Assignment 07

Due Time : 8:15, April 22, 2020 (Wednesday)

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Score : ________

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 edge of the square. The eigenfunctions $\psi_{mn}(z,x)$ of the Hamiltonian of the particle are of the form

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

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

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

Solution: Suppose the dimension of irreducible representation Γ^p is d_p. Since the order of D_4 is 8, we have

$$\begin{aligned}&d_1^2+d_2^2+d_3^2+d_4^2+d_5^2=8, && (1)\\ \Longrightarrow\ & d_1=d_2=d_3=d_4=1,\quad d_5=2. && (2)\end{aligned}$$

Γ_1, Γ_2, Γ_3, and Γ_4 are 1-dimensional representations and Γ_5 is 2-dimensional representation.
For 1-dimensional representations Γ_1, Γ_2, Γ_3, and Γ_4 of D_4, the basis functions transform for every coordinate transformation T of D_4 according to

$$Q(T)\psi(\vec{r})=\Gamma(T)_{11}\psi(\vec{r})=\chi(T)\psi. \tag{3}$$

We first calculate $Q(T)\psi_{11}(z,x)$ and $Q(T)\psi_{22}(z,x)$ for every coordinate transformation T of D_4. We already know the transformation matrices of D_4 in two dimensions are

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

Since

$$R(T)^{-1}=R(T)^T \tag{4}$$

for every $T\in G$, we have

$$Q(T)\psi(\vec{r})=\psi(R(T)^{-1}\vec{r})=\psi(R(T)^T\vec{r}). \tag{5}$$

Since

$$R(E)^T\vec{r}=\begin{pmatrix}1&0\\0&1\end{pmatrix}\begin{pmatrix}z\\x\end{pmatrix}=\begin{pmatrix}z\\x\end{pmatrix}, \tag{6}$$

$$R(C_{2x})^T\vec{r}=\begin{pmatrix}1&0\\0&-1\end{pmatrix}\begin{pmatrix}z\\x\end{pmatrix}=\begin{pmatrix}z\\-x\end{pmatrix}, \tag{7}$$

$$R(C_{2y})^T\vec{r}=\begin{pmatrix}-1&0\\0&-1\end{pmatrix}\begin{pmatrix}z\\x\end{pmatrix}=\begin{pmatrix}-z\\-x\end{pmatrix}, \tag{8}$$

$$R(C_{2z})^T\vec{r} = \begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix}\begin{pmatrix}z\\ x\end{pmatrix} = \begin{pmatrix}-z\\ x\end{pmatrix}, \tag{9}$$

$$R(C_{4y})^T\vec{r} = \begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}\begin{pmatrix}z\\ x\end{pmatrix} = \begin{pmatrix}x\\ -z\end{pmatrix}, \tag{10}$$

$$R(C_{4y}^{-1})^T\vec{r} = \begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}\begin{pmatrix}z\\ x\end{pmatrix} = \begin{pmatrix}-x\\ z\end{pmatrix}, \tag{11}$$

$$R(C_{2c})^T\vec{r} = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}z\\ x\end{pmatrix} = \begin{pmatrix}x\\ z\end{pmatrix}, \tag{12}$$

$$R(C_{2d})^T\vec{r} = \begin{pmatrix}0 & -1\\ -1 & 0\end{pmatrix}\begin{pmatrix}z\\ x\end{pmatrix} = \begin{pmatrix}-x\\ -z\end{pmatrix}, \tag{13}$$

for $\psi_{11}(z,x)$, we have

$$\begin{aligned}&Q(E)\psi_{11}(z,x) = R(C_{2x})\psi_{11}(z,x) = R(C_{2y})\psi_{11}(z,x) = R(C_{2z})\psi_{11}(z,x)\\ =&Q(C_{4y})\psi_{11}(z,x) = Q(C_{4y}^{-1})\psi_{11}(z,x) = Q(C_{2c})\psi_{11}(z,x) = Q(C_{2d})\psi_{11}(z,x) = \psi_{11}(z,x) = \sin(k_1z)\sin(k_2x) = \psi_{11}(z,x),\end{aligned} \tag{14}$$

