi_{22}(z, x), \\ Q(C_{2z})\psi_{22}(z, x) &= -\psi_{22}(z, x), & Q(C_{4y})\psi_{22}(z, x) &= -\psi_{22}(z, x), & Q(C_{4y}^{-1})\psi_{22}(z, x) &= -\psi_{22}(z, x), \\ Q(C_{2c})\psi_{22}(z, x) &= \psi_{22}(z, x), & Q(C_{2d})\psi_{22}(z, x) &= \psi_{22}(z, x). \end{aligned}$$

Since $\psi_{22}(z, x)$ is a complete basis set by itself, $\psi_{22}(z, x)$ is the basis of a one-dimensional irreducible representation. From the above results, we can infer the characters of the elements of D_4 . We have

$$\chi(E) = 1, \chi(C_{2x}) = -1, \chi(C_{2y}) = 1, \chi(C_{2z}) = -1, \chi(C_{4y}) = -1, \chi(C_{4y}^{-1}) = -1, \chi(C_{2c}) = 1, \chi(C_{2d}) = 1.$$

Comparing the above characters of the elements with those in the given character table, we see that $\psi_{22}(z, x)$ forms the basis for the one-dimensional parity representation Γ^4 .

- Find the matrices representing all the elements of D_4 in the space spanned by the degenerate eigenfunctions $\psi_{12}(z, x)$ and $\psi_{21}(z, x)$. And then calculate the characters for all the classes of D_4 in this representation. For which irreducible representation do $\psi_{12}(z, x)$ and $\psi_{21}(z, x)$ form a basis?

Note that $\psi_{12}(z, x) \propto \cos(\pi z/2) \sin(\pi x)$ and $\psi_{21}(z, x) \propto \sin(\pi z) \cos(\pi x/2)$. For $\psi_{12}(z, x) \propto \cos(\pi z/2) \sin(\pi x)$, we have

$$\begin{aligned} Q(E)\psi_{12}(z, x) &= \psi_{12}(z, x), & Q(C_{2x})\psi_{12}(z, x) &= \psi_{12}(z, x), & Q(C_{2y})\psi_{12}(z, x) &= -\psi_{12}(z, x), \\ Q(C_{2z})\psi_{12}(z, x) &= -\psi_{12}(z, x), & Q(C_{4y})\psi_{12}(z, x) &= -\psi_{21}(z, x), & Q(C_{4y}^{-1})\psi_{12}(z, x) &= \psi_{21}(z, x), \\ Q(C_{2c})\psi_{12}(z, x) &= \psi_{21}(z, x), & Q(C_{2d})\psi_{12}(z, x) &= -\psi_{21}(z, x). \end{aligned}$$

For $\psi_{21}(z, x) \propto \sin(\pi z) \cos(\pi x/2)$, we have

$$\begin{aligned} Q(E)\psi_{21}(z, x) &= \psi_{21}(z, x), & Q(C_{2x})\psi_{21}(z, x) &= -\psi_{21}(z, x), & Q(C_{2y})\psi_{21}(z, x) &= -\psi_{21}(z, x), \\ Q(C_{2z})\psi_{21}(z, x) &= \psi_{21}(z, x), & Q(C_{4y})\psi_{21}(z, x) &= \psi_{12}(z, x), & Q(C_{4y}^{-1})\psi_{21}(z, x) &= -\psi_{12}(z, x), \\ Q(C_{2c})\psi_{21}(z, x) &= \psi_{12}(z, x), & Q(C_{2d})\psi_{21}(z, x) &= -\psi_{12}(z, x). \end{aligned}$$

