Assignment 04

Due Time : 8:15, March 31, 2020 (Wednesday)

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Score : ________

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

	E	D	F	A	B	C
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

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

(b) Find the character table for D_3.

Solution: (a) The inverse of each element in D_3 are

$$E^{-1} = E, \qquad D^{-1} = F, \qquad F^{-1} = D, \tag{1}$$
$$A^{-1} = A, \qquad B^{-1} = B, \qquad C^{-1} = C. \tag{2}$$

Constructing a class from D: For $X = E, D, F$,

$$XDX^{-1} = D. \tag{3}$$

For $X = A, B, C$,

$$XDX^{-1} = F. \tag{4}$$

The class of D_3 constructed from D is $\{D, F\}$.
Using the similar method, we construct all the three classes of D_3:

$$\mathcal{C}_1 = \{E\}, \quad \mathcal{C}_2 = \{D, F\}, \quad \mathcal{C}_3 = \{A, B, C\}.$$

The number of inequivalent irreducible representations of D_3 is equal to the number of classes of G, so D_3 has three inequivalent irreducible representations. Suppose the dimensions of the three inequivalent irreducible representations $\Gamma^1, \Gamma^2, \Gamma^3$ are d_1, d_2, d_3, respectively. The order of D_3 is $g = 6$. The sum of the squares of the dimensions of the inequivalent irreducible representations of D_3 is equal to the order of D_3:

$$d_1^2 + d_2^2 + d_3^2 = 6. \tag{5}$$

Solving the above equation, we get

$$d_1 = 1, \quad d_2 = 1, \quad d_3 = 2. \tag{6}$$

(b) Since the character of identity in a representation is equal to the dimension of the representation, we have

$$\chi^1(\mathcal{C}_1) = \chi^2(\mathcal{C}_1) = 1, \quad \chi^3(\mathcal{C}_1) = 2. \tag{7}$$

Since $A^2 = B^2 = C^2 = E$, we have

$$\chi^p(\mathcal{C}_3) = \pm 1, \quad p = 1, 2. \tag{8}$$

Since $AB = F$ and $AC = D$, we have

$$\chi^p(\mathcal{C}_2) = \chi^p(\mathcal{C}_3)^2 = 1. \quad p = 1, 2. \tag{9}$$

There are two possibilities of $\chi^p(\mathcal{C}_3)$. Without loss of generality, we set Γ^1 to be the identity representation so that

$$\chi^1(\mathcal{C}_j) = 1, \quad j = 1, 2, 3. \tag{10}$$

As for Γ^2, we have

$$\chi^2(\mathcal{C}_1) = 1, \quad \chi^2(\mathcal{C}_2) = 1, \quad \chi^3(\mathcal{C}_3) = -1. \tag{11}$$

Using the orthogonality relation for characters

$$\frac{1}{g} \sum_{T \in G} \chi^q(T)^* \chi^q(T) = \delta_{pq}, \tag{12}$$

we have

$$
\begin{aligned}
\chi^3(\mathcal{C}_1)+2\chi^3(\mathcal{C}_2)+3\chi^3(\mathcal{C}_3)=&0 \qquad (13)\\
\chi^3(\mathcal{C}_1)+2\chi^3(\mathcal{C}_2)-3\chi^3(\mathcal{C}_3)=&0, \qquad (14)\\
|\chi^3(\mathcal{C}_1)|^2+2|\chi^3(\mathcal{C}_2)|^2+3|\chi^3(\mathcal{C}_3)|^2=&6. \qquad (15)
\end{aligned}
$$

Adding up the two equations (13) and (14) above, we get

$$\chi^3(\mathcal{C}_1)+2\chi^3(\mathcal{C}_2)=0, \qquad (16)$$

so

$$\chi^3(\mathcal{C}_2)=-1. \qquad (17)$$

Using the equation (15), we get

$$\chi^3(\mathcal{C}_3)=0. \qquad (18)$$

Now we have the character table for D_3 as shown in table 1.

Table 1: character table for D_3

	$\mathcal{C}_1=\{E\}$	$\mathcal{C}_2=\{D,F\}$	$\mathcal{C}_2=\{A,B,C\}$
Γ^1	1	1	1
Γ^2	1	1	-1
Γ^3	2	-1	0

□

Problem 2 Score: _________. 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

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

The basis function 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 function as normalizable. Using

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

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.

