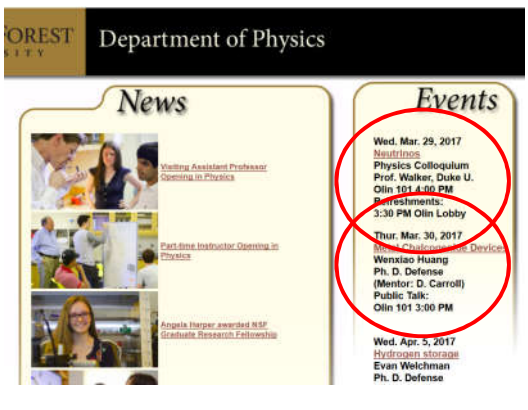
PHY 745 Group Theory
11-11:50 AM MWF Olin 102

Plan for Lecture 27:

Topics involving angular momentum
Chap. 14 in DDJ

1. **"Addition" of angular momenta**
2. **Rotation of angular momenta**
3. **Double group representations**

23	Mon: 03/20/2017	Chap. 7.7	Jahn-Teller Effect	#15	03/24/2017
24	Wed: 03/22/2017	Chap. 7.7	Jahn-Teller Effect		
25	Fri: 03/24/2017		Spin 1/2	#16	03/27/2017
26	Mon: 03/27/2017		Dirac equation for H-like atoms	#17	03/29/2017
27	Wed: 03/29/2017	Chap. 14	Angular momenta	#18	03/31/2017
28	Fri: 03/31/2017				
29	Mon: 04/03/2017				
30	Wed: 04/05/2017				
31	Fri: 04/07/2017				
32	Mon: 04/10/2017				
33	Wed: 04/12/2017				
	Fri: 04/14/2017		*Good Friday Holiday -- no class*		
34	Mon: 04/17/2017				
35	Wed: 04/19/2017				
36	Fri: 04/21/2017				
	Mon: 04/24/2017		Presentations I		
	Wed: 04/26/2017		Presentations II		



On March 29-30, 2017, the Sustainability Graduate Programs and the Center for Energy, Environment, and Sustainability will host several distinguished Wake Forest alumni and guests who have dedicated their lives to the environmental sector through jobs in leadership, policy, and protection.

Wednesday, March 29

Join as experts share insights from their own impact careers in environmental leadership, policy and protection at the Environmental Futures: Pathways to Impact event. The panel will also discuss both the current and future states of environmental and sustainability fields. The event will take place on March 29 at the Wake Forest Byrum Welcome Center at 6:00 p.m. This event is free and open to the public. RSVP on Eventbrite.

Speakers include:

Stanley Meiburg ('75): *Former Acting Deputy Administrator, EPA*
Benjamin H. Grumbles ('82): *Secretary of the Environment, State of Maryland and former Assistant Administrator, Office of Water, EPA*
Lyons Gray: *North Carolina Utilities Commission and former Chief Financial Officer, EPA*
Jim Perdue ('73, P'07): *Chairman of Perdue Farms*
Laura Vaught ('93): *former Associate Administrator, Office of Policy, EPA*

Addition of angular momenta

$\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2$

Eigenstates: $|jm\rangle$, $|j_1 m_1\rangle$, $|j_2 m_2\rangle$,

where $J^2|jm\rangle = \hbar^2 j(j+1)|jm\rangle$ and $J_z|jm\rangle = \hbar m|jm\rangle$

$J_1^2|j_1 m_1\rangle = \hbar^2 j_1(j_1+1)|j_1 m_1\rangle$ and $J_{1z}|j_1 m_1\rangle = \hbar m_1|j_1 m_1\rangle$ etc.

Clebsch-Gordon coefficients:

$$|jm\rangle = \sum_{m_1 m_2} C(j_1 j_2 j; m_1 m_2 m)|j_1 m_1\rangle|j_2 m_2\rangle$$

$$|j_1 m_1\rangle|j_2 m_2\rangle = \sum_{j} C(j_1 j_2 j; m_1 m_2 m)|jm\rangle$$

$m = m_1 + m_2$ $\qquad |j_1 - j_2| \le j \le j_1 + j_2$

For more information on the Clebsch-Gordon coefficients:
http://dlmf.nist.gov/34

For the case of coupling of orbit and spin angular momentum:

$$\mathcal{Y}_{jm}^{l} = \sqrt{\frac{l+m+\frac{1}{2}}{2l+1}} Y_{l\left(m-\frac{1}{2}\right)}(\hat{\mathbf{r}})\begin{pmatrix}1\\0\end{pmatrix} + \sqrt{\frac{l-m+\frac{1}{2}}{2l+1}} Y_{l\left(m+\frac{1}{2}\right)}(\hat{\mathbf{r}})\begin{pmatrix}0\\1\end{pmatrix} \quad \text{for } j = l+\tfrac{1}{2}$$

