PHY 745 Group Theory
11-11:50 AM MWF Olin 102

Plan for Lecture 14:

Properties of direct product groups

Reading: Chapter 6 in DDJ

1. **Definition of direct product group**
2. **Representations of direct product groups**
3. **Examples**

[illegible]	[illegible]	Notes	Continuous groups	[illegible]	[illegible]
11	Mon: 02/06/2017	Notes	Group of three-dimensional rotations	#9	02/08/2017
12	Wed: 02/08/2017	Notes	Continuous groups	#10	02/10/2017
13	Fri: 02/10/2017	Chap. 5	Atomic orbitals	#11	02/13/2017
14	Mon: 02/13/2017	Chap. 6	Direct product groups	#12	02/15/2017
15	Wed: 02/15/2017				
16	Fri: 02/17/2017				
17	Mon: 02/20/2017				
18	Wed: 02/22/2017				
19	Fri: 02/24/2017				
20	Mon: 02/27/2017				Exam
21	Wed: 03/01/2017				Exam
22	Fri: 03/03/2017				Exam Due
	Mon: 03/06/2017		*Spring break - no class*		
	Wed: 03/08/2017		*Spring break - no class*		
	Fri: 03/10/2017		*Spring break - no class*		
	Mon: 03/13/2017		*APS Meeting - no class*		
	Wed: 03/15/2017		*APS Meeting - no class*		
	Fri: 03/17/2017		*APS Meeting - no class*		
23	Mon: 03/20/2017				

Definition of direct product group

Consider two groups:

G_A having order h_a and G_B having order h_b

$E, A_2, A_3, \ldots A_{h_a}$ and $E, B_2, B_3, \ldots B_{h_b}$

Also suppose that for all i and j, $A_i B_j = B_j A_i$

Then it is possible form the direct product group

$G_A \otimes G_B$ having the order $h_a h_b$:

$E, A_2, A_3, \ldots A_{h_a}, B_2, B_3, \ldots B_{h_b}, (A_2B_2), (A_2B_3), \ldots (A_2B_{h_b}), \ldots (A_{h_a}B_{h_b})$

Checking group properties of $G_A \otimes G_B$:

Consider $(A_iB_j)(A_kB_l) = A_i\left(B_jA_k\right)B_l = A_i\left(A_kB_j\right)B_l$

$=(A_iA_k)(B_jB_l)$

$=A_{ik}B_{jl}$ for $A_{ik} \equiv A_iA_k$ and $B_{jl} \equiv B_jB_l$

Irreducible representations of direct product groups

Direct products of matrices

$$\begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \otimes \begin{pmatrix} n_{11} & n_{12} & n_{13} \\ n_{21} & n_{22} & n_{23} \\ n_{31} & n_{32} & n_{33} \end{pmatrix} = \begin{pmatrix} m_{11}n_{11} & m_{11}n_{12} & m_{11}n_{13} & m_{12}n_{11} & m_{12}n_{12} & m_{12}n_{13} \\ m_{11}n_{21} & m_{11}n_{22} & m_{11}n_{23} & m_{12}n_{21} & m_{12}n_{22} & m_{12}n_{23} \\ m_{11}n_{31} & m_{11}n_{32} & m_{11}n_{33} & m_{12}n_{31} & m_{12}n_{32} & m_{12}n_{33} \\ m_{21}n_{11} & m_{21}n_{12} & m_{21}n_{13} & m_{22}n_{11} & m_{22}n_{12} & m_{22}n_{13} \\ m_{21}n_{21} & m_{21}n_{22} & m_{21}n_{23} & m_{22}n_{21} & m_{22}n_{22} & m_{22}n_{23} \\ m_{21}n_{31} & m_{21}n_{32} & m_{21}n_{33} & m_{22}n_{31} & m_{22}n_{32} & m_{22}n_{33} \end{pmatrix}$$

$$m_{ij}n_{kl} = o_{ik,jl}$$

$$= \begin{pmatrix} o_{11,11} & o_{11,12} & o_{11,13} & o_{11,21} & o_{11,22} & o_{11,23} \\ o_{12,11} & o_{12,12} & o_{12,13} & o_{12,21} & o_{12,22} & o_{12,23} \\ o_{13,11} & o_{13,12} & o_{13,13} & o_{13,21} & o_{13,22} & o_{13,23} \\ o_{21,11} & o_{21,12} & o_{21,13} & o_{21,21} & o_{21,22} & o_{21,23} \\ o_{22,11} & o_{22,12} & o_{22,13} & o_{22,21} & o_{22,22} & o_{22,23} \\ o_{23,11} & o_{23,12} & o_{23,13} & o_{23,21} & o_{23,22} & o_{23,23} \end{pmatrix}$$

Theorem: The direct product of the representations of groups G_A and G_B forms a representation of their direct product group

$$D^{A_n}_{pq}(A_i)D^{B_m}_{st}(B_j) = D^{(A\otimes B)_l}_{ps,qt}(A_iB_j)$$

Proof:

First consider

$$D^{(A\otimes B)_l}_{ps,qt}(A_iB_jA_kB_l) = D^{(A\otimes B)_l}_{ps,qt}(A_iA_kB_jB_l)$$

$$D^{(A\otimes B)_l}_{ps,qt}(A_iB_jA_kB_l) = \sum_{uv} D^{(A\otimes B)_l}_{ps,uv}(A_iB_j)D^{(A\otimes B)_l}_{uv,qt}(A_kB_l)$$

If the identity is correct then:

$$D^{A_n}_{pq}(A_iA_k)D^{B_m}_{st}(B_jB_l) = \sum_{uv} D^{A_n}_{pu}(A_i)D^{B_m}_{sv}(B_j)D^{A_n}_{uq}(A_k)D^{B_m}_{vt}(B_l)$$

$$D^{(A\otimes B)_l}_{ps,qt}(A_iB_jA_kB_l) = \sum_{uv} D^{(A\otimes B)_l}_{ps,uv}(A_iB_j)D^{(A\otimes B)_l}_{uv,qt}(A_kB_l)$$

If the identity is correct then:

$$D^{A_n}_{pq}(A_iA_k)D^{B_m}_{st}(B_jB_l) = \sum_{uv} D^{A_n}_{pu}(A_i)D^{B_m}_{sv}(B_j)D^{A_n}_{uq}(A_k)D^{B_m}_{vt}(B_l)$$

$$= \sum_{u} D^{A_n}_{pu}(A_i)D^{A_n}_{uq}(A_k)\sum_{v} D^{B_m}_{sv}(B_j)D^{B_m}_{vt}(B_l)$$

$$= D^{A_n}_{pq}(A_iA_k)D^{B_m}_{st}(B_jB_l)$$

$$D^{A_n}_{pq}(A_i)D^{B_m}_{st}(B_j) = D^{(A\otimes B)_l}_{ps,qt}(A_iB_j)$$

Construction of direct product representations:

$$D^{(A\otimes B)_l}_{ps,qt}(A_iB_j) = D^{A_n}_{pq}(A_i)D^{B_m}_{st}(B_j)$$

Construction of direct product characters:

$$\sum_{ps} D^{(A\otimes B)_l}_{ps,ps}(A_iB_j) = \sum_{p} D^{A_n}_{pp}(A_i)\sum_{s} D^{B_m}_{ss}(B_j)$$

$$\Rightarrow \chi^{(A\otimes B)_l}(A_iB_j) = \chi^{A_n}(A_i)\chi^{B_m}(B_j)$$

Example $D_3 \otimes i$

D_3 (32)			E	$2C_3$	$3C_2'$
x^2+y^2, z^2		A_1	1	1	1
	R_z, z	A_2	1	1	−1
(xz, yz), (x^2-y^2, xy)	(x,y), (R_x, R_y)	E	2	−1	0

h_{D3}=6

S_2 ($\bar{1}$)			E	i
$x^2, y^2, z^2, xy, xz, yz$	R_x, R_y, R_z	A_g	1	1
	x, y, z	A_u	1	−1

h_i=2

$D_{3d} = D_3 \otimes i$ ($\bar{3}m$)			E	$2C_3$	$3C_2''$	i	$2iC_3$	$3iC_2''$
x^2+y^2, z^2		A_{1g}	1	1	1	1	1	1
	R_z	A_{2g}	1	1	−1	1	1	−1
$(xz, yz), (x^2-y^2, xy)$	(R_x, R_y)	E_g	2	−1	0	2	−1	0
		A_{1u}	1	1	1	−1	−1	−1
	z	A_{2u}	1	1	−1	−1	−1	1
	(x,y)	E_u	2	−1	0	−2	1	0

h=12

Example $O \otimes i$

O (432)	E	$8C_3$	$3C_2$	$6C_4$	$6C_2'$
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
E	2	−1	2	0	0
T_1	3	0	−1	1	−1
T_2	3	0	−1	−1	1

O_h ($m3m$)	E	$8C_3$	$6C_2$	$6C_4$	$3C_2$ ($=C_4^2$)	i	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	−1	−1	1	1	−1	1	1	−1
E_g	2	−1	0	0	2	2	0	−1	2	0
T_{1g}	3	0	−1	1	−1	3	1	0	−1	−1
T_{2g}	3	0	1	−1	−1	3	−1	0	−1	1
A_{1u}	1	1	1	1	1	−1	−1	−1	−1	−1
A_{2u}	1	1	−1	−1	1	−1	1	−1	−1	1
E_u	2	−1	0	0	2	−2	0	1	−2	0
T_{1u}	3	0	−1	1	−1	−3	−1	0	1	1
T_{2u}	3	0	1	−1	−1	−3	1	0	1	−1