$$\Longrightarrow \chi(C_1) = \chi(C_2) = \chi(C_3) = \chi(C_4) = \chi(C_5) = 1. \tag{15}$$

and for $\psi_{22}(z,x)$, we have

$$Q(E)\psi_{22}(z,x) = Q(C_{2y})\psi_{22}(z,x) = Q(C_{2c})\psi_{22}(z,x) = Q(C_{2d})\psi_{22}(z,x) = \sin(k_1z)\sin(k_1x) = \psi_{22}(z,x), \tag{16}$$

$$Q(C_{2x})\psi_{22}(z,x) = Q(C_{2z})\psi_{22}(z,x) = Q(C_{4y})\psi_{22}(z,x) = Q(C_{4y}^{-1})\psi_{22}(z,x) = -\sin(k_1z)\sin(k_1x) = -\psi_{22}(z,x). \tag{17}$$

$$\Longrightarrow \chi(C_1) = \chi(C_3) = \chi(C_5) = 1, \quad \chi(C_2) = \chi(C_4) = -1. \tag{18}$$

Therefore, the eigenfunction $\psi_{11}(z,x)$ forms the basis of Γ_1 and the eigenfunction $\psi_{22}(z,x)$ forms the basis of Γ_4. □

Problem 2 Score: _________. 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?

Solution: Since

$$Q(E)\psi_{12}(z,x) = \cos(k_1z)\sin(k_2x) = \psi_{12}(z,x) = \Gamma(E)_{11}\psi_{12}(z,x) + \Gamma(E)_{21}\psi_{21}(z,x), \tag{19}$$

$$Q(E)\psi_{21}(z,x) = \sin(k_2z)\cos(k_1x) = \psi_{21}(z,x) = \Gamma(E)_{12}\psi_{12}(z,x) + \Gamma(E)_{22}\psi_{21}(z,x), \tag{20}$$

we have

$$\Gamma(E)_{11} = 1, \quad \Gamma(E)_{21} = 0, \quad \Gamma(E)_{12} = 0, \quad \Gamma(E)_{22} = 1, \tag{21}$$

$$\Longrightarrow \Gamma(E) = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}. \tag{22}$$

Since

$$Q(C_{2x})\psi_{12}(z,x) = -\cos(k_1z)\sin(k_2x) = -\psi_{12}(z,x) = \Gamma(C_{2x})_{11}\psi_{12}(z,x) + \Gamma(C_{2x})_{21}\psi_{21}(z,x), \tag{23}$$

$$Q(C_{2x})\psi_{21}(z,x) = \sin(k_2z)\cos(k_1x) = \psi_{21}(z,x) = \Gamma(C_{2x})_{12}\psi_{12}(z,x) + \Gamma(C_{2x})_{22}\psi_{21}(z,x), \tag{24}$$

we have

$$\Gamma(C_{2x})_{11} = -1, \quad \Gamma(C_{2x})_{21} = 0, \quad \Gamma(C_{2x})_{12} = 0, \quad \Gamma(C_{2x})_{22} = 1, \tag{25}$$

$$\Longrightarrow \Gamma(C_{2x}) = \begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix}. \tag{26}$$

Since

$$Q(C_{2y})\psi_{12}(z,x) = -\cos(k_1z)\sin(k_2x) = -\psi_{12}(z,x) = \Gamma(C_{2y})_{11}\psi_{12}(z,x) + \Gamma(C_{2y})_{21}\psi_{21}(z,x), \tag{27}$$

$$Q(C_{2y})\psi_{21}(z,x) = -\sin(k_2z)\cos(k_1x) = -\psi_{21}(z,x) = \Gamma(C_{2z})_{12}\psi_{12}(z,x) + \Gamma(C_{2y})_{22}\psi_{21}(z,x), \tag{28}$$

we have

$$\Gamma(C_{2y})_{11}=-1,\quad \Gamma(C_{2y})_{21}=0,\quad \Gamma(C_{2y})_{12}=0,\quad \Gamma(C_{2y})_{22}=-1, \tag{29}$$

$$\Longrightarrow \Gamma(C_{2y})=\begin{pmatrix}-1 & 0\\ 0 & -1\end{pmatrix}. \tag{30}$$