Let $\phi_1 = \psi_{12}(z, x)$ and $\phi_2 = \psi_{21}(z, x)$. Making use of

$$Q(T)\phi_i^p(z, x) = \phi_i^p(z', x') = \sum_{j=1}^{d_p} \Gamma^p(T)_{ji} \phi_j^p(z, x),$$

we have

$$\begin{aligned} \Gamma_{11}(E) &= 1, & \Gamma_{21}(E) &= 0, & \Gamma_{11}(C_{2x}) &= 1, & \Gamma_{21}(C_{2x}) &= 0, & \Gamma_{11}(C_{2y}) &= -1, & \Gamma_{21}(C_{2y}) &= 0, \\ \Gamma_{11}(C_{2z}) &= -1, & \Gamma_{21}(C_{2z}) &= 0, & \Gamma_{11}(C_{4y}) &= 0, & \Gamma_{21}(C_{4y}) &= -1, & \Gamma_{11}(C_{4y}^{-1}) &= 0, & \Gamma_{21}(C_{4y}^{-1}) &= 1, \\ \Gamma_{11}(C_{2c}) &= 0, & \Gamma_{21}(C_{2c}) &= 1, & \Gamma_{11}(C_{2d}) &= 0, & \Gamma_{21}(C_{2d}) &= -1, \end{aligned}$$

and

$$\begin{aligned} \Gamma_{12}(E) &= 0, & \Gamma_{22}(E) &= 1, & \Gamma_{12}(C_{2x}) &= 0, & \Gamma_{22}(C_{2x}) &= -1, & \Gamma_{12}(C_{2y}) &= 0, & \Gamma_{22}(C_{2y}) &= -1, \\ \Gamma_{12}(C_{2z}) &= 0, & \Gamma_{22}(C_{2z}) &= 1, & \Gamma_{12}(C_{4y}) &= 1, & \Gamma_{22}(C_{4y}) &= 0, & \Gamma_{12}(C_{4y}^{-1}) &= -1, & \Gamma_{22}(C_{4y}^{-1}) &= 0, \\ \Gamma_{12}(C_{2c}) &= 1, & \Gamma_{22}(C_{2c}) &= 0, & \Gamma_{12}(C_{2d}) &= -1, & \Gamma_{22}(C_{2d}) &= 0, \end{aligned}$$

From the above results, we obtain the following matrices representing all the elements

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

The characters are given by

	$C_1 = \{E\}$	$C_2 = \{C_{2x}, C_{2z}\}$	$C_3 = \{C_{2y}\}$	$C_4 = \{C_{4y}, C_{4y}^{-1}\}$	$C_5 = \{C_{2c}, C_{2d}\}$
Γ	2	0	-2	0	0

From the given character table, we see that the above character system is identical with that of the irreducible representation Γ^5 . Thus, $\psi_{12}(z, x)$ and $\psi_{21}(z, x)$ form a basis for the two-dimensional coordinate irreducible representation Γ^5 .

3. What is the degeneracy corresponding to $(m = 6, n = 7)$ and $(m = 2, n = 9)$? Is this degeneracy normal or accidental?

For $(m = 6, n = 7)$, the energy is given by

$$E_{6,7} = \frac{\pi^2 \hbar^2}{8m} (6^2 + 7^2) = \frac{85\pi^2 \hbar^2}{8m}.$$

For $(m = 2, n = 9)$, the energy is given by

$$E_{6,7} = \frac{\pi^2 \hbar^2}{8m} (2^2 + 9^2) = \frac{85\pi^2 \hbar^2}{8m}.$$

Thus, the energy $85\pi^2 \hbar^2 / 8m$ is four-fold degenerate. Because the elements of D_4 transform $\psi_{6,7}(z, x)$ and $\psi_{7,6}(z, x)$ only between them, $\psi_{6,7}(z, x)$ and $\psi_{7,6}(z, x)$ give rise to a two-fold degeneracy of the energy $85\pi^2 \hbar^2 / 8m$. Similarly, the elements of D_4 transform $\psi_{2,9}(z, x)$ and $\psi_{9,2}(z, x)$ only between them. $\psi_{2,9}(z, x)$ and $\psi_{9,2}(z, x)$ also give rise to a two-fold degeneracy of the energy $85\pi^2 \hbar^2 / 8m$. Since the elements of D_4 can not transform $\psi_{6,7}(z, x)$ and $\psi_{7,6}(z, x)$ into $\psi_{2,9}(z, x)$ or $\psi_{9,2}(z, x)$, the four-fold degeneracy is accidental.

