Lecture 6 What we did last time

- Defined RR : reducible representation $\Gamma^{(red)}(\gamma_i)$ as one that can be put into block-diagonal form

$$\Gamma^{(red)}(\gamma_i) = \begin{pmatrix} \Gamma^{(j)}(\gamma_i) & & \\ & \Gamma^{(k)}(\gamma_i) & \\ & & \Gamma^{(l)}(\gamma_h) \end{pmatrix}$$

This can be accomplished through a similarity transformation

$$\Gamma^{(red)}(\gamma_k) = D^{-1}\,\Gamma^{(mess)}(\gamma_k)\,D$$

If it cannot $\rightarrow$ the representation is irreducible, IRR

- "Orthogonality" was introduced on page 84

- The character of an IRR was introduced.

$$\chi^{(i)}(\gamma_p) \equiv \sum_{n=1}^{d_i} \Gamma^{(i)}(\gamma_p)^{n}{}_{n}$$

ie, the TRACE of the i^{th} IRR of dimension d_i

Because the group elements in each class are related by a similarity transformation, their characters are all the same.

χ for a given IRR and given class: a number

- The character table can be constructed by:

a) brute force -- looking at the matrix IRR and calculating the traces explicitly

b) calculating one or two and using 2 orthogonality relations "row orthogonality" and "column orthogonality" to fill them out.

I had a typo in the character table for D_3 (not fixed on page 88

elements in class

group type

	C_1	$2C_3$	$3C_2$	$\leftarrow nX$
A_1	1	1	1	
A_2	1	1	-1	
E	2	-1	0	

- operations on functions is a critically important concept.

$\Gamma(\gamma)$ operates on $|x\rangle$, which in turn causes the functional form to change:

$$f(|x\rangle) \xrightarrow{\Gamma(\gamma)} f'(|x\rangle) = \Gamma(\gamma_i)\, f(|x\rangle)$$

$$= f(\,|x\rangle\, \Gamma^{-1}(\gamma_i)\,)$$

or

$$\Gamma(\gamma) f_j(|x\rangle) = f_i(|x\rangle)\, \Gamma(\gamma)^i{}_j$$

now the $f_i(x)$ are a set of basis functions which span a functional vector space

- We explicitly calculated and found

$\Gamma^{-1}(\gamma)|x\rangle = |x'\rangle$ for each γ of D_3

eg $\quad \Gamma^{-1}(b)|x\rangle = \Gamma^{-1}(b)\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} -\frac{1}{2}x - \frac{\sqrt{3}}{2}y \\ -\frac{\sqrt{3}x}{2} - \frac{1}{2}y \end{pmatrix}$

and so on.

So, for example $\qquad f = f(x)$

$$\Gamma(e) f(x) = f_1$$

$$\Gamma(a) f_1 = f_1$$
$$\Gamma(b) f_1 = f_1\left(\tfrac{1}{2}x - \tfrac{\sqrt{3}}{2}y\right) \equiv f_3$$
$$\Gamma(c) f_1 = f_2$$
$$\Gamma(d) f_1 = f_3$$
$$\Gamma(f) f_1 = f_2$$

and $\qquad \Gamma(e) f_2 = f_2$
$$\Gamma(a) f_2 = f_3$$
$$\vdots$$
and so on

f_1, f_2, and f_3 form a closed set — a basis of $\Gamma_{D_3}(6)$.