$$\mathcal{Y}_{jm}^{l} = -\sqrt{\frac{l-m+\frac{1}{2}}{2l+1}} Y_{l\left(m-\frac{1}{2}\right)}(\hat{\mathbf{r}})\begin{pmatrix}1\\0\end{pmatrix} + \sqrt{\frac{l+m+\frac{1}{2}}{2l+1}} Y_{l\left(m+\frac{1}{2}\right)}(\hat{\mathbf{r}})\begin{pmatrix}0\\1\end{pmatrix} \quad \text{for } j = l-\tfrac{1}{2}$$

$$|jm\rangle = \sqrt{\frac{l+m+\frac{1}{2}}{2l+1}}\left|l\left(m-\tfrac{1}{2}\right)\right\rangle\left|\tfrac{1}{2}\tfrac{1}{2}\right\rangle + \sqrt{\frac{l-m+\frac{1}{2}}{2l+1}}\left|l\left(m+\tfrac{1}{2}\right)\right\rangle\left|\tfrac{1}{2}\left(-\tfrac{1}{2}\right)\right\rangle \quad \text{for } l = j-\tfrac{1}{2}$$

$$|jm\rangle = -\sqrt{\frac{l-m+\frac{1}{2}}{2l+1}}\left|l\left(m-\tfrac{1}{2}\right)\right\rangle\left|\tfrac{1}{2}\tfrac{1}{2}\right\rangle + \sqrt{\frac{l+m+\frac{1}{2}}{2l+1}}\left|l\left(m+\tfrac{1}{2}\right)\right\rangle\left|\tfrac{1}{2}\left(-\tfrac{1}{2}\right)\right\rangle \quad \text{for } l = j+\tfrac{1}{2}$$

Rotations of angular momentum

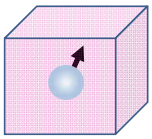
Irreducible representations in terms of angular momentum-spin eigenfunctions

$$O_R(\alpha, \mathbf{z}) = e^{-i\alpha J_z/\hbar}$$

$$\chi^j(\alpha) = \sum_{m=-j}^{j} \langle jm | O_R(\alpha, \hat{\mathbf{z}}) | jm \rangle = \sum_{m=-j}^{j} e^{-i\alpha m} = \frac{\sin\left[\alpha\left(j+\frac{1}{2}\right)\right]}{\sin(\alpha/2)}$$

Note that: $\chi^j(\alpha + 2\pi) = (-1)^{2j}\chi^j(\alpha)$

$$\chi^j(\alpha + 4\pi) = \chi^j(\alpha)$$



Octahedral symmetry

	E	$8C_3$	$3C_2 = 3C_4^2$	$6C_2'$	$6C_4$
Γ_1	1	1	1	1	1
Γ_2	1	1	1	−1	−1
Γ_{12}	2	−1	2	0	0
$\Gamma_{15'}$	3	0	−1	−1	1
$\Gamma_{25'}$	3	0	−1	1	−1

Introduce rotation by $2\pi \equiv R$ and construct direct product character table for $O \times R$

$$\chi^j(\alpha) = \frac{\sin\left[\alpha\left(j+\frac{1}{2}\right)\right]}{\sin(\alpha/2)}$$

Special cases for $j = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}$.....

$\chi^j(\pi) = \chi^j(C_2) = 0 \quad \Rightarrow R$ does not change C_2

	E	$8C_3$	$3C_2 = 3C_4^2$ (+3R)	$6C_2'$ (+6R)	$6C_4$	R	$8RC_3$	$6RC_4$
Γ_1	1	1	1	1	1	1	1	1
Γ_2	1	1	1	−1	−1	1	1	−1
Γ_{12}	2	−1	2	0	0	2	−1	0
$\Gamma_{15'}$	3	0	−1	−1	1	3	0	1
$\Gamma_{25'}$	3	0	−1	1	−1	3	0	−1

Note that complete group is now of order 48
and there are 8 classes and 8 representations
➔need to find three more representations

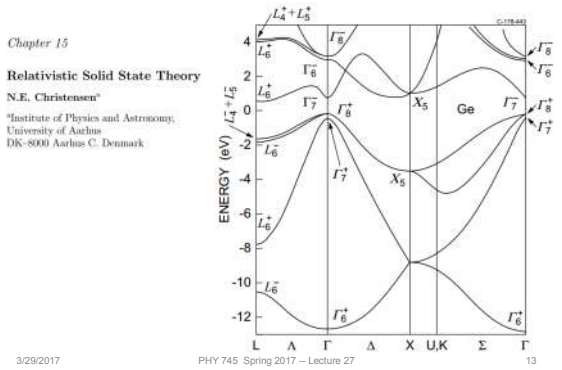
	E	$8C_3$	$3C_2 = 3C_4^2$ (+3R)	$6C_2'$ (+6R)	$6C_4$	R	$8RC_3$	$6RC_4$
Γ_1	1	1	1	1	1	1	1	1
Γ_2	1	1	1	−1	−1	1	1	−1
Γ_{12}	2	−1	2	0	0	2	−1	0
$\Gamma_{15'}$	3	0	−1	−1	1	3	0	1
$\Gamma_{25'}$	3	0	−1	1	−1	3	0	−1
Γ_6	2	1	0	0	$\sqrt{2}$	-2	-1	$-\sqrt{2}$
Γ_7	2	1	0	0	$-\sqrt{2}$	-2	-1	$\sqrt{2}$
Γ_8	4	-1	0	0	0	-4	1	0