4. Find the matrices representing all the elements of D_4 in the space spanned by the degenerate eigenfunctions $\psi_{mn}(z, x)$ and $\psi_{nm}(z, x)$. Here both m and n are odd integers but they are not equal. And then calculate the characters for all the classes of D_4 in this representation. Is this representation reducible or irreducible? If this representation is reducible, write it as a direct sum of irreducible representations.

For odd m and n , we have $\psi_{mn}(z, x) \propto \cos(m\pi z/2) \cos(n\pi x/2)$ and $\psi_{nm}(z, x) \propto \cos(n\pi z/2) \cos(m\pi x/2)$.

The elements of D_4 transform $\psi_{mn}(z, x)$ as follows

$$\begin{aligned} Q(E)\psi_{mn}(z, x) &= \psi_{mn}(z, x), & Q(C_{2x})\psi_{mn}(z, x) &= \psi_{mn}(z, x), & Q(C_{2y})\psi_{mn}(z, x) &= \psi_{mn}(z, x), \\ Q(C_{2z})\psi_{mn}(z, x) &= \psi_{mn}(z, x), & Q(C_{4y})\psi_{mn}(z, x) &= \psi_{nm}(z, x), & Q(C_{4y}^{-1})\psi_{mn}(z, x) &= \psi_{nm}(z, x), \\ Q(C_{2c})\psi_{mn}(z, x) &= \psi_{nm}(z, x), & Q(C_{2d})\psi_{mn}(z, x) &= \psi_{nm}(z, x). \end{aligned}$$

The elements of D_4 transform $\psi_{nm}(z, x)$ as follows

$$\begin{aligned} Q(E)\psi_{nm}(z, x) &= \psi_{nm}(z, x), & Q(C_{2x})\psi_{nm}(z, x) &= \psi_{nm}(z, x), & Q(C_{2y})\psi_{nm}(z, x) &= \psi_{nm}(z, x), \\ Q(C_{2z})\psi_{nm}(z, x) &= \psi_{nm}(z, x), & Q(C_{4y})\psi_{nm}(z, x) &= \psi_{mn}(z, x), & Q(C_{4y}^{-1})\psi_{nm}(z, x) &= \psi_{mn}(z, x), \\ Q(C_{2c})\psi_{nm}(z, x) &= \psi_{mn}(z, x), & Q(C_{2d})\psi_{nm}(z, x) &= \psi_{mn}(z, x). \end{aligned}$$

Making use of

$$Q(T)\phi_i^p(z, x) = \phi_i^p(z', x') = \sum_{j=1}^{d_p} \Gamma^p(T)_{ji} \phi_j^p(z, x)$$

with $\phi_1 = \psi_{mn}$ and $\phi_2 = \psi_{nm}$, we have

$$\begin{aligned} \Gamma_{11}(E) &= 1, & \Gamma_{21}(E) &= 0, & \Gamma_{11}(C_{2x}) &= 1, & \Gamma_{21}(C_{2x}) &= 0, & \Gamma_{11}(C_{2y}) &= 1, & \Gamma_{21}(C_{2y}) &= 0, \\ \Gamma_{11}(C_{2z}) &= 1, & \Gamma_{21}(C_{2z}) &= 0, & \Gamma_{11}(C_{4y}) &= 0, & \Gamma_{21}(C_{4y}) &= 1, & \Gamma_{11}(C_{4y}^{-1}) &= 0, & \Gamma_{21}(C_{4y}^{-1}) &= 1, \\ \Gamma_{11}(C_{2c}) &= 0, & \Gamma_{21}(C_{2c}) &= 1, & \Gamma_{11}(C_{2d}) &= 0, & \Gamma_{21}(C_{2d}) &= 1, \end{aligned}$$