Since

$$Q(C_{2z})\psi_{12}(z,x)=\cos(k_1z)\sin(k_2x)=\psi_{12}(z,x)=\Gamma(C_{2z})_{11}\psi_{12}(z,x)+\Gamma(C_{2z})_{21}\psi_{21}(z,x), \tag{31}$$

$$Q(C_{2z})\psi_{21}(z,x)=-\sin(k_2z)\cos(k_1x)=-\psi_{21}(z,x)=\Gamma(C_{2z})_{12}\psi_{12}(z,x)+\Gamma(C_{2z})_{22}\psi_{21}(z,x), \tag{32}$$

we have

$$\Gamma(C_{2z})_{11}=1,\quad \Gamma(C_{2z})_{21}=0,\quad \Gamma(C_{2z})_{12}=0,\quad \Gamma(C_{2z})_{22}=-1, \tag{33}$$

$$\Longrightarrow \Gamma(C_{2z})=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{34}$$

Since

$$Q(C_{4y})\psi_{12}(z,x)=-\cos(k_1x)\sin(k_2z)=-\psi_{21}(z,x)=\Gamma(C_{4y})_{11}\psi_{12}(z,x)+\Gamma(C_{4y})_{21}\psi_{21}(z,x), \tag{35}$$

$$Q(C_{4y})\psi_{21}(z,x)=\sin(k_2x)\cos(k_1z)=\psi_{12}(z,x)=\Gamma(C_{4y})_{12}\psi_{12}(z,x)+\Gamma(C_{4y})_{22}\psi_{21}(z,x), \tag{36}$$

we have

$$\Gamma(C_{4y})_{11}=0,\quad \Gamma(C_{4y})_{21}=-1,\quad \Gamma(C_{4y})_{12}=1,\quad \Gamma(C_{4y})_{22}=0, \tag{37}$$

$$\Longrightarrow \Gamma(C_{4y})=\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}. \tag{38}$$

Since

$$Q(C_{4y}^{-1})\psi_{12}(z,x)=\cos(k_1x)\sin(k_2z)=\psi_{21}(z,x)=\Gamma(C_{4y}^{-1})_{11}\psi_{12}(z,x)+\Gamma(C_{4y}^{-1})_{21}\psi_{21}(z,x), \tag{39}$$

$$Q(C_{4y}^{-1})\psi_{21}(z,x)=-\sin(k_2x)\cos(k_1z)=-\psi_{12}(z,x)=\Gamma(C_{4y}^{-1})_{12}\psi_{12}(z,x)+\Gamma(C_{4y}^{-1})_{22}\psi_{21}(z,x), \tag{40}$$

we have

$$\Gamma(C_{4y}^{-1})_{11}=0,\quad \Gamma(C_{4y}^{-1})_{21}=1,\quad \Gamma(C_{4y}^{-1})_{12}=-1,\quad \Gamma(C_{4y}^{-1})_{22}=0, \tag{41}$$

$$\Longrightarrow \Gamma(C_{4y}^{-1})=\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}. \tag{42}$$

Since

$$Q(C_{2c})\psi_{12}(z,x)=\cos(k_1x)\sin(k_2z)=\psi_{21}(z,x)=\Gamma(C_{2c})_{11}\psi_{12}(z,x)+\Gamma(C_{2c})_{21}\psi_{21}(z,x), \tag{43}$$

$$Q(C_{2c})\psi_{21}(z,x)=\sin(k_2x)\cos(k_1z)=\psi_{12}(z,x)=\Gamma(C_{2c})_{12}\psi_{12}(z,x)+\Gamma(C_{2c})_{22}\psi_{21}(z,x), \tag{44}$$

we have

$$\Gamma(C_{2c})_{11}=0,\quad \Gamma(C_{2c})_{21}=1,\quad \Gamma(C_{2c})_{12}=1,\Gamma(C_{2c})_{22}=0, \tag{45}$$

$$\Longrightarrow \Gamma(C_{2c})=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}. \tag{46}$$