Summary of results

O	E	$\mathcal{R}$	$3C_4^2 + 3\bar{\mathcal{R}}C_4^2$	$6C_4$	$6\mathcal{R}C_4$	$6C_2 + 6\bar{\mathcal{R}}C_2$	$8C_3$	$8\mathcal{R}C_3$
Γ_1	1	1	1	1	1	1	1	1
Γ_2	1	1	1	−1	−1	−1	1	1
Γ_{12}	2	2	2	0	0	0	−1	−1
$\Gamma_{15'}$	3	3	−1	1	1	−1	0	0
$\Gamma_{25'}$	3	3	−1	−1	−1	1	0	0
Γ_6	2	−2	0	$\sqrt{2}$	$-\sqrt{2}$	0	1	−1
Γ_7	2	−2	0	$-\sqrt{2}$	$\sqrt{2}$	0	1	−1
Γ_8	4	−4	0	0	0	0	−1	1

valid double group representations

Double group band structure of Ge



PHYSICAL REVIEW B VOLUME 3, NUMBER 10 15 MAY 1971

Comparison of the Energy-Band Structure of Ge-Si with Those of Si and Ge

D. J. Stukel

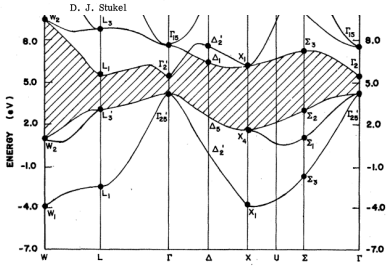


FIG. 5. Self-consistent OPW energy-band structure of Ge obtained using Slater's exchange. The solid dots denote SCOPW energy levels. The solid lines were obtained by fitting a pseudopotential-type interpolation scheme to the SCOPW energy levels.

Crystal field splitting of atom in octahedral field

O	E	$\mathcal{R}$	$3C_4^2+3\bar{\mathcal{R}}C_4^2$	$6C_4$	$6\mathcal{R}C_4$	$6C_2+6\bar{\mathcal{R}}C_2$	$8C_3$	$8\mathcal{R}C_3$
Γ_1	1	1	1	1	1	1	1	1
Γ_2	1	1	1	−1	−1	−1	1	1
Γ_{12}	2	2	2	0	0	0	−1	−1
$\Gamma_{15'}$	3	3	−1	1	1	−1	0	0
$\Gamma_{25'}$	3	3	−1	−1	−1	1	0	0
Γ_6	2	−2	0	$\sqrt{2}$	$-\sqrt{2}$	0	1	−1
Γ_7	2	−2	0	$-\sqrt{2}$	$\sqrt{2}$	0	1	−1
Γ_8	4	−4	0	0	0	0	−1	1
$j=\frac{1}{2}$	2	-2	0	$\sqrt{2}$	$-\sqrt{2}$	0	1	-1

Γ_6

Crystal field splitting of atom in octahedral field

O	E	$\mathcal{R}$	$3C_4^2+3\bar{\mathcal{R}}C_4^2$	$6C_4$	$6\mathcal{R}C_4$	$6C_2+6\bar{\mathcal{R}}C_2$	$8C_3$	$8\mathcal{R}C_3$
Γ_1	1	1	1	1	1	1	1	1
Γ_2	1	1	1	−1	−1	−1	1	1
Γ_{12}	2	2	2	0	0	0	−1	−1
$\Gamma_{15'}$	3	3	−1	1	1	−1	0	0
$\Gamma_{25'}$	3	3	−1	−1	−1	1	0	0
Γ_6	2	−2	0	$\sqrt{2}$	$-\sqrt{2}$	0	1	−1
Γ_7	2	−2	0	$-\sqrt{2}$	$\sqrt{2}$	0	1	−1
Γ_8	4	−4	0	0	0	0	−1	1
$j=\frac{3}{2}$	4	-4	0	0	0	0	-1	1

Γ_8

PHYSICAL REVIEW VOLUME 96, NUMBER 2 OCTOBER 15, 1954

Spin-Orbit Coupling in Band Theory—Character Tables for Some "Double" Space Groups

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(Received May 26, 1954)

To take account of the electron spin in band theory, a method is outlined which allows us to construct character tables for the double space groups of the simple, face-centered, and body-centered cubic, diamond, and hexagonal close packed lattices. The effects of time reversal are also considered. Particular attention is given to the splitting of otherwise degenerate bands by the spin-orbit coupling.