and

$$\begin{aligned}\Gamma_{12}(E) &= 0, & \Gamma_{22}(E) &= 1, & \Gamma_{12}(C_{2x}) &= 0, & \Gamma_{22}(C_{2x}) &= 1, & \Gamma_{12}(C_{2y}) &= 0, & \Gamma_{22}(C_{2y}) &= 1, \\ \Gamma_{12}(C_{2z}) &= 0, & \Gamma_{22}(C_{2z}) &= 1, & \Gamma_{12}(C_{4y}) &= 1, & \Gamma_{22}(C_{4y}) &= 0, & \Gamma_{12}(C_{4y}^{-1}) &= 1, & \Gamma_{22}(C_{4y}^{-1}) &= 0, \\ \Gamma_{12}(C_{2c}) &= 1, & \Gamma_{22}(C_{2c}) &= 0, & \Gamma_{12}(C_{2d}) &= 1, & \Gamma_{22}(C_{2d}) &= 0.\end{aligned}$$

From the above results, we obtain the following matrices representing all the elements

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

The characters are given by

	$C_1 = \{E\}$	$C_2 = \{C_{2x}, C_{2z}\}$	$C_3 = \{C_{2y}\}$	$C_4 = \{C_{4y}, C_{4y}^{-1}\}$	$C_5 = \{C_{2c}, C_{2d}\}$
Γ	2	2	2	0	0

Because the above character system is not identical with the character system of any irreducible representation of D_4 , the representation Γ is reducible. For the convenience of reducing the Γ representation, we list in the following the characters for all the irreducible representations of D_4 and the representation Γ .

	$C_1 = \{E\}$	$C_2 = \{C_{2x}, C_{2z}\}$	$C_3 = \{C_{2y}\}$	$C_4 = \{C_{4y}, C_{4y}^{-1}\}$	$C_5 = \{C_{2c}, C_{2d}\}$
Γ^1	1	1	1	1	1
Γ^2	1	1	1	-1	-1
Γ^3	1	-1	1	1	-1
Γ^4	1	-1	1	-1	1
Γ^5	2	0	-2	0	0
Γ	2	2	2	0	0

We now calculate the number of times that each irreducible representation occurs in the reduction of Γ .

For Γ^1 , we have

$$n_1 = \frac{1}{g} \sum_{T \in D_4} \chi(T) \chi^1(T)^* = \frac{1}{8} (2 \times 1 + 2 \times 2 \times 1 + 2 \times 1) = 1.$$

For Γ^2 , we have

$$n_2 = \frac{1}{g} \sum_{T \in D_4} \chi(T) \chi^2(T)^* = \frac{1}{8} (2 \times 1 + 2 \times 2 \times 1 + 2 \times 1) = 1.$$

For Γ^3 , we have

$$n_3 = \frac{1}{g} \sum_{T \in D_4} \chi(T) \chi^3(T)^* = \frac{1}{8} [2 \times 1 + 2 \times 2 \times (-1) + 2 \times 1] = 0.$$

For Γ^4 , we have

$$n_4 = \frac{1}{g} \sum_{T \in D_4} \chi(T) \chi^4(T)^* = \frac{1}{8} [2 \times 1 + 2 \times 2 \times (-1) + 2 \times 1] = 0.$$

For Γ^5 , we have

$$n_5 = \frac{1}{g} \sum_{T \in D_4} \chi(T) \chi^5(T)^* = \frac{1}{8} [2 \times 2 + 2 \times (-2)] = 0.$$

Thus,

$$\Gamma \approx \Gamma^1 \oplus \Gamma^2.$$

5. Consider the case in which the particle is subject to an interaction given by Ax with A a constant.

- (a) For which irreducible representation of D_4 is x an irreducible tensor operator?
- (b) Consider the transitions caused by the interaction. If the particle is initially in the state $\psi_{mn}(z, x)$ or $\psi_{nm}(z, x)$ with m and n respectively even and odd integers, through reducing the direct product of irreducible representations find the irreducible representations which the allowed final states transform as.