Since

$$Q(C_{2d})\psi_{12}(z,x)=-\cos(k_1x)\sin(k_2z)=-\psi_{21}(z,x)=\Gamma(C_{2d})_{11}\psi_{12}(z,x)+\Gamma(C_{2d})_{21}\psi_{21}(z,x), \tag{47}$$

$$Q(C_{2d})\psi_{21}(z,x)=-\sin(k_2x)\cos(k_1z)=-\psi_{12}(z,x)=\Gamma(C_{2d})_{12}\psi_{12}(z,x)+\Gamma(C_{2d})_{22}\psi_{21}(z,x), \tag{48}$$

we have

$$\Gamma(C_{2d})_{11}=0,\quad \Gamma(C_{2d})_{21}=-1,\quad \Gamma(C_{2d})_{12}=-1,\quad \Gamma(C_{2d})_{22}=0, \tag{49}$$

$$\Longrightarrow \Gamma(C_{2d})=\begin{pmatrix}0 & -1\\ -1 & 0\end{pmatrix}. \tag{50}$$

The characters for all the classes of D_4 in this representation are

$$\chi(C_1)=2,\quad \chi(C_2)=\chi(C_4)=\chi(C_5)=0,\quad \chi(C_3)=-2. \tag{51}$$

Therefore, $\psi_{12}(z,x)$ and $\psi_{21}(z,x)$ form a basis of Γ_5. □

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

Solution: Similar to last problem, both $(m = 6, n = 7)$ and $(m = 2, n = 9)$ form the basis of the representation Γ^5 respectively, so their corresponding representation is irreducible, $\Gamma = \Gamma^5 \oplus \Gamma^5$. Therefore, the corresponding degeneracy is accidental. □

Problem 4 Score: _________. 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.

Solution: Since

$$\begin{aligned} Q(E)\psi_{mn}(z,x) &= \cos(k_m z)\cos(k_n x) = \psi_{mn}(z,x) = \Gamma(E)_{11}\psi_{mn}(z,x) + \Gamma(E)_{21}\psi_{nm}(z,x), && (52)\\ Q(E)\psi_{nm}(z,x) &= \cos(k_n z)\cos(k_m x) = \psi_{nm}(z,x) = \Gamma(E)_{12}\psi_{mn}(z,x) + \Gamma(E)_{22}\psi_{nm}(z,x), && (53) \end{aligned}$$

we have

$$\begin{gathered} \Gamma(E)_{11} = 1, \quad \Gamma(E)_{21} = 0, \quad \Gamma(E)_{12} = 0, \quad \Gamma(E)_{22} = 1, \qquad (54)\\ \Longrightarrow \Gamma(E) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \qquad (55) \end{gathered}$$

Since

$$\begin{aligned} Q(C_{2x})\psi_{mn}(z,x) &= \cos(k_m z)\cos(k_n x) = \psi_{mn}(z,x) = \Gamma(C_{2x})_{11}\psi_{mn}(z,x) + \Gamma(C_{2x})_{21}\psi_{nm}(z,x), && (56)\\ Q(C_{2y})\psi_{nm}(z,x) &= \cos(k_n z)\cos(k_m x) = \psi_{nm}(z,x) = \Gamma(C_{2x})_{12}\psi_{mn}(z,x) + \Gamma(C_{2x})_{22}\psi_{nm}(z,x), && (57) \end{aligned}$$

we have

$$\begin{gathered} \Gamma(C_{2x})_{11} = 1, \quad \Gamma(C_{2x})_{21} = 0, \quad \Gamma(C_{2x})_{12} = 0, \quad \Gamma(C_{2x})_{22} = 1, \qquad (58)\\ \Longrightarrow \Gamma(C_{2x}) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \qquad (59) \end{gathered}$$