Further, the matrices that transform

$$|f_i\rangle \Gamma \rightarrow (f_1, f_2, f_3)\begin{pmatrix} & & \end{pmatrix}$$

the $\Gamma^{(5)}$ matrices

- Important claim: any arbitrary function in which $\Gamma(\gamma)$ can operate can be written as

$$\psi(x) = \sum_{\ell=1}^{N_\ell} \sum_{j=1}^{n_\ell} f_j^{(\ell)}(x)$$

IRR of group

dimensionality of ℓ^{th} IRR

for which a set of projection operators can be formed. that

$$P^{(\ell)}\psi(x) = f^{(\ell)} = \frac{d_\ell}{g} \sum_k \chi^{*(\ell)}(\gamma_k)\,\Gamma(\gamma_k)\,\psi(x)$$

decompose the general $\psi(x)$ into basis functions

$$P^{(1)}x^2 = \frac{1}{6}\sum_k \chi^{(1)*}(\gamma_k)\Gamma(\gamma_k)\psi$$

$$= \frac{1}{6}\left[\chi^{(1)*}(e)\Gamma(e) + \chi^{(1)*}(a)\Gamma(a) + \cdots\right]\psi$$

$$= \frac{1}{6}\Big[\overset{e}{(1)x^2}\ \overset{a}{(1)x^2} + \overset{b}{(1)\left(\tfrac{1}{2}x - \tfrac{\sqrt{3}}{2}y\right)^2} + \overset{c}{(1)\left(\tfrac{1}{2}x + \tfrac{\sqrt{3}}{2}y\right)^2}$$

$$+ (1)\left(-\tfrac{1}{2}x + \tfrac{\sqrt{3}}{2}y\right)^2 + (1)\left(-\tfrac{1}{2}x - \tfrac{\sqrt{3}}{2}y\right)^2\Big]$$

d

$$= \frac{1}{6}\Big[x^2 + x^2 + \underline{\tfrac{1}{4}x^2} + \underline{\tfrac{3}{4}y^2} - \underline{\underline{2\cdot\tfrac{\sqrt{3}}{4}xy}}$$

$$+ \underline{\tfrac{1}{4}x^2} + \underline{\tfrac{3}{4}y^2} + \underline{\underline{2\cdot\tfrac{\sqrt{3}}{4}xy}}$$

$$+ \underline{\tfrac{1}{4}x^2} + \underline{\tfrac{3}{4}y^2} - \underline{\underline{2\cdot\tfrac{\sqrt{3}}{4}xy}} + \underline{\tfrac{1}{4}x^2} + \underline{\tfrac{3}{4}y^2} + \underline{\underline{2\cdot\tfrac{\sqrt{3}}{4}xy}}\Big]$$

$$= \frac{1}{6}\left[2x^2 + x^2 + 3y^2\right]$$

$$= \frac{1}{2}(x^2+y^2) = P^{(A_1)}$$

also, $\quad P^{(2)}\psi = 0 = P(A_2)$

$$P^{(3)}\psi = \frac{1}{2}(x^2-y^2) = P^{(E)}$$

so, the decomposition

$$\psi = \underbrace{\tfrac{1}{2}(x^2+y^2)}_{\text{IRR of } A_1} \oplus \underbrace{\tfrac{1}{2}(x^2-y^2)}_{\text{IRR of } E}$$

one more step. Since E is 2 dimensional, there must be 2 basis functions.

We stay within $\Gamma^{(3)}$

$$\mathbb{P}^{(E)i}{}_{j}\,\psi \rightarrow \quad \mathbb{P}^{(E)1}{}_{1}\,\psi = 0$$

$$\mathbb{P}^{(E)2}{}_{2}\,\psi = \tfrac{1}{2}(x^2 - y^2) \quad \text{one}$$

$$\mathbb{P}^{(E)1}{}_{2}\,\psi = 0$$

$$\mathbb{P}^{(E)2}{}_{1}\,\psi = -xy. \quad \text{the other}$$

Let $\psi_1 = xy.$

$$\psi_2 = \tfrac{1}{2}(x^2 - y^2)$$

$$\psi_3 = \tfrac{1}{2}(x^2 + y^2)$$

This same procedure can be done for many functions — for all groups. What you find is that particular IRRs have possible functions in 3-space which can act as bases:

For D_3

	E	$2C_3$	$3C_2$	
A_1	1	1	1	$\underline{x^2+y^2}$; z^2
A_2	1	1	−1	z
E	2	−1	0	$\underline{x^2-y^2}$; $\underline{xy}$; xz; yz; x; y

possible basis functions

One. More. Concept. before physics. Product representations

If we have a group $\mathcal{G} = \mathcal{A} \otimes \mathcal{B}$

we can relate the IIR of the product to the subgroups

$$\Gamma^{(i \otimes j)}(\alpha \beta) = \Gamma^{(i)}(\alpha) \otimes \Gamma^{(j)}(\beta)$$ $\longrightarrow$ page 105a

The characters:

$$\chi^{(i \otimes j)}(\alpha \beta) = \sum_n \sum_m \Gamma^{(i)}(\alpha)^n{}_n \, \Gamma^{(j)}(\beta)^m{}_m$$

$$= \chi^{(i)}(\alpha) \chi^{(j)}(\beta)$$

so, can get the character table of the product group directly.

Just like we had matrix representations of the direct sum

$$\mathbb{G} = \mathbb{A} \oplus \mathbb{B} \qquad \mathbb{A} = \begin{pmatrix} a \end{pmatrix}$$

$$\mathbb{B} = \begin{pmatrix} b \end{pmatrix}$$

$$\mathbb{G} = \left(\begin{array}{c|c} (a) & 0 \\ \hline 0 & (b) \end{array}\right)$$

we have direct products

$$\mathbb{G} = \mathbb{A} \otimes \mathbb{B} \qquad \mathbb{A} = \begin{pmatrix} a_1 & a_2 \\ a_3 & a_4 \end{pmatrix}$$

replace every element of $\mathbb{A}$ by the matrix $\mathbb{B}$

$$\mathbb{B} = \begin{pmatrix} b_1 & b_2 & b_3 \\ b_4 & b_5 & b_6 \\ b_7 & b_8 & b_9 \end{pmatrix}$$

$$\mathbb{G} = \begin{pmatrix} a_1b_1 & a_1b_2 & a_1b_3 & a_2b_1 & a_2b_2 & a_2b_3 \\ a_1b_4 & a_1b_5 & a_1b_6 & a_2b_4 & a_2b_5 & a_2b_6 \\ a_1b_7 & a_1b_8 & a_1b_9 & a_2b_7 & a_2b_8 & a_2b_9 \\ & & & & & \\ & & \text{etc} & & & \end{pmatrix}$$

$$G^{ij}_{kl} = A^i{}_k B^j{}_l$$

Basis functions for direct product representations.

We know $\Gamma^{(i)}(\gamma) f_m^{(i)}(x) = f_n^{(i)}(x)\, \Gamma^{(i)}(\gamma)^n{}_m$

and $\Gamma^{(j)}(\gamma) f_{m'}^{(j)}(x) = f_{n'}^{(j)} \,\Gamma^{(j)}(\gamma)^{n'}{}_{m'}$

Both $\mathcal{G}$.

So,

$$\Gamma(\gamma) \underbrace{f_m^{(i)} f_{m'}^{(j)}}_{\substack{\text{basis functions}\\ \text{of direct product}\\ \text{representation}}} = \sum_{n,n'} f_n^{(i)} f_{n'}^{(j)} \underbrace{\Gamma^{(i)n}{}_m \Gamma^{(j)n'}{}_{m'}}_{\Gamma^{(i\otimes j)nn'}{}_{mm'}}$$

If same group, then $\Gamma^{(i\otimes j)}$ is just another representation of the group. It must be a

a) RR of $\mathcal{G}$

or

b) IRR of $\mathcal{G}$

Remember the frequency of the j^{th} IRR inside of $\Gamma^{(red)}$ is (page 89)

$$n_j = \frac{1}{g} \sum_m \chi^{(j)}(\gamma_m)\, \chi^{(red)}(\gamma_m)$$

So, $$\Gamma^{(i \otimes j)} = \sum_k n_{ijk} \Gamma^{(k)}$$

where

$$n_{ijk} = \frac{1}{g} \sum_m \chi^{k*}(\gamma_m) \{ \chi^i(\gamma_m) \chi^j(\gamma_m) \}$$

Q.M.