Solution: The inverse of $R(F)$ is equal to its transpose

$$R(F)^{-1}=R(F)^T=\frac{1}{2}\begin{pmatrix}-1&-\sqrt{3}\\\sqrt{3}&-1\end{pmatrix}. \qquad (19)$$

Making $R(F)^{-1}$ operate on $\vec{\rho}$, we get

$$R(F)^{-1}\vec{\rho}=\frac{1}{2}\begin{pmatrix}-1&-\sqrt{3}\\\sqrt{3}&-1\end{pmatrix}\begin{pmatrix}x\\y\end{pmatrix}=\frac{1}{2}\begin{pmatrix}-x-\sqrt{3}y\\\sqrt{3}x-y\end{pmatrix} \qquad (20)$$

Making $Q(F)$ operating on $\psi_n(\vec{\rho})$, we get

$$
\begin{aligned}
Q(F)\psi_1(\vec{\rho})=&\psi_1(R(F)^{-1}\vec{\rho})=\frac{1}{4}(x^2+2\sqrt{3}xy+3y^2)F(\rho)=\frac{1}{4}\psi_1(\vec{\rho})+\frac{\sqrt{3}}{2}\psi_2(\vec{\rho})+\frac{3}{4}\psi_3(\vec{\rho}), \qquad (21)\\
Q(F)\psi_2(\vec{\rho})=&\psi_2(R(F)^{-1}\vec{\rho})=\frac{1}{4}(-\sqrt{3}x^2-2xy+\sqrt{3}y^2)F(\rho)=-\frac{\sqrt{3}}{4}\psi_1(\vec{\rho})-\frac{1}{2}\psi_2(\vec{\rho})+\frac{\sqrt{3}}{4}\psi_3(\vec{\rho}), \qquad (22)
\end{aligned}
$$

$$Q(F)\psi_3(\vec{\rho}) = \psi_3(R(F)^{-1}\vec{\rho}) = \frac{1}{4}(3x^2 - 2\sqrt{3}xy + y^2)F(\rho) = \frac{3}{4}\psi_1(\vec{\rho}) - \frac{\sqrt{3}}{2}\psi_2(\vec{\rho}) + \frac{1}{4}\psi_3(\vec{\rho}). \tag{23}$$

Using

$$Q(T)\psi_n(\vec{\rho}) = \psi_n(R(T)^{-1}\vec{\rho}) = \sum_{m=1}^{3}\Gamma(T)_{mn}\psi_m(\vec{\rho}), \quad n = 1, 2, 3, \tag{24}$$

we find the representation matrix $\Gamma(F)$ of the element F of D_3:

$$\Gamma(F) = \begin{pmatrix} \frac{1}{4} & \frac{\sqrt{3}}{2} & \frac{3}{4} \\ -\frac{\sqrt{3}}{4} & -\frac{1}{2} & \frac{\sqrt{3}}{4} \\ \frac{3}{4} & -\frac{\sqrt{3}}{2} & \frac{1}{4} \end{pmatrix}. \tag{25}$$

□

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

Solution: The inverse of $R(B)$ is its transpose

$$R(T)^{-1} = R(T)^T = \frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ \sqrt{3} & 1 \end{pmatrix}. \tag{26}$$

Making $R(B)^{-1}$ operate on $\vec{\rho}$, we get

$$R(F)^{-1}\vec{\rho} = \frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ \sqrt{3} & 1 \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} = \frac{1}{2}\begin{pmatrix} -x + \sqrt{3}y \\ \sqrt{3}x + y \end{pmatrix}. \tag{27}$$

Making $Q(B)$ operating on $\psi_n(\vec{\rho})$, we get

$$Q(B)\psi_1(\vec{\rho}) = \psi_1(R(B)^{-1}\vec{\rho}) = \frac{1}{4}(x^2 - 2\sqrt{3}xy + 3y^2)F(\rho) = \frac{1}{4}\psi_1(\vec{\rho}) - \frac{\sqrt{3}}{2}\psi_2(\vec{\rho}) + \frac{3}{4}\psi_3(\vec{\rho}), \tag{28}$$

$$Q(F)\psi_2(\vec{\rho}) = \psi_2(R(F)^{-1}\vec{\rho}) = \frac{1}{4}(-\sqrt{3}x^2 + 2xy + \sqrt{3}y^2)F(\rho) = -\frac{\sqrt{3}}{4}\psi_1(\vec{\rho}) + \frac{1}{2}\psi_2(\vec{\rho}) + \frac{\sqrt{3}}{4}\psi_3(\vec{\rho}), \tag{29}$$

$$Q(F)\psi_3(\vec{\rho}) = \psi_3(R(F)^{-1}\vec{\rho}) = \frac{1}{4}(3x^2 + 2\sqrt{3}xy + y^2)F(\rho) = \frac{3}{4}\psi_1(\vec{\rho}) + \frac{\sqrt{3}}{2}\psi_2(\vec{\rho}) + \frac{1}{4}\psi_3(\vec{\rho}). \tag{30}$$