Application of symmetry analysis to point group analysis
Recall the Fermi Golden Rule for transitions between initial and final states of a quantum mechanical system

$$R_{i\to f} = \frac{2\pi}{\hbar}\left|\langle \Psi_i | \Delta H | \Psi_f \rangle\right|^2 \rho_f$$

density of final states

Example of electronic states $|\Psi_i\rangle \to |\Psi_f\rangle$ due to coupling with an electromagnetic field characterized by vector potential $\mathbf{A}$

$$H = H_0 + \Delta H = \frac{\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2}{2m} + V(\mathbf{r})$$

$$H_0 = \frac{p^2}{2m} + V(\mathbf{r})$$

$$\Delta H = -\frac{e}{2mc}(\mathbf{p}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{p}) + \frac{e^2}{2mc^2}A^2 \approx -\frac{e}{mc}\mathbf{A}\cdot\mathbf{p}$$

Prediction of electromagnetic transitions

$\langle \Psi_i |$ unitial state

ΔH coupling to electromagnetic field $\propto p_x, p_y, p_z$

$|\Psi_j\rangle$ final state

$$\langle \Psi_i | \Delta H | \Psi_j \rangle \Leftrightarrow \sum_k N(\mathcal{C}_k)\left(\chi^i(\mathcal{C}_k)\right)^* \chi^{\Delta H}(\mathcal{C}_k)\chi^f(\mathcal{C}_k)$$

Example D_3

D_3 (32)			E	$2C_3$	$3C_2'$
x^2+y^2, z^2		A_1	1	1	1
	R_z, z	A_2	1	1	−1
(xz, yz), (x^2-y^2, xy)	(x, y), (R_x, R_y)	E	2	−1	0

Example D_3

D_3 (32)			E	$2C_3$	$3C_2'$
x^2+y^2, z^2		A_1	1	1	1
	R_z, z	A_2	1	1	−1
(xz, yz), (x^2-y^2, xy)	(x, y), (R_x, R_y)	E	2	−1	0

$$\langle \Psi_i | \Delta H | \Psi_j \rangle \Leftrightarrow \sum_k N(\mathcal{C}_k)\left(\chi^i(\mathcal{C}_k)\right)^* \chi^{\Delta H}(\mathcal{C}_k)\chi^f(\mathcal{C}_k)$$

For $\mathbf{A}=A_0\hat{\mathbf{z}}$ $\chi^{\Delta H}(\mathcal{C}_k) = \chi^{A_2}(\mathcal{C}_k)$

$\lvert\Psi_i\rangle$	$\to$	$\lvert\Psi_f\rangle$
A_1		A_2
A_2		A_1
E		no transition

Example D_3

D_3 (32)			E	$2C_3$	$3C_2'$
x^2+y^2, z^2		A_1	1	1	1
	R_z, z	A_2	1	1	−1
(xz, yz), (x^2-y^2, xy)	(x, y), (R_x, R_y)	E	2	−1	0

$$\langle \Psi_i | \Delta H | \Psi_j \rangle \Leftrightarrow \sum_k N(\mathcal{C}_k)\left(\chi^i(\mathcal{C}_k)\right)^* \chi^{\Delta H}(\mathcal{C}_k)\chi^f(\mathcal{C}_k)$$

For $\mathbf{A}=A_0\hat{\mathbf{x}}$ or $A_0\hat{\mathbf{y}}$ $\quad \chi^{\Delta H}(\mathcal{C}_k) = \chi^E(\mathcal{C}_k)$

$\|\Psi_i\rangle$	$\rightarrow$	$\|\Psi_f\rangle$
A_1		E
A_2		no transition
E		A_1

2/13/2017 PHY 745 Spring 2017 -- Lecture 13

Example $D_3 \otimes i$

$D_{3d} = D_3 \otimes i$ ($\bar{3}m$)			E	$2C_3$	$3C_2'$	i	$2iC_3$	$3iC_2'$
x^2+y^2, z^2		A_{1g}	1	1	1	1	1	1
	R_z	A_{2g}	1	1	−1	1	1	−1
(xz, yz), (x^2-y^2, xy)	(R_x, R_y)	E_g	2	−1	0	2	−1	0
		A_{1u}	1	1	1	−1	−1	−1
	z	A_{2u}	1	1	−1	−1	−1	1
	(x, y)	E_u	2	−1	0	−2	1	0

For $\mathbf{A}=A_0\hat{\mathbf{z}}$ $\quad \chi^{\Delta H}(\mathcal{C}_k) = \chi^{A_{2u}}(\mathcal{C}_k)$

For $\mathbf{A}=A_0\hat{\mathbf{x}}$ or $A_0\hat{\mathbf{y}}$ $\quad \chi^{\Delta H}(\mathcal{C}_k) = \chi^{E_u}(\mathcal{C}_k)$

2/13/2017 PHY 745 Spring 2017 -- Lecture 14