Suppose we have the Sch. Eq.

$$H_0 \psi_i(x) = E_i \psi_i(x) \qquad \text{or!}$$

$$H_0 | \psi_i(x) \rangle = E_i | \psi_i(x) \rangle$$

Suppose we have some group $\mathcal{G} \in \{ \Gamma(\gamma_1), \Gamma(\gamma_2 \ldots \}$
and find that

$$[H_0, \Gamma(\gamma)] = 0$$ → would say Γ is a constant of the motion

But for symmetry, it means that if we transform

$$\Gamma(g) | \psi \rangle$$

and operate

$$H_0 \Gamma(\gamma_i) | \psi \rangle = \Gamma(\gamma) H_0 | \psi \rangle = \Gamma(\gamma) E_i | \psi_i \rangle$$

$$H_0 \Gamma(\gamma) | \psi \rangle = E_i \Gamma(\gamma) | \psi \rangle$$

$|\psi_i\rangle$ is an eigenstate of H_0 with energy E_i

$\Gamma(\gamma) | \psi_i \rangle$ is <u>also</u> with the same energy

→ degenerate

Earlier I said

$$\Gamma(\gamma_k) f_m^{(\ell)}(x) = \sum_n \underbrace{f_n^{(\ell)}(x) \Gamma^{(\ell)}(\gamma_k)^n{}_m}$$

and we've seen that we can create a closed set of functions that transform as an IRR of Γ

So, any degeneracy for a "group of the Hamiltonian" will be determined by the dimensionality of the matrix representation of that IRR.

remarkable

remember D_3, It has

2 1d IRR

1 2d IRR

$\Rightarrow$ energy levels of a system respecting D_3 can only be non-degenerate or have a 2 fold degeneracy.

THIS - WITHOUT KNOWING ANYTHING ABOUT THE SYSTEM!

LIFTING OF DEGENERACIES

What about perturbations?

Suppose $\quad H = H_0 + H'$

let $\mathcal{G}_0$ be the group of H_0 and
$\mathcal{G}'$ " H'

If $\mathcal{G}_0 = \mathcal{G}'$ then H' will not lift any degeneracy in H. But, if $\mathcal{G}' \subseteq \mathcal{G}_0$ .. technically a proper subgroup, some degeneracy may be lifted by H'

$$\mathcal{G}_0 = \{ \Gamma(\gamma_1), \Gamma(\gamma_2), \underbrace{\Gamma(\gamma_3), \ldots \Gamma(e)}_{\mathcal{G}'} \}$$

the Γ's are all IRR in $\mathcal{G}_0$

BUT

they may not be IRR in $\mathcal{G}'$

$$\Gamma^{(red)}(\gamma) = n_1 \Gamma^{(1)}(\gamma) \oplus n_2 \Gamma^{(2)}(\gamma) \oplus \ldots$$

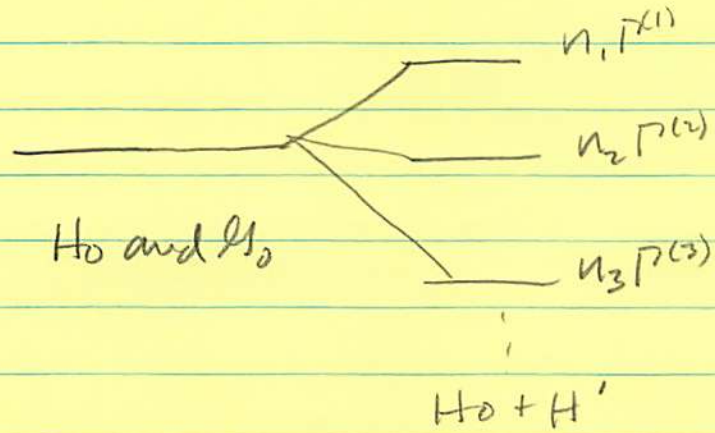
in $\mathcal{G}'$
but in the rep of $\mathcal{G}_0$