Using

$$Q(T)\psi_n(\vec{\rho}) = \psi_n(R(T)^{-1}\vec{\rho}) = \sum_{m=1}^{3}\Gamma(T)_{mn}\psi_m(\vec{\rho}), \quad n = 1, 2, 3, \tag{31}$$

we find the representation matrix $\Gamma(F)$ of the element F of D_3:

$$\Gamma(F) = \begin{pmatrix} \frac{1}{4} & -\frac{\sqrt{3}}{2} & \frac{3}{4} \\ -\frac{\sqrt{3}}{4} & \frac{1}{2} & \frac{\sqrt{3}}{4} \\ \frac{3}{4} & \frac{\sqrt{3}}{2} & \frac{1}{4} \end{pmatrix}. \tag{32}$$

□

Problem 4 Score: _________. 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 $P^p_{mn}P^q_{jk} = \delta_{pq}\delta_{nj}P^q_{mk}$.

Solution: Using the definition of the projection operators

$$P^p_{mn} = \frac{d_p}{g}\sum_{T\in G}\Gamma^p(T)^*_{mn}Q(T), \tag{33}$$

$$P^q_{jk} = \frac{d_q}{g}\sum_{T'\in G}\Gamma^p(T')^*_{jk}Q(T'), \tag{34}$$

we have

$$P^p_{mn}P^q_{jk} = \frac{d_p d_q}{g^2}\sum_{T,T'\in G}\Gamma^p(T)^*_{mn}\Gamma^q(T')^*_{jk}Q(T)Q(T'). \tag{35}$$

Since
$$Q(T)Q(T')=Q(TT'),\tag{36}$$
we have
$$P^p_{mn}P^q_{jk}=\frac{d_pd_q}{g^2}\sum_{T,T'\in G}\Gamma^p(T)^*_{mn}\Gamma^q(T')^*_{jk}Q(TT').\tag{37}$$
Setting $T''=TT'\in G$ and replacing T' with $T'=T^{-1}T''$, we get
$$P^p_{mn}P^q_{jk}=\frac{d_pd_q}{g^2}\sum_{T,T''\in G}\Gamma^p(T)^*_{mn}\Gamma^q(T^{-1}T'')^*_{jk}Q(T'').\tag{38}$$
Since Γ^p and Γ^q are two unitary representations,
$$\Gamma^q(T^{-1}T'')^*=[\Gamma^q(T^{-1})\Gamma^q(T'')]^*=[\Gamma^q(T)^{-1}\Gamma^q(T'')]^*=[\Gamma^q(T)^\dagger\Gamma^q(T'')]^*=\Gamma^q(T)^T\Gamma^q(T'')^*,\tag{39}$$
we have
$$P^p_{mn}P^q_{jk}=\frac{d_pd_q}{g^2}\sum_{T,T''\in G}\sum_l\Gamma^p(T)^*_{mn}\Gamma^q(T)_{lj}\Gamma^q(T'')_{lk}Q(T'').\tag{40}$$
Using the orthogonality relation for unitary irreducible representations
$$\frac{1}{g}\sum_{T\in G}\Gamma^p(T)^*_{mn}\Gamma^q(T)_{lj}=\frac{1}{d_p}\delta_{pq}\delta_{ml}\delta_{nj},\tag{41}$$
we get
$$P^p_{mn}P^q_{jk}=\frac{d_q}{g}\delta_{pq}\delta_{nj}\sum_{T''\in G}\sum_l\delta_{ml}\Gamma^q(T'')_{lk}Q(T'')=\frac{d_q}{g}\delta_{pq}\delta_{nj}\sum_{T''\in G}\Gamma^q(T'')_{mk}Q(T'')=\delta_{pq}\delta_{nj}P^q_{mk}.\tag{42}$$
□