Since

$$\begin{aligned} Q(C_{2y})\psi_{mn}(z,x) &= \cos(k_m z)\cos(k_n x) = \psi_{mn}(z,x) = \Gamma(C_{2y})_{11}\psi_{mn}(z,x) + \Gamma(C_{2y})_{21}\psi_{nm}(z,x), && (60)\\ Q(C_{2y})\psi_{nm}(z,x) &= \cos(k_n z)\cos(k_m x) = \psi_{nm}(z,x) = \Gamma(C_{2y})_{12}\psi_{mn}(z,x) + \Gamma(C_{2y})_{22}\psi_{nm}(z,x), && (61) \end{aligned}$$

we have

$$\begin{gathered} \Gamma(C_{2y})_{11} = 1, \quad \Gamma(C_{2y})_{21} = 0, \quad \Gamma(C_{2y})_{12} = 0, \quad \Gamma_{22}(C_{2y}) = 1, \qquad (62)\\ \Longrightarrow \Gamma(C_{2y}) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \qquad (63) \end{gathered}$$

Since

$$\begin{aligned} Q(C_{2z})\psi_{mn}(z,x) &= \cos(k_m z)\cos(k_n x) = \psi_{mn}(z,x) = \Gamma(C_{2z})_{11}\psi_{mn}(z,x) + \Gamma(C_{2z})_{21}\psi_{nm}(z,x), && (64)\\ Q(C_{2z})\psi_{nm}(z,x) &= \cos(k_n z)\cos(k_m x) = \psi_{nm}(z,x) = \Gamma(C_{2z})_{12}\psi_{mn}(z,x) + \Gamma(C_{2z})_{12}\psi_{nm}(z,x), && (65) \end{aligned}$$

we have

$$\begin{gathered} \Gamma(C_{2z})_{11} = 1, \quad \Gamma(C_{2z})_{21} = 0, \quad \Gamma(C_{2z})_{12} = 0, \quad \Gamma(C_{2z})_{22} = 1, \qquad (66)\\ \Longrightarrow \Gamma(C_{2z}) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \qquad (67) \end{gathered}$$

Since

$$\begin{aligned} Q(C_{4y})\psi_{mn}(z,x) &= \cos(k_m x)\cos(k_n z) = \psi_{nm}(z,x) = \Gamma(C_{4y})_{11}\psi_{mn}(z,x) + \Gamma(C_{4y})_{21}\psi_{nm}(z,x), && (68)\\ Q(C_{4y})\psi_{nm}(z,x) &= \cos(k_n x)\cos(k_m z) = \psi_{mn}(z,x) = \Gamma(C_{4y})_{12}\psi_{mn}(z,x) + \Gamma(C_{4y})_{22}\psi_{nm}(z,x), && (69) \end{aligned}$$

we have

$$\Gamma(C_{4y})_{11}=0,\quad \Gamma(C_{4y})_{21}=1,\quad \Gamma(C_{4y})_{12}=1,\quad \Gamma(C_{4y})_{22}=0, \tag{70}$$

$$\Longrightarrow \Gamma(C_{4y})=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}. \tag{71}$$

Since

$$Q(C_{4y}^{-1})\psi_{mn}(z,x)=\cos(k_m x)\cos(k_n z)=\psi_{nm}(z,x)=\Gamma(C_{4y}^{-1})_{11}\psi_{mn}(z,x)+\Gamma(C_{4y}^{-1})_{21}\psi_{nm}(z,x), \tag{72}$$

$$Q(C_{4y}^{-1})\psi_{nm}(z,x)=\cos(k_n x)\cos(k_m z)=\psi_{mn}(z,x)=\Gamma(C_{4y}^{-1})_{12}\psi_{mn}(z,x)+\Gamma(C_{4y}^{-1})_{22}\psi_{nm}(z,x), \tag{73}$$

we have

$$\Gamma(C_{4y}^{-1})_{11}=-1,\quad \Gamma(C_{4y}^{-1})_{21}=1,\quad \Gamma(C_{4y}^{-1})_{12}=1,\quad \Gamma(C_{4y}^{-1})_{22}=0, \tag{74}$$

$$\Longrightarrow \Gamma(C_{4y}^{-1})=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}. \tag{75}$$