the number comes from:

$$n_j = \frac{1}{g} \sum_p \chi^{(j)}(\gamma_p) \chi^{(red)}(\gamma_p)$$

in rep of $\mathcal{G}_0$

$$= \frac{1}{g} \sum_r N_r \chi^{(j)}(\mathcal{C}_r) \chi^{(red)}(\mathcal{C}_r)$$



neither magnitudes nor signs predicted

Suppose $\mathcal{G}_0 \equiv D_3$ maybe in a crystal.

and the perturbation is electric diple.

Then $H' \sim x f(\vec{r})$ or $y f(\vec{r})$ or $z f(\vec{r})$

Look at subgroups of D_3 for any which have electric dipole-like functional forms in the character table

Subgroups are C_2 and C_3

Their character tables – and characteristic functions – are

C_2	E	C_2	
A	1	1	$x^2; y^2; z^2; xy; z$
B	1	-1	$x; y; xz; yz$

	E	C_3	C_3^2	
A	1	1	1	$x^2+y^2; z^2$
E	1	θ	θ^2	$xz; yz$
	1	θ^2	θ	$x^2-y^2; xy$

$$\theta = e^{2\pi i/3}$$

notice that only C_2 has IRR that transform like x, y, or z → like the perturbation of electric dipole

So, here, $\mathcal{G}_0 = D_3$
$\mathcal{G}' = C_2$

How much of the A & B IRRs?

$$\Gamma_{D_3}^{(k)}(\gamma) = n_A^{C_2}\,\Gamma^{(A)}(\gamma) \oplus n_B^{C_2}\,\Gamma^{(B)}(\gamma)$$

$$n_A = \frac{1}{g_A}\sum_{r=1}^{N_r(C_2)} N_r\,\chi^{(A)}(\mathcal{C}_r)^*\,\chi^{(A_1)}(\mathcal{C}_r)$$

$$\begin{array}{c|ccc} D_3 & E & 2C_3 & 3C_2 \\ \hline A_1 & 1 & 1 & 1 \end{array}$$

$$\begin{array}{c|cc} C_2 & E & \mathcal{C}_2 \\ \hline A & 1 & 1 \\ B & & \end{array}$$

$$= \frac{1}{2}\Big[\underbrace{(1)(1)(1)}_{E} + \underbrace{(1)(1)(1)}_{\mathcal{C}_2}\Big] = 1 \qquad \#\underbrace{A\text{'s}}_{C_2} \text{ in } \underbrace{A_1}_{D_3}$$

#A's in A_2

$$n_A = \frac{1}{2}\Big[\underbrace{(1)(1)(1)}_{E} + \underbrace{(1)(1)(-1)}_{C_2}\Big] = 0$$