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

Solution: The transformation matrices of D_4 are
$$R(E)=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix},\quad R(C_{2x})=\begin{pmatrix}1&0&0\\0&-1&0\\0&0&-1\end{pmatrix},\quad R(C_{2y})=\begin{pmatrix}-1&0&0\\0&1&0\\0&0&-1\end{pmatrix},\quad R(C_{2z})=\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&1\end{pmatrix},\tag{43}$$
$$R(C_{4z})=\begin{pmatrix}0&0&-1\\0&1&0\\1&0&0\end{pmatrix},\quad R(C_{4y}^{-1})=\begin{pmatrix}0&0&1\\0&1&0\\-1&0&0\end{pmatrix},\quad R(C_{2c})=\begin{pmatrix}0&0&1\\0&-1&0\\1&0&0\end{pmatrix},\quad R(C_{2d})=\begin{pmatrix}0&0&-1\\0&-1&0\\-1&0&0\end{pmatrix}.\tag{44}$$
The inverses of these transformation operators are their transposes respectively
$$R(E)^{-1}=R(E)^T=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix},\qquad R(C_{2x})^{-1}=R(C_{2x})=\begin{pmatrix}1&0&0\\0&-1&0\\0&0&-1\end{pmatrix},\tag{45}$$
$$R(C_{2y})^{-1}=R(C_{2y})^T=\begin{pmatrix}-1&0&0\\0&1&0\\0&0&-1\end{pmatrix},\qquad R(C_{2z})^{-1}=R(C_{2z})^T=\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&1\end{pmatrix},\tag{46}$$
$$R(C_{4y})^{-1}=R(C_{4y})^T=\begin{pmatrix}0&0&1\\0&1&0\\-1&0&0\end{pmatrix},\qquad R(C_{4y}^{-1})^{-1}=R(C_{4y}^{-1})^T=\begin{pmatrix}0&0&-1\\0&1&0\\1&0&0\end{pmatrix},\tag{47}$$
$$R(C_{2c})^{-1}=R(C_{2c})^T=\begin{pmatrix}0&0&1\\0&-1&0\\1&0&0\end{pmatrix},\qquad R(C_{2d})^{-1}=R(C_{2d})^T=\begin{pmatrix}0&0&-1\\0&-1&0\\-1&0&0\end{pmatrix}.\tag{48}$$
Making the inverse of transformation operators operate on $\vec{r}$, we get
$$R(E)^{-1}\vec{r}=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}\begin{pmatrix}x\\y\\z\end{pmatrix}=\begin{pmatrix}x\\y\\z\end{pmatrix},\tag{49}$$

$$R(C_{2x})^{-1}\vec{r} = \begin{pmatrix}1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & -1\end{pmatrix}\begin{pmatrix}x\\ y\\ z\end{pmatrix} = \begin{pmatrix}x\\ -y\\ -z\end{pmatrix}, \tag{50}$$

$$R(C_{2y})^{-1}\vec{r} = \begin{pmatrix}-1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & -1\end{pmatrix}\begin{pmatrix}x\\ y\\ z\end{pmatrix} = \begin{pmatrix}-x\\ y\\ -z\end{pmatrix}, \tag{51}$$

$$R(C_{2z})^{-1}\vec{r} = \begin{pmatrix}-1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & 1\end{pmatrix}\begin{pmatrix}x\\ y\\ z\end{pmatrix} = \begin{pmatrix}-x\\ -y\\ z\end{pmatrix}, \tag{52}$$

$$R(C_{4y})^{-1}\vec{r} = \begin{pmatrix}0 & 0 & 1\\ 0 & 1 & 0\\ -1 & 0 & 0\end{pmatrix}\begin{pmatrix}x\\ y\\ z\end{pmatrix} = \begin{pmatrix}z\\ y\\ -x\end{pmatrix}, \tag{53}$$

$$R(C_{4y}^{-1})^{-1}\vec{r} = \begin{pmatrix}0 & 0 & -1\\ 0 & 1 & 0\\ 1 & 0 & 0\end{pmatrix}\begin{pmatrix}x\\ y\\ z\end{pmatrix} = \begin{pmatrix}-z\\ y\\ x\end{pmatrix}, \tag{54}$$

$$R(C_{2c})^{-1}\vec{r} = \begin{pmatrix}0 & 0 & 1\\ 0 & -1 & 0\\ 1 & 0 & 0\end{pmatrix}\begin{pmatrix}x\\ y\\ z\end{pmatrix} = \begin{pmatrix}z\\ -y\\ x\end{pmatrix}, \tag{55}$$

$$R(C_{2d})^{-1}\vec{r} = \begin{pmatrix}0 & 0 & -1\\ 0 & -1 & 0\\ -1 & 0 & 0\end{pmatrix}\begin{pmatrix}x\\ y\\ z\end{pmatrix} = \begin{pmatrix}-z\\ -y\\ -x\end{pmatrix}. \tag{56}$$