Since

$$Q(C_{2c})\psi_{mn}(z,x)=\cos(k_m x)\cos(k_n z)=\psi_{nm}(z,x)=\Gamma(C_{2c})_{11}\psi_{mn}(z,x)+\Gamma(C_{2c})_{21}\psi_{nm}(z,x), \tag{76}$$

$$Q(C_{2c})\psi_{nm}(z,x)=\cos(k_n x)\cos(k_m z)=\psi_{mn}(z,x)=\Gamma(C_{2c})_{12}\psi_{mn}(z,x)+\Gamma(C_{2c})_{22}\psi_{nm}(z,x), \tag{77}$$

we have

$$\Gamma(C_{2c})_{11}=0,\quad \Gamma(C_{2c})_{21}=1,\quad \Gamma(C_{2c})_{12}=1,\quad \Gamma(C_{2c})_{22}=0, \tag{78}$$

$$\Longrightarrow \Gamma(C_{2c})=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}. \tag{79}$$

Since

$$Q(C_{2c})\psi_{mn}(z,x)=\cos(k_m x)\cos(k_n z)=\psi_{nm}(z,x)=\Gamma(C_{2d})_{11}\psi_{mn}(z,x)+\Gamma(C_{2d})_{21}\psi_{nm}(z,x), \tag{80}$$

$$Q(C_{2c})\psi_{nm}(z,x)=\cos(k_n x)\cos(k_m z)=\psi_{mn}(z,x)=\Gamma(C_{2d})_{12}\psi_{mn}(z,x)+\Gamma(C_{2d})_{22}\psi_{nm}(z,x), \tag{81}$$

we have

$$\Gamma(C_{2d})_{11}=0,\quad \Gamma(C_{2d})_{21}=1,\quad \Gamma(C_{2d})_{12}=1,\quad \Gamma(C_{2d})_{22}=0, \tag{82}$$

$$\Longrightarrow \Gamma(C_{2d})=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}. \tag{83}$$

The characters for all the classes of D_4 in this representation is

$$\chi(C_1)=\chi(C_2)=\chi(C_3)=2,\quad \chi(C_4)=\chi(C_5)=0. \tag{84}$$

This representation is similar to such a representation

$$\Gamma'=S^{-1}\Gamma S=\frac{\sqrt{2}}{2}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\Gamma\frac{\sqrt{2}}{2}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix} \tag{85}$$

that

$$\Gamma'(E)=\Gamma'(C_{2x})=\Gamma'(C_{2y})=\Gamma'(C_{2z})=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}, \tag{86}$$

$$\Gamma'(C_{4y})=\Gamma'(C_{4y}^{-1})=\Gamma'(C_{2c})=\Gamma'(C_{2d})=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{87}$$

Therefore, this representation is reducible:

$$\Gamma\cong\Gamma_1\oplus\Gamma_2. \tag{88}$$

□

Problem 5 Score: ________. 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 state transform as.

Solution: (a) Let $Q(T)xQ(T)^{-1}$ operate on an arbitrary wavefunction $f(z,x)$, we have

$$Q(T)xQ(T^{-1})f(z,x)=Q(T)\{x[Q(T)^{-1}\psi(z,x)]\}=[Q(T)x][Q(X)Q(X)^{-1}\psi(z,x)]=[Q(T)x]\psi(z,x). \tag{89}$$