#A's in E

$$n_A = \frac{1}{2}\Big[(1)(1)(2) + (1)(1)(0)\Big] = 1$$

#B's in A_1

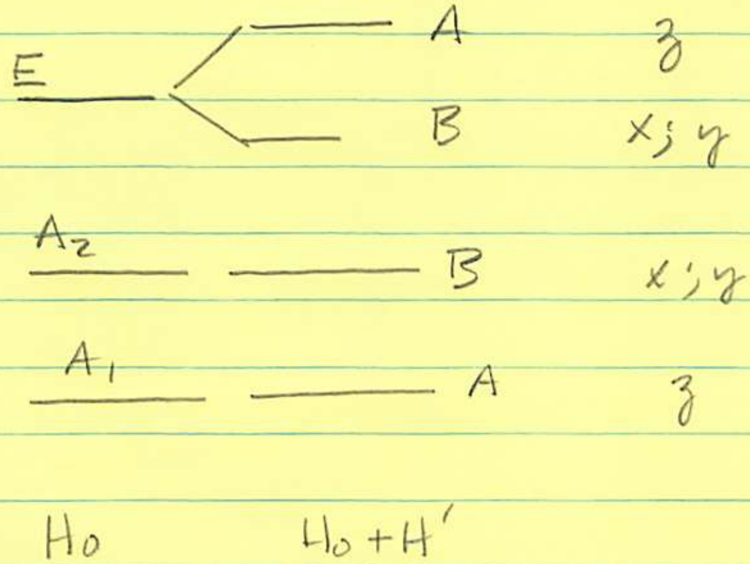
$$n_B = \frac{1}{2}\Big[(1)(1)(1) + (-1)(-1)(1)\Big] = 0$$

#B's in A_2 $\qquad n_B = 1$

#B's in E

$$n_B = \frac{1}{2}\Big[(1)(1)(2) + (1)(-1)(0)\Big] = 1$$

So, the splittings are



SELECTION RULES

Suppose we have a perturbation H' ...
we know that its effect is determined by forming the matrix element

$$M^f{}_i = \langle \psi^f | H' | \psi_i \rangle$$

ψ's are eigenfunctions which belong to particular representations of a group

say ψ_i belongs to $\Gamma^{(l)}$

ψ^f belongs to $\Gamma^{(k)}$

But, the perturbation has some functional form which in turn can be associated with an IRR of a group

H' belongs to $\Gamma^{(m)}$

If $M^f{}_i = 0$, then the transition from $i \to f$ is forbidden

$\neq 0$ allowed

$$H' \, |\psi_i\rangle$$

$$\uparrow \quad \Gamma^{(\ell)}$$

$$\uparrow$$

$$\underbrace{\Gamma^{(m)}}$$

will belong to the direct product group

$$\Gamma^{(m \otimes \ell)} = \Gamma^{(m)} \otimes \Gamma^{(\ell)}$$

$$\langle \psi^f |$$

$$\uparrow$$

$$\Gamma^{(k^*)}$$

For $M^f_i \neq 0$, $\Gamma^{(m)} \otimes \Gamma^{(\ell)}$ must either

a) <u>be</u> $\Gamma^{(k)}$

or

b) contain $\Gamma^{(k)}$

If $\Gamma^{(m \otimes l)}$ contains $\Gamma^{(k)}$

then

$$\Gamma^{(k^* \otimes m \otimes l)} \text{ must contain } \Gamma^{(k^* \otimes k)} .$$

$\Gamma^{(k^* \otimes k)} = \Gamma^{(k^*)} \otimes \Gamma^{(k)}$ always contains Γ^1,
the totally symmetric representation

That is $$n_{kks} = \frac{1}{g} \sum_h \chi^{s^*}(\gamma_h) \{ \underbrace{\chi^{k^*}(\gamma_h) \chi^{k}(\gamma_h)}_{1 \text{ orthogonality}} \}$$

$$n_{kks} = 1 \text{ if } \chi^{s^*} = \chi^1 = g$$

So,

$$\langle \psi^f | H' | \psi_i \rangle \neq 0$$

if $\Gamma^{(k^* \otimes m \otimes l)}$ contains Γ^1

so, the investigation is to find how many times

$$\Gamma^{(h^* \otimes m \otimes l)} \text{ contains } \Gamma^1$$

again, calculate

$$a_1 = \frac{1}{g} \sum_h \chi^{1*}(\gamma_h)\, \chi^{h^* \otimes m \otimes l}$$

$$= \frac{1}{g} \sum_h \chi^{1*}(\gamma_h)\, \chi^{h^*} \chi^{m} \chi^{l}$$

But, there's a brute force way

Let's suppose we're talking about a system which is classified according to D_3 and ask what the allowed transitions are for Electric Dipole transitions