- (a) The transformation matrices for the elements of D_4 are given by

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

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

x , y , and z are transformed by the rotation corresponding to the element X of D_4 as follows

$$\begin{aligned} Q(X)xQ(X)^{-1} &= R_{11}(X)x + R_{21}(X)y + R_{31}(X)z, \\ Q(X)yQ(X)^{-1} &= R_{12}(X)x + R_{22}(X)y + R_{32}(X)z, \\ Q(X)zQ(X)^{-1} &= R_{13}(X)x + R_{23}(X)y + R_{33}(X)z. \end{aligned}$$

Noticing that $R(X)_{21} = R(X)_{23} = 0$ for all $X \in D_4$, we have

$$\begin{aligned} Q(X)xQ(X)^{-1} &= R_{11}(X)x + R_{31}(X)z, \\ Q(X)zQ(X)^{-1} &= R_{13}(X)x + R_{33}(X)z. \end{aligned}$$

Let $T_1 = x$ and $T_2 = z$. We can then rewrite the above transformation in the form

$$Q(X)T_jQ(X)^{-1} = \sum_{k=1}^2 \Gamma(X)_{kj}T_k,$$

where

$$\Gamma(X) = \begin{pmatrix} R_{11}(X) & R_{31}(X) \\ R_{13}(X) & R_{33}(X) \end{pmatrix}.$$

From the above-given transformation matrices for the elements of D_4 , we have the following matrices for all the elements of D_4 in the representation Γ

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

The characters of the classes of D_4 in the representation Γ are given by

	$C_1 = \{E\}$	$C_2 = \{C_{2x}, C_{2z}\}$	$C_3 = \{C_{2y}\}$	$C_4 = \{C_{4y}, C_{4y}^{-1}\}$	$C_5 = \{C_{2c}, C_{2d}\}$
Γ	2	0	-2	0	0

Comparing the characters in the representation Γ with those in the irreducible representation Γ^5 , we see that the representation Γ is equivalent to the irreducible representation Γ^5 . Hence, x and z are a set of irreducible tensor operators for the irreducible representation Γ^5 . Therefore, x is an irreducible tensor operator for the irreducible representation Γ^5 .

- (b) From the solution to Problem 2 in the above, we know that the degenerate eigenfunctions $\psi_{mn}(z, x)$ and $\psi_{nm}(z, x)$ with m and n respectively even and odd integers form a basis for Γ^5 . Thus, $\psi_{mn}(z, x)$ and $\psi_{nm}(z, x)$ transform as Γ^5 . Because x is an irreducible tensor operator for the irreducible representation Γ^5 and $\psi_{mn}(z, x)$ and $\psi_{nm}(z, x)$ transform as Γ^5 , we must consider the direct product $\Gamma^5 \otimes \Gamma^5$ to find the allowed final states. The characters for $\Gamma^5 \otimes \Gamma^5$ are given by

	$C_1 = \{E\}$	$C_2 = \{C_{2x}, C_{2z}\}$	$C_3 = \{C_{2y}\}$	$C_4 = \{C_{4y}, C_{4y}^{-1}\}$	$C_5 = \{C_{2c}, C_{2d}\}$
$\Gamma^5 \otimes \Gamma^5$	4	0	4	0	0

Using

$$n_{pq}^r = \frac{1}{g} \sum_{T \in G} \chi^p(T) \chi^q(T) \chi^r(T)^*,$$

we have

$$\begin{aligned} n_{55}^1 &= \frac{1}{8}(4 + 4) = 1, \\ n_{55}^2 &= \frac{1}{8}(4 + 4) = 1, \\ n_{55}^3 &= \frac{1}{8}(4 + 4) = 1, \\ n_{55}^4 &= \frac{1}{8}(4 + 4) = 1, \\ n_{55}^5 &= \frac{1}{8}(8 - 8) = 0. \end{aligned}$$

We thus have

$$\Gamma^5 \otimes \Gamma^5 \approx \Gamma^1 \oplus \Gamma^2 \oplus \Gamma^3 \oplus \Gamma^4.$$

The eigenfunctions that transform as Γ^1 through Γ^4 may be the final states while the eigenfunctions that transform as Γ^5 can not be the final states.