Due to the arbitrariness of the wavefunction $\psi(z,x)$, we have

$$Q(T)xQ(T)^{-1}=Q(T)x. \tag{90}$$

Now that x is an irreducible tensor operator, let z also be in the set of irreducible operators. To make x an irreducible tensor operator, we need

$$Q(T)x=\Gamma^q(T)_{12}z+\Gamma^q(T)_{22}x, \tag{91}$$
$$Q(T)z=\Gamma^q(T)_{11}z+\Gamma^q(T)_{21}x. \tag{92}$$

for every $T\in D_4$.
For $T=E$, we need

$$Q(E)x=x=\Gamma^q(E)_{12}z+\Gamma^q(E)_{22}x, \tag{93}$$
$$Q(E)z=z=\Gamma^q(E)_{11}z+\Gamma^q(E)_{21}x, \tag{94}$$

$$\Longrightarrow \Gamma^q(E)_{12}=0,\quad \Gamma^q(E)_{22}=1,\quad \Gamma^q(E)_{11}=1,\quad \Gamma^q(E)_{11}=0, \tag{95}$$
$$\Longrightarrow \Gamma^q(E)=\begin{pmatrix}1&0\\0&1\end{pmatrix}. \tag{96}$$

For $T=C_{2x}$, we need

$$Q(C_{2x})x=-x=\Gamma^q(C_{2x})_{12}z+\Gamma^q(C_{2x})_{22}x, \tag{97}$$
$$Q(C_{2x})z=z=\Gamma^q(C_{2x})_{11}z+\Gamma^q(C_{2x})_{21}x, \tag{98}$$

$$\Longrightarrow \Gamma^q(C_{2x})_{12}=0,\quad \Gamma^q(C_{2z})_{22}=-1,\quad \Gamma^q(C_{2x})_{11}=1,\quad \Gamma^q(C_{2x})_{21}=0 \tag{99}$$
$$\Longrightarrow \Gamma^q(C_{2x})=\begin{pmatrix}1&0\\0&-1\end{pmatrix}. \tag{100}$$

For $T=C_{2y}$, we need

$$Q(C_{2y})x=-x=\Gamma^q(C_{2y})_{12}z+\Gamma^q(C_{2y})_{22}x, \tag{101}$$
$$Q(C_{2y})z=-z=\Gamma^q(C_{2y})_{11}z+\Gamma^q(C_{2y})_{21}x, \tag{102}$$

$$\Longrightarrow \Gamma^q(C_{2y})_{12}=0,\quad \Gamma^q(C_{2y})_{22}=-1,\quad \Gamma^q(C_{2y})_{11}=-1,\quad \Gamma^q(C_{2y})_{21}=0, \tag{103}$$
$$\Longrightarrow \Gamma^q(C_{2y})=\begin{pmatrix}-1&0\\0&-1\end{pmatrix}. \tag{104}$$

For $T=C_{2z}$, we need

$$Q(C_{2z})x=x=\Gamma^q(C_{2z})_{12}z+\Gamma^q(C_{2z})_{22}x, \tag{105}$$
$$Q(C_{2z})z=-z=\Gamma^q(C_{2z})_{11}z+\Gamma^q(C_{2z})_{21}x, \tag{106}$$

$$\Longrightarrow \Gamma^q(C_{2z})_{12}=0,\quad \Gamma^q(C_{2z})_{22}=1,\quad \Gamma^q(C_{2z})_{11}=-1,\quad \Gamma^q(C_{2z})_{12}=0, \tag{107}$$

$$\Longrightarrow \Gamma^q(C_{2z}) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{108}$$

For $T = C_{4y}$, we need

$$Q(C_{4y})x = -z = \Gamma^q(C_{4y})_{12}z + \Gamma^q(C_{4y})_{22}x, \tag{109}$$
$$Q(C_{4y})z = x = \Gamma^q(C_{4y})_{11}z + \Gamma^q(C_{4y})_{21}x, \tag{110}$$

$$\Longrightarrow \Gamma^q(C_{4y})_{12} = -1, \quad \Gamma^q(C_{4y})_{22} = 0, \quad \Gamma^q(C_{4y})_{11} = 0, \quad \Gamma^q(C_{4y})_{21} = 1, \tag{111}$$
$$\Longrightarrow \Gamma^q(C_{4y}) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{112}$$