Remember, we're asking if

$$H^{'(m)} | \psi_i^{(l)} \rangle$$

contains

$$\langle \psi^{+(h)}$$

$$n_k = \frac{1}{g} \sum_r N_r \chi^{(k)*}(\mathcal{C}_r) \chi^{(m)}(\mathcal{C}_r) \chi^{(l)}(\mathcal{C}_r)$$

writing in terms of classes

If m and l are different or if either $\Gamma^{(m)}$ or $\Gamma^{(l)}$ are the identity, then

$\Gamma^{(m \otimes l)}$ is IRR $\rightarrow$ just look for $\Gamma^{(k)}$.

But, if $l = m$, then $\Gamma^{(m \otimes l)}$ is RR and can be decomposed to look for non-zero n_k.

So, $$n_k = \frac{1}{g} \sum_r N_r \chi^{(k)*}(\mathcal{C}_r) \left[\chi^{m}(\mathcal{C}_r)\right]^2$$

Look at the character table for D_3

H' must be like $x f(\vec{r})$, $y f(\vec{r})$, $z f(\vec{r})$

so, the IRR to which H' belongs are only

A_2 if $\vec{E}$ along $\hat{z}$

E if $\vec{E}$ along $\hat{x}$ or $\hat{y}$

Calculate $\chi^{(l)} \chi^{(m)}$ in general

	E	$2C_3$	$3C_2$	
$\chi^{(A_1)}\chi^{(A_1)}$	1	1	1	A_1
$\chi^{(A_1)}\chi^{(A_2)}$	1	1	-1	A_2
$\chi^{(A_1)}\chi^{(E)}$	2	-1	0	E
$\chi^{(A_2)}\chi^{(A_2)}$	1	1	1	A_1
$\chi^{(A_2)}\chi^{(E)}$	2	-1	0	E
$\chi^{(E)}\chi^{(E)}$	4	1	0	$E + A_1 + A_2$

Suppose we have $\vec{E} = \hat{z} f(\vec{r})$, then $H' \sim A_2$ and the only ones above that count are $\chi^{(A_2)}\chi^{(any)}$

$A_1 \to A_1$ $\quad n_{A_1} = \frac{1}{6} \sum_r 1\, \chi^{(A_1)}(\mathcal{G}_r)\, \chi^{(A_2 \cdot A_1)}(\mathcal{G}_r)$

$$= \frac{1}{6}\left[1(1)(1) + 2(1)(1) + 3(1)(-1)\right] = 0$$

$A_1 \to A_2$ $\quad n_{A_2} = \frac{1}{6}\left[1(1)(1) + 2(1)(1) + 3(-1)(-1)\right] = 1$

$A_2 \to A_2$ $\quad n_{A_2} = \frac{1}{6}\left[1(1)(1) + 2(1)(1) + 3(-1)(1)\right] = 0$

$A_2 \to A_1$ $\quad n_{A_1} = \frac{1}{6}\left[1(1)(1) + 2(1)(1) + 3(1)(1)\right] = 1$

$E \to A_1$ $\quad n_{A_1} = \frac{1}{6}\left[1(1)(2) + 2(1)(-1) + 3(1)(0)\right] = 0$

$E \to A_2$ $\quad n_{A_2} = 1/6\left[1(1)(2) + 2(1)(-1) + 3(-1)(0)\right] = 0$

$E \to E \qquad n_E = \frac{1}{6}\left[1(2)(2) + 2(-1)(-1) + 3(0)(0) \right] = 1$

So, allowed transitions are

$A_1 \leftrightarrow A_1$

$A_2 \leftrightarrow A_1$

$E \leftrightarrow E$

$\left.\begin{array}{l} E \leftrightarrow A_1 \\ E \leftrightarrow A_2 \end{array}\right\}$ forbidden

For $\vec{E} = \hat{x}\, f(\vec{r})$ or $\hat{y}\, f(\vec{r})$