Making the scalar transformation operators operate on $\phi(\vec{r})$, we get

$$\begin{aligned}
Q(E)\phi(\vec{r}) =&\phi(R(E)^{-1}\vec{r}) = (xy+yz)e^{-r}, &(57)\\
Q(R_{2x})\phi(\vec{r}) =&\phi(R(C_{2x})^{-1}\vec{r}) = (-xy+yz)e^{-r}, &(58)\\
Q(R_{2y})\phi(\vec{r}) =&\phi(R(C_{2y})^{-1}\vec{r}) = (-xy-yz)e^{-r}, &(59)\\
Q(R_{2z})\phi(\vec{r}) =&\phi(R(C_{2z})^{-1}\vec{r}) = (xy-yz)e^{-r}, &(60)\\
Q(R_{4y})\phi(\vec{r}) =&\phi(R(C_{4y})^{-1}\vec{r}) = (-xy+yz)e^{-r}, &(61)\\
Q(R_{4y}^{-1})\phi(\vec{r}) =&\phi(R(C_{4y}^{-1})^{-1}\vec{r}) = (xy-yz)e^{-r}, &(62)\\
Q(R_{2c})\phi(\vec{r}) =&\phi(R(C_{2c})^{-1}\vec{r}) = (-xy-yz)e^{-r}, &(63)\\
Q(R_{2d})\phi(\vec{r}) =&\phi(R(C_{2d})^{-1}\vec{r}) = (xy+yz)e^{-r}. &(64)
\end{aligned}$$

The two-dimensional irreducible representation Γ^5 of D_4 is

$$\Gamma^5(E) = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}, \quad \Gamma^5(C_{2x}) = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, \quad \Gamma^5(C_{2y}) = \begin{pmatrix}-1 & 0\\ 0 & -1\end{pmatrix}, \quad \Gamma^5(C_{2z}) = \begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix}, \tag{65}$$

$$\Gamma^5(C_{4y}) = \begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}, \quad \Gamma^5(C_{4y}^{-1}) = \begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}, \quad \Gamma^5(C_{2c}) = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \quad \Gamma^5(C_{2d}) = \begin{pmatrix}0 & -1\\ -1 & 0\end{pmatrix}. \tag{66}$$

Using

$$P_{mn}^p(\vec{r}) = \frac{d_p}{g}\sum_{T\in D_4}\Gamma^p(T)_{mn}Q(T)\phi(\vec{r}), \tag{67}$$

we have

$$\begin{aligned}
P_{11}^5\phi(\vec{r}) =&\frac{1}{4}[(xy+yz)+(-xy+yz)-(-xy-yz)-(xy-yz)]e^{-r} = yze^{-r}, &(68)\\
P_{22}^5\phi(\vec{r}) =&\frac{1}{4}[(xy+yz)-(-xy+yz)-(-xy-yz)+(xy-yz)]e^{-r} = xye^{-r}. &(69)
\end{aligned}$$

We calculate the coefficients

$$\begin{aligned}
(c_1^5)^2 =&(P_{11}^5\phi(\vec{r}), P_{11}^5\phi(\vec{r}))^{1/2} = \iiint_{-\infty}^{+\infty} dx\,dy\,dz\,y^2z^2e^{-2r}\\
=&\int_0^{2\pi}d\varphi\int_0^{\pi}\sin\theta\,d\theta\int_0^{+\infty}r^2\,dr\,(r\sin\theta\sin\varphi)^2(r\cos\theta)^2e^{-2r} = \frac{3}{2}\pi, &(70)
\end{aligned}$$

$$c_2^5 =(P_{11}^5(\vec{r}), P_{22}^5\phi(\vec{r})) = \iiint_{-\infty}^{+\infty} dx\, dy\, dz\, x^2y^2e^{-2r} = (c_1^5)^2 = \frac{3}{2}\pi. \tag{71}$$

Without loss of generality, we set $c_1^5 = \left(\frac{3}{2}\pi\right)^{1/2}$. The basis functions for Γ^5 of D_4 are

$$\psi_1^5(\vec{r}) =\frac{P_{11}^p\phi(\vec{r})}{c_1^5} = \left(\frac{2}{3\pi}\right)^{1/2} yze^{-r}, \tag{72}$$

$$\psi_2^5(\vec{r}) =P_{21}^5\psi_1^5(\vec{r}) = \frac{2}{8}\sum_{T\in G}\Gamma^5(T)_{21}^*Q(T)\psi(\vec{r}) = \frac{1}{4}\left(\frac{2}{3\pi}\right)^{1/2}[(-xy) - xy + (-xy) - xy]e^{-1} = -\left(\frac{2}{3\pi}\right)^{1/2} xye^{-r}. \tag{73}$$

□