For $T = C_{4y}^{-1}$, we need

$$Q(C_{4y}^{-1}) = z = \Gamma^q(C_{4y}^{-1})_{12}z + \Gamma^q(C_{4y}^{-1})_{22}x, \tag{113}$$
$$Q(C_{4y}^{-1}) = -x = \Gamma^q(C_{4y}^{-1})_{11}z + \Gamma^q(C_{4y}^{-1})_{21}x, \tag{114}$$

$$\Longrightarrow \Gamma^q(C_{4y})_{12} = 1, \quad \Gamma^q(C_{4y})_{22} = 0, \quad \Gamma^q(C_{4y}^{-1})_{11} = 0, \quad \Gamma^q(C_{4y}^{-1})_{21} = -1, \tag{115}$$
$$\Longrightarrow \Gamma^q(C_{4y}^{-1}) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{116}$$

For $T = C_{2c}$, we need

$$Q(C_{2c})x = z = \Gamma^q(C_{2c})_{12}z + \Gamma^q(C_{2c})_{22}x, \tag{117}$$
$$Q(C_{2c})x = x = \Gamma^q(C_{2c})_{11}z + \Gamma^q(C_{2c})_{21}x, \tag{118}$$

$$\Longrightarrow \Gamma^q(C_{2c})_{12} = 1, \quad \Gamma^q(C_{2c})_{22} = 0, \quad \Gamma^q(C_{2c})_{11} = 0, \quad \Gamma^q(C_{2c})_{21} = 1, \tag{119}$$
$$\Longrightarrow \Gamma^q(C_{2c}) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{120}$$

For $T = C_{2d}$, we need

$$Q(C_{2d})x = -z = \Gamma^q(C_{2c})_{12}z + \Gamma^q(C_{2d})_{22}x, \tag{121}$$
$$Q(C_{2d})z = -x = \Gamma^q(C_{2c})_{11}z + \Gamma^q(C_{2d})_{21}x, \tag{122}$$

$$\Longrightarrow \Gamma^q(C_{2d})_{12} = 0, \quad \Gamma^q(C_{2d})_{22} = -1, \quad \Gamma^q(C_{2d})_{11} = 0, \quad \Gamma^q(C_{2d})_{21} = -1, \tag{123}$$
$$\Longrightarrow \Gamma^q(C_{2c}) = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}. \tag{124}$$

We find that the Γ^q is exactly Γ^5. Therefore, x is a irreducible tensor operator for irreducible representation Γ^5 of D_4.

(b) The Hamiltonian under the interaction is

$$H = H_0 + Ax \tag{125}$$

whose symmetry group is

$$D_1 = \{E, C_{2x}\} \tag{126}$$

D_1, with order of 2, has two classes:

$$\{E\}, \quad \{C_{2x}\}, \tag{127}$$

so D_1 has two inequivalent irreducible 1-dimensional representation, one of which is the identity representation, $\Gamma^1_{D_1}$:

$$\Gamma^1_{D_1}(E) = \Gamma^1_{D_1}(C_{2x}) = 1, \tag{128}$$

another is

$$\Gamma^2_{D_1}(E) = \Gamma^2_{D_1}(C_{2x}) = -1. \tag{129}$$

From problem 2, we know that the representation of D_4 corresponding to ψ_{mn} and ψ_{nm} is Γ^5. We write the characters of Γ^5 with character table of D_1 together:

	$\{E\}$	$\{C_{2x}\}$
Γ^5	2	0
$\Gamma^1_{D_1}$	1	1
$\Gamma^2_{D_1}$	1	-1

We can easily find that

$$\Gamma^5 = \Gamma^1_{D_1} \oplus \Gamma^2_{D_1}. \tag{130}$$

Therefore, the irreducible representations which the allowed final transform as are $\Gamma^1_{D_1}$ and $\Gamma^2_{D_1}$.